

Supporting Information

Bond analysis in *meta*-, and *para*-substituted thiophenols: overlap descriptors, local mode analysis, and QTAIM

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1 H–S–C–C dihedral profiles for OP/TOP descriptors

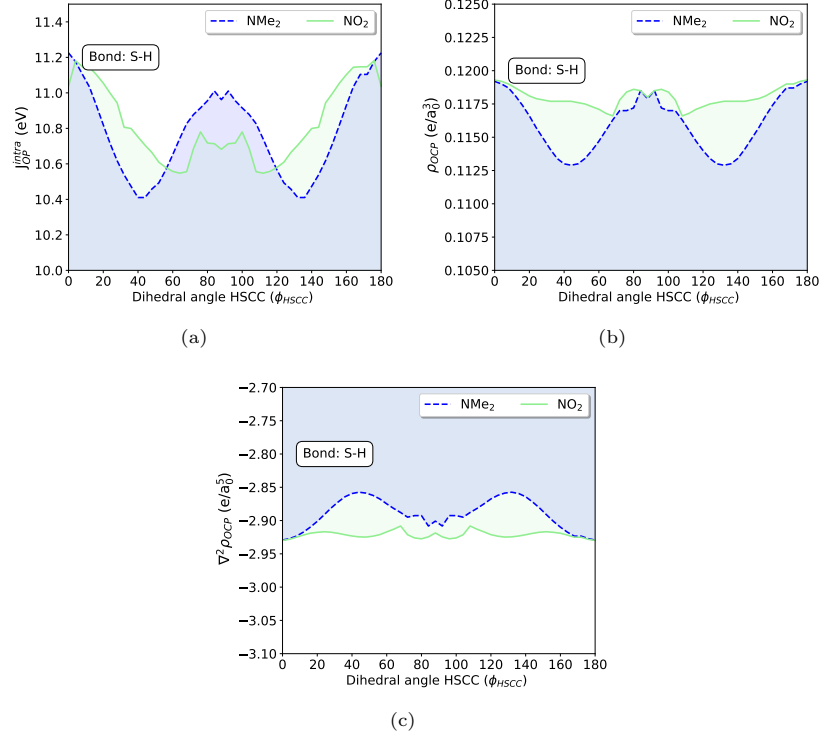


Fig. 1 Plots of intra-overlap repulsion J_{OP}^{intra} (in E_h)(a), overlap critical point density ρ_{OCP} (in e/a_0^3)(b), and Laplacian of ρ_{OCP} at OCP $\nabla^2 \rho_{OCP}$ (in e/a_0^5)(c) versus H–S–C–C dihedral angle for S–H bonds in *para*-substituted thiophenols.

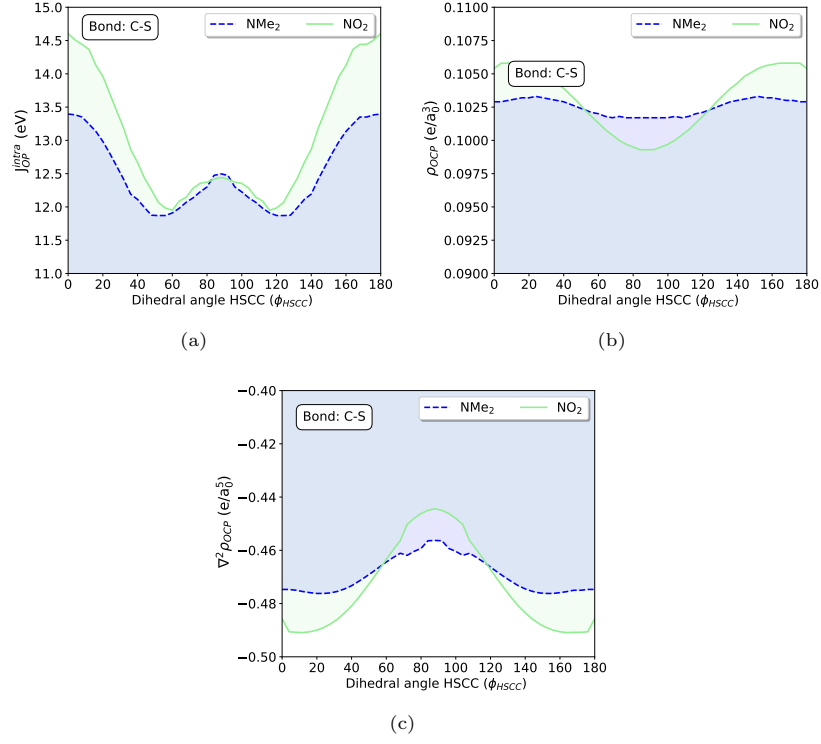


Fig. 2 Plots of intra-overlap repulsion J_{OCP}^{intra} (in E_h)(a), overlap critical point density ρ_{OCP} (in e/a_0^3)(b), and Laplacian of ρ_{OCP} at OCP $\nabla^2 \rho_{OCP}$ (in e/a_0^5)(c) versus H–S–C–C dihedral angle for S–H bonds in *para*-substituted thiophenols.

2 Cartesian coordinates for the studied complexes

PhSH

C	0.507262000000	0.000340000000	-0.000418000000
C	-0.192589000000	1.202658000000	0.000201000000
C	-1.577949000000	1.199395000000	0.000152000000
C	-2.280209000000	0.004062000000	0.000079000000
C	-1.582080000000	-1.193594000000	0.000003000000
C	-0.196970000000	-1.199994000000	-0.000475000000
H	0.341279000000	2.144812000000	0.000704000000
H	-2.110421000000	2.142223000000	0.000335000000
H	-3.362221000000	0.006208000000	0.000145000000
H	-2.117324000000	-2.134776000000	-0.000113000000
H	0.338502000000	-2.141559000000	-0.001173000000
S	2.271693000000	-0.083101000000	0.000684000000
H	2.498306000000	1.235514000000	-0.008107000000

meta-NMe2PhSH

C	-1.454033000000	-0.204070000000	-0.002638000000
C	-0.175622000000	-0.739241000000	-0.073183000000
C	0.956946000000	0.088379000000	-0.064859000000
C	0.753966000000	1.474361000000	0.042479000000
C	-0.526941000000	1.987395000000	0.113770000000
C	-1.643511000000	1.168981000000	0.088831000000
H	-0.066728000000	-1.812447000000	-0.133081000000
H	1.591540000000	2.154576000000	0.071162000000
H	-0.658118000000	3.059681000000	0.193472000000
H	-2.636946000000	1.593406000000	0.143544000000
S	-2.800922000000	-1.349071000000	-0.036326000000
H	-3.780705000000	-0.451918000000	0.120628000000
N	2.224002000000	-0.444108000000	-0.162018000000
C	3.368392000000	0.408528000000	0.051847000000
H	3.379050000000	0.857562000000	1.053493000000
H	4.277123000000	-0.177184000000	-0.067284000000
H	3.402105000000	1.217345000000	-0.682441000000
C	2.403151000000	-1.873391000000	-0.078226000000
H	1.876592000000	-2.386329000000	-0.887164000000
H	3.460561000000	-2.107377000000	-0.178728000000
H	2.049560000000	-2.288188000000	0.874730000000

meta-NH2PhSH

C	0.846421973168	0.049293178357	-0.000668913487
C	-0.193705914091	-0.870198012801	-0.008088827159
C	-1.520213098281	-0.442556134093	-0.008993764441
C	-1.788895279226	0.927250940396	-0.003594789690
C	-0.745212273373	1.833325128055	0.003995124291
C	0.575269804496	1.413236250197	0.005501061669
H	0.023437154523	-1.932553069636	-0.017838808485
H	-2.814810365179	1.275129846636	-0.010064742145
H	-0.963633410878	2.894077185292	0.009172105324
H	1.378196794530	2.138160402312	0.011667994743
S	2.491447187822	-0.595188681744	0.001595012144
H	3.126517090683	0.582126481113	0.014837941781
N	-2.553588048831	-1.366004328459	-0.068164682488
H	-2.333112909833	-2.292217367057	0.254638359163
H	-3.446624134591	-1.041782391679	0.260320385057

meta-OHPhSH

C	0.748236000000	-0.249859000000	0.011361000000
C	-0.369830000000	-1.063849000000	0.130312000000
C	-1.638711000000	-0.502606000000	0.105509000000
C	-1.798296000000	0.870380000000	-0.037808000000
C	-0.674166000000	1.671095000000	-0.155439000000
C	0.597932000000	1.127284000000	-0.132535000000
H	-0.275609000000	-2.136270000000	0.243048000000

H	-2.789957000000	1.307778000000	-0.057333000000
H	-0.792944000000	2.741441000000	-0.267313000000
H	1.463372000000	1.769702000000	-0.225740000000
S	2.328108000000	-1.036400000000	0.051883000000
H	3.063447000000	0.072405000000	-0.088356000000
O	-2.690360000000	-1.350032000000	0.226074000000
H	-3.510067000000	-0.853543000000	0.196522000000

meta-MeOPhSH

C	1.189809000000	-0.279794000000	0.009679000000
C	-0.004638000000	-0.975313000000	0.087109000000
C	-1.218041000000	-0.293263000000	0.046647000000
C	-1.236634000000	1.091905000000	-0.071979000000
C	-0.029387000000	1.774024000000	-0.148410000000
C	1.180438000000	1.109836000000	-0.109348000000
H	-0.022931000000	-2.053735000000	0.179851000000
H	-2.165331000000	1.641820000000	-0.105586000000
H	-0.039142000000	2.852902000000	-0.240867000000
H	2.107190000000	1.664771000000	-0.170610000000
S	2.683691000000	-1.219898000000	0.068228000000
H	3.527740000000	-0.186818000000	-0.032708000000
O	-2.323105000000	-1.067906000000	0.129555000000
C	-3.583222000000	-0.440977000000	0.095014000000
H	-3.736886000000	0.098300000000	-0.844830000000
H	-4.319559000000	-1.237241000000	0.174795000000
H	-3.709544000000	0.251189000000	0.933277000000

meta-FPhSH

C	-0.828487150763	0.053546999201	0.000079016694
C	0.181074929417	-0.903895046331	0.000112016081
C	1.494762000984	-0.482993979824	0.000000918228
C	1.850907020986	0.850909126359	-0.000024179326
C	0.832934885541	1.790895172345	-0.000023177223
C	-0.497624155927	1.405418106144	-0.000030080604
H	-0.038885002611	-1.963381136961	0.000326090186
H	2.894152079748	1.133463175585	0.000001746073
H	1.080378908021	2.844651257637	-0.000042504469
H	-1.274723221546	2.158372142126	-0.000128081109
S	-2.494575260377	-0.526688089710	-0.000127856579
H	-3.082897327554	0.674877991681	0.001373106427
F	2.459308136782	-1.411584026532	-0.000019081655

meta-MePhSH

C	-0.865376943474	0.038841957005	0.000185914361
C	0.206743148140	-0.847325088228	-0.011039079542
C	1.517948219655	-0.388756033647	-0.012334026436
C	1.745401195694	0.983558077326	-0.008213979590
C	0.681176111129	1.869735126338	0.002391014320
C	-0.624361948309	1.407761064873	0.007936961650
H	0.017856133748	-1.915216169896	-0.021188116712
H	2.761541266586	1.359284126654	-0.015609938308
H	0.867244092479	2.936527207404	0.003597050811
H	-1.447236010156	2.111264106073	0.014443957306
S	-2.492937033449	-0.648588127277	0.001737845074
H	-3.160340089566	0.510922952764	-0.009767142703
C	2.664414328019	-1.361014086457	0.009843981885
H	2.952706336116	-1.592119126362	1.038372055980
H	2.399358334173	-2.299793153222	-0.477098092236
H	3.540197383342	-0.950266028436	-0.493180017438

meta-ClPhSH

C	1.192976978475	0.002125819629	0.000196906431
C	-0.006146023323	-0.701910286474	-0.000093933777
C	-1.200899185234	-0.003371280248	-0.000000905634

C	-1.235178229070	1.379911826244	-0.000013032419
C	-0.032696168849	2.069191927101	0.000031808844
C	1.175265892210	1.394087923816	0.000292777367
H	-0.020325010204	-1.783238369143	-0.000490831372
H	-2.181025304679	1.902519831832	-0.000033007219
H	-0.038734187095	3.151516006021	0.000082707970
H	2.105308983443	1.948224008269	0.000734652647
S	2.764582130729	-0.799094175095	-0.000507141726
H	2.308824150363	-2.057057289519	0.006320012199
Cl	-2.692194228554	-0.895098411210	-0.000057705403

meta-BrPhSH

C	1.782839321871	-0.045718956834	0.000144144602
C	0.495548246497	-0.572231062353	-0.000097042905
C	-0.588474840649	0.288442949557	-0.000018098550
C	-0.425131847080	1.662662057351	-0.000053972428
C	0.863120161260	2.174329164563	0.000026213853
C	1.962779271925	1.334478154633	0.000275272872
H	0.333567302249	-1.641559151299	-0.000427144890
H	-1.284032983970	2.318612066766	-0.000085018516
H	1.010581116808	3.246543253932	0.000062314590
H	2.962130347908	1.751011236549	0.000698418981
S	3.224327514584	-1.062545962820	-0.000407771288
H	2.593684496918	-2.242584081297	0.005049065027
Br	-2.335692913510	-0.442373194343	-0.000012354225

meta-CF₃PhSH

C	-1.733961071501	-0.008157173047	-0.000088862354
C	-0.456896928559	-0.549700155619	0.000040991975
C	0.650997079701	0.286701963287	-0.000047049414
C	0.502467979876	1.662435061478	-0.000010947090
C	-0.776285085174	2.199954043669	-0.000019801601
C	-1.886744121396	1.377442928621	-0.000163759139
H	-0.315021862216	-1.623002222828	0.000249910041
H	1.369900036114	2.306335149297	-0.000024980182
H	-0.907988147684	3.274036118143	-0.000043720360
H	-2.879322257769	1.810701916934	-0.000431645225
S	-3.195185141387	-0.995819315273	0.000295199835
H	-2.587260020526	-2.187750380207	-0.003753930487
C	2.016947178075	-0.348741020647	0.000008791222
F	2.195961332532	-1.130242142463	1.076803807694
F	2.195458137886	-1.131508998089	-1.075948355629
F	3.002303209190	0.554326096128	-0.000748235357

meta-CNPhSH

C	1.092424199316	-0.032416915082	0.000103984017
C	-0.112500807675	-0.721559076946	-0.000116946584
C	-1.312779955927	-0.016096134828	-0.000020916154
C	-1.323423086265	1.375368966564	-0.000021954506
C	-0.116954045896	2.053278127861	0.000051976160
C	1.081377042148	1.360927184969	0.000253945441
H	-0.135119695418	-1.803104169913	-0.000442915325
H	-2.263474189301	1.908957923954	-0.000026930201
H	-0.107691115659	3.135225210326	0.000121945510
H	2.017115086017	1.906170308167	0.000664891158
S	2.658416368490	-0.841753836066	-0.000430058911
H	2.195075489817	-2.097049971240	0.005633995862
C	-2.550658946922	-0.740363300529	-0.000042844360
N	-3.540782018366	-1.322424438836	-0.000044786916

meta-MeSO₂PhSH

C	-2.069164272298	-0.138472139655	-0.011554873051
C	-0.755210177891	-0.477255164744	-0.303570002459
C	0.236483809135	0.483179934826	-0.183750167008

C	-0.045719115111	1.780802058255	0.195390791168
C	-1.360979218968	2.112211084635	0.486350922067
C	-2.364447293949	1.165361980155	0.385343088046
H	-0.498698174072	-1.483874258463	-0.611514974649
H	0.756928892678	2.503044128401	0.263758659198
H	-1.608247184178	3.120283181603	0.793121896539
H	-3.387487306990	1.438917999982	0.612764187506
S	-3.405232366434	-1.286488255278	-0.120996658448
H	-2.678816310193	-2.347657351813	-0.490521678594
S	1.922715950333	0.060608899223	-0.623212337195
O	2.726396965030	1.255545017817	-0.402649494476
O	2.087630071155	-0.949998079536	0.653025818271
C	3.318296164575	-1.670950110801	0.653885747176
H	4.154353248803	-1.004183030486	0.870620629627
H	3.231777271896	-2.417491111204	1.439889876334
H	3.482676133882	-2.168611219176	-0.306358300356

meta-NO₂PhSH

C	1.426305197838	0.013011999279	0.000383145760
C	0.196674122199	-0.631297128372	-0.000348904394
C	-0.954682959807	0.133264865659	0.000079025319
C	-0.937299063835	1.514141969414	0.000252002514
C	0.296051969112	2.144428094068	0.000227052918
C	1.466894098273	1.406440106165	0.000612123772
H	0.113068191522	-1.708280216026	-0.001604890084
H	-1.863946160072	2.067519959832	0.000529947043
H	0.345905916493	3.225118184771	0.000316036877
H	2.422546140376	1.915988202460	0.001490162551
S	2.960012368887	-0.855920974668	-0.001288763246
H	2.446557399296	-2.091397098778	0.016146233626
N	-2.255451015523	-0.563366263910	-0.000165027524
O	-2.244061956934	-1.775188355494	0.000247993838
O	-3.255917120887	0.118864728727	-0.000539088898

para-NMe2PhSH

C	1.768268108813	0.000006044686	-0.014037017409
C	1.053849929586	1.191413085075	-0.027421028558
C	-0.327699096982	1.199955995581	-0.040793045323
C	-1.058759054007	0.000001856460	-0.054989052713
C	-0.327691953089	-1.199957186230	-0.040779041494
C	1.053850088339	-1.191411095369	-0.027398024853
H	1.589798954006	2.132149192185	-0.024138023542
H	-0.836165195139	2.152751030883	-0.043089052906
H	-0.836162919677	-2.152749289890	-0.043062045975
H	1.589810225481	-2.132140127379	-0.024086016901
S	3.546476230154	0.000002160948	-0.038983999080
H	3.747689211453	-0.000083823634	1.287299102993
N	-2.433526197869	-0.000001233830	-0.090006071265
C	-3.150592327133	1.242811811974	0.062599930209
H	-4.219133381340	1.048555728172	0.006004913976
H	-2.942669325399	1.732586866979	1.022411001212
H	-2.901992316952	1.945622885128	-0.737115131198
C	-3.150603175266	-1.242812378194	0.062556934558
H	-4.219139255208	-1.048556431978	0.005865917581
H	-2.901943103468	-1.945628415030	-0.737132123080
H	-2.942764101044	-1.732582400723	1.022390008751

para-NH2PhSH

C	0.973650154107	-0.000025084060	-0.010750083040
C	0.262898114860	1.195086030276	-0.011412060230
C	-1.119079968620	1.199311060809	0.004253928743
C	-1.833758026795	-0.000007015091	0.012810893614
C	-1.119110978407	-1.199294127137	0.004271869916
C	0.262904041646	-1.195094158438	-0.011286118797
H	0.801835191535	2.133799087471	-0.024553033339

H	-1.653715945532	2.142133147591	0.010187947415
H	-1.653749072028	-2.142116182169	0.010107842574
H	0.801825084249	-2.133818238396	-0.024222137906
S	2.751718308066	-0.000083130306	-0.075833072554
H	2.979891282669	0.001343831283	1.245913034075
N	-3.217173144013	0.000026016947	0.077349886112
H	-3.674188132017	0.838334096887	-0.236584120503
H	-3.674199191821	-0.838388025341	-0.236300160816

para-OHPhSH

C	0.955302097188	-0.002088962857	-0.010808879236
C	0.253928084230	1.200474134192	-0.016404728562
C	-1.127751966624	1.215951145239	-0.002919791776
C	-1.831441077128	0.017267064377	0.005518990617
C	-1.142326037239	-1.189291031389	-0.000797162239
C	0.242843037971	-1.193897043082	-0.010794097040
H	0.801069101631	2.134143200853	-0.031793559629
H	-1.676097021019	2.148519226882	-0.004193674823
H	-1.686222086831	-2.127683094957	0.000348667322
H	0.777192094979	-2.134934125044	-0.017767216572
S	2.734910262777	-0.016085970868	-0.070080800497
H	2.953291182812	0.063564829889	1.250632321450
O	-3.184498142255	0.085299081440	0.015659936720
H	-3.555137168353	-0.799118977633	0.016020782845

para-MeOPhSH

C	1.402512012862	-0.018280102305	-0.010090135880
C	0.825195932863	1.250919982202	-0.017487136389
C	-0.544902121378	1.400873971147	-0.004617135475
C	-1.373542151448	0.278941878445	0.001762864997
C	-0.808692111574	-0.991386206954	-0.004574135484
C	0.573472983147	-1.128188193889	-0.010302135875
H	1.462386989808	2.125650054176	-0.034307137591
H	-0.999503161525	2.382734035100	-0.006452135587
H	-1.425247107929	-1.878577275994	-0.004684135453
H	1.010276998643	-2.118447258595	-0.013812136129
S	3.171157160466	-0.215323090469	-0.067928140257
H	3.404711179761	-0.075550077029	1.245136953305
O	-2.701613266079	0.525344876453	0.009788865588
C	-3.586697299484	-0.570238217875	0.010403865597
H	-3.452331258304	-1.192909259662	0.900281929911
H	-4.589260375533	-0.149290199587	0.016523866047
H	-3.460725279498	-1.187058257947	-0.884724198167

para-MePhSH

C	0.997321046221	0.000662986702	0.001186002211
C	0.292783929175	1.197813034101	-0.004192023948
C	-1.092858124660	1.191456953869	-0.009779006116
C	-1.814164127879	0.003980816079	-0.010317962190
C	-1.095399974658	-1.187204236783	-0.008933936773
C	0.288096053761	-1.196358156507	-0.002073954014
H	0.821199903784	2.143213134855	-0.007573058627
H	-1.621864237738	2.137687989907	-0.016458027401
H	-1.627629994290	-2.131701333604	-0.014711902767
H	0.818998156005	-2.140656198014	-0.001856933450
S	2.762632165484	-0.082451916808	0.003331981800
H	2.988170154894	1.235962194581	0.033875942696
C	-3.317139224356	0.002064729555	0.013775059325
H	-3.690253265366	-0.125911272554	1.033085151921
H	-3.720900301153	0.939294771161	-0.370032993263
H	-3.721673217443	-0.813155372412	-0.587624955529

para-FPhSH

C	0.945122049860	0.000290239275	0.004254873801
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C	0.242515900596	1.200348290551	-0.008068997565
C	-1.142862146709	1.206035204984	-0.003817922516
C	-1.816330103277	0.001795071466	-0.000694978324
C	-1.145031985101	-1.203960983630	0.004628893952
C	0.239688083213	-1.199242897487	0.012673820779
H	0.773105894098	2.143785397716	-0.024144955288
H	-1.698616264686	2.133882242384	-0.008447821958
H	-1.702268963565	-2.130850088498	0.010204853358
H	0.773654174645	-2.141067934956	0.030432721488
S	2.711805166978	-0.079479657319	-0.020815228894
H	2.937726121963	1.203708433788	0.282987881435
F	-3.156788251870	0.003402989925	-0.001315906388

para-ClPhSH

C	-1.382807992160	0.000723017786	0.000166934890
C	-0.678469898678	1.199734074518	-0.000195082357
C	0.706359180150	1.202175999976	-0.000084138918
C	1.393076147500	0.000894872490	0.000006821571
C	0.707162047872	-1.201443179446	0.000139838051
C	-0.676820029851	-1.198591109869	0.000374894564
H	-1.206077872546	2.144978173819	-0.000667051788
H	1.249406270681	2.137319047529	-0.000223152141
H	1.250716037290	-2.136220279764	0.000290806976
H	-1.208860074850	-2.141726152078	0.000889907325
S	-3.146116122619	-0.081087898947	-0.000595994026
H	-3.370385092068	1.237825216003	0.007576028528
Cl	3.130121316926	0.002015784470	-0.000046249457

para-BrPhSH

C	-2.054832141521	0.000714084480	0.000123786994
C	-1.350360113277	1.199632170855	-0.000184137701
C	0.034479972437	1.201523164587	-0.000069957550
C	0.721959007944	0.000275072843	0.000009148310
C	0.034753927499	-1.201710011782	0.000158075246
C	-1.349276093682	-1.198796007300	0.000360895074
H	-1.877458119030	2.145110245877	-0.000635219078
H	0.573175003438	2.139313236116	-0.000193900175
H	0.573532991847	-2.139379081641	0.000313158206
H	-1.881217129619	-2.141943077707	0.000870838741
S	-3.817795301331	-0.080642914328	-0.000578441323
H	-4.041906311372	1.238327182958	0.007374512170
Br	2.614807135989	0.001115064677	-0.000024605472

para-CF₃PhSH

C	2.005990033958	0.004106103132	-0.000008817363
C	1.313048883805	1.208780137335	-0.000057013874
C	-0.071847188863	1.218156020456	-0.000135031693
C	-0.776453098951	0.026726868290	-0.000180853680
C	-0.087763993829	-1.179955164652	-0.000140656794
C	1.291999059523	-1.193689044673	-0.000055470741
H	1.849554867279	2.148812248200	-0.000038515478
H	-0.599812304456	2.161581046505	-0.000184185380
H	-0.633271917322	-2.114955276138	-0.000196516957
H	1.819424202651	-2.139215073737	-0.000039309191
S	3.764837200207	-0.093592755812	0.000069218713
H	4.001649099236	1.223369368878	0.000059819943
C	-2.279013214629	0.005519740144	-0.000002868141
F	-2.808637406734	1.234007794830	-0.002123066902
F	-2.765284190186	-0.636717517392	-1.074758855133
F	-2.765045213740	-0.632843183206	1.077190308173

para-CNPhSH

C	-1.263886147746	0.001241010927	0.000101753059
C	-0.561583111210	1.203874119184	-0.000082102803

C	0.819417952316	1.204136157174	-0.000025051357
C	1.520319039566	0.000574082331	-0.000010143322
C	0.819463038218	-1.203746026539	0.000084712387
C	-0.560652023840	-1.202213063550	0.000244661132
H	-1.092118176113	2.147138174806	-0.000363029986
H	1.360898942779	2.140550240854	-0.000090939269
H	1.360941065289	-2.140084083323	0.000169640679
H	-1.096506060944	-2.142902153262	0.000615548977
S	-3.021357241477	-0.081006043694	-0.000366320411
H	-3.246732297212	1.237996055586	0.004307800998
C	2.951834146174	0.001567121486	-0.000040089992
N	4.100822207471	0.002971153032	-0.000060047118

para-MeSO₂PhSH

C	-2.372360240106	-0.055977817757	0.030519928365
C	-1.649076172331	-1.146426822245	-0.452805254927
C	-0.281447047463	-1.051691801886	-0.620762167155
C	0.370634898516	0.128625222635	-0.297104894780
C	-0.337106069266	1.220276232606	0.169940289725
C	-1.707845221744	1.126728209734	0.339701202650
H	-2.159471227397	-2.069334842000	-0.698223466246
H	0.276348953846	-1.901956808406	-0.994072310670
H	0.194540902873	2.134358253195	0.402598500840
H	-2.258114258781	1.981753218527	0.711349348067
S	-4.113813403099	-0.251820849624	0.213586798001
H	-4.368034439854	0.976057164450	0.680627036816
S	2.130090089425	0.285655259155	-0.563255776993
O	2.496021078456	1.636083283336	-0.153142488249
O	2.494607011012	-0.763656037289	0.639446145792
C	3.883380100794	-1.077030089177	0.720761183490
H	3.968342048171	-1.898935275108	1.427843098051
H	4.273055167153	-1.390763944553	-0.252124918046
H	4.450800142895	-0.218965097851	1.084775397274

para-NO₂PhSH

C	-1.646205068249	0.001245131524	0.000008341421
C	-0.944385911389	1.205247148933	0.000034935171
C	0.436821160840	1.207370012261	0.000061823778
C	1.111774094603	0.000384848441	0.000008120437
C	0.436786923072	-1.207390173914	-0.000014474321
C	-0.943551134279	-1.203706036615	0.000017476714
H	-1.475231815008	2.148144273050	0.000004363649
H	0.993848320524	2.132803022427	0.000123510129
H	0.993503879053	-2.132928299849	-0.000056557935
H	-1.479885293901	-2.143934054189	0.000099776053
S	-3.401955224648	-0.081064698758	-0.000083493957
H	-3.627992069451	1.237883420209	0.000848140794
N	2.579038193609	0.001294701674	-0.000003997511
O	3.142228151535	-1.072519435225	0.000095269368
O	3.141063379492	1.075906725254	-0.000139355018