Theoretical Research of Substituted Bay Region with Helical Chirality: Structures and Enantiomerization

Huimin Zhou,[1][0009-0006-3977-7695] Yijian Ma,[1][0009-0000-6632-4153] Jiaxin Shi,[1]

Na Yang, *[2,3] Chengshuo Shen, *[1,3][0000-0003-2422-3922]

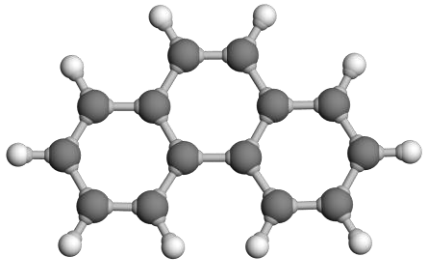
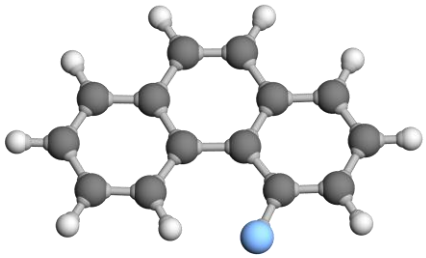
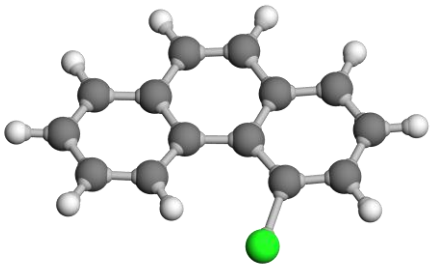
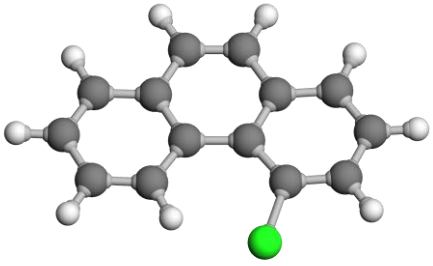
Supplementary Materials

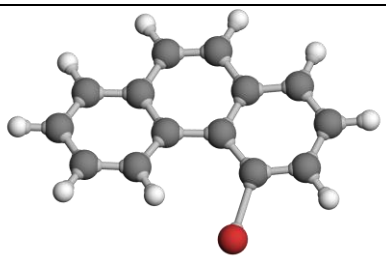
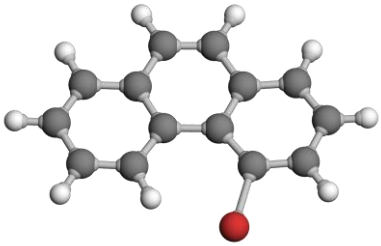
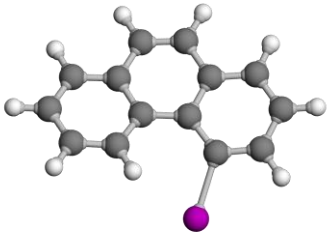
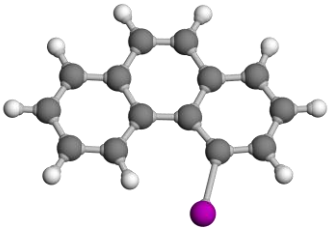
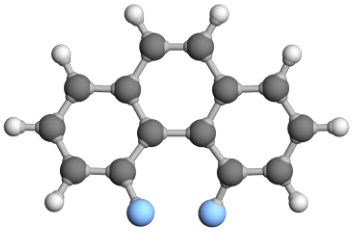
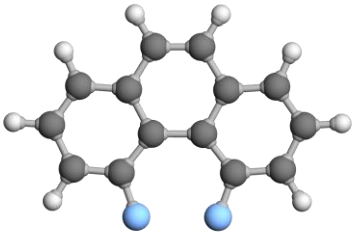
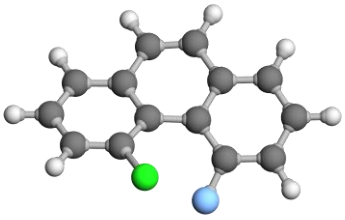
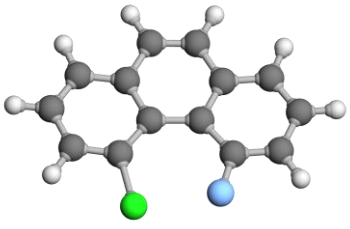
1. Funding

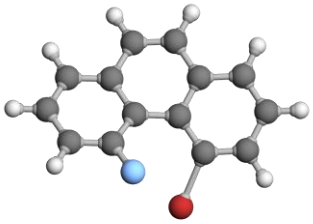
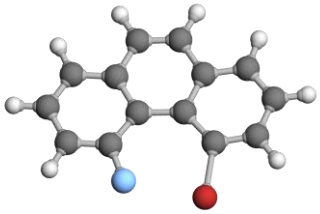
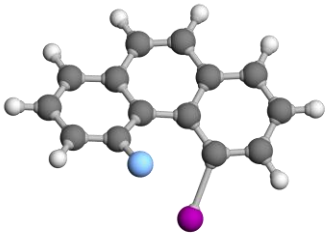
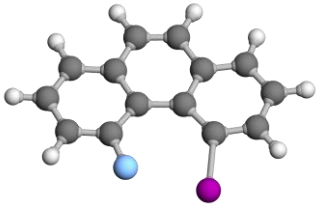
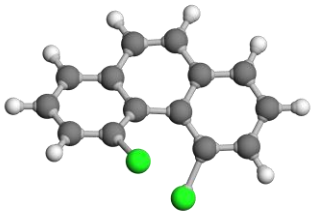
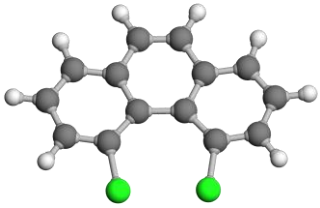
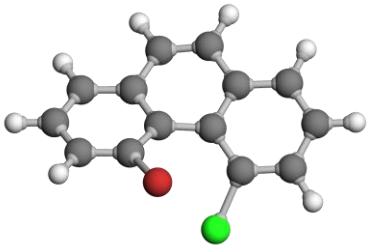
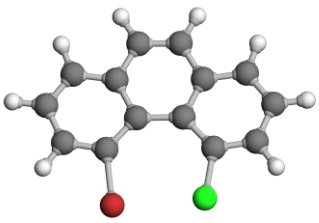
This work was financially supported by the Zhejiang Provincial Natural Science Foundation, China (LY23B040003), and the National Natural Science Foundation of China (22561160131).

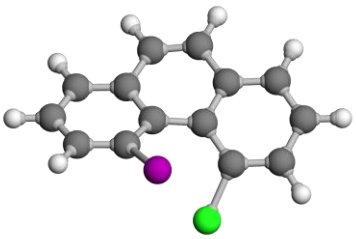
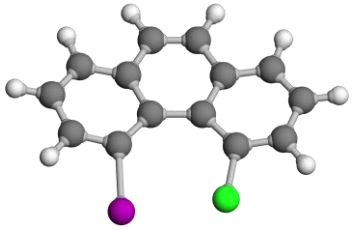
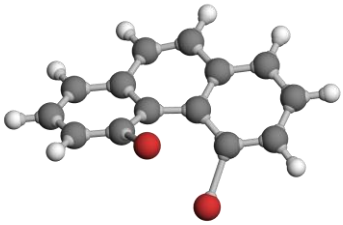
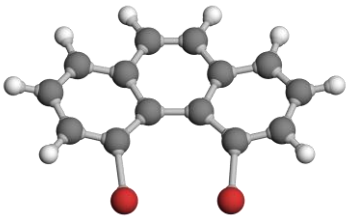
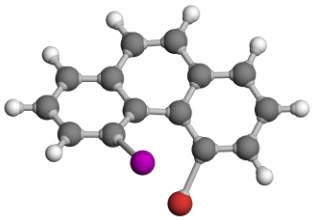
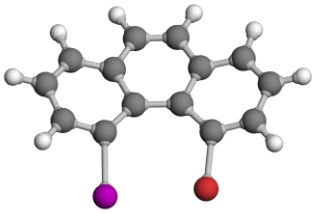
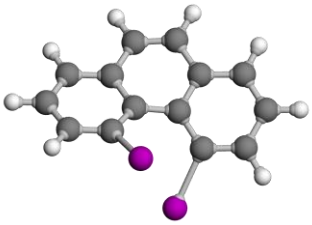
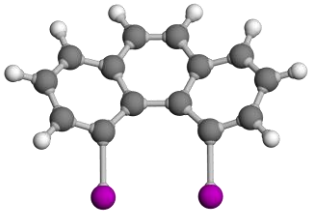
2. The enantiomerization energy barriers (in kcal mol^{-1}) and angle of Phenanthrene derivative.

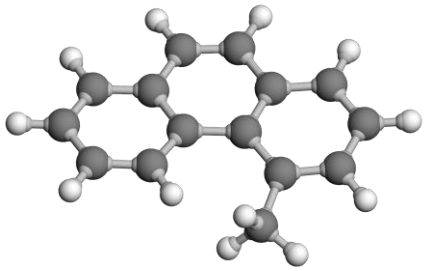
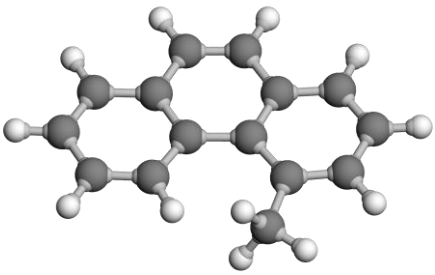
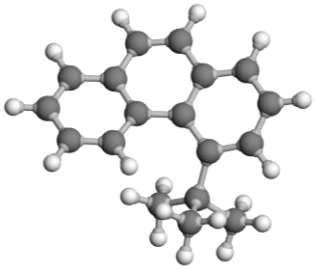
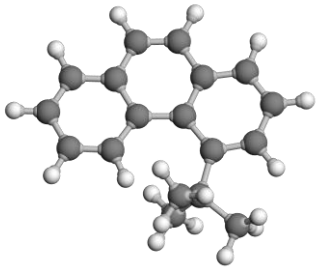
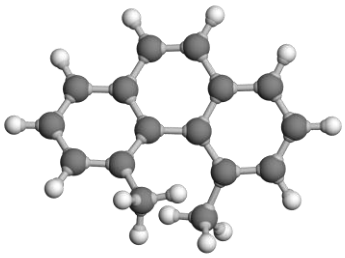
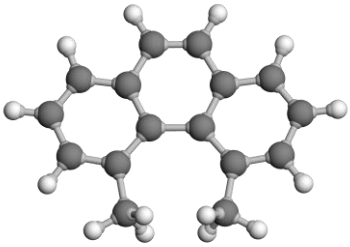
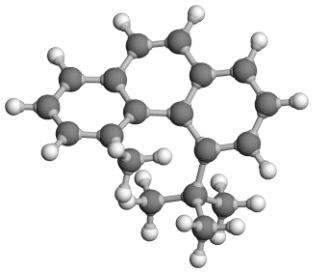
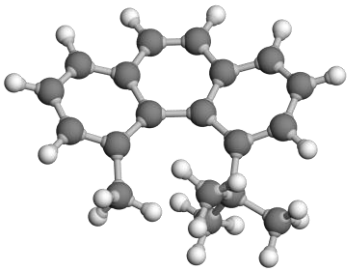
Figure S1. The enantiomerization energy barriers (in kcal mol^{-1}) and angle of Phenanthrene derivative.

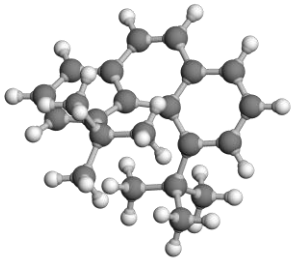
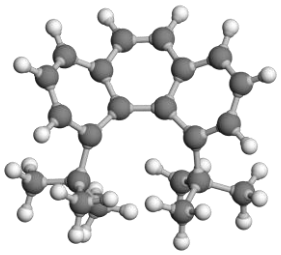
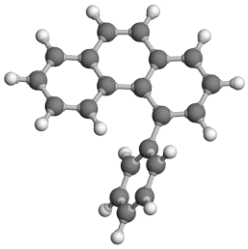
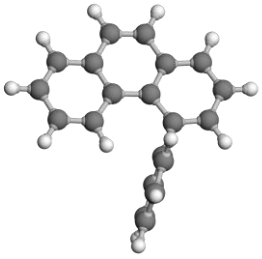
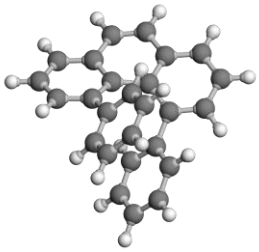
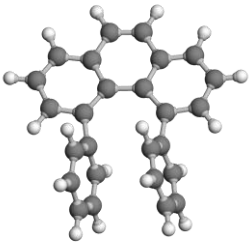
	
Phenanthrene ∠A: 0° ∠B: 58.24°	
	
$Phen_{F,H}$ ∠A: 0° ∠B: 57.78°	
	
$Phen_{Cl,H}$ ∠A: 9.41° ∠B: 56.96°	+1.12 kcal mol^{-1} ∠A: 0° ∠B: 56.57°

	
$Phen_{Br,H}$ ∠A: 13.80° ∠B: 57.27°	+1.19 kcal mol^{-1} ∠A: 0° ∠B: 56.38°
	
$Phen_{I,H}$ ∠A: 17.21° ∠B: 57.69°	+1.53 kcal mol^{-1} ∠A: 0° ∠B: 56.23°
	
$Phen_{F,F}$ ∠A: 22.39° ∠B: 58.77°	+2.31 kcal mol^{-1} ∠A: 0° ∠B: 56.35°
	
$Phen_{F,Cl}$ ∠A: 29.06° ∠B: 59.32°	+6.98 kcal mol^{-1} ∠A: 0° ∠B: 54.93°

	
$Phen_{F,Br}$ ∠A: 29.72° ∠B: 59.45°	+8.28 kcal mol^{-1} ∠A: 0° ∠B: 54.78°
	
$Phen_{F,I}$ ∠A: 29.77° ∠B:59.49°	+9.32 kcal mol^{-1} ∠A: 0° ∠B: 54.79°
	
$Phen_{Cl,Cl}$ ∠A: 34.27° ∠B: 59.91°	+16.17 kcal mol^{-1} ∠A: 0° ∠B: 53.11°
	
$Phen_{Cl,Br}$ ∠A: 34.84° ∠B: 60.03°	+18.57 kcal mol^{-1} ∠A: 0° ∠B: 52.83°

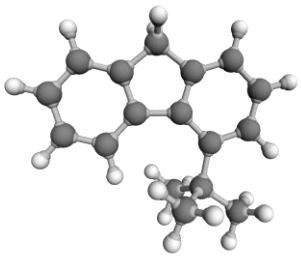
	
$Phen_{Cl,I}$ ∠A: 34.99° ∠B: 60.10°	+20.83 kcal mol^{-1} ∠A: 2.43° ∠B: 52.81°
	
$Phen_{Br,Br}$ ∠A: 35.39° ∠B: 60.17°	+22.16 kcal mol^{-1} ∠A: 0° ∠B: 52.51°
	
$Phen_{Br,I}$ ∠A: 35.58° ∠B: 60.25°	+25.17 kcal mol^{-1} ∠A: 3.56° ∠B: 52.51°
	
$Phen_{I,I}$ ∠A: 35.80° ∠B: 60.35°	+28.90 kcal mol^{-1} ∠A: 0° ∠B: 52.34°

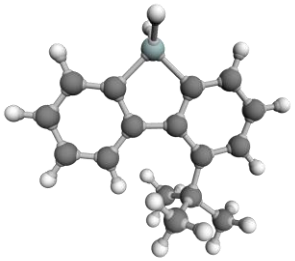
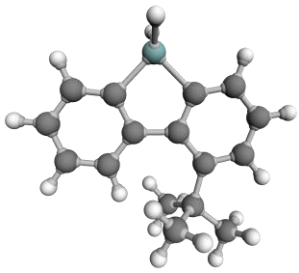
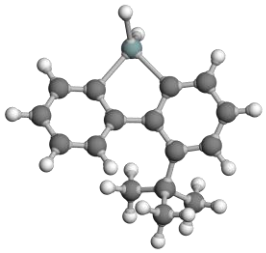
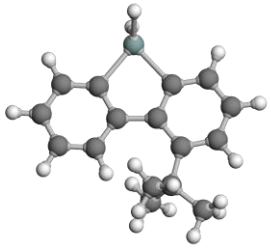
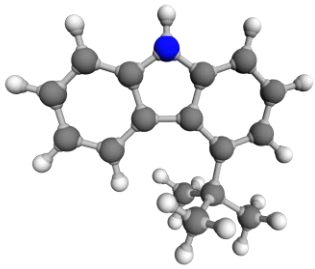
	
$Phen_{Me,H}$ ∠A: 9.87° ∠B: 56.94°	+1.08 kcal mol^{-1} ∠A: 0° ∠B: 56.52°
	
$Phen_{tBu,H}$ ∠A: 23.94° ∠B: 58.51°	+1.10 kcal mol^{-1} ∠A: 3.52° ∠B: 55.19°
	
$Phen_{Me,Me}$ ∠A: 33.03° ∠B: 59.34°	+16.20 kcal mol^{-1} ∠A: 0° ∠B: 52.63°
	
$Phen_{Me,tBu}$ ∠A: 36.87° ∠B: 60.15°	+29.39 kcal mol^{-1} ∠A: 2.09° ∠B: 51.29°

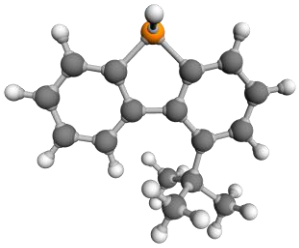
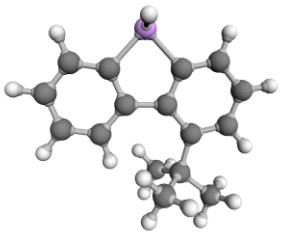
	
$Phen_{tBu,tBu}$ ∠A: 43.88° ∠B: 61.50°	+54.23 kcal mol^{-1} ∠A: 14.15° ∠B: 49.78°
	
$Phen_{Ph,H}$ ∠A: 13.12° ∠B: 57.67°	+1.52 kcal mol^{-1} ∠A: 0° ∠B: 56.76°
	
$Phen_{Ph,Ph}$ ∠A: 28.23° ∠B: 59.05°	+21.96 kcal mol^{-1} ∠A: 1.15° ∠B: 53.20°

3. The enantiomerization energy barriers (in kcal mol^{-1}) and angle of H3X derivatives (X = C, Si, Ge Sn N, P, As, Sb, O, S, Se, and Te).

Figure S2. The enantiomerization energy barriers (in kcal mol^{-1}) and angle of H3X derivatives (X = C, Si, Ge , Sn, N, P, As, Sb, O, S, Se, and Te).

	
$H3C_{tBu,H}$	

∠A: 0° ∠B: 35.07°	
	
H3Si $_{tBu,H}$ ∠A: 0° ∠B: 47.16°	
	
H3Ge $_{tBu,H}$ ∠A: 0° ∠B: 49.18°	
	
H3Sn $_{tBu,H}$ ∠A: 30.09° ∠B: 59.29°	+1.20 kcal mol^{-1} ∠A: 0° ∠B: 53.17°
	
H3N $_{tBu,H}$ ∠A: 0° ∠B: 31.93°	

	
H3P $_{tBu,H}$ ∠A: 0° ∠B: 43.35°	
	
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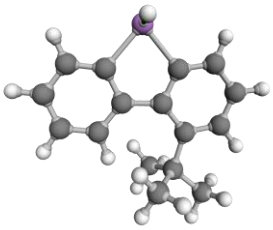
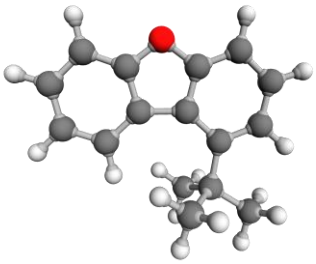
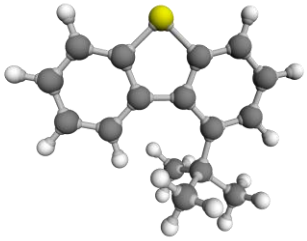
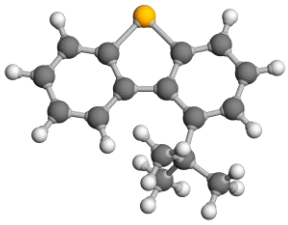
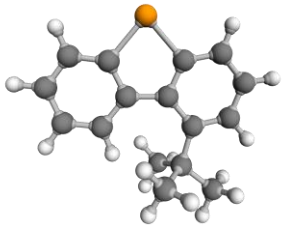
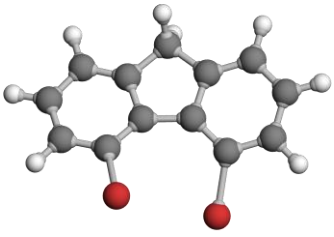
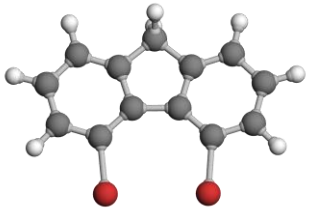
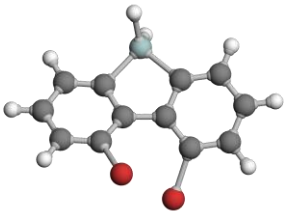
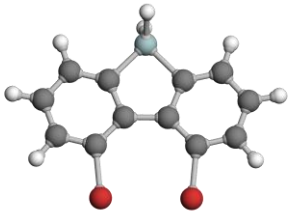
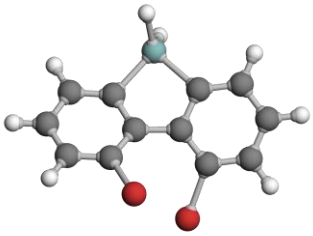
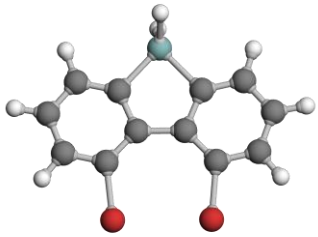
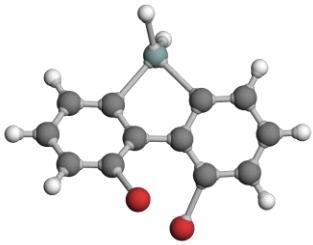
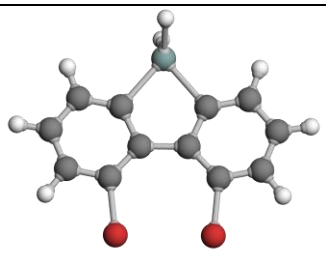
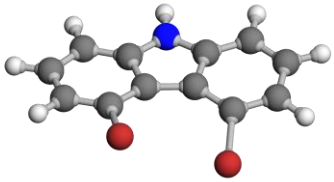
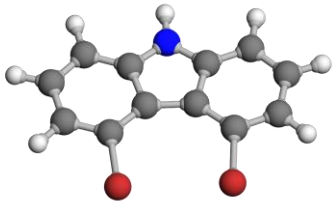
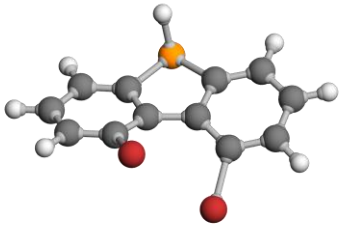
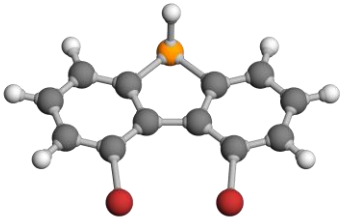
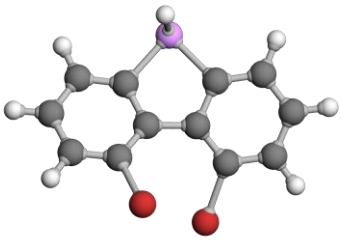
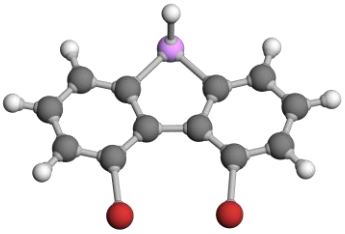
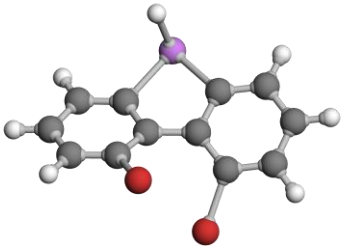
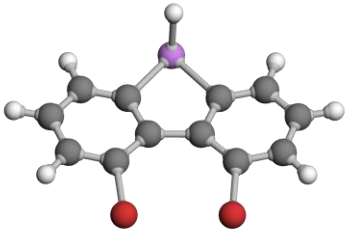
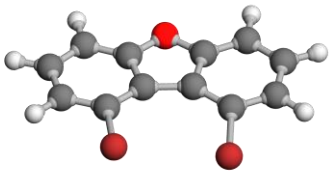
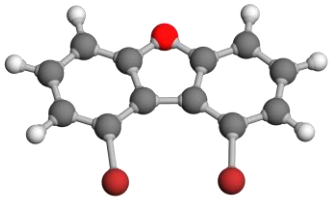
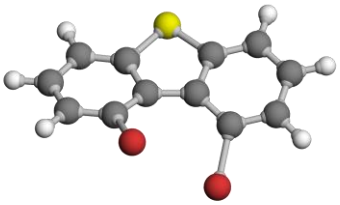
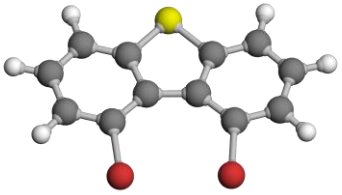
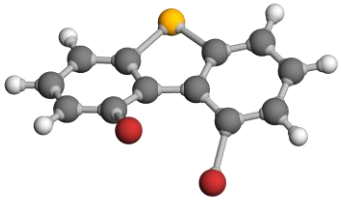
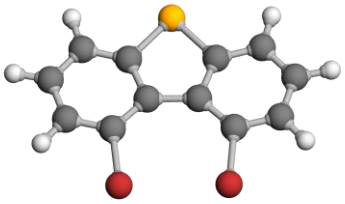
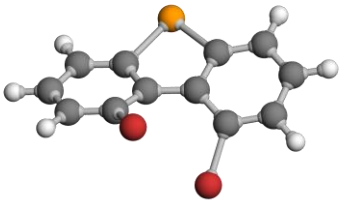
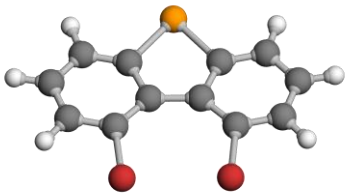
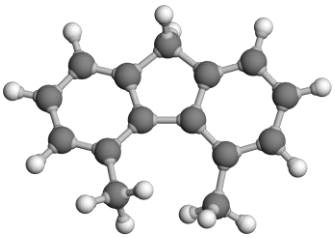
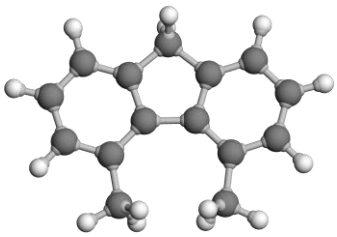
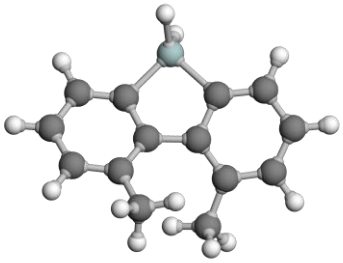
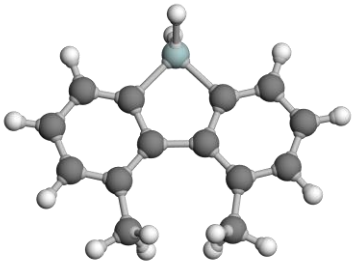
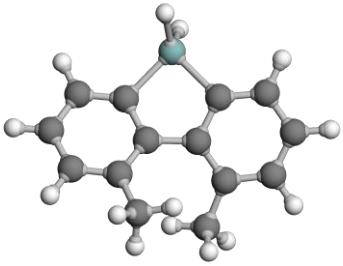
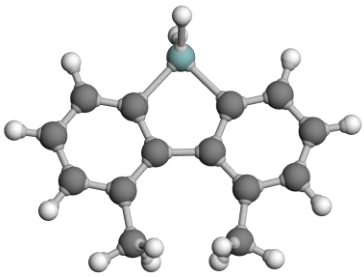
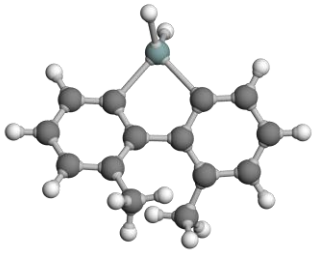
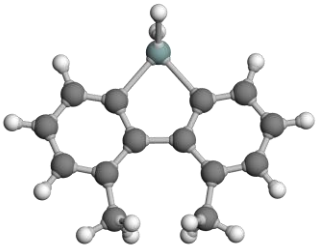
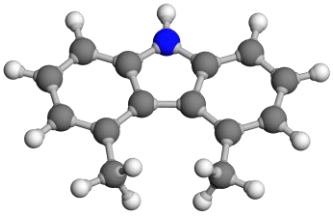
	
H3Sb $_{tBu,H}$ ∠A: 0° ∠B: 50.61°	
	
H3O $_{tBu,H}$ ∠A: 0° ∠B: 29.45°	

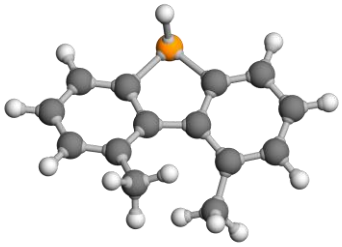
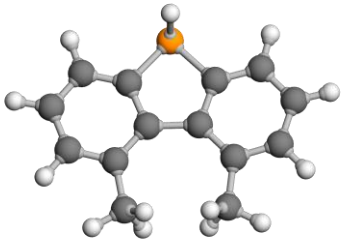
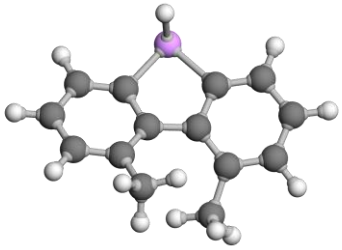
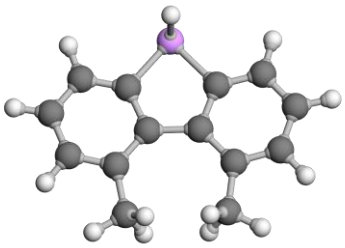
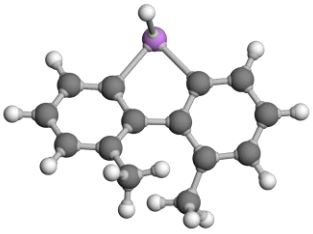
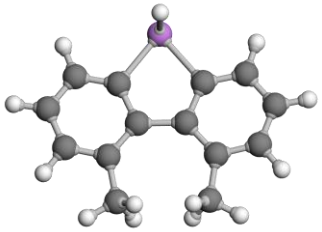
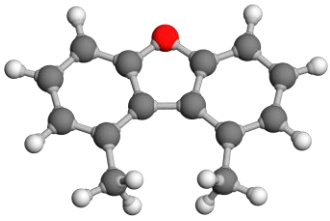
	
H3S $_{tBu,H}$ ∠A: 0° ∠B: 41.38°	
	
H3Se $_{tBu,H}$ ∠A: 0° ∠B: 45.39°	
	
H3Te $_{tBu,H}$ ∠A: 0° ∠B: 50.03°	
	
H3C$_{Br,Br}$ ∠A: 23.03° ∠B: 36.58°	+3.10 kcal mol^{-1} ∠A: 0° ∠B: 34.06°

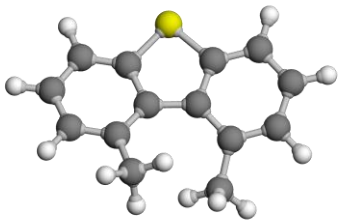
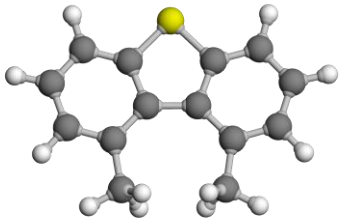
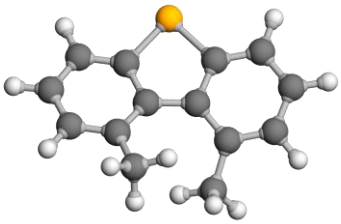
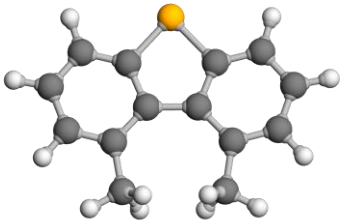
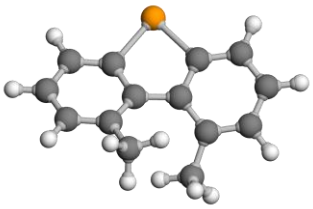
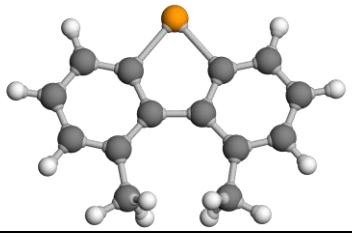
	
$H3Si_{Br,Br}$ ∠A: 37.23° ∠B: 53.06°	+12.53 kcal mol^{-1} ∠A: 0° ∠B: 44.53°
	
$H3Ge_{Br,Br}$ ∠A: 38.0° ∠B: 55.48°	+14.14 kcal mol^{-1} ∠A: 0° ∠B: 46.37°
	
$H3Sn_{Br,Br}$ ∠A: 42.13° ∠B: 61.75°	+19.02 kcal mol^{-1} ∠A: 0° ∠B: 49.55°
	
$H3N_{Br,Br}$ ∠A: 14.82° ∠B: 31.98°	+1.56 kcal mol^{-1} ∠A: 0.24° ∠B: 31.28°

	
H3P$_{Br,Br}$ ∠A: 30.94° ∠B: 46.82°	+7.98 kcal mol^{-1} ∠A: 0° ∠B: 41.44°
	
H3As$_{Br,Br}$ ∠A: 33.68° ∠B: 50.99°	+10.59 kcal mol^{-1} ∠A: 0° ∠B: 44.11°
	
H3Sb$_{Br,Br}$ ∠A: 38.34° ∠B: 60.45°	+15.48 kcal mol^{-1} ∠A: 0° ∠B: 47.48°
	
H3O$_{Br,Br}$ ∠A: 5.53° ∠B: 29.09°	+1.81 kcal mol^{-1} ∠A: −0.22° ∠B: 56.35°

	
$H3S_{Br,Br}$ ∠A: 26.53° ∠B: 43.23°	+5.30 kcal mol^{-1} ∠A: 0° ∠B: 39.88°
	
$H3Se_{Br,Br}$ ∠A: 29.82° ∠B: 48.22°	+8.11 kcal mol^{-1} ∠A: 0° ∠B: 43.41°
	
$H3Te_{Br,Br}$ ∠A: 33.99° ∠B: 54.55°	+12.81 kcal mol^{-1} ∠A: 0° ∠B: 47.27°
	
$H3C_{Me,Me}$ ∠A: 18.59° ∠B: 35.82°	+1.24 kcal mol^{-1} ∠A: 0° ∠B: 34.27°

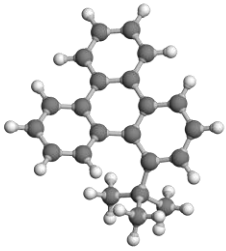
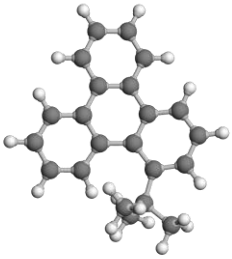
	
$H3Si_{Me,Me}$ ∠A: 33.75° ∠B: 52.10°	+8.79 kcal mol^{-1} ∠A: 0° ∠B: 44.92°
	
$H3Ge_{Me,Me}$ ∠A: 34.52° ∠B: 54.46°	+10.13 kcal mol^{-1} ∠A: 0° ∠B: 46.76°
	
$H3Sn_{Me,Me}$ ∠A: 38.37° ∠B: 60.45°	+14.64 kcal mol^{-1} ∠A: 0° ∠B: 50.02°
	
$H3N_{Me,Me}$ ∠A: 0° ∠B: 31.48°	

	
$H3P_{Me,Me}$ ∠A: 27.90° ∠B: 46.09°	+4.80 kcal mol^{-1} ∠A: 0° ∠B: 41.78°
	
$H3As_{Me,Me}$ ∠A: 30.56° ∠B: 50.15°	+6.99 kcal mol^{-1} ∠A: 0° ∠B: 44.47°
	
$H3Sb_{Me,Me}$ ∠A: 34.92° ∠B: 56.34°	+11.28 kcal mol^{-1} ∠A: 0° ∠B: 47.90°
	
$H3O_{Me,Me}$ ∠A: 0° ∠B: 29.17°	

	
$H3S_{Me,Me}$ ∠A: 23.28° ∠B: 42.65°	+2.53 kcal mol^{-1} ∠A: 0° ∠B: 40.22°
	
$H3Se_{Me,Me}$ ∠A: 27.04° ∠B: 47.63°	+4.73 kcal mol^{-1} ∠A: 0° ∠B: 43.81°
	
$H3Te_{Me,Me}$ ∠A: 31.17° ∠B: 53.86°	+8.70 kcal mol^{-1} ∠A: 0° ∠B: 47.74°

4. The enantiomerization energy barriers (in kcal mol^{-1}) and angle of PAH1-PAH7.

Figure S3. The enantiomerization energy barriers (in kcal mol^{-1}) and angle of PAH1 derivatives.

	
$PAH1_{tBu,H}$ ∠A: 26.90° ∠B: 60.90°	+7.05 kcal mol^{-1} ∠A: -9.72° ∠B: 56.88°

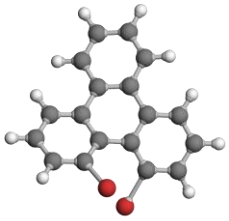
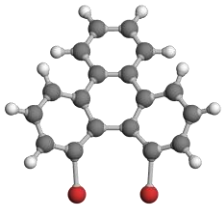
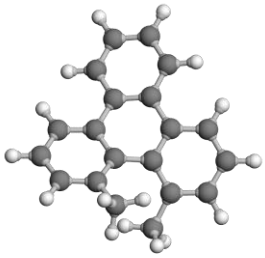
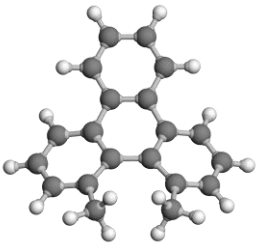
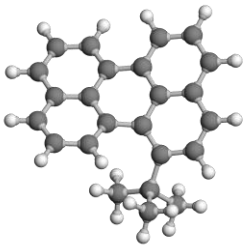
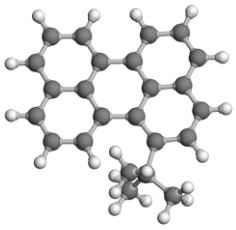
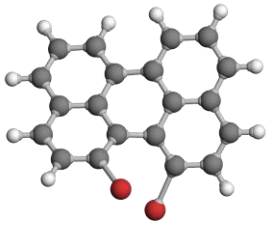
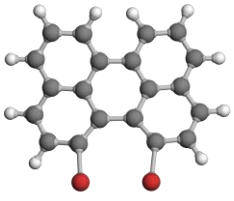
	
$PAH1_{Br,Br}$ ∠A: 39.14° ∠B: 63.27°	+25.14 kcal mol^{-1} ∠A: 0° ∠B: 52.19°
	
$PAH1_{Me,Me}$ ∠A: 36.49° ∠B: 62.39°	+20.17 kcal mol^{-1} ∠A: 0° ∠B: 52.55°

Figure S4. The enantiomerization energy barriers (in kcal mol^{-1}) and angle of PAH2 derivatives.

	
$PAH2_{tBu,H}$ ∠A: 29.24° ∠B: 60.89°	+7.50 kcal mol^{-1} ∠A: 0° ∠B: 56.37°
	
$PAH2_{Br,Br}$ ∠A: 37.44° ∠B: 61.88°	+31.09 kcal mol^{-1} ∠A: −4.23° ∠B: 54.16°

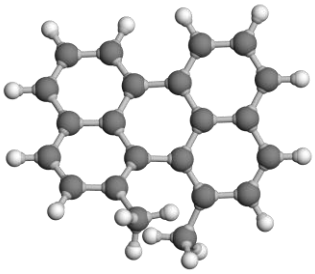
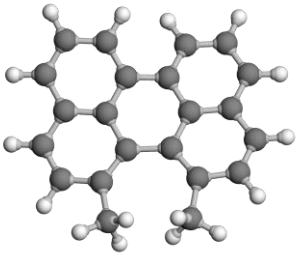
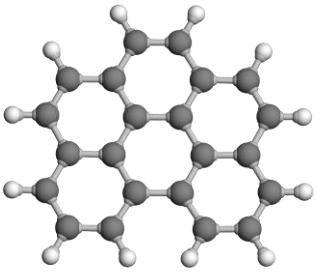
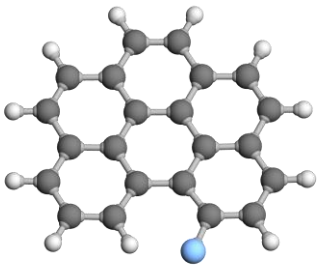
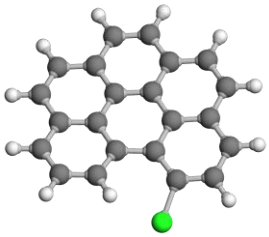
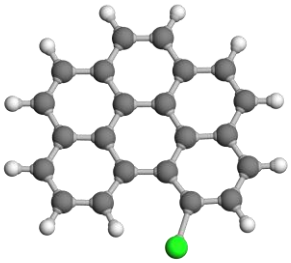
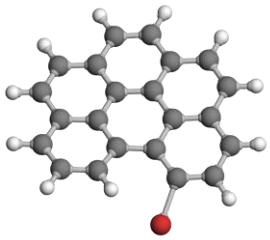
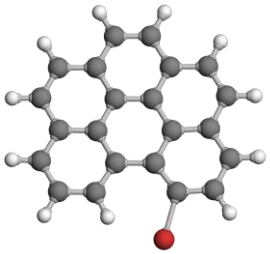
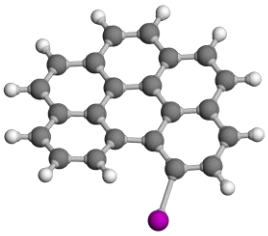
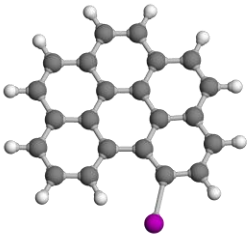
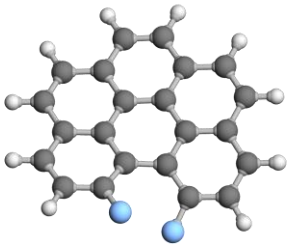
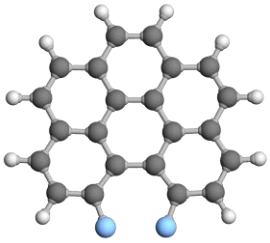
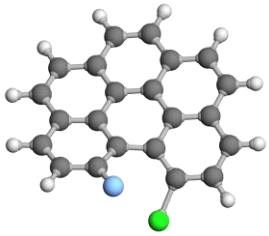
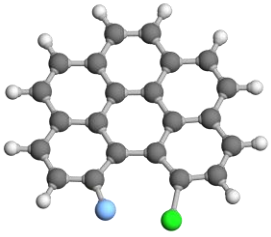
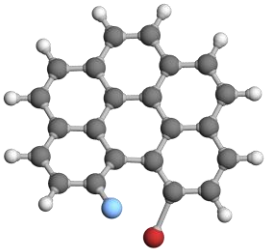
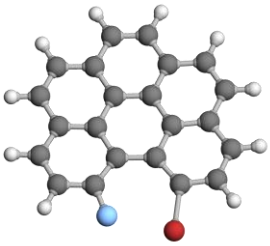
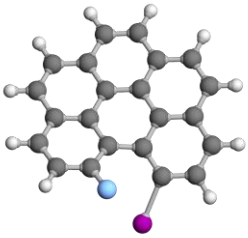
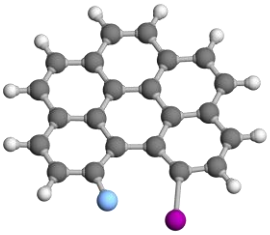
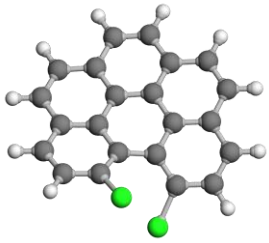
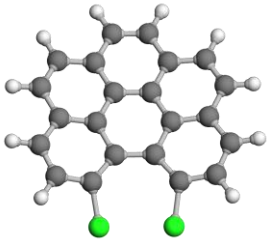
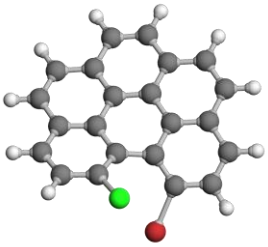
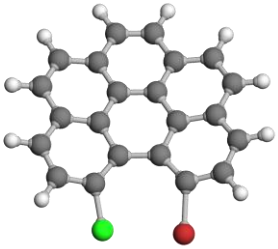
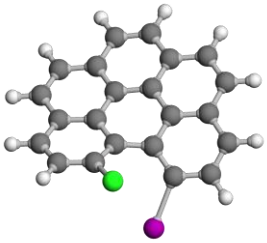
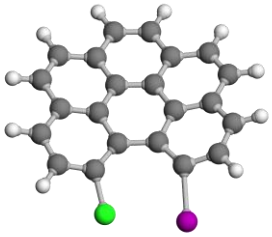
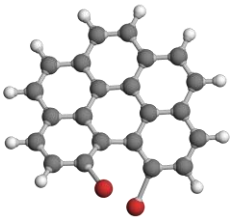
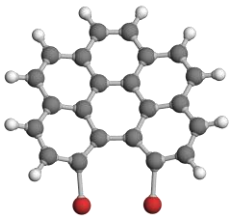
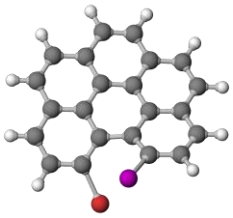
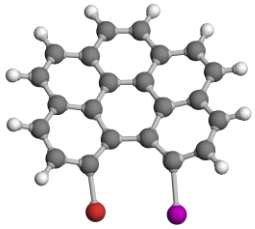
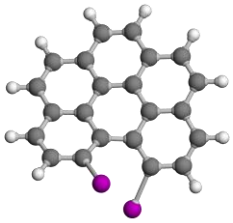
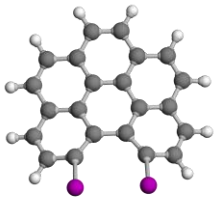
	
$PAH2_{Me,Me}$ ∠A: 34.76° ∠B: 61.12°	+26.74 kcal mol^{-1} ∠A: −4.72° ∠B: 54.16°

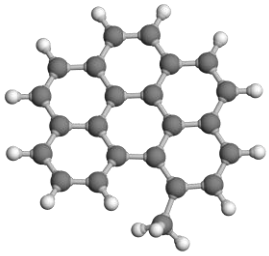
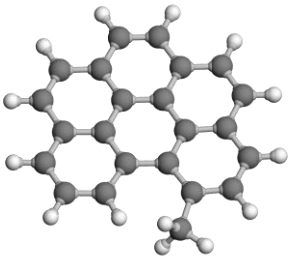
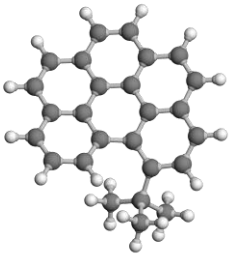
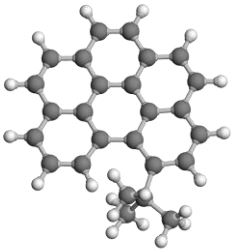
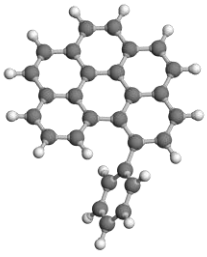
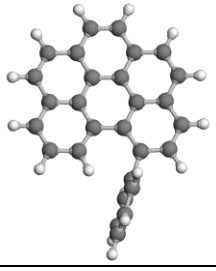
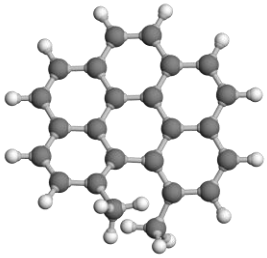
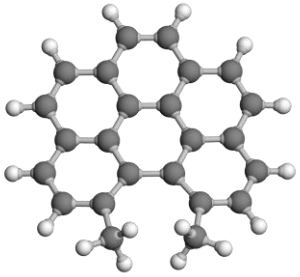
Figure S5. The enantiomerization energy barriers (in kcal mol^{-1}) and angle of PAH3 derivatives.

	
$PAH3_{H,H}$ ∠A: 0° ∠B: 58.42°	
	
$PAH3_{F,H}$ ∠A: 0° ∠B: 58.20°	
	
$PAH3_{Cl,H}$ ∠A: 15.22° ∠B: 58.24°	+1.30kcal mol^{-1} ∠A: 0° ∠B: 57.32°

	
$PAH3_{Br,H}$ ∠A: 17.87° ∠B: 58.49°	+1.72kcal mol^{-1} ∠A: 0° ∠B: 57.19°
	
$PAH3_{I,H}$ ∠A: 20.05° ∠B: 58.78°	+2.38kcal mol^{-1} ∠A: 0° ∠B: 57.08°
	
$PAH3_{F,F}$ ∠A: 23.62° ∠B: 59.56°	+3.76kcal mol^{-1} ∠A: 0° ∠B: 57.13°
	
$PAH3_{F,Cl}$ ∠A: 29.42° ∠B: 60.04°	+10.25kcal mol^{-1} ∠A: 0° ∠B: 56.13°

	
$PAH3_{F,Br}$ ∠A: 30.03° ∠B: 60.13°	+11.76kcal mol^{-1} ∠A: 0° ∠B: 55.94°
	
$PAH3_{F,I}$ ∠A: 30.17° ∠B: 60.16°	+12.76kcal mol^{-1} ∠A: 0° ∠B: 55.98°
	
$PAH3_{Cl,Cl}$ ∠A: 34.29° ∠B: 60.59°	+22.69 kcal mol^{-1} ∠A: 0° ∠B: 54.46°
	
$PAH3_{Cl,Br}$ ∠A: 34.91° ∠B: 60.70°	+25.59 kcal mol^{-1} ∠A: −2.53° ∠B: 54.30°

	
$PAH3_{Cl,I}$ ∠A: 35.16° ∠B: 60.77°	+27.55 kcal mol^{-1} ∠A: −6.1° ∠B: 54.41°
	
$PAH3_{Br,Br}$ ∠A: 35.52° ∠B: 60.82°	+28.55 kcal mol^{-1} ∠A: 0° ∠B: 54.04°
	
$PAH3_{Br,I}$ ∠A: 35.79° ∠B: 60.91°	+31.53 kcal mol^{-1} ∠A: −4.46° ∠B: 54.04°
	
$PAH3_{I,I}$ ∠A: 36.07° ∠B: 61.01°	+35.13 kcal mol^{-1} ∠A: 0° ∠B: 53.82°

	
$PAH3_{Me,H}$ ∠A: 16.23° ∠B: 58.28°	+1.47 kcal mol^{-1} ∠A: 0° ∠B: 57.24°
	
$PAH3_{tBu,H}$ ∠A: 26.31° ∠B: 59.66°	+5.54 kcal mol^{-1} ∠A: 0° ∠B: 56.26°
	
$PAH3_{Ph,H}$ ∠A: 15.63° ∠B: 58.52°	+2.00 kcal mol^{-1} ∠A: 0° ∠B: 57.41°
	
$PAH3_{Me,Me}$ ∠A: 33.12° ∠B: 60.10°	+23.87 kcal mol^{-1} ∠A: 0° ∠B: 53.96°

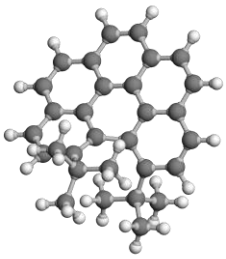
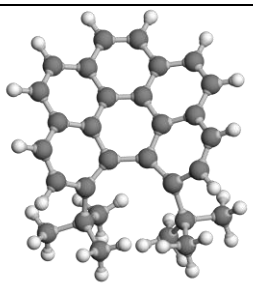
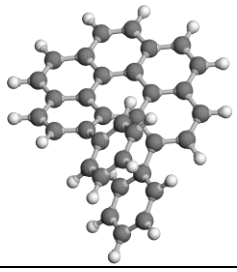
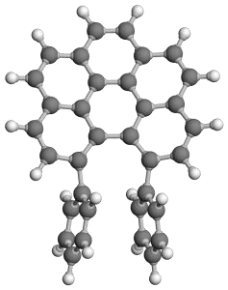
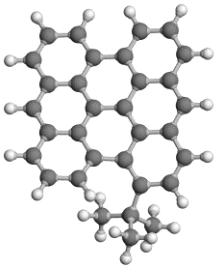
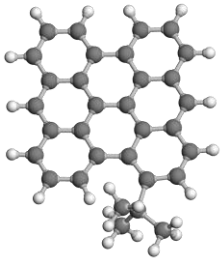
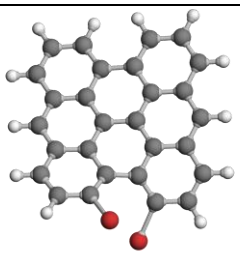
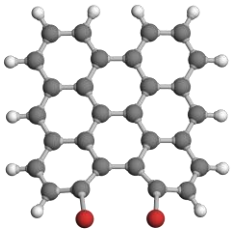
	
$PAH3_{tBu,tBu}$ ∠A: 44.35° ∠B: 62.46°	+63.90 kcal mol^{-1} ∠A: −12.37° ∠B: 51.03°
	
$PAH3_{Ph,\ Ph}$ ∠A: 29.43° ∠B: 60.06°	+27.21 kcal mol^{-1} ∠A: 0.19° ∠B: 54.68°

Figure S6. The enantiomerization energy barriers (in kcal mol^{-1}) and angle of PAH4 derivatives.

	
$PAH4_{tBu,H}$ ∠A: 28.39° ∠B: 59.83°	+7.27 kcal mol^{-1} ∠A: 0° ∠B: 55.75°
	
$PAH4_{Br,Br}$ ∠A: 36.53° ∠B: 60.70°	+30.62 kcal mol^{-1} ∠A: 0° ∠B: 53.51°

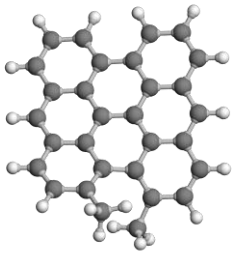
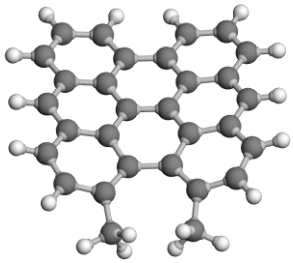
	
$PAH4_{Me,Me}$ ∠A: 34.11° ∠B: 60.04°	+26.99 kcal mol^{-1} ∠A: −0.84° ∠B: 53.40°

Figure S7. The enantiomerization energy barriers (in kcal mol^{-1}) and angle of PAH5 derivatives.

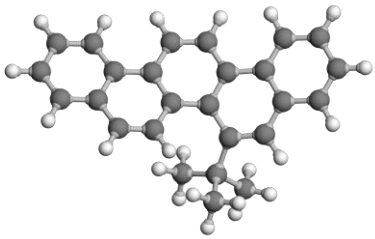
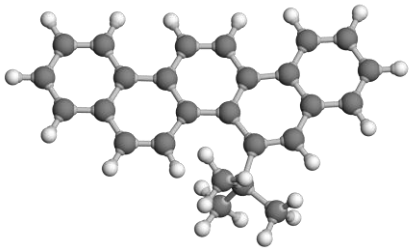
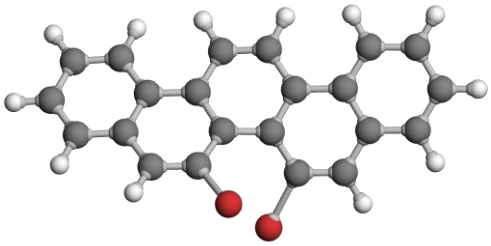
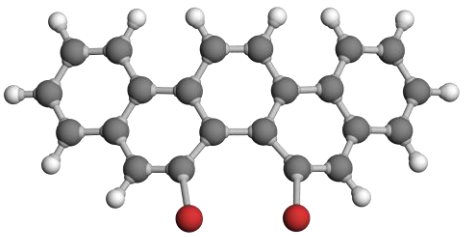
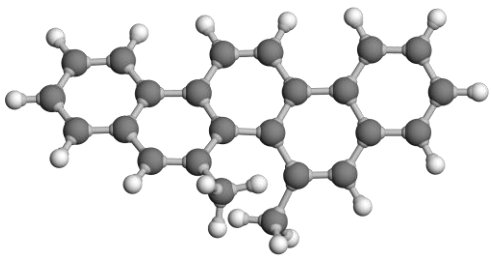
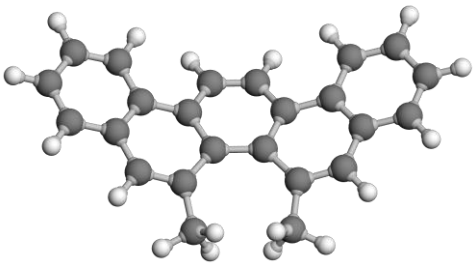
	
$PAH5_{tBu,H}$ ∠A: 26.65° ∠B: 60.55°	+5.08 kcal mol^{-1} ∠A: 0° ∠B: 57.35°
	
$PAH5_{Br,Br}$ ∠A: 35.24° ∠B: 61.85°	+26.94 kcal mol^{-1} ∠A: 0° ∠B: 54.53°
	
$PAH5_{Me,Me}$ ∠A: 33.86° ∠B: 61.04°	+21.09 kcal mol^{-1} ∠A: 0° ∠B: 54.19°

Figure S8. The enantiomerization energy barriers (in kcal mol^{-1}) and angle of PAH6 derivatives.

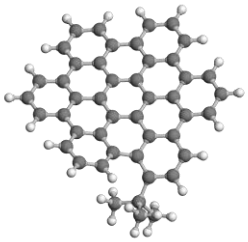
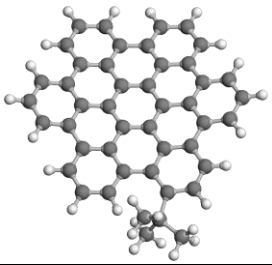
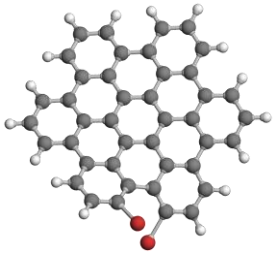
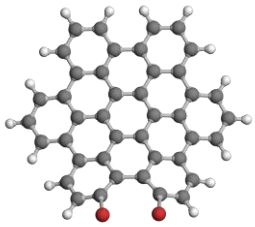
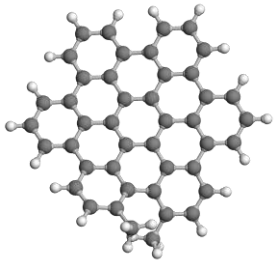
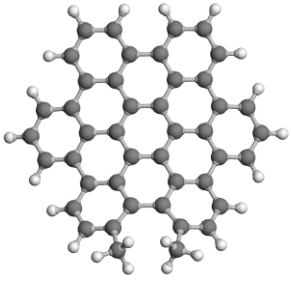
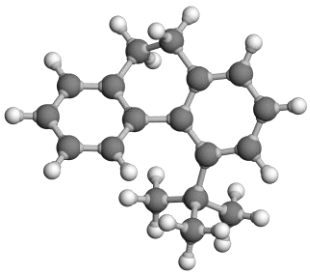
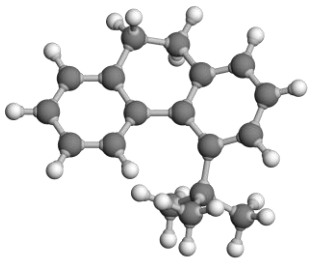
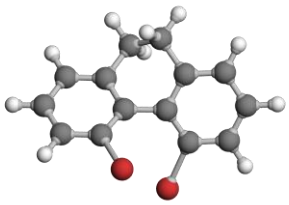
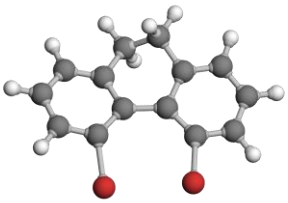
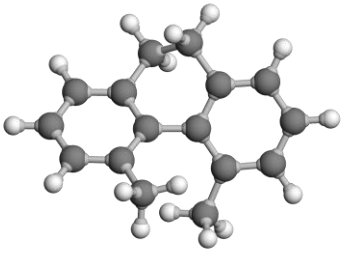
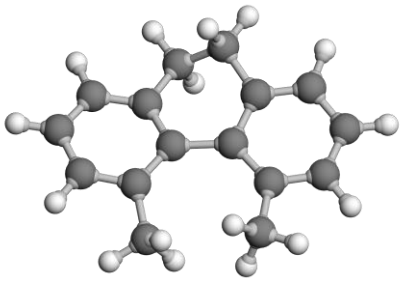
	
$PAH6_{tBu,H}$ ∠A: 28.83° ∠B: 60.96°	+9.43 kcal mol^{-1} ∠A: −2.62° ∠B:56.92°
	
$PAH6_{Br,Br}$ ∠A: 38.33° ∠B: 62.17°	+31.58 kcal mol^{-1} ∠A: 0° ∠B: 54.59°
	
$PAH6_{Me,Me}$ ∠A: 36.02° ∠B: 61.46°	+26.24 kcal mol^{-1} ∠A: 0° ∠B: 54.42°

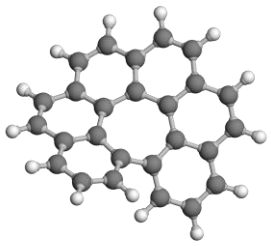
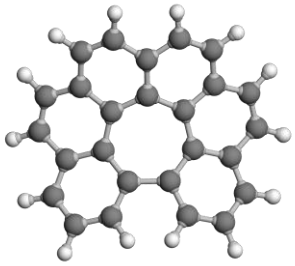
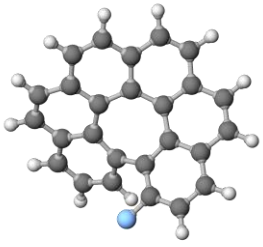
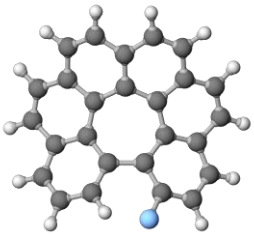
Figure S9. The enantiomerization energy barriers (in kcal mol^{-1}) and angle of PAH7 derivatives.

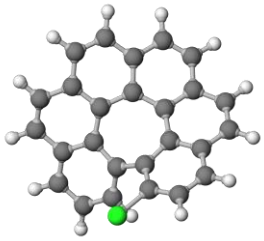
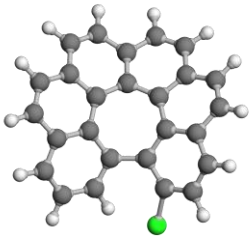
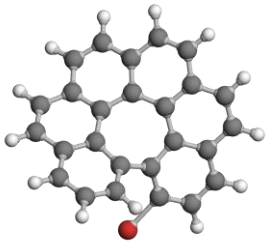
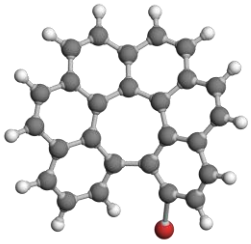
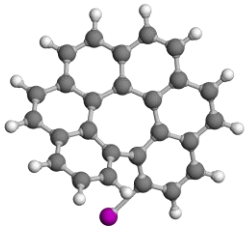
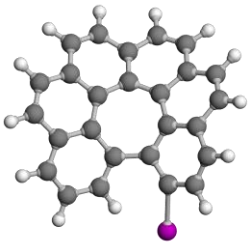
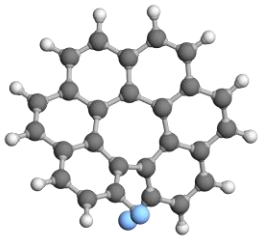
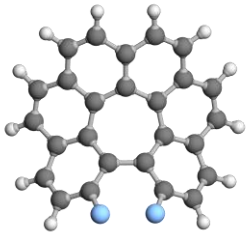
	
$PAH7_{tBu,H}$ ∠A: 40.09° ∠B: 63.67°	+12.12kcal mol^{-1} ∠A: 10.19° ∠B: 57.32°

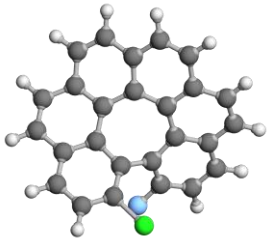
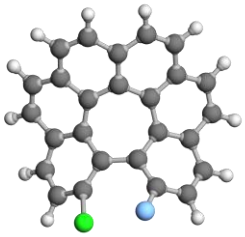
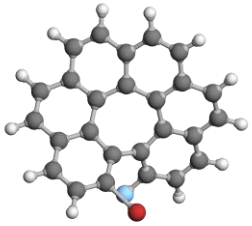
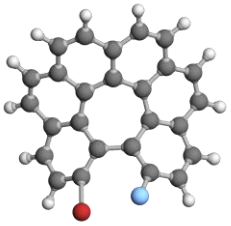
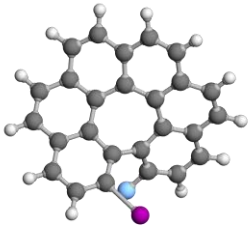
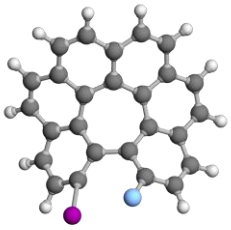
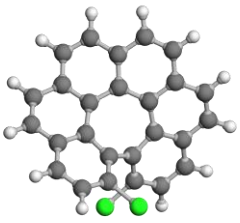
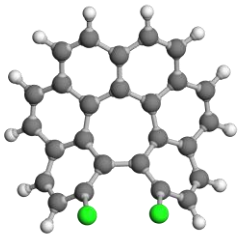
	
$PAH7_{Br,Br}$ ∠A: 48.62° ∠B: 64.96°	+30.19kcal mol^{-1} ∠A: 15.51° ∠B: 53.30°
	
$PAH7_{Me,Me}$ ∠A: 36.22° ∠B: 63.91°	+25.03kcal mol^{-1} ∠A: 10.15° ∠B: 53.35°

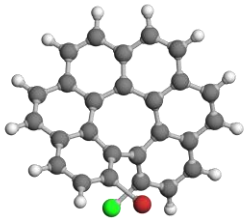
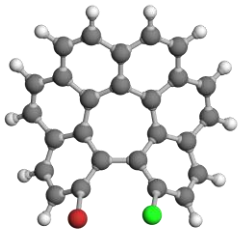
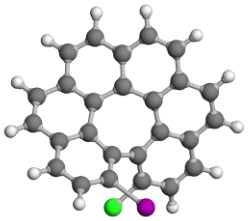
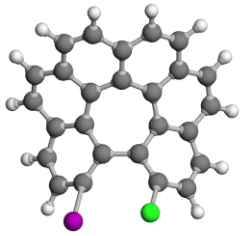
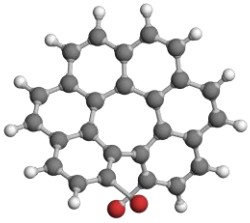
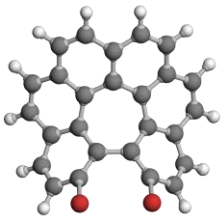
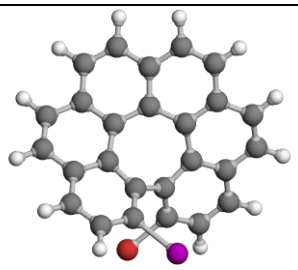
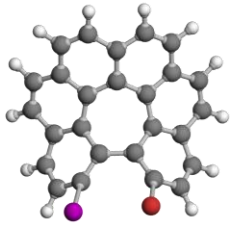
5. The enantiomerization energy barriers (in kcal mol^{-1}) and angle of PAH8.

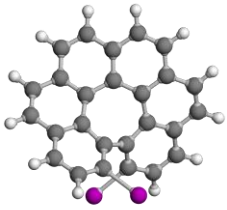
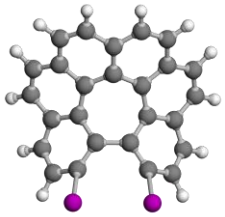
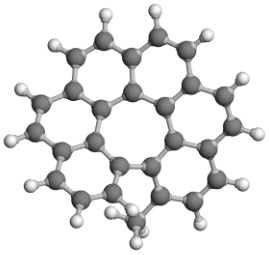
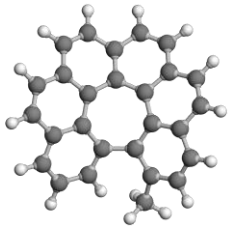
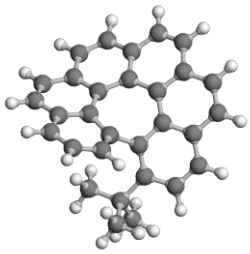
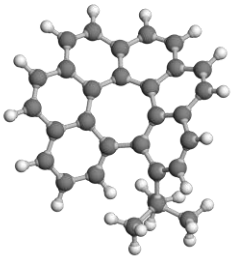
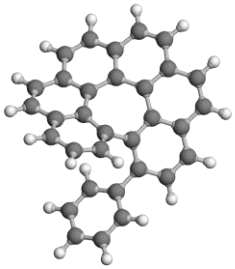
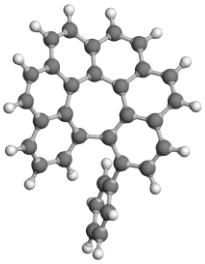
Figure S10. The enantiomerization energy barriers (in kcal mol^{-1}) and angle of PAH8.

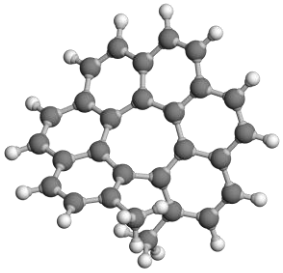
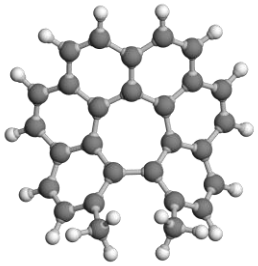
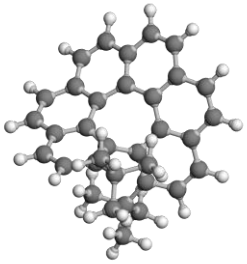
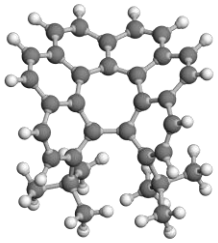
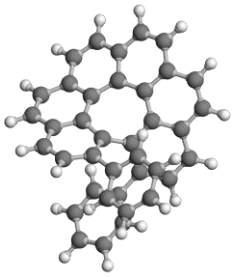
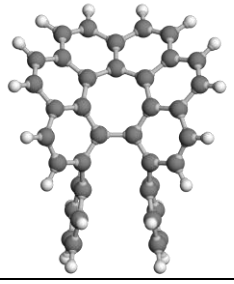
	
$PAH8_{H,H}$ ∠A: 40.02° ∠B: 85.87°	+15.88 kcal mol^{-1} ∠A: 0° ∠B: 73.28°
	
$PAH8_{F,H}$ ∠A: 43.34° ∠B: 86.96°	+20.01 kcal mol^{-1} ∠A: −3.86° ∠B: 70.82°

	
$PAH8_{Cl,H}$ ∠A: 46.87° ∠B: 87.85°	+26.56 kcal mol^{-1} ∠A: −7.43° ∠B: 69.11°
	
$PAH8_{Br,H}$ ∠A: 47.26° ∠B: 88.0°	+27.92 kcal mol^{-1} ∠A: −8.44° ∠B: 69.08°
	
$PAH8_{I,H}$ ∠A: 47.71° ∠B: 88.14°	+29.27 kcal mol^{-1} ∠A: −9.35° ∠B: 69.21°
	
$PAH8_{F,F}$ ∠A: 45.17° ∠B: 87.82°	+33.27 kcal mol^{-1} ∠A: 0° ∠B: 66.85°

	
$PAH8_{F,Cl}$ ∠A: 49.10° ∠B: 88.85°	+41.21 kcal mol^{-1} ∠A: −5.2° ∠B: 65.30°
	
$PAH8_{F,Br}$ ∠A: 49.77° ∠B: 89.07°	+42.40 kcal mol^{-1} ∠A: −8.08° ∠B: 65.61°
	
$PAH8_{F,I}$ ∠A: 50.57° ∠B: 89.28°	+42.75 kcal mol^{-1} ∠A: −10.23° ∠B: 66.28°
	
$PAH8_{Cl,Cl}$ ∠A: 52.75° ∠B: 89.94°	+52.04 kcal mol^{-1} ∠A: 0° ∠B: 62.45°

	
$PAH8_{Cl,Br}$ ∠A: 53.37° ∠B: 89.83°	+54.15 kcal mol^{-1} ∠A: −3.48° ∠B: 62.36°
	
$PAH8_{Cl,I}$ ∠A: 54.04° ∠B: 89.63°	+55.36 kcal mol^{-1} ∠A: −7.55° ∠B: 62.87°
	
$PAH8_{Br,Br}$ ∠A: 53.98° ∠B: 89.61°	+56.72 kcal mol^{-1} ∠A: 0° ∠B: 61.96°
	
$PAH8_{Br,I}$ ∠A: 54.62° ∠B: 89.42°	+58.52 kcal mol^{-1} ∠A: −4.71° ∠B: 62.16°

	
$PAH8_{I,I}$ ∠A: 55.22° ∠B: 89.23°	+61.23 kcal mol^{-1} ∠A: 0° ∠B: 61.79°
	
$PAH8_{Me,H}$ ∠A: 46.65° ∠B: 87.65°	+27.37 kcal mol^{-1} ∠A: −6.59° ∠B: 69.32°
	
$PAH8_{tBu,H}$ ∠A: 48.98° ∠B: 88.76°	+36.04 kcal mol^{-1} ∠A: −16.07° ∠B: 69.06°
	
$PAH8_{Ph,H}$ ∠A: 44.77° ∠B: 87.78°	+25.93 kcal mol^{-1} ∠A: −9.06° ∠B: 69.90°

	
$PAH8_{Me,Me}$ ∠A: 52.86° ∠B: 89.75°	+51.47 kcal mol^{-1} ∠A: 0° ∠B: 62.07°
	
$PAH8_{tBu,tBu}$ ∠A: 61.88° ∠B: 87.53°	+80.05 kcal mol^{-1} ∠A: −10.28° ∠B: 57.31°
	
$PAH8_{Ph,Ph}$ ∠A: 49.33° ∠B: 89.53°	+51.11 kcal mol^{-1} ∠A: 0° ∠B: 63.14°

6. Cartesian coordinates of the optimized geometries (in Å)

$Phen_{H,H}$

C	2.859901	-1.520896	0.000080	C	-1.486374	-1.556356	-0.000084
C	1.486359	-1.556378	0.000084	C	-2.859929	-1.520862	-0.000080
C	0.723533	-0.376162	0.000004	C	-3.535938	-0.296004	0.000008
C	1.412442	0.860169	-0.000044	C	-2.817917	0.872847	0.000065
C	2.817930	0.872819	-0.000064	H	3.421050	-2.447452	0.000159
C	3.535929	-0.296030	-0.000007	H	3.327397	1.829980	-0.000119
C	-0.723537	-0.376164	-0.000005	H	4.618776	-0.272985	-0.000020
C	-1.412441	0.860188	0.000043	H	-1.227435	3.014824	0.000073
C	-0.675393	2.081742	0.000033	H	1.227465	3.014810	-0.000079
C	0.675412	2.081734	-0.000037	H	-3.421056	-2.447431	-0.000160

H	-4.618783	-0.272914	0.000025	H	0.991593	-2.518130	0.000168
H	-3.327394	1.830003	0.000120	H	-0.991644	-2.518128	-0.000168

$Phen_{F,H}$

C	2.913903	-1.077221	-0.000083	C	-3.620492	-0.310004	-0.000022
C	1.550464	-1.217229	-0.000058	C	-2.963088	0.893525	0.000061
C	0.651340	-0.134598	-0.000048	H	3.524619	-1.970401	-0.000082
C	1.256412	1.152014	-0.000040	H	3.068856	2.295880	-0.000038
C	2.653100	1.295471	-0.000061	H	4.552011	0.313626	-0.000118
C	3.475546	0.198595	-0.000086	H	-1.527121	3.115401	0.000155
C	-0.795631	-0.240592	-0.000046	H	0.923137	3.284778	0.000046
C	-1.560070	0.955068	0.000042	H	-3.383752	-2.449206	-0.000214
C	-0.910548	2.223787	0.000088	H	-4.703010	-0.344434	-0.000005
C	0.434493	2.317509	0.000028	H	-3.518985	1.824374	0.000131
C	-1.501777	-1.460041	-0.000149	H	-0.965025	-2.393013	-0.000242
C	-2.876798	-1.491894	-0.000133	F	1.089037	-2.477893	-0.000034

$Phen_{Cl,H}$

C	2.943068	-0.408749	0.080479	C	-3.682983	-0.540002	0.029448
C	1.618261	-0.786165	0.017017	C	-3.170533	0.723451	-0.111041
C	0.556177	0.153912	0.037255	H	3.699788	-1.181311	0.065557
C	0.967298	1.520454	0.034755	H	2.568923	2.938054	0.107256
C	2.320400	1.883506	0.099049	H	4.349178	1.209360	0.193614
C	3.303979	0.932534	0.140115	H	-2.039807	3.096297	-0.251799
C	-0.874750	-0.126536	0.046401	H	0.364385	3.587278	-0.078456
C	-1.785774	0.956678	-0.087201	H	-3.186995	-2.607590	0.363327
C	-1.313409	2.297766	-0.154594	H	-4.753077	-0.706162	0.012902
C	0.002098	2.566097	-0.062243	H	-3.830503	1.575549	-0.228336
C	-1.441902	-1.403527	0.225526	H	-0.807930	-2.255070	0.390960
C	-2.802388	-1.605509	0.217240	Cl	1.405659	-2.502347	-0.160253

$Phen_{Br,H}$

C	2.555069	0.985841	0.192103	C	-3.558034	-1.549158	0.061422
C	1.461342	0.151985	0.093475	C	-3.535367	-0.200236	-0.182291
C	0.131032	0.641449	0.082148	H	3.544958	0.550705	0.202921
C	0.015196	2.063186	0.039658	H	0.988449	3.967811	0.120443
C	1.139704	2.895050	0.139161	H	3.268457	3.006247	0.327037
C	2.398345	2.367537	0.243415	H	-3.337377	2.416118	-0.460180
C	-1.101038	-0.136231	0.092936	H	-1.292885	3.760230	-0.200532
C	-2.334458	0.527181	-0.145443	H	-2.366656	-3.252768	0.621055
C	-2.377939	1.943398	-0.284863	H	-4.491337	-2.098037	0.035417
C	-1.258628	2.678407	-0.146618	H	-4.454020	0.337928	-0.386794
C	-1.172754	-1.509127	0.393423	H	-0.282297	-2.046290	0.668062
C	-2.363353	-2.197307	0.377469	Br	1.958243	-1.668954	-0.159560

$Phen_{I,H}$

C	1.705564	1.960482	0.314629	C	-3.157316	-2.499364	0.097314
C	0.967967	0.800621	0.185496	C	-3.581562	-1.241674	-0.247819
C	-0.448542	0.818603	0.126957	H	2.784293	1.900818	0.364608
C	-1.040348	2.112361	0.029113	H	-0.773144	4.235926	0.098800
C	-0.270795	3.277552	0.157435	H	1.681496	4.103577	0.446867
C	1.084247	3.207131	0.337343	H	-4.270012	1.278863	-0.675536
C	-1.344546	-0.327759	0.139881	H	-2.832415	3.249860	-0.352487
C	-2.709379	-0.141655	-0.202481	H	-1.507609	-3.648181	0.869838
C	-3.221942	1.168783	-0.422269	H	-3.841155	-3.338595	0.064800
C	-2.433614	2.247290	-0.250325	H	-4.612013	-1.068353	-0.536757
C	-0.965905	-1.615674	0.556480	H	0.026914	-1.786808	0.937596
C	-1.842976	-2.674558	0.533944	I	2.198321	-0.880612	-0.145742

$Phen_{F,Cl}$

C	2.943176	-0.568021	0.063253	C	-3.617762	-0.095685	-0.135992
C	1.592607	-0.791217	-0.108996	C	-2.993364	1.100709	-0.389475
C	0.643808	0.243052	0.060315	H	3.627093	-1.395699	-0.067433
C	1.172679	1.558983	0.157483	H	2.907661	2.784901	0.436149
C	2.547115	1.768428	0.332756	H	4.482585	0.868569	0.477982
C	3.420978	0.710490	0.335919	H	-1.629677	3.369120	-0.538776
C	-0.798666	0.097112	0.053567	H	0.748138	3.671264	0.010604
C	-1.602958	1.226176	-0.256976	H	-3.333898	-2.098195	0.645203
C	-0.996714	2.516982	-0.321310	H	-4.691596	-0.189684	-0.236598
C	0.308378	2.681515	-0.027265	H	-3.569307	1.977352	-0.660085
C	-1.505945	-1.052387	0.446645	F	-0.865300	-2.049938	1.058461
C	-2.868601	-1.173861	0.329351	Cl	1.165815	-2.342068	-0.739967

$Phen_{F,Br}$

C	2.677619	0.787009	0.291431	C	-3.612061	-1.097126	-0.117523
C	1.503522	0.090991	0.093762	C	-3.430268	0.214305	-0.482006
C	0.245217	0.732724	0.139191	H	3.617655	0.253480	0.257222
C	0.274401	2.154299	0.128634	H	1.452277	3.930303	0.350557
C	1.475361	2.847254	0.331145	H	3.588412	2.700619	0.631936
C	2.660069	2.168766	0.466154	H	-2.932387	2.798499	-0.830535
C	-1.054353	0.091839	0.111756	H	-0.848029	3.961937	-0.239148
C	-2.181073	0.833551	-0.331773	H	-2.696142	-2.790805	0.879807
C	-2.058180	2.244540	-0.509883	H	-4.578179	-1.572038	-0.231795
C	-0.913043	2.881166	-0.192972	H	-4.259282	0.802952	-0.855580
C	-1.338279	-1.190829	0.609909	F	-0.423674	-1.834158	1.338660
C	-2.563448	-1.795414	0.477270	Br	1.724772	-1.690757	-0.507628

$Phen_{F,I}$

C	1.812442	1.945697	0.448030	C	1.027410	0.830216	0.234195

C	-0.383178	0.927245	0.181510	C	-3.514689	-1.030752	-0.547976
C	-0.916857	2.241555	0.082710	H	2.887946	1.838703	0.491565
C	-0.103001	3.361272	0.301675	H	-0.551585	4.346419	0.252108
C	1.239324	3.212983	0.540896	H	1.869544	4.074504	0.722694
C	-1.324602	-0.173380	0.143070	H	-4.048096	1.522408	-1.058990
C	-2.621418	0.039525	-0.394101	H	-2.630379	3.440049	-0.455714
C	-3.050168	1.374001	-0.663918	H	-1.746957	-3.428072	1.051443
C	-2.269522	2.424584	-0.340563	H	-3.883021	-3.110257	-0.214485
C	-1.112854	-1.436908	0.718608	H	-4.482889	-0.838120	-0.993981
C	-1.990889	-2.482951	0.584820	F	-0.062394	-1.625573	1.522218
C	-3.189892	-2.286865	-0.097710	I	2.098304	-0.870037	-0.372435

Phen$_{Cl,Cl}$

C	-2.925398	-0.719036	0.077069	C	3.523277	0.450899	0.383488
C	-1.564227	-0.768419	0.294106	C	2.765608	1.589003	0.508190
C	-0.724293	0.322969	-0.019680	H	-3.524475	-1.585190	0.323538
C	-1.382883	1.553702	-0.283062	H	-3.228946	2.539172	-0.745698
C	-2.765546	1.589055	-0.508196	H	-4.590863	0.474433	-0.561818
C	-3.523239	0.450965	-0.383486	H	1.177908	3.704302	0.357515
C	0.724332	0.322958	0.019666	H	-1.177807	3.704321	-0.357548
C	1.382942	1.553677	0.283048	H	3.524479	-1.585254	-0.323553
C	0.646246	2.774781	0.191542	H	4.590900	0.474340	0.561830
C	-0.646163	2.774792	-0.191564	H	3.229021	2.539112	0.745698
C	1.564249	-0.768444	-0.294127	Cl	0.985296	-2.135643	-1.176907
C	2.925418	-0.719090	-0.077078	Cl	-0.985303	-2.135641	1.176869

Phen$_{Cl,Br}$

C	2.754492	0.641984	0.270219	C	-3.635073	-0.671940	-0.427975
C	1.526759	0.074861	0.001937	C	-3.326579	0.639260	-0.693898
C	0.327549	0.809284	0.130422	H	3.647512	0.040693	0.166844
C	0.475346	2.217343	0.249562	H	1.797303	3.855002	0.654798
C	1.727417	2.780972	0.530012	H	3.816658	2.424034	0.822130
C	2.849009	1.992672	0.598901	H	-2.615926	3.192322	-0.794943
C	-1.017290	0.277584	0.040773	H	-0.489321	4.136856	0.010168
C	-2.046883	1.140423	-0.419722	H	-2.969630	-2.461487	0.573023
C	-1.805086	2.547774	-0.476703	H	-4.621694	-1.062633	-0.642736
C	-0.637474	3.064770	-0.044445	H	-4.077523	1.316483	-1.082899
C	-1.434600	-0.996084	0.485227	Cl	-0.478639	-1.929794	1.579588
C	-2.700334	-1.475144	0.220242	Br	1.581839	-1.622343	-0.833697

Phen$_{Cl,I}$

C	1.859207	1.950147	0.501878	C	-0.865049	2.333421	0.174514
C	1.046606	0.875335	0.203133	C	-0.027602	3.413032	0.487268
C	-0.360870	1.005203	0.182445	C	1.311478	3.215245	0.712270

C	-1.319243	-0.074646	0.064354	H	-0.452248	4.409631	0.513122
C	-2.571632	0.203434	-0.544035	H	1.959961	4.045210	0.963477
C	-2.969751	1.563253	-0.729574	H	-3.943817	1.755873	-1.163442
C	-2.200159	2.573336	-0.276278	H	-2.545787	3.599537	-0.319886
C	-1.174778	-1.367384	0.613056	H	-1.907081	-3.355788	0.762892
C	-2.065868	-2.379411	0.325568	H	-3.874851	-2.929294	-0.690458
C	-3.188359	-2.124813	-0.458685	H	-4.393407	-0.594407	-1.343947
C	-3.464206	-0.835415	-0.841561	Cl	-0.016496	-1.695579	1.852706
H	2.932926	1.819548	0.515995	I	2.044249	-0.780723	-0.610895

Phen$_{Br,Br}$

C	2.913925	0.206463	-0.253818	C	-3.448489	-0.957310	0.803456
C	1.589462	0.250947	0.125626	C	-2.682242	-2.095449	0.844180
C	0.717154	-0.835429	-0.101271	H	3.546058	1.063989	-0.068062
C	1.337507	-2.064394	-0.450559	H	3.113998	-3.042589	-1.144752
C	2.682229	-2.095440	-0.844210	H	4.485789	-0.976860	-1.112908
C	3.448475	-0.957307	-0.803477	H	-1.123323	-4.215087	0.504049
C	-0.717163	-0.835426	0.101270	H	1.123310	-4.215081	-0.504095
C	-1.337522	-2.064400	0.450540	H	-3.546055	1.064001	0.068072
C	-0.617001	-3.285731	0.271523	H	-4.485805	-0.976875	1.112879
C	0.616989	-3.285728	-0.271557	H	-3.114022	-3.042598	1.144702
C	-1.589464	0.250951	-0.125615	Br	-1.105292	1.709230	-1.230899
C	-2.913934	0.206462	0.253820	Br	1.105292	1.709198	1.230944

Phen$_{Br,I}$

C	1.816943	2.082283	0.626622	C	-3.145081	-1.870770	-1.007316
C	1.020445	1.058273	0.156488	C	-3.448820	-0.541165	-1.163521
C	-0.388768	1.161598	0.170744	H	2.893009	1.973702	0.608034
C	-0.918087	2.461094	0.390222	H	-0.539665	4.457248	1.075248
C	-0.097509	3.487985	0.877226	H	1.882962	4.069400	1.439087
C	1.247405	3.281297	1.055092	H	-3.986808	2.056458	-1.030312
C	-1.325346	0.096710	-0.123333	H	-2.627905	3.756994	0.122388
C	-2.581376	0.449908	-0.683826	H	-1.855545	-3.267163	0.005269
C	-3.008345	1.812977	-0.633393	H	-3.810871	-2.638238	-1.381445
C	-2.260142	2.746367	-0.010985	H	-4.381020	-0.237274	-1.624658
C	-1.157982	-1.266488	0.201723	Br	0.062817	-1.831107	1.534341
C	-2.024105	-2.232938	-0.262271	I	2.031706	-0.415213	-0.942177

Phen$_{I,I}$

C	0.163499	2.801088	-0.823672	C	1.322276	3.209032	-1.484695
C	0.119311	1.581160	-0.180693	C	1.207577	-0.683837	0.239167
C	1.208172	0.682877	-0.239150	C	2.434805	-1.219153	0.711824
C	2.435880	1.217155	-0.711723	C	3.656979	-0.550355	0.391937
C	2.462100	2.452767	-1.373535	C	3.657469	0.547330	-0.391751

C	0.117967	-1.581201	0.180631	H	4.586039	-0.998954	0.723560
C	0.161082	-2.801170	0.823609	H	4.586930	0.995146	-0.723309
C	1.319467	-3.210094	1.484708	H	-0.689375	-3.467005	0.765004
C	2.459937	-2.454787	1.373630	H	1.333688	-4.161428	2.001678
H	-0.686397	3.467643	-0.765126	H	3.404159	-2.817813	1.762041
H	3.406655	2.814991	-1.761884	I	-1.445213	1.360389	1.200195
H	1.337329	4.160351	-2.001670	I	-1.446288	-1.359106	-1.200351

$Phen_{Cl,H}^{‡}$

C	2.948247	-0.379941	-0.000260	C	-3.691138	-0.556994	0.000340
C	1.626080	-0.773235	-0.000135	C	-3.183268	0.715723	0.000269
C	0.551879	0.155106	-0.000055	H	3.711503	-1.146114	-0.000315
C	0.953058	1.526096	-0.000116	H	2.539716	2.961064	-0.000284
C	2.303621	1.903670	-0.000243	H	4.342313	1.252384	-0.000414
C	3.298727	0.964659	-0.000315	H	-2.071162	3.094402	0.000124
C	-0.879278	-0.134501	0.000079	H	0.337936	3.591695	-0.000099
C	-1.798680	0.951297	0.000141	H	-3.180688	-2.647575	0.000336
C	-1.336978	2.297116	0.000074	H	-4.761090	-0.724774	0.000439
C	-0.019631	2.568767	-0.000048	H	-3.846461	1.573355	0.000312
C	-1.443245	-1.426031	0.000155	H	-0.807450	-2.290908	0.000116
C	-2.803197	-1.632207	0.000282	Cl	1.444329	-2.502069	-0.000090

$Phen_{Br,H}^{‡}$

C	2.525000	1.058079	0.000023	C	-3.562738	-1.620714	-0.000030
C	1.453567	0.188522	0.000012	C	-3.570252	-0.250537	-0.000024
C	0.104972	0.634648	0.000005	H	3.525969	0.649292	0.000028
C	-0.045062	2.057037	0.000010	H	0.871876	3.989167	0.000024
C	1.058497	2.921917	0.000021	H	3.191696	3.098478	0.000037
C	2.336280	2.435053	0.000028	H	-3.437809	2.370399	-0.000012
C	-1.114860	-0.170377	-0.000007	H	-1.392542	3.738129	0.000008
C	-2.376030	0.488825	-0.000013	H	-2.301705	-3.364906	-0.000029
C	-2.457241	1.908807	-0.000007	H	-4.491031	-2.178564	-0.000039
C	-1.339265	2.655823	0.000004	H	-4.507059	0.295083	-0.000028
C	-1.153832	-1.578119	-0.000014	H	-0.240440	-2.142253	-0.000010
C	-2.335353	-2.282169	-0.000025	Br	2.043252	-1.624871	0.000008

$Phen_{I,H}^{‡}$

C	1.671038	1.976648	0.000027	C	-1.378221	-0.362779	-0.000003
C	0.945574	0.799744	0.000016	C	-2.784785	-0.145349	-0.000008
C	-0.477298	0.789409	0.000009	C	-3.319418	1.172117	-0.000003
C	-1.081753	2.086802	0.000014	C	-2.499904	2.237692	0.000008
C	-0.320254	3.263811	0.000026	C	-0.965283	-1.707572	-0.000010
C	1.045443	3.218295	0.000032	C	-1.855189	-2.755986	-0.000021

C	-3.230140	-2.525071	-0.000026	H	-2.897203	3.245898	0.000013
C	-3.677431	-1.229966	-0.000020	H	-1.473414	-3.769747	-0.000025
H	2.751300	1.929246	0.000032	H	-3.929681	-3.351838	-0.000035
H	-0.844233	4.212193	0.000029	H	-4.739905	-1.014442	-0.000023
H	1.640210	4.122898	0.000041	H	0.080645	-1.952386	-0.000006
H	-4.396278	1.294106	-0.000007	I	2.274830	-0.846103	0.000011

Phen$_{F,Cl}$‡

C	3.028821	-0.282311	0.000056	C	-3.734875	-0.145845	0.000089
C	1.703661	-0.684064	0.000059	C	-3.108619	1.069618	0.000056
C	0.620509	0.250513	0.000038	H	3.783748	-1.055906	0.000076
C	1.059179	1.617921	0.000000	H	2.645290	3.047185	-0.000036
C	2.410979	1.989789	-0.000007	H	4.448217	1.327671	0.000022
C	3.401787	1.051066	0.000024	H	-1.885056	3.320362	-0.000022
C	-0.842764	0.029247	0.000050	H	0.544005	3.707507	-0.000060
C	-1.708698	1.172585	0.000037	H	-3.364815	-2.277537	0.000122
C	-1.185056	2.493923	-0.000006	H	-4.814236	-0.225913	0.000102
C	0.137612	2.703443	-0.000026	H	-3.681903	1.988361	0.000046
C	-1.569099	-1.186530	0.000082	F	-0.969545	-2.373363	0.000097
C	-2.941103	-1.281967	0.000098	Cl	1.610369	-2.414008	0.000086

Phen$_{F,Br}$‡

C	2.525889	1.211272	-0.000005	C	-3.720981	-1.400100	-0.000009
C	1.481528	0.300607	-0.000011	C	-3.638037	-0.035288	-0.000001
C	0.109729	0.713886	-0.000006	H	3.534615	0.824296	-0.000008
C	-0.044714	2.143478	0.000002	H	0.819503	4.095491	0.000012
C	1.037253	3.034558	0.000006	H	3.167615	3.258938	0.000005
C	2.323497	2.581455	0.000003	H	-3.426353	2.519466	0.000010
C	-1.145151	-0.071747	-0.000009	H	-1.356218	3.848733	0.000014
C	-2.398915	0.624626	0.000000	H	-2.520400	-3.201043	-0.000022
C	-2.453252	2.044127	0.000007	H	-4.676378	-1.908637	-0.000011
C	-1.325759	2.765981	0.000008	H	-4.533274	0.574031	0.000008
C	-1.321496	-1.475047	-0.000013	F	-0.288946	-2.311760	-0.000014
C	-2.536067	-2.119193	-0.000017	Br	2.231319	-1.452750	-0.000026

Phen$_{F,I}$‡

C	1.697148	2.006613	0.000023	C	-3.315408	1.395976	-0.000007
C	0.962730	0.828517	0.000012	C	-2.435664	2.405261	0.000004
C	-0.473403	0.844287	0.000005	C	-1.228759	-1.649533	-0.000014
C	-1.030364	2.170603	0.000010	C	-2.202015	-2.618956	-0.000025
C	-0.248266	3.333407	0.000021	C	-3.543964	-2.269410	-0.000030
C	1.112417	3.263346	0.000028	C	-3.856911	-0.938150	-0.000024
C	-1.460500	-0.257478	-0.000007	H	2.775435	1.941612	0.000029
C	-2.860349	0.051046	-0.000013	H	-0.758980	4.288561	0.000024

H	1.730858	4.151731	0.000036	H	-4.313302	-3.030649	-0.000039
H	-4.383015	1.577778	-0.000012	H	-4.889728	-0.612449	-0.000027
H	-2.769469	3.435798	0.000008	F	0.007383	-2.140747	-0.000010
H	-1.875317	-3.650386	-0.000029	I	2.393555	-0.743622	0.000011

Phen$_{Cl,Cl}$‡

C	3.083262	-0.529647	0.000078	C	-3.643270	0.733279	0.000082
C	1.713569	-0.747919	0.000054	C	-2.785052	1.791184	0.000023
C	0.749420	0.315324	0.000020	H	3.721044	-1.401884	0.000112
C	1.394414	1.605889	-0.000017	H	3.155273	2.808580	-0.000036
C	2.785138	1.791064	-0.000005	H	4.717688	0.862901	0.000067
C	3.643311	0.733122	0.000051	H	-1.229827	3.751611	-0.000087
C	-0.749397	0.315357	0.000028	H	1.229998	3.751558	-0.000102
C	-1.394335	1.605950	-0.000002	H	-3.721095	-1.401723	0.000138
C	-0.667079	2.826646	-0.000058	H	-4.717641	0.863104	0.000106
C	0.667210	2.826618	-0.000066	H	-3.155143	2.808717	-0.000002
C	-1.713592	-0.747845	0.000069	Cl	-1.440093	-2.457089	0.000077
C	-3.083275	-0.529514	0.000101	Cl	1.439997	-2.457152	0.000060

Phen$_{Cl,Br}$‡

C	2.565842	1.335905	0.027755	C	-3.868664	-1.034066	0.009097
C	1.511821	0.431605	0.029858	C	-3.669113	0.313438	-0.003065
C	0.132108	0.843200	0.016660	H	3.568953	0.936584	0.038352
C	0.018970	2.284188	0.001507	H	0.898073	4.226670	-0.012130
C	1.110466	3.165089	-0.000117	H	3.244309	3.371968	0.011862
C	2.391103	2.706307	0.012902	H	-3.334424	2.793530	-0.025662
C	-1.164114	0.085771	0.015701	H	-1.216483	4.044536	-0.024228
C	-2.378657	0.864935	-0.000085	H	-2.841798	-2.909021	0.034606
C	-2.378984	2.284565	-0.014283	H	-4.859078	-1.470134	0.006938
C	-1.230391	2.962037	-0.013496	H	-4.506240	0.999990	-0.015441
C	-1.455151	-1.317187	0.027815	Cl	-0.336102	-2.631131	0.048319
C	-2.742129	-1.833049	0.024502	Br	2.325760	-1.297491	0.052505

Phen$_{Cl,I}$‡

C	1.685259	2.088997	-0.266124	C	-1.412492	-1.575051	-0.095849
C	0.954173	0.911576	-0.142074	C	-2.491998	-2.435770	-0.200092
C	-0.486431	0.925062	-0.019408	C	-3.799253	-1.986902	-0.190436
C	-1.002230	2.272945	0.067786	C	-3.990745	-0.645055	-0.046937
C	-0.214136	3.430139	-0.011344	H	2.755184	2.017520	-0.388852
C	1.127556	3.353466	-0.211207	H	-0.714772	4.386820	0.069102
C	-1.527445	-0.153956	-0.018045	H	1.751110	4.232988	-0.305234
C	-2.910800	0.247669	0.039105	H	-4.361471	1.822584	0.272281
C	-3.304646	1.602033	0.191245	H	-2.668375	3.608883	0.317210
C	-2.385830	2.568613	0.215671	H	-2.278241	-3.492918	-0.271898

H	-4.625919	-2.680405	-0.272703	Cl	0.048400	-2.479583	-0.028756
H	-4.988764	-0.227541	-0.000912	I	2.487679	-0.581353	-0.094134

Phen$_{Br,Br}$‡

C	-3.079950	0.120667	0.317513	C	3.623221	1.392677	0.298751
C	-1.727276	-0.127590	0.131788	C	2.769459	2.423481	0.052483
C	-0.750979	0.918433	-0.001426	H	-3.732554	-0.729936	0.447783
C	-1.390364	2.211275	-0.085087	H	-3.131666	3.440235	-0.022510
C	-2.770517	2.422290	0.052515	H	-4.686027	1.540573	0.441745
C	-3.623834	1.391119	0.298792	H	1.230227	4.331574	-0.420906
C	0.750567	0.918756	-0.001435	H	-1.232112	4.331045	-0.420892
C	1.389395	2.211872	-0.085103	H	3.732855	-0.728331	0.447741
C	0.665889	3.416051	-0.296753	H	4.685351	1.542588	0.441691
C	-0.667379	3.415765	-0.296745	H	3.130169	3.441581	-0.022547
C	1.727315	-0.126847	0.131768	Br	1.549555	-2.016859	-0.003519
C	3.079884	0.121992	0.317478	Br	-1.548706	-2.017525	-0.003501

Phen$_{Br,I}$‡

C	-1.594118	2.376725	0.510685	C	3.797511	-1.682358	0.461247
C	-0.917328	1.199208	0.215337	C	3.992370	-0.379196	0.115252
C	0.506186	1.185930	-0.019729	H	-2.645390	2.316955	0.749788
C	1.029657	2.522872	-0.171418	H	0.780672	4.641744	-0.113796
C	0.280268	3.691955	0.027553	H	-1.591495	4.518061	0.667782
C	-1.012705	3.631464	0.443889	H	4.353138	2.008461	-0.603368
C	1.527616	0.091371	-0.011342	H	2.674027	3.812977	-0.684629
C	2.911055	0.486246	-0.111286	H	2.297211	-3.193174	0.625551
C	3.301431	1.811955	-0.437236	H	4.620219	-2.349704	0.682286
C	2.392183	2.787454	-0.481433	H	4.990206	0.032356	0.028418
C	1.414135	-1.323584	0.170643	Br	-0.103798	-2.423821	-0.083646
C	2.493069	-2.144432	0.454165	I	-2.485563	-0.224954	-0.012041

Phen$_{I,I}$‡

C	0.654006	3.009217	0.660054	C	1.944157	-3.530155	0.600334
C	0.350908	1.710367	0.278031	C	2.913289	-2.730339	0.077262
C	1.376472	0.748312	-0.020398	H	-0.157531	3.661607	0.948281
C	2.656083	1.385634	-0.204726	H	3.910241	3.109190	-0.087316
C	2.906494	2.737476	0.077240	H	2.124639	4.558781	0.895235
C	1.935376	3.534884	0.600306	H	4.696351	-1.229324	-0.889204
C	1.378328	-0.744986	-0.020392	H	4.693281	1.240890	-0.889214
C	2.659519	-1.379127	-0.204715	H	-0.148429	-3.662077	0.948312
C	3.808396	-0.662918	-0.637499	H	2.135964	-4.553576	0.895272
C	3.806737	0.672280	-0.637505	H	3.917957	-3.099559	-0.087292
C	0.355158	-1.709584	0.278046	I	-1.737092	1.710625	-0.056532
C	0.661485	-3.007674	0.660079	I	-1.732835	-1.715035	-0.056518

Phen$_{Me,H}$

C	2.938736	0.968061	0.000911	H	3.615302	1.813385	0.054208
C	1.578840	1.217175	0.054520	H	2.991586	-2.398497	-0.137661
C	0.667158	0.122947	-0.011404	H	4.541924	-0.459693	-0.143952
C	1.226708	-1.186182	-0.042192	H	-1.577305	-3.111018	0.177915
C	2.614668	-1.382915	-0.101349	H	0.868931	-3.312959	0.008853
C	3.469526	-0.315310	-0.098246	H	-3.369447	2.442037	-0.289091
C	-0.787057	0.229829	-0.025221	H	-4.710046	0.366493	0.006800
C	-1.572128	-0.951961	0.074187	H	-3.534307	-1.801123	0.188836
C	-0.948304	-2.231014	0.107698	H	-0.974152	2.361461	-0.327455
C	0.390760	-2.340178	0.017587	C	1.195401	2.658328	0.235201
C	-1.498981	1.437246	-0.174291	H	0.778601	3.098390	-0.674355
C	-2.873871	1.486579	-0.165781	H	0.466888	2.792894	1.035914
C	-3.627999	0.323439	-0.009427	H	2.082583	3.236848	0.491791
C	-2.974593	-0.876907	0.098013				

Phen$_{tBu,H}$

C	-2.456594	0.980806	-0.552429	H	1.303396	3.685782	0.513450
C	-1.457217	0.096560	-0.174316	H	2.405470	-3.080817	-1.251480
C	-0.130530	0.623842	-0.094616	H	4.470975	-2.121202	-0.249090
C	0.017837	2.037875	-0.022624	H	4.416766	0.180686	0.644861
C	-1.053156	2.888055	-0.324933	H	0.318541	-1.826259	-1.187467
C	-2.263497	2.354570	-0.678021	C	-1.936032	-1.302724	0.285272
C	1.106889	-0.137817	-0.131968	C	-0.993582	-1.977520	1.287736
C	2.320047	0.458560	0.293418	H	-0.731259	-1.287756	2.092529
C	2.349391	1.846413	0.616871	H	-1.509054	-2.830488	1.733804
C	1.263748	2.610351	0.381916	H	-0.069934	-2.347623	0.856922
C	1.197137	-1.407277	-0.724497	C	-3.255893	-1.132146	1.065696
C	2.378770	-2.108245	-0.775151	H	-4.087657	-0.813419	0.439068
C	3.543164	-1.562795	-0.228634	H	-3.536022	-2.093027	1.501495
C	3.509574	-0.288984	0.281384	H	-3.142203	-0.409823	1.875753
H	-3.458928	0.604718	-0.701599	C	-2.245073	-2.228753	-0.895495
H	-0.899082	3.960246	-0.288070	H	-1.369330	-2.475145	-1.494537
H	-3.089451	2.990649	-0.971712	H	-2.668004	-3.167893	-0.529750
H	3.279736	2.284068	0.959822	H	-2.976782	-1.766957	-1.561530

Phen$_{Me,Me}$

C	2.903811	1.027098	0.191009	C	0.654563	-2.465031	-0.160473
C	1.530168	1.109271	0.354616	C	-1.530119	1.109333	-0.354604
C	0.727855	-0.007312	0.011178	C	-2.903768	1.027196	-0.191024
C	1.391899	-1.242292	-0.221427	C	-3.531027	-0.138677	0.236497
C	2.781586	-1.279509	-0.390289	C	-2.781623	-1.279423	0.390242
C	3.531027	-0.138787	-0.236542	H	3.507271	1.888777	0.455860
C	-0.727846	-0.007286	-0.011183	H	3.255564	-2.230635	-0.604029
C	-1.391933	-1.242246	0.221398	H	4.605938	-0.162312	-0.367666
C	-0.654639	-2.465011	0.160431	H	-1.194091	-3.394782	0.300239

H	1.193983	-3.394819	-0.300293	H	-0.019042	2.183028	1.413966
H	-3.507198	1.888898	-0.455870	H	1.629402	2.519460	1.935449
H	-4.605942	-0.162169	0.367602	C	-1.001362	2.324073	-1.064069
H	-3.255632	-2.230538	0.603965	H	-1.027748	3.220741	-0.442915
C	1.001457	2.324001	1.064135	H	0.019111	2.183051	-1.413958
H	1.027940	3.220707	0.443041	H	-1.629338	2.519637	-1.935338

Phen$_{Me,tBu}$

C	-2.554389	0.791946	-0.600693	H	4.592846	-1.658278	0.269966
C	-1.474121	0.044218	-0.148198	H	4.222882	0.635890	1.138856
C	-0.200767	0.681131	-0.148596	C	-1.841813	-1.270334	0.577925
C	-0.182536	2.103698	-0.169149	C	0.473106	-1.801229	-1.803008
C	-1.316402	2.822923	-0.562698	H	0.143427	-2.800297	-1.512326
C	-2.474423	2.154041	-0.872529	H	-0.408661	-1.192604	-1.986299
C	1.100704	0.026395	-0.117629	H	1.010704	-1.908233	-2.747799
C	2.188354	0.728068	0.467501	C	-2.610767	-2.243079	-0.318961
C	2.065434	2.128678	0.724929	H	-2.921265	-3.112100	0.266135
C	0.976215	2.799786	0.300290	H	-3.512230	-1.787518	-0.731046
C	1.392936	-1.183658	-0.789187	H	-2.005685	-2.598485	-1.151133
C	2.640786	-1.762281	-0.626929	C	-0.692239	-2.007791	1.261666
C	3.636239	-1.166678	0.141590	H	-0.021647	-2.512570	0.574130
C	3.423897	0.093369	0.646575	H	-0.095357	-1.335244	1.878660
H	-3.525166	0.317433	-0.670495	H	-1.119006	-2.770159	1.917324
H	-1.263366	3.904532	-0.607955	C	-2.778409	-0.845610	1.728618
H	-3.348039	2.688287	-1.225303	H	-3.686637	-0.365791	1.365453
H	2.911008	2.650021	1.158447	H	-3.067468	-1.724645	2.309617
H	0.927863	3.881043	0.361504	H	-2.272992	-0.144721	2.396015
H	2.852781	-2.690254	-1.147240				

Phen$_{tBu,tBu}$

C	2.840354	-0.250273	0.663324	H	2.797031	2.923618	1.786446
C	1.637807	-0.317298	-0.032088	H	4.159910	0.843640	1.957413
C	0.709110	0.738193	0.175657	H	-0.990528	4.114063	-0.739097
C	1.224197	1.962149	0.690519	H	0.990872	4.113865	0.739062
C	2.452187	1.989752	1.357796	H	-3.547411	-1.064003	-0.564683
C	3.219658	0.851707	1.419883	H	-4.160404	0.844435	-1.956951
C	-0.709311	0.738334	-0.175821	H	-2.797088	2.924152	-1.786245
C	-1.224245	1.962390	-0.690580	C	1.590419	-1.375642	-1.156959
C	-0.544544	3.187488	-0.396565	C	-1.590486	-1.375358	1.156881
C	0.544744	3.187380	0.396473	C	1.852588	-2.794031	-0.644631
C	-1.638169	-0.316951	0.032103	H	1.909279	-3.482002	-1.491545
C	-2.840840	-0.249722	-0.663072	H	2.793764	-2.868689	-0.098832
C	-3.220057	0.852326	-1.419582	H	1.057317	-3.143741	0.012663
C	-2.452345	1.990221	-1.357656	C	0.333740	-1.394742	-2.019877
H	3.546801	-1.064677	0.565046	H	-0.538425	-1.776691	-1.499700

H	0.084743	-0.403279	-2.399549	H	-0.517626	-2.045415	2.877329
H	0.518234	-2.045652	-2.877826	C	-2.738335	-0.994097	2.113688
C	2.738423	-0.994166	-2.113485	H	-3.709862	-1.021546	1.620741
H	3.709845	-1.021500	-1.620324	H	-2.762548	-1.690431	2.955488
H	2.762927	-1.690454	-2.955315	H	-2.590400	0.013872	2.506261
H	2.590428	0.013801	-2.506041	C	-1.852511	-2.793761	0.644501
C	-0.333567	-1.394277	2.019462	H	-2.793820	-2.868575	0.098958
H	0.538579	-1.775846	1.498961	H	-1.057348	-3.143252	-0.013044
H	-0.084761	-0.402817	2.399265	H	-1.908824	-3.481810	1.491375

Phen$_{Ph,H}$

C	-0.797910	2.633521	-0.193740	H	4.443852	-0.383835	0.548703
C	-0.589362	1.268024	-0.113828	H	3.901306	2.010604	0.402738
C	0.736785	0.757911	-0.065889	H	-0.141851	-3.729223	-0.917877
C	1.792286	1.700532	0.058565	H	2.167794	-4.408813	-0.292198
C	1.534004	3.078847	-0.006936	H	3.815940	-2.666230	0.302452
C	0.256303	3.544964	-0.167526	C	-1.811220	0.440962	0.028565
C	1.091076	-0.651176	-0.147159	C	-2.793445	0.438450	-0.957626
C	2.429899	-1.041373	0.115085	C	-2.030037	-0.290010	1.195546
C	3.429755	-0.054390	0.353092	C	-3.958536	-0.297142	-0.793336
C	3.131041	1.258155	0.277757	H	-2.630231	1.003880	-1.867665
C	0.197560	-1.663631	-0.546404	C	-3.194481	-1.018857	1.362388
C	0.577102	-2.983638	-0.600643	H	-1.272149	-0.287615	1.969686
C	1.877418	-3.365769	-0.261028	C	-4.161421	-1.030068	0.365479
C	2.789185	-2.399530	0.078034	H	-4.708438	-0.297817	-1.575328
H	-1.819010	2.994219	-0.228512	H	-3.349880	-1.580935	2.275439
H	2.368382	3.765847	0.076309	H	-5.070472	-1.604626	0.494867
H	0.057166	4.607737	-0.228441	H	-0.807990	-1.409495	-0.838700

Phen$_{Ph,Ph}$

C	-0.373753	2.910180	0.027192	H	0.488275	3.529016	-0.188771
C	-0.290591	1.552427	-0.233971	H	-3.648811	3.214705	0.772017
C	-1.420104	0.727338	0.023520	H	-1.576129	4.573523	0.669968
C	-2.655323	1.377603	0.281618	H	-4.807255	-1.181610	-0.350016
C	-2.693890	2.755990	0.542628	H	-4.807253	1.181508	0.350136
C	-1.551383	3.509605	0.469087	H	0.488289	-3.529078	0.188882
C	-1.420099	-0.727415	-0.023502	H	-1.576130	-4.573629	-0.669777
C	-2.655323	-1.377693	-0.281548	H	-3.648815	-3.214817	-0.771855
C	-3.878229	-0.647889	-0.186102	C	0.924859	-1.089500	0.936358
C	-3.878228	0.647794	0.186190	C	2.186686	-1.548047	0.562510
C	-0.290581	-1.552490	0.234000	C	0.821159	-0.273649	2.063020
C	-0.373747	-2.910257	-0.027089	C	3.313791	-1.191407	1.282501
C	-1.551382	-3.509701	-0.468944	H	2.286512	-2.159067	-0.325961
C	-2.693891	-2.756090	-0.542505	C	1.948399	0.085797	2.781659

H	-0.154286	0.073896	2.379126	C	3.313770	1.191351	-1.282509
C	3.200775	-0.369597	2.393669	H	2.286526	2.158776	0.326116
H	4.287083	-1.544551	0.963797	C	1.948330	-0.085524	-2.781901
H	1.846775	0.717982	3.655773	H	-0.154355	-0.073596	-2.379384
H	4.082475	-0.086718	2.955913	C	3.200724	0.369744	-2.393823
C	0.924832	1.089487	-0.936393	H	4.287076	1.544397	-0.963738
C	2.186677	1.547915	-0.562462	H	1.846682	-0.717546	-3.656130
C	0.821102	0.273842	-2.063203	H	4.082415	0.086926	-2.956113

Phen$_{Me,H}^{‡}$

C	-2.948356	0.953237	−0.000307	H	-3.629829	1.796068	−0.000348
C	-1.589617	1.215121	−0.000113	H	-2.978301	-2.414925	−0.000531
C	-0.667414	0.125378	−0.000054	H	-4.545443	-0.488745	−0.000602
C	-1.222149	-1.187342	−0.000220	H	1.591115	-3.110219	−0.000018
C	-2.609911	-1.395603	−0.000413	H	-0.860977	-3.313430	−0.000337
C	-3.473264	-0.335980	−0.000454	H	3.374887	2.461811	0.000724
C	0.788641	0.236076	0.000156	H	4.717611	0.365607	0.000699
C	1.576659	-0.949397	0.000158	H	3.537239	-1.807868	0.000343
C	0.957821	-2.230525	−0.000027	H	0.987243	2.389798	0.000397
C	-0.383504	-2.340312	−0.000202	C	-1.225103	2.672189	0.000008
C	1.505409	1.450797	0.000371	H	-0.649228	2.955725	0.883466
C	2.880415	1.497837	0.000562	H	-0.648924	2.955794	−0.883229
C	3.635354	0.325374	0.000550	H	-2.135370	3.270935	−0.000123
C	2.979613	-0.877960	0.000352				

Phen$_{Me,Me}^{‡}$

C	-3.059352	0.899822	−0.001983	H	-3.157630	-2.439150	−0.002010
C	-1.692563	1.147995	−0.001104	H	-4.708548	-0.484968	−0.003029
C	-0.752163	0.051389	−0.000486	H	1.231186	-3.386501	0.000802
C	-1.390278	-1.238982	−0.000885	H	-1.231210	-3.386491	−0.000769
C	-2.783802	-1.422392	−0.001779	H	3.720587	1.756900	0.002397
C	-3.633006	-0.361299	−0.002337	H	4.708547	-0.485005	0.003028
C	0.752166	0.051383	0.000483	H	3.157614	-2.439175	0.002031
C	1.390271	-1.238993	0.000895	C	-1.436999	2.631208	−0.000958
C	0.667661	-2.461535	0.000438	H	-0.904015	2.969152	0.881780
C	-0.667678	-2.461530	−0.000415	H	-0.902875	2.969129	−0.883015
C	1.692575	1.147982	0.001090	H	-2.394604	3.147468	−0.001582
C	3.059362	0.899799	0.001970	C	1.437021	2.631197	0.000930
C	3.633006	-0.361327	0.002337	H	0.904041	2.969137	−0.881811
C	2.783794	-1.422414	0.001790	H	0.902900	2.969130	0.882984
H	-3.720571	1.756929	−0.002419	H	2.394631	3.147450	0.001550

Phen$_{Me,tBu}^{‡}$

C	2.719092	-1.908171	-0.407694	C	1.119186	-0.097165	0.059763
C	1.420205	-1.506248	-0.103676	C	2.319552	0.703162	0.156005

C	3.615884	0.214020	-0.061437	C	-2.140143	-1.139483	0.137125
C	3.825706	-1.082980	-0.419244	C	-1.655988	-1.574281	1.538392
C	-0.182438	0.677867	0.034578	H	-1.862354	-2.629610	1.732517
C	-0.057701	2.111187	0.085621	H	-0.605673	-1.379148	1.732252
C	1.158047	2.775778	0.403501	H	-2.221047	-0.991142	2.268946
C	2.303649	2.095254	0.444024	C	-1.880590	-2.008484	-1.111377
C	-1.564074	0.252760	-0.123847	H	-0.878238	-1.907393	-1.517902
C	-2.530328	1.176045	-0.488834	H	-2.084870	-3.067237	-0.931771
C	-2.327880	2.544529	-0.572872	H	-2.567650	-1.666650	-1.888205
C	-1.104369	3.003166	-0.202207	C	-3.671513	-1.171226	0.298898
H	2.870703	-2.966946	-0.583687	H	-4.020230	-0.466199	1.054829
H	4.438910	0.912892	0.024731	H	-4.210253	-0.985061	-0.630830
H	4.810808	-1.466597	-0.652363	H	-3.947771	-2.176356	0.627197
H	1.129491	3.848253	0.551733	C	0.625582	-2.776960	0.133603
H	3.250202	2.588569	0.627283	H	1.032810	-3.251904	1.030849
H	-3.528741	0.817703	-0.679214	H	-0.426417	-2.698295	0.277000
H	-3.131729	3.210095	-0.861032	H	0.790966	-3.467274	-0.694872
H	-0.890622	4.063986	-0.153088				

Phen$_{tBu,H}$‡

C	-2.523495	1.110558	-0.053172	H	1.389937	3.726020	0.055607
C	-1.511033	0.167617	-0.013183	H	2.328916	-3.359559	-0.161614
C	-0.140470	0.628361	-0.014493	H	4.513991	-2.160506	-0.018895
C	0.044117	2.046883	-0.008696	H	4.491982	0.313009	0.096944
C	-1.033093	2.945964	-0.045640	H	0.285661	-2.173781	-0.157955
C	-2.313656	2.485775	-0.078977	C	-1.974034	-1.295960	0.034719
C	1.095922	-0.173956	-0.020713	C	-1.454334	-1.968907	1.324520
C	2.361704	0.482734	0.038638	H	-2.111572	-1.690652	2.150416
C	2.454012	1.898877	0.078902	H	-1.482529	-3.057905	1.233072
C	1.337505	2.643611	0.042135	H	-0.449912	-1.676207	1.613568
C	1.172877	-1.581792	-0.096834	C	-3.497911	-1.456320	0.138636
C	2.358391	-2.278316	-0.099064	H	-4.024111	-1.069636	-0.735394
C	3.579906	-1.612609	-0.021683	H	-3.717192	-2.524957	0.201246
C	3.564447	-0.245894	0.044329	H	-3.905086	-0.985173	1.034717
H	-3.547301	0.773355	-0.059106	C	-1.617968	-1.992630	-1.298797
H	-0.816510	4.007755	-0.045708	H	-0.667086	-1.684487	-1.724463
H	-3.157215	3.164232	-0.112664	H	-1.610797	-3.080089	-1.184565
H	3.435842	2.355166	0.125831	H	-2.382364	-1.743847	-2.037059

Phen$_{tBu,tBu}$‡

C	-2.857805	-0.075318	-1.120348	C	-3.356399	1.210198	-1.308049
C	-1.767196	-0.378849	-0.326688	C	0.618795	0.818500	0.178520
C	-0.878773	0.706580	0.058373	C	1.087113	2.139616	0.497814
C	-1.592972	1.948416	0.138996	C	0.242894	3.126383	1.090285
C	-2.804165	2.185696	-0.532927	C	-1.072253	3.057932	0.863495

C	1.713888	-0.039663	-0.303128	H	-0.486938	-1.075536	1.888458
C	2.726815	0.620423	-0.984590	H	-2.182318	-1.160879	2.296487
C	3.038987	1.967443	-0.856556	H	-1.237541	-2.648568	2.202290
C	2.310181	2.670050	0.054448	C	-3.275798	-2.296430	0.397377
H	-3.440180	-0.897497	-1.511926	H	-3.713502	-2.585653	-0.558292
H	-3.239519	3.175371	-0.462982	H	-3.269684	-3.191079	1.025723
H	-4.222671	1.388179	-1.932232	H	-3.923374	-1.555419	0.867513
H	0.704169	3.996828	1.540808	C	2.286371	-2.334330	-1.316289
H	-1.745077	3.866371	1.123380	H	1.367169	-2.322172	-1.898161
H	3.430532	0.011597	-1.534269	H	3.075856	-1.956694	-1.968022
H	3.888047	2.393652	-1.375315	H	2.528669	-3.373363	-1.080351
H	2.565024	3.684724	0.334494	C	3.643786	-1.396568	0.535497
C	-1.823632	-1.790244	0.279412	H	3.660022	-0.764402	1.425229
C	2.200282	-1.507770	-0.025825	H	3.988943	-2.392887	0.821349
C	-1.122218	-2.822802	-0.604089	H	4.362254	-0.993614	-0.174092
H	-1.044555	-3.794351	-0.108257	C	1.506820	-2.277347	1.089740
H	-1.716452	-2.959512	-1.510487	H	1.502953	-1.692249	2.010420
H	-0.136565	-2.514080	-0.919307	H	0.501813	-2.585893	0.874053
C	-1.384163	-1.666040	1.747959	H	2.083080	-3.184433	1.283932

Phen$_{Ph,H}^{‡}$

C	0.794087	2.628117	0.000000	H	-4.525692	-0.353177	-0.000001
C	0.581299	1.261288	0.000000	H	-3.932983	2.033952	-0.000001
C	-0.743075	0.742001	0.000000	H	0.189905	-3.825849	0.000000
C	-1.802218	1.693694	0.000000	H	-2.224849	-4.431105	0.000000
C	-1.539977	3.072530	0.000000	H	-3.912925	-2.624612	-0.000001
C	-0.255586	3.543778	0.000000	C	1.828480	0.451183	0.000000
C	-1.101385	-0.673068	0.000000	C	2.441139	0.098492	1.199058
C	-2.475504	-1.036674	0.000000	C	2.441140	0.098492	-1.199057
C	-3.488916	-0.036629	-0.000001	C	3.627311	-0.619311	1.199331
C	-3.163839	1.270135	-0.000001	H	1.971801	0.378071	2.134740
C	-0.172348	-1.732618	0.000000	C	3.627311	-0.619311	-1.199330
C	-0.566262	-3.050095	0.000000	H	1.971802	0.378071	-2.134739
C	-1.919454	-3.391910	0.000000	C	4.220768	-0.985567	0.000001
C	-2.854358	-2.389790	0.000000	H	4.089745	-0.893180	2.140046
H	1.817577	2.983585	0.000000	H	4.089746	-0.893179	-2.140044
H	-2.381395	3.755970	0.000000	H	5.146201	-1.548426	0.000001
H	-0.051776	4.607357	0.000000	H	0.883135	-1.528205	0.000000

Phen$_{Ph,Ph}^{‡}$

C	0.723792	-3.043066	0.082759	C	3.050854	-2.782361	0.083501
C	0.493306	-1.668058	0.049544	C	1.979971	-3.623203	0.100869
C	1.593220	-0.745814	0.027095	C	1.593208	0.745842	-0.027126
C	2.880971	-1.390390	0.045765	C	2.880949	1.390438	-0.045827

C	4.104073	0.667589	-0.022017	H	-1.129027	0.804941	-2.083245
C	4.104083	-0.667523	0.021920	C	-3.084263	2.107560	0.973059
C	0.493280	1.668070	-0.049545	H	-1.173399	2.243517	1.932915
C	0.723744	3.043082	-0.082756	C	-3.762820	1.779282	-0.190105
C	1.979914	3.623238	-0.100894	H	-3.577497	1.034733	-2.192383
C	3.050810	2.782412	-0.083560	H	-3.625189	2.484861	1.832792
H	-0.146200	-3.685312	0.113097	H	-4.838167	1.895730	-0.247886
H	4.063849	-3.166330	0.097283	C	-0.987380	-1.479746	0.057588
H	2.094744	-4.699210	0.133044	C	-1.677950	-1.153621	1.217326
H	5.028888	1.231149	-0.039805	C	-1.709388	-1.961475	-1.034199
H	5.028908	-1.231069	0.039683	C	-3.055170	-1.296388	1.280215
H	-0.146258	3.685315	-0.113070	H	-1.128980	-0.804955	2.083273
H	2.094670	4.699246	-0.133064	C	-3.084247	-2.107606	-0.972998
H	4.063799	3.166396	-0.097367	H	-1.173397	-2.243531	-1.932886
C	-0.987403	1.479734	-0.057562	C	-3.762789	-1.779339	0.190178
C	-1.677987	1.153598	-1.217288	H	-3.577444	-1.034787	2.192453
C	-1.709401	1.961452	1.034237	H	-3.625181	-2.484916	-1.832721
C	-3.055211	1.296342	-1.280154	H	-4.838133	-1.895805	0.247977

H3O$_{tBu,H}$

C	2.342018	1.333052	-0.000216	H	-4.247766	1.179316	0.000152
C	1.496995	0.229496	-0.000099	C	2.065151	-1.183369	-0.000038
C	0.109185	0.495803	-0.000041	C	1.613498	-1.909747	-1.272940
C	-0.311668	1.835594	-0.000105	H	1.911381	-2.960619	-1.235666
C	0.530656	2.927552	-0.000221	H	0.538884	-1.864090	-1.432161
C	1.881833	2.648988	-0.000276	H	2.088168	-1.455420	-2.145057
C	-1.135567	-0.270251	0.000077	C	3.592537	-1.203532	-0.000110
C	-2.159991	0.688311	0.000070	H	4.007762	-0.720801	-0.886833
C	-1.523682	-1.612972	0.000185	H	4.007848	-0.720691	0.886513
C	-2.869877	-1.936326	0.000280	H	3.932358	-2.241360	-0.000063
C	-3.854079	-0.949622	0.000269	C	1.613621	-1.909586	1.272999
C	-3.507268	0.390522	0.000163	H	0.539024	-1.863905	1.432321
H	3.410721	1.176743	-0.000263	H	1.911497	-2.960465	1.235828
H	0.138340	3.935371	-0.000266	H	2.088379	-1.455153	2.145013
H	2.599140	3.460485	-0.000367	H	-0.796996	-2.410740	0.000198
H	-3.161371	-2.979207	0.000363	O	-1.667453	1.953112	-0.000039
H	-4.899409	-1.232209	0.000344				

H3S$_{tBu,H}$

C	2.402751	1.365852	-0.000237	C	-0.993288	-0.426126	0.000031
C	1.575311	0.251585	-0.000066	C	-2.210539	0.290584	0.000341
C	0.167840	0.474009	0.000038	C	-1.109001	-1.824952	-0.000323
C	-0.272397	1.818334	0.000278	C	-2.343596	-2.443750	-0.000322
C	0.579059	2.914850	0.000182	C	-3.521456	-1.701525	0.000075
C	1.930840	2.675138	-0.000172	C	-3.456872	-0.324669	0.000405

H	3.472420	1.222649	-0.000385	C	3.747319	-1.085763	0.000196
H	0.180141	3.921371	0.000354	H	4.144684	-0.590281	-0.887379
H	2.633653	3.499255	-0.000340	H	4.144438	-0.589512	0.887455
H	-2.388393	-3.525787	-0.000614	H	4.125324	-2.110578	0.000649
H	-4.482713	-2.200132	0.000131	C	1.833314	-1.873756	1.292485
H	-4.358524	0.275306	0.000691	H	0.780603	-1.796682	1.548537
C	2.217333	-1.134268	0.000057	H	2.095877	-2.932488	1.221404
C	1.833442	-1.873919	-1.292346	H	2.392851	-1.446659	2.127105
H	2.095151	-2.932843	-1.220881	H	-0.237033	-2.454425	-0.000617
H	0.780902	-1.796065	-1.548912	S	-1.992311	2.001567	0.000581
H	2.393668	-1.447482	-2.126834				

H3Se$_{tBu,H}$

C	-2.279957	-1.783763	-0.000048	H	3.939346	1.239914	0.001155
C	-1.762969	-0.494726	-0.000059	C	-2.751361	0.671834	-0.000455
C	-0.342759	-0.344969	0.000309	C	-2.584644	1.482030	-1.298857
C	0.417858	-1.536442	0.000625	H	-3.090651	2.447698	-1.218675
C	-0.125667	-2.811746	0.000644	H	-1.551231	1.657351	-1.582910
C	-1.493894	-2.929526	0.000307	H	-3.046821	0.931857	-2.120756
C	0.524397	0.849802	0.000395	C	-4.215708	0.221830	-0.000717
C	1.904858	0.554826	0.000751	H	-4.469984	-0.360022	-0.888257
C	0.206124	2.217818	0.000227	H	-4.470418	-0.359728	0.886891
C	1.183826	3.193742	0.000399	H	-4.847890	1.112702	-0.001008
C	2.532913	2.858430	0.000732	C	-2.585181	1.482404	1.297783
C	2.895137	1.527617	0.000904	H	-1.551875	1.657832	1.582158
H	-3.350638	-1.916311	-0.000325	H	-3.091204	2.448027	1.217173
H	0.515346	-3.684428	0.000907	H	-3.047613	0.932427	2.119671
H	-1.962780	-3.905913	0.000329	H	-0.815842	2.548327	-0.000063
H	0.884891	4.234649	0.000273	Se	2.272485	-1.275686	0.001027
H	3.292441	3.630312	0.000849				

H3Te$_{tBu,H}$

C	2.245603	-2.073107	0.000080	H	1.583293	-4.113936	-0.000062
C	1.950821	-0.715009	0.000086	H	0.417308	4.407416	0.000074
C	0.573227	-0.322211	-0.000053	H	-2.069786	4.402476	-0.000373
C	-0.372415	-1.375516	-0.000248	H	-3.262705	2.238771	-0.000637
C	-0.043468	-2.722499	-0.000257	C	3.137780	0.252762	0.000206
C	1.284130	-3.072825	-0.000070	C	3.130130	1.073028	1.305565
C	-0.044268	1.028863	-0.000096	H	3.773330	1.952396	1.215086
C	-1.457405	1.076839	-0.000347	H	2.143841	1.398972	1.622119
C	0.583321	2.286517	0.000043	H	3.527888	0.453402	2.111444
C	-0.127428	3.471295	-0.000045	C	4.498837	-0.453452	0.000188
C	-1.515308	3.472187	-0.000293	H	4.647552	-1.070092	0.888083
C	-2.179549	2.263024	-0.000445	H	4.647339	-1.070428	-0.887509
H	3.279150	-2.381031	0.000182	H	5.277973	0.312407	-0.000035
H	-0.817778	-3.479937	-0.000407	C	3.130197	1.073259	-1.305004

H	2.143961	1.399477	-1.621432	H	1.652400	2.368699	0.000216
H	3.773586	1.952475	-1.214403	Te	-2.351336	-0.778866	-0.000519
H	3.527774	0.453698	-2.111023				

H3N$_{tBu,H}$

C	2.374550	1.293418	0.000316	H	-4.304375	1.120739	-0.000352
C	1.494227	0.219650	0.000299	C	2.031871	-1.206182	0.000328
C	0.110599	0.519415	0.000127	C	1.570684	-1.921068	-1.276195
C	-0.278794	1.882578	0.000180	H	1.824110	-2.983209	-1.230194
C	0.617636	2.941295	0.000318	H	0.503138	-1.829989	-1.457716
C	1.956216	2.624107	0.000343	H	2.081097	-1.490536	-2.140059
C	-1.138170	-0.238516	-0.000278	C	3.558755	-1.264178	-0.000860
C	-2.188633	0.711612	-0.000177	H	3.985522	-0.792806	-0.887940
C	-1.506672	-1.588116	-0.000750	H	3.986915	-0.792346	0.885303
C	-2.842074	-1.946930	-0.001011	H	3.871080	-2.310660	-0.000831
C	-3.849513	-0.982349	-0.000843	C	1.572759	-1.920262	1.278052
C	-3.531918	0.361102	-0.000435	H	0.505562	-1.828859	1.461417
H	3.437342	1.103697	0.000360	H	1.825893	-2.982479	1.232210
H	0.273807	3.968337	0.000368	H	2.084776	-1.489349	2.140777
H	2.698454	3.412893	0.000410	H	-0.765862	-2.371773	-0.000914
H	-3.107193	-2.996580	-0.001352	N	-1.646621	1.966934	0.000121
H	-4.888367	-1.288009	-0.001070	H	-2.168036	2.822321	0.000005

H3P$_{tBu,H}$

C	-2.411797	1.366191	-0.045731	H	4.379717	0.155494	0.024533
C	-1.568597	0.257974	-0.008527	C	-2.211723	-1.129519	0.010798
C	-0.167341	0.501290	0.006534	C	-1.823206	-1.855035	1.311001
C	0.264669	1.847747	0.009145	H	-2.065956	-2.918920	1.245723
C	-0.606715	2.923340	-0.007702	H	-0.774923	-1.756937	1.577080
C	-1.961197	2.676851	-0.052160	H	-2.398055	-1.433118	2.137808
C	1.003311	-0.421830	0.007254	C	-3.742877	-1.084595	0.025440
C	2.240036	0.259742	0.010628	H	-4.132847	-0.572049	0.906601
C	1.066742	-1.820124	-0.007843	H	-4.152926	-0.610438	-0.867944
C	2.281403	-2.485982	-0.035634	H	-4.116308	-2.110865	0.050730
C	3.481421	-1.791461	-0.036475	C	-1.846105	-1.880226	-1.282134
C	3.454295	-0.408753	0.000808	H	-0.802679	-1.786303	-1.568427
H	-3.479214	1.207549	-0.064339	H	-2.086511	-2.942924	-1.192354
H	-0.223882	3.937021	0.016137	H	-2.435853	-1.474338	-2.106440
H	-2.673693	3.492405	-0.078381	H	0.177409	-2.423194	-0.001327
H	2.283317	-3.569261	-0.051813	H	2.315066	2.370542	-1.232032
H	4.425022	-2.322650	-0.054976	P	2.057504	2.050256	0.130112

H3As$_{tBu,H}$

C	2.266287	-1.817223	-0.035658	C	0.340661	-0.366071	-0.005275
C	1.757191	-0.519899	-0.009443	C	-0.435439	-1.545969	-0.011211

C	0.106484	-2.817547	-0.019488	C	2.602165	1.431868	1.316973
C	1.477668	-2.954608	-0.044707	H	3.114708	2.394947	1.246651
C	-0.513258	0.862327	-0.004080	H	1.569856	1.611390	1.602085
C	-1.901193	0.611641	-0.008947	H	3.060106	0.871457	2.134386
C	-0.138945	2.211978	-0.007276	C	4.224341	0.159187	0.026328
C	-1.080010	3.229268	-0.024020	H	4.457762	-0.438795	0.908935
C	-2.436343	2.950279	-0.028259	H	4.485585	-0.412270	-0.865954
C	-2.842352	1.626613	-0.010051	H	4.868313	1.041391	0.048836
H	3.336401	-1.955352	-0.044221	C	2.632954	1.452530	-1.284554
H	-0.538794	-3.688279	-0.005804	H	1.607427	1.635761	-1.591196
H	1.939879	-3.934254	-0.061793	H	3.142813	2.414721	-1.187109
H	-0.737294	4.257049	-0.029431	H	3.110522	0.905085	-2.099491
H	-3.165812	3.750796	-0.037950	H	0.893049	2.507528	0.001628
H	-3.898643	1.382745	0.003773	H	-2.591284	-1.428004	-1.421111
C	2.766137	0.631049	0.011663	As	-2.343779	-1.260869	0.077051

H3Sb$_{tBu,H}$

C	2.235444	-2.103244	-0.018142	H	-3.192450	2.343197	0.006444
C	1.950978	-0.737722	-0.005318	C	3.155084	0.211344	0.004800
C	0.578328	-0.341116	-0.003386	C	3.156198	1.025691	1.314518
C	-0.381406	-1.379616	-0.006041	H	3.808955	1.898574	1.228979
C	-0.055825	-2.723457	-0.004509	H	2.173649	1.360753	1.633067
C	1.271750	-3.093494	-0.019764	H	3.547593	0.397760	2.117168
C	-0.023528	1.037916	-0.003139	C	4.506352	-0.514833	0.010978
C	-1.433743	1.120490	-0.007797	H	4.640238	-1.138519	0.896376
C	0.645734	2.269142	-0.002700	H	4.654356	-1.128375	-0.879211
C	-0.028809	3.480112	-0.010650	H	5.295751	0.240480	0.021186
C	-1.410653	3.526931	-0.012268	C	3.171788	1.034652	-1.299359
C	-2.108116	2.330108	-0.003248	H	2.192955	1.371112	-1.627713
H	3.267185	-2.417708	-0.023170	H	3.822951	1.907297	-1.200056
H	-0.834736	-3.477536	0.007531	H	3.573200	0.412283	-2.101349
H	1.563281	-4.136978	-0.026865	H	1.716193	2.322579	0.002816
H	0.547953	4.397360	-0.012212	H	-2.608267	-0.841383	-1.657572
H	-1.935807	4.474282	-0.015587	Sb	-2.408256	-0.755398	0.045224

H3C$_{tBu,H}$

C	-2.411569	1.248214	0.000284	C	1.474653	-1.554341	0.000080
C	-1.485618	0.206539	0.000011	C	2.800809	-1.962018	0.000282
C	-0.118343	0.568284	-0.000096	C	3.836325	-1.039079	0.000315
C	0.226321	1.933981	-0.000116	C	3.543087	0.316523	0.000091
C	-0.717067	2.941547	0.000141	H	-3.465520	1.012556	0.000425
C	-2.052359	2.588103	0.000384	H	-0.412276	3.981771	0.000166
C	1.157995	-0.194611	-0.000082	H	-2.823681	3.348891	0.000650
C	2.223199	0.723805	-0.000126	H	3.024765	-3.022046	0.000430

H	4.865909	-1.375432	0.000528	H	-3.793225	-2.392232	-0.000403
H	4.340197	1.051629	0.000094	C	-1.520196	-1.935532	-1.284619
C	-1.987003	-1.235113	-0.000144	H	-0.465772	-1.788804	-1.501469
C	-1.520245	-1.935784	1.284211	H	-1.715277	-3.009660	-1.227507
H	-1.715301	-3.009906	1.226883	H	-2.078330	-1.538622	-2.135151
H	-0.465831	-1.789074	1.501127	H	0.713051	-2.316087	0.000057
H	-2.078417	-1.539050	2.134801	C	1.708645	2.123418	-0.000462
C	-3.513408	-1.336384	-0.000208	H	2.046273	2.683776	0.877405
H	-3.956069	-0.879615	0.886895	H	2.045627	2.682712	-0.879297
H	-3.955995	-0.879289	-0.887180				

H3Si$_{tBu,H}$

C	-2.432688	1.350276	0.000133	C	-2.189612	-1.135424	0.000151
C	-1.559427	0.260626	0.000060	C	-1.813839	-1.867566	1.302789
C	-0.164080	0.538502	-0.000061	H	-2.013942	-2.938946	1.216763
C	0.233594	1.899529	-0.000141	H	-0.779864	-1.733699	1.606254
C	-0.671586	2.945810	-0.000095	H	-2.431252	-1.479553	2.115290
C	-2.023123	2.670502	0.000053	C	-3.722634	-1.111331	0.000280
C	1.021380	-0.400863	-0.000094	H	-4.131005	-0.625100	0.887891
C	2.288941	0.232490	-0.000162	H	-4.131167	-0.625602	-0.887530
C	1.031209	-1.798674	-0.000062	H	-4.079136	-2.144027	0.000596
C	2.217571	-2.519135	-0.000112	C	-1.814108	-1.867599	-1.302543
C	3.444592	-1.881193	-0.000188	H	-0.780227	-1.733644	-1.606291
C	3.467888	-0.495546	-0.000213	H	-2.014090	-2.938992	-1.216409
H	-3.495272	1.161991	0.000265	H	-2.431773	-1.479682	-2.114900
H	-0.320465	3.971844	-0.000161	H	0.122801	-2.369842	0.000003
H	-2.758518	3.466066	0.000113	H	2.626158	2.751078	-1.203352
H	2.168722	-3.601738	-0.000088	Si	2.077554	2.067786	-0.000221
H	4.365205	-2.451766	-0.000224	H	2.626188	2.751182	1.202838
H	4.419935	0.024148	-0.000267				

H3Ge$_{tBu,H}$

C	2.279397	-1.813830	0.000127	H	1.999069	-3.936353	0.000355
C	1.746249	-0.523436	0.000003	H	-0.656524	4.250921	0.000874
C	0.326649	-0.394874	0.000101	H	-3.100858	3.823089	0.000336
C	-0.428734	-1.592165	0.000117	H	-3.902465	1.479806	-0.000200
C	0.142522	-2.850430	0.000196	C	2.748799	0.635740	-0.000212
C	1.516961	-2.966095	0.000257	C	2.600819	1.442694	1.304998
C	-0.535420	0.849529	0.000173	H	3.086095	2.418305	1.215508
C	-1.934136	0.638712	-0.000057	H	1.573152	1.597001	1.619842
C	-0.124390	2.186940	0.000525	H	3.096715	0.899388	2.111642
C	-1.033675	3.235044	0.000591	C	4.212615	0.177860	-0.000785
C	-2.396071	3.000612	0.000303	H	4.467680	-0.403408	0.886871
C	-2.838054	1.686820	-0.000007	H	4.466931	-0.403436	-0.888637
H	3.351846	-1.930942	0.000096	H	4.846149	1.067968	-0.001056
H	-0.482816	-3.736018	0.000216	C	2.599980	1.443086	-1.305086

H	1.572122	1.597301	-1.619334	H	-3.063352	-1.748243	-1.252036
H	3.085106	2.418765	-1.215535	H	-3.063728	-1.748106	1.251606
H	3.095574	0.900150	-2.112165	Ge	-2.326514	-1.244979	-0.000133
H	0.913480	2.456520	0.000755				

H3Sn$_{tBu,H}$

C	2.305697	-1.892856	-0.629818	C	3.035313	0.257497	0.409350
C	1.918139	-0.618374	-0.199436	C	2.527537	1.333304	1.374070
C	0.532969	-0.336732	-0.247708	H	3.371805	1.711319	1.954251
C	-0.369297	-1.419667	-0.371252	H	2.064433	2.183758	0.885705
C	0.060736	-2.692621	-0.687121	H	1.800932	0.916571	2.074607
C	1.412361	-2.906496	-0.913563	C	3.934690	-0.645786	1.276331
C	-0.099694	1.014827	-0.244689	H	3.347145	-1.172289	2.030693
C	-1.442845	1.149044	0.154788	H	4.485231	-1.386325	0.698227
C	0.530107	2.133313	-0.788665	H	4.672347	-0.026009	1.789841
C	-0.100015	3.366601	-0.825433	C	3.922436	0.877322	-0.673858
C	-1.387992	3.509461	-0.334088	H	3.381671	1.576292	-1.311754
C	-2.064951	2.388157	0.127049	H	4.750832	1.421355	-0.212952
H	3.360961	-2.116157	-0.709103	H	4.344727	0.103550	-1.318203
H	-0.642824	-3.512091	-0.777943	H	1.517822	2.032555	-1.213857
H	1.775750	-3.872764	-1.242730	H	-3.601145	-0.991325	-0.841103
H	0.417142	4.217861	-1.252018	H	-2.741249	-1.413324	1.773097
H	-1.878341	4.475365	-0.353240	Sn	-2.303290	-0.785846	0.247493
H	-3.097721	2.486636	0.442397				

H3O$_{Br,Br}$

C	-3.115782	0.445324	-0.166429	C	2.357305	2.736332	0.182462
C	-1.817658	-0.031845	-0.058007	H	-3.926992	-0.269058	-0.181106
C	-0.734012	0.861241	-0.040706	H	-2.536938	3.795612	-0.212401
C	-1.088279	2.226205	-0.081182	H	-4.419552	2.134530	-0.318836
C	-2.367317	2.728209	-0.182493	H	3.927254	-0.255565	0.181383
C	-3.391760	1.804949	-0.236624	H	4.411565	2.149710	0.318866
C	0.730414	0.863757	0.040867	H	2.523263	3.804314	0.212261
C	1.079996	2.229932	0.081203	Br	1.693150	-1.896460	-0.120166
C	1.817118	-0.025604	0.058261	Br	-1.687266	-1.902244	0.120612
C	3.113597	0.456026	0.166634	O	-0.005525	3.035085	-0.000031
C	3.384910	1.816598	0.236688				

H3S$_{Br,Br}$

C	-3.022872	-0.017369	-0.373710	C	1.714244	-0.248317	0.020656
C	-1.709825	-0.278304	-0.021007	C	3.022496	0.035580	0.373438
C	-0.726558	0.722785	-0.108512	C	3.401684	1.323544	0.731305
C	-1.217406	2.034419	-0.313728	C	2.492316	2.357741	0.649450
C	-2.533454	2.313714	-0.649814	H	-3.748787	-0.816282	-0.310157
C	-3.424573	1.263746	-0.731597	H	-2.851986	3.333849	-0.820902
C	0.713587	0.735401	0.108068	H	-4.456850	1.443700	-1.003844
C	1.181378	2.055427	0.313312	H	3.762291	-0.750503	0.309961

H	4.430645	1.521553	1.003574	Br	-1.418672	-1.938234	0.826968
H	2.792925	3.383308	0.820489	S	-0.028562	3.253438	-0.000338
Br	1.452235	-1.913199	-0.827122				

H3Se$_{Br,Br}$

C	0.406419	-2.998136	-0.366361	C	-1.924536	2.558070	0.720333
C	0.617045	-1.681648	0.008423	H	1.220468	-3.704256	-0.277066
C	-0.401612	-0.720519	-0.113967	H	-2.927438	-2.906611	-0.924520
C	-1.690957	-1.241732	-0.362503	H	-0.993969	-4.457841	-1.070323
C	-1.922888	-2.559193	-0.720035	H	1.218160	3.705122	0.277819
C	-0.848313	-3.425327	-0.778772	H	-0.996814	4.457213	1.071033
C	-0.402101	0.720416	0.114156	H	-2.929317	2.904867	0.924741
C	-1.691782	1.240784	0.362657	Br	2.222395	1.355960	-0.944479
C	0.615973	1.682200	-0.008058	Br	2.223256	-1.354352	0.944818
C	0.404544	2.998482	0.366945	Se	-3.052700	-0.000887	-0.000031
C	-0.850496	3.424839	0.779318				

H3Te$_{Br,Br}$

C	0.819792	-2.965834	-0.335027	C	-1.502163	2.615680	0.800843
C	0.951853	-1.643472	0.055291	H	1.657586	-3.637347	-0.206705
C	-0.095492	-0.721905	-0.118196	H	-2.478824	-3.010713	-1.051792
C	-1.350808	-1.290573	-0.427158	H	-0.481121	-4.473347	-1.124142
C	-1.502552	-2.615536	-0.800848	H	1.658159	3.636989	0.206812
C	-0.391740	-3.438899	-0.816603	H	-0.480445	4.473331	1.124169
C	-0.095379	0.721825	0.118233	H	-2.478382	3.011009	1.051752
C	-1.350613	1.290694	0.427158	Br	2.488777	1.248493	-1.082197
C	0.952116	1.643228	-0.055215	Br	2.488531	-1.248978	1.082339
C	0.820252	2.965610	0.335102	Te	-2.920245	0.000190	-0.000033
C	-0.391221	3.438869	0.816635				

H3N$_{Br,Br}$

C	-3.095229	0.380914	-0.262499	C	2.408655	2.680794	0.357018
C	-1.793429	-0.043626	-0.051611	H	-3.888276	-0.353536	-0.250459
C	-0.727351	0.871238	-0.069426	H	-2.629375	3.738206	-0.434504
C	-1.109053	2.239652	-0.159155	H	-4.428613	2.022088	-0.596529
C	-2.408433	2.680981	-0.357028	H	3.888268	-0.353833	0.250404
C	-3.399185	1.727124	-0.436962	H	4.428787	2.021748	0.596492
C	0.727434	0.871181	0.069402	H	2.629675	3.738002	0.434508
C	1.109240	2.239566	0.159149	Br	1.630900	-1.864675	-0.410382
C	1.793443	-0.043762	0.051574	Br	-1.631025	-1.864554	0.410330
C	3.095276	0.380677	0.262457	N	0.000121	3.020898	0.000015
C	3.399336	1.726863	0.436931	H	0.000170	4.023366	-0.000045

H3P$_{Br,Br}$

C	-2.955854	0.479823	-0.390888	C	-0.830142	2.222182	-0.378625
C	-1.704365	0.031671	0.010524	C	-2.084227	2.681615	-0.737996
C	-0.579121	0.855719	-0.111766	C	-3.137869	1.785087	-0.816196

C	0.848168	0.590932	0.122037	H	-4.121624	2.116025	-1.124639
C	1.567943	1.775510	0.389324	H	3.501517	-1.521261	0.251019
C	1.607914	-0.576686	-0.014736	H	4.632287	0.522666	1.045675
C	2.949502	-0.595856	0.345478	H	3.417443	2.692161	0.968629
C	3.587390	0.559306	0.763973	Br	0.992088	-2.108310	-0.931302
C	2.905321	1.765488	0.739060	Br	-1.689807	-1.602990	0.955872
H	-3.800330	-0.191808	-0.313866	P	0.571010	3.267991	0.103301
H	-2.245314	3.735512	-0.930188	H	1.112826	3.558091	-1.179575

H3As$_{Br,Br}$

C	0.450040	-2.980467	-0.366713	C	-1.853950	2.575020	0.783975
C	0.623132	-1.662009	0.034635	H	1.274276	-3.672551	-0.258498
C	-0.402701	-0.722659	-0.126885	H	-2.858207	-2.932005	-1.027542
C	-1.677430	-1.241977	-0.439313	H	-0.894694	-4.450466	-1.144121
C	-1.865908	-2.562211	-0.798992	H	1.289066	3.675355	0.229053
C	-0.775953	-3.419667	-0.834226	H	-0.881480	4.468270	1.097921
C	-0.396911	0.729618	0.114922	H	-2.842345	2.941277	1.034398
C	-1.667805	1.257361	0.416914	Br	2.211795	1.294890	-1.016145
C	0.634688	1.662734	-0.043072	Br	2.187085	-1.313118	1.035887
C	0.461442	2.987592	0.338477	H	-3.369082	0.560940	-1.330627
C	-0.764586	3.434338	0.797793	As	-3.094612	-0.013982	0.057417

H3Sb$_{Br,Br}$

C	0.855127	-2.956347	-0.313336	C	-1.432175	2.617350	0.874907
C	0.958054	-1.630324	0.086617	H	1.697360	-3.617497	-0.159923
C	-0.088825	-0.725897	-0.130293	H	-2.407784	-3.023700	-1.154359
C	-1.327104	-1.285340	-0.510143	H	-0.395631	-4.472388	-1.156940
C	-1.445117	-2.614711	-0.871067	H	1.710612	3.614763	0.151439
C	-0.327705	-3.437734	-0.843934	H	-0.379164	4.474850	1.150703
C	-0.083895	0.728611	0.120595	H	-2.390542	3.023444	1.176698
C	-1.318096	1.293604	0.496780	Br	2.477309	1.200607	-1.147157
C	0.967326	1.628405	-0.091570	Br	2.462517	-1.211763	1.154193
C	0.866096	2.956376	0.303942	H	-3.153362	0.737414	-1.495464
C	-0.314509	3.440264	0.836654	Sb	-2.949993	-0.010891	0.034931

H3C$_{Br,Br}$

C	-3.055707	0.269271	-0.349465	C	1.745208	-0.068895	0.033405
C	-1.745441	-0.072147	-0.033282	C	3.054842	0.274985	0.349578
C	-0.732667	0.889194	-0.096702	C	3.396651	1.582684	0.646856
C	-1.142536	2.228998	-0.267789	C	2.438861	2.581662	0.558319
C	-2.444013	2.577073	-0.558424	H	-3.815686	-0.499442	-0.315513
C	-3.399941	1.576313	-0.646854	H	-2.715681	3.616729	-0.696447
C	0.730651	0.890554	0.096737	H	-4.427935	1.815835	-0.888078
C	1.138042	2.231135	0.267702	H	3.816239	-0.492328	0.315716

H	4.424195	1.824130	0.888078	C	-0.003104	3.158344	-0.000111
H	2.708586	3.621838	0.696231	H	0.220856	3.810770	-0.849783
Br	1.524474	-1.798375	-0.688062	H	-0.228257	3.810508	0.849445
Br	-1.521455	-1.801147	0.688339				

H3Si$_{Br,Br}$

C	-2.974641	-0.162534	-0.333508	H	-3.648642	-0.998679	-0.202879
C	-1.648943	-0.299929	0.063076	H	-2.989035	3.116947	-1.116060
C	-0.736213	0.739756	-0.128210	H	-4.473546	1.128310	-1.143231
C	-1.269965	2.002005	-0.482780	H	3.663843	-0.939894	0.203714
C	-2.597500	2.143456	-0.844756	H	4.454380	1.200233	1.143781
C	-3.439281	1.039534	-0.834570	H	2.938145	3.164785	1.116032
C	0.723873	0.751522	0.128489	Br	1.282558	-1.820263	-1.083716
C	1.237256	2.022257	0.482828	Br	-1.253428	-1.840509	1.084415
C	1.653205	-0.273393	-0.062557	Si	-0.026717	3.304731	-0.000188
C	2.976487	-0.114658	0.334127	H	0.486135	4.178756	-1.087997
C	3.421710	1.094808	0.835020	H	-0.553469	4.170910	1.087251
C	2.562314	2.185078	0.844898				

H3Ge$_{Br,Br}$

C	0.504500	-2.966275	-0.322368	H	1.342440	-3.635622	-0.180573
C	0.628024	-1.640016	0.075565	H	-2.765547	-2.996621	-1.143077
C	-0.413356	-0.730137	-0.128476	H	-0.769031	-4.470683	-1.149561
C	-1.663804	-1.273991	-0.497347	H	1.345216	3.634269	0.181358
C	-1.797356	-2.600205	-0.860960	H	-0.765712	4.470887	1.150190
C	-0.688670	-3.436343	-0.838597	H	-2.763377	2.998384	1.143332
C	-0.412817	0.730145	0.128878	Br	2.152575	1.234431	-1.119665
C	-1.662896	1.274945	0.497615	Br	2.151529	-1.236339	1.120360
C	0.629285	1.639233	-0.074992	H	-3.928802	0.554267	-1.127237
C	0.506745	2.965561	0.323014	H	-3.929688	-0.551425	1.126838
C	-0.686120	3.436512	0.839147	Ge	-3.043809	0.001033	-0.000039
C	-1.795459	2.601234	0.861311				

H3Sn$_{Br,Br}$

C	0.897770	-2.940918	-0.269122	H	1.748318	-3.582799	-0.082976
C	0.957178	-1.610423	0.125927	H	-2.320125	-3.073459	-1.259227
C	-0.100043	-0.731174	-0.130544	H	-0.286726	-4.484122	-1.156477
C	-1.311503	-1.310853	-0.564602	H	1.749492	3.581972	0.083645
C	-1.382412	-2.643892	-0.926851	H	-0.285346	4.483945	1.157004
C	-0.252616	-3.447360	-0.844457	H	-2.319239	3.073977	1.259479
C	-0.099820	0.730961	0.131013	Br	2.423908	1.143343	-1.227875
C	-1.311139	1.311039	0.564941	Br	2.423497	-1.144376	1.228480
C	0.957702	1.609868	-0.125372	H	-3.868300	0.689342	-1.215403
C	0.898712	2.940374	0.269703	H	-3.868654	-0.688340	1.215496
C	-0.251555	3.447184	0.844949	Sn	-2.891762	0.000337	0.000096
C	-1.381634	2.644095	0.927203				

H3O$_{Me,Me}$

C	-3.083739	-0.547278	0.000035	H	-4.422865	1.128457	0.000143
C	-1.782537	-1.036541	-0.000034	H	3.897223	-1.263207	0.000065
C	-0.733475	-0.096358	-0.000002	H	4.422857	1.128488	-0.000078
C	-1.087212	1.263234	0.000020	H	2.566566	2.816313	-0.000084
C	-2.377269	1.751480	0.000070	O	-0.000007	2.076241	-0.000012
C	-3.387554	0.811123	0.000093	C	1.599781	-2.522041	0.000190
C	0.733479	-0.096351	-0.000022	H	1.055602	-2.864614	0.880230
C	1.087205	1.263245	-0.000040	H	1.055233	-2.864784	-0.879543
C	1.782542	-1.036530	0.000039	H	2.571786	-3.014464	0.000046
C	3.083744	-0.547258	0.000018	C	-1.599758	-2.522049	-0.000229
C	3.387549	0.811143	-0.000048	H	-2.571755	-3.014488	-0.000126
C	2.377258	1.751496	-0.000066	H	-1.055551	-2.864576	-0.880268
H	-3.897215	-1.263231	0.000025	H	-1.055228	-2.864824	0.879505
H	-2.566576	2.816297	0.000074				

H3S$_{Me,Me}$

C	-3.025655	-0.899694	0.049477	H	-4.541155	0.576743	-0.313374
C	-1.677744	-1.206475	0.190059	H	3.749035	-1.693385	-0.199475
C	-0.731770	-0.177732	-0.009544	H	4.541188	0.576413	0.313262
C	-1.231952	1.139273	-0.128078	H	2.915093	2.456480	0.366856
C	-2.581376	1.432494	-0.257719	S	0.000076	2.349121	0.000019
C	-3.479735	0.387192	-0.211452	C	1.338374	-2.577562	-0.695940
C	0.731738	-0.177789	0.009566	H	1.172173	-3.302619	0.101616
C	1.232019	1.139181	0.128076	H	0.448447	-2.558403	-1.323155
C	1.677631	-1.206601	-0.190069	H	2.165764	-2.947774	-1.302075
C	3.025569	-0.899915	-0.049541	C	-1.338602	-2.577462	0.695934
C	3.479750	0.386938	0.211376	H	-2.166043	-2.947620	1.302033
C	2.581468	1.432304	0.257677	H	-1.172417	-3.302524	-0.101622
H	-3.749183	-1.693114	0.199382	H	-0.448703	-2.558368	1.323188
H	-2.914925	2.456694	-0.366905				

H3Se$_{Me,Me}$

C	2.999240	1.312084	0.075779	H	4.566274	-0.090224	-0.352086
C	1.639295	1.556553	0.234113	H	-3.691059	2.127545	-0.255359
C	0.732815	0.502801	-0.008630	H	-4.566271	-0.090189	0.352051
C	1.281957	-0.788649	-0.161671	H	-3.016340	-2.028021	0.441831
C	2.638753	-1.022410	-0.305897	Se	-0.000008	-2.151392	-0.000042
C	3.499423	0.056251	-0.235808	C	-1.245197	2.881960	-0.817876
C	-0.732807	0.502808	0.008608	H	-1.160080	3.672875	-0.071256
C	-1.281961	-0.788641	0.161619	H	-0.298084	2.817079	-1.350608
C	-1.639276	1.556574	-0.234110	H	-2.009177	3.193501	-1.531523
C	-2.999224	1.312115	-0.075781	C	1.245229	2.881929	0.817909
C	-3.499419	0.056279	0.235777	H	2.009215	3.193448	1.531560
C	-2.638759	-1.022391	0.305840	H	1.160117	3.672861	0.071306
H	3.691083	2.127503	0.255376	H	0.298118	2.817045	1.350644
H	3.016323	-2.028040	-0.441913				

H3Te$_{Me,Me}$

C	1.706232	-2.963029	0.123847	H	0.402208	-4.593007	-0.372184
C	1.873098	-1.591577	0.291653	H	2.547817	3.612393	-0.341077
C	0.791701	-0.735015	-0.004648	H	0.403835	4.592855	0.372010
C	-0.467524	-1.342367	-0.204366	H	-1.598500	3.142936	0.526641
C	-0.621755	-2.709462	-0.355493	Te	-2.037621	0.000355	-0.000078
C	0.493439	-3.521016	-0.245799	C	3.145034	1.131097	-0.945242
C	0.791968	0.734713	0.004622	H	3.994421	1.113154	-0.260463
C	-0.467051	1.342522	0.204250	H	3.039276	0.139617	-1.381339
C	1.873687	1.590878	-0.291650	H	3.395137	1.825348	-1.749308
C	1.707302	2.962396	-0.123905	C	3.144578	-1.132273	0.945318
C	0.494691	3.520828	0.245665	H	3.394396	-1.826643	1.749372
C	-0.620799	2.709677	0.355329	H	3.994003	-1.114611	0.260577
H	2.546504	-3.613334	0.341037	H	3.039156	-0.140773	1.381449
H	-1.599603	-3.142364	-0.526867				

H3N$_{Me,Me}$

C	-3.084706	-0.580397	0.002867	H	-4.465329	1.063890	0.003978
C	-1.772530	-1.036701	0.001726	H	3.880089	-1.316307	-0.003666
C	-0.734325	-0.079471	0.000670	H	4.465330	1.063882	-0.003967
C	-1.119426	1.286735	0.000981	H	2.666676	2.787820	-0.002299
C	-2.435170	1.729525	0.002139	N	0.000002	2.070531	0.000000
C	-3.422571	0.771107	0.003065	H	0.000003	3.072667	0.000002
C	0.734325	-0.079473	-0.000677	C	1.577159	-2.521335	-0.001849
C	1.119428	1.286732	-0.000982	H	1.032286	-2.861676	0.878216
C	1.772527	-1.036704	-0.001733	H	1.030832	-2.861277	-0.881178
C	3.084704	-0.580403	-0.002866	H	2.546220	-3.019475	-0.002771
C	3.422572	0.771100	-0.003059	C	-1.577164	-2.521332	0.001836
C	2.435172	1.729520	-0.002134	H	-2.546227	-3.019470	0.002759
H	-3.880092	-1.316300	0.003668	H	-1.032294	-2.861671	-0.878231
H	-2.666671	2.787825	0.002307	H	-1.030836	-2.861279	0.881164

H3P$_{Me,Me}$

C	-3.001732	-0.947175	0.058158	H	-3.700888	-1.759279	0.227053
C	-1.642852	-1.199422	0.242281	H	-2.990663	2.390575	-0.440851
C	-0.738001	-0.151456	-0.000703	H	-4.553463	0.458791	-0.398189
C	-1.259066	1.151542	-0.173227	H	3.691191	-1.773409	-0.294757
C	-2.615165	1.381469	-0.317834	H	4.566733	0.441142	0.311703
C	-3.489093	0.307212	-0.266166	H	3.003497	2.367783	0.477725
C	0.739106	-0.158716	0.016069	P	-0.004581	2.429256	0.109854
C	1.269507	1.137689	0.185518	H	0.253156	2.821549	-1.233458
C	1.634457	-1.211020	-0.242238	C	1.233912	-2.539908	-0.812535
C	2.999509	-0.959550	-0.105361	H	1.157208	-3.325282	-0.058742
C	3.498619	0.292195	0.210182	H	0.279712	-2.478747	-1.333201
C	2.626897	1.364209	0.317864	H	1.988166	-2.858246	-1.533706

C	-1.262367	-2.523062	0.838991	H	-1.195014	-3.323920	0.100732
H	-2.023433	-2.816757	1.563683	H	-0.309523	-2.465353	1.362125

H3As$_{Me,Me}$

C	2.978466	1.358076	0.094893	H	4.574681	0.015064	-0.394201
C	1.609855	1.560818	0.274230	H	-3.656223	2.179068	-0.319747
C	0.737738	0.495508	-0.010589	H	-4.580256	0.000789	0.348704
C	1.300432	-0.781435	-0.220674	H	-3.065168	-1.962054	0.518693
C	2.661813	-0.966273	-0.359816	H	-0.309122	-2.486801	-1.405330
C	3.505397	0.131526	-0.265405	As	0.012789	-2.202202	0.060930
C	-0.741099	0.496520	0.004946	C	-1.183574	2.863248	-0.887715
C	-1.302905	-0.780568	0.199378	H	-1.150150	3.684451	-0.169539
C	-1.613563	1.562731	-0.274228	H	-0.203416	2.782108	-1.354228
C	-2.984220	1.351668	-0.118145	H	-1.900350	3.142299	-1.661913
C	-3.510155	0.121692	0.231007	C	1.183134	2.850058	0.913770
C	-2.662067	-0.971062	0.345264	H	1.901748	3.112866	1.692044
H	3.649997	2.186207	0.295375	H	1.150063	3.685162	0.211802
H	3.070403	-1.958253	-0.513191	H	0.203786	2.761579	1.380469

H3Sb$_{Me,Me}$

C	1.706762	-2.967635	0.157719	H	0.432438	-4.605059	-0.376226
C	1.859997	-1.591088	0.328867	H	2.629935	3.553315	-0.405802
C	0.784663	-0.749962	-0.009160	H	0.541546	4.593617	0.376232
C	-0.466844	-1.348712	-0.269950	H	-1.490037	3.192541	0.623364
C	-0.600956	-2.717668	-0.400901	H	-2.284989	0.468453	-1.605210
C	0.513948	-3.532008	-0.250602	Sb	-2.074443	0.015327	0.037439
C	0.804020	0.732579	0.000943	C	3.142842	1.047154	-1.008702
C	-0.431213	1.360903	0.257621	H	4.011977	1.045842	-0.348222
C	1.899573	1.548248	-0.332677	H	3.013349	0.040395	-1.401319
C	1.776221	2.928659	-0.164916	H	3.377840	1.706120	-1.846757
C	0.597900	3.519250	0.247804	C	3.111967	-1.119683	1.010506
C	-0.533599	2.729492	0.408643	H	3.328654	-1.784481	1.848933
H	2.546041	-3.611570	0.398722	H	3.983412	-1.138066	0.353383
H	-1.570726	-3.161171	-0.595697	H	3.004687	-0.110287	1.403017

H3C$_{Me,Me}$

C	-3.053721	-0.655807	0.019786	C	1.716212	-1.033090	-0.140415
C	-1.716314	-1.032954	0.140410	C	3.053649	-0.656045	-0.019814
C	-0.742118	-0.032016	-0.010113	C	3.449194	0.655469	0.183280
C	-1.164573	1.308354	-0.105490	C	2.494520	1.659353	0.210651
C	-2.494409	1.659547	-0.210672	H	-3.811862	-1.423895	0.126238
C	-3.449162	0.655736	-0.183312	H	-2.784071	2.700715	-0.293273
C	0.742096	-0.032074	0.010112	H	-4.501894	0.895743	-0.268764
C	1.164655	1.308262	0.105480	H	3.811728	-1.424193	-0.126274

H	4.501945	0.895393	0.268718	H	0.619028	-2.509534	-1.251794
H	2.784262	2.700499	0.293251	H	2.325712	-2.871086	-1.019063
C	0.000075	2.238188	-0.000009	C	-1.440976	-2.451930	0.539593
H	0.098172	2.892032	-0.872540	H	-2.325955	-2.870883	1.019092
H	-0.097974	2.892064	0.872503	H	-1.195006	-3.095858	-0.305458
C	1.440762	-2.452050	-0.539581	H	-0.619238	-2.509465	1.251799
H	1.194731	-3.095946	0.305479				

H3Si$_{Me,Me}$

C	-2.969026	-1.009627	0.137107	H	3.627035	-1.843104	-0.359975
C	-1.594318	-1.190984	0.305760	H	4.587607	0.296532	0.372871
C	-0.744761	-0.119974	-0.008947	H	3.113002	2.280952	0.577752
C	-1.316823	1.152079	-0.252797	Si	-0.000071	2.442535	0.000098
C	-2.684732	1.302982	-0.388108	H	0.309255	3.320698	-1.161248
C	-3.515690	0.198917	-0.249695	H	-0.309478	3.320446	1.161617
C	0.744770	-0.119937	0.009009	C	1.140957	-2.464618	-0.957432
C	1.316767	1.152143	0.252860	H	1.132278	-3.313304	-0.270852
C	1.594378	-1.190904	-0.305707	H	0.144963	-2.365568	-1.385303
C	2.969078	-1.009476	-0.137071	H	1.829762	-2.713457	-1.766865
C	3.515685	0.199100	0.249719	C	-1.140838	-2.464677	0.957486
C	2.684671	1.303120	0.388149	H	-1.829639	-2.713554	1.766911
H	-3.626941	-1.843290	0.360003	H	-1.132108	-3.313360	0.270904
H	-3.113113	2.280792	-0.577719	H	-0.144853	-2.365578	1.385366
H	-4.587614	0.296294	-0.372868				

H3Ge$_{Me,Me}$

C	2.958904	1.385805	0.147174	H	-3.604081	2.226761	-0.378663
C	1.581566	1.543684	0.317122	H	-4.595919	0.107554	0.375713
C	0.744856	0.464244	-0.008575	H	-3.149228	-1.896171	0.595748
C	1.339667	-0.792238	-0.262346	H	-0.333501	-3.065077	-1.205756
C	2.707414	-0.925838	-0.398639	H	0.333960	-3.064517	1.206400
C	3.522735	0.189517	-0.251017	Ge	0.000130	-2.170548	0.000137
C	-0.744922	0.464169	0.008705	C	-1.111087	2.803113	-0.984256
C	-1.339608	-0.792390	0.262368	H	-1.112255	3.664046	-0.313060
C	-1.581730	1.543534	-0.316995	H	-0.108208	2.693630	-1.392866
C	-2.959063	1.385481	-0.147182	H	-1.785333	3.039043	-1.809764
C	-3.522791	0.189102	0.250889	C	1.110830	2.803166	0.984496
C	-2.707352	-0.926160	0.398537	H	1.785088	3.039092	1.809996
H	3.603842	2.227149	0.378646	H	1.111895	3.664151	0.313365
H	3.149390	-1.895785	-0.595943	H	0.107980	2.693559	1.393140
H	4.595860	0.108104	-0.375961				

H3Sn$_{Me,Me}$

C	1.758966	-2.928756	0.203014	C	-0.533173	-2.762261	-0.443015
C	1.856600	-1.545678	0.368532	C	0.602886	-3.537260	-0.243008
C	0.762438	-0.746770	-0.005964	C	0.763054	0.746138	0.005955
C	-0.458926	-1.388148	-0.312636	C	-0.457772	1.388522	0.312662

C	1.857871	1.544145	-0.368540	H	-3.024920	-0.439780	1.320234
C	1.761398	2.927297	-0.202964	Sn	-2.036298	0.000831	0.000065
C	0.605832	3.536749	0.243095	C	3.076029	1.021812	-1.074077
C	-0.530872	2.762692	0.443084	H	3.967743	1.048003	-0.444758
H	2.613871	-3.539961	0.472986	H	2.938425	0.001007	-1.425101
H	-1.474883	-3.243841	-0.680453	H	3.278757	1.651456	-1.942756
H	0.565070	-4.613083	-0.366714	C	3.075224	-1.024337	1.073997
H	2.616809	3.537798	-0.472925	H	3.277530	-1.654179	1.942632
H	0.568917	4.612599	0.366845	H	3.966868	-1.051197	0.444608
H	-1.472179	3.245050	0.680541	H	2.938449	-0.003439	1.425077
H	-3.024811	0.442213	-1.319922				

H3Sn$_{tBu,H}^{‡}$

C	2.240954	-2.107373	0.002870	C	3.140524	0.209522	-0.000541
C	1.937831	-0.744353	0.001074	C	3.153878	1.024105	1.310556
C	0.558535	-0.365552	0.000862	H	3.788815	1.908942	1.213597
C	-0.386486	-1.420899	0.001028	H	2.172429	1.340558	1.650779
C	-0.037501	-2.759048	0.002543	H	3.573505	0.402393	2.103653
C	1.295035	-3.112533	0.003897	C	4.496558	-0.509622	-0.003913
C	-0.045320	1.029986	0.000452	H	4.645021	-1.126696	0.883716
C	-1.455985	1.153720	-0.002569	H	4.640134	-1.127039	-0.892116
C	0.655354	2.242692	0.003423	H	5.280293	0.251749	-0.006110
C	0.017963	3.474673	0.002991	C	3.149090	1.026411	-1.310191
C	-1.360281	3.563851	-0.000483	H	2.166595	1.344226	-1.645977
C	-2.089993	2.385396	-0.003139	H	3.784958	1.910658	-1.214052
H	3.276994	-2.406616	0.003357	H	3.565302	0.405875	-2.106009
H	-0.803347	-3.526514	0.002666	H	1.725630	2.269639	0.006131
H	1.603181	-4.151350	0.005365	H	-3.289598	-1.122207	-1.395717
H	0.623862	4.373115	0.005407	H	-3.295530	-1.119317	1.386141
H	-1.857604	4.526197	-0.000935	Sn	-2.383761	-0.735540	-0.003250
H	-3.173341	2.433303	-0.005571				

H3O$_{Br,Br}^{‡}$

C	3.121239	0.460912	-0.006992	C	-2.368022	2.741346	0.021880
C	1.820624	-0.021904	0.002651	H	3.933980	-0.251820	-0.009072
C	0.733871	0.868213	0.005637	H	2.534544	3.809618	-0.014717
C	1.086953	2.234292	-0.000255	H	4.427003	2.155437	-0.021561
C	2.367994	2.741325	-0.010273	H	-3.933937	-0.251806	0.035283
C	3.397150	1.822198	-0.013801	H	-4.427016	2.155471	0.036461
C	-0.733855	0.868215	0.014679	H	-2.534599	3.809643	0.020927
C	-1.086969	2.234301	0.014444	Br	-1.692361	-1.901036	0.018088
C	-1.820592	-0.021902	0.021591	Br	1.692381	-1.901008	0.011702
C	-3.121213	0.460928	0.029829	O	-0.000017	3.041024	0.005507
C	-3.397155	1.822222	0.030227				

H3S$_{Br,Br}^{‡}$

C	0.177998	-3.120199	-0.001106	C	-0.194108	-1.783141	-0.001586

C	0.768451	-0.742360	-0.000426	H	-0.605558	-3.864290	-0.002098
C	2.107132	-1.228011	0.001187	H	3.535677	-2.824791	0.003256
C	2.485312	-2.562727	0.001845	H	1.751112	-4.575467	0.001065
C	1.503803	-3.521726	0.000671	H	-0.605641	3.864276	-0.002104
C	0.768435	0.742375	-0.000424	H	1.751013	4.575504	0.001067
C	2.107105	1.228055	0.001190	H	3.535616	2.824867	0.003265
C	-0.194147	1.783136	-0.001587	Br	-2.077525	1.617620	-0.003927
C	0.177931	3.120201	-0.001109	Br	-2.077490	-1.617666	-0.003927
C	1.503727	3.521758	0.000672	S	3.308527	0.000035	0.002187
C	2.485256	2.562780	0.001852				

H3Se$_{Br,Br}^{‡}$

C	0.211996	-3.120788	0.000984	C	-2.099318	2.615437	-0.001955
C	0.552844	-1.773527	0.001913	H	1.014298	-3.844332	0.002019
C	-0.429950	-0.747499	0.000464	H	-3.143184	-2.902940	-0.003393
C	-1.752916	-1.274114	-0.001599	H	-1.323615	-4.615443	-0.001244
C	-2.099320	-2.615436	-0.001963	H	1.014302	3.844330	0.002007
C	-1.100170	-3.556370	-0.000793	H	-1.323611	4.615444	-0.001244
C	-0.429950	0.747499	0.000465	H	-3.143181	2.902942	-0.003380
C	-1.752915	1.274115	-0.001594	Br	2.438117	1.599799	0.005797
C	0.552846	1.773526	0.001910	Br	2.438115	-1.599801	0.005798
C	0.211999	3.120788	0.000977	Se	-3.107170	0.000001	-0.004344
C	-1.100167	3.556371	-0.000793				

H3Te$_{Br,Br}^{‡}$

C	0.778845	-3.050805	-0.649029	C	-1.544251	2.615917	0.565252
C	1.079634	-1.719650	-0.375663	H	1.603695	-3.731036	-0.802581
C	0.071439	-0.737373	-0.156571	H	-2.569537	-2.947806	-0.579858
C	-1.234738	-1.303135	-0.255920	H	-0.707452	-4.566012	-0.943925
C	-1.535928	-2.628140	-0.527939	H	1.591882	3.746236	0.755770
C	-0.515016	-3.522704	-0.729070	H	-0.721927	4.561107	0.958664
C	0.069052	0.739155	0.151187	H	-2.578854	2.926557	0.644810
C	-1.238891	1.293511	0.285359	Br	2.962775	1.559679	0.280940
C	1.074091	1.730229	0.343293	Br	2.967884	-1.533087	-0.363227
C	0.769156	3.058828	0.624364	Te	-2.802614	-0.011689	0.035741
C	-0.526183	3.519448	0.738858				

H3N$_{Br,Br}^{‡}$

C	3.123357	0.430514	0.010641	C	-3.123355	0.430526	0.014274
C	1.812305	-0.019559	0.013520	C	-3.432825	1.785693	0.003329
C	0.734534	0.886481	0.010635	C	-2.425659	2.722447	-0.002345
C	1.118862	2.259151	0.002787	H	3.918242	-0.301704	0.013212
C	2.425656	2.722466	-0.000346	H	2.633997	3.785115	-0.006052
C	3.432826	1.785709	0.004030	H	4.470319	2.094937	0.001858
C	-0.734533	0.886484	0.011260	H	-3.918241	-0.301670	0.020323
C	-1.118864	2.259144	0.002056	H	-4.470319	2.094910	0.000095
C	-1.812302	-0.019533	0.018777	H	-2.634003	3.785085	-0.009693

Br	-1.671889	-1.900561	0.037090	N	-0.000003	3.038056	-0.001581
Br	1.671897	-1.900672	0.018425	H	-0.000003	4.040453	-0.012286

H3P$_{Br,Br}^{‡}$

C	-0.155317	3.120989	0.101441	C	-2.457922	-2.597483	0.004738
C	0.195122	1.772503	0.044151	H	0.643892	3.847339	0.143492
C	-0.784589	0.754605	0.001903	H	-3.503003	2.882661	-0.041266
C	-2.115834	1.258050	-0.023663	H	-1.695599	4.605416	0.133430
C	-2.458756	2.596718	0.004948	H	0.645108	-3.847102	0.143778
C	-1.466024	3.548355	0.091527	H	-1.694138	-4.605930	0.133412
C	-0.784343	-0.754837	0.001869	H	-3.502071	-2.883761	-0.041611
C	-2.115424	-1.258706	-0.023802	Br	2.082643	-1.606105	0.016144
C	0.195689	-1.772417	0.044226	Br	2.082119	1.606766	0.016178
C	-0.154328	-3.121010	0.101593	P	-3.388920	-0.000526	-0.176149
C	-1.464898	-3.548797	0.091504	H	-3.825885	-0.000693	1.177985

H3As$_{Br,Br}^{‡}$

C	-0.226245	-3.122480	0.116473	C	2.080291	2.635026	0.051933
C	-0.552935	-1.766024	0.067960	H	-1.039217	-3.833765	0.145577
C	0.441388	-0.758680	0.040737	H	3.120693	-2.938280	0.020976
C	1.759644	-1.292605	0.029727	H	1.285693	-4.635256	0.150118
C	2.080874	-2.634643	0.052042	H	-1.040063	3.833455	0.145640
C	1.073902	-3.574167	0.115474	H	1.284671	4.635463	0.150054
C	0.441222	0.758700	0.040719	H	3.120041	2.938894	0.020819
C	1.759358	1.292916	0.029664	Br	-2.441796	1.593410	0.029596
C	-0.553323	1.765823	0.067973	Br	-2.441451	-1.594042	0.029596
C	-0.226934	3.122351	0.116494	H	3.495522	0.000390	1.404666
C	1.073113	3.574327	0.115420	As	3.172224	0.000309	-0.088530

H3Sb$_{Br,Br}^{‡}$

C	0.602145	3.122208	0.414070	C	-1.705904	-2.689348	0.303509
C	0.896440	1.756119	0.366056	H	1.432800	3.811363	0.461682
C	-0.117072	0.764786	0.318382	H	-2.735927	3.023934	0.255870
C	-1.420814	1.338463	0.282419	H	-0.868983	4.674736	0.425175
C	-1.705875	2.689289	0.303291	H	1.432819	-3.811406	0.461347
C	-0.682094	3.608909	0.389693	H	-0.868980	-4.674799	0.425061
C	-0.117122	-0.764846	0.318434	H	-2.735957	-3.024013	0.256234
C	-1.420875	-1.338512	0.282624	Br	2.788646	-1.576996	0.354432
C	0.896394	-1.756165	0.366007	Br	2.788839	1.577328	0.354296
C	0.602143	-3.122265	0.413896	H	-3.338065	0.000187	1.840221
C	-0.682097	-3.608967	0.389660	Sb	-3.043460	-0.000002	0.149021

H3C$_{Br,Br}^{‡}$

C	3.124910	0.397004	0.000447	C	1.794254	-0.015350	-0.000195

C	0.749716	0.925002	-0.000423	H	2.717130	3.745383	0.000278
C	1.164465	2.279027	-0.000336	H	4.523643	2.012962	0.001242
C	2.480334	2.688039	0.000218	H	-3.893431	-0.363416	0.000669
C	3.478049	1.731966	0.000706	H	-4.523643	2.012962	0.001186
C	-0.749716	0.925002	-0.000425	H	-2.717130	3.745382	0.000252
C	-1.164466	2.279027	-0.000343	Br	-1.644978	-1.899724	-0.000954
C	-1.794254	-0.015350	-0.000206	Br	1.644978	-1.899724	-0.000971
C	-3.124910	0.397003	0.000415	C	0.000000	3.201483	-0.000759
C	-3.478049	1.731965	0.000666	H	-0.000003	3.854446	0.877815
C	-2.480334	2.688039	0.000193	H	0.000002	3.853339	-0.880177
H	3.893431	-0.363415	0.000711				

H3Si$_{Br,Br}^{‡}$

C	0.119157	-3.127012	0.001230	H	-0.701113	-3.830682	0.002230
C	-0.198424	-1.763951	0.001237	H	3.463654	-2.972322	-0.002355
C	0.802683	-0.767970	0.000111	H	1.612384	-4.656263	0.000020
C	2.124227	-1.308989	-0.001157	H	-0.701113	3.830682	0.002236
C	2.426525	-2.655959	-0.001251	H	1.612385	4.656262	0.000020
C	1.412147	-3.592338	0.000044	H	3.463655	2.972322	-0.002362
C	0.802683	0.767970	0.000110	Br	-2.088703	1.589699	0.002690
C	2.124227	1.308989	-0.001160	Br	-2.088704	-1.589699	0.002689
C	-0.198424	1.763951	0.001239	Si	3.416829	0.000000	-0.001840
C	0.119158	3.127012	0.001234	H	4.286818	0.000001	1.204154
C	1.412148	3.592338	0.000044	H	4.286737	-0.000002	-1.207883
C	2.426526	2.655959	-0.001256				

H3Ge$_{Br,Br}^{‡}$

C	-0.247822	3.127325	0.000261	H	-1.075222	3.822329	0.000546
C	-0.550873	1.760961	0.000560	H	3.095743	3.004610	-0.001138
C	0.458634	0.769554	0.000245	H	1.229950	4.671944	-0.000683
C	1.769607	1.331062	-0.000300	H	-1.075198	-3.822338	0.000230
C	2.061922	2.678877	-0.000673	H	1.229979	-4.671939	-0.000758
C	1.039471	3.606172	-0.000411	H	3.095762	-3.004594	-0.000787
C	0.458639	-0.769553	0.000291	Br	-2.442255	-1.582878	0.001363
C	1.769615	-1.331053	-0.000102	Br	-2.442266	1.582861	0.001350
C	-0.550862	-1.760967	0.000485	H	4.032694	-0.000122	-1.255400
C	-0.247802	-3.127329	0.000098	H	4.032295	0.000146	1.255369
C	1.039493	-3.606168	-0.000433	Ge	3.148400	0.000009	-0.000161
C	2.061939	-2.678867	-0.000472				

H3Sn$_{Br,Br}^{‡}$

C	-0.623740	3.127070	-0.198260	C	1.426004	1.373103	-0.119107
C	-0.895920	1.753103	-0.208844	C	1.686719	2.728750	-0.109048
C	0.130694	0.774763	-0.169078	C	0.648679	3.636825	-0.149064

C	0.130722	-0.774787	-0.168797	H	-1.466144	-3.802456	-0.229775
C	1.426051	-1.373062	-0.118547	H	0.816197	-4.706533	-0.141181
C	-0.895855	-1.753177	-0.208287	H	2.711133	-3.081374	-0.068393
C	-0.623618	-3.127131	-0.197352	Br	-2.789175	-1.568079	-0.281760
C	0.648819	-3.636822	-0.147967	Br	-2.789227	1.567902	-0.282405
C	1.686820	-2.728695	-0.108097	H	4.039035	-0.000246	-1.415240
H	-1.466295	3.802352	-0.230835	H	3.931548	0.000413	1.374786
H	2.711021	3.081481	-0.069533	Sn	3.011075	0.000060	-0.057759
H	0.816013	4.706544	-0.142547				

H3O$_{Me,Me}^{‡}$

C	3.084156	-0.551935	0.000240	H	4.423297	1.123998	0.000119
C	1.782978	-1.041382	0.000257	H	-3.897775	-1.267801	-0.000315
C	0.733634	-0.101062	0.000053	H	-4.423297	1.123998	-0.000120
C	1.087307	1.258686	0.000035	H	-2.567223	2.811778	-0.000020
C	2.377655	1.746976	0.000070	O	0.000000	2.070998	0.000001
C	3.387942	0.806658	0.000141	C	-1.600410	-2.526927	-0.000961
C	-0.733634	-0.101062	-0.000053	H	-1.058730	-2.869493	-0.882673
C	-1.087307	1.258686	-0.000034	H	-1.052546	-2.869934	0.876613
C	-1.782978	-1.041382	-0.000258	H	-2.572170	-3.019694	0.002207
C	-3.084156	-0.551935	-0.000241	C	1.600410	-2.526927	0.000962
C	-3.387942	0.806658	-0.000142	H	1.058732	-2.869492	0.882674
C	-2.377655	1.746976	-0.000070	H	1.052544	-2.869934	-0.876612
H	3.897775	-1.267801	0.000313	H	2.572170	-3.019694	-0.002208
H	2.567223	2.811778	0.000021				

H3S$_{Me,Me}^{‡}$

C	-3.078436	-0.840502	-0.000100	H	-4.567115	0.709193	-0.000225
C	-1.740709	-1.217283	0.000186	H	3.822575	-1.627774	-0.001300
C	-0.741966	-0.204666	0.000296	H	4.567115	0.709194	-0.001193
C	-1.229503	1.126711	0.000522	H	2.857473	2.527094	0.000043
C	-2.572269	1.482501	0.000427	S	0.000000	2.331558	0.000917
C	-3.508884	0.479758	0.000002	C	1.516799	-2.700171	-0.000752
C	0.741967	-0.204666	0.000131	H	0.971019	-3.037478	0.877753
C	1.229503	1.126711	0.000290	H	0.978506	-3.037689	-0.883985
C	1.740710	-1.217283	-0.000401	H	2.481004	-3.206617	0.003276
C	3.078436	-0.840502	-0.000908	C	-1.516799	-2.700171	0.001093
C	3.508884	0.479759	-0.000820	H	-0.971060	-3.037866	-0.877290
C	2.572270	1.482502	-0.000130	H	-0.978466	-3.037301	0.884448
H	-3.822575	-1.627774	-0.000324	H	-2.481004	-3.206618	-0.002687
H	-2.857473	2.527093	0.000591				

H3Se$_{Me,Me}^{‡}$

C	-3.078194	-1.234548	0.000410	C	-1.730430	-1.580138	-0.000244

C	-0.747236	-0.547724	-0.000361	H	3.801922	-2.040241	0.001588
C	-1.276065	0.767515	-0.000461	H	4.605930	0.276661	0.000977
C	-2.624932	1.091328	0.000006	H	2.934740	2.129108	-0.000674
C	-3.542805	0.071251	0.000610	Se	-0.000065	2.124809	-0.001188
C	0.747194	-0.547708	-0.000273	C	1.497043	-3.062711	0.000694
C	1.275977	0.767550	-0.000624	H	0.958017	-3.399399	0.882975
C	1.730429	-1.580090	0.000473	H	0.955177	-3.399412	-0.879719
C	3.078179	-1.234436	0.000973	H	2.459506	-3.572045	-0.000809
C	3.542741	0.071383	0.000602	C	-1.496929	-3.062726	-0.001309
C	2.624831	1.091420	-0.000308	H	-0.958047	-3.398757	-0.883908
H	-3.801901	-2.040388	0.000634	H	-0.954851	-3.399942	0.878793
H	-2.934885	2.129003	-0.000022	H	-2.459343	-3.572152	0.000007
H	-4.606002	0.276492	0.001158				

H3Te$_{Me,Me}^{‡}$

C	1.607348	-3.077206	0.001375	H	0.144360	-4.651121	0.003983
C	1.915205	-1.718518	0.000288	H	2.433847	3.776322	-0.003532
C	0.859134	-0.754233	0.001082	H	0.143616	4.650932	-0.001175
C	-0.439883	-1.329127	0.003013	H	-1.747844	3.031630	0.002182
C	-0.720026	-2.688205	0.004051	C	3.397580	1.475067	-0.003429
C	0.319987	-3.582581	0.003218	H	3.734816	0.937030	0.878159
C	0.859012	0.754158	0.000246	H	3.732550	0.936114	-0.885328
C	-0.440097	1.328846	0.001556	H	3.910374	2.435346	-0.004578
C	1.914927	1.718609	-0.001656	C	3.397819	-1.474741	-0.001687
C	1.606856	3.077249	-0.002075	H	3.732741	-0.936668	-0.884141
C	0.319415	3.582420	-0.000756	H	3.734938	-0.935723	0.879348
C	-0.720455	2.687879	0.001094	H	3.910763	-2.434940	-0.001810
H	2.434447	-3.776152	0.000727	Te	-2.007469	-0.000265	0.004325
H	-1.747360	-3.032117	0.005508				

H3N$_{Me,Me}^{‡}$

C	-3.084579	0.583667	0.000441	H	-2.666602	-2.784615	0.000235
C	-1.772403	1.039914	0.000154	H	-4.465364	-1.060474	0.000748
C	-0.734292	0.082613	-0.000056	H	3.879914	1.319629	0.000077
C	-1.119466	-1.283534	-0.000050	H	4.465364	-1.060474	-0.000154
C	-2.435217	-1.726285	0.000257	H	2.666601	-2.784615	-0.000499
C	-3.422573	-0.767821	0.000537	N	0.000000	-2.067435	-0.000446
C	0.734292	0.082613	-0.000208	H	0.000000	-3.069573	0.000211
C	1.119465	-1.283534	-0.000352	C	1.576821	2.524563	-0.000505
C	1.772403	1.039914	-0.000141	H	1.034854	2.864840	-0.882493
C	3.084579	0.583667	-0.000084	H	1.028515	2.864872	0.877316
C	3.422572	-0.767821	-0.000219	H	2.546030	3.022467	0.002800
C	2.435217	-1.726285	-0.000393	C	-1.576820	2.524563	0.000387
H	-3.879914	1.319629	0.000533	H	-1.034962	2.864947	0.882407

H	-1.028407	2.864765	-0.877402	H	-2.546029	3.022467	-0.003101

H3P$_{Me,Me}^{‡}$

C	-3.079288	0.867121	0.048952	H	-4.598064	-0.647393	0.095732
C	-1.730040	1.221260	0.001900	H	3.806241	1.670738	0.068409
C	-0.754892	0.190250	-0.013913	H	4.598156	-0.646919	0.096457
C	-1.260231	-1.134051	-0.012670	H	2.916638	-2.491355	-0.010420
C	-2.607413	-1.452896	0.011850	P	0.000159	-2.411567	-0.135372
C	-3.536200	-0.437411	0.062122	H	0.000148	-2.825169	1.226397
C	0.754919	0.190331	-0.013897	C	-1.502380	2.704985	-0.028926
C	1.260395	-1.133919	-0.012559	H	-0.961338	3.062632	0.843937
C	1.729964	1.221441	0.001942	H	-0.963826	3.024444	-0.917809
C	3.079240	0.867441	0.049209	H	-2.466004	3.212447	-0.038296
C	3.536277	-0.437045	0.062641	C	1.502182	2.705153	-0.028872
C	2.607602	-1.452625	0.012286	H	0.961747	3.024450	-0.916617
H	-3.806372	1.670342	0.068185	H	0.962962	3.062925	0.845121
H	-2.916338	-2.491656	-0.010985	H	2.465768	3.212648	-0.040298

H3As$_{Me,Me}^{‡}$

C	-3.079979	1.254462	0.037051	H	-4.626732	-0.231018	0.084378
C	-1.723023	1.585329	0.000346	H	3.792463	2.069991	0.044132
C	-0.759035	0.540305	0.002507	H	4.626440	-0.232154	0.088196
C	-1.295070	-0.770455	0.019599	H	2.970827	-2.102007	0.031691
C	-2.645218	-1.067594	0.035916	H	-0.000915	-2.478528	1.439734
C	-3.561218	-0.038741	0.059854	As	-0.000329	-2.186562	-0.060316
C	0.759004	0.540114	0.003105	C	1.489061	3.068261	-0.039531
C	1.294703	-0.770778	0.020583	H	0.950880	3.380992	-0.930459
C	1.723247	1.584901	0.001784	H	0.949749	3.431404	0.831524
C	3.080090	1.253707	0.039628	H	2.451276	3.577914	-0.053374
C	3.560994	-0.039615	0.062778	C	-1.488465	3.068641	-0.040747
C	2.644764	-1.068245	0.038015	H	-0.949869	3.431656	0.830805
H	-3.792157	2.070919	0.040920	H	-0.949406	3.381278	-0.931176
H	-2.971526	-2.101277	0.029373	H	-2.450557	3.578503	-0.055460

H3Sb$_{Me,Me}^{‡}$

C	-1.626684	3.079494	-0.026748	C	-1.621671	-3.080149	-0.027850
C	-1.921703	1.712539	0.016908	C	-0.347757	-3.595275	-0.120019
C	-0.858306	0.765936	-0.050046	C	0.697171	-2.698553	-0.165521
C	0.434731	1.343028	-0.140817	H	-2.460403	3.769392	0.021099
C	0.692752	2.701721	-0.164938	H	1.715065	3.058839	-0.221033
C	-0.353626	3.596723	-0.118973	H	-0.189234	4.666925	-0.145701
C	-0.857053	-0.765334	-0.050254	H	-2.454277	-3.771417	0.019602
C	0.436938	-1.340289	-0.141049	H	-0.181617	-4.665199	-0.147070
C	-1.918916	-1.713691	0.016239	H	1.720072	-3.053993	-0.221552

H	2.173302	0.002907	-1.905456	H	-3.912872	2.427704	0.179102
Sb	2.061662	0.002716	-0.191587	C	-3.398284	-1.471568	0.136180
C	-3.400669	1.467979	0.136841	H	-3.663203	-0.934830	1.042494
H	-3.808367	0.930958	-0.714791	H	-3.806802	-0.934766	-0.715191
H	-3.664671	0.930343	1.042884	H	-3.908943	-2.432140	0.177916

H3C$_{Me,Me}^{‡}$

C	-3.083822	-0.618742	0.000354	H	3.853192	-1.382462	-0.000747
C	-1.752970	-1.036913	0.000751	H	4.516647	0.975242	0.000688
C	-0.749563	-0.045141	0.000046	H	2.750580	2.741812	0.000842
C	-1.165013	1.302212	-0.000270	C	0.000000	2.228808	0.000000
C	-2.489970	1.689591	-0.000533	H	0.000285	2.882747	-0.878256
C	-3.465988	0.711912	-0.000376	H	-0.000285	2.882746	0.878257
C	0.749563	-0.045141	-0.000046	C	1.545208	-2.521944	-0.002877
C	1.165013	1.302212	0.000270	H	0.998938	-2.863983	0.874421
C	1.752970	-1.036913	-0.000751	H	1.006177	-2.861681	-0.885844
C	3.083822	-0.618742	-0.000354	H	2.512397	-3.023747	0.000229
C	3.465988	0.711912	0.000377	C	-1.545208	-2.521944	0.002876
C	2.489970	1.689591	0.000533	H	-0.998937	-2.863983	-0.874422
H	-3.853192	-1.382462	0.000746	H	-1.006177	-2.861681	0.885843
H	-2.750580	2.741812	-0.000841	H	-2.512397	-3.023747	-0.000230
H	-4.516647	0.975242	-0.000688				

H3Si$_{Me,Me}^{‡}$

C	-3.083507	-0.902719	0.001310	H	3.786976	-1.729872	-0.000129
C	-1.720885	-1.225587	0.001006	H	4.646883	0.559661	-0.001771
C	-0.768746	-0.173418	0.000036	H	3.009711	2.445181	-0.002705
C	-1.311411	1.141224	-0.000557	Si	0.001530	2.431453	-0.001900
C	-2.666601	1.418521	-0.000224	H	0.001562	3.307679	-1.205377
C	-3.578104	0.383410	0.000730	H	0.002458	3.309336	1.200367
C	0.768963	-0.174262	-0.000464	C	1.482632	-2.711599	0.001024
C	1.313062	1.139788	-0.001471	H	0.945240	-3.048840	0.883266
C	1.719958	-1.227470	-0.000012	H	0.943257	-3.049843	-0.879585
C	3.082930	-0.906082	-0.000500	H	2.443728	-3.223574	0.000248
C	3.578927	0.379508	-0.001431	C	-1.485144	-2.709961	0.001779
C	2.668554	1.415609	-0.001943	H	-0.947889	-3.048814	-0.879921
H	-3.788448	-1.725743	0.002064	H	-0.946353	-3.047724	0.882933
H	-3.006638	2.448464	-0.000712	H	-2.446783	-3.220915	0.002913
H	-4.645863	0.564727	0.001025				

H3Ge$_{Me,Me}^{‡}$

C	3.083619	-1.272327	-0.000023	C	0.770327	-0.521182	0.000151
C	1.717814	-1.581234	-0.000341	C	1.333197	0.782748	0.000773

C	2.688849	1.050569	0.001017	H	-3.040585	2.073654	-0.000281
C	3.591383	0.007884	0.000658	H	-0.002728	3.051713	1.252597
C	-0.770431	-0.522150	-0.000009	H	-0.001705	3.052426	-1.250571
C	-1.334849	0.781123	-0.000034	Ge	-0.001659	2.159276	0.000758
C	-1.716682	-1.583334	0.000010	C	1.477513	-3.065298	-0.001580
C	-3.082851	-1.275961	-0.000035	H	0.937773	-3.403535	0.878428
C	-3.592119	0.003646	-0.000213	H	0.941993	-3.402358	-0.884747
C	-2.690806	1.047378	-0.000216	H	2.438084	-3.577949	0.000312
H	3.780009	-2.102335	-0.000375	C	-1.474997	-3.067230	0.000293
H	3.037440	2.077248	0.001503	H	-0.935043	-3.404516	-0.879958
H	4.660767	0.179623	0.000882	H	-0.939164	-3.404508	0.883193
H	-3.778289	-2.106765	0.000007	H	-2.435151	-3.580666	-0.001876
H	-4.661705	0.174124	-0.000314				

H3Sn$_{Me,Me}^{‡}$

C	1.645531	-3.082889	-0.001891	H	2.493344	3.758706	0.003658
C	1.923631	-1.709485	-0.000811	H	0.234604	4.695489	0.003108
C	0.845428	-0.775989	-0.000695	H	-1.694374	3.116515	0.000765
C	-0.443344	-1.376815	-0.001804	H	-3.011980	0.002099	-1.392962
C	-0.678654	-2.739828	-0.002824	H	-3.013562	0.000024	1.388449
C	0.380302	-3.622076	-0.002873	Sn	-2.025778	0.000799	-0.001695
C	0.845832	0.776100	0.000437	C	3.407632	-1.460229	0.000096
C	-0.442630	1.377592	0.000190	H	3.744841	-0.923284	-0.881291
C	1.924518	1.709038	0.001721	H	3.743987	-0.924639	0.882637
C	1.647122	3.082586	0.002658	H	3.923651	-2.418663	-0.000389
C	0.382171	3.622426	0.002360	C	3.408395	1.459026	0.002211
C	-0.677240	2.740726	0.001068	H	3.744519	0.921889	0.883896
H	2.491409	-3.759441	-0.001933	H	3.745300	0.923285	-0.880027
H	-1.695982	-3.115093	-0.003612	H	3.924901	2.417197	0.003195
H	0.232180	-4.695062	-0.003651				

PAH1$_{tBu,H}$

C	-2.237556	0.310811	0.208163	C	2.148802	-2.061940	-0.676911
C	-1.887794	-1.012440	-0.119926	C	1.856302	-0.804498	-0.165378
C	-0.507581	-1.343112	-0.464526	C	0.928387	2.015732	-0.783944
C	0.504909	-0.373930	-0.263412	C	0.527848	3.327904	-0.894054
C	0.073642	1.018921	-0.296487	C	-0.768032	3.683812	-0.530683
C	-1.266479	1.364097	-0.035141	C	-1.652160	2.707376	-0.129853
C	-3.527461	0.578880	0.682227	C	2.993698	-0.105886	0.614466
C	-4.469233	-0.418031	0.798379	H	-3.790298	1.586700	0.974913
C	-4.137650	-1.722333	0.439852	H	-5.459118	-0.188452	1.173170
C	-2.866337	-2.009391	-0.003645	H	-4.868776	-2.516284	0.530914
C	-0.157300	-2.613303	-0.927239	H	-2.616186	-3.036771	-0.229208
C	1.165367	-2.937560	-1.115783	H	-0.923461	-3.338754	-1.162073

H	1.441427	-3.899701	-1.529395	C	4.107404	0.389633	-0.311522
H	3.177343	-2.396924	-0.700945	H	4.938820	0.778846	0.281431
H	1.212345	4.071952	-1.282787	H	4.489733	-0.421149	-0.934456
H	-1.097221	4.712468	-0.611775	H	3.775141	1.187951	-0.975814
H	-2.680506	2.981285	0.063530	C	3.607489	-1.162509	1.555767
C	2.538221	1.020308	1.546763	H	4.072075	-1.990167	1.022268
H	2.300345	1.948136	1.036538	H	4.380021	-0.693010	2.168233
H	1.660515	0.722662	2.123603	H	2.847011	-1.574654	2.221563
H	3.344147	1.234674	2.251678	H	1.914418	1.730554	-1.118228

PAH1$_{Br,Br}$

C	-2.572690	-0.634127	-0.307197	C	0.986747	-2.894613	-0.068072
C	-2.572688	0.634146	0.307144	C	-0.140807	-3.465299	-0.644304
C	-1.315696	1.363886	0.439569	C	-1.292177	-2.722525	-0.771519
C	-0.113011	0.724110	0.065869	H	-3.820928	-2.168533	-1.159477
C	-0.113008	-0.724065	-0.065979	H	-5.929589	-1.080523	-0.615245
C	-1.315690	-1.363843	-0.439686	H	-5.929579	1.080452	0.615407
C	-3.800134	-1.215348	-0.650095	H	-3.820908	2.168509	1.159523
C	-4.995169	-0.606918	-0.340844	H	-2.198280	3.217119	1.089855
C	-4.995163	0.606875	0.340943	H	-0.136183	4.514970	0.909965
C	-3.800125	1.215333	0.650122	H	1.849154	3.498579	-0.178556
C	-1.292205	2.722582	0.771341	H	1.849187	-3.498521	0.178366
C	-0.140845	3.465367	0.644098	H	-0.136129	-4.514890	-0.910220
C	0.986719	2.894672	0.067897	H	-2.198240	-3.217060	-1.090068
C	0.980625	1.552768	-0.249078	Br	2.392212	0.962357	-1.363433
C	0.980637	-1.552721	0.248947	Br	2.392207	-0.962316	1.363325

PAH1$_{Me,Me}$

C	-1.648811	-0.675176	-0.200568	C	0.782272	-3.521027	-0.133789
C	-1.648824	0.675157	0.200521	C	-0.372486	-2.804426	-0.354753
C	-0.390034	1.413004	0.225470	C	3.122800	-0.888262	1.166759
C	0.819832	0.729351	-0.037724	C	3.122947	0.888245	-1.166420
C	0.819831	-0.729341	0.037797	H	-2.899066	-2.326677	-0.792156
C	-0.390003	-1.412995	-0.225541	H	-5.007545	-1.167061	-0.431107
C	-2.877755	-1.303649	-0.443698	H	-5.007563	1.166938	0.431219
C	-4.073300	-0.654489	-0.237437	H	-2.899096	2.326607	0.792210
C	-4.073311	0.654399	0.237497	H	-1.282425	3.340230	0.583873
C	-2.877775	1.303592	0.443714	H	0.782629	4.599067	0.238980
C	-0.372572	2.804449	0.354529	H	2.780676	3.433868	-0.634242
C	0.782185	3.521060	0.133596	H	2.780679	-3.433861	0.634278
C	1.912659	2.862251	-0.324093	H	0.782761	-4.599021	-0.239303
C	1.944285	1.481704	-0.447848	H	-1.282294	-3.340210	-0.584265
C	1.944254	-1.481701	0.447980	H	2.961529	0.152397	1.439230
C	1.912680	-2.862237	0.324094	H	3.290105	-1.453272	2.085985

H	4.042442	-0.949708	0.582517	H	4.042467	0.949578	-0.581976
H	3.290491	1.453310	-2.085567	H	2.961665	-0.152387	-1.438994

PAH3$_{fBu,H}$

C	1.883663	-0.232712	0.144764	H	4.333385	2.758277	0.435914
C	1.400954	1.087058	-0.034975	H	-2.142914	3.871226	-0.888672
C	0.013257	1.321857	-0.266678	H	-3.734310	2.091656	-0.468851
C	-0.921889	0.243258	-0.230640	H	-1.155895	-4.229277	-1.430990
C	-0.360406	-1.097046	-0.376343	H	1.130160	-4.695086	-0.605902
C	1.007984	-1.325898	-0.087239	H	3.282210	-3.859922	0.242328
C	3.243887	-0.460428	0.426841	H	4.758359	-1.967133	0.760732
C	4.110379	0.644416	0.555578	H	2.538096	4.308076	-0.153445
C	3.654534	1.916518	0.358100	H	0.160095	4.724141	-0.632402
C	2.302179	2.168580	0.043681	C	-3.399777	-0.331358	0.524819
C	-0.421446	2.651784	-0.467378	C	-2.891361	-1.509080	1.362309
C	-1.788454	2.874767	-0.651470	H	-2.554384	-2.358027	0.777363
C	-2.679202	1.857236	-0.428446	H	-2.067126	-1.203233	2.009408
C	-2.292167	0.546587	-0.099364	H	-3.705235	-1.858799	2.000472
C	-1.083925	-2.148868	-0.921864	C	-4.406720	-0.813339	-0.523161
C	-0.553822	-3.432194	-1.011766	H	-5.228844	-1.342492	-0.034786
C	0.723282	-3.691188	-0.567343	H	-4.830057	0.028133	-1.075215
C	1.536285	-2.640303	-0.126718	H	-3.961409	-1.492996	-1.250082
C	2.901086	-2.845112	0.228990	C	-4.168956	0.547512	1.534308
C	3.716603	-1.800212	0.511250	H	-4.698023	1.376859	1.068286
C	1.829735	3.488399	-0.191977	H	-4.914105	-0.065313	2.045034
C	0.520673	3.717326	-0.454831	H	-3.491638	0.957809	2.285537
H	5.154778	0.465907	0.785019	H	-2.078230	-1.959996	-1.296862

PAH3$_{Br,Br}$

C	-2.194873	0.688209	0.168789	C	1.317571	2.915784	-0.214521
C	-2.194873	-0.688209	-0.168789	C	0.185767	3.536677	0.250267
C	-0.965985	-1.404164	-0.225729	C	-0.997989	2.806861	0.409865
C	0.262035	-0.728139	0.024436	C	-2.239281	3.447661	0.679856
C	0.262035	0.728139	-0.024436	C	-3.403275	2.754261	0.655307
C	-0.965984	1.404164	0.225729	C	-3.403275	-2.754260	-0.655307
C	-3.416348	1.366039	0.349245	C	-2.239282	-3.447660	-0.679856
C	-4.625373	0.659259	0.176182	H	-5.561109	1.189066	0.313098
C	-4.625373	-0.659258	-0.176182	H	-5.561109	-1.189065	-0.313098
C	-3.416348	-1.366038	-0.349245	H	0.178901	-4.608544	-0.408810
C	-0.997990	-2.806861	-0.409865	H	2.195466	-3.492032	0.473370
C	0.185767	-3.536676	-0.250267	H	2.195467	3.492032	-0.473370
C	1.317571	-2.915784	0.214521	H	0.178901	4.608544	0.408810
C	1.340856	-1.532174	0.397157	H	-2.236327	4.514976	0.868426
C	1.340856	1.532174	-0.397157	H	-4.347933	3.255951	0.830505

H	-4.347933	-3.255951	-0.830505	Br	2.803011	-0.879204	1.398442
H	-2.236327	-4.514975	-0.868426	Br	2.803011	0.879204	-1.398442

PAH3$_{Me,Me}$

C	1.274253	-0.701637	0.102765	C	2.485409	2.801872	-0.396280
C	1.274495	0.701178	-0.102787	C	1.320125	3.493266	-0.365535
C	0.044091	1.416808	-0.099790	H	4.642004	-1.214482	0.199828
C	-1.189134	0.727116	0.081479	H	4.642423	1.212847	-0.199925
C	-1.189390	-0.726711	-0.081434	H	-1.100090	4.623462	-0.017370
C	0.043599	-1.416836	0.099801	H	-3.123734	3.435762	0.718350
C	2.496875	-1.392776	0.218717	H	-3.124964	-3.434678	-0.718233
C	3.706516	-0.673472	0.113038	H	-1.101709	-4.623088	0.017416
C	3.706749	0.672163	-0.113116	H	1.315013	-4.573885	0.458234
C	2.497357	1.391890	-0.218768	H	3.429611	-3.318905	0.520221
C	0.078167	2.829548	-0.163898	H	3.430759	3.317691	-0.520300
C	-1.109655	3.541330	0.044710	H	1.316603	4.573411	-0.458265
C	-2.242507	2.873109	0.429182	C	-3.507555	0.883624	1.163393
C	-2.300008	1.472977	0.497463	H	-3.698899	1.436050	2.086031
C	-2.300538	-1.472182	-0.497381	H	-4.409148	0.964359	0.552609
C	-2.243528	-2.872335	-0.429098	H	-3.364491	-0.163673	1.421290
C	-1.110898	-3.540953	-0.044663	C	-3.507901	-0.882414	-1.163279
C	0.077181	-2.829587	0.163907	H	-3.699437	-1.434756	-2.085927
C	1.318911	-3.493740	0.365509	H	-4.409508	-0.962876	-0.552479
C	2.484438	-2.802755	0.396225	H	-3.364501	0.164841	-1.421155

PAH2$_{tBu,H}$

C	0.290433	-0.914252	-0.428169	C	4.260383	-0.347630	0.843696
C	-0.698044	0.141317	-0.200677	C	0.799740	4.105575	-0.187671
C	1.197027	1.722766	0.056726	C	-0.537218	3.889059	-0.389526
C	-0.182559	1.476848	-0.190686	H	3.733411	1.711111	1.108912
C	1.644068	-0.699024	-0.056086	H	2.708138	3.224397	0.204622
C	2.093283	0.594799	0.309009	H	-3.104373	3.136768	-0.748717
C	3.381098	0.740089	0.786346	H	-3.977018	0.908180	-0.363424
C	1.656469	3.026573	0.045007	H	0.622299	-4.032631	-1.733438
C	-1.052416	2.580162	-0.375366	H	2.876928	-3.812033	-0.748335
C	-2.428312	2.318254	-0.530311	H	4.576142	-2.404364	0.353949
C	-2.906476	1.060191	-0.326380	H	5.261919	-0.201155	1.229613
C	-2.074260	-0.055107	-0.057714	H	1.199795	5.112061	-0.200487
C	-0.021436	-2.082993	-1.090060	H	-1.217140	4.717421	-0.551992
C	0.911276	-3.121114	-1.224233	H	-1.011263	-2.202097	-1.506547
C	2.165128	-2.996604	-0.692298	C	-1.903881	-2.313104	1.210822
C	2.569525	-1.774732	-0.112240	H	-1.356026	-2.964111	0.537459
C	-2.799965	-1.295772	0.499518	H	-1.178101	-1.817285	1.858013
C	3.878102	-1.575381	0.371792	H	-2.531590	-2.949800	1.837580

C	-3.635165	-1.994168	-0.576848	C	-3.763404	-0.796702	1.597213
H	-4.215602	-2.805897	-0.131241	H	-4.534525	-0.126643	1.221293
H	-4.334858	-1.301241	-1.048107	H	-4.267068	-1.654044	2.047919
H	-3.013613	-2.422976	-1.363854	H	-3.214586	-0.272261	2.381793

PAH2$_{Br,Br}$

C	-0.038802	0.728011	-0.063753	C	-2.479787	3.462464	0.722950
C	-0.038802	-0.728011	0.063753	C	-3.639706	2.742652	0.835525
C	-2.491495	-0.700279	-0.209013	C	-3.639707	-2.742651	-0.835525
C	-1.263275	-1.411931	-0.202811	C	-2.479788	-3.462464	-0.722950
C	-1.263275	1.411931	0.202811	H	-4.587832	0.838723	0.595459
C	-2.491495	0.700279	0.209013	H	-4.587832	-0.838723	-0.595459
C	-3.648594	1.374031	0.550380	H	-0.087460	-4.618354	-0.264824
C	-3.648594	-1.374031	-0.550381	H	1.886372	-3.466356	0.662519
C	-1.277565	-2.819952	-0.372799	H	1.886373	3.466356	-0.662519
C	-0.091536	-3.543635	-0.127260	H	-0.087459	4.618354	0.264824
C	1.009520	-2.907828	0.364611	H	-2.473303	4.534255	0.882578
C	1.023476	-1.507416	0.493399	H	-4.563232	3.235508	1.112952
C	1.023477	1.507416	-0.493399	H	-4.563232	-3.235508	-1.112952
C	1.009521	2.907828	-0.364611	H	-2.473303	-4.534255	-0.882578
C	-0.091536	3.543634	0.127261	Br	2.490018	0.806004	-1.451216
C	-1.277565	2.819952	0.372799	Br	2.490017	-0.806005	1.451216

PAH2$_{Me,Me}$

C	0.723780	0.852700	0.118225	C	2.805371	-2.759221	-0.580984
C	-0.723780	0.852700	-0.118225	C	-2.805373	-2.759219	0.580984
C	-0.716753	-1.606906	0.142983	C	-3.511240	-1.596644	0.415503
C	-1.422205	-0.376854	0.079739	H	0.887394	-3.705660	-0.508657
C	1.422204	-0.376855	-0.079739	H	-0.887397	-3.705659	0.508657
C	0.716752	-1.606907	-0.142984	H	-4.620984	0.800902	-0.112361
C	1.417273	-2.766526	-0.418395	H	-3.396602	2.783432	-0.892325
C	-1.417275	-2.766525	0.418395	H	3.396604	2.783430	0.892326
C	-2.839395	-0.392779	0.133229	H	4.620985	0.800899	0.112361
C	-3.537969	0.799180	-0.156147	H	-0.238820	3.010962	1.426580
C	-2.853496	1.902644	-0.566757	H	1.328219	3.348187	2.168834
C	-1.440855	1.950183	-0.583460	H	0.930096	4.056666	0.614041
C	1.440857	1.950182	0.583460	H	-1.328217	3.348188	-2.168834
C	2.853497	1.902642	0.566758	H	-0.930093	4.056667	-0.614041
C	3.537969	0.799177	0.156147	H	0.238822	3.010962	-1.426580
C	2.839395	-0.392781	-0.133229	H	4.593039	-1.589087	-0.483015
C	0.819998	3.155001	1.221139	H	3.321237	-3.684232	-0.807857
C	-0.819995	3.155002	-1.221139	H	-3.321240	-3.684229	0.807857
C	3.511239	-1.596647	-0.415503	H	-4.593040	-1.589084	0.483015

PAH6$_{tBu,H}$

C	-0.429809	-0.839777	-0.192199	C	5.198293	3.379167	0.111378
C	-0.607458	0.557848	-0.210365	C	2.437775	-4.775038	0.039785
C	-1.932671	1.118592	-0.219502	C	2.300233	-3.389422	0.092925
C	-3.064842	0.264207	-0.110349	C	-0.078664	-3.657033	-0.411446
C	-2.854937	-1.125016	-0.481276	C	0.106368	-5.037009	-0.438299
C	-1.562953	-1.687461	-0.409297	C	0.031287	5.568130	-0.681508
C	0.858529	-1.395571	-0.088133	C	-2.455573	-3.806625	-1.147057
C	0.520996	1.404079	-0.173595	H	-3.582898	4.076739	-0.286300
C	-2.097782	2.513844	-0.278140	H	-5.408045	2.646335	0.305784
C	-3.394418	3.016620	-0.195125	H	-4.475790	-3.773484	-1.848525
C	-4.444013	2.189552	0.125771	H	-2.058637	5.188116	-0.715322
C	-4.307481	0.807990	0.276541	H	2.145740	5.704429	-0.583708
C	-3.875070	-1.881054	-1.048270	H	1.478416	-6.664587	-0.239350
C	-3.674316	-3.205733	-1.391974	H	3.851877	4.990268	-0.187469
C	-1.077189	4.749923	-0.604101	H	4.829712	-4.103726	0.765697
C	-0.940631	3.378329	-0.401693	H	6.740408	-2.627431	1.113126
C	-5.462351	0.092403	1.010128	H	6.501999	-0.212782	0.877260
C	1.485498	3.673197	-0.323726	H	6.344398	1.618152	0.403148
C	1.025878	-2.820217	-0.126315	H	6.066593	4.026010	0.138220
C	0.355843	2.823980	-0.293807	H	3.404880	-5.233220	0.187725
C	-1.382382	-3.064577	-0.653786	H	-0.732931	-5.693128	-0.621176
C	1.297311	5.038090	-0.530549	H	-0.091701	6.630322	-0.854035
C	1.351695	-5.589210	-0.213726	H	-2.325187	-4.850015	-1.397697
C	3.942951	3.919449	-0.079581	H	-4.826033	-1.409973	-1.246699
C	2.811188	3.108764	-0.128810	C	-5.110123	-1.278416	1.594741
C	1.979752	-0.549379	0.037805	H	-5.087737	-2.078453	0.861954
C	1.813695	0.850044	-0.032806	H	-4.139961	-1.257015	2.094635
C	3.280249	-1.116201	0.252485	H	-5.863858	-1.541832	2.339498
C	4.402951	-0.271974	0.408427	C	-6.716341	-0.010165	0.137919
C	4.248513	1.163624	0.239668	H	-7.543598	-0.421252	0.721819
C	2.960969	1.710913	0.029372	H	-7.020954	0.971215	-0.230760
C	3.438380	-2.519413	0.343825	H	-6.569214	-0.657456	-0.727197
C	4.692210	-3.037575	0.658353	C	-5.817738	0.955662	2.238859
C	5.776561	-2.206150	0.855078	H	-6.193178	1.942872	1.974836
C	5.636629	-0.839924	0.720198	H	-6.597096	0.454032	2.815846
C	5.349571	2.016668	0.268042	H	-4.946717	1.087050	2.883520

PAH6$_{Br,Br}$

C	-0.019626	-0.704184	-0.019100	C	1.220135	-1.418327	0.104404
C	-0.019626	0.704184	0.019101	C	-1.237971	-1.409757	-0.064190
C	1.220135	1.418327	-0.104404	C	-1.237971	1.409757	0.064190
C	2.433959	0.694312	-0.210285	C	1.212921	2.819148	-0.243713
C	2.433959	-0.694312	0.210285	C	2.384106	3.454269	-0.655317

C	3.498646	2.723102	-0.999183	C	-6.106167	2.783178	0.523591
C	3.517116	1.350590	-0.802371	C	-2.399995	-4.943004	-0.377344
C	3.517116	-1.350590	0.802371	C	-2.443004	-3.553142	-0.286052
C	3.498646	-2.723102	0.999183	C	-0.015522	-3.551236	0.004376
C	-0.021628	4.939554	0.103327	C	-0.021629	-4.939554	-0.103327
C	-0.015521	3.551236	-0.004376	C	-1.202476	5.626560	0.301261
C	-2.443004	3.553142	0.286052	C	2.384106	-3.454269	0.655317
C	-1.232900	-2.843120	-0.119959	H	2.402851	4.524550	-0.804526
C	-1.232900	2.843120	0.119959	H	4.354402	3.206702	-1.450004
C	1.212921	-2.819148	0.243713	H	4.354401	-3.206702	1.450004
C	-2.399995	4.943004	0.377344	H	0.906009	5.492197	0.051508
C	-1.202477	-5.626560	-0.301262	H	-3.310350	5.509888	0.506340
C	-4.914018	3.478897	0.520260	H	-1.191311	-6.705789	-0.391007
C	-3.699986	2.823117	0.330448	H	-4.938220	4.547504	0.675896
C	-2.460507	-0.703753	-0.050001	H	-4.938220	-4.547504	-0.675896
C	-2.460507	0.703753	0.050001	H	-7.038165	-3.309864	-0.687670
C	-3.700201	-1.418907	-0.156323	H	-7.059636	-0.897143	-0.328226
C	-4.926826	-0.717082	-0.117879	H	-7.059636	0.897143	0.328226
C	-4.926826	0.717082	0.117879	H	-7.038165	3.309864	0.687670
C	-3.700201	1.418907	0.156323	H	-3.310350	-5.509888	-0.506340
C	-3.699987	-2.823117	-0.330448	H	0.906009	-5.492197	-0.051508
C	-4.914018	-3.478897	-0.520260	H	-1.191310	6.705789	0.391007
C	-6.106168	-2.783177	-0.523591	H	2.402851	-4.524550	0.804526
C	-6.113814	-1.418937	-0.315938	Br	4.949742	-0.421988	1.610845
C	-6.113814	1.418938	0.315938	Br	4.949742	0.421988	-1.610845

PAH6$_{Me,Me}$

C	0.886211	-0.704678	-0.006397	C	5.649645	0.598431	-1.340111
C	0.886210	0.704679	0.006398	C	-1.540220	3.556955	0.229512
C	2.127661	1.415235	-0.123019	C	-0.329816	-2.843825	-0.076339
C	3.347174	0.696058	-0.213968	C	-0.329818	2.843825	0.076340
C	3.347175	-0.696055	0.213968	C	2.117758	-2.813676	0.275486
C	2.127662	-1.415233	0.123020	C	-1.497871	4.947912	0.300113
C	-0.333619	-1.409888	-0.041113	C	-0.299798	-5.629905	-0.216977
C	-0.333620	1.409888	0.041114	C	-4.011577	3.486776	0.461028
C	2.117756	2.813677	-0.275486	C	-2.797249	2.827860	0.283620
C	3.293022	3.445304	-0.683358	C	-1.556660	-0.704269	-0.038529
C	4.408466	2.705330	-0.994533	C	-1.556660	0.704268	0.038529
C	4.461292	1.327814	-0.787104	C	-2.796713	-1.420922	-0.133064
C	4.461293	-1.327810	0.787103	C	-4.023686	-0.718937	-0.105765
C	4.408469	-2.705327	0.994529	C	-4.023687	0.718935	0.105763
C	0.881273	4.939497	0.033647	C	-2.796714	1.420920	0.133063
C	0.888363	3.549338	-0.053784	C	-2.797247	-2.827862	-0.283619
C	5.649646	-0.598428	1.340110	C	-4.011574	-3.486779	-0.461029

C	-5.203863	-2.791496	-0.475232	H	6.562664	-0.796567	0.775211
C	-5.210980	-1.423904	-0.290995	H	5.496084	-0.478162	-1.371626
C	-5.210982	1.423900	0.290992	H	6.562662	0.796569	-0.775210
C	-5.203865	2.791493	0.475230	H	5.826040	0.944323	-2.360909
C	-1.497867	-4.947913	-0.300111	H	-2.408590	5.516641	0.418290
C	-1.540218	-3.556956	-0.229511	H	-0.288619	-6.710515	-0.290144
C	0.888365	-3.549338	0.053786	H	-4.035528	4.557929	0.598375
C	0.881277	-4.939496	-0.033643	H	-4.035525	-4.557932	-0.598374
C	-0.299803	5.629905	0.216981	H	-6.136080	-3.320905	-0.629438
C	3.293026	-3.445302	0.683356	H	-6.156678	-0.902065	-0.311457
H	3.310060	4.513729	-0.847152	H	-6.156679	0.902062	0.311453
H	5.268399	3.197591	-1.435601	H	-6.136082	3.320901	0.629436
H	5.268404	-3.197588	1.435596	H	-2.408586	-5.516643	-0.418288
H	1.809324	5.490875	-0.023609	H	1.809328	-5.490873	0.023615
H	5.826039	-0.944318	2.360909	H	-0.288625	6.710514	0.290150
H	5.496086	0.478166	1.371624	H	3.310065	-4.513727	0.847147

PAH5$_{t\mathrm{Bu,H}}$

C	0.302518	-2.247367	0.620453	H	-3.198256	2.045466	-1.747110
C	-1.047039	-2.108634	0.698033	H	3.444926	1.842770	-0.417688
C	-1.670572	-0.926931	0.240603	H	5.274798	0.403816	-0.996998
C	-0.850986	0.146807	-0.155233	H	6.314834	-1.833055	-0.888154
C	0.573281	0.097509	0.040310	H	4.958081	-3.784013	-0.171928
C	1.147160	-1.177821	0.238957	H	2.608975	-3.520131	0.383941
C	-3.102286	-0.833469	0.090638	H	-3.599468	-2.649203	1.151300
C	-3.655089	0.268887	-0.603819	H	-6.001284	-2.444112	0.845343
C	-2.780011	1.250214	-1.140504	H	-6.955914	-0.518601	-0.397222
C	-1.447166	1.198152	-0.906582	H	-5.450363	1.208073	-1.316342
C	1.451349	1.251769	-0.011440	C	1.104781	2.687361	0.459415
C	2.758904	1.011519	-0.313223	C	2.229037	3.151951	1.407199
C	3.333907	-0.282149	-0.379155	H	3.188946	3.266697	0.905702
C	2.552922	-1.389549	0.012863	H	1.965065	4.124799	1.827047
C	4.691029	-0.461288	-0.702566	H	2.359084	2.447689	2.230641
C	5.269793	-1.702191	-0.635335	C	1.057251	3.686047	-0.700471
C	4.503480	-2.802476	-0.229300	H	0.239827	3.496572	-1.395740
C	3.176745	-2.647932	0.090312	H	0.926979	4.699037	-0.311482
C	-3.986149	-1.803187	0.599480	H	1.988308	3.661558	-1.270018
C	-5.344017	-1.688470	0.432518	C	-0.169263	2.778210	1.304732
C	-5.883992	-0.600368	-0.265151	H	-1.087874	2.680173	0.735283
C	-5.048220	0.359077	-0.774853	H	-0.175498	2.014103	2.084399
H	0.741072	-3.203786	0.868402	H	-0.193456	3.754018	1.794180
H	-1.643544	-2.950110	1.021240	H	-0.798470	1.937940	-1.348756

PAH5$_{\mathrm{Br,Br}}$

C	-0.674151	2.695746	-0.085997	C	3.603127	2.628254	0.498202
C	0.674151	2.695746	0.085997	C	4.971470	2.574365	0.601301
C	1.416614	1.491589	0.069867	C	5.656076	1.378533	0.350336
C	0.711267	0.282810	-0.094035	C	4.954151	0.253231	0.003547
C	-0.711267	0.282810	0.094035	H	-1.193478	3.640840	-0.158735
C	-1.416614	1.491589	-0.069867	H	1.193478	3.640840	0.158735
C	2.855062	1.488531	0.154448	H	3.364646	-1.703398	-0.924444
C	3.551674	0.284030	-0.094604	H	-3.364646	-1.703398	0.924444
C	2.822846	-0.850723	-0.535987	H	-5.470197	-0.677858	0.200446
C	1.467738	-0.844520	-0.555188	H	-6.735564	1.345163	-0.430819
C	-1.467738	-0.844520	0.555188	H	-5.523538	3.462397	-0.883513
C	-2.822846	-0.850723	0.535987	H	-3.100119	3.560872	-0.714673
C	-3.551674	0.284030	0.094604	H	3.100119	3.560872	0.714673
C	-2.855062	1.488531	-0.154448	H	5.523538	3.462397	0.883513
C	-4.954151	0.253231	-0.003547	H	6.735564	1.345163	0.430819
C	-5.656076	1.378533	-0.350336	H	5.470197	-0.677858	-0.200446
C	-4.971470	2.574365	-0.601301	Br	0.632563	-2.226952	-1.546898
C	-3.603127	2.628254	-0.498202	Br	-0.632563	-2.226952	1.546898

PAH5$_{Me,Me}$

C	-0.676122	-1.965400	0.065092	C	4.980291	-1.868025	-0.445675
C	0.676122	-1.965401	-0.065092	C	5.662544	-0.673776	-0.175642
C	1.415871	-0.760263	-0.032760	C	4.954161	0.455772	0.140437
C	0.713322	0.455161	0.108017	H	-1.196986	-2.911026	0.119531
C	-0.713322	0.455162	-0.108016	H	1.196986	-2.911026	-0.119531
C	-1.415871	-0.760263	0.032760	H	3.348629	2.429467	0.965668
C	2.854653	-0.768108	-0.075782	H	-3.348629	2.429467	-0.965669
C	3.547737	0.434286	0.190658	H	-1.229305	2.926855	-2.223413
C	2.802999	1.571705	0.584462	H	0.293647	2.607407	-1.403413
C	1.440966	1.607138	0.572803	H	-0.888826	3.702534	-0.685185
C	-1.440966	1.607138	-0.572802	H	1.229305	2.926854	2.223413
C	-2.802999	1.571705	-0.584462	H	-0.293646	2.607408	1.403413
C	-3.547737	0.434286	-0.190658	H	0.888827	3.702534	0.685186
C	-2.854653	-0.768107	0.075782	H	-5.467880	1.385774	-0.356957
C	-0.769447	2.774392	-1.245396	H	-6.744546	-0.646615	0.218105
C	0.769448	2.774391	1.245396	H	-5.537168	-2.760223	0.704920
C	-4.954161	0.455773	-0.140437	H	-3.109718	-2.844974	0.619536
C	-5.662544	-0.673776	0.175642	H	3.109718	-2.844975	-0.619536
C	-4.980291	-1.868025	0.445675	H	5.537168	-2.760223	-0.704920
C	-3.609508	-1.913727	0.389654	H	6.744546	-0.646616	-0.218105
C	3.609508	-1.913727	-0.389654	H	5.467880	1.385773	0.356956

PAH4$_{tBu,H}$

C	0.678709	0.710202	-0.175201	C	0.920949	-0.704606	-0.061133

C	-0.140304	-1.598348	-0.267968	C	1.391907	-3.472297	-0.059994
C	-1.460255	-1.110669	-0.489279	H	-0.721571	-4.925978	-0.861105
C	-1.756960	0.297621	-0.249946	H	-2.884860	-3.992188	-1.593031
C	-0.636804	1.193773	-0.316746	H	-4.214118	2.606488	-0.236851
C	0.117467	-3.000965	-0.352591	H	-2.373647	4.108166	-0.718958
C	-0.920336	-3.862991	-0.790347	H	2.448219	4.955380	-0.405830
C	-2.118942	-3.345127	-1.182635	H	4.739184	4.108532	-0.048439
C	-2.383256	-1.970426	-1.041823	H	5.143075	1.722715	0.272349
C	-3.025486	0.821528	0.005937	H	5.410483	-0.166925	0.744967
C	-3.208462	2.207657	-0.260312	H	5.761270	-2.573829	0.946286
C	-2.185306	3.059468	-0.521146	H	3.903320	-4.151517	0.569400
C	-0.849126	2.597718	-0.443577	H	0.057806	4.528537	-0.582745
C	-4.218654	0.129462	0.691473	H	1.583000	-4.539590	-0.087366
C	1.765863	1.605081	-0.119154	H	-3.334568	-1.577405	-1.369944
C	3.094448	1.136657	0.110494	C	-3.900161	-1.195924	1.387719
C	3.322496	-0.295817	0.301769	H	-3.834644	-2.043633	0.713233
C	2.222138	-1.190207	0.157329	H	-2.961110	-1.137692	1.940925
C	1.536792	3.004515	-0.293009	H	-4.697187	-1.411945	2.101982
C	2.633524	3.896761	-0.266172	C	-4.678367	1.062802	1.832655
C	3.898330	3.425823	-0.064993	H	-5.026720	2.032473	1.481643
C	4.124815	2.054940	0.123307	H	-5.504731	0.592475	2.368966
C	4.563149	-0.822562	0.597806	H	-3.865132	1.233547	2.540688
C	4.769763	-2.205694	0.711937	C	-5.396457	-0.053875	-0.269820
C	3.742579	-3.081374	0.511144	H	-6.260900	-0.447969	0.270314
C	2.443936	-2.601565	0.218911	H	-5.690195	0.893668	-0.725477
C	0.232812	3.464564	-0.465465	H	-5.161762	-0.750067	-1.076024

PAH4$_{Br,Br}$

C	-1.345980	0.713019	0.099632	C	-3.811967	-0.715749	-0.148970
C	-1.345980	-0.713019	-0.099632	C	-2.566123	-1.404499	-0.228486
C	-0.130702	-1.419276	-0.090976	C	-2.557811	2.818701	0.431020
C	1.105623	-0.721380	0.101109	C	-3.782176	3.498088	0.627845
C	1.105623	0.721380	-0.101109	C	-4.960602	2.810238	0.604718
C	-0.130702	1.419276	0.090976	C	-4.974325	1.429821	0.358718
C	-0.148384	-2.845444	-0.152885	C	-4.974325	-1.429821	-0.358718
C	1.055841	-3.551861	0.092126	C	-4.960601	-2.810238	-0.604718
C	2.163134	-2.885559	0.509682	C	-3.782175	-3.498088	-0.627845
C	2.172870	-1.474355	0.562318	C	-2.557811	-2.818701	-0.431020
C	2.172870	1.474355	-0.562318	C	-1.346866	3.506587	0.377513
C	2.163134	2.885559	-0.509682	C	-1.346866	-3.506587	-0.377513
C	1.055841	3.551861	-0.092126	H	1.057667	-4.633029	0.023004
C	-0.148384	2.845444	0.152885	H	3.052554	-3.420769	0.813453
C	-2.566123	1.404499	0.228486	H	3.052553	3.420769	-0.813453
C	-3.811967	0.715749	0.148970	H	1.057667	4.633029	-0.023004

H	-3.764536	4.568884	0.793059	H	-3.764536	-4.568884	-0.793059
H	-5.898126	3.328384	0.765249	H	-1.348176	4.587712	0.461624
H	-5.930348	0.924759	0.339878	H	-1.348176	-4.587712	-0.461624
H	-5.930348	-0.924759	-0.339878	Br	3.643051	-0.730653	1.476840
H	-5.898126	-3.328384	-0.765248	Br	3.643051	0.730653	-1.476840

PAH4$_{Me,Me}$

C	0.380578	0.717847	-0.057678	C	4.010995	-1.448626	0.269957
C	0.380577	-0.717848	0.057678	C	3.997412	-2.841085	0.433899
C	-0.836366	-1.420096	0.014786	C	2.818330	-3.528348	0.420582
C	-2.076491	-0.718731	-0.132071	C	1.593544	-2.838472	0.267475
C	-2.076491	0.718733	0.132071	C	0.381206	3.521096	-0.183882
C	-0.836364	1.420097	-0.014786	C	0.381203	-3.521096	0.183882
C	-0.817940	-2.847430	0.004898	H	-2.027855	-4.621517	-0.251425
C	-2.027617	-3.537807	-0.261025	H	-4.028014	-3.371694	-0.934448
C	-3.135803	-2.841215	-0.619329	H	-4.028011	3.371697	0.934447
C	-3.177821	-1.422798	-0.604932	H	-2.027851	4.621518	0.251425
C	-3.177820	1.422801	0.604932	H	-4.229569	-0.269441	1.428813
C	-3.135800	2.841218	0.619329	H	-5.281046	0.896297	0.620936
C	-2.027614	3.537808	0.261025	H	-4.583056	1.292036	2.180529
C	-0.817937	2.847430	-0.004898	H	-4.583057	-1.292032	-2.180530
C	-4.380317	0.790251	1.231191	H	-4.229568	0.269445	-1.428813
C	-4.380318	-0.790247	-1.231191	H	-5.281046	-0.896293	-0.620937
C	1.601685	1.415062	-0.145793	H	2.800448	4.607019	-0.523766
C	2.847924	0.723473	-0.105796	H	4.935151	3.368310	-0.560881
C	2.847923	-0.723476	0.105796	H	4.967064	0.943314	-0.278434
C	1.601684	-1.415064	0.145793	H	4.967063	-0.943319	0.278434
C	1.593546	2.838470	-0.267475	H	4.935147	-3.368315	0.560881
C	2.818333	3.528345	-0.420582	H	2.800444	-4.607022	0.523766
C	3.997415	2.841081	-0.433899	H	0.381752	4.605406	-0.210740
C	4.010996	1.448622	-0.269957	H	0.381748	-4.605407	0.210740

PAH7$_{tBu,H}$

C	1.366426	2.561512	0.090387	C	-2.525984	0.961182	-0.481091
C	2.092431	1.676982	1.096249	C	-2.319382	2.312141	-0.680278
C	2.202085	0.318032	0.481569	C	-1.059753	2.843470	-0.467400
C	1.065756	-0.183673	-0.167916	H	1.264197	3.583049	0.462077
C	-0.185897	0.602763	-0.135580	H	1.959191	2.611366	-0.831091
C	0.000514	2.000636	-0.190328	H	1.514730	1.643063	2.027171
C	3.396752	-0.384815	0.428221	H	3.081883	2.070418	1.334484
C	3.499042	-1.559233	-0.302043	H	4.264772	0.010151	0.944895
C	2.403559	-2.011729	-1.021418	H	4.438883	-2.096536	-0.339594
C	1.204537	-1.321871	-0.958875	H	2.483628	-2.897605	-1.639753
C	-1.497367	0.080167	-0.136577	H	-3.536043	0.584512	-0.565891

H	-3.151731	2.954028	-0.942626	C	-0.889705	-2.065161	1.169818
H	-0.893476	3.913582	-0.521712	H	-0.059096	-2.461922	0.595409
H	0.361542	-1.659617	-1.545949	H	-0.478441	-1.413970	1.943855
C	-1.929882	-1.327528	0.322340	H	-1.376218	-2.907669	1.665882
C	-2.345029	-2.193621	-0.870088	C	-3.156594	-1.179317	1.242403
H	-1.510702	-2.393979	-1.542577	H	-2.933587	-0.521859	2.084877
H	-2.728569	-3.155417	-0.519778	H	-4.032617	-0.785393	0.729462
H	-3.131314	-1.707620	-1.451090	H	-3.427995	-2.160248	1.637758

PAH7$_{Br,Br}$

C	0.406285	3.170260	0.646835	C	2.615057	2.004853	1.004574
C	-0.406260	3.170263	-0.646835	H	1.025590	4.064868	0.727060
C	-1.279748	1.950957	-0.643350	H	-0.279793	3.165073	1.501221
C	-0.725189	0.763992	-0.130064	H	0.279818	3.165072	-1.501221
C	0.725196	0.763986	0.130063	H	-1.025558	4.064877	-0.727059
C	1.279764	1.950947	0.643349	H	-3.017539	2.924764	-1.412524
C	-2.615041	2.004873	-1.004575	H	-4.480476	0.944418	-1.107966
C	-3.438286	0.905710	-0.816090	H	-3.596010	-1.048125	0.063354
C	-2.945413	-0.219596	-0.181006	H	3.596003	-1.048153	-0.063357
C	-1.608777	-0.270957	0.186429	H	4.480484	0.944383	1.107964
C	1.608775	-0.270969	-0.186430	H	3.017562	2.924740	1.412524
C	2.945412	-0.219618	0.181004	Br	1.098915	-1.708850	-1.303371
C	3.438294	0.905684	0.816089	Br	-1.098928	-1.708841	1.303370

PAH7$_{Me,Me}$

C	0.520960	2.370368	0.557113	H	1.145293	3.264732	0.520015
C	-0.520952	2.370370	-0.557111	H	0.006691	2.367470	1.525289
C	-1.373717	1.147954	-0.393483	H	-0.006683	2.367472	-1.525287
C	-0.739856	-0.047002	-0.001420	H	-1.145282	3.264736	-0.520012
C	0.739856	-0.047004	0.001423	H	-3.220164	2.130948	-0.825036
C	1.373721	1.147950	0.393483	H	-4.604105	0.141986	-0.286559
C	-2.750861	1.205671	-0.509819	H	-3.522365	-1.865850	0.647707
C	-3.525668	0.099897	-0.192090	H	3.522358	-1.865860	-0.647711
C	-2.915564	-1.031369	0.312894	H	4.604107	0.141973	0.286550
C	-1.529691	-1.119112	0.442184	H	3.220172	2.130938	0.825031
C	1.529687	-1.119117	-0.442183	H	1.565802	-2.514093	-2.048203
C	2.915560	-1.031378	-0.312896	H	1.006992	-3.216246	-0.538959
C	3.525669	0.099887	0.192084	H	-0.061796	-2.160421	-1.464285
C	2.750866	1.205663	0.509816	H	0.061790	-2.160422	1.464285
C	0.970412	-2.315229	-1.155035	H	-1.565808	-2.514075	2.048215
C	-0.970422	-2.315223	1.155042	H	-1.007014	-3.216244	0.538973

PAH1$_{tBu,H}^{‡}$

C	-2.326399	0.334791	-0.093178	C	-1.953086	-1.007272	0.045898

C	-0.545216	-1.384698	-0.018489	H	-2.706609	-2.996011	0.430478
C	0.503959	-0.420602	0.030853	H	-1.078863	-3.451955	-0.278741
C	0.079361	0.999143	0.067740	H	1.226701	-4.260462	-0.352471
C	-1.286491	1.346412	-0.119625	H	3.054258	-2.677976	-0.184363
C	-3.692999	0.661044	-0.119020	H	1.304361	4.182682	0.320979
C	-4.665633	-0.297787	0.023229	H	-1.071445	4.750182	-0.231483
C	-4.295374	-1.625360	0.225897	H	-2.683773	2.943600	-0.451462
C	-2.964535	-1.965126	0.238997	C	4.432613	-0.940645	-0.116989
C	-0.268109	-2.748835	-0.170159	H	4.561313	-1.665223	0.688373
C	1.015270	-3.205649	-0.226932	H	4.476288	-1.462005	-1.074435
C	2.050123	-2.290722	-0.137844	H	5.285215	-0.258279	-0.077363
C	1.858638	-0.923704	-0.021295	C	3.306715	0.525293	1.446462
C	0.953264	2.086872	0.252938	H	3.977846	1.388336	1.426843
C	0.566567	3.404236	0.168903	H	2.369070	0.826042	1.906455
C	-0.751310	3.721104	-0.125294	H	3.748311	-0.218624	2.111765
C	-1.652356	2.694604	-0.252757	C	3.231588	0.872409	-1.164853
C	3.156531	-0.097427	0.036739	H	2.281884	1.310133	-1.454141
H	-4.005225	1.689010	-0.227564	H	3.935270	1.684720	-0.965138
H	-5.711075	-0.015357	0.005281	H	3.601373	0.322025	-2.031792
H	-5.048666	-2.387425	0.383722	H	1.984442	1.918069	0.467515

PAH1$_{Br,Br}$‡

C	2.669067	0.694381	-0.092222	C	-0.709613	2.965007	0.818796
C	2.669071	-0.694369	-0.092208	C	0.540375	3.447227	1.150093
C	1.459017	-1.381247	0.318090	C	1.620869	2.671672	0.824537
C	0.177958	-0.750721	0.192210	H	3.805787	2.463320	-0.564259
C	0.177953	0.750721	0.192196	H	5.812969	1.241370	-1.248157
C	1.459008	1.381258	0.318064	H	5.812978	-1.241359	-1.248133
C	3.815178	1.382884	-0.510602	H	3.805803	-2.463311	-0.564211
C	4.940529	0.696870	-0.908701	H	2.623585	-3.037829	0.992356
C	4.940534	-0.696859	-0.908687	H	0.656007	-4.427773	1.593292
C	3.815188	-1.382873	-0.510575	H	-1.579779	-3.596074	0.929855
C	1.620886	-2.671651	0.824587	H	-1.579802	3.596075	0.929797
C	0.540397	-3.447208	1.150153	H	0.655979	4.427801	1.593215
C	-0.709594	-2.965003	0.818845	H	2.623566	3.037860	0.992297
C	-0.890398	-1.691931	0.297787	Br	-2.657238	-1.573602	-0.387296
C	-0.890409	1.691926	0.297758	Br	-2.657246	1.573576	-0.387325

PAH1$_{Me,Me}$‡

C	-1.655945	0.695348	0.026178	C	-0.399856	1.385987	-0.197415
C	-1.655931	-0.695394	0.026173	C	-2.852975	1.380741	0.278588
C	-0.399827	-1.386005	-0.197424	C	-4.024871	0.696838	0.508915
C	0.854480	-0.753053	0.068018	C	-4.024857	-0.696937	0.508909
C	0.854464	0.753061	0.068023	C	-2.852947	-1.380814	0.278577

C	-0.490659	-2.700690	-0.663844	H	0.566789	-4.490244	-1.185500
C	0.622595	-3.484782	-0.787917	H	2.688995	-3.606166	-0.297118
C	1.815156	-2.966118	-0.321641	H	2.688917	3.606216	-0.297095
C	1.961961	-1.661981	0.136713	H	0.566692	4.490253	-1.185474
C	1.961925	1.662012	0.136724	H	-1.458780	3.083138	-0.954591
C	1.815091	2.966149	-0.321622	C	3.325528	-1.447762	0.738188
C	0.622520	3.484789	-0.787896	H	4.017958	-0.931266	0.078951
C	-0.490717	2.700673	-0.663828	H	3.284080	-0.919943	1.684691
H	-2.853292	2.460813	0.336648	H	3.759054	-2.425188	0.944912
H	-4.936770	1.242347	0.718860	C	3.325495	1.447821	0.738201
H	-4.936744	-1.242467	0.718849	H	3.284056	0.920001	1.684704
H	-2.853242	-2.460887	0.336628	H	4.017937	0.931338	0.078966
H	-1.458713	-3.083174	-0.954609	H	3.759002	2.425255	0.944926

PAH3$_{t\mathrm{Bu,H}}^{\ddagger}$

C	1.944146	-0.262989	-0.000984	H	4.469914	2.685515	-0.001761
C	1.460913	1.066684	-0.000168	H	-1.981846	4.061331	0.003350
C	0.052963	1.328802	0.000929	H	-3.650111	2.325197	0.003930
C	-0.928445	0.274764	0.001268	H	-1.361157	-4.387968	-0.000042
C	-0.394603	-1.110507	0.000400	H	1.098568	-4.764608	-0.001943
C	1.017971	-1.339708	-0.000689	H	3.303975	-3.904803	-0.003229
C	3.335960	-0.510395	-0.002068	H	4.885882	-2.014351	-0.003705
C	4.236640	0.568881	-0.002335	H	2.689793	4.268842	0.000072
C	3.777310	1.851633	-0.001557	H	0.268064	4.765877	0.001984
C	2.397383	2.127838	-0.000468	C	-3.536747	-0.263463	0.002936
C	-0.331402	2.697591	0.001688	C	-3.585172	-1.069565	-1.318127
C	-1.679337	3.020513	0.002766	H	-2.612217	-1.360098	-1.703901
C	-2.615658	2.025416	0.003086	H	-4.052336	-0.450045	-2.085414
C	-2.306355	0.661921	0.002384	H	-4.194922	-1.970237	-1.206544
C	-1.182707	-2.262438	0.000568	C	-3.583296	-1.070484	1.323506
C	-0.671105	-3.552818	-0.000249	H	-4.193194	-1.971086	1.212159
C	0.682075	-3.764146	-0.001294	H	-4.049380	-0.451504	2.091884
C	1.541000	-2.664922	-0.001530	H	-2.609793	-1.361274	1.707701
C	2.947865	-2.881032	-0.002616	C	-4.879301	0.485902	0.004150
C	3.815098	-1.846204	-0.002877	H	-5.016901	1.103730	0.892785
C	1.952055	3.474933	0.000323	H	-5.673662	-0.264528	0.004450
C	0.631596	3.744780	0.001365	H	-5.018159	1.104351	-0.883858
H	5.300510	0.361274	-0.003171	H	-2.245704	-2.195730	0.001356

PAH3$_{\mathrm{Br,Br}}^{\ddagger}$

C	2.292720	0.705231	-0.104173	C	-0.213775	0.752274	0.145783
C	2.292488	-0.705594	-0.103999	C	1.081144	1.412393	0.153623
C	1.080681	-1.412294	0.153981	C	3.515330	1.394219	-0.294502
C	-0.214022	-0.751753	0.145971	C	4.690352	0.679206	-0.588515

C	4.690129	-0.680476	-0.588347	C	2.474893	-3.471316	0.249460
C	3.514872	-1.395031	-0.294154	H	5.601929	1.234821	-0.774841
C	1.226647	-2.808565	0.390656	H	5.601523	-1.236437	-0.774534
C	0.119921	-3.565840	0.752444	H	0.235033	-4.608294	1.022211
C	-1.110960	-2.997627	0.665098	H	-1.993637	-3.595445	0.838782
C	-1.289605	-1.669383	0.258825	H	-1.992460	3.596725	0.837868
C	-1.289058	1.670285	0.258404	H	0.236543	4.608889	1.021047
C	-1.109978	2.998574	0.664338	H	2.502312	4.538891	0.429733
C	0.121089	3.566405	0.751544	H	4.527838	3.301996	-0.280136
C	1.227568	2.808675	0.389951	H	4.526754	-3.303136	-0.279314
C	2.476032	3.470982	0.248591	H	2.500823	-4.539188	0.430869
C	3.579572	2.798953	-0.133610	Br	-3.113201	1.543207	-0.268626
C	3.578653	-2.799745	-0.132913	Br	-3.113708	-1.541842	-0.268234

PAH3$_{Me,Me}$‡

C	-1.288312	0.690471	0.074785	C	-2.530151	-2.834673	0.022337
C	-1.271011	-0.721203	0.077426	C	-1.381971	-3.502417	-0.195776
C	-0.027883	-1.414499	-0.039528	H	-4.659887	1.180361	0.369721
C	1.253414	-0.740739	0.045111	H	-4.629650	-1.292284	0.375206
C	1.234560	0.771962	0.044493	H	0.936791	-4.641826	-0.618935
C	-0.062226	1.413689	-0.042765	H	3.114979	-3.577513	-0.332782
C	-2.533914	1.363196	0.140153	H	3.026602	3.654859	-0.326115
C	-3.726645	0.635128	0.289089	H	0.824374	4.663520	-0.620762
C	-3.710021	-0.724745	0.292139	H	-1.484295	4.542351	-0.344595
C	-2.499862	-1.424033	0.145919	H	-3.565241	3.259887	0.059784
C	-0.132927	-2.824020	-0.223714	H	-3.484217	-3.345781	0.073826
C	1.012645	-3.580472	-0.415621	H	-1.373061	-4.577529	-0.331998
C	2.219352	-2.973206	-0.262053	C	3.785174	1.460604	0.424327
C	2.380479	-1.614119	0.044285	H	3.889546	0.986809	1.394675
C	2.340632	1.672697	0.046969	H	4.361523	0.905663	-0.306607
C	2.147024	3.027493	-0.258355	H	4.256967	2.436780	0.515004
C	0.925607	3.604494	-0.416369	C	3.825580	-1.371430	0.403377
C	-0.201363	2.820301	-0.228612	H	4.403386	-0.919031	-0.398537
C	-1.467025	3.467671	-0.205820	H	3.946369	-0.785603	1.303989
C	-2.598742	2.772360	0.011574	H	4.285448	-2.336716	0.606353

PAH2$_{t\text{Bu},H}$‡

C	-0.697855	0.191065	0.006693	C	3.616214	0.563785	-0.016102
C	0.207421	-0.996293	0.005387	C	2.497671	-1.964919	-0.003537
C	2.235927	0.456460	-0.008737	C	1.961849	-3.265932	0.002677
C	1.634178	-0.825459	-0.002244	C	0.611910	-3.425222	0.009891
C	-0.045890	1.481567	-0.000070	C	-0.232543	-2.310313	0.011121
C	1.374027	1.632435	-0.007487	C	-2.118052	0.173792	0.013853
C	1.932217	2.898576	-0.013494	C	-2.809353	1.402141	0.013808

C	-2.199779	2.613851	0.007435	H	4.518029	-2.689999	-0.011817
C	-0.804584	2.688970	0.000405	C	-3.043625	-1.058187	0.022026
C	-0.191516	3.956057	-0.005972	C	-2.858767	-1.841950	1.344955
C	1.167201	4.062623	-0.012835	H	-3.189070	-2.878622	1.236863
C	4.447896	-0.553935	-0.017294	H	-1.842362	-1.844241	1.728274
C	3.895558	-1.802882	-0.011066	H	-3.480576	-1.378177	2.112373
H	3.006208	3.007842	-0.018965	C	-2.872383	-1.849264	-1.298380
H	4.085573	1.536170	-0.021201	H	-1.859975	-1.853711	-1.692121
H	2.635965	-4.114315	0.001569	H	-3.201538	-2.885311	-1.181165
H	0.168163	-4.413526	0.014780	H	-3.502061	-1.389717	-2.061914
H	-3.886049	1.391978	0.019141	C	-4.542896	-0.715137	0.028820
H	-2.782729	3.527527	0.007772	H	-4.845273	-0.158638	0.917153
H	-0.826766	4.834037	-0.005219	H	-4.854505	-0.163717	-0.859490
H	1.653614	5.030153	-0.017734	H	-5.093845	-1.658882	0.034372
H	5.523084	-0.423622	-0.023146	H	-1.272862	-2.536611	0.016935

PAH2$_{Br,Br}^{‡}$

C	-0.049750	0.720905	0.141525	C	-2.576309	3.577435	-0.048839
C	-0.118324	-0.791651	0.044630	C	-3.648378	2.943914	-0.609826
C	-2.629169	-0.619004	-0.133304	C	-4.065491	-2.566553	0.122740
C	-1.454072	-1.388247	0.054927	C	-2.959530	-3.350158	0.272043
C	-1.312738	1.450178	0.064291	H	-4.479071	1.046331	-1.115727
C	-2.525171	0.813473	-0.295582	H	-4.759198	-0.572926	-0.139758
C	-3.615090	1.557599	-0.715446	H	-0.734554	-4.703555	0.559372
C	-3.884385	-1.202567	-0.071377	H	1.525588	-3.787590	0.333640
C	-1.670924	-2.787283	0.239988	H	1.770260	3.441930	1.134635
C	-0.576351	-3.645874	0.389149	H	-0.400239	4.586391	1.082720
C	0.666838	-3.135937	0.274213	H	-2.578452	4.647545	0.120192
C	0.902821	-1.757194	0.070045	H	-4.521515	3.496463	-0.932922
C	1.039718	1.585054	0.361572	H	-5.062721	-2.985664	0.166782
C	0.880308	2.910341	0.830870	H	-3.043194	-4.419243	0.426396
C	-0.309386	3.547001	0.792789	Br	2.882148	1.465450	-0.109405
C	-1.411701	2.858121	0.270618	Br	2.775902	-1.613177	-0.211924

PAH2$_{Me,Me}^{‡}$

C	0.757346	0.927048	-0.024413	C	-3.651594	0.651948	-0.009727
C	-0.767532	0.931299	0.085965	C	-3.047321	1.850478	0.146053
C	-0.725528	-1.591861	0.005683	C	-1.644466	2.036071	0.177713
C	-1.432303	-0.362300	0.002875	C	1.646423	2.019017	-0.151432
C	1.415091	-0.372802	-0.005504	C	3.003759	1.798279	-0.493641
C	0.707306	-1.584381	0.193736	C	3.600871	0.586607	-0.486534
C	1.372567	-2.754653	0.516653	C	2.828793	-0.524355	-0.134096
C	-1.373502	-2.794378	-0.219497	C	3.474782	-1.753662	0.096699
C	-2.852315	-0.489759	-0.092624	C	2.760748	-2.850432	0.482479

C	-2.755546	-2.881985	-0.357290	H	-3.229229	-3.840305	-0.529812
C	-3.486610	-1.735448	-0.266944	H	-4.567412	-1.748289	-0.344854
H	0.797128	-3.627647	0.790790	C	1.474129	3.496822	0.110853
H	-0.786407	-3.696662	-0.312485	H	1.064818	4.046263	-0.735734
H	-4.729877	0.564510	-0.066913	H	0.885429	3.706221	0.990838
H	-3.667399	2.733562	0.226534	H	2.460314	3.917465	0.299698
H	3.606689	2.673653	-0.701001	C	-1.357445	3.508065	0.315401
H	4.659654	0.473675	-0.685927	H	-0.883808	3.753367	1.262994
H	4.553269	-1.789201	-0.003067	H	-0.761053	3.905929	-0.494173
H	3.251790	-3.783478	0.729107	H	-2.300542	4.049457	0.298766

$PAH6_{tBu,H}^{‡}$

C	-0.375242	-0.873930	-0.062464	C	5.970498	-2.058996	0.359990
C	-0.602381	0.515719	-0.071348	C	5.759659	-0.696894	0.424131
C	-1.953490	1.034899	-0.081769	C	5.305190	2.167343	0.540148
C	-3.099530	0.179191	0.064769	C	5.095199	3.531137	0.532842
C	-2.826155	-1.269866	0.112339	C	2.680752	-4.660524	-0.510517
C	-1.496510	-1.766628	-0.029978	C	2.491791	-3.309266	-0.232325
C	0.946116	-1.384017	-0.057930	C	0.083251	-3.672397	-0.296122
C	0.513704	1.393594	-0.063746	C	0.317677	-5.015479	-0.587334
C	-2.105257	2.435145	-0.224297	C	-0.043372	5.515738	-0.767469
C	-3.374990	2.975254	-0.168671	C	-2.310120	-4.059349	0.066940
C	-4.467305	2.171167	0.007697	H	-3.526748	4.042363	-0.228872
C	-4.398366	0.789597	0.125400	H	-5.425497	2.659302	0.059896
C	-3.824146	-2.232817	0.277837	H	-4.406238	-4.276673	0.424238
C	-3.582975	-3.589908	0.269848	H	-2.111384	5.068295	-0.902306
C	-1.130141	4.669148	-0.692572	H	2.063538	5.714092	-0.567398
C	-0.967557	3.319167	-0.382998	H	1.767621	-6.541828	-0.958266
C	1.431470	3.691808	-0.210130	H	3.684592	5.102346	0.291580
C	1.177248	-2.793576	-0.180991	H	5.091857	-3.976341	0.111115
C	0.329230	2.808438	-0.201822	H	6.971172	-2.457422	0.473785
C	-1.260138	-3.163259	-0.097587	H	6.611150	-0.049316	0.572013
C	1.224241	5.036339	-0.505874	H	6.305508	1.800362	0.716173
C	1.603592	-5.500642	-0.709108	H	5.922007	4.207034	0.713273
C	3.833023	4.032044	0.290307	H	3.679466	-5.062117	-0.603092
C	2.754951	3.177121	0.074737	H	-0.509893	-5.690709	-0.748892
C	2.046852	-0.507391	0.023550	H	-0.185775	6.556679	-1.030522
C	1.829044	0.884376	0.027969	H	-2.126467	-5.123381	0.073907
C	3.383857	-1.030060	0.105528	C	-5.769414	0.111146	0.319330
C	4.480183	-0.159584	0.298915	C	-5.833821	-0.556135	1.717147
C	4.255096	1.274379	0.336033	H	-6.125511	0.198316	2.449455
C	2.949499	1.780243	0.139349	H	-6.589447	-1.345991	1.741187
C	3.612536	-2.420410	0.004062	H	-4.891359	-0.972257	2.061967
C	4.907690	-2.912408	0.147600	C	-6.101399	-0.777152	-0.906520

H	-6.834366	-1.545770	-0.647189	H	-6.883022	1.804110	1.186379
H	-6.544759	-0.148782	-1.680556	H	-7.066100	1.653184	-0.574653
H	-5.241280	-1.264251	-1.356515	H	-7.859511	0.511717	0.501862
C	-6.948871	1.098209	0.357200	H	-4.836544	-1.946063	0.428855

PAH6$_{Br,Br}$‡

C	-0.062453	-0.700446	0.280092	C	-3.730351	-2.829130	-0.193956
C	-0.062456	0.700451	0.280092	C	-4.887649	-3.518361	-0.545947
C	1.180909	1.407084	0.417555	C	-6.012992	-2.838915	-0.968400
C	2.438065	0.744989	0.161408	C	-6.011439	-1.459210	-1.023204
C	2.438067	-0.744976	0.161414	C	-6.011447	1.459191	-1.023199
C	1.180914	-1.407073	0.417564	C	-6.013006	2.838896	-0.968391
C	-1.288738	-1.399912	0.198679	C	-2.590379	-4.860726	0.666220
C	-1.288743	1.399912	0.198677	C	-2.551968	-3.520199	0.295240
C	1.098701	2.771309	0.791655	C	-0.168681	-3.476574	0.832518
C	2.272915	3.454617	1.065191	C	-0.254138	-4.820908	1.195416
C	3.464680	2.903503	0.691406	C	-1.454724	5.498323	1.127529
C	3.539792	1.639301	0.121457	C	2.272925	-3.454590	1.065239
C	3.539799	-1.639284	0.121481	H	2.266771	4.457235	1.463877
C	3.464691	-2.903475	0.691455	H	4.368972	3.492226	0.751616
C	-0.254160	4.820908	1.195429	H	4.368985	-3.492191	0.751684
C	-0.168695	3.476579	0.832515	H	0.619593	5.358107	1.533098
C	-2.551984	3.520192	0.295249	H	-3.519801	5.410685	0.621788
C	-1.337312	-2.810413	0.420571	H	-1.503648	-6.537374	1.428983
C	-1.337324	2.810413	0.420571	H	-4.908929	4.598394	-0.508508
C	1.098710	-2.771295	0.791674	H	-4.908908	-4.598409	-0.508519
C	-2.590403	4.860715	0.666241	H	-6.902565	-3.388708	-1.250089
C	-1.454697	-5.498331	1.127504	H	-6.913960	-0.953007	-1.333383
C	-4.887665	3.518346	-0.545938	H	-6.913966	0.952985	-1.333375
C	-3.730364	2.829119	-0.193950	H	-6.902581	3.388686	-1.250079
C	-2.487320	-0.702550	-0.055066	H	-3.519773	-5.410703	0.621759
C	-2.487323	0.702545	-0.055066	H	0.619619	-5.358106	1.533079
C	-3.703821	-1.421694	-0.306524	H	-1.503682	6.537361	1.429021
C	-4.874129	-0.726938	-0.688335	H	2.266784	-4.457199	1.463945
C	-4.874133	0.726923	-0.688332	Br	5.172001	-1.554788	-0.845967
C	-3.703827	1.421684	-0.306523	Br	5.171999	1.554788	-0.845981

PAH6$_{Me,Me}$‡

C	0.896789	0.700844	-0.040501	C	-0.333674	1.399413	-0.068538
C	0.896798	-0.700830	-0.040436	C	-0.333655	-1.399419	-0.068392
C	2.148753	-1.408121	-0.050728	C	2.097396	-2.782842	-0.393315
C	3.380222	-0.748976	0.305436	C	3.283146	-3.491703	-0.470674
C	3.380208	0.749049	0.305405	C	4.427267	-2.918290	0.004657
C	2.148733	1.408154	-0.050825	C	4.496270	-1.616274	0.492144

C	4.496232	1.616374	0.492106	C	0.783464	4.814555	-0.986154
C	4.427203	2.918392	0.004623	C	-0.420430	-5.486789	-1.052363
C	0.783516	-4.814662	-0.985605	C	3.283090	3.491760	-0.470773
C	0.838023	-3.479172	-0.586452	H	3.306825	-4.521134	-0.793748
C	-1.587043	-3.517207	-0.300020	H	5.320947	-3.527337	0.069416
C	-0.364243	2.810277	-0.296007	H	5.320861	3.527467	0.069423
C	-0.364206	-2.810310	-0.295700	H	1.684364	-5.345507	-1.255946
C	2.097362	2.782851	-0.393495	H	-2.525455	-5.397500	-0.748699
C	-1.593697	-4.852502	-0.691729	H	-0.443426	6.518026	-1.383045
C	-0.420494	5.486648	-1.053050	H	-4.007826	-4.597348	0.276161
C	-3.990552	-3.517389	0.320479	H	-4.007912	4.597325	0.275500
C	-2.805151	-2.827555	0.080637	H	-6.061994	3.388800	0.836273
C	-1.551087	0.702502	0.069360	H	-6.079044	0.952931	0.926977
C	-1.551077	-0.702510	0.069440	H	-6.079012	-0.952902	0.927176
C	-2.787004	1.420900	0.202508	H	-6.061916	-3.388784	0.836819
C	-3.987973	0.726911	0.475207	H	-2.525525	5.397366	-0.749427
C	-3.987959	-0.726905	0.475315	H	1.684308	5.345369	-1.256570
C	-2.786981	-1.420910	0.202694	H	-0.443352	-6.518218	-1.382198
C	-2.805198	2.827528	0.080255	H	3.306746	4.521194	-0.793836
C	-3.990618	3.517373	0.319972	C	5.779769	-1.421224	1.257550
C	-5.149734	2.838843	0.640202	H	6.564082	-0.924083	0.694139
C	-5.151990	1.459277	0.700464	H	5.630802	-0.899137	2.194959
C	-5.151955	-1.459262	0.700707	H	6.160539	-2.408477	1.515307
C	-5.149673	-2.838837	0.640644	C	5.779771	1.421347	1.257449
C	-1.593760	4.852393	-0.692353	H	5.630970	0.898951	2.194700
C	-1.587092	3.517151	-0.300462	H	6.564158	0.924538	0.693830
C	0.837984	3.479127	-0.586795	H	6.160359	2.408601	1.515470

PAH5$_{t\mathrm{Bu,H}}^{\ddagger}$

C	0.262907	-2.309059	0.000028	C	5.334927	-1.823443	-0.000020
C	-1.083400	-2.198062	0.000031	C	4.468357	-2.924318	-0.000023
C	-1.699696	-0.935842	0.000008	C	3.107196	-2.745842	-0.000018
C	-0.888063	0.230545	-0.000007	C	-3.972182	-2.005795	0.000004
C	0.572380	0.129082	-0.000011	C	-5.340678	-1.900018	0.000001
C	1.118568	-1.188431	0.000001	C	-5.960305	-0.643520	-0.000003
C	-3.145666	-0.863487	0.000003	C	-5.186281	0.486135	-0.000006
C	-3.782723	0.394937	-0.000004	H	0.690244	-3.299375	0.000052
C	-2.964022	1.546342	-0.000011	H	-1.677717	-3.098977	0.000056
C	-1.612550	1.463413	-0.000014	H	-3.435744	2.522805	-0.000016
C	1.539548	1.239245	-0.000023	H	3.590300	1.737170	-0.000024
C	2.867777	0.936343	-0.000018	H	5.457669	0.310691	-0.000017
C	3.416630	-0.362838	-0.000013	H	6.407354	-1.974919	-0.000023
C	2.538843	-1.455168	-0.000009	H	4.873825	-3.928843	-0.000030
C	4.809888	-0.558916	-0.000016	H	2.484546	-3.628226	-0.000025

H	-3.540655	-2.996118	0.000004	C	2.461899	3.641172	-0.000062
H	-5.945269	-2.798857	0.000001	H	3.080005	3.502839	0.888293
H	-7.040903	-0.569996	-0.000004	H	3.079998	3.502807	-0.888418
H	-5.642167	1.469887	-0.000011	H	2.119590	4.678917	-0.000079
C	1.216183	2.741705	-0.000042	C	0.502831	3.121685	-1.320347
C	0.502847	3.121721	1.320261	H	-0.170490	2.360271	-1.703259
H	-0.058143	4.053668	1.210113	H	-0.058164	4.053631	-1.210216
H	-0.170475	2.360321	1.703199	H	1.259776	3.282189	-2.089931
H	1.259801	3.282239	2.089834	H	-1.093215	2.393582	-0.000022

$PAH5_{Br,Br}^{‡}$

C	-0.672693	-2.427959	-1.147300	C	3.354198	-2.950625	-0.305452
C	0.672857	-2.427915	-1.147300	C	4.623937	-3.197077	0.155120
C	1.392415	-1.390561	-0.523572	C	5.358959	-2.195595	0.803547
C	0.736905	-0.148823	-0.248996	C	4.803041	-0.955580	0.973368
C	-0.736891	-0.148871	-0.248996	H	-1.203177	-3.262794	-1.578501
C	-1.392319	-1.390652	-0.523572	H	1.203394	-3.262716	-1.578501
C	2.754774	-1.684944	-0.145137	H	3.586759	1.415462	0.861794
C	3.504996	-0.691304	0.502125	H	-3.586847	1.415226	0.861795
C	2.946373	0.599895	0.553694	H	-5.353519	-0.161095	1.463131
C	1.687816	0.891543	0.126069	H	-6.357868	-2.404276	1.165856
C	-1.687870	0.891433	0.126070	H	-5.056095	-4.181598	0.023054
C	-2.946408	0.599701	0.553695	H	-2.816575	-3.763897	-0.770917
C	-3.504946	-0.691533	0.502126	H	2.816825	-3.763713	-0.770916
C	-2.754660	-1.685125	-0.145137	H	5.056373	-4.181268	0.023055
C	-4.802973	-0.955895	0.973369	H	6.358030	-2.403859	1.165855
C	-5.358811	-2.195946	0.803548	H	5.353535	-0.160743	1.463129
C	-4.623724	-3.197379	0.155120	Br	1.562441	2.770441	-0.134704
C	-3.354001	-2.950844	-0.305452	Br	-1.562619	2.770339	-0.134704

$PAH5_{Me,Me}^{‡}$

C	-0.672504	-1.692894	-0.840984	C	-2.788483	-0.800374	-0.090880
C	0.672507	-1.692893	-0.840984	C	-4.943258	0.119881	0.599577
C	1.394308	-0.571484	-0.392603	C	-5.499660	-1.131480	0.605400
C	0.742336	0.695262	-0.254191	C	-4.706029	-2.238028	0.273556
C	-0.742337	0.695261	-0.254191	C	-3.384849	-2.078363	-0.064119
C	-1.394307	-0.571485	-0.392604	C	3.384852	-2.078358	-0.064119
C	2.788484	-0.800370	-0.090880	C	4.706032	-2.238021	0.273557
C	3.590022	0.293616	0.258726	C	5.499661	-1.131473	0.605401
C	2.991819	1.564404	0.195291	C	4.943257	0.119887	0.599578
C	1.675592	1.812941	-0.072886	H	-1.202291	-2.574937	-1.166379
C	-1.675595	1.812939	-0.072886	H	1.202295	-2.574935	-1.166379
C	-2.991821	1.564400	0.195290	H	3.647157	2.415028	0.343764
C	-3.590022	0.293611	0.258726	H	-3.647160	2.415023	0.343763

H	-5.533646	0.992153	0.856798	C	-1.432683	3.289212	-0.230473
H	-6.540696	-1.269630	0.870538	H	-0.895034	3.734349	0.601035
H	-5.134326	-3.232792	0.294032	H	-0.911294	3.528384	-1.151690
H	-2.804597	-2.964346	-0.277043	H	-2.398779	3.787475	-0.281871
H	2.804601	-2.964343	-0.277043	C	1.432679	3.289214	-0.230473
H	5.134331	-3.232785	0.294033	H	0.911289	3.528385	-1.151690
H	6.540697	-1.269621	0.870539	H	0.895029	3.734350	0.601035
H	5.533644	0.992161	0.856799	H	2.398774	3.787478	-0.281871

PAH4$_{t\mathrm{Bu,H}}$‡

C	0.705569	0.711126	0.000001	C	1.513257	-3.455658	-0.000001
C	0.979868	-0.702449	-0.000001	H	-0.590529	-5.020733	0.000005
C	-0.095612	-1.607036	0.000004	H	-2.951955	-4.244175	0.000017
C	-1.465614	-1.163952	0.000004	H	-4.163649	2.724798	-0.000006
C	-1.779226	0.287269	0.000003	H	-2.261294	4.194149	-0.000002
C	-0.633335	1.177042	-0.000001	H	2.427265	4.997309	0.000006
C	0.199118	-3.013730	0.000000	H	4.759380	4.163400	0.000004
C	-0.843535	-3.967230	0.000006	H	5.198107	1.764516	-0.000004
C	-2.129358	-3.539241	0.000011	H	5.549559	-0.110507	0.000003
C	-2.419732	-2.167394	0.000011	H	5.976138	-2.510724	-0.000007
C	-3.072116	0.871916	-0.000002	H	4.088933	-4.110717	-0.000008
C	-3.182583	2.281247	-0.000003	H	0.053838	4.541366	0.000002
C	-2.122003	3.119493	-0.000001	H	1.707048	-4.522616	-0.000003
C	-0.819817	2.597404	0.000001	C	-4.430964	0.147056	-0.000004
C	1.794840	1.616699	0.000004	C	-4.601394	-0.641143	1.322761
C	3.148856	1.164171	-0.000003	H	-4.979838	0.040979	2.085580
C	3.417416	-0.268313	0.000001	H	-5.332599	-1.446160	1.209952
C	2.314834	-1.168748	-0.000005	H	-3.681610	-1.066703	1.714633
C	1.560573	3.024757	0.000003	C	-4.601385	-0.641155	-1.322762
C	2.642876	3.935362	0.000005	H	-5.332596	-1.446166	-1.209953
C	3.924168	3.473756	0.000003	H	-4.979818	0.040962	-2.085592
C	4.168999	2.094477	0.000001	H	-3.681600	-1.066725	-1.714622
C	4.700587	-0.779284	-0.000003	C	-5.645716	1.090532	-0.000013
C	4.952296	-2.157121	-0.000005	H	-5.690814	1.722239	0.888345
C	3.914826	-3.041168	-0.000007	H	-5.690805	1.722233	-0.888376
C	2.581187	-2.571097	-0.000005	H	-6.543032	0.466814	-0.000016
C	0.252661	3.475381	0.000002	H	-3.457369	-1.931351	0.000015

PAH4$_{\mathrm{Br,Br}}$‡

C	-1.427971	-0.717628	0.116069	C	-0.216433	-1.409055	0.318445
C	-1.428563	0.717513	0.116253	C	-0.331255	2.819644	0.564760
C	-0.217587	1.409888	0.318763	C	0.815064	3.565206	0.894818
C	1.086292	0.751582	0.227161	C	2.021070	2.992357	0.730732
C	1.086907	-0.749662	0.227023	C	2.157868	1.659243	0.270860

C	2.159223	-1.656456	0.270589	C	-1.536928	-3.485740	0.466474
C	2.023498	-2.989752	0.730255	C	-1.539797	3.485438	0.467417
C	0.817955	-3.563632	0.894141	H	0.717673	4.598978	1.201625
C	-0.328953	-2.818960	0.564115	H	2.924583	3.564116	0.884649
C	-2.654876	-1.412574	-0.032336	H	2.927475	-3.560787	0.884141
C	-3.871679	-0.728792	-0.316162	H	0.721395	-4.597541	1.200751
C	-3.872302	0.726765	-0.315862	H	-3.905886	-4.612892	0.011503
C	-2.656057	1.411478	-0.031880	H	-5.971825	-3.391247	-0.603741
C	-2.701701	-2.829163	0.107315	H	-5.948675	-0.957519	-0.760807
C	-3.908656	-3.534856	-0.096834	H	-5.949575	0.953872	-0.760040
C	-5.044282	-2.859445	-0.431070	H	-5.974770	3.387527	-0.602162
C	-5.022022	-1.462939	-0.528959	H	-3.909763	4.610726	0.013123
C	-5.023310	1.460004	-0.528193	H	-1.556481	-4.554838	0.644719
C	-5.046744	2.856458	-0.429829	H	-1.560225	4.554473	0.645945
C	-3.911638	3.532722	-0.095556	Br	3.927869	1.549488	-0.410821
C	-2.704060	2.827984	0.108211	Br	3.929121	-1.545193	-0.411115

PAH4$_{Me,Me}$‡

C	-0.386949	0.717190	-0.018160	C	-2.859883	-3.548537	0.014043
C	-0.380728	-0.719697	-0.017750	C	-1.641780	-2.838870	-0.091308
C	0.848818	-1.406224	-0.112131	C	-0.475504	3.492257	-0.330824
C	2.140212	-0.745596	0.053846	C	-0.447608	-3.495312	-0.328180
C	2.132689	0.763637	0.065757	H	1.867281	-4.612713	-0.817359
C	0.838012	1.414474	-0.102405	H	4.028538	-3.548258	-0.394423
C	0.762123	-2.821760	-0.336480	H	3.998846	3.595697	-0.293526
C	1.935009	-3.566318	-0.546266	H	1.836767	4.640158	-0.746040
C	3.117952	-2.966584	-0.316200	H	-2.885004	4.600893	-0.140860
C	3.250025	-1.614729	0.094186	H	-5.000831	3.364023	0.224300
C	3.235360	1.641456	0.136259	H	-4.978462	0.929598	0.377347
C	3.095707	3.000397	-0.243489	H	-4.962066	-0.974039	0.454976
C	1.909964	3.590479	-0.489504	H	-4.961102	-3.410269	0.330469
C	0.741730	2.831279	-0.316167	H	-2.841569	-4.628284	-0.075479
C	-1.625709	1.405159	0.015480	H	-0.482113	4.565832	-0.482503
C	-2.863160	0.715587	0.171695	H	-0.446283	-4.568703	-0.481354
C	-2.855311	-0.739809	0.189380	C	4.630413	1.427423	0.665741
C	-1.613163	-1.418975	0.028219	H	4.622028	0.977903	1.654122
C	-1.666662	2.824055	-0.116084	H	5.276744	0.849550	0.015727
C	-2.894204	3.521884	-0.041538	H	5.099382	2.402368	0.784821
C	-4.055955	2.838814	0.156605	C	4.659304	-1.416030	0.594872
C	-4.034941	1.441648	0.253158	H	5.340370	-1.043808	-0.169517
C	-4.016647	-1.477354	0.310891	H	4.722617	-0.786703	1.468829
C	-4.024165	-2.875601	0.232987	H	5.040560	-2.391509	0.894714

PAH7$_{tBu,H}$‡

C	1.357162	2.487270	0.715427	H	4.326294	-2.470339	-0.268271
C	2.586802	1.776248	0.217891	H	2.094254	-3.432957	-0.830895
C	2.381850	0.295937	0.119488	H	-3.398154	0.799655	-0.860290
C	1.099648	-0.260647	-0.059668	H	-2.844208	3.151361	-1.115109
C	-0.122333	0.590884	-0.034629	H	-0.645871	3.959958	-0.238860
C	0.097652	1.984999	0.072038	C	-2.094215	-1.196425	0.231502
C	3.511382	-0.512400	0.064233	C	-2.297473	-2.155138	-0.949998
C	3.432133	-1.860180	-0.232706	H	-2.941090	-1.685677	-1.696957
C	2.190750	-2.396615	-0.530431	H	-2.793444	-3.066187	-0.605502
C	1.062596	-1.602374	-0.452269	H	-1.384812	-2.451119	-1.463363
C	-1.471378	0.159409	-0.189025	C	-1.353538	-1.842420	1.410351
C	-2.390256	1.114851	-0.633339	H	-1.878349	-2.754472	1.703424
C	-2.096121	2.457245	-0.752301	H	-1.367447	-1.162781	2.265279
C	-0.867239	2.900554	-0.301955	H	-0.319254	-2.104835	1.221911
H	1.442394	3.565736	0.571197	C	-3.508776	-0.948698	0.798551
H	1.260033	2.322812	1.795818	H	-4.238360	-0.682712	0.034393
H	2.835405	2.137660	-0.788371	H	-3.500943	-0.163859	1.556277
H	3.451513	1.999359	0.846851	H	-3.862462	-1.870082	1.265454
H	4.479876	-0.053775	0.233950	H	0.121315	-2.037739	-0.728253

PAH7$_{Br,Br}$‡

C	0.562738	3.362763	0.494935	C	2.739869	2.372462	0.089478
C	-0.559681	3.363237	-0.494993	H	1.187701	4.252680	0.422759
C	-1.377516	2.146421	-0.204506	H	0.155893	3.322802	1.512136
C	-0.763589	0.866377	-0.017470	H	-0.152872	3.322855	-1.512192
C	0.764416	0.865696	0.017544	H	-1.183849	4.253716	-0.422866
C	1.379486	2.145200	0.204518	H	-3.101476	3.385043	-0.230524
C	-2.737694	2.374905	-0.089465	H	-4.668282	1.531996	0.363528
C	-3.609541	1.356532	0.222514	H	-3.748333	-0.756566	0.436190
C	-3.091249	0.088091	0.288187	H	3.747713	-0.759939	-0.436001
C	-1.731525	-0.168883	0.101504	H	4.669708	1.527802	-0.363444
C	1.731427	-0.170436	-0.101372	H	3.104552	3.382282	0.230487
C	3.091384	0.085313	-0.288049	Br	1.550351	-2.045402	0.153250
C	3.610809	1.353293	-0.222435	Br	-1.552133	-2.044022	-0.153049

PAH7$_{Me,Me}$‡

C	-0.579304	-2.404443	0.473224	C	3.057186	0.932793	0.169822
C	0.579085	-2.404481	-0.473335	C	1.688668	1.186295	0.036887
C	1.383016	-1.175092	-0.194571	C	-1.688529	1.186465	-0.036856
C	0.765283	0.098940	-0.027106	C	-3.057073	0.933105	-0.169791
C	-0.765253	0.099015	0.027095	C	-3.607620	-0.325894	-0.137740
C	-1.383112	-1.174962	0.194515	C	-2.751613	-1.375060	0.103755
C	2.751496	-1.375331	-0.103809	H	-1.206165	-3.290375	0.366116
C	3.607606	-0.326260	0.137730	H	-0.207447	-2.387227	1.505136

H	0.207230	-2.387180	-1.505247	C	1.436035	2.660697	-0.137568
H	1.205857	-3.290480	-0.366268	H	0.758612	2.862270	-0.959048
H	3.133459	-2.382673	-0.219875	H	1.061088	3.157154	0.754851
H	4.674533	-0.475116	0.247559	H	2.381473	3.139647	-0.387707
H	3.715168	1.788130	0.265761	C	-1.435747	2.660836	0.137648
H	-3.714970	1.788512	-0.265696	H	-0.758304	2.862314	0.959134
H	-4.674562	-0.474639	-0.247566	H	-1.060751	3.157285	-0.754756
H	-3.133677	-2.382367	0.219785	H	-2.381137	3.139873	0.387802

$PAH3_{H,H}$

C	-3.518097	0.931866	0.000010	H	1.230697	4.255830	-0.000006
C	-2.840305	-0.322589	0.000003	H	-4.602103	0.929185	0.000012
C	-1.421707	-0.343231	0.000002	H	-3.357522	3.047063	0.000016
C	-0.708949	0.888762	0.000003	H	4.602103	0.929185	-0.000012
C	-1.408427	2.112084	0.000007	H	3.357523	3.047063	-0.000016
C	-2.832197	2.098732	0.000012	C	-3.544932	-1.530021	-0.000004
C	-0.729742	-1.580785	-0.000003	C	-2.866409	-2.729005	-0.000015
C	0.708949	0.888762	-0.000003	C	-1.477361	-2.753228	-0.000015
C	1.421707	-0.343231	-0.000002	H	-4.628601	-1.508630	-0.000003
C	0.729742	-1.580785	0.000003	H	-3.414913	-3.663087	-0.000025
C	2.840305	-0.322589	-0.000003	C	1.477361	-2.753228	0.000016
C	3.518097	0.931866	-0.000009	C	3.544932	-1.530021	0.000005
C	2.832197	2.098732	-0.000011	H	4.628601	-1.508630	0.000004
C	1.408427	2.112084	-0.000006	C	2.866408	-2.729005	0.000016
C	0.683237	3.320111	-0.000003	H	3.414912	-3.663088	0.000026
C	-0.683237	3.320111	0.000004	H	0.980309	-3.713429	0.000028
H	-1.230697	4.255830	0.000006	H	-0.980309	-3.713429	-0.000028

$PAH3_{F,H}$

				C	1.713313	3.167844	0.000002
C	3.746058	0.077304	0.000003	H	2.507167	3.906103	0.000003
C	2.740340	-0.931332	0.000002	H	0.148017	4.612031	0.000001
C	1.371326	-0.555675	0.000001	H	4.783935	-0.235490	0.000003
C	1.040504	0.828460	0.000001	H	4.192725	2.151768	0.000004
C	2.060453	1.802670	0.000002	H	-4.029008	2.407458	-0.000003
C	3.421124	1.390358	0.000003	H	-2.221049	4.076619	-0.000001
C	0.358315	-1.554217	0.000000	C	3.086676	-2.285414	0.000001
C	-0.318070	1.234347	0.000000	C	2.103957	-3.245935	0.000000
C	-1.356457	0.259268	-0.000001	C	0.760281	-2.889565	-0.000001
C	-1.040857	-1.131395	-0.000001	H	4.134747	-2.561846	0.000002
C	-2.704510	0.704011	-0.000002	H	2.369132	-4.296214	0.000000
C	-2.989985	2.098640	-0.000002	C	-2.133771	-1.994424	-0.000002
C	-1.996538	3.016251	-0.000001	C	-3.740308	-0.233871	-0.000003
C	-0.634712	2.609480	0.000000	H	-4.768331	0.107827	-0.000004
C	0.406014	3.559171	0.000001	C	-3.454104	-1.575258	-0.000003

H	-4.230468	-2.329095	-0.000004	F	-1.962970	-3.325450	-0.000002
H	0.027237	-3.676375	-0.000001				

PAH3$_{Cl,H}$

C	3.093008	-2.288915	0.152959	H	3.308135	3.491131	0.077317
C	1.682261	-2.399441	-0.008304	H	3.677170	-3.201534	0.182113
C	0.883497	-1.225660	-0.013513	H	4.770617	-1.004706	0.354535
C	1.528797	0.038707	0.057655	H	-1.280223	4.529671	-0.261091
C	2.932299	0.116443	0.172890	H	1.179292	4.618975	-0.163559
C	3.694850	-1.081076	0.245759	C	1.081524	-3.647213	-0.195144
C	-0.529751	-1.322411	-0.144706	C	-0.270704	-3.726530	-0.424602
C	0.761038	1.225493	-0.040745	C	-1.061579	-2.583777	-0.402163
C	-0.662694	1.158815	-0.101910	H	1.699251	-4.537807	-0.188535
C	-1.338143	-0.102397	-0.064597	H	-0.735944	-4.684459	-0.622301
C	-1.385668	2.378497	-0.152936	C	-2.732152	-0.043070	0.069353
C	-0.693470	3.620507	-0.199603	C	-2.781228	2.350084	-0.125577
C	0.656525	3.669713	-0.144777	H	-3.336718	3.278891	-0.175140
C	1.417670	2.475114	-0.042109	C	-3.437997	1.158118	0.015946
C	2.821162	2.522701	0.074279	H	-4.515497	1.125162	0.102559
C	3.556203	1.379061	0.187202	H	-2.111451	-2.696063	-0.603693
H	4.635386	1.425961	0.277830	Cl	-3.750957	-1.409255	0.401613

PAH3$_{Br,H}$

C	-2.735100	-3.025297	-0.191478	H	-4.585212	2.456416	-0.193441
C	-1.360574	-2.729460	0.036659	H	-3.035169	-4.066288	-0.227759
C	-0.929897	-1.377087	0.046614	H	-4.696380	-2.272103	-0.491806
C	-1.902708	-0.348346	-0.072457	H	-0.495949	4.753329	0.324384
C	-3.263732	-0.672741	-0.246576	H	-2.873890	4.141806	0.134789
C	-3.649661	-2.038453	-0.334442	C	-0.439703	-3.750030	0.289703
C	0.443450	-1.066116	0.240442	C	0.862781	-3.435391	0.595708
C	-1.507642	1.006920	0.048180	C	1.294962	-2.114385	0.575751
C	-0.126837	1.347312	0.161720	H	-0.776054	-4.780363	0.279091
C	0.879367	0.329373	0.151362	H	1.567417	-4.216563	0.853357
C	0.219823	2.720907	0.228690	C	2.200464	0.779128	0.033088
C	-0.797679	3.715298	0.246404	C	1.567157	3.086603	0.240382
C	-2.103343	3.379552	0.140839	H	1.837463	4.133809	0.305077
C	-2.490790	2.018851	0.014191	C	2.537954	2.130165	0.105763
C	-3.843804	1.666216	-0.162459	H	3.579670	2.411656	0.036235
C	-4.218741	0.361385	-0.298641	H	2.317619	-1.913847	0.843582
H	-5.262137	0.101003	-0.435059	Br	3.701537	-0.315174	-0.376523

PAH3$_{I,H}$

C	-2.936484	-3.136916	-0.221921	C	-2.254375	-0.418487	-0.086951
C	-1.589783	-2.767472	0.059637	C	-3.588622	-0.815011	-0.308529
C	-1.234256	-1.394065	0.072092	C	-3.895964	-2.200250	-0.406514

C	0.109917	-1.007331	0.317157	H	-1.130338	4.748130	0.371104
C	-1.935829	0.955075	0.050765	H	-3.464768	4.013700	0.103995
C	-0.579191	1.367913	0.207604	C	-0.625062	-3.731944	0.366355
C	0.478802	0.405313	0.219307	C	0.641341	-3.341828	0.733677
C	-0.304983	2.756439	0.287971	C	0.999200	-1.998500	0.716361
C	-1.373719	3.695965	0.279949	H	-0.902101	-4.779751	0.353577
C	-2.656224	3.292351	0.131666	H	1.372736	-4.079518	1.040125
C	-2.968721	1.913929	-0.013570	C	1.780129	0.913347	0.112906
C	-4.294047	1.490382	-0.239490	C	1.022315	3.186878	0.334924
C	-4.594412	0.167875	-0.392723	H	1.239568	4.245541	0.413773
H	-5.617338	-0.146109	-0.566221	C	2.043699	2.281805	0.205443
H	-5.075154	2.239979	-0.294635	H	3.067048	2.627422	0.151367
H	-3.180242	-4.192334	-0.262951	H	1.990800	-1.732879	1.043378
H	-4.921656	-2.490713	-0.602898	I	3.501728	-0.179646	-0.415961

$PAH3_{F,F}$

C	1.313794	-3.509596	0.248549	H	4.633878	1.215218	-0.140660
C	0.066022	-2.840329	0.105977	H	1.310841	-4.591700	0.310121
C	0.033195	-1.423860	0.068523	H	3.426030	-3.338630	0.363823
C	1.263478	-0.707557	0.072032	H	1.323954	4.587941	-0.310129
C	2.486525	-1.404080	0.153564	H	3.435553	3.328831	-0.363863
C	2.478395	-2.820197	0.275767	C	-1.126170	-3.556808	-0.045491
C	-1.201765	-0.725259	-0.052308	C	-2.298652	-2.895428	-0.308384
C	1.265494	0.703949	-0.072040	C	-2.315218	-1.507559	-0.341886
C	0.037263	1.423766	-0.068514	H	-1.105000	-4.639212	-0.006481
C	-1.199686	0.728697	0.052336	H	-3.221208	-3.422782	-0.512318
C	0.074138	2.840135	-0.105968	C	-2.310895	1.514176	0.341929
C	1.323815	3.505833	-0.248558	C	-1.116000	3.560019	0.045516
C	2.486441	2.813109	-0.275793	H	-1.091736	4.642357	0.006505
C	2.490526	1.396974	-0.153591	C	-2.290363	2.901993	0.308426
C	3.697744	0.672197	-0.079664	H	-3.211406	3.431980	0.512372
C	3.695809	-0.682756	0.079617	F	-3.459732	-0.949565	-0.735684
H	4.630389	-1.228451	0.140598	F	-3.456994	0.959455	0.735741

$PAH3_{F,Cl}$

C	2.184208	-3.147634	0.350529	C	-1.147922	0.464276	-0.047820
C	0.837714	-2.757101	0.106159	C	-0.333563	2.788436	-0.247066
C	0.512570	-1.379429	0.052400	C	0.753325	3.697060	-0.374976
C	1.561786	-0.421119	0.111084	C	2.035521	3.263663	-0.326378
C	2.895769	-0.843109	0.279940	C	2.329442	1.885651	-0.141891
C	3.174211	-2.227800	0.441519	C	3.655756	1.434737	0.024251
C	-0.828253	-0.952921	-0.160206	C	3.929453	0.115732	0.241071
C	1.273905	0.953006	-0.089057	H	4.952797	-0.217324	0.370972
C	-0.077501	1.398382	-0.161087	H	4.459098	2.161656	-0.012661

H	2.404769	-4.205749	0.432356	H	-2.182789	-4.002239	-0.818245
H	4.200841	-2.535313	0.603128	C	-2.407508	0.995251	0.244342
H	0.530077	4.752450	-0.480169	C	-1.653178	3.243210	-0.146633
H	2.858955	3.964898	-0.397198	H	-1.860289	4.303415	-0.230630
C	-0.162802	-3.704665	-0.140510	C	-2.661976	2.364781	0.150621
C	-1.415801	-3.297847	-0.524149	H	-3.666033	2.716902	0.345364
C	-1.715987	-1.942603	-0.567304	F	-2.896394	-1.619762	-1.096513
H	0.078582	-4.759605	-0.089762	Cl	-3.692039	0.050925	0.903358

$PAH3_{F,Br}$

C	-2.485822	-3.174227	-0.411970	H	-4.851764	2.104563	-0.233861
C	-1.168528	-2.765464	-0.061004	H	-2.685744	-4.235311	-0.507105
C	-0.866963	-1.383454	0.011221	H	-4.483174	-2.589071	-0.828629
C	-1.920349	-0.439267	-0.132391	H	-1.007756	4.744865	0.555286
C	-3.230960	-0.878902	-0.405587	H	-3.311605	3.926983	0.284398
C	-3.477011	-2.267556	-0.585965	C	-0.179254	-3.697764	0.273761
C	0.446472	-0.938277	0.327285	C	1.032318	-3.271853	0.757610
C	-1.666916	0.937760	0.091923	C	1.310014	-1.912476	0.814269
C	-0.331242	1.401040	0.270417	H	-0.401490	-4.756208	0.210257
C	0.758218	0.481819	0.234019	H	1.781115	-3.964107	1.119457
C	-0.101525	2.793753	0.381974	C	2.027205	1.031888	0.034502
C	-1.207525	3.687201	0.428350	C	1.215463	3.266127	0.385622
C	-2.475751	3.236999	0.276265	H	1.401834	4.328179	0.492202
C	-2.735706	1.856109	0.063931	C	2.256021	2.403535	0.155145
C	-4.038478	1.388310	-0.208234	H	3.263914	2.776820	0.034609
C	-4.276903	0.066367	-0.448249	F	2.437602	-1.566691	1.436685
H	-5.282368	-0.279509	-0.658962	Br	3.492602	0.046454	-0.639404

$PAH3_{F,I}$

C	-2.784788	-3.184645	-0.451410	C	-4.587229	0.047242	-0.596601
C	-1.490646	-2.767870	-0.030326	H	-5.578119	-0.303551	-0.861283
C	-1.200618	-1.383948	0.050345	H	-5.182750	2.082701	-0.415028
C	-2.249036	-0.445739	-0.152995	H	-2.974474	-4.247059	-0.552456
C	-3.540616	-0.892795	-0.495455	H	-4.758750	-2.611239	-0.980364
C	-3.769114	-2.283485	-0.684010	H	-1.402953	4.741554	0.593781
C	0.091309	-0.929947	0.433656	H	-3.683367	3.912234	0.191626
C	-2.014489	0.932324	0.083886	C	-0.516657	-3.692788	0.364636
C	-0.692668	1.402526	0.334976	C	0.664624	-3.257498	0.911748
C	0.403810	0.490718	0.352008	C	0.931595	-1.896509	0.972543
C	-0.477498	2.795946	0.464232	H	-0.729716	-4.752779	0.295779
C	-1.589362	3.683307	0.452318	H	1.396139	-3.943372	1.318220
C	-2.844571	3.226726	0.228019	C	1.681567	1.044071	0.218228
C	-3.085040	1.844954	-0.001414	C	0.834623	3.274134	0.543529
C	-4.368484	1.370535	-0.344879	H	1.009728	4.336367	0.667326

C	1.891356	2.418702	0.359905	F	2.024891	-1.537486	1.649243
H	2.898413	2.807898	0.293717	I	3.340991	0.003169	-0.523561

PAH3$_{Cl,Cl}$

C	1.650574	-3.484822	0.452423	H	4.970876	1.207516	-0.232023
C	0.408584	-2.827737	0.230674	H	1.647631	-4.562175	0.571129
C	0.375070	-1.416119	0.135492	H	3.759933	-3.303115	0.608651
C	1.604094	-0.698230	0.122073	H	1.647868	4.562048	-0.571114
C	2.826134	-1.386293	0.256339	H	3.760128	3.302909	-0.608392
C	2.814619	-2.791462	0.469573	C	-0.776226	-3.547708	0.035515
C	-0.854464	-0.725824	-0.063381	C	-1.913564	-2.899371	-0.370828
C	1.604134	0.698105	-0.122066	C	-1.940035	-1.506574	-0.467658
C	0.375139	1.416039	-0.135627	H	-0.766366	-4.627434	0.125366
C	-0.854444	0.725790	0.063102	H	-2.799757	-3.453018	-0.650511
C	0.408717	2.827657	-0.230802	C	-1.940029	1.506583	0.467255
C	1.650758	3.484695	-0.452407	C	-0.776088	3.547673	-0.035779
C	2.814778	2.791292	-0.469423	H	-0.766174	4.627399	-0.125626
C	2.826216	1.386123	-0.256188	C	-1.913497	2.899379	0.370430
C	4.035298	0.669410	-0.131013	H	-2.799702	3.453057	0.650012
C	4.035258	-0.669626	0.131306	Cl	-3.307819	-0.841003	-1.278645
H	4.970803	-1.207767	0.232427	Cl	-3.307942	0.841062	1.278073

PAH3$_{Cl,Br}$

C	-2.321772	-3.310771	-0.534210	H	-5.153532	1.711594	-0.015978
C	-1.037969	-2.797525	-0.199299	H	-2.427299	-4.380600	-0.672474
C	-0.858495	-1.399183	-0.077435	H	-4.378216	-2.895074	-0.858144
C	-1.998314	-0.549968	-0.147836	H	-1.522430	4.671305	0.669153
C	-3.273106	-1.096972	-0.392894	H	-3.755351	3.653562	0.508489
C	-3.397424	-2.492503	-0.632935	C	0.040334	-3.644936	0.082710
C	0.418026	-0.850617	0.232175	C	1.202552	-3.128882	0.595189
C	-1.865054	0.833948	0.127874	C	1.372665	-1.748202	0.715439
C	-0.569980	1.411477	0.253890	H	-0.079462	-4.716338	-0.025591
C	0.589220	0.592765	0.130075	H	1.995339	-3.778837	0.940297
C	-0.456420	2.816273	0.381582	C	1.779112	1.255576	-0.177794
C	-1.633209	3.603061	0.523155	C	0.811513	3.403162	0.295245
C	-2.863441	3.042602	0.431061	H	0.913674	4.475435	0.413001
C	-3.011322	1.650964	0.182296	C	1.898759	2.640377	-0.047627
C	-4.277305	1.074614	-0.055346	H	2.854939	3.103323	-0.250596
C	-4.402647	-0.252338	-0.347955	Cl	2.728849	-1.238973	1.649621
H	-5.380262	-0.681757	-0.534807	Br	3.236229	0.403863	-1.025346

PAH3$_{Cl,I}$

C	2.705305	3.252542	-0.589540	C	1.212951	1.388757	-0.041013
C	1.427995	2.780680	-0.177383	C	2.319661	0.504169	-0.172851

C	3.594363	1.010136	-0.494170	H	4.725018	2.771811	-1.032319
C	3.747182	2.400487	-0.748114	H	1.730878	-4.693110	0.721026
C	-0.059345	0.880101	0.343463	H	3.980478	-3.747240	0.419734
C	2.159334	-0.872955	0.120778	C	0.395231	3.661164	0.166929
C	0.856167	-1.409014	0.325269	C	-0.749875	3.181569	0.749332
C	-0.283514	-0.557132	0.255666	C	-0.955228	1.806877	0.880597
C	0.707027	-2.808315	0.474823	H	0.541393	4.728370	0.049600
C	1.865446	-3.630165	0.557277	H	-1.499956	3.855936	1.140048
C	3.104833	-3.109196	0.387704	C	-1.511216	-1.180815	0.015702
C	3.281075	-1.724905	0.116714	C	-0.581366	-3.354586	0.467566
C	4.548268	-1.190035	-0.198829	H	-0.710822	-4.421681	0.605314
C	4.697765	0.130655	-0.508687	C	-1.661779	-2.561838	0.170256
H	5.675937	0.527867	-0.754648	H	-2.637037	-3.006110	0.022891
H	5.405235	-1.853903	-0.205001	Cl	-2.270898	1.337230	1.891834
H	2.836271	4.318211	-0.737990	I	-3.123370	-0.232101	-0.922653

PAH3$_{Br,I}$

C	2.677561	3.344120	-0.751573	H	5.762863	-1.480455	0.101120
C	1.418978	2.784873	-0.394150	H	2.728833	4.407719	-0.953739
C	1.312948	1.388579	-0.191077	H	4.756101	3.019389	-1.034167
C	2.496132	0.597856	-0.201367	H	2.280372	-4.581907	0.928263
C	3.743046	1.196013	-0.467900	H	4.458936	-3.459354	0.733042
C	3.795610	2.579263	-0.792201	C	0.295146	3.587850	-0.166212
C	0.064786	0.791903	0.144487	C	-0.839750	3.041986	0.378913
C	2.431838	-0.771250	0.158378	C	-0.935676	1.663761	0.577468
C	1.166855	-1.408026	0.303384	H	0.357315	4.656010	-0.337344
C	-0.030758	-0.661804	0.112509	H	-1.661704	3.673461	0.687728
C	1.123319	-2.806705	0.513287	C	-1.180512	-1.397966	-0.185756
C	2.337194	-3.520041	0.718646	C	-0.111506	-3.461371	0.441391
C	3.537990	-2.901769	0.607412	H	-0.162728	-4.528480	0.623158
C	3.617886	-1.521803	0.274767	C	-1.227906	-2.778670	0.025979
C	4.854899	-0.894714	0.013964	H	-2.148519	-3.311654	-0.170400
C	4.914490	0.416716	-0.359628	Br	-2.367514	1.106038	1.676939
H	5.870821	0.884742	-0.563190	I	-2.784215	-0.628492	-1.288283

PAH3$_{I,I}$

C	2.727440	-3.408105	0.857555	C	1.457784	1.390249	-0.296026
C	1.486894	-2.781635	0.551891	C	0.231285	0.728660	-0.005985
C	1.457347	-1.390426	0.295899	C	1.487768	2.781449	-0.552018
C	2.686482	-0.678576	0.204388	C	2.728508	3.407525	-0.857701
C	3.907220	-1.346699	0.420180	C	3.892870	2.716396	-0.798428
C	3.892020	-2.717346	0.798263	C	3.907641	1.345745	-0.420345
C	0.231054	-0.728448	0.005877	C	5.116522	0.648643	-0.210476
C	2.686694	0.678009	-0.204534	C	5.116320	-0.649982	0.210291

H	6.052142	-1.171859	0.374431	H	0.304910	-4.577789	0.639606
H	6.052507	1.170223	-0.374631	H	-1.695978	-3.515292	-0.320457
H	2.723976	-4.464131	1.101510	C	-0.848563	1.545355	0.339071
H	4.835945	-3.210174	1.000612	C	0.303094	3.515796	-0.424956
H	2.725375	4.463552	-1.101655	H	0.306353	4.577978	-0.639714
H	4.836948	3.208925	-1.000791	C	-0.824163	2.919265	0.084172
C	0.301984	-3.515606	0.424848	H	-1.694857	3.516115	0.320380
C	-0.825091	-2.918718	-0.084262	I	-2.420494	-0.908369	-1.567244
C	-0.849059	-1.544800	-0.339162	I	-2.420183	0.909422	1.567175

PAH3$_{Me,H}$

C	-2.923471	2.186129	-0.188051	H	-2.102660	4.143937	-0.208896
C	-2.674958	0.786846	-0.110722	H	4.774015	-0.344860	0.170226
C	-1.343657	0.300854	-0.065844	H	4.241452	2.052494	0.294433
C	-0.281901	1.252891	-0.038614	C	-3.730542	-0.122862	-0.041111
C	-0.560568	2.636189	-0.068629	C	-3.470087	-1.455994	0.140218
C	-1.907513	3.078499	-0.166850	C	-2.170050	-1.971295	0.186629
C	-1.079841	-1.100274	0.001664	H	-4.750967	0.240203	-0.082606
C	1.063331	0.818123	0.056397	H	-4.296541	-2.146065	0.267814
C	1.358322	-0.571765	0.012167	C	0.694221	-2.854294	-0.331979
C	0.316270	-1.534812	-0.090761	C	3.031864	-2.335090	-0.149937
C	2.717200	-0.982706	0.012825	H	4.071732	-2.640740	-0.147554
C	3.744920	-0.005169	0.143575	C	2.027282	-3.249581	-0.356529
C	3.452093	1.314246	0.209791	H	2.266364	-4.289875	-0.541520
C	2.105447	1.764645	0.139943	C	-2.074085	-3.435086	0.508031
C	1.793769	3.138084	0.125534	H	-1.959994	-4.058156	-0.383778
C	0.500451	3.559762	0.015582	H	-1.239947	-3.655904	1.174418
H	0.268567	4.618605	-0.003487	H	-2.993945	-3.753634	0.999282
H	2.602477	3.857044	0.191296	H	-0.050145	-3.602086	-0.537668
H	-3.953332	2.519791	-0.244907				

PAH3$_{Ph,H}$

C	-2.930334	2.125474	-0.276794	C	2.094708	1.782869	0.216833
C	-2.662859	0.729301	-0.195328	C	1.761504	3.151363	0.201092
C	-1.324756	0.271292	-0.088649	C	0.465004	3.554854	0.057026
C	-0.278692	1.238209	-0.026949	H	0.218665	4.610376	0.035595
C	-0.578772	2.615941	-0.063429	H	2.556790	3.882551	0.291343
C	-1.930182	3.033830	-0.208704	H	-3.961708	2.443931	-0.376242
C	-1.038986	-1.121031	0.000786	H	-2.142445	4.095942	-0.253344
C	1.069452	0.821808	0.104583	H	4.794212	-0.287908	0.283767
C	1.386530	-0.563600	0.059533	H	4.223534	2.099098	0.419008
C	0.363081	-1.540338	-0.065705	C	-3.702731	-0.202378	-0.191125
C	2.750321	-0.956472	0.081231	C	-3.429588	-1.532615	0.003484
C	3.760596	0.036036	0.240013	C	-2.120398	-2.008109	0.140635
C	3.446805	1.350413	0.312310	H	-4.725989	0.141366	-0.288260

H	-4.241780	-2.243514	0.096966	C	-1.409716	-3.775466	1.748796
C	0.754158	-2.853960	-0.312452	C	-2.480386	-5.767095	0.148080
C	3.081964	-2.303563	-0.087345	H	-3.011758	-4.182618	-1.199108
H	4.125118	-2.597664	-0.069491	C	-1.347796	-5.097143	2.153032
C	2.091468	-3.230610	-0.318029	H	-0.990683	-2.993988	2.371111
H	2.346855	-4.266673	-0.504087	C	-1.877435	-6.099881	1.350847
H	0.012314	-3.609972	-0.511065	H	-2.899550	-6.541846	-0.482728
C	-2.002133	-3.431203	0.534073	H	-0.885636	-5.347497	3.100385
C	-2.548357	-4.440744	-0.253897	H	-1.824696	-7.134724	1.666287

PAH3$_{tBu,tBu}$

C	2.125430	-3.341326	1.072245	H	-0.314581	4.519278	-0.852982
C	0.893831	-2.741306	0.692603	C	-1.359132	2.911207	0.085758
C	0.861974	-1.371643	0.355126	H	-2.200334	3.546034	0.333228
C	2.091622	-0.662942	0.250022	C	-2.457588	1.218871	1.542111
C	3.311071	-1.312227	0.520126	C	-2.457728	-1.218759	-1.542079
C	3.291947	-2.652893	0.990866	C	-2.463602	0.214786	-2.060203
C	-0.358900	-0.733602	-0.020296	H	-2.854299	0.928161	-1.341410
C	2.091658	0.662858	-0.250037	H	-1.465718	0.547993	-2.347758
C	0.862057	1.371632	-0.355142	H	-3.099586	0.255509	-2.947636
C	-0.358857	0.733664	0.020255	C	-2.077406	-2.095022	-2.753825
C	0.893990	2.741286	-0.692615	H	-2.098855	-3.158230	-2.514928
C	2.125615	3.341243	-1.072257	H	-2.779422	-1.915040	-3.571508
C	3.292095	2.652743	-0.990884	H	-1.072490	-1.850008	-3.103001
C	3.311144	1.312073	-0.520145	C	-3.880483	-1.592833	-1.117679
C	4.521552	0.630210	-0.260936	H	-4.221190	-1.002561	-0.268078
C	4.521518	-0.630437	0.260909	H	-4.566930	-1.408589	-1.947383
H	5.457583	-1.137840	0.465377	H	-3.969462	-2.646053	-0.849314
H	5.457642	1.137568	-0.465399	C	-3.880364	1.592973	1.117767
H	2.118699	-4.380165	1.382426	H	-4.566803	1.408561	1.947439
H	4.232652	-3.130130	1.240891	H	-3.969417	2.646243	0.849595
H	2.118929	4.380086	-1.382422	H	-4.221046	1.002831	0.268066
H	4.232826	3.129926	-1.240908	C	-2.463514	-0.214699	2.060164
C	-0.290501	-3.477268	0.555352	H	-2.854342	-0.928002	1.341364
C	-1.359295	-2.911104	-0.085754	H	-1.465630	-0.548012	2.347599
C	-1.404825	-1.555042	-0.469436	H	-3.099409	-0.255419	2.947663
H	-0.314822	-4.519232	0.852989	C	-2.077183	2.095061	2.753876
H	-2.200517	-3.545895	-0.333238	H	-2.098510	3.158273	2.515014
C	-1.404724	1.555134	0.469417	H	-2.779220	1.915130	3.571554
C	-0.290313	3.477308	-0.555358	H	-1.072296	1.849917	3.103055

PAH3$_{Ph,Ph}$

C	-2.749656	3.499335	0.304644	C	-1.472863	1.416735	0.065098
C	-1.506427	2.831924	0.117598	C	-2.704560	0.702837	0.086805

C	-3.927201	1.395887	0.190221	H	-0.327514	-4.622880	0.028819
C	-3.914809	2.809915	0.342002	C	0.823403	-2.870176	0.440435
C	-0.241532	0.725032	-0.102556	H	1.701277	-3.431256	0.735377
C	-2.704557	-0.702841	-0.086801	C	2.084199	0.891286	-1.132044
C	-1.472857	-1.416735	-0.065097	C	3.352857	1.395056	-0.849924
C	-0.241529	-0.725026	0.102558	C	1.966009	-0.101443	-2.105620
C	-1.506415	-2.831923	-0.117603	C	4.471682	0.913384	-1.508201
C	-2.749642	-3.499339	-0.304648	H	3.466726	2.144872	-0.076920
C	-3.914798	-2.809924	-0.342001	C	3.084147	-0.586092	-2.761046
C	-3.927195	-1.395897	-0.190216	H	0.985086	-0.487308	-2.352992
C	-5.135854	-0.675442	-0.099474	C	4.343490	-0.081946	-2.464383
C	-5.135856	0.675428	0.099481	H	5.449806	1.307911	-1.261005
H	-6.071478	1.217701	0.175542	H	2.970490	-1.354000	-3.516923
H	-6.071474	-1.217719	-0.175535	H	5.217955	-0.461332	-2.979006
H	-2.744766	4.580499	0.383275	C	2.084205	-0.891277	1.132042
H	-4.860175	3.328018	0.455597	C	3.352867	-1.395030	0.849904
H	-2.744748	-4.580503	-0.383282	C	1.966013	0.101427	2.105643
H	-4.860162	-3.328030	-0.455596	C	4.471691	-0.913363	1.508185
C	-0.317508	3.540202	-0.077664	H	3.466737	-2.144828	0.076882
C	0.823389	2.870185	-0.440449	C	3.084150	0.586071	2.761073
C	0.880002	1.471108	-0.505590	H	0.985088	0.487277	2.353031
H	-0.327534	4.622885	-0.028837	C	4.343496	0.081943	2.464391
H	1.701261	3.431267	-0.735395	H	5.449817	-1.307876	1.260974
C	0.880010	-1.471099	0.505585	H	2.970491	1.353959	3.516969
C	-0.317492	-3.540197	0.077652	H	5.217961	0.461325	2.979017

PAH8$_{H,H}$

C	2.989446	-1.013420	-0.254578	C	-2.374410	1.539549	-0.655760
C	1.621425	-0.646348	-0.086240	C	-1.288417	0.724077	-0.249277
C	0.678913	-1.680568	-0.280387	C	-3.706730	1.048960	-0.716544
C	1.060940	-2.859598	-0.902677	C	-4.020031	-0.155977	-0.204072
C	2.387201	-3.132180	-1.227953	C	-2.989499	-1.013279	0.254553
C	3.346986	-2.240014	-0.838814	C	-1.621457	-0.646269	0.086247
C	4.020030	-0.156142	0.203975	C	-3.347108	-2.239829	0.838840
C	3.706797	1.048816	0.716435	C	-2.387372	-3.132008	1.228068
C	2.374493	1.539455	0.655699	C	-1.061088	-2.859498	0.902821
C	1.288454	0.724024	0.249255	C	-0.678995	-1.680522	0.280473
C	2.226522	2.925445	0.877920	H	0.298312	-3.599519	-1.107723
C	1.088191	3.536772	0.496403	H	2.649769	-4.058404	-1.723546
C	0.000058	2.784609	0.000001	H	4.400309	-2.453716	-0.978304
C	0.000031	1.358688	-0.000004	H	5.047596	-0.493394	0.137134
C	-1.088042	3.536818	-0.496406	H	4.476174	1.716386	1.085873
C	-2.226381	2.925537	-0.877965	H	3.072953	3.487778	1.253175

H	0.983459	4.614001	0.547163	H	-5.047613	-0.493187	-0.137267
H	-0.983270	4.614044	-0.547147	H	-4.400445	-2.453483	0.978301
H	-3.072781	3.487903	-1.253242	H	-2.649994	-4.058192	1.723709
H	-4.476066	1.716552	-1.086025	H	-0.298498	-3.599441	1.107928

$PAH8_{F,H}$

C	-2.935735	-1.010834	0.384616	C	3.037830	-0.657315	-0.122103
C	-1.595695	-0.578275	0.165822	C	1.646819	-0.381974	0.015291
C	-0.589758	-1.535650	0.409364	C	3.478985	-1.871229	-0.673536
C	-0.883004	-2.685506	1.122556	C	2.586763	-2.826197	-1.068844
C	-2.183879	-3.010688	1.495946	C	1.245409	-2.613187	-0.776258
C	-3.205264	-2.210764	1.062168	C	0.761044	-1.468959	-0.165141
C	-4.018904	-0.247382	-0.117913	H	-0.078591	-3.373432	1.347690
C	-3.780675	0.933638	-0.720063	H	-2.380422	-3.915139	2.057557
C	-2.479673	1.506913	-0.704293	H	-4.240245	-2.482032	1.234955
C	-1.347114	0.786730	-0.250296	H	-5.024595	-0.637071	-0.013725
C	-2.412283	2.881765	-1.015724	H	-4.590805	1.526764	-1.127419
C	-1.314948	3.583000	-0.668142	H	-3.287566	3.368182	-1.428988
C	-0.191377	2.931843	-0.111144	H	-1.274373	4.659260	-0.786485
C	-0.104301	1.512013	-0.024841	H	0.664785	4.847346	0.348847
C	0.836054	3.777562	0.364827	H	2.795077	3.897000	1.178630
C	1.996782	3.261916	0.814282	H	4.312741	2.210688	1.143691
C	2.237878	1.877612	0.674547	H	5.048718	0.009518	0.288874
C	1.215837	0.975090	0.287012	H	4.544195	-2.028330	-0.792676
C	3.597321	1.479324	0.787385	H	2.888178	-3.752779	-1.538598
C	4.000022	0.279645	0.326255	F	0.405509	-3.609439	-1.092678

$PAH8_{Cl,H}$

C	-1.227043	2.770255	0.537151	C	2.387214	-1.894425	0.651681
C	-0.618387	1.511691	0.265369	C	1.324294	-1.025879	0.298616
C	-1.392222	0.372536	0.557481	C	2.193991	-3.291355	0.826870
C	-2.505774	0.479216	1.371453	C	1.042977	-3.878453	0.444148
C	-2.988091	1.714118	1.796872	C	-0.039155	-3.076732	0.008318
C	-2.394240	2.848818	1.313545	C	0.035257	-1.658944	0.101149
C	-0.670510	3.954762	-0.007554	C	-1.190602	-3.696437	-0.503325
C	0.485476	3.894706	-0.698106	C	-2.257723	-2.954702	-0.918854
C	1.245863	2.693627	-0.738459	C	-2.251020	-1.581282	-0.665002
C	0.733713	1.468867	-0.245291	C	-1.174855	-0.943766	-0.059835
C	2.590543	2.822990	-1.146288	H	-3.044874	-0.423239	1.629388
C	3.465749	1.839058	-0.854496	H	-3.860002	1.768140	2.436302
C	3.027085	0.639139	-0.250435	H	-2.805969	3.828635	1.526062
C	1.644465	0.349265	-0.065838	H	-1.193995	4.892354	0.137683
C	4.041645	-0.246351	0.178415	H	0.919932	4.784710	-1.137710
C	3.728654	-1.454235	0.688210	H	2.916455	3.756806	-1.588307

H	4.525362	1.954218	-1.049507	H	0.926473	-4.955673	0.450664
H	5.072506	0.073638	0.083669	H	-1.202686	-4.776173	-0.592663
H	4.494969	-2.142300	1.023954	H	-3.122583	-3.407492	-1.383639
H	3.037895	-3.882324	1.162171	Cl	-3.668253	-0.711661	-1.152949

$PAH8_{Br,H}$

C	-0.483240	2.897093	0.713286	C	-0.052480	-3.047218	0.149447
C	-0.053752	1.575863	0.400801	C	0.199556	-1.648599	0.214166
C	-0.930035	0.536630	0.765653	C	-1.307157	-3.525221	-0.261416
C	-1.948305	0.771525	1.672132	C	-2.305365	-2.661594	-0.609795
C	-2.240973	2.053963	2.129235	C	-2.111473	-1.298325	-0.377276
C	-1.561528	3.111314	1.586904	C	-0.925757	-0.793075	0.138977
C	0.161956	4.007596	0.113383	H	-2.566006	-0.061782	1.981590
C	1.239687	3.811202	-0.672263	H	-3.041604	2.209558	2.841077
C	1.845451	2.528082	-0.767334	H	-1.834409	4.132469	1.826724
C	1.234746	1.372643	-0.221995	H	-0.231567	5.000819	0.294631
C	3.155863	2.495176	-1.289699	H	1.737794	4.643918	-1.154531
C	3.928351	1.412245	-1.065671	H	3.552517	3.383562	-1.766196
C	3.402992	0.273208	-0.414676	H	4.973273	1.399399	-1.352114
C	2.016724	0.151939	-0.109522	H	5.386711	-0.535156	-0.251233
C	4.336979	-0.727888	-0.064268	H	4.631079	-2.662320	0.764427
C	3.926597	-1.887832	0.486475	H	2.991816	-4.212152	1.056801
C	2.543964	-2.162946	0.571345	H	0.714367	-5.026417	0.542220
C	1.566530	-1.173932	0.297177	H	-1.456948	-4.596009	-0.332754
C	2.199631	-3.525212	0.783986	H	-3.247942	-3.013000	-1.005703
C	0.958043	-3.971206	0.508687	Br	-3.567616	-0.172329	-0.835097

$PAH8_{I,H}$

C	-0.153178	2.883450	0.820581	C	2.912466	-2.142427	0.508333
C	0.273887	1.568072	0.482139	C	1.912076	-1.163255	0.286925
C	-0.570065	0.518385	0.890553	C	2.592386	-3.506716	0.745206
C	-1.538431	0.738616	1.853974	C	1.341365	-3.965191	0.541988
C	-1.818043	2.016812	2.332103	C	0.304565	-3.052256	0.232415
C	-1.183316	3.082924	1.754328	C	0.547536	-1.651407	0.277465
C	0.446011	4.001798	0.188596	C	-0.965009	-3.541872	-0.113323
C	1.482221	3.818441	-0.654349	C	-1.984696	-2.687565	-0.423416
C	2.095957	2.542350	-0.785442	C	-1.794856	-1.319466	-0.206237
C	1.527856	1.379523	-0.210591	C	-0.589116	-0.807489	0.256093
C	3.376007	2.523235	-1.378922	H	-2.127177	-0.103486	2.195021
C	4.169778	1.446958	-1.201235	H	-2.578719	2.161541	3.088597
C	3.692426	0.301400	-0.525057	H	-1.453807	4.100293	2.012269
C	2.326516	0.166507	-0.143696	H	0.052148	4.990423	0.392766
C	4.653521	-0.691483	-0.228835	H	1.944288	4.657503	-1.160902
C	4.285383	-1.854810	0.344560	H	3.737518	3.416403	-1.874079

H	5.197247	1.444852	-1.545318	H	1.109780	-5.022357	0.594196
H	5.689277	-0.489458	-0.474663	H	-1.109841	-4.614302	-0.171168
H	5.011621	-2.622472	0.582639	H	-2.936940	-3.055943	-0.779185
H	3.404651	-4.185441	0.976476	I	-3.427730	-0.090268	-0.684172

PAH8$_{F,F}$

C	2.994842	-0.686025	-0.251826	C	-2.994960	-0.685416	0.251804
C	1.627471	-0.334480	-0.069224	C	-1.627516	-0.334149	0.069216
C	0.673636	-1.351233	-0.289894	C	-3.346604	-1.892301	0.878161
C	1.068879	-2.486114	-0.973811	C	-2.388381	-2.766786	1.305513
C	2.387831	-2.767334	-1.305406	C	-1.069366	-2.485844	0.973931
C	3.346235	-1.893011	-0.878127	C	-0.673887	-1.351081	0.289957
C	4.018985	0.164800	0.230239	H	2.621450	-3.686489	-1.825351
C	3.696686	1.355459	0.772304	H	4.396770	-2.111602	-1.027074
C	2.362690	1.842013	0.707414	H	5.048905	-0.163715	0.156369
C	1.283885	1.028758	0.279298	H	4.460696	2.018669	1.159697
C	2.205312	3.226312	0.935896	H	3.041369	3.789428	1.332445
C	1.075103	3.836675	0.528104	H	0.968143	4.913671	0.579918
C	0.000318	3.086032	-0.000048	H	-0.967147	4.913849	-0.580053
C	0.000179	1.661364	-0.000032	H	-3.040575	3.789994	-1.332604
C	-1.074316	3.836874	-0.528222	H	-4.460247	2.019511	-1.159861
C	-2.204636	3.226724	-0.936026	H	-5.048910	-0.162721	-0.156469
C	-2.362288	1.842460	-0.707518	H	-4.397185	-2.110678	1.027095
C	-1.283652	1.029005	-0.279357	H	-2.622193	-3.685866	1.825504
C	-3.696377	1.356164	-0.772425	F	-0.156183	-3.403415	1.311500
C	-4.018924	0.165589	-0.230324	F	0.155509	-3.403524	-1.311313

PAH8$_{F,Cl}$

C	0.887110	-2.877680	0.409154	C	-2.311190	2.087433	0.678975
C	0.377569	-1.570991	0.170941	C	-1.344677	1.128135	0.287204
C	1.239186	-0.488919	0.442420	C	-1.995567	3.468101	0.801088
C	2.348127	-0.715749	1.235066	C	-0.826948	3.949558	0.332252
C	2.768943	-1.981990	1.621528	C	0.162283	3.051051	-0.135210
C	2.072667	-3.055373	1.140774	C	-0.021577	1.648933	0.010776
C	0.212805	-4.006403	-0.117562	C	1.331783	3.553964	-0.727626
C	-0.965586	-3.844447	-0.752494	C	2.310123	2.711792	-1.171011
C	-1.624390	-2.584529	-0.745000	C	2.203539	1.352959	-0.868625
C	-0.987924	-1.409120	-0.276068	C	1.113353	0.831524	-0.186163
C	-2.997583	-2.601396	-1.071865	H	3.661381	-2.084645	2.223858
C	-3.771862	-1.555008	-0.719416	H	2.417017	-4.064631	1.331855
C	-3.203039	-0.396581	-0.142627	H	0.662484	-4.985360	-0.000881
C	-1.793502	-0.218557	-0.043549	H	-1.493725	-4.691129	-1.174275
C	-4.115424	0.569756	0.338372	H	-3.423397	-3.501578	-1.498250
C	-3.678016	1.756420	0.805622	H	-4.847271	-1.584401	-0.848806

H	-5.172190	0.331906	0.311516	H	1.430451	4.625556	-0.853796
H	-4.366185	2.508077	1.172796	H	3.185527	3.075828	-1.690631
H	-2.767506	4.134648	1.166640	Cl	3.516158	0.345382	-1.369835
H	-0.625887	5.013671	0.297107	F	3.103624	0.317488	1.621888

PAH8$_{F,Br}$

C	-0.477657	2.890149	0.611189	C	0.098896	-3.046172	0.007578
C	-0.013187	1.577294	0.321806	C	0.318585	-1.646928	0.127240
C	-0.860131	0.507130	0.672918	C	-1.126873	-3.531117	-0.475821
C	-1.880652	0.745129	1.573579	C	-2.124277	-2.673426	-0.842843
C	-2.241748	2.015902	2.003607	C	-1.967094	-1.315753	-0.558834
C	-1.582262	3.081292	1.457345	C	-0.816587	-0.811134	0.028547
C	0.159306	4.010025	0.022724	H	-3.068239	2.129000	2.691969
C	1.268018	3.832121	-0.724031	H	-1.891991	4.094429	1.683865
C	1.905571	2.562589	-0.782367	H	-0.261666	4.995405	0.183893
C	1.299586	1.395936	-0.255092	H	1.765265	4.672096	-1.194011
C	3.240548	2.558229	-1.241150	H	3.637433	3.452323	-1.706472
C	4.028588	1.498665	-0.966525	H	5.086549	1.511345	-1.200327
C	3.500788	0.348648	-0.336281	H	5.492810	-0.411678	-0.074947
C	2.105016	0.193037	-0.100363	H	4.740155	-2.571705	0.870670
C	4.440021	-0.631953	0.056003	H	3.120870	-4.171069	1.034392
C	4.031401	-1.810059	0.569117	H	0.892576	-5.019197	0.379476
C	2.653638	-2.119077	0.578470	H	-1.255342	-4.601421	-0.585559
C	1.669196	-1.145686	0.276633	H	-3.042968	-3.028578	-1.288286
C	2.328449	-3.493586	0.739579	Br	-3.420615	-0.193221	-1.016465
C	1.112793	-3.958360	0.387855	F	-2.608469	-0.279387	2.030217

PAH8$_{F,I}$

C	-0.176977	2.872226	0.757982	C	3.007828	-2.090322	0.483369
C	0.282844	1.567752	0.427515	C	1.991560	-1.130201	0.253437
C	-0.521310	0.484021	0.832763	C	2.711782	-3.467940	0.672719
C	-1.472585	0.701394	1.811402	C	1.479449	-3.949329	0.412696
C	-1.816078	1.964848	2.276916	C	0.430050	-3.051496	0.100334
C	-1.216538	3.042539	1.687241	C	0.640738	-1.649527	0.200090
C	0.399586	4.003041	0.129513	C	-0.819173	-3.551039	-0.300624
C	1.452741	3.843210	-0.697811	C	-1.845334	-2.704584	-0.613427
C	2.101489	2.582933	-0.809704	C	-1.689561	-1.341985	-0.343891
C	1.551372	1.406258	-0.244952	C	-0.509436	-0.828596	0.174892
C	3.398743	2.597113	-1.366031	H	-2.588954	2.062564	3.027100
C	4.217954	1.546261	-1.155827	H	-1.522825	4.049765	1.942927
C	3.753442	0.387659	-0.492242	H	-0.021140	4.982044	0.326248
C	2.381226	0.213771	-0.153712	H	1.902541	4.691967	-1.198822
C	4.731304	-0.581603	-0.172939	H	3.749165	3.497797	-1.855353
C	4.376959	-1.764194	0.369808	H	5.255270	1.573273	-1.467874

H	5.768524	-0.348625	-0.382546	H	-0.943519	-4.623241	-0.397197
H	5.115932	-2.516499	0.617508	H	-2.780374	-3.078330	-1.007013
H	3.531866	-4.134586	0.911326	I	-3.329593	-0.119072	-0.795162
H	1.272762	-5.012848	0.424571	F	-2.149806	-0.336332	2.314466

PAH8$_{Cl,Cl}$

C	0.402379	2.978366	-0.295763	C	0.402432	-2.978359	0.295739
C	0.047405	1.617589	-0.092907	C	0.047433	-1.617587	0.092888
C	1.045042	0.651665	-0.338190	C	1.579616	-3.301946	0.989460
C	2.132817	0.998086	-1.125667	C	2.394869	-2.322499	1.481537
C	2.394824	2.322539	-1.481564	C	2.132837	-0.998050	1.125643
C	1.579556	3.301972	-0.989488	C	1.045055	-0.651646	0.338170
C	-0.427788	4.006978	0.212157	H	3.265527	2.551699	-2.080147
C	-1.613303	3.691205	0.773133	H	1.813116	4.346487	-1.158294
C	-2.114034	2.361819	0.711356	H	-0.096021	5.035393	0.132364
C	-1.308004	1.279610	0.281001	H	-2.264282	4.460668	1.170677
C	-3.499113	2.207627	0.937236	H	-4.061540	3.044750	1.332691
C	-4.113100	1.078229	0.527811	H	-5.190634	0.976076	0.578952
C	-3.366821	-0.000029	0.000002	H	-5.190620	-0.976167	-0.578935
C	-1.942936	-0.000016	-0.000004	H	-4.061494	-3.044819	-1.332688
C	-4.113084	-1.078300	-0.527803	H	-2.264210	-4.460704	-1.170693
C	-3.499080	-2.207686	-0.937236	H	-0.095933	-5.035393	-0.132392
C	-2.113996	-2.361853	-0.711366	H	1.813196	-4.346456	1.158262
C	-1.307983	-1.279631	-0.281014	H	3.265577	-2.551645	2.080117
C	-1.613242	-3.691231	-0.773150	Cl	3.249760	0.196711	1.681822
C	-0.427718	-4.006984	-0.212180	Cl	3.249759	-0.196655	-1.681847

PAH8$_{Cl,Br}$

C	-0.057511	3.013025	-0.165479	C	-2.169792	-2.487493	-0.743606
C	-0.343756	1.633566	0.017516	C	-1.482934	-1.348966	-0.255929
C	0.732513	0.732269	-0.122218	C	-1.579348	-3.781005	-0.730411
C	1.859866	1.142324	-0.816082	C	-0.437279	-4.010049	-0.049555
C	2.071460	2.478352	-1.161101	C	0.269111	-2.922184	0.518586
C	1.156519	3.407156	-0.750599	C	-0.152815	-1.591366	0.255657
C	-0.997006	3.988175	0.249151	C	1.388896	-3.155785	1.333133
C	-2.210107	3.598788	0.692845	C	2.082146	-2.116930	1.886947
C	-2.616928	2.239641	0.596577	C	1.771078	-0.817864	1.480325
C	-1.704132	1.209452	0.262784	C	0.749457	-0.557728	0.579237
C	-4.005098	1.997354	0.683315	H	2.972331	2.763342	-1.686341
C	-4.500880	0.827261	0.229944	H	1.339605	4.463571	-0.907629
C	-3.637561	-0.204865	-0.203160	H	-0.725482	5.035546	0.191570
C	-2.223965	-0.111336	-0.060986	H	-2.945122	4.326607	1.015272
C	-4.255590	-1.335884	-0.783766	H	-4.657249	2.798941	1.008331
C	-3.532243	-2.427575	-1.108626	H	-5.569309	0.655747	0.173711

H	-5.326789	-1.305585	-0.944218	H	1.673418	-4.179679	1.544656
H	-3.997282	-3.304531	-1.542418	H	2.900368	-2.278884	2.574835
H	-2.135634	-4.597188	-1.175706	Cl	2.742662	0.458190	2.121617
H	-0.048890	-5.013036	0.081728	Br	3.203706	-0.087263	-1.323731

PAH8$_{Cl,I}$

C	-0.419677	3.027157	-0.088317	C	0.057012	-2.883420	0.685163
C	-0.673064	1.639807	0.081684	C	-0.390760	-1.572266	0.372043
C	0.440813	0.775622	0.025691	C	1.116534	-3.065536	1.588929
C	1.599737	1.213382	-0.597086	C	1.724454	-1.995387	2.182304
C	1.787611	2.556312	-0.935817	C	1.401018	-0.713368	1.732830
C	0.819403	3.457753	-0.588677	C	0.446484	-0.502813	0.748779
C	-1.419895	3.971156	0.249470	H	2.706685	2.874909	-1.407857
C	-2.650178	3.542090	0.599916	H	0.979915	4.519093	-0.737996
C	-3.002988	2.169589	0.481125	H	-1.180419	5.027030	0.206921
C	-2.032503	1.169768	0.227699	H	-3.431928	4.245862	0.859854
C	-4.384631	1.880080	0.459973	H	-5.087333	2.660752	0.725061
C	-4.803269	0.690374	-0.019845	H	-5.857552	0.481867	-0.158220
C	-3.874196	-0.314966	-0.372402	H	-5.461230	-1.482161	-1.228652
C	-2.480131	-0.170620	-0.121832	H	-4.022116	-3.439802	-1.693964
C	-4.405480	-1.473026	-0.984784	H	-2.148913	-4.662291	-1.166430
C	-3.622252	-2.542491	-1.237401	H	-0.152320	-4.989013	0.252739
C	-2.291135	-2.550662	-0.767272	H	1.420672	-4.075567	1.836715
C	-1.684298	-1.383094	-0.243631	H	2.490641	-2.119040	2.934988
C	-1.657978	-3.821627	-0.690828	Cl	2.273159	0.606139	2.427085
C	-0.564273	-4.002067	0.078676	I	3.151333	-0.103510	-1.086133

PAH8$_{Br,Br}$

C	0.114191	2.959364	0.429898	C	2.631833	-2.391982	0.604998
C	0.473239	1.610373	0.167212	C	1.827317	-1.290579	0.223758
C	-0.520610	0.631584	0.374743	C	2.127127	-3.721446	0.609476
C	-1.596974	0.936078	1.192718	C	0.940317	-4.010596	0.036336
C	-1.862138	2.241869	1.609283	C	0.113732	-2.959361	-0.429712
C	-1.059082	3.246503	1.146021	C	0.472995	-1.610421	-0.167056
C	0.940896	4.010482	-0.036203	C	-1.059632	-3.246330	-1.145754
C	2.127619	3.721161	-0.609436	C	-1.862571	-2.241581	-1.608968
C	2.632131	2.391624	-0.605005	C	-1.597184	-0.935827	-1.192429
C	1.827486	1.290336	-0.223702	C	-0.520725	-0.631488	-0.374525
C	4.017628	2.248661	-0.835335	H	-2.722353	2.444868	2.231745
C	4.631998	1.101829	-0.477262	H	-1.297135	4.281514	1.361155
C	3.886347	-0.000272	-0.000062	H	0.607328	5.033975	0.087116
C	2.462640	-0.000167	0.000001	H	2.776757	4.508641	-0.973342
C	4.631878	-1.102483	0.477074	H	4.580194	3.103081	-1.191674
C	4.017370	-2.249222	0.835208	H	5.709650	1.003019	-0.532280

H	5.709550	-1.003831	0.531994	H	-1.297853	-4.281307	-1.360865
H	4.579842	-3.103723	1.191501	H	-2.722860	-2.444455	-2.231368
H	2.776178	-4.509019	0.973336	Br	-2.794957	0.403907	-1.779791
H	0.606591	-5.034042	-0.086952	Br	-2.794892	-0.403481	1.780185

$PAH8_{Br,I}$

C	0.457010	-2.977146	-0.395273	C	0.230411	2.904748	0.644164
C	0.770500	-1.618175	-0.126705	C	0.636395	1.585860	0.308314
C	-0.283973	-0.687327	-0.231298	C	-0.891531	3.105224	1.464847
C	-1.402648	-1.019824	-0.979885	C	-1.597525	2.044546	1.960456
C	-1.632437	-2.329826	-1.409754	C	-1.301797	0.768172	1.477793
C	-0.753047	-3.305244	-1.027387	C	-0.284885	0.548939	0.561987
C	1.369230	-3.994780	-0.023723	H	-2.519932	-2.567446	-1.979745
C	2.584498	-3.657772	0.456421	H	-0.958564	-4.345840	-1.249679
C	3.021662	-2.304515	0.445534	H	1.077234	-5.031080	-0.145466
C	2.134241	-1.237530	0.163458	H	3.299577	-4.419116	0.744518
C	4.412965	-2.095630	0.562629	H	5.045565	-2.928395	0.845174
C	4.937202	-0.909605	0.188742	H	6.009422	-0.756565	0.156478
C	4.100054	0.164690	-0.189970	H	5.819044	1.278223	-0.837471
C	2.683262	0.089653	-0.072527	H	4.534443	3.334045	-1.330461
C	4.746221	1.318119	-0.690516	H	2.684250	4.635230	-0.918742
C	4.047169	2.441101	-0.958017	H	0.585872	5.012031	0.330566
C	2.680313	2.503774	-0.610530	H	-1.164755	4.118701	1.733921
C	1.967516	1.350340	-0.201810	H	-2.410964	2.181430	2.659150
C	2.109041	3.803566	-0.529618	Br	-2.374471	-0.653159	2.113122
C	0.960207	4.011932	0.147059	I	-2.825092	0.413880	-1.527659

$PAH8_{I,I}$

C	0.524621	-2.912182	-0.663787	C	3.045986	2.432922	-0.410411
C	0.889338	-1.589678	-0.296967	C	2.243022	1.303489	-0.118902
C	-0.101037	-0.594693	-0.430742	C	2.536774	3.757181	-0.311897
C	-1.170051	-0.820028	-1.284710	C	1.347849	3.998411	0.279514
C	-1.434084	-2.090131	-1.805637	C	0.525178	2.911960	0.664996
C	-0.645401	-3.134612	-1.407851	C	0.889616	1.589426	0.297995
C	1.347257	-3.998717	-0.278467	C	-0.644622	3.134508	1.409370
C	2.536396	-3.757603	0.312563	C	-1.433353	2.090114	1.807290
C	3.045816	-2.433406	0.410823	C	-1.169620	0.820004	1.286236
C	2.242899	-1.303888	0.119518	C	-0.100850	0.594567	0.431982
C	4.431969	-2.310757	0.648519	H	-2.282757	-2.244952	-2.457368
C	5.047064	-1.138789	0.384187	H	-0.889074	-4.148349	-1.703578
C	4.302251	-0.000331	-0.000064	H	1.010728	-5.008864	-0.479327
C	2.878689	-0.000237	0.000188	H	3.183447	-4.573062	0.613154
C	5.047073	1.138038	-0.384557	H	4.994526	-3.191612	0.933377
C	4.432037	2.310103	-0.648603	H	6.124910	-1.046051	0.445749

H	6.124884	1.045160	-0.446518	H	-0.888080	4.148263	1.705216
H	4.994610	3.190899	-0.933613	H	-2.281846	2.245017	2.459236
H	3.183840	4.572573	-0.612633	I	-2.461391	-0.722909	1.859823
H	1.011516	5.008588	0.480550	I	-2.461770	0.723032	-1.858022

PAH8$_{Me,H}$

C	3.011459	-0.774135	-0.074563	C	-3.246542	-2.063316	1.148148
C	1.632683	-0.441655	0.029352	C	-2.241295	-2.880412	1.590168
C	0.712989	-1.493998	-0.186569	C	-0.936516	-2.605417	1.186548
C	1.104476	-2.658422	-0.844833	C	-0.621885	-1.488079	0.432375
C	2.465809	-2.878038	-1.101069	H	2.766714	-3.784499	-1.614197
C	3.401695	-1.998000	-0.641427	H	4.460513	-2.209335	-0.736915
C	4.000748	0.119725	0.400844	H	5.037372	-0.196233	0.394938
C	3.639710	1.343324	0.835449	H	4.377755	2.047408	1.200931
C	2.302948	1.800024	0.680726	H	2.938104	3.805703	1.144657
C	1.252226	0.932697	0.288973	H	0.863558	4.827534	0.261098
C	2.118660	3.196545	0.782619	H	-1.090441	4.691674	-0.869251
C	0.987650	3.751970	0.304041	H	-3.160841	3.471306	-1.463200
C	-0.071940	2.939478	-0.159101	H	-4.536157	1.678450	-1.102933
C	-0.040898	1.519537	-0.043486	H	-5.031704	-0.446055	0.057269
C	-1.172448	3.620659	-0.726408	H	-4.286094	-2.298816	1.344708
C	-2.301980	2.957583	-1.048330	H	-2.456353	-3.760922	2.182623
C	-2.421113	1.593450	-0.707745	C	0.134405	-3.705883	-1.314782
C	-1.310843	0.840997	-0.252211	H	-0.144070	-3.306413	1.416203
C	-3.741335	1.065081	-0.695093	H	0.106805	-4.575569	-0.653454
C	-4.013706	-0.096183	-0.067571	H	-0.881023	-3.323023	-1.393678
C	-2.951721	-0.888103	0.437391	H	0.446432	-4.062692	-2.298894
C	-1.601827	-0.504587	0.191500				

PAH8$_{tBu,H}$

C	-0.373351	3.003740	-0.350670	C	3.291260	-2.231651	1.326765
C	0.016917	1.641269	-0.287789	C	2.026054	-2.382670	0.721974
C	-1.021421	0.687680	-0.135153	C	1.325461	-1.273032	0.189871
C	-2.261121	1.052202	0.393045	C	1.562323	-3.714980	0.537497
C	-2.574905	2.425138	0.418429	C	0.539404	-3.983185	-0.299531
C	-1.694249	3.361701	-0.036424	C	-0.202081	-2.916160	-0.868404
C	0.559070	3.999135	-0.725466	C	0.088096	-1.577193	-0.487876
C	1.858830	3.670826	-0.873103	C	-1.244979	-3.191258	-1.769749
C	2.318656	2.365105	-0.553975	C	-2.016347	-2.177641	-2.273858
C	1.423265	1.295166	-0.301645	C	-1.856832	-0.895143	-1.751178
C	3.711155	2.235147	-0.351153	C	-0.885579	-0.613121	-0.805560
C	4.195725	1.134546	0.257997	H	-3.553586	2.742306	0.753256
C	3.348291	0.038790	0.541601	H	-1.980592	4.404905	-0.103798
C	1.980060	0.023011	0.147148	H	0.214388	5.018334	-0.855630
C	3.948178	-1.059290	1.198517	H	2.598059	4.419974	-1.130932

H	4.353035	3.072274	-0.598021	H	-4.384468	-0.474846	-0.779332
H	5.242569	1.054682	0.525945	H	-5.328684	-0.565205	0.708597
H	4.964560	-0.945278	1.556671	H	-4.980987	1.005829	-0.019879
H	3.756481	-3.091844	1.793086	C	-2.772005	-1.320420	1.283795
H	2.125701	-4.515544	1.002407	H	-2.661378	-1.919621	0.383696
H	0.258678	-5.001948	-0.539566	H	-1.811259	-1.297335	1.801195
H	-1.413801	-4.220662	-2.063944	H	-3.485985	-1.834493	1.931362
H	-2.786330	-2.376228	-3.008950	C	-3.653616	0.666708	2.398351
C	-3.291276	0.093574	1.015643	H	-4.133620	1.643059	2.342026
H	-2.536207	-0.103057	-2.037219	H	-4.348210	-0.011514	2.898441
C	-4.569226	0.014068	0.177311	H	-2.762916	0.763860	3.022137

PAH8$_{Ph,H}$

C	0.680682	-3.104821	0.049420	C	-0.666071	0.281254	0.865704
C	0.735644	-1.687385	0.159033	H	-2.551822	-3.497537	-0.898871
C	-0.504242	-1.010440	0.180019	H	-0.518401	-4.821484	-0.409742
C	-1.668004	-1.639863	-0.270704	H	1.742395	-4.966910	0.303381
C	-1.650840	-3.017881	-0.537401	H	3.909067	-3.855154	0.732999
C	-0.520516	-3.743404	-0.298190	H	5.290861	-2.072579	0.454544
C	1.832414	-3.887037	0.306358	H	5.683907	0.190150	-0.469890
C	3.012712	-3.279016	0.536347	H	4.945363	2.091849	-1.445508
C	3.147083	-1.872904	0.378544	H	3.231569	3.857885	-1.714485
C	2.024980	-1.025510	0.200900	H	1.277561	4.805420	-0.995406
C	4.470008	-1.395957	0.249753	H	-0.675807	4.812200	0.517634
C	4.683130	-0.162726	-0.250861	H	-2.090016	3.669030	2.042312
C	3.598804	0.706577	-0.507076	H	-2.961533	1.558341	3.028604
C	2.260580	0.369200	-0.153115	H	-2.157369	-0.588757	2.101210
C	3.923436	1.938188	-1.119659	C	-2.932790	-0.906062	-0.495277
C	2.991461	2.902134	-1.264401	C	-2.940121	0.309877	-1.179770
C	1.713959	2.718581	-0.693475	C	-4.151498	-1.437173	-0.076600
C	1.304892	1.466309	-0.172766	C	-4.126010	0.979855	-1.421573
C	0.927243	3.891727	-0.529876	H	-2.002822	0.728849	-1.524193
C	-0.141398	3.896962	0.291586	C	-5.340228	-0.765268	-0.315535
C	-0.588930	2.683796	0.872271	H	-4.163756	-2.375965	0.465155
C	0.030096	1.453309	0.510015	C	-5.332327	0.447478	-0.987112
C	-1.667605	2.708285	1.771786	H	-4.108557	1.922526	-1.955193
C	-2.161225	1.546219	2.299702	H	-6.275612	-1.189508	0.029595
C	-1.682072	0.336739	1.804249	H	-6.260270	0.974149	-1.173705

PAH8$_{Me,Me}$

C	-3.056613	-0.042136	0.272583	C	-2.828993	-2.114262	1.472117
C	-1.649743	0.019588	0.087203	C	-3.622872	-1.124729	0.966021
C	-0.921785	-1.160513	0.348650	C	-3.884226	0.983537	-0.246036
C	-1.466924	-2.168211	1.138439	C	-3.322469	2.077538	-0.800815

C	-1.918092	2.288169	-0.727898	H	-4.695340	-1.135794	1.123168
C	-1.033128	1.272855	-0.287998	H	-4.960269	0.874037	-0.176981
C	-1.473717	3.608483	-0.957079	H	-3.934860	2.875621	-1.203651
C	-0.240712	3.971688	-0.547210	H	-2.172038	4.333576	-1.357564
C	0.654108	3.016292	-0.013731	H	0.087617	5.002903	-0.602854
C	0.351612	1.624615	-0.005978	H	1.995416	4.594715	0.555542
C	1.865934	3.519717	0.511780	H	3.774739	3.055941	1.323585
C	2.837679	2.681898	0.928861	H	4.772939	0.996139	1.190130
C	2.693460	1.293862	0.714789	H	4.873340	-1.260976	0.186588
C	1.466118	0.732845	0.283055	H	3.795977	-2.992427	-1.094800
C	3.883842	0.520102	0.793734	H	1.750012	-4.012778	-2.038946
C	3.939915	-0.714054	0.251576	C	-0.661781	-3.326928	1.647623
C	2.760402	-1.308920	-0.259075	H	-0.914694	-3.506899	2.694818
C	1.506373	-0.667016	-0.077995	H	-0.880422	-4.251380	1.106528
C	2.825092	-2.535707	-0.940541	H	0.409166	-3.147301	1.579240
C	1.691298	-3.111404	-1.439135	C	-0.784088	-3.316975	-1.608233
C	0.430230	-2.591911	-1.108371	H	-0.966908	-4.244167	-1.058616
C	0.353843	-1.441161	-0.329781	H	-1.684044	-2.708967	-1.542853
H	-3.254996	-2.904135	2.080658	H	-0.631215	-3.594628	-2.653470

PAH8$_{rBu,rBu}$

C	0.007295	2.932130	-0.524287	C	1.914298	-2.135936	1.741652
C	-0.352938	1.593872	-0.236789	C	1.654395	-0.801306	1.367104
C	0.626029	0.592783	-0.442617	C	0.626024	-0.592688	0.442181
C	1.654421	0.801444	-1.367493	H	2.752166	2.345446	-2.394154
C	1.914244	2.136101	-1.742037	H	1.470200	4.203666	-1.453507
C	1.185355	3.178591	-1.246443	H	-0.459109	5.016341	-0.204558
C	-0.801338	3.997897	-0.062027	H	-2.627000	4.529145	0.880766
C	-1.986674	3.729736	0.526904	H	-4.446588	3.132013	1.121110
C	-2.499882	2.404039	0.550046	H	-5.582907	1.021836	0.508007
C	-1.699696	1.292206	0.187644	H	-5.582920	-1.022114	-0.507932
C	-3.885949	2.268341	0.783931	H	-4.446554	-3.132226	-1.121173
C	-4.504763	1.115467	0.450841	H	-2.626876	-4.529248	-0.881024
C	-3.762329	-0.000077	-0.000115	H	-0.458921	-5.016319	0.204257
C	-2.339756	-0.000036	-0.000219	H	1.470352	-4.203531	1.453172
C	-4.504760	-1.115667	-0.450946	H	2.752074	-2.345191	2.394008
C	-3.885917	-2.268507	-0.784111	C	2.460953	-0.272117	-2.119485
C	-2.499814	-2.404123	-0.550402	C	3.958596	-0.194990	-1.821795
C	-1.699640	-1.292240	-0.188129	H	4.175873	-0.571675	-0.823566
C	-1.986551	-3.729804	-0.527240	H	4.508099	-0.813237	-2.536049
C	-0.801187	-3.997897	0.061661	H	4.342806	0.823968	-1.896336
C	0.007423	-2.932079	0.523848	C	2.001372	-1.707691	-1.894799
C	-0.352851	-1.593843	0.236266	H	2.184719	-2.058572	-0.882204
C	1.185487	-3.178475	1.246034	H	0.941207	-1.828296	-2.118616

H	2.559292	-2.358153	-2.572899	H	4.177036	0.571762	0.826602
C	2.244949	0.006560	-3.619224	C	2.001005	1.707903	1.894884
H	2.650187	0.967868	-3.934177	H	2.185056	2.058685	0.882377
H	2.741828	-0.770509	-4.204493	H	0.940725	1.828779	2.118009
H	1.181375	-0.007798	-3.864786	H	2.558621	2.358253	2.573344
C	2.460085	0.272251	2.119970	C	2.241904	-0.006802	3.619298
C	3.958179	0.195039	1.824463	H	2.646036	-0.968574	3.934295
H	4.506584	0.813243	2.539595	H	2.738503	0.769702	4.205571
H	4.342326	-0.823892	1.899550	H	1.178003	0.008149	3.863401

PAH8$_{Ph,Ph}$

C	-0.480571	2.783449	-1.077347	H	-4.959952	3.296221	0.429302
C	-0.851242	1.520352	-0.543580	H	-6.093299	1.101512	0.277207
C	0.150409	0.527375	-0.514279	H	-6.093310	-1.101455	-0.277266
C	1.275857	0.628712	-1.334981	H	-4.959991	-3.296180	-0.429333
C	1.530089	1.838728	-2.000255	H	-3.156084	-4.610284	0.092483
C	0.718929	2.916886	-1.795435	H	-0.966466	-4.883109	1.207028
C	-1.309115	3.912630	-0.867674	H	0.963414	-3.883653	2.219969
C	-2.505411	3.760721	-0.263103	H	2.401117	-1.917227	2.638212
C	-3.012653	2.464760	0.028016	C	2.224609	-0.486722	-1.526086
C	-2.208016	1.304886	-0.090735	C	1.768719	-1.791836	-1.719569
C	-4.399008	2.381080	0.282453	C	3.598314	-0.252581	-1.578687
C	-5.015438	1.183747	0.202044	C	2.657286	-2.829247	-1.939436
C	-4.269689	0.000017	-0.000024	H	0.704687	-1.989596	-1.706247
C	-2.846052	0.000008	-0.000018	C	4.489284	-1.290365	-1.801824
C	-5.015451	-1.183703	-0.202094	H	3.972079	0.749463	-1.408698
C	-4.399036	-2.381045	-0.282487	C	4.023212	-2.583999	-1.978671
C	-3.012686	-2.464741	-0.028033	H	2.279882	-3.833890	-2.087392
C	-2.208035	-1.304877	0.090715	H	5.553316	-1.087081	-1.828082
C	-2.505466	-3.760706	0.263113	H	4.718961	-3.396381	-2.150524
C	-1.309184	-3.912622	0.867709	C	2.224579	0.486699	1.526100
C	-0.480628	-2.783449	1.077382	C	1.768694	1.791830	1.719471
C	-0.851271	-1.520357	0.543584	C	3.598279	0.252546	1.578775
C	0.718853	-2.916888	1.795501	C	2.657263	2.829246	1.939312
C	1.530021	-1.838734	2.000322	H	0.704664	1.989602	1.706076
C	1.275820	-0.628730	1.335015	C	4.489250	1.290334	1.801887
C	0.150393	-0.527395	0.514287	H	3.972040	-0.749514	1.408866
H	2.401199	1.917223	-2.638126	C	4.023184	2.583985	1.978630
H	0.963511	3.883657	-2.219880	H	2.279864	3.833904	2.087181
H	-0.966377	4.883118	-1.206970	H	5.553279	1.087040	1.828207
H	-3.156020	4.610306	-0.092470	H	4.718934	3.396370	2.150463

PAH3$_{Cl,H}^{‡}$

C	1.543014	0.029621	-0.000004	C	0.773335	1.218858	0.000004

C	-0.653157	1.156470	0.000014	C	3.111115	-2.296795	-0.000012
C	-1.341332	-0.104208	0.000015	C	3.720128	-1.090265	-0.000023
C	-0.532774	-1.333391	0.000020	C	0.683492	3.669016	0.000007
C	0.889905	-1.232747	0.000005	C	-0.666464	3.626904	0.000017
C	2.952780	0.104932	-0.000017	H	4.665143	1.405236	-0.000033
C	3.581973	1.364146	-0.000023	H	3.331890	3.478737	-0.000017
C	2.844606	2.510503	-0.000014	H	-3.298398	3.318134	0.000028
C	1.436787	2.466645	-0.000001	H	-4.511337	1.167322	0.000015
C	-1.362584	2.386918	0.000019	H	-0.761609	-4.732327	0.000061
C	-2.757167	2.379750	0.000023	H	1.712704	-4.551790	0.000020
C	-3.430294	1.191710	0.000017	H	3.692866	-3.211370	-0.000015
C	-2.744248	-0.022551	0.000011	H	4.801244	-1.012697	-0.000034
C	-1.070945	-2.619765	0.000043	H	1.212616	4.614860	0.000004
C	-0.280037	-3.762102	0.000043	H	-1.252189	4.538739	0.000021
C	1.088209	-3.665942	0.000021	Cl	-3.847364	-1.366836	-0.000012
C	1.691783	-2.406515	0.000004	H	-2.133313	-2.761426	0.000062

$PAH3_{Br,H}^{‡}$

C	-1.941216	-0.323399	0.000006	C	-1.454858	-2.714413	-0.000025
C	-1.504282	1.023820	0.000017	C	-2.854137	-2.975917	-0.000043
C	-0.109587	1.333149	0.000006	C	-3.754748	-1.968356	-0.000027
C	0.885357	0.294011	0.000019	C	-2.054822	3.413756	0.000024
C	0.416769	-1.102114	0.000022	C	-0.740586	3.723440	-0.000006
C	-0.983637	-1.372991	-0.000002	H	-5.313236	0.197033	0.000025
C	-3.322556	-0.615508	0.000001	H	-4.560887	2.544970	0.000054
C	-4.256338	0.437586	0.000023	H	1.877951	4.111281	-0.000091
C	-3.840177	1.735352	0.000038	H	3.608315	2.362443	-0.000060
C	-2.468952	2.056958	0.000030	H	1.516184	-4.326754	0.000024
C	0.253215	2.706369	-0.000019	H	-0.922006	-4.792592	-0.000045
C	1.600258	3.064173	-0.000056	H	-3.179061	-4.009979	-0.000067
C	2.561158	2.093972	-0.000040	H	-4.819108	-2.173106	-0.000036
C	2.218230	0.741521	0.000012	H	-2.811788	4.189368	0.000039
C	1.266138	-2.206456	0.000038	H	-0.410962	4.755799	-0.000018
C	0.799245	-3.514829	0.000014	H	2.329473	-2.071266	0.000072
C	-0.547135	-3.775648	-0.000022	Br	3.803187	-0.320367	0.000099

$PAH3_{I,H}^{‡}$

C	-2.319063	-0.383795	0.000000	C	-4.665421	0.274177	0.000001
C	-1.940403	0.980645	0.000000	C	-4.305972	1.588755	0.000001
C	-0.559909	1.351021	-0.000001	C	-2.950175	1.970016	0.000000
C	0.483509	0.358647	-0.000001	C	-0.261055	2.739433	-0.000001
C	0.070581	-1.056099	-0.000001	C	1.067546	3.157157	-0.000001
C	-1.316250	-1.389452	-0.000001	C	2.072324	2.232068	-0.000002
C	-3.686226	-0.736560	0.000000	C	1.799235	0.860931	-0.000002

C	0.964629	-2.122376	-0.000002	H	1.298341	4.215702	-0.000001
C	0.559187	-3.450746	-0.000003	H	3.101628	2.562573	-0.000002
C	-0.774234	-3.771183	-0.000002	H	1.312594	-4.228957	-0.000003
C	-1.727495	-2.750665	-0.000001	H	-1.103873	-4.803659	-0.000002
C	-3.113860	-3.073838	-0.000001	H	-3.392623	-4.121281	-0.000001
C	-4.058177	-2.107176	0.000000	H	-5.112449	-2.358752	0.000000
C	-2.597636	3.344030	0.000000	H	-3.388719	4.084818	0.000001
C	-1.298730	3.711744	0.000000	H	-1.014732	4.757550	0.000000
H	-5.710779	-0.012347	0.000001	H	2.022223	-1.944789	-0.000002
H	-5.061127	2.366346	0.000001	I	3.646502	-0.172586	-0.000001

$PAH3_{F,F}^{‡}$

C	1.260329	0.708877	-0.000084	C	0.099729	2.847241	0.000832
C	1.260319	-0.708894	-0.000295	C	1.355792	3.513013	0.001353
C	0.028197	-1.426532	0.000135	C	2.513514	2.819463	0.000645
C	-1.233929	-0.739419	-0.000113	C	2.513477	-2.819496	-0.000377
C	-1.233918	0.739435	-0.000181	C	1.355745	-3.513031	0.000625
C	0.028216	1.426532	0.000241	H	4.634667	1.233168	-0.002203
C	2.492982	1.401442	-0.000379	H	4.634650	-1.233228	-0.002803
C	3.702265	0.680541	-0.001503	H	-1.008269	-4.687324	0.001603
C	3.702256	-0.680589	-0.001832	H	-3.215810	-3.516005	0.000721
C	2.492963	-1.401475	-0.000944	H	-3.215763	3.516047	-0.000888
C	0.099691	-2.847242	0.000741	H	-1.008207	4.687338	0.000655
C	-1.070899	-3.606004	0.000927	H	1.355069	4.596793	0.002367
C	-2.279595	-2.973666	0.000565	H	3.471052	3.326741	0.000730
C	-2.348622	-1.586662	0.000048	H	3.471007	-3.326787	-0.000735
C	-2.348600	1.586693	-0.000437	H	1.355008	-4.596811	0.001459
C	-2.279555	2.973697	-0.000527	F	-3.602995	1.142960	-0.000269
C	-1.070851	3.606019	0.000232	F	-3.603014	-1.142917	-0.000107

$PAH3_{F,Cl}^{‡}$

C	-1.640185	-0.267654	0.015452	C	2.553220	0.787611	0.175671
C	-1.181448	1.071982	0.021490	C	1.471600	-2.274299	0.160500
C	0.218462	1.359615	0.075601	C	0.953406	-3.562536	0.151342
C	1.219139	0.312588	0.126026	C	-0.390999	-3.764693	0.098671
C	0.719102	-1.093634	0.118908	C	-1.237478	-2.658681	0.054124
C	-0.702195	-1.338033	0.063515	C	-2.638720	-2.886909	-0.000500
C	-3.030746	-0.527992	-0.038510	C	-3.511214	-1.860382	-0.045475
C	-3.947292	0.537922	-0.085730	C	-1.719799	3.471908	-0.022900
C	-3.510145	1.824882	-0.080111	C	-0.406047	3.765645	0.027688
C	-2.134852	2.118469	-0.027047	H	-5.006100	0.310579	-0.126539
C	0.573059	2.738082	0.077051	H	-4.212503	2.649467	-0.116368
C	1.911121	3.113354	0.127782	H	2.177977	4.163030	0.128716
C	2.868476	2.151470	0.175621	H	3.913887	2.421134	0.215436

H	1.663891	-4.377480	0.187690	H	-2.472439	4.250384	-0.060749
H	-0.809464	-4.763483	0.090905	H	-0.059845	4.792383	0.032122
H	-2.982988	-3.914437	-0.004821	F	2.798408	-2.293335	0.214764
H	-4.580456	-2.030176	-0.087200	Cl	4.046301	-0.096422	0.244585

PAH3$_{F,Br}^{‡}$

C	-2.071801	-0.252025	0.013653	C	-1.697999	-2.647366	0.071574
C	-1.594763	1.080647	0.033173	C	-3.099039	-2.859589	-0.031892
C	-0.193050	1.351598	0.135803	C	-3.957545	-1.823194	-0.109631
C	0.796856	0.293307	0.224051	C	-2.104857	3.486930	-0.035402
C	0.270844	-1.103361	0.201653	C	-0.790754	3.765611	0.060384
C	-1.149405	-1.332210	0.096873	H	-5.423230	0.366393	-0.247430
C	-3.462523	-0.496246	-0.088531	H	-4.599843	2.694969	-0.214008
C	-4.363693	0.580300	-0.169990	H	1.790218	4.134232	0.250762
C	-3.910041	1.861408	-0.151561	H	3.500222	2.392009	0.402309
C	-2.533899	2.138108	-0.050981	H	1.179078	-4.396577	0.311369
C	0.173635	2.726474	0.146281	H	-1.295325	-4.756784	0.128174
C	1.511696	3.087585	0.242978	H	-3.454906	-3.883062	-0.046249
C	2.458675	2.117516	0.326967	H	-5.026524	-1.980942	-0.188568
C	2.135692	0.754337	0.319769	H	-2.847129	4.273442	-0.101269
C	1.005016	-2.291428	0.272063	H	-0.432264	4.787980	0.074663
C	0.478048	-3.575140	0.248040	F	2.328094	-2.312396	0.372605
C	-0.866112	-3.762754	0.148447	Br	3.807475	-0.167438	0.458295

PAH3$_{F,I}^{‡}$

C	-2.461678	-0.263678	0.006655	C	-2.062298	-2.656417	0.053753
C	-1.993110	1.071605	0.025231	C	-3.462554	-2.881664	-0.035152
C	-0.591599	1.353564	0.113649	C	-4.331853	-1.853042	-0.100666
C	0.410611	0.305060	0.188015	C	-2.523852	3.473880	-0.030507
C	-0.112749	-1.090568	0.166455	C	-1.211240	3.763092	0.052039
C	-1.529614	-1.334798	0.076633	H	-5.820020	0.327245	-0.216486
C	-3.850757	-0.520591	-0.081217	H	-5.013736	2.661596	-0.184813
C	-4.761300	0.548651	-0.149751	H	1.370189	4.148064	0.215935
C	-4.316737	1.833334	-0.132267	H	3.089492	2.439953	0.342706
C	-2.941917	2.121363	-0.045625	H	0.840247	-4.371458	0.257427
C	-0.237764	2.731092	0.124335	H	-1.633370	-4.761020	0.100236
C	1.097744	3.099681	0.207639	H	-3.809325	-3.908277	-0.048585
C	2.055227	2.137368	0.278339	H	-5.399964	-2.021620	-0.168500
C	1.753578	0.766614	0.271048	H	-3.273289	4.254398	-0.086031
C	0.633406	-2.267846	0.225360	H	-0.860645	4.788191	0.065667
C	0.128065	-3.558976	0.203984	F	1.958838	-2.255111	0.311328
C	-1.215894	-3.761968	0.118504	I	3.673100	-0.160649	0.404032

PAH3$_{Cl,Cl}^{‡}$

C	1.624179	0.706375	-0.050042	C	0.530528	2.829269	0.277393
C	1.624144	-0.706432	-0.050030	C	1.784564	3.489116	0.188294
C	0.398900	-1.419118	0.119929	C	2.913807	2.802404	-0.068111
C	-0.894471	-0.753518	0.109865	C	2.913669	-2.802524	-0.068063
C	-0.894434	0.753588	0.109853	C	1.784393	-3.489177	0.188353
C	0.398970	1.419124	0.119905	H	4.973399	1.236144	-0.502419
C	2.857551	1.393243	-0.177666	H	4.973339	-1.236373	-0.502398
C	4.052418	0.679025	-0.377017	H	-0.487152	-4.676800	0.685437
C	4.052384	-0.679207	-0.377005	H	-2.711100	-3.627152	0.544847
C	2.857483	-1.393362	-0.177642	H	-2.710923	3.627318	0.544786
C	0.530389	-2.829266	0.277441	H	-0.486923	4.676859	0.685359
C	-0.592513	-3.613752	0.508079	H	1.795712	4.565538	0.311162
C	-1.815414	-3.032357	0.440566	H	3.871626	3.299162	-0.165321
C	-1.978114	-1.667187	0.173499	H	3.871464	-3.299331	-0.165265
C	-1.978032	1.667310	0.173471	H	1.795488	-4.565597	0.311240
C	-1.815265	3.032477	0.440515	Cl	-3.665376	-1.422328	-0.134246
C	-0.592336	3.613813	0.508018	Cl	-3.665306	1.422529	-0.134271

PAH3$_{Cl,Br}^{‡}$

C	2.129909	0.388317	-0.070456	C	1.551467	2.697174	0.317575
C	1.804373	-0.985494	-0.076067	C	2.922392	3.054192	0.218185
C	0.456574	-1.400195	0.152022	C	3.859660	2.135595	-0.085740
C	-0.656571	-0.461952	0.153642	C	2.581421	-3.319288	-0.119662
C	-0.303327	1.001077	0.126526	C	1.344195	-3.727245	0.221110
C	1.104442	1.356624	0.136475	H	5.493639	0.145789	-0.632649
C	3.482864	0.778840	-0.225497	H	4.923805	-2.259355	-0.659833
C	4.473482	-0.186269	-0.479839	H	-1.096567	-4.339015	0.948750
C	4.160027	-1.508505	-0.494764	H	-3.028952	-2.840214	0.838864
C	2.842462	-1.934563	-0.247962	H	-1.430737	4.203552	0.576923
C	0.279877	-2.797593	0.361106	H	0.976593	4.717639	0.771975
C	-0.970713	-3.291161	0.706049	H	3.182764	4.095668	0.364866
C	-2.037648	-2.453780	0.655179	H	4.902863	2.405242	-0.198501
C	-1.916876	-1.107360	0.284635	H	3.393900	-4.022510	-0.257640
C	-1.146724	2.136036	0.177655	H	1.119461	-4.775656	0.376654
C	-0.689193	3.423982	0.476698	Cl	-2.823196	2.251161	-0.211263
C	0.634076	3.710277	0.570578	Br	-3.705650	-0.569764	-0.130034

PAH3$_{Cl,I}^{‡}$

C	2.526416	0.307727	-0.076228	C	3.902481	0.625667	-0.177344
C	2.122422	-1.044042	-0.113627	C	4.843937	-0.389756	-0.421695
C	0.749080	-1.384935	0.089257	C	4.454683	-1.691372	-0.479355
C	-0.313591	-0.391068	0.069552	C	3.108843	-2.047432	-0.276889
C	0.130337	1.043375	0.030514	C	0.497546	-2.767932	0.310194
C	1.549115	1.327413	0.101223	C	-0.769825	-3.175485	0.698205

C	-1.789737	-2.278111	0.651944	H	5.179382	-2.480927	-0.640271
C	-1.616037	-0.953135	0.219500	H	-0.952457	-4.206859	0.973876
C	-0.651727	2.216220	0.018119	H	-2.787702	-2.618885	0.882764
C	-0.156550	3.486408	0.323478	H	-0.864892	4.301821	0.366166
C	1.173314	3.705801	0.496450	H	1.555090	4.696655	0.708985
C	2.051834	2.644861	0.302799	H	3.754905	3.950243	0.438922
C	3.444042	2.925708	0.272241	H	5.403223	2.174186	-0.063517
C	4.343301	1.959097	0.000688	H	3.537722	-4.164408	-0.313112
C	2.765988	-3.417014	-0.173110	H	1.222549	-4.791505	0.311977
C	1.506222	-3.756771	0.161115	Cl	-2.290295	2.352173	-0.479463
H	5.886133	-0.115361	-0.535359	I	-3.614812	-0.422618	-0.340273

PAH3$_{Br,I}^{‡}$

C	2.668434	0.461605	-0.101059	C	1.933977	2.701202	0.412711
C	2.439804	-0.929568	-0.133534	C	3.276074	3.156774	0.313890
C	1.133878	-1.438313	0.137534	C	4.267175	2.324825	-0.064514
C	-0.044159	-0.587497	0.140750	C	3.373401	-3.201117	-0.210102
C	0.204800	0.892947	0.118229	C	2.188761	-3.690627	0.206319
C	1.582216	1.345461	0.158113	H	6.020940	0.470914	-0.756519
C	3.985806	0.952077	-0.267465	H	5.618181	-1.965130	-0.840268
C	5.030391	0.065807	-0.585826	H	-0.158574	-4.424129	1.162389
C	4.808412	-1.275676	-0.631909	H	-2.192796	-3.089340	1.059921
C	3.534448	-1.801121	-0.349134	H	-1.145464	3.982845	0.713040
C	1.069622	-2.836204	0.394314	H	1.210781	4.636171	1.010585
C	-0.119403	-3.388112	0.849096	H	3.468886	4.203516	0.516820
C	-1.249429	-2.632116	0.800771	H	5.285391	2.675309	-0.183845
C	-1.255665	-1.314437	0.316719	H	4.224015	-3.848465	-0.386719
C	-0.712753	1.965277	0.182659	H	2.050213	-4.749518	0.389338
C	-0.356375	3.255356	0.587278	I	-3.273620	-1.080443	-0.329836
C	0.944744	3.623488	0.734092	Br	-2.495003	2.047529	-0.442898

PAH3$_{I,I}^{‡}$

C	2.792236	0.704946	-0.144034	C	-0.599929	-2.954562	0.754746
C	2.792237	-0.704357	-0.145604	C	-0.787350	-1.659798	0.251036
C	1.585812	-1.406170	0.142812	C	-0.787410	1.659574	0.254197
C	0.292615	-0.749675	0.115273	C	-0.600026	2.953303	0.760584
C	0.292586	0.749704	0.116812	C	0.635078	3.515591	0.875440
C	1.585791	1.406134	0.145851	C	1.735813	2.790239	0.438598
C	4.010105	1.396817	-0.345352	C	2.981092	3.457213	0.286074
C	5.176800	0.681557	-0.670824	C	4.073661	2.798499	-0.151059
C	5.176794	-0.679813	-0.672363	C	4.073641	-2.797901	-0.157301
C	4.010096	-1.395789	-0.348484	C	2.981101	-3.457559	0.278479
C	1.735847	-2.790902	0.432592	H	6.085609	1.236015	-0.873709
C	0.635178	-3.517147	0.868122	H	6.085598	-1.233821	-0.876495

H	0.750695	-4.540716	1.202692	H	5.016652	3.308493	-0.307800
H	-1.473073	-3.552395	0.972941	H	5.016617	-3.307558	-0.315219
H	-1.473187	3.550751	0.979751	H	3.014771	-4.518844	0.494248
H	0.750549	4.538462	1.212149	I	-2.745183	-1.702141	-0.546645
H	3.014750	4.518027	0.504147	I	-2.745169	1.703810	-0.543671

PAH3$_{H,Me}^{‡}$

C	1.105597	0.766645	0.000000	C	3.521190	1.162090	-0.000002
C	-0.220871	1.263076	-0.000001	C	-1.754714	3.175660	-0.000003
C	-1.327698	0.360923	0.000001	C	-2.812520	2.336023	-0.000001
C	-1.138522	-1.058395	0.000003	H	2.794219	3.731201	-0.000006
C	0.244584	-1.560726	0.000003	H	0.487892	4.602041	-0.000006
C	1.332138	-0.636820	0.000002	H	-4.735313	0.506793	0.000004
C	2.193553	1.666743	-0.000002	H	-4.425859	-1.923796	0.000007
C	1.948855	3.052642	-0.000004	H	2.085891	-4.431582	0.000007
C	0.672959	3.533916	-0.000005	H	3.968157	-2.816181	0.000005
C	-0.431572	2.660326	-0.000003	H	4.762399	-0.558350	0.000001
C	-2.631194	0.924696	0.000001	H	4.344187	1.867605	-0.000003
C	-3.738786	0.080798	0.000003	H	-1.894473	4.250498	-0.000004
C	-3.557616	-1.275404	0.000005	H	-3.826760	2.718520	-0.000001
C	-2.292978	-1.873477	0.000005	H	-0.179048	-3.668961	0.000006
C	0.580995	-2.915307	0.000005	C	-2.333080	-3.374793	0.000006
C	1.896113	-3.364999	0.000006	H	-1.856479	-3.805464	-0.883712
C	2.939547	-2.474802	0.000004	H	-1.856478	-3.805462	0.883725
C	2.675150	-1.103290	0.000002	H	-3.371258	-3.705579	0.000007
C	3.750360	-0.170060	0.000000				

PAH3$_{H,Ph}^{‡}$

C	-2.187524	0.582568	0.000041	C	-0.162981	3.708757	0.000208
C	-2.011832	-0.823368	-0.000030	C	-1.258393	2.842340	0.000160
C	-0.699634	-1.384298	-0.000058	C	-2.585040	3.360612	0.000185
C	0.464348	-0.553585	-0.000023	C	-3.658319	2.538641	0.000141
C	0.271451	0.905087	0.000056	C	-2.985449	-3.071557	-0.000136
C	-1.050186	1.436376	0.000085	C	-1.749615	-3.617297	-0.000162
C	-3.489446	1.127381	0.000068	H	-5.596398	0.698132	0.000047
C	-4.602424	0.265489	0.000026	H	-5.296397	-1.748121	-0.000073
C	-4.436129	-1.088475	-0.000041	H	0.769415	-4.465348	-0.000202
C	-3.149226	-1.660435	-0.000069	H	2.782762	-3.041393	-0.000151
C	-0.584152	-2.799701	-0.000125	H	1.968414	3.857281	0.000222
C	0.680979	-3.385224	-0.000154	H	-0.334975	4.778969	0.000267
C	1.797244	-2.591556	-0.000125	H	-2.712165	4.437167	0.000242
C	1.716900	-1.195118	-0.000064	H	-4.665254	2.940128	0.000161
C	1.321210	1.822440	0.000108	H	-3.870642	-3.697209	-0.000165
C	1.110772	3.195564	0.000183	H	-1.617068	-4.693110	-0.000213

H	2.340311	1.483648	0.000090	C	4.973907	0.289192	-1.199342
C	3.050924	-0.538118	-0.000058	H	3.203571	-0.486066	-2.135042
C	3.704948	-0.269283	1.199168	C	5.609809	0.575722	-0.000056
C	3.704883	-0.269128	-1.199284	H	5.468173	0.500034	2.140007
C	4.973973	0.289038	1.199228	H	5.468056	0.500310	-2.140120
H	3.203688	-0.486342	2.134925	H	6.600456	1.013706	-0.000054

PAH3$_{tBu,tBu}^{‡}$

C	-2.239191	0.487395	0.141630	H	-4.802912	2.749800	0.021396
C	-2.038760	-0.895619	0.287202	H	-3.866859	-3.755212	0.737596
C	-0.790423	-1.443500	-0.128928	H	-1.925322	-4.668297	-0.503509
C	0.429089	-0.657681	-0.161638	C	2.363654	2.219996	0.557126
C	0.211391	0.841968	-0.201254	C	3.056332	-1.669634	0.121591
C	-1.159976	1.284835	-0.328021	C	3.098183	-3.138641	0.633012
C	-3.529101	1.029351	0.333138	H	2.989005	-3.881158	-0.153162
C	-4.543978	0.213212	0.869374	H	4.059203	-3.313708	1.121452
C	-4.345640	-1.127432	1.027478	H	2.308566	-3.309330	1.367088
C	-3.128925	-1.721713	0.639143	C	2.512480	3.730801	0.837446
C	-0.862880	-2.796389	-0.550860	H	3.252688	3.851518	1.632836
C	0.181147	-3.261176	-1.340882	H	2.874021	4.299365	-0.019366
C	1.357635	-2.575788	-1.283583	H	1.574837	4.171980	1.177316
C	1.600768	-1.464473	-0.452903	C	2.062636	1.644597	1.950200
C	1.132521	1.932600	-0.310035	H	2.943576	1.673792	2.594954
C	0.770495	3.023140	-1.109305	H	1.293428	2.270127	2.408444
C	-0.519055	3.328349	-1.440139	H	1.671605	0.634755	1.930224
C	-1.517825	2.551537	-0.862966	C	3.658379	1.823532	-0.152294
C	-2.846935	3.045857	-0.760561	H	4.529153	1.919688	0.501966
C	-3.805402	2.347465	-0.111149	H	3.630097	0.821056	-0.553071
C	-3.035097	-3.124112	0.447404	H	3.805437	2.500149	-0.997418
C	-1.969844	-3.623198	-0.219655	C	3.470298	-0.917239	1.379785
H	-5.508226	0.657268	1.088887	H	3.623449	0.138100	1.257003
H	-5.150675	-1.766620	1.371784	H	2.746505	-1.078100	2.178871
H	0.097611	-4.192167	-1.888355	H	4.420462	-1.336963	1.716390
H	2.213939	-3.019457	-1.771116	C	4.132973	-1.548143	-0.968454
H	1.545260	3.732741	-1.365438	H	4.073427	-0.621929	-1.536034
H	-0.763529	4.225379	-1.995901	H	5.124180	-1.603300	-0.512718
H	-3.054552	4.026254	-1.173677	H	4.065938	-2.365113	-1.687861

PAH3$_{Ph,Ph}^{‡}$

C	-2.855098	0.726874	0.090301	C	-1.628752	1.412326	-0.159310
C	-2.878460	-0.685278	0.104213	C	-4.066602	1.437387	0.273072
C	-1.673406	-1.414872	-0.121625	C	-5.260402	0.743423	0.539558
C	-0.378690	-0.771933	-0.172566	C	-5.282876	-0.616685	0.550230
C	-0.353693	0.725749	-0.205422	C	-4.112023	-1.353316	0.296941

C	-1.821625	-2.822187	-0.275015	C	2.177896	-1.482492	-0.015797
C	-0.711746	-3.602065	-0.571560	C	2.621101	-1.236066	1.278109
C	0.517335	-3.019880	-0.560007	C	3.109304	-1.896297	-0.969005
C	0.726203	-1.655029	-0.287794	C	3.958399	-1.389368	1.607530
C	0.772995	1.571206	-0.361516	H	1.904850	-0.942805	2.035947
C	0.604489	2.936016	-0.661267	C	4.443945	-2.049866	-0.642548
C	-0.604633	3.558802	-0.667526	H	2.771818	-2.107329	-1.977161
C	-1.734179	2.819843	-0.341604	C	4.874060	-1.801303	0.652472
C	-2.968719	3.507378	-0.187431	H	4.284226	-1.191072	2.621453
C	-4.095297	2.847751	0.145923	H	5.150937	-2.365783	-1.400415
C	-4.185039	-2.764468	0.196711	H	5.917482	-1.924492	0.915457
C	-3.078266	-3.466707	-0.115933	C	2.242088	1.399373	-0.131682
H	-6.165948	1.315220	0.706233	C	3.143111	1.195601	-1.167384
H	-6.206683	-1.155675	0.725735	C	2.729953	1.837183	1.099554
H	-0.825744	-4.665822	-0.742266	C	4.500486	1.401203	-0.971314
H	1.394921	-3.638869	-0.685787	H	2.776565	0.886154	-2.138430
H	1.500962	3.514713	-0.840829	C	4.083467	2.047666	1.296035
H	-0.688606	4.619877	-0.869410	H	2.027539	2.039572	1.899691
H	-2.967748	4.581877	-0.328548	C	4.975858	1.833301	0.256733
H	-5.035045	3.368079	0.288773	H	5.189830	1.228620	-1.789141
H	-5.141613	-3.251591	0.344827	H	4.440281	2.390825	2.259877
H	-3.110965	-4.543457	-0.234263	H	6.035841	2.002328	0.401801

PAH8$_{H,H}^{‡}$

C	2.939284	-1.041829	-0.448074	C	-3.645780	1.215798	-0.707612
C	1.603910	-0.665456	-0.078999	C	-3.893023	-0.090135	-0.886547
C	0.747850	-1.726411	0.367168	C	-2.939285	-1.041826	-0.448073
C	1.361029	-2.940111	0.669796	C	-1.603911	-0.665455	-0.078998
C	2.672770	-3.266538	0.362197	C	-3.433500	-2.342596	-0.284738
C	3.433497	-2.342600	-0.284739	C	-2.672773	-3.266535	0.362198
C	3.893023	-0.090139	-0.886548	C	-1.361032	-2.940109	0.669797
C	3.645781	1.215795	-0.707612	C	-0.747852	-1.726410	0.367168
C	2.397894	1.641231	-0.190117	H	0.796356	-3.734449	1.120551
C	1.296192	0.757181	-0.032264	H	3.053132	-4.251428	0.602235
C	2.340428	2.997763	0.192845	H	4.446353	-2.557252	-0.602829
C	1.185291	3.518473	0.642259	H	4.848904	-0.445411	-1.251496
C	0.000001	2.756948	0.543522	H	4.395468	1.969520	-0.916561
C	0.000001	1.371155	0.205613	H	3.244696	3.590679	0.127514
C	-1.185287	3.518475	0.642258	H	1.112698	4.549984	0.964263
C	-2.340425	2.997765	0.192844	H	-1.112693	4.549985	0.964262
C	-2.397892	1.641234	-0.190117	H	-3.244692	3.590683	0.127513
C	-1.296191	0.757183	-0.032264	H	-4.395466	1.969525	-0.916561

H	-4.848905	-0.445406	-1.251495	H	-3.053136	-4.251424	0.602236
H	-4.446355	-2.557247	-0.602828	H	-0.796359	-3.734448	1.120552

PAH8$_{F,H}^{‡}$

C	-2.450910	-1.844618	0.570711	C	2.929491	0.234968	0.745380
C	-1.346968	-1.034490	0.153381	C	1.609916	0.084093	0.217536
C	-0.182590	-1.735267	-0.325782	C	3.844246	-0.827190	0.778829
C	-0.364174	-3.075578	-0.661192	C	3.553176	-1.964325	0.100730
C	-1.475794	-3.830594	-0.304944	C	2.288378	-2.100287	-0.452232
C	-2.469390	-3.238093	0.408095	C	1.215042	-1.222234	-0.260443
C	-3.659996	-1.274483	1.041750	H	0.411787	-3.608210	-1.166663
C	-3.898333	0.030608	0.833535	H	-1.510102	-4.881341	-0.563979
C	-2.903075	0.847168	0.244959	H	-3.327926	-3.792825	0.766629
C	-1.569168	0.396022	0.065519	H	-4.416918	-1.933297	1.449587
C	-3.332483	2.114834	-0.205088	H	-4.859382	0.475957	1.061348
C	-2.449872	2.965743	-0.760647	H	-4.382830	2.364584	-0.115156
C	-1.069327	2.671680	-0.689029	H	-2.755331	3.930265	-1.147281
C	-0.581767	1.406836	-0.256768	H	-0.633823	4.687088	-1.310864
C	-0.214575	3.776543	-0.900638	H	1.691614	4.597141	-0.446788
C	1.047461	3.726133	-0.436181	H	3.268334	3.592998	0.843803
C	1.557824	2.522455	0.097124	H	4.434453	1.529243	1.585130
C	0.835842	1.300854	0.020992	H	4.812955	-0.676013	1.237541
C	2.828588	2.611635	0.713406	H	4.258557	-2.773283	-0.033206
C	3.461386	1.496106	1.110700	F	2.188869	-3.232297	-1.174121

PAH8$_{Cl,H}^{‡}$

C	0.916780	-2.911289	-0.634852	C	-0.303477	3.874481	-0.632995
C	0.568942	-1.587766	-0.217138	C	-1.407702	3.412012	-1.243567
C	-0.787145	-1.392094	0.238133	C	-1.819409	2.078917	-0.996298
C	-1.478004	-2.544177	0.589000	C	-0.980193	1.123519	-0.351565
C	-1.085492	-3.836250	0.256517	C	-3.169582	1.808265	-1.251300
C	0.055429	-4.006241	-0.462739	C	-3.754436	0.772390	-0.601293
C	2.214890	-3.222979	-1.111392	C	-2.972369	-0.111347	0.143820
C	3.223420	-2.359544	-0.901127	C	-1.561843	-0.125966	0.089672
C	2.966885	-1.113396	-0.281474	H	-2.421058	-2.460643	1.084508
C	1.646431	-0.631751	-0.094433	H	-1.717840	-4.671869	0.528854
C	4.091524	-0.415984	0.214142	H	0.371804	-4.979728	-0.817275
C	3.928744	0.759632	0.851594	H	2.388499	-4.208274	-1.526734
C	2.668089	1.398797	0.814371	H	4.249150	-2.616831	-1.136875
C	1.510297	0.753289	0.301043	H	5.068648	-0.871132	0.105243
C	2.671134	2.771949	1.145275	H	4.766568	1.290565	1.286833
C	1.666544	3.552996	0.702564	H	3.546785	3.190619	1.626111
C	0.559147	2.977626	0.041718	H	1.701133	4.631285	0.802813
C	0.359337	1.571837	0.008098	H	-0.033816	4.923327	-0.661740

H	-2.071339	4.064642	-1.797187	H	-4.825833	0.628104	-0.613248
H	-3.757076	2.513299	-1.825429	Cl	-4.005430	-1.092004	1.153649

PAH8$_{Br,H}^{‡}$

C	-0.832122	-2.993390	0.717539	C	0.941175	2.402487	1.204910
C	-0.688348	-1.630193	0.306709	C	0.347535	1.309502	0.508219
C	0.644982	-1.201938	-0.043001	C	2.281754	2.365615	1.605648
C	1.550280	-2.214942	-0.320597	C	3.100014	1.442517	1.040384
C	1.363527	-3.556445	-0.006345	C	2.561966	0.437194	0.236168
C	0.216203	-3.922334	0.624904	C	1.176746	0.178443	0.152626
C	-2.088556	-3.522907	1.105188	H	2.502899	-1.967768	-0.738449
C	-3.212862	-2.846421	0.812716	H	2.151324	-4.268500	-0.217565
C	-3.130393	-1.578964	0.188579	H	0.046988	-4.935825	0.967957
C	-1.902358	-0.878259	0.084994	H	-2.119892	-4.522131	1.522370
C	-4.317959	-1.092044	-0.402873	H	-4.193267	-3.275678	0.981328
C	-4.309886	0.082382	-1.063097	H	-5.208852	-1.706294	-0.350125
C	-3.182053	0.928771	-0.958588	H	-5.190588	0.453110	-1.573207
C	-1.975442	0.502911	-0.339352	H	-4.281068	2.524311	-1.900789
C	-3.388871	2.272638	-1.340515	H	-2.774489	4.277960	-0.998590
C	-2.567676	3.224170	-0.854645	H	-1.251368	4.894945	0.596842
C	-1.439949	2.862411	-0.085733	H	0.772571	4.415788	1.958063
C	-1.009820	1.512724	0.015478	H	2.679253	3.163265	2.220236
C	-0.808535	3.906861	0.631858	H	4.172250	1.493632	1.167463
C	0.288435	3.650132	1.364640	Br	3.988868	-0.357972	-0.766572

PAH8$_{I,H}^{‡}$

C	-1.123734	-3.002651	0.753747	C	-1.302997	3.904835	0.602341
C	-1.004823	-1.633211	0.354448	C	-0.254761	3.687376	1.414971
C	0.329393	-1.160421	0.075290	C	0.437116	2.453958	1.323025
C	1.279114	-2.141060	-0.157291	C	-0.075894	1.338693	0.597862
C	1.122196	-3.490762	0.134771	C	1.742110	2.449427	1.826202
C	-0.043568	-3.897782	0.704995	C	2.625300	1.546131	1.326819
C	-2.378813	-3.570644	1.087424	C	2.180559	0.525158	0.483505
C	-3.510134	-2.925410	0.753902	C	0.809123	0.234177	0.305864
C	-3.440134	-1.655979	0.132049	H	2.246048	-1.861088	-0.520613
C	-2.230125	-0.919836	0.076384	H	1.943227	-4.174522	-0.040288
C	-4.615567	-1.207108	-0.511720	H	-0.196659	-4.918459	1.034016
C	-4.610879	-0.041027	-1.186700	H	-2.397598	-4.572046	1.500138
C	-3.510953	0.836744	-1.048629	H	-4.483421	-3.383343	0.883880
C	-2.323399	0.454360	-0.366898	H	-5.490828	-1.845209	-0.489297
C	-3.731855	2.166640	-1.468903	H	-5.478446	0.298575	-1.739249
C	-2.956930	3.148723	-0.967442	H	-4.602416	2.384147	-2.075613
C	-1.862927	2.831842	-0.133094	H	-3.181664	4.193628	-1.145358
C	-1.405771	1.496035	0.018919	H	-1.765803	4.880833	0.519238

H	0.167405	4.473921	2.028056	H	3.681230	1.636456	1.540616
H	2.073122	3.258157	2.465463	I	3.881116	-0.210753	-0.558031

PAH8$_{F,F}^{‡}$

C	-0.646804	2.804268	0.880859	C	-0.645893	-2.804445	0.882670
C	-0.338900	1.547248	0.282497	C	-0.338297	-1.547619	0.283632
C	-1.428686	0.746691	-0.248170	C	-1.958227	-3.300263	0.923896
C	-2.587278	1.497025	-0.481791	C	-2.895565	-2.699497	0.152213
C	-2.896507	2.698058	0.150770	C	-2.586678	-1.498690	-0.480924
C	-1.959363	3.299509	0.922172	C	-1.428337	-0.747843	-0.247739
C	0.359331	3.715748	1.287131	H	-3.885607	3.106635	-0.007403
C	1.618646	3.541458	0.848856	H	-2.163544	4.225348	1.444495
C	1.960659	2.363370	0.144609	H	0.060311	4.610325	1.819600
C	1.063179	1.269994	0.038528	H	2.384822	4.291231	1.004812
C	3.238596	2.329738	-0.458701	H	3.838356	3.231894	-0.439932
C	3.687777	1.197716	-1.035785	H	4.660240	1.149377	-1.510388
C	2.958239	-0.000046	-0.855036	H	4.661361	-1.149516	-1.507425
C	1.640121	0.000012	-0.330242	H	3.840904	-3.230314	-0.432507
C	3.688838	-1.197598	-1.032920	H	2.386887	-4.288671	1.012057
C	3.240419	-2.328690	-0.453457	H	0.061443	-4.609270	1.823512
C	1.962074	-2.362226	0.149043	H	-2.162114	-4.225872	1.446739
C	1.063795	-1.269737	0.040502	H	-3.884570	-3.108395	-0.005725
C	1.620246	-3.539759	0.854264	F	-3.551826	-1.120749	-1.315931
C	0.360437	-3.714836	1.290789	F	-3.552300	1.118393	-1.316651

PAH8$_{F,Cl}^{‡}$

C	0.399064	2.885219	0.919402	C	0.706600	-3.860046	0.754102
C	0.312959	1.580767	0.350085	C	-0.422129	-3.618091	1.446392
C	-0.977742	1.127294	-0.144677	C	-1.137215	-2.420074	1.197276
C	-1.840340	2.186623	-0.422625	C	-0.582080	-1.340473	0.456529
C	-1.766525	3.455347	0.144760	C	-2.497091	-2.430938	1.536279
C	-0.695937	3.764692	0.916803	C	-3.328709	-1.625338	0.830988
C	1.632805	3.440670	1.339915	C	-2.817109	-0.665565	-0.050694
C	2.785092	2.874742	0.935226	C	-1.454822	-0.282872	-0.019881
C	2.753500	1.659369	0.213271	H	-2.580575	4.141486	-0.046820
C	1.561612	0.903451	0.087913	H	-0.609326	4.724986	1.408803
C	3.950630	1.253946	-0.422729	H	1.619123	4.390698	1.860180
C	4.003327	0.085675	-1.094207	H	3.743173	3.348963	1.110693
C	2.931891	-0.830192	-0.970215	H	4.807283	1.915453	-0.372256
C	1.706253	-0.458967	-0.362071	H	4.899881	-0.229057	-1.614381
C	3.216059	-2.176478	-1.293412	H	4.121517	-2.402566	-1.843313
C	2.455177	-3.151857	-0.754375	H	2.729745	-4.196243	-0.844392
C	1.298863	-2.826066	-0.009977	H	1.197354	-4.825385	0.784819
C	0.792920	-1.501757	0.015737	H	-0.882453	-4.374716	2.069782

H	-2.882386	-3.194071	2.200389	Cl	-4.045205	-0.207642	-1.188449
H	-4.402447	-1.744005	0.879271	F	-2.878573	2.054046	-1.240629

PAH8$_{F,Br}$‡

C	1.067084	2.881498	0.915518	C	-0.823644	-2.293733	1.462611
C	0.832895	1.572643	0.399306	C	-0.274817	-1.267191	0.645956
C	-0.527776	1.212379	0.035538	C	-2.116815	-2.170109	1.986135
C	-1.328300	2.325562	-0.201152	C	-2.960660	-1.294708	1.382792
C	-1.106111	3.604677	0.298617	C	-2.492275	-0.403492	0.410553
C	0.050210	3.849320	0.963605	C	-1.107582	-0.145645	0.256460
C	2.370099	3.339250	1.231187	H	-1.878164	4.347802	0.151217
C	3.439702	2.663777	0.770874	H	0.255492	4.814651	1.408320
C	3.254382	1.443588	0.080837	H	2.473722	4.300143	1.720474
C	1.996943	0.791521	0.055191	H	4.444477	3.056606	0.869337
C	4.361453	0.933759	-0.638220	H	5.274614	1.516685	-0.654739
C	4.257862	-0.229373	-1.312685	H	5.079833	-0.617739	-1.901756
C	3.120401	-1.046776	-1.111342	H	4.080586	-2.702557	-2.103845
C	1.987241	-0.577421	-0.399923	H	2.616666	-4.382176	-1.014530
C	3.249871	-2.406070	-1.475058	H	1.205219	-4.899628	0.757388
C	2.449202	-3.319279	-0.886326	H	-0.644837	-4.273976	2.296073
C	1.403306	-2.904997	-0.031363	H	-2.478640	-2.888598	2.710594
C	1.025195	-1.541202	0.055098	H	-4.022726	-1.321535	1.583403
C	0.806814	-3.892700	0.789490	Br	-3.965898	0.084170	-0.702086
C	-0.198466	-3.556105	1.619075	F	-2.452326	2.231344	-0.901670

PAH8$_{F,I}$‡

C	1.496139	2.891149	0.874124	C	1.084736	-3.910453	0.754164
C	1.223330	1.571295	0.405249	C	0.155875	-3.559010	1.663000
C	-0.157107	1.223095	0.118218	C	-0.432652	-2.272328	1.579681
C	-0.956272	2.336560	-0.104987	C	0.080620	-1.253326	0.730612
C	-0.694004	3.630562	0.329494	C	-1.663563	-2.100249	2.222779
C	0.498227	3.878285	0.927927	C	-2.528201	-1.189550	1.702580
C	2.816282	3.329397	1.141984	C	-2.129166	-0.318430	0.680563
C	3.859913	2.615620	0.679805	C	-0.751394	-0.114779	0.405920
C	3.631127	1.386955	0.018196	H	-1.462699	4.379692	0.196148
C	2.359511	0.763011	0.034326	H	0.739027	4.854623	1.328649
C	4.706253	0.847894	-0.727744	H	2.952960	4.301139	1.600820
C	4.551157	-0.306838	-1.406542	H	4.875286	2.987209	0.747041
C	3.396034	-1.093205	-1.183063	H	5.633672	1.406575	-0.768219
C	2.301537	-0.604467	-0.424687	H	5.344342	-0.712277	-2.022956
C	3.468280	-2.446280	-1.582513	H	4.266532	-2.753341	-2.247258
C	2.657363	-3.348247	-0.989981	H	2.784054	-4.412194	-1.151809
C	1.664220	-2.922851	-0.080016	H	1.444529	-4.929107	0.673152
C	1.334745	-1.550381	0.055081	H	-0.262866	-4.275651	2.358668

H	-1.984827	-2.808435	2.976136	I	-3.875611	0.119342	-0.446432
H	-3.564189	-1.187167	2.012509	F	-2.128225	2.216424	-0.720891

PAH8$_{Cl,Cl}$‡

C	0.210845	-2.697521	1.226131	C	0.210839	2.697524	1.226129
C	-0.001540	-1.501495	0.487182	C	-0.001543	1.501496	0.487181
C	1.147765	-0.746852	0.008907	C	1.510740	3.140544	1.512984
C	2.303406	-1.549723	-0.089502	C	2.522267	2.640685	0.759497
C	2.522273	-2.640678	0.759499	C	2.303403	1.549728	-0.089503
C	1.510746	-3.140538	1.512987	C	1.147764	0.746855	0.008906
C	-0.841240	-3.600868	1.517894	H	3.502673	-3.097187	0.752214
C	-2.008305	-3.485854	0.854209	H	1.661990	-3.986404	2.171271
C	-2.250335	-2.349072	0.047674	H	-0.628619	-4.454120	2.150245
C	-1.353362	-1.253299	0.034748	H	-2.777196	-4.246072	0.922067
C	-3.430250	-2.329841	-0.732831	H	-4.026820	-3.233189	-0.781391
C	-3.805569	-1.206137	-1.380684	H	-4.708612	-1.172533	-1.978025
C	-3.113793	-0.000003	-1.119654	H	-4.708615	1.172523	-1.978026
C	-1.876246	-0.000002	-0.432001	H	-4.026827	3.233181	-0.781393
C	-3.805571	1.206129	-1.380685	H	-2.777205	4.246068	0.922064
C	-3.430255	2.329834	-0.732833	H	-0.628629	4.454121	2.150242
C	-2.250340	2.349068	0.047672	H	1.661982	3.986410	2.171267
C	-1.353365	1.253297	0.034747	H	3.502666	3.097197	0.752212
C	-2.008312	3.485851	0.854206	Cl	3.533863	1.461563	-1.299227
C	-0.841248	3.600869	1.517891	Cl	3.533866	-1.461556	-1.299226

PAH8$_{Cl,Br}$‡

C	0.877141	2.773578	1.195221	C	1.461659	-3.804399	0.875804
C	0.744619	1.533076	0.512035	C	0.404516	-3.596781	1.685481
C	-0.584432	1.070613	0.139116	C	-0.402496	-2.449304	1.484383
C	-1.505040	2.130447	0.042736	C	0.008491	-1.370492	0.655195
C	-1.394706	3.291476	0.815381	C	-1.717254	-2.511102	1.967239
C	-0.250718	3.552234	1.497156	C	-2.659847	-1.793793	1.302075
C	2.138531	3.381522	1.411848	C	-2.290173	-0.852110	0.335351
C	3.208017	2.943598	0.718531	C	-0.964363	-0.369435	0.246280
C	3.108851	1.766658	-0.059662	H	-2.227922	3.980965	0.816156
C	1.960457	0.940939	0.002284	H	-0.146907	4.440224	2.107428
C	4.194822	1.437197	-0.905293	H	2.181090	4.281989	2.012294
C	4.217425	0.259667	-1.565647	H	4.149850	3.478900	0.731018
C	3.249546	-0.723733	-1.251626	H	5.003367	2.152124	-1.002240
C	2.109427	-0.406190	-0.474726	H	5.038221	-0.005347	-2.221028
C	3.572073	-2.065812	-1.560192	H	4.401054	-2.264655	-2.228540
C	2.964525	-3.059340	-0.875905	H	3.294519	-4.087609	-0.965994
C	1.899097	-2.774138	0.009666	H	2.005338	-4.741486	0.881209
C	1.322847	-1.481458	0.056794	H	0.061713	-4.354467	2.379318

H	-1.992633	-3.257308	2.701487	Br	-3.725849	-0.641057	-0.895540
H	-3.713520	-1.986470	1.450736	Cl	-2.803916	2.243025	-1.082634

PAH8$_{Cl,I}$‡

C	1.444727	2.780329	1.120120	C	-0.175264	-2.348189	1.598304
C	1.210153	1.523666	0.494144	C	0.258689	-1.315479	0.723168
C	-0.158300	1.148935	0.171311	C	-1.425557	-2.256574	2.222625
C	-0.997650	2.264973	0.036861	C	-2.356697	-1.454150	1.638974
C	-0.781752	3.466619	0.717726	C	-2.011623	-0.588712	0.592819
C	0.389614	3.670999	1.372496	C	-0.653782	-0.245343	0.367070
C	2.753888	3.280081	1.328636	H	-1.558486	4.218460	0.685668
C	3.787403	2.718660	0.670671	H	0.574636	4.581328	1.928256
C	3.585275	1.538998	-0.082727	H	2.872250	4.196126	1.894451
C	2.367000	0.821790	-0.009706	H	4.774509	3.165131	0.680020
C	4.631604	1.110737	-0.934621	H	5.504719	1.745132	-1.031795
C	4.530622	-0.051603	-1.613839	H	5.313388	-0.384060	-2.284859
C	3.471668	-0.939560	-1.308324	H	4.432391	-2.557419	-2.362923
C	2.384164	-0.530926	-0.498458	H	3.173135	-4.297810	-1.127767
C	3.645161	-2.296271	-1.666116	H	1.918180	-4.867350	0.770565
C	2.954104	-3.244647	-0.996305	H	0.164597	-4.304059	2.439005
C	1.959556	-2.879702	-0.060062	H	-1.698914	-2.957105	3.001453
C	1.518716	-1.537686	0.040596	H	-3.399178	-1.544417	1.912966
C	1.476311	-3.879322	0.818977	I	-3.707784	-0.477385	-0.676556
C	0.521061	-3.576459	1.720333	Cl	-2.345671	2.348415	-1.023932

PAH8$_{Br,Br}$‡

C	-0.533163	-2.681331	1.435314	C	-2.672540	3.481223	0.750599
C	-0.639355	-1.495353	0.658420	C	-1.613645	3.586863	1.577926
C	0.564996	-0.746333	0.332879	C	-0.533031	2.681334	1.435312
C	1.721578	-1.550406	0.405348	C	-0.639287	1.495356	0.658425
C	1.821403	-2.618451	1.302858	C	0.713074	3.106700	1.918405
C	0.712910	-3.106718	1.918472	C	1.821527	2.618390	1.302758
C	-1.613804	-3.586835	1.577875	C	1.721644	1.550313	0.405292
C	-2.672662	-3.481163	0.750504	C	0.565030	0.746285	0.332868
C	-2.802257	-2.348791	-0.087938	H	2.788885	-3.080880	1.443298
C	-1.914410	-1.251433	0.020205	H	0.772571	-3.938162	2.609074
C	-3.863558	-2.331019	-1.023573	H	-1.493358	-4.434479	2.241273
C	-4.149161	-1.207313	-1.716492	H	-3.440639	-4.244412	0.712143
C	-3.500889	0.000071	-1.364884	H	-4.447061	-3.234939	-1.153264
C	-2.368242	0.000041	-0.515937	H	-4.962893	-1.175476	-2.430850
C	-4.149135	1.207483	-1.716441	H	-4.962873	1.175692	-2.430796
C	-3.863502	2.331155	-1.023480	H	-4.446985	3.235094	-1.153132
C	-2.802186	2.348871	-0.087860	H	-3.440500	4.244491	0.712277
C	-1.914366	1.251486	0.020239	H	-1.493149	4.434498	2.241326

H	0.772784	3.938156	2.608988	Br	3.195388	1.578173	-0.786739
H	2.789030	3.080788	1.443156	Br	3.195299	-1.578413	-0.786712

PAH8$_{Br,I}^{‡}$

C	-1.280522	-2.714734	1.351652	C	-0.426876	2.576539	1.564615
C	-1.184943	-1.491699	0.631045	C	-0.675795	1.453780	0.728856
C	0.132311	-0.944375	0.342940	C	0.813738	2.716441	2.200450
C	1.129534	-1.935214	0.354847	C	1.870006	2.050634	1.658910
C	1.046206	-3.074394	1.160015	C	1.678694	1.086696	0.661279
C	-0.125932	-3.393464	1.769353	C	0.398852	0.520174	0.444744
C	-2.509701	-3.404135	1.498186	H	1.918127	-3.707959	1.248869
C	-3.551662	-3.067170	0.712206	H	-0.210928	-4.264375	2.406618
C	-3.475971	-1.914276	-0.103997	H	-2.535803	-4.284619	2.128479
C	-2.395194	-1.007206	0.008103	H	-4.452527	-3.668085	0.677621
C	-4.513082	-1.693729	-1.041681	H	-5.262704	-2.466196	-1.166932
C	-4.561391	-0.548360	-1.755545	H	-5.344029	-0.368392	-2.482602
C	-3.686909	0.511683	-1.417334	H	-4.846577	1.928645	-2.558169
C	-2.595397	0.305995	-0.539503	H	-3.961436	3.875645	-1.307622
C	-4.064715	1.814556	-1.817108	H	-2.885162	4.691265	0.615212
C	-3.577350	2.876499	-1.138432	H	-1.097300	4.478293	2.326785
C	-2.578355	2.701740	-0.152701	H	0.959429	3.485490	2.948346
C	-1.930370	1.452946	0.004935	H	2.881711	2.321524	1.929560
C	-2.289959	3.790454	0.705282	I	3.373685	1.153955	-0.601727
C	-1.316191	3.677846	1.630806	Br	2.607316	-2.045279	-0.813872

PAH8$_{I,I}^{‡}$

C	-1.096412	-2.670225	1.504324	C	-3.179773	3.481930	0.674159
C	-1.152825	-1.491477	0.710407	C	-2.180164	3.580709	1.573553
C	0.067913	-0.745565	0.458064	C	-1.096596	2.670238	1.504385
C	1.224704	-1.539695	0.616068	C	-1.152921	1.491508	0.710438
C	1.261932	-2.588219	1.541693	C	0.112675	3.072810	2.087701
C	0.112892	-3.072734	2.087609	C	1.261755	2.588381	1.541793
C	-2.179921	-3.580767	1.573483	C	1.224612	1.539882	0.616134
C	-3.179545	-3.482030	0.674101	C	0.067871	0.745681	0.458087
C	-3.259959	-2.350660	-0.172564	H	2.213369	-3.053570	1.761847
C	-2.384333	-1.250804	-0.009115	H	0.129223	-3.891400	2.795780
C	-4.261912	-2.333328	-1.171442	H	-2.103167	-4.425396	2.247140
C	-4.508441	-1.208375	-1.877947	H	-3.939676	-4.249042	0.585844
C	-3.884481	-0.000053	-1.487771	H	-4.834569	-3.238119	-1.338321
C	-2.804803	-0.000026	-0.572245	H	-5.278313	-1.177382	-2.639434
C	-4.508514	1.208235	-1.877932	H	-5.278383	1.177205	-2.639420
C	-4.262055	2.333193	-1.171410	H	-4.834768	3.237950	-1.338276
C	-3.260107	2.350572	-0.172529	H	-3.939953	4.248894	0.585912
C	-2.384410	1.250769	-0.009096	H	-2.103470	4.425327	2.247232

H	0.128940	3.891461	2.795889	I	2.872653	1.734681	-0.676966
H	2.213158	3.053786	1.761976	I	2.872711	-1.734322	-0.677093

PAH8$_{Me,H}^{‡}$

C	2.211049	-2.103264	-0.514825	C	-3.807376	-0.373904	-0.981826
C	1.214935	-1.153660	-0.121031	C	-3.695105	-1.522743	-0.269011
C	-0.017467	-1.690448	0.405123	C	-2.532009	-1.842689	0.442305
C	0.040061	-3.011742	0.831152	C	-1.363745	-1.058558	0.272767
C	1.062702	-3.904680	0.529746	H	0.994478	-4.930528	0.869962
C	2.091343	-3.476194	-0.248903	H	2.874976	-4.143902	-0.585567
C	3.449951	-1.693800	-1.068770	H	4.114794	-2.453143	-1.462399
C	3.833428	-0.410422	-0.957975	H	4.823216	-0.086279	-1.256814
C	2.967059	0.535851	-0.360617	H	4.616693	1.896514	-0.128464
C	1.605385	0.239261	-0.098284	H	3.242457	3.619668	1.013590
C	3.554684	1.758421	0.035642	H	1.207199	4.575143	1.392571
C	2.808519	2.695575	0.651430	H	-1.161347	4.742370	0.669577
C	1.402458	2.549547	0.685765	H	-2.844463	3.971315	-0.673231
C	0.756779	1.353170	0.268491	H	-4.142737	2.087466	-1.646091
C	0.676670	3.723551	0.984290	H	-4.711956	-0.130589	-1.525253
C	-0.610540	3.812139	0.595685	H	-4.530373	-2.211486	-0.215726
C	-1.258447	2.694497	0.026525	C	-2.757582	-3.021754	1.359415
C	-0.666667	1.403307	0.036619	H	-2.484969	-3.984863	0.918752
C	-2.501421	2.945924	-0.604478	H	-2.246435	-2.918368	2.316417
C	-3.205460	1.928074	-1.127094	H	-3.825323	-3.068468	1.577499
C	-2.814158	0.598676	-0.827935	H	-0.778115	-3.426494	1.373078
C	-1.562437	0.282694	-0.223201				

PAH8$_{tBu,H}^{‡}$

C	-0.836374	2.997331	-0.554658	C	-0.990699	-1.522007	0.078531
C	-0.704026	1.613670	-0.216445	C	-0.683600	-3.937121	-0.391982
C	0.603756	1.177205	0.216490	C	0.347225	-3.660648	-1.211077
C	1.442149	2.181372	0.668185	C	0.927089	-2.367352	-1.171924
C	1.242064	3.543973	0.465649	C	0.354786	-1.292321	-0.436552
C	0.163247	3.939243	-0.261878	C	2.194388	-2.217272	-1.737271
C	-2.046819	3.514765	-1.079900	C	3.012006	-1.260237	-1.222433
C	-3.177234	2.790318	-0.992203	C	2.590887	-0.346465	-0.248251
C	-3.143374	1.506880	-0.396778	C	1.182190	-0.168446	-0.086183
C	-1.920005	0.838513	-0.146682	H	1.979178	4.252561	0.823051
C	-4.381035	0.985020	0.047494	H	0.005173	4.973779	-0.541399
C	-4.413561	-0.162622	0.753776	H	-2.055420	4.535712	-1.442507
C	-3.251685	-0.965580	0.835875	H	-4.136838	3.200871	-1.283158
C	-2.004661	-0.531337	0.310373	H	-5.278822	1.564135	-0.132800
C	-3.432659	-2.282939	1.309060	H	-5.336668	-0.543890	1.173562
C	-2.522771	-3.227552	0.990060	H	-4.362370	-2.536462	1.804066
C	-1.366673	-2.878183	0.259580	H	-2.695359	-4.274247	1.211554

H	-1.064531	-4.944537	-0.274333	H	4.054765	0.924264	2.637699
H	0.835004	-4.429470	-1.797974	C	4.953998	-0.754802	0.594030
H	2.567132	-2.959575	-2.432451	H	5.509634	-0.766987	-0.343524
H	4.050537	-1.258958	-1.518006	H	5.652205	-0.430341	1.369189
H	2.361084	1.913992	1.134195	H	4.637762	-1.772133	0.827886
C	3.761013	0.227369	0.591389	C	4.361237	1.524445	0.013028
C	3.374851	0.267279	2.089625	H	5.146606	1.896545	0.676310
H	2.354921	0.572759	2.302931	H	4.824614	1.294893	-0.948716
H	3.482625	-0.736047	2.505494	H	3.654520	2.328140	-0.164640

PAH8$_{Ph,H}^{‡}$

C	-0.723912	3.016744	-0.712269	C	0.808478	-0.439065	-0.306591
C	-0.760719	1.639145	-0.321935	H	2.483077	3.804816	-0.002376
C	0.511413	1.007962	-0.074628	H	0.417207	4.810538	-1.004493
C	1.584526	1.865665	0.129785	H	-1.813570	4.731634	-1.429699
C	1.580598	3.226051	-0.154079	H	-4.016845	3.788798	-0.796374
C	0.455803	3.775881	-0.685794	H	-5.182581	2.376312	0.569166
C	-1.907395	3.731740	-1.023463	H	-5.419387	0.237116	1.805537
C	-3.101911	3.219936	-0.681117	H	-4.802654	-1.931776	2.125047
C	-3.174492	1.945277	-0.069706	H	-3.610392	-3.900453	1.196909
C	-2.059620	1.069904	-0.031261	H	-2.275748	-4.762425	-0.447244
C	-4.390751	1.636920	0.580594	H	-0.298238	-4.603536	-1.942964
C	-4.521559	0.474369	1.247864	H	1.724524	-3.621258	-2.394791
C	-3.535593	-0.527452	1.095644	H	3.505027	-2.131649	-1.533399
C	-2.314592	-0.287996	0.405696	H	2.522810	1.469313	0.456615
C	-3.913900	-1.821374	1.515666	C	3.362309	-0.307910	0.172164
C	-3.263603	-2.890173	1.014725	C	3.462835	-0.397201	1.561559
C	-2.140833	-2.707293	0.179405	C	4.463744	0.149270	-0.549458
C	-1.531340	-1.435238	0.016988	C	4.622373	-0.010163	2.211416
C	-1.703248	-3.847229	-0.539663	H	2.615551	-0.768049	2.125951
C	-0.631147	-3.763833	-1.345294	C	5.621846	0.542227	0.102764
C	0.194073	-2.613192	-1.273918	H	4.396272	0.221435	-1.628553
C	-0.195187	-1.435434	-0.566612	C	5.704959	0.467470	1.485341
C	1.488680	-2.759387	-1.782975	H	4.683096	-0.085887	3.290461
C	2.461839	-1.928943	-1.325187	H	6.463002	0.910312	-0.472461
C	2.152775	-0.840781	-0.501672	H	6.610737	0.772997	1.994462

PAH8$_{Me,Me}^{‡}$

C	0.611200	2.696452	-1.019517	C	-0.398866	3.602432	-1.430492
C	0.313043	1.499666	-0.311805	C	-1.636118	3.487841	-0.909359
C	1.400618	0.750597	0.293947	C	-1.973043	2.349775	-0.138241
C	2.555403	1.523561	0.547708	C	-1.083464	1.254059	-0.020620
C	2.841476	2.625831	-0.272259	C	-3.237443	2.330395	0.495703
C	1.936387	3.136029	-1.146137	C	-3.688171	1.206142	1.093154

C	-2.970242	0.000133	0.915934	H	-2.391702	4.248313	-1.067316
C	-1.659036	0.000073	0.379714	H	-3.835634	3.233926	0.473213
C	-3.688329	-1.205799	1.093042	H	-4.656834	1.172019	1.577178
C	-3.237718	-2.330064	0.495529	H	-4.657004	-1.171591	1.577036
C	-1.973265	-2.349579	-0.138312	H	-3.836018	-3.233521	0.472953
C	-1.083565	-1.253971	-0.020605	H	-2.392040	-4.248089	-1.067391
C	-1.636373	-3.487722	-0.909328	H	-0.112819	-4.456910	-2.031688
C	-0.399021	-3.602554	-1.430167	H	2.166625	-3.986046	-1.775867
C	0.611093	-2.696695	-1.019044	H	3.810879	-3.098281	-0.153726
C	0.312954	-1.499756	-0.311576	C	3.523156	-1.425026	1.697983
C	1.936231	-3.136522	-1.145263	H	4.486354	-0.987846	1.442070
C	2.841198	-2.626301	-0.271267	H	3.111695	-0.912634	2.558193
C	2.555162	-1.523752	0.548338	H	3.722765	-2.450784	2.015409
C	1.400535	-0.750683	0.294166	C	3.523487	1.425150	1.697302
H	3.811265	3.097672	-0.155041	H	3.112658	0.911964	2.557305
H	2.166776	3.985387	-1.776968	H	4.487103	0.989063	1.441031
H	-0.112671	4.456686	-2.032161	H	3.722133	2.450956	2.015178

PAH8$_{tBu,tBu}$‡

C	0.814277	2.502840	1.591579	C	-0.763874	-0.583972	0.279169
C	0.774500	1.390812	0.713322	H	-2.355323	3.484817	1.374024
C	-0.516015	0.891454	0.250878	H	-0.393480	3.809247	2.828953
C	-1.491419	1.921589	0.201609	H	2.005565	4.000724	2.582784
C	-1.479850	2.859961	1.247490	H	3.980619	3.605616	1.135781
C	-0.391720	3.070427	2.037682	H	4.920360	2.569529	-0.790396
C	2.019816	3.198892	1.854144	H	5.109557	0.588530	-2.258743
C	3.097264	2.981550	1.067739	H	4.633166	-1.743433	-2.526774
C	3.087451	1.919967	0.131665	H	3.712541	-3.760983	-1.433008
C	2.017703	0.996516	0.100399	H	2.564083	-4.677799	0.458445
C	4.172658	1.784876	-0.769577	H	0.843793	-4.457783	2.238213
C	4.279846	0.699584	-1.570736	H	-1.163741	-3.262653	3.082194
C	3.403208	-0.395256	-1.371846	H	-3.114799	-2.252435	2.002112
C	2.263419	-0.258571	-0.548786	C	-3.182675	-1.610735	-0.509237
C	3.811339	-1.673697	-1.824019	C	-2.422053	2.259490	-0.964189
C	3.302619	-2.778408	-1.228613	C	-3.151602	-1.045346	-1.922179
C	2.265183	-2.670165	-0.270918	H	-2.162043	-1.169304	-2.363392
C	1.596451	-1.437283	-0.092612	H	-3.851352	-1.624078	-2.528759
C	1.976093	-3.774200	0.568419	H	-3.443955	-0.009934	-2.004686
C	1.033263	-3.658241	1.532049	C	-4.589388	-1.486509	0.095389
C	0.151224	-2.550889	1.507695	H	-5.333920	-1.668185	-0.682472
C	0.343009	-1.464886	0.621983	H	-4.759353	-2.230417	0.874077
C	-1.051747	-2.601765	2.232031	H	-4.790258	-0.509575	0.530839
C	-2.123276	-2.003530	1.645264	C	-2.930297	-3.126323	-0.740282
C	-2.035492	-1.226960	0.468818	H	-3.015252	-3.701449	0.179831

H	-3.664173	-3.505821	-1.455731	H	-1.454135	0.685807	-2.166978
H	-1.932472	-3.292711	-1.151019	H	-2.509221	1.768624	-3.086302
C	-3.878746	1.889521	-0.690944	H	-0.932291	2.314505	-2.509306
H	-4.500880	2.054350	-1.574748	C	-2.411607	3.787142	-1.177619
H	-3.997259	0.864862	-0.370207	H	-2.916707	4.003931	-2.122820
H	-4.266257	2.523969	0.109445	H	-2.939455	4.333373	-0.396230
C	-1.803038	1.706724	-2.254994	H	-1.392502	4.171018	-1.239756

PAH8$_{Ph,Ph}^{‡}$

C	-1.165337	2.698720	-1.500058	H	-4.739073	3.241143	1.548580
C	-1.187890	1.502428	-0.728614	H	-5.113637	1.169962	2.856413
C	0.035159	0.745551	-0.583463	H	-5.113637	-1.169962	2.856413
C	1.217801	1.490402	-0.818788	H	-4.739073	-3.241143	1.548580
C	1.182739	2.570294	-1.713654	H	-3.944498	-4.274539	-0.394641
C	0.008638	3.101582	-2.150015	H	-2.196083	-4.479344	-2.144476
C	-2.242446	3.620137	-1.486395	H	-0.012299	-3.950610	-2.821712
C	-3.194031	3.506386	-0.539088	H	2.123075	-3.037508	-1.977607
C	-3.236034	2.358225	0.289101	C	2.479995	-1.442056	-0.052649
C	-2.376727	1.256706	0.060032	C	2.399674	-1.545396	1.336044
C	-4.180425	2.335805	1.341581	C	3.727711	-1.598485	-0.655902
C	-4.388844	1.206075	2.052017	C	3.529762	-1.789887	2.096596
C	-3.789513	0.000000	1.619528	H	1.429930	-1.460420	1.811356
C	-2.766256	0.000000	0.638687	C	4.858423	-1.836264	0.103979
C	-4.388844	-1.206075	2.052017	H	3.811524	-1.514520	-1.733053
C	-4.180425	-2.335804	1.341581	C	4.764518	-1.939287	1.484615
C	-3.236034	-2.358225	0.289101	H	3.442675	-1.872640	3.173327
C	-2.376727	-1.256706	0.060033	H	5.820475	-1.939209	-0.383620
C	-3.194031	-3.506386	-0.539088	H	5.649095	-2.133025	2.078745
C	-2.242446	-3.620137	-1.486394	C	2.479995	1.442056	-0.052649
C	-1.165337	-2.698720	-1.500058	C	3.727711	1.598485	-0.655902
C	-1.187890	-1.502428	-0.728614	C	2.399674	1.545396	1.336044
C	0.008638	-3.101582	-2.150015	C	4.858423	1.836264	0.103979
C	1.182739	-2.570294	-1.713653	H	3.811524	1.514520	-1.733053
C	1.217801	-1.490402	-0.818788	C	3.529762	1.789887	2.096596
C	0.035159	-0.745551	-0.583463	H	1.429930	1.460420	1.811355
H	2.123075	3.037508	-1.977607	C	4.764518	1.939287	1.484615
H	-0.012299	3.950610	-2.821712	H	5.820475	1.939209	-0.383620
H	-2.196083	4.479344	-2.144476	H	3.442675	1.872640	3.173327
H	-3.944498	4.274540	-0.394641	H	5.649095	2.133025	2.078745