

Ground-state Baird aromaticity in a stable reduced carbon macrocycle

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Additional Details

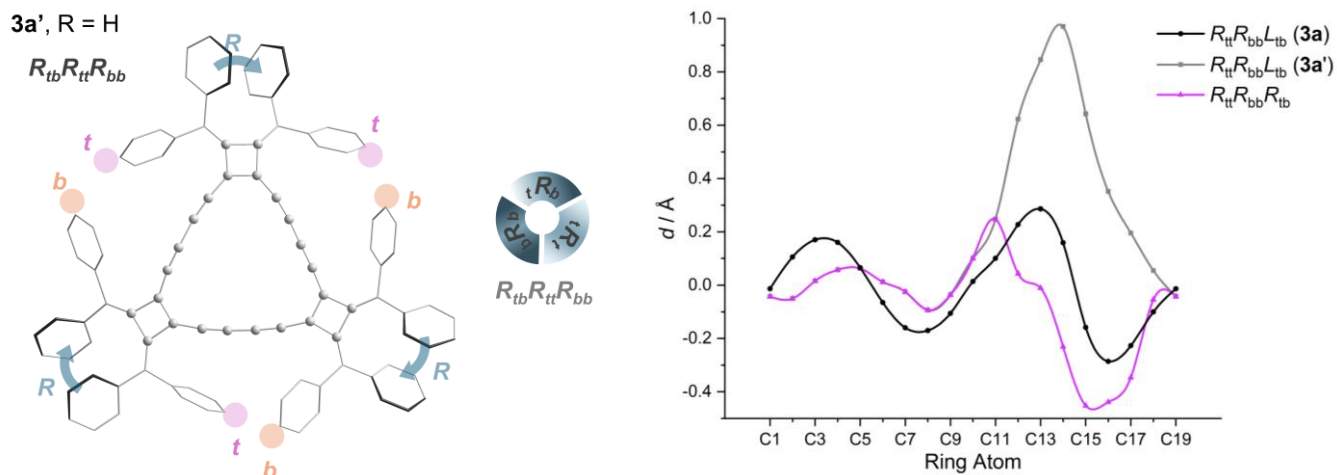


Fig. S1. Left: X-Ray structure (Ball-and-Stick/wireframe mole) of **3a'** showing the $R_{tb}R_{tt}R_{bb}$ -set of sites (50:50 occupation). H-atoms are omitted for clarity. Right: Out-of-plane shift of individual atoms of the C_{18} motif. For $R_{tt}R_{bb}L_{tb}$ -**3a'** and $R_{tt}R_{bb}R_{tb}$ -**3a'** only the non-disordered parts (C_{10}) were used to calculate the mean plane. The Sum of the differences $\Sigma(\text{abs}(d(\mathbf{3a}')-\mathbf{3a}))$ for various labeling possibilities only includes this C_{10} motif to highlight the variations along the perimeter.

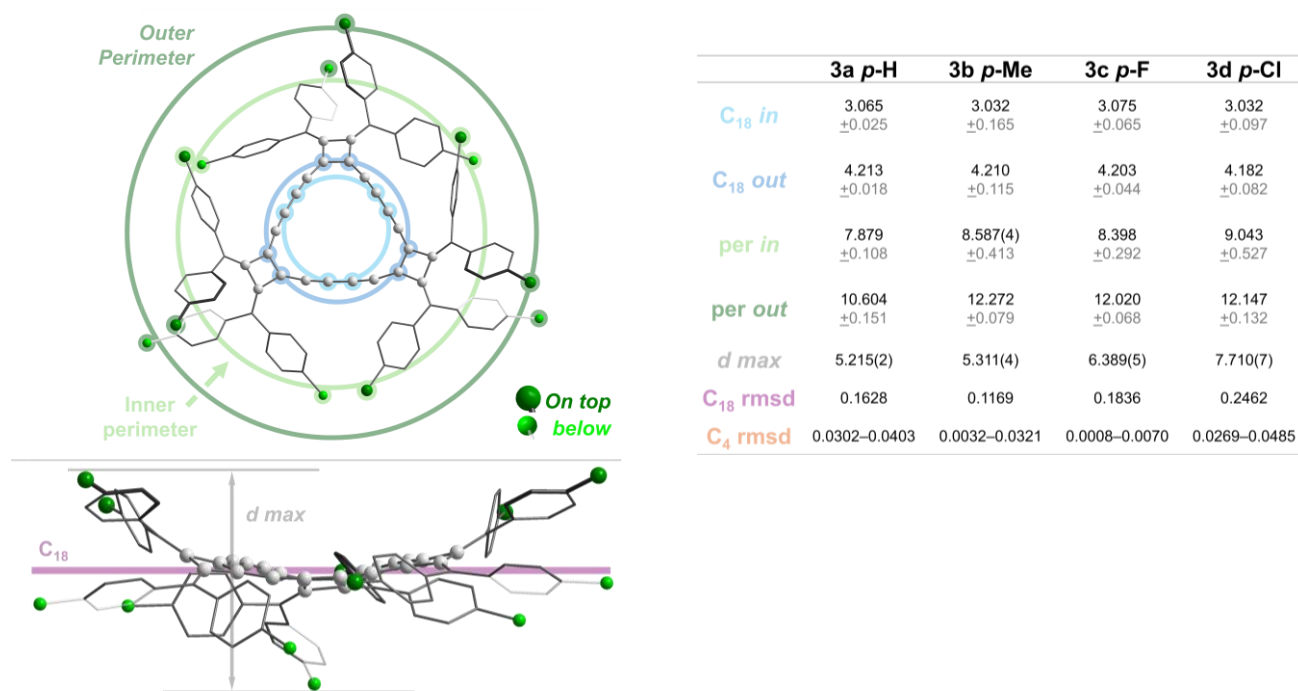


Fig. S2. Selected geometric features of the C_{18} macrocycles **3a-d**.

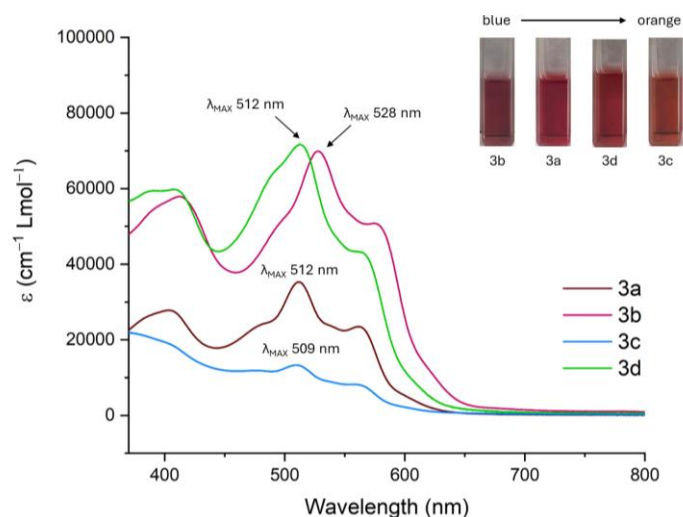


Fig. S3. UV-Vis Spectra of **3a–d** in CHCl_3 .

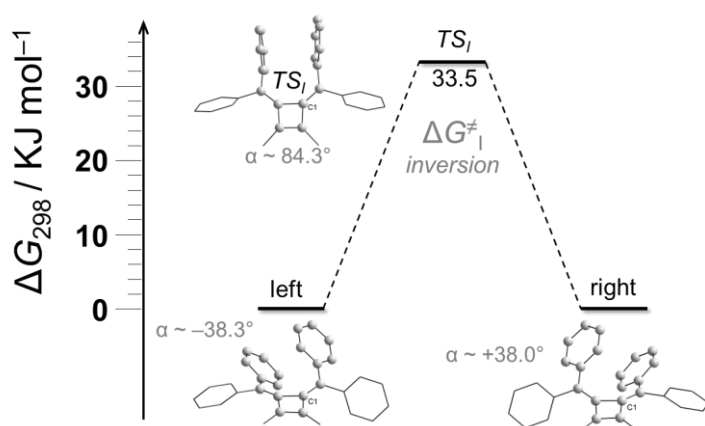


Fig. S4. Calculation of the inversion barrier of the butafulvene backbone between *L* (left) and *R* (right) isomers.

Aromaticity and electronic structure of the 20π electron systems

Two exchange–correlation functionals, M06-2X¹ and CAM-B3LYP², which have been shown to reliably describe electronic structure, were used to optimize the geometries of compounds **3a–d** and a simplified model system, **3m**, in which the terminal phenyl rings were replaced by hydrogen atoms. This simplification serves two purposes. First, removal of the twelve phenyl rings significantly improves computational efficiency and accuracy. Second, elimination of their steric effects allows the preferred geometric and electronic structure of the bare scaffold to be revealed.

The stability of all wavefunctions was examined to ensure that the DFT results are free from instabilities. Geometry optimizations were carried out using the def2-SVP and def2-TZVPP³ basis sets (only for **3m**) in combination with both functionals. The nature of each stationary point was confirmed by analyzing the eigenvalues of the Hessian matrix. All DFT and ab initio calculations were performed using the Gaussian suite of programs.⁴ The ground-state

¹ Zhao, Y. & Truhlar, D. G. The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06-class functionals and 12 other functionals. *Theor. Chem. Acc.* **120**, 215–241 (2008). DOI: 10.1007/s00214-007-0310-x.

² Yanai, T., *et al.* A new hybrid exchange–correlation functional using the Coulomb-attenuating method (CAM-B3LYP). *Chem. Phys. Lett.* **393**, 51–57 (2004). DOI: 10.1016/j.cplett.2004.06.011.

³ (a) Weigend, F. & Ahlrichs, R. Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: design and assessment of accuracy. *Phys. Chem. Chem. Phys.* **7**, 3297–3305 (2005). DOI: 10.1039/B508541A. (b) Weigend, F. Accurate Coulomb-fitting basis sets for H to Rn. *Phys. Chem. Chem. Phys.* **8**, 1057–1065 (2006). DOI: 10.1039/B515623H.

⁴ M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G.

electronic structures of the neutral species and their dianions were investigated using DFT for all systems. DFT predicts relatively large singlet–triplet energy gaps for the neutral species, whereas a small negative singlet–triplet gap, favoring a triplet dianion, was obtained for **3a–d** and **3m**. Notably, the computed DFT energy gaps are consistent with the experimental observations. However, because DFT results may benefit from error cancellation, we re-examined the electronic structure of **3m** at the FIC-NEVPT2⁵/ma-def2-TZVPP⁶ level of theory using ORCA suite of programs.⁷ The S–T energy gap evaluated at the FIC-NEVPT2 level consistently identifies the triplet dianion $T[3m]^{2-}$ as the ground state across multiple choices of active space.

The DFT wavefunctions, saved as formatted checkpoint files, were analyzed with MultiWFN software¹ to compute the multicenter index (MCI).² NMR shielding calculations were carried out using the gauge-including atomic orbital (GIAO) formalism, and the corresponding wavefunctions were saved in WFX format for the ring current analysis. These wavefunctions were subsequently analyzed with AIMAll³ to evaluate magnetic aromaticity by computing the magnetically induced current density passing through interatomic (zero-flux) surfaces shared between neighboring atoms of the quantum theory of atoms in molecules (QTAIM).⁴ The use of interatomic surfaces provides a unique and reproducible measure of current intensity free from user-dependent parameter selection. Notably, the current-density data are automatically generated and stored in atomic files by AIMAll. To ensure the quality of the QTAIM analysis, the integrated Laplacian of the electron density over each atomic basin was verified to be smaller than 10^{-4} a.u., and the total electronic energy difference between the QTAIM and DFT calculations was kept below $0.1 \text{ kcal mol}^{-1}$.

Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, D. J. Fox 2016.

⁵ (a) Angeli, C., *et al.* Introduction of n -electron valence states for multireference perturbation theory. *J. Chem. Phys.* **114**, 10252–10264 (2001). DOI: 10.1063/1.1361246. (b) Angeli, C., *et al.* n -Electron valence state perturbation theory: a spinless formulation and an efficient implementation of the strongly contracted and of the partially contracted variants. *J. Chem. Phys.* **117**, 9138–9153 (2002). DOI: 10.1063/1.1515317.

⁶ Zheng, J., *et al.* Minimally augmented Karlsruhe basis sets. *Theor. Chem. Acc.* **128**, 295–305 (2011). DOI: 10.1007/s00214-010-0846-z.

⁷ Neese, F. Software update: The ORCA program system—Version 5.0. *WIREs Comput. Mol. Sci.* **12**, e1606 (2022). DOI: 10.1002/wcms.1606.

Experimental

General. Unless otherwise noted, reactions were carried out under an atmosphere of nitrogen (UWA) or argon (UALbany) using standard Schlenk techniques. For neutral organic precursors, no particular care was taken to exclude air upon work-up of reaction products. Reaction flasks were heated at reduced pressure with a heat gun and flushed with nitrogen. This procedure was repeated three times. If necessary, solvents were deoxygenated by standard procedures. For column chromatography silica with a particle size of 60 μm was used.

Reagents. Tetrahydrofuran, dichloromethane, hexane and toluene were dried and purified with an Innovative Technologies Solvent Purification System and stored over molecular sieve (4 Å). The 1,2-dibromo cyclobutene precursors **1a–d** were synthesized according to a recently published procedure.^[8] Further starting materials were purchased from commercial suppliers and used without further purification, except otherwise noted.

Instruments.

FT-IR spectra were recorded on an Agilent Cary 630 FTIR spectrometer using ATR or transmission mode from solutions between CaF₂ plates.

NMR spectra were recorded on a Bruker Avance Neo 400 MHz (¹H: 400.13 MHz, ¹³C: 100.63 MHz, ³¹P: 161.97 MHz, ¹⁹F: 376.46 MHz), and Bruker Avance IIIHD 500 MHz (¹H: 500.10 MHz, ¹³C: 125.8 MHz, ³¹P: 202.4 MHz, ¹⁹F: 470.6 MHz) spectrometers at room temperature.

They are reported with chemical shifts in δ (ppm) units downfield from tetramethylsilane with the solvent as the reference signal (chloroform-*d*₁: ¹H at 7.26 ppm and ¹³C{¹H} at 77.16 ppm) or by the ²H solvent lock signal^[9] unless otherwise noted. For all NMR spectra, multiplets are reported according to their closest first order approximation. The description *o*-, *m*-, *p*- refers to the *ipso* carbon closest to the cyclobutene core.

High-resolution Mass spectra (HRMS) were recorded on a Thermo Fusion Orbitrap Exploris 120, using positive mode electrospray ionization (ESI(+)). Samples were prepared in MeCN and inserted by direct injection via the on-board injector.

Electrochemistry. Cyclic voltammetry was carried out by using a PalmSens Emstat³⁺ potentiostat, with a glassy-carbon working, platinum counter and pseudo-reference electrodes, from solutions in oxygen-free anhydrous dichloromethane containing 0.1 M [NBu₄][BAr^F₄] as the electrolyte, scan rate = 100 mV·s⁻¹. The presented results are reported against the ferrocene/ferrocenium redox couple as an internal standard as required by IUPAC.^{Error!} ^{Bookmark not defined.} Referencing was achieved by addition of decamethylferrocene as an internal standard.¹⁰ The latter has been measured together with ferrocene and its redox potential was set to -626 mV (± 1 mV; $E_{\text{step}} = 2$ mV) for [NBu₄][BAr^F₄] electrolyte solution. These values represent the average of 5 consecutive measurements, which were all found within the given precision. Data have been processed with the PStTrace 4.8 software and Microsoft Excel to set the formal reduction potentials of the FcH/FcH⁺ couple to 0.0 V.¹¹

Spectro-electrochemical FT-IR measurements were conducted in an OTTLE cell using CH₂Cl₂ solutions containing 0.1 M [NBu₄][BAr^F₄] supporting electrolyte. Spectra were recorded on an Agilent Technologies Cary 660 FTIR. Electrolysis in the cell was performed using a PalmSens Emstat³⁺ potentiostat at a scan rate of 0.0025 V s⁻¹.

Single crystal X-ray diffraction analysis. Data for **3a–c**, **5** were collected with a Rigaku-Oxford Diffraction XtaLAB Synergy-S diffractometer using a micro-focus sealed Cu K α radiation ($\lambda = 1.54184$ Å) X-ray source at 100 K. Data for **3d** were collected the MX2 beamline at the Australian Synchrotron.^[12] Single crystals were transferred from the mother liquor into immersion oil, frozen in liquid nitrogen and measured under a stream of nitrogen at 100 K.

⁸ M. Korb et al, dibromocyclobutene manuscript

⁹ R. K. Harris, E. D. Becker, S. M. Cabral de Menezes, R. Goodfellow, P. Granger, *Pure Appl. Chem.* **2001**, *73*, 1795.

¹⁰ a) I. Noviadri, K. N. Brown, D. S. Fleming, P. T. Gulyas, P. A. Lay, A. F. Masters, L. Phillips, *J. Phys. Chem. B* **1999**, *103*, 6713–6722;

b) A. Nafady, W. E. Geiger, *Organometallics* **2008**, *27*, 5624–5631.

¹¹ a) F. Barrière, N. Camire, W. E. Geiger, U. T. Mueller-Westerhoff, R. Sanders, *J. Am. Chem. Soc.* **2002**, *124*, 7262–7263.

¹² D. Aragão, J. Aishima, H. Cherukuvada, R. Clarken, M. Clift, N. P. Cowieson, D.J. Ericsson, C. L. Gee, S. Macedo, N. Mudie, S. Panjkar, J. R. Price, A. Riboldi-Tunnicliffe, R. Rostan, R. Williamson, T. Tudor Caradoc-Davies, MX2: a high-flux undulator microfocuss beamline serving both the chemical and macromolecular crystallography communities at the Australian Synchrotron, *J. Synchrotron Rad.* **2018**, *25*, 885.

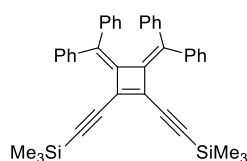
The molecular structures were solved by direct methods using SHELXS-18/3^[13] and refined by full-matrix least-squares procedures on F^2 using SHELXL-18.^[14,15] All non-hydrogen atoms were refined anisotropically and a riding model was employed in the treatment of the hydrogen atom positions, except otherwise noted. Graphics of the molecular structures have been created by using ORTEP.^[16] Crystallographic data have been deposited at the Cambridge Crystallographic Data Centre. Copies of the data with CCDC numbers listed in Tables S1 and S2 (below), that can be obtained free of charge via <https://www.ccdc.cam.ac.uk/structures/>, or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, U.KCB21EZ, UK (fax +441223336033; email deposit@ccdc.cam.ac.uk). (The usage of SQUEEZE procedures, which is implemented in the PLATON program package, is mentioned individually.¹⁷⁾

Synthesis of Starting Materials

GP1. General procedure for conversion of 1,2-dibromocyclobutene via Sonogashira C,C cross-coupling reactions.

The respective 1,2-dibromocyclobutene (1 equiv), $[\text{PdCl}_2(\text{PPh}_3)_2]$ (2.5 mol%) and CuI (5 mol%) were weighed into a screwcap vial (21 mL size). To the solid materials, dry NEt_3 (ca 5 mL) was added and the remainder of the vial was filled with toluene. The suspension was sonicated to remove dissolved air and nitrogen gas was bubbled through the suspension for ca 10 min, followed by additional sonication. In the final step trimethylsilyl acetylene (3 equiv) were added (Note: more toluene was added if the vial was not filled completely), the vial was closed, placed in an oil bath and stirred at 85 °C for 18h. Afterwards the content was poured into a separatory funnel and the mixture, washed with HCl-acidified water and extracted using Et_2O (3 x 50 mL). The combined organic extract were dried over MgSO_4 followed by removal of all volatiles in vacuo. Purification was realized via column chromatography (silica 3.5 x 15 cm) using solvent mixtures outlined below.

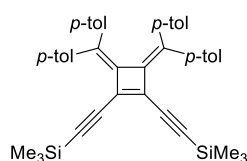
1,2-Bis(trimethylsilylethynyl)-3,4-bis(diphenylmethylene)cyclobut-1-ene (2a)



Compound **1a** (1.416 g, 2.62 mmol), $[\text{PdCl}_2(\text{PPh}_3)_2]$ (84 mg, 0.12 mmol), CuI (100 mg, 0.53 mmol), and TMSA (1.20 mL, 8.45 mmol) were reacted according to GP1. A 95:5 hexane/ CH_2Cl_2 solvent mixture eluted the product as a yellow solid.

Yield of the crude: 770 mg (99%, quant). **$^1\text{H NMR}$** (CDCl_3 , δ): 0.03 (s, 18, CH_3), 6.66–6.71 (m, 4H), 6.70 (tt, $J_{\text{H,H}} = 7.5, 1.3$ Hz, 2H, *p*-Ph), 6.83–6.86 (m, 4H), 7.26–7.31 (m, 10H) ppm. **$^{13}\text{C}\{^1\text{H}\}$ NMR** (CDCl_3 , δ): –0.3 (CH_3), 96.1 ($\text{C}\equiv\text{CSi}$), 112.3 ($\text{C}\equiv\text{CSi}$), 127.1 (CH), 127.41 (*p*-Ph), 127.48 (CH), 127.8 (*p*-Ph), 130.8 (CH), 131.9 (CH), 133.7, 138.7, 140.0, 140.6, 141.4 ppm. ESI(+)-**HRMS** (m/z): calcd. for $\text{C}_{40}\text{H}_{38}\text{Si}_2 + \text{H}$ 575.2585; found 575.2584 [$\text{M} + \text{H}$]⁺.

1,2-Bis(trimethylsilylethynyl)-3,4-bis(bis(4-tolyl)methylene)cyclobut-1-ene (2b)



Compound **1b** (1.200 g, 2.012 mmol), $[\text{PdCl}_2(\text{PPh}_3)_2]$ (84 mg, 0.12 mmol), CuI (100 mg, 0.53 mmol), and TMSA (1.00 mL, 7.041 mmol) were reacted according to GP1. A 9:1 hexane/ CH_2Cl_2 solvent mixture eluted the product as a yellow solid.

Yield: 914 mg (1.449 mmol, 72%). $M = 631.02$ g/mol. **$^1\text{H NMR}$** (CDCl_3 , δ): 0.02 (s, 18H, SiCH_3), 2.09 (s, 6H, CH_3), 2.36 (s, 6H, CH_3), 6.47 (d, $^3J_{\text{H,H}} = 7.8$ Hz, *m*-4H), 6.70 (d, $^3J_{\text{H,H}} = 8.1$ Hz, *o*-4H, CH), 7.08 (d, $^3J_{\text{H,H}} = 7.7$ Hz, *m*-4H, CH), 7.16 (d, $^3J_{\text{H,H}} = 8.1$ Hz, *o*-4H, CH) ppm. **$^{13}\text{C}\{^1\text{H}\}$ NMR** (CDCl_3 , δ): –0.4 (CH_3), 21.2 (CH_3), 21.5 (CH_3), 96.5 ($\text{C}\equiv\text{CSi}$), 111.6 ($\text{C}\equiv\text{CSi}$), 127.7 (*m*-C), 128.2 (*m*-C), 130.7 (*o*-C), 131.8 (*o*-C), 133.5 ($\text{C}^{\text{Cybu}} = \text{C}^{\text{Vinyl}}$), 136.8 ($^q\text{C}^{\text{Ar}}$), 137.2 ($^q\text{C}^{\text{Ar}}$), 137.5 ($^q\text{C}^{\text{Ar}}$), 137.8 ($^q\text{C}^{\text{Ar}}$), 138.1 (C– $\text{C}\equiv\text{C}$), 140.8 ($\text{C}^{\text{Cybu}} = \text{C}^{\text{Vinyl}}$) ppm. APCI(–)-**HRMS** (m/z): calcd. for $\text{C}_{44}\text{H}_{46}\text{Si}_2$ 630.3144; found 630.3144 [M][–].

¹³ Sheldrick, G. M.; Phase annealing in SHELX-90: direct methods for larger structures; *Acta Crystallogr. Sect. A Found. Crystallogr.* **1990**, *46*, 467–473.

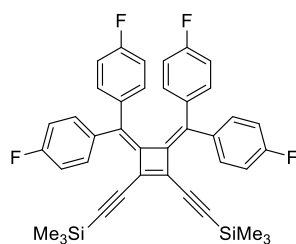
¹⁴ Sheldrick, G. M.; Program for Crystal Structure Refinement; University of Gottingen, Gottingen, Germany, 1997.

¹⁵ Sheldrick, G. M.; A short history of SHELX; *Acta Crystallogr. Sect. A Found. Crystallogr.* **2008**, *64*, 112–122; Sheldrick, G. M., *Acta Crystallogr. Sect. C Struct. Chem.* **2015**, *71*, 3–8.

¹⁶ L. J. Farrugia, *J. Appl. Crystallogr.* **2012**, *45*, 849–854.

¹⁷ A. L. Spek, *Acta Cryst. Sect. C* **2015**, *71*, 9–18.

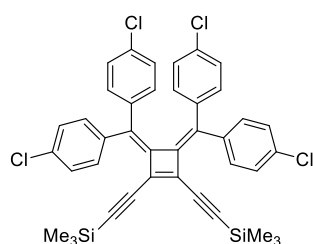
1,2-Bis(trimethylsilylethynyl)-3,4-bis(bis(4-fluorophenyl)methylene)cyclobut-1-ene (2c)



Compound **1c** (1.400 g, 2.287 mmol), [PdCl₂(PPh₃)₂] (84 mg, 0.12 mmol), CuI (200 mg, 1.053 mmol), and TMSA (1.00 mL, 7.041 mmol) were reacted according to GP1. A 85:15 hexane/CH₂Cl₂ solvent mixture eluted the product as a yellow solid.

Yield: 962 mg (1.487 mmol, 65%). M = 646.88 g/mol. ¹H NMR (CDCl₃, δ): 0.06 (s, 18H, CH₃), 6.46 (dd, ³J_{H,H} = ³J_{H,F} = 8.8 Hz, *m*-4H), 6.80 (dd, ³J_{H,H} = 8.8 Hz, ⁴J_{H,F} = 5.5 Hz, *o*-4H, CH), 6.98 (dd, ³J_{H,H} = ³J_{H,F} = 8.7 Hz, *m*-4H, CH), 7.22 (dd, ³J_{H,H} = 8.7 Hz, ⁴J_{H,F} = 5.5 Hz, *o*-4H, CH) ppm. ¹³C{¹H} NMR (CDCl₃, δ): -0.4 (CH₃), 95.8 (C≡CSi), 113.2 (C≡CSi), 114.3 (d, ²J_{C,F} = 21.6 Hz, *m*-C), 114.6 (d, ²J_{C,F} = 21.4 Hz, *m*-C), 131.3 (C^{Cybu}=C^{Vinyl}), 132.3 (d, ³J_{C,F} = 8.5 Hz, *o*-C), 133.3 (d, ³J_{C,F} = 8.2 Hz, *o*-C), 135.8 (d, ⁴J_{C,F} = 3.3 Hz, *i*-C), 136.1 (d, ⁴J_{C,F} = 3.3 Hz, *i*-C), 138.6 (C-C≡C), 141.0 (C^{Cybu}=C^{Vinyl}), 162.5 (d, ¹J_{C,F} = 248.6 Hz, *p*-CF), 162.9 (d, ¹J_{C,F} = 247.0 Hz, *p*-CF) ppm. ¹⁹F{¹H} NMR (CDCl₃, δ): -114.43 (s), -114.24 (s) ppm. APCI(-)-HRMS (*m/z*): calcd. for C₄₀H₃₄F₄Si₂ 646.2141; found 646.2139 [M]⁻.

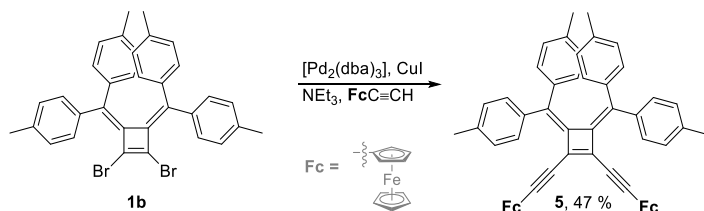
1,2-Bis(trimethylsilylethynyl)-3,4-bis(bis(4-chlorophenyl)methylene)cyclobut-1-ene (2d)



Compound **1d** (600 mg, 0.885 mmol), [PdCl₂(PPh₃)₂] (31 mg, 0.04 mmol), CuI (100 mg, 0.05 mmol), and TMSA (1.00 mL, 7.041 mmol) were reacted according to GP1. A 85:15 hexane/CH₂Cl₂ solvent mixture eluted the product as a pale yellow solid.

Yield: 422 mg (0.593 mmol, 67%). M = 712.68 g/mol. ¹H NMR (CDCl₃, δ): 0.07 (s, 18H, CH₃), 6.72 (d, ³J_{H,H} = 9.1 Hz, *m*-4H), 6.76 (d, ³J_{H,H} = 8.8 Hz, *o*-4H), 7.18 (d, ³J_{H,H} = 8.4 Hz, *m*-4H), 7.27 (d, ³J_{H,H} = 8.4 Hz, *o*-4H) ppm. ¹³C{¹H} NMR (CDCl₃, δ): -0.5 (CH₃), 95.6 (C≡CSi), 114.1 (C≡CSi), 127.6 (CH), 127.9 (CH), 131.2, 131.8 (CH), 133.0 (CH), 134.20, 134.26, 137.92, 138.02, 139.2, 141.3 ppm. APCI(-)-HRMS (*m/z*): calcd. for C₄₀H₃₄³⁵Cl₃³⁷ClSi₂ 712.0929; found 712.0924 [M]⁻.

1,2-Bis(ferrocenylethynyl)-3,4-bis(bis-4-tolylmethylene)cyclobut-1-ene (5) – MK-U-387-F2



Compound **1b** (200 mg, 0.335 mmol), [Pd₂(dba)₃] (30 mg, 0.033 mmol), CuI (100 mg, 0.053 mmol), dppf (18 mg, 0.032 mmol), and ethynyl ferrocene (211 mg, 1.091 mmol) were reacted according to GP1. A 60:40 hexane/CH₂Cl₂ solvent mixture eluted the product as an orange solid.

Yield: 136 mg (0.159 mmol, 47%). M = 854.70 g/mol. ¹H NMR (CDCl₃, δ): 2.11 (s, 6H, Me^{out}), 2.46 (s, 6H, Meⁱⁿ), 4.12 (s, 10H, C₅H₅), 4.20 (s br, 8H, C₅H₄), 6.50 (d, ³J_{H,H} = 7.6 Hz, 4H, *m*-C₆H₄^o), 6.76 (d, ³J_{H,H} = 8.1 Hz, 4H, *o*-C₆H₄^o), 7.17 (d, ³J_{H,H} = 7.8 Hz, 4H, *m*-C₆H₄ⁱ), 7.27 (d, ³J_{H,H} = 8.1 Hz, 4H, *o*-C₆H₄ⁱ) ppm. ¹³C{¹H} NMR (CDCl₃, δ): 21.2 (Me^o), 21.7 (Meⁱ), 65.1 (^qC₅H₄), 69.4 (C₅H₄), 70.3 (C₅H₅), 71.6 (C₅H₄), 80.0 (C≡C), 105.0 (C≡C), 127.7 (*m*-C₆H₄^o), 128.2 (*m*-C₆H₄ⁱ), 130.7 (*o*-C₆H₄^o), 131.76 (^qC₆H₄-C^{vinyl}), 131.85 (*o*-C₆H₄ⁱ), 136.5 (C-CH₃^o), 136.8 (C-CH₃ⁱ), 137.9 (^qC₆H₄^o), 138.3 (^qC₆H₄ⁱ), 139.0, 139.2 ppm. ESI(+)-HRMS (*m/z*): calcd. for C₅₈H₄₆Fe₂ 854.2293; found 854.2285 [M]⁺.

GP2. General procedure for the formation of macrocycles 3 via oxidative coupling.

A two necked round bottom flask, equipped with a stirrer bar, was charged with 10 ml of methanol, 30 ml of toluene and 40 ml of pyridine. Compounds **2** (200 mg, 1 eq.) were added, resulting in a transparent yellow solution, followed by addition of KF (72 mg, 1.24 mmol, 4 eq.) and Cu(OAc)₂·H₂O in crystal form (926 mg, 4.638 mmol, 15 eq.). The mixture was stoppered, stirred, and heated to 50–60 °C for 72h. During that time, the colour of the solution changed from dark green to dark purple. The reaction mixture was evaporated to dryness using a cold trap. To remove polymers, the black crude product was dissolved in CH₂Cl₂ and filtered through a 4 cm plug of silica using CH₂Cl₂

until the eluent remained colourless. The resulting dark purple/red crude product was adsorbed onto silica and chromatographed on a pre-packed silica column (3.5 cm × 30 cm) with a 9:1 hexanes/CH₂Cl₂ solvent mixture, that was gradually changed to 4:6 hexanes/CH₂Cl₂. The major red fraction eluted as a mixture of trimeric and tetrameric cyclic products (~300 mg), which was re-adsorbed to silica and loaded onto another pre-packed silica column (3.5 cm × 40 cm), and subsequently eluted with a 8:2 hexanes/CH₂Cl₂ solvent mixture that was changed gradually over the course of several hours to 3:1 hexanes/CH₂Cl₂

Macrocycle 3a (R = H)

Macrocycle **3a** was prepared from compound **2a** (727 mg, 1.69 mmol) according to GP2. A total of 185 fractions were eluted. The purity of the fractions was determined via HRMS (APCI (-)), as the tetramer and trimer produced identical ¹H NMR. The fractions containing pure trimer were combined to give **3a** as a deep red solid.

Yield: 134 mg (0.104 mmol, 6.2%). M = 1285.602 g/mol. M = 1313.66 g / mol. ¹H NMR (CDCl₃, δ): 7.55 (dt, J = 8.8, 4.2 Hz, 6H), 7.48 (d, J = 4.4 Hz, 24H), 7.01 – 6.96 (m, 12H), 6.89 (ddt, J = 7.9, 6.9, 1.3 Hz, 6H), 6.83 – 6.77 (m, 12H) ppm. ¹³C{¹H} NMR (CDCl₃, δ): 142.5, 140.4, 140.1, 136.8, 131.5, 131.5, 129.0, 128.0, 127.9, 127.4, 93.8, 85.4, 77.4, 77.2, 77.0 ppm. APCI(-)-HRMS (m/z): calcd. for [C₁₀₁¹³CH₆₀]⁻ 1285.4734; found 1285.4735 [M]⁻.

Macrocycle 3b (R = Me)

Macrocycle **3b** was prepared from compound **2b** (840 mg, 0.578 mmol) according to GP2. Work-up is similar to compound **3a**, whereas the fraction sizes differ slightly.

Yield: 87 mg (0.060 mmol, 10.4 %). M = 1453.93 g/mol. ¹H NMR (CDCl₃, δ): 7.33 (d, J = 8.1 Hz, 12H), 7.15 (d, J = 7.9 Hz, 12H), 6.82 (d, J = 8.0 Hz, 12H), 6.57 (d, J = 7.9 Hz, 12H), 2.42 (s, 18H), 2.16 (s, 18H) ppm. ¹³C{¹H} NMR (CDCl₃, δ): 140.81, 136.85, 136.15, 136.07, 136.00, 135.95, 133.57, 130.32, 129.80, 127.09, 126.61, 89.97, 80.95, 28.68, 20.34, 20.03 ppm. APCI(-)-HRMS (m/z): calcd. for [C₁₁₃¹³CH₆₀]⁻ 1453.66121; found 1453.6613 [M]⁻.

Macrocycle 3c (R = F)

Deep red solid. As a mixture of isomers (Major isomer noted as superscript a, minor isomer noted as superscript b). ¹H NMR (CDCl₃, δ): 7.46 (d, J = 8.1 Hz, 4H^a), 7.37 (d, J = 8.2 Hz, 4H^a), 7.29 (d, J = 8.3 Hz, 4H^b), 7.14 (d, J = 8.1 Hz, 4H^b), 6.86 (s, 8H^a), 6.77 (q, J = 8.4 Hz, 8H^b) ppm. ¹³C{¹H} NMR (CDCl₃, δ): 142.29, 142.16, 139.00, 137.95, 137.80, 137.47, 137.40, 135.18, 134.94, 134.88, 134.77, 134.47, 133.20, 132.73, 132.63, 132.48, 131.97, 128.59, 128.12, 127.93, 127.79, 93.83 (≡C^a), 91.39 (≡C^b), 85.61 (≡C^a), 81.95 (≡C^b) ppm. APCI(-)-HRMS (m/z): calcd. for [C₁₀₁¹³CH₄₈³⁵Cl₉³⁷Cl₃-H]⁻ 1697.9891; found 1697.9960 [M-H]⁻.

Macrocycle 3d (R = Cl)

¹H NMR (CDCl₃, δ): 7.44 – 7.38 (m, 12H), 7.20 – 7.13 (m, 12H), 6.97 – 6.90 (m, 12H), 6.60 – 6.53 (m, 12H) ppm. ¹³C{¹H} NMR (CDCl₃, δ): 164.34 (d, J = 54.3 Hz), 161.86 (d, J = 54.0 Hz), 141.90, 138.36, 135.76 (d, J = 3.2 Hz), 134.70, 133.09 (d, J = 7.8 Hz), 115.28 (d, J = 10.0 Hz), 115.28 (d, J = 23.2 Hz), 114.64 (d, J = 21.7 Hz), 93.45, 85.33 ppm. ¹⁹F{¹H} NMR (CDCl₃, δ): -111.10, -113.27 ppm. ESI(+)-HRMS (m/z): calcd. for [C₁₀₁¹³CH₄₈F₁₂+H]⁺ 1502.3671; found 1502.3710 [M+H]⁺.

Table S1. Crystallographic data precursor **2a**, and macrocycles **3a–d**, isomorph **3a'**, and diferrocenyl derivative **5**.

Compound	2a	3a · 2toluene	3a'	3b · 2CH ₃ CN	3c · 0.9CHCl ₃	3d · CHCl ₃	5 · CHCl ₃
CCDC numbers	2550375	2550376	2550377	2550378	2550379	2550380	2550381
Empirical formula	C ₄₀ H ₃₈ Si ₂	C ₁₁₆ H ₇₆	C ₁₀₂ H ₆₀	C ₁₁₈ H ₉₀ N ₂	C _{102.9} H _{48.90} Cl _{2.70} F ₁₂	C ₅₉ H ₄₇ Cl ₃ Fe ₂	C ₅₉ H ₄₇ Cl ₃ Fe ₂
Formula weight	1469.76	1469.76	1285.50	1535.91	1608.83	974.01	974.01
Temperature (K)	100.00(10)	100.00(10)	100.00(10)	100.00(10)	100.00(10)	100.00(10)	100.00(10)
Wavelength (Å)	1.54184	1.54184	1.54184	1.54184	1.54184	1.54184	1.54184
Crystal system	Monoclinic	Monoclinic	Triclinic	Monoclinic	Triclinic	Triclinic	Triclinic
Space group	<i>P</i> 2 ₁ / <i>n</i>	<i>I</i> 2/ <i>a</i>	<i>P</i> -1	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> -1	<i>P</i> -1	<i>P</i> -1
<i>a</i> (Å)	12.1937(6)	21.4999(2)	10.3845(7)	12.65630(10)	15.0766(7)	5.80560(10)	5.80560(10)
<i>b</i> (Å)	5.9510(2)	20.89980(10)	18.1721(11)	36.6318(3)	16.3859(8)	15.9743(6)	15.9743(6)
<i>c</i> (Å)	47.117(3)	21.7375(2)	23.6809(16)	18.7282(2)	22.1854(13)	25.2401(5)	25.2401(5)
α (°)	90.00	90.00	71.279(6)	90.00	75.966(5)	83.365(2)	83.365(2)
β (°)	90.923(5)	117.3860(10)	85.550(6)	95.1360(10)	76.006(4)	86.052(2)	86.052(2)
γ (°)	90.00	90.00	87.146(5)	90.00	68.247(4)	87.760(3)	87.760(3)
<i>V</i> (Å ³)	3394.1(3)	8672.93(14)	4218.1(5)	8647.96(14)	4867.8(5)	2318.44(11)	2318.44(11)
<i>Z</i>	4	4	2	4	2	2	2
ρ_{calcd} (g·cm ⁻³)	1.125	1.126	1.012	1.180	1.098	1.395	1.395
μ (mm ⁻¹)	1.127	0.483	0.437	0.509	1.319	6.906	6.906
<i>F</i> (000)	1244	3088	1344	3248	1640	1008	1008
Crystal size/mm	0.177·0.055·0.032	0.225·0.100·0.046	0.141·0.028·0.025	0.161·0.064·0.051	0.217·0.047·0.037	0.212·0.037·0.028	0.212·0.037·0.028
θ range / °	3.660–66.489	3.117–55.491	3.706–66.500	2.658–66.499	2.946–66.496	2.786–66.497	2.786–66.497
Refl. collected	41346	57852	50526	104525	52749	22201	22201
Indep. Refl.	5903	7641	14711	15171	16946	8011	8011
<i>R</i> _{int}	0.1577	0.0346	0.3661	0.0466	0.0912	0.0847	0.0847
Transmission factors (min/max)	0.863/1.000	0.604/1.000	1.000/1.000		0.809/1.000	0.680/1.000	0.680/1.000
Data/restraints/param.	5903/64/418	7641/0/563	14711/1224/1077	15171/2/1095	16946/0/1099	8011/120/637	8011/120/637
<i>R</i> 1, ^a <i>wR</i> 2 ^b (<i>I</i> > 2 σ (<i>I</i>))	0.1069, 0.2796	0.0375, 0.0943	0.1074, 0.2297	0.0646, 0.1799	0.0762, 0.1994	0.0664, 0.1610	0.0664, 0.1610
<i>R</i> 1, ^a <i>wR</i> 2 ^b (all data)	0.1428, 0.3012	0.0409, 0.0962	0.2799, 0.2872	0.0786, 0.1885	0.1204, 0.2188	0.0901, 0.1705	0.0901, 0.1705
Quality-of-fit ^c	1.049	1.019	0.835	1.038	0.997	1.061	1.061

$$R_{\text{int}} = \frac{\sum |F_o^2 - \langle F_o^2 \rangle|}{\sum |F_o^2|}$$

$$^a R1 = \frac{\sum ||F_o| - |F_c||}{\sum |F_o|}, \quad ^b wR2 = \frac{[\sum [w(F_o^2 - F_c^2)^2]]}{[\sum [w(F_o^2)^2]]}$$

$$^c \text{Quality-of-fit} = \frac{[\sum [w(F_o^2 - F_c^2)^2]]}{(N_{\text{obs}} - N_{\text{params}})}^{1/2}, \text{ based on all data.}$$

Chemical Reduction of 3a

All manipulations were carried out using break-and-seal and glove-box techniques under an atmosphere of argon.¹⁸ Tetrahydrofuran (THF) and hexanes (Sigma Aldrich) were dried over Na/benzophenone and distilled prior to use. THF-*d*₈ (Sigma Aldrich) was dried over NaK₂ alloy and vacuum-transferred. Rubidium (99.5 %), [2.2.2]cryptand (99.0%), and 18-crown-6 ether (99.0 %) were purchased from Sigma Aldrich and used as received. The UV-Vis absorption spectra were recorded on a Shimadzu UV-2600i UV-Vis spectrophotometer. The ¹H NMR spectra were recorded on a JEOL ECZR 600 spectrometer (600 MHz for ¹H). Chemical shifts (δ) are reported in parts per million (ppm) and referenced to the resonances of the corresponding solvent used. The EPR spectra were collected with an ADANI SPINSCAN X EPR spectrometer with the following parameters: center field = 335.00 mT, sweep width = 15 mT, sweep time = 60 s, modulation amplitude = 100 uT, attenuation = 20 dB. The oxygen- and moisture sensitivity of the reduced products, [Rb_{crypt}]₂[3a] and [Rb_{crown}]₂[3a], prevented obtaining elemental analysis data.

Preparation of [Rb(cryptand)]₂[3a]·2THF·C₆H₁₄ ([Rb_{crypt}]₂[3a]·2THF·C₆H₁₄)

THF (1.0 mL) was added to a customized glass system containing Rb metal (2.0 mg, 0.023 mmol), **3a** (2.0 mg, 0.002 mmol), and [2.2.2]cryptand (1.5 mg, 0.004 mmol). The mixture was allowed to stir under argon at 25 °C for 40 minutes in a closed system. The initial red color of the suspension changed to red purple after 20 minutes, blue-violet after 35 minutes and remained the same until the reaction was stopped. After 40 minutes, the violet suspension was filtered, and the violet filtrate was layered with 1.0 mL hexanes. The ampule was sealed and kept at 5 °C. After 5 days, black plates formed in the ampule. Yield: 1.5 mg, 39%. UV-vis (THF): λ_{max} 382, 516, 690 nm.

Preparation of [Rb(18-crown-6)]₂[3a]·3.5THF ([Rb_{crypt}]₂[3a]·3.5THF)

THF (1.0 mL) was added to a customized glass system containing Rb metal (2.0 mg, 0.023 mmol), **3a** (2.0 mg, 0.002 mmol), and 18-crown-6 (1.0 mg, 0.004 mmol). The mixture was allowed to stir under argon at 25 °C for 30 minutes in a closed system. The initial red color of the suspension changed to red purple after 10 minutes, blue after 20 minutes and remained the same until the reaction was stopped. After 30 minutes, the blue suspension was filtered, and the blue filtrate was layered with 1.0 mL hexanes. The ampule was sealed and kept at 5 °C. After 5 days, black needles formed in the ampule. Yield: 2.1 mg, 60%. UV-vis (THF): λ_{max} 328, 364, 570, 720 nm.

UV-vis Spectroscopic Investigation

Sample preparation (in situ 3a/Rb): THF (3.0 mL) was added to a quartz cuvette containing **3a** (0.3 mg, 0.0002 mmol) and Rb metal (1.0 mg, 0.0117 mmol) under argon atmosphere. The ampule was sealed with a Teflon stopper under argon. UV-vis absorption spectra were monitored at different reaction times at room temperature.

Sample preparation (crystals): THF (3.0 mL) was added to a quartz cuvette containing crystalline solids [Rb_{crypt}]₂[3a] (0.5 mg, 0.0002 mmol) or [Rb_{crown}]₂[3a] (0.3 mg, 0.0001 mmol) under argon atmosphere. The ampule was sealed with a Teflon stopper under argon. UV-vis absorption spectra were collected at room temperature.

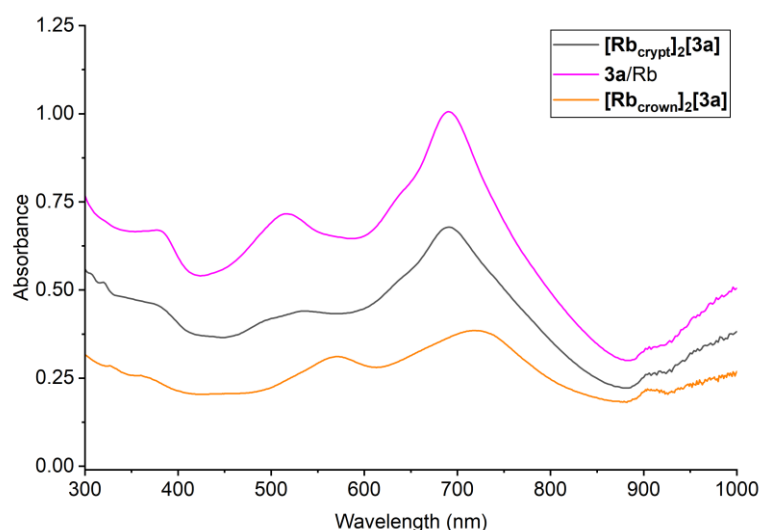


Fig. S5. UV-Vis spectra of crystalline samples of [Rb_{crypt}]₂[3a] and [Rb_{crown}]₂[3a] dissolved in THF in comparison to the in situ generated 3a²⁻/Rb at room temperature.

¹⁸ W. Stawski, Y. Zhu, Z. Wei, M. A. Petrukhina, H. L. Anderson, *Chem. Sci.* **2023**, *14*, 14109–14114.

NMR and EPR Spectroscopic Investigation

Sample preparation (solution): Crystals of $[\text{Rb}_{\text{crypt}}]_2[\mathbf{3a}]$ (2.0 mg, 0.0009 mmol) or $[\text{Rb}_{\text{crown}}]_2[\mathbf{3a}]$ (1.0 mg, 0.0003 mmol) were washed with fresh hexanes, dried under vacuum, dissolved in $\text{THF-}d_8$ (~0.7 mL), and transferred into an NMR tube (O.D. 5 mm). The tube was sealed under argon, and the NMR and EPR spectra were collected at room temperature.

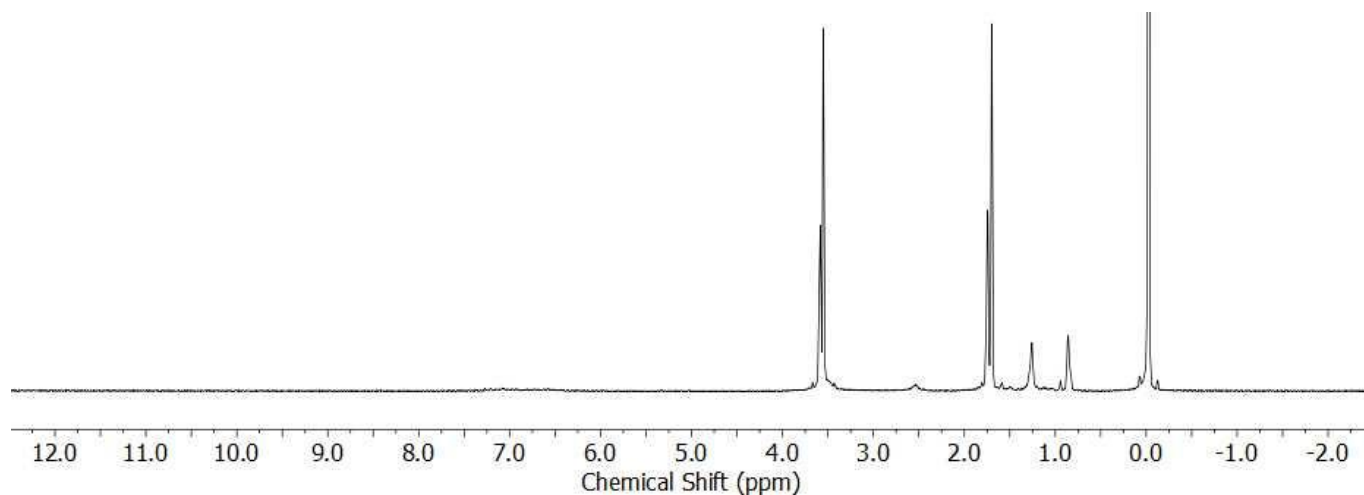


Fig. S6. ^1H NMR spectrum of crystals of $[\text{Rb}_{\text{crypt}}]_2[\mathbf{3a}]$ dissolved in $\text{THF-}d_8$ at 25 °C.

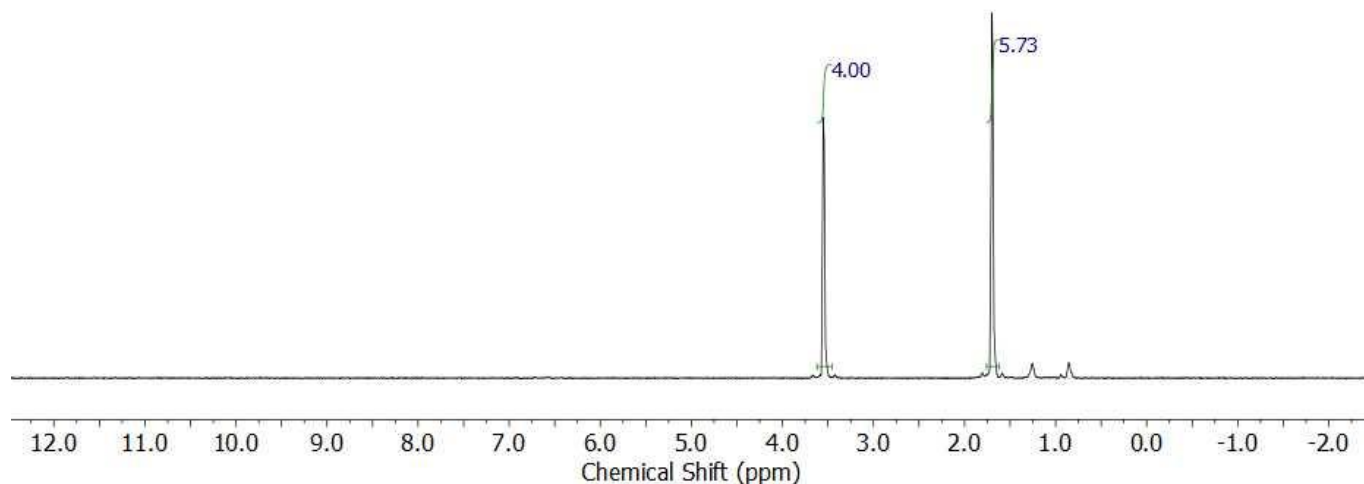


Fig. S7. ^1H NMR spectrum of crystals of $[\text{Rb}_{\text{crown}}]_2[\mathbf{3a}]$ dissolved in $\text{THF-}d_8$ at 25 °C.

Sample preparation (solid): Crystals of $[\text{Rb}_{\text{crypt}}]_2[\mathbf{3a}]$ (1.5 mg, 0.0006 mmol) were washed with fresh hexanes, dried under vacuum, and transferred into an NMR tube (O.D. 5 mm). The tube was sealed under argon, and the EPR spectra were collected at variable temperature.

Sample preparation (in situ): THF (0.8 mL) was added to an NMR tube containing excess Rb metal (2.0 mg, 0.0233 mmol), $\mathbf{3a}$ (1.0 mg, 0.0008 mmol), and [2.2.2]cryptand (1.0 mg, 0.0026 mmol). The tube was sealed under argon. EPR spectra was monitored at different reaction time at 30 °C.

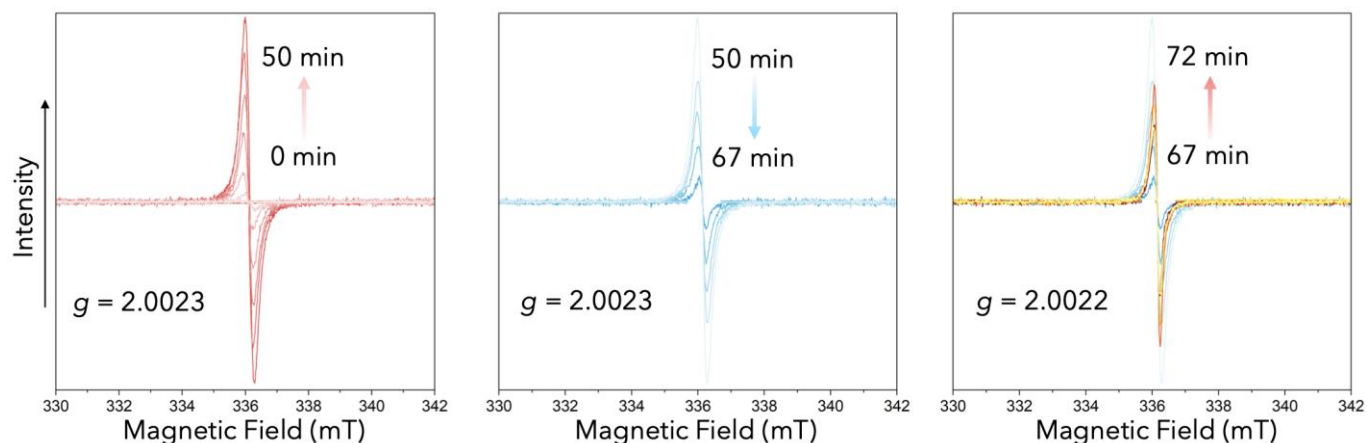


Fig. S8. EPR spectra of **3a**/Rb/crypt at different reaction time in THF at 30 °C.

Crystal Structure Solution and Refinement

Data collections of **[Rb_{crypt}]₂[3a]** and **[Rb_{crypt}]₂[3a]** were performed at 100.00(10) K on a Rigaku XtaLAB Synergy-S X-ray diffractometer equipped with a HyPix-6000HE hybrid photon counting (HPC) detector and a microfocus Cu-K α radiation ($\lambda = 1.54184 \text{ \AA}$). Data collection strategy to ensure completeness and desired redundancy was determined using CrysAlisPro.¹⁹ Data processing was performed also using CrysAlisPro. Empirical absorption correction was applied using the SCALE3 ABSPACK scaling algorithm.²⁰ The structures were solved by SHELXT (version 2018/2)²¹ and refined by full-matrix least-squares procedures using the SHELXL (version 2019/3)²² software through the OLEX2 graphical interface.²³ All non-hydrogen atoms, including those in disordered parts, were refined anisotropically. Hydrogen atoms were included in idealized positions for structure factor calculations with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ and $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{C})$ for methyl groups. In **[Rb_{crypt}]₂[3a]**, one THF molecule and two phenyl groups were found to be disordered. In **[Rb_{crypt}]₂[3a]**, one diphenylmethylene group was found to be disordered. The disordered parts were modeled with two orientations with their relative occupancies refined. The geometries of the disordered parts were restrained to be similar. They were also restrained to have the same U_{ij} components, with a standard uncertainty of 0.01 \AA^2 . In each unit cell of **[Rb_{crypt}]₂[3a]**, four hexanes solvent molecules were found to be severely disordered and removed by the Olex2's solvent mask subroutine.¹⁴ The total void volume was 1182.4 \AA^3 , equivalent to 9.21 % of the unit cell's total volume. In each unit cell of **[Rb_{crypt}]₂[3a]**, seven THF solvent molecules were found to be severely disordered and removed by the Olex2's solvent mask subroutine.¹⁴ The total void volume was 1187.9 \AA^3 , equivalent to 20.30 % of the unit cell's total volume. Besides, the structure of **[Rb_{crypt}]₂[3a]** was refined as a 2-component non-merohedral twin. Crystallographic data have been deposited at the Cambridge Crystallographic Data Centre. Further crystal and data collection details, along with CCDC numbers are listed in Table S1. These data can be obtained free of charge via <https://www.ccdc.cam.ac.uk/structures/>, or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, U.KCB21EZ, UK (fax +441223336033; email deposit@ccdc.cam.ac.uk). The ORTEP drawings and additional structural figures, along with the key bond distances and angles, are also shown below.

¹⁹ Rigaku Corporation. Rigaku Oxford Diffraction, CrysAlisPro Software System, Version 1.171.43.92a. 2023.

²⁰ Rigaku Oxford Diffraction. SCALE3 ABSPACK; A Rigaku Oxford Diffraction Program (1.0.11,Gui:1.0.7) (C). 2005.

²¹ G. M. Sheldrick, *Acta Crystallogr. Sect. Found. Adv.* **2015**, *71*, 3–8.

²² G. M. Sheldrick, *Acta Crystallogr. Sect. C Struct. Chem.* **2015**, *71*, 3–8.

²³ O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard, JH. Puschmann, *J. Appl. Crystallogr.* **2009**, *42*, 339–341.

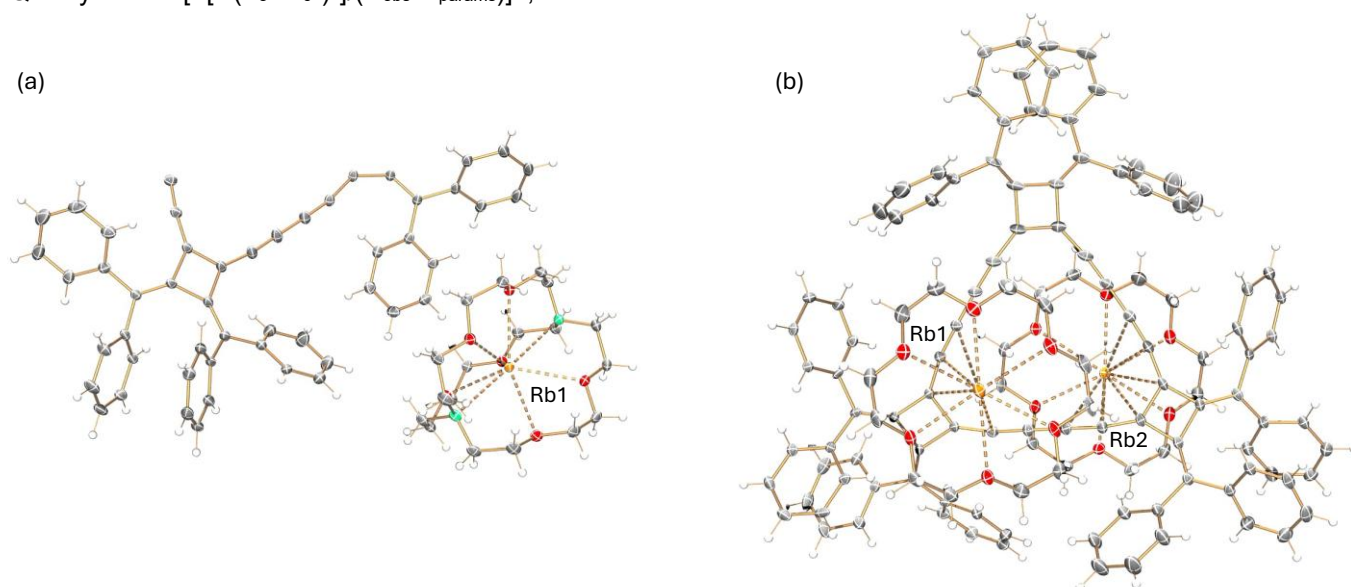
Table S2. Crystallographic data of **[Rb_{crypt}]₂[3a]**·2THF·C₆H₁₄ and **[Rb_{crown}]₂[3a]**·3.5THF.

Compound	[Rb_{crypt}]₂[3a] ·2THF·C ₆ H ₁₄	[Rb_{crown}]₂[3a] ·3.5THF
CCDC numbers	2551069	2551070
Empirical formula	C ₁₅₂ H ₁₆₂ N ₄ O ₁₄ Rb ₂	C ₁₄₀ H ₁₃₆ O _{15.50} Rb ₂
Formula weight	2439.79	2237.42
Temperature (K)	100.00(10)	100.00(10)
Wavelength (Å)	1.54184	1.54184
Crystal system	Monoclinic	Triclinic
Space group	<i>C2/c</i>	<i>P-1</i>
<i>a</i> (Å)	23.90607(12)	13.01556(12)
<i>b</i> (Å)	26.15504(9)	18.7307(2)
<i>c</i> (Å)	22.71299(9)	25.82470(16)
α (°)	90.00	96.6869(7)
β (°)	115.3036(6)	90.9842(6)
γ (°)	90.00	110.3305(9)
<i>V</i> (Å ³)	12839.05(11)	5852.20(10)
<i>Z</i>	4	2
ρ_{calcd} (g·cm ⁻³)	1.262	1.270
μ (mm ⁻¹)	1.505	1.606
<i>F</i> (000)	5152	2348
Crystal size (mm)	0.09×0.11×0.21	0.05×0.10×0.32
θ range for data collection (°)	3.380–79.864	2.537–79.719
Reflections collected	80954	135186
Independent reflections	13826 [<i>R</i> _{int} = 0.0201]	135186 [<i>R</i> _{int} = 0.0542]
Transmission factors (min/max)	0.80074/1.00000	0.79974/1.00000
Data/restraints/params.	13826/550/904	135186/493/1374
<i>R</i> 1, ^a <i>wR</i> 2 ^b (<i>I</i> > 2 σ (<i>I</i>))	0.0320, 0.0853	0.0919, 0.2526
<i>R</i> 1, ^a <i>wR</i> 2 ^b (all data)	0.0331, 0.0861	0.0982, 0.2562
Quality-of-fit ^c	1.050	1.026

$$R_{\text{int}} = \frac{\sum |F_o^2 - \langle F_o^2 \rangle|}{\sum |F_o^2|}$$

$${}^a R1 = \frac{\sum ||F_o| - |F_c||}{\sum |F_o|}, \quad {}^b wR2 = \frac{[\sum [w(F_o^2 - F_c^2)^2]]}{[\sum [w(F_o^2)^2]]}$$

$${}^c \text{Quality-of-fit} = \frac{[\sum [w(F_o^2 - F_c^2)^2]]}{(N_{\text{obs}} - N_{\text{params}})}^{1/2}, \text{ based on all data.}$$

**Fig. S9.** ORTEP drawing of the asymmetric unit of (a) **[Rb_{crypt}]₂[3a]** and (b) **[Rb_{crown}]₂[3a]**, drawn with thermal ellipsoids at the 30% probability level. The interstitial solvent molecules are omitted for clarity. Color key: C grey, O red, N spring green, H white, and Rb orange. Due to symmetry, only one cation moiety and half of the dianion were shown in the asymmetric unit of **[Rb_{crypt}]₂[3a]**.

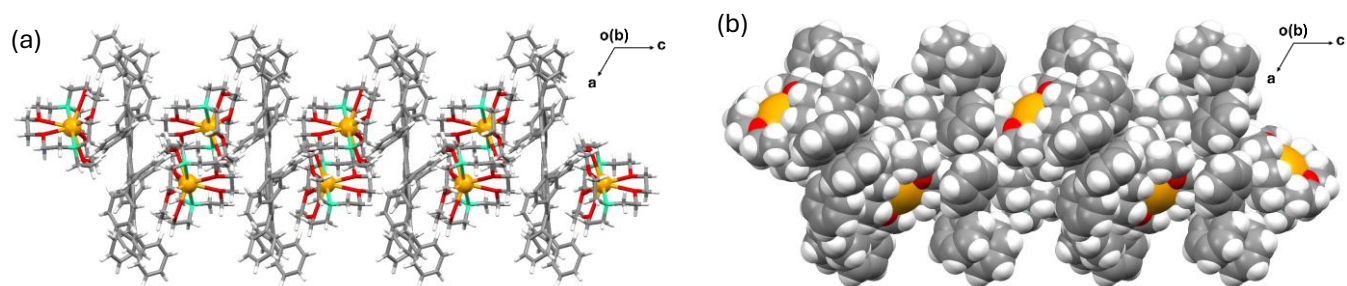
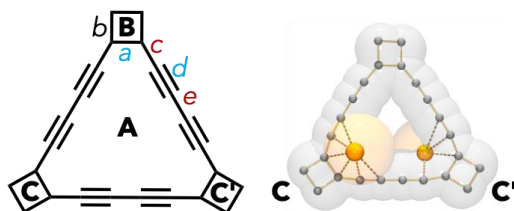


Fig. S10. 1D column packing of $[\text{Rb}_{\text{crypt}}]_2[\mathbf{3a}]$, (a) mixed and (c) space-filling models.

Table S3. Selected distances (Å) and angles (°) in $\mathbf{3a}$ and its dianions, along with the labeling schemes.



Bonds	$\mathbf{3a}$	$[\text{Rb}_{\text{crypt}}]_2[\mathbf{3a}]$	$[\text{Rb}_{\text{crown}}]_2[\mathbf{3a}]$
<i>a</i>	1.399(2)/1.400(2)	1.438(2)/1.439(3)	1.420(5)–1.452(5)
<i>b</i>	1.484(2)–1.491(2)	1.475(2)–1.481(2)	1.458(5)–1.490(5)
<i>c</i>	1.386(2)–1.390(2)	1.365(2)–1.372(2)	1.342(5)–1.386(5)
<i>d</i>	1.218(2)–1.222(2)	1.216(2)–1.230(2)	1.218(5)–1.266(5)
<i>e</i>	1.350(2)	1.330(3)/1.341(2)	1.305(5)–1.358(5)
RMSD/A	$\mathbf{3a}$	$[\text{Rb}_{\text{crypt}}]_2[\mathbf{3a}]$	$[\text{Rb}_{\text{crown}}]_2[\mathbf{3a}]$
A	0.163	0.124	0.222
B	0.040	0.019	0.045
C(C')	0.030	0.022	0.043/0.054

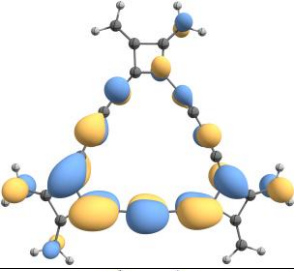
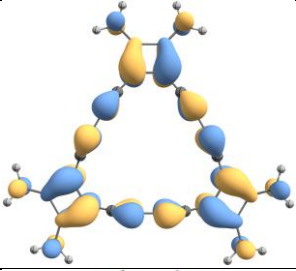
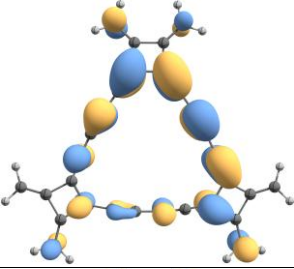
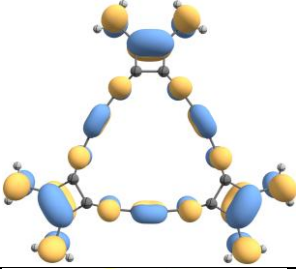
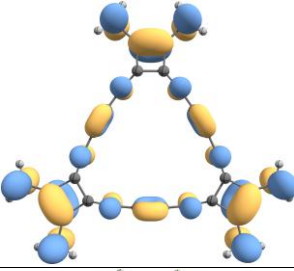
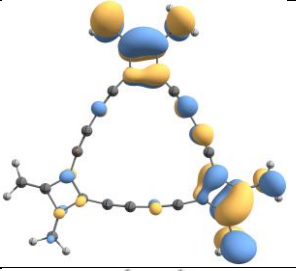
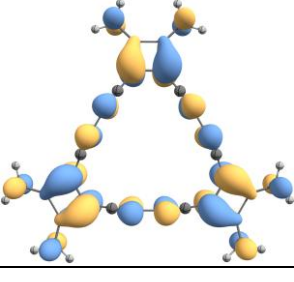
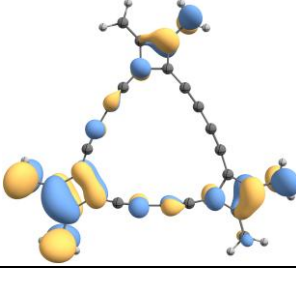
Quantum Chemical Computations.

Table S4. Singlet-Triplet Gibbs free energy gap of neutral **3m**.

Functional	3m (neutral)	
CAM-B3LYP/def2-TZVPP	41.1 kcal/mol	1.78 eV
M06-2X/def2-TZVPP	47.0 kcal/mol	2.04 eV

Table S5. Frontier Orbitals of **3m** and **3m²⁻**.

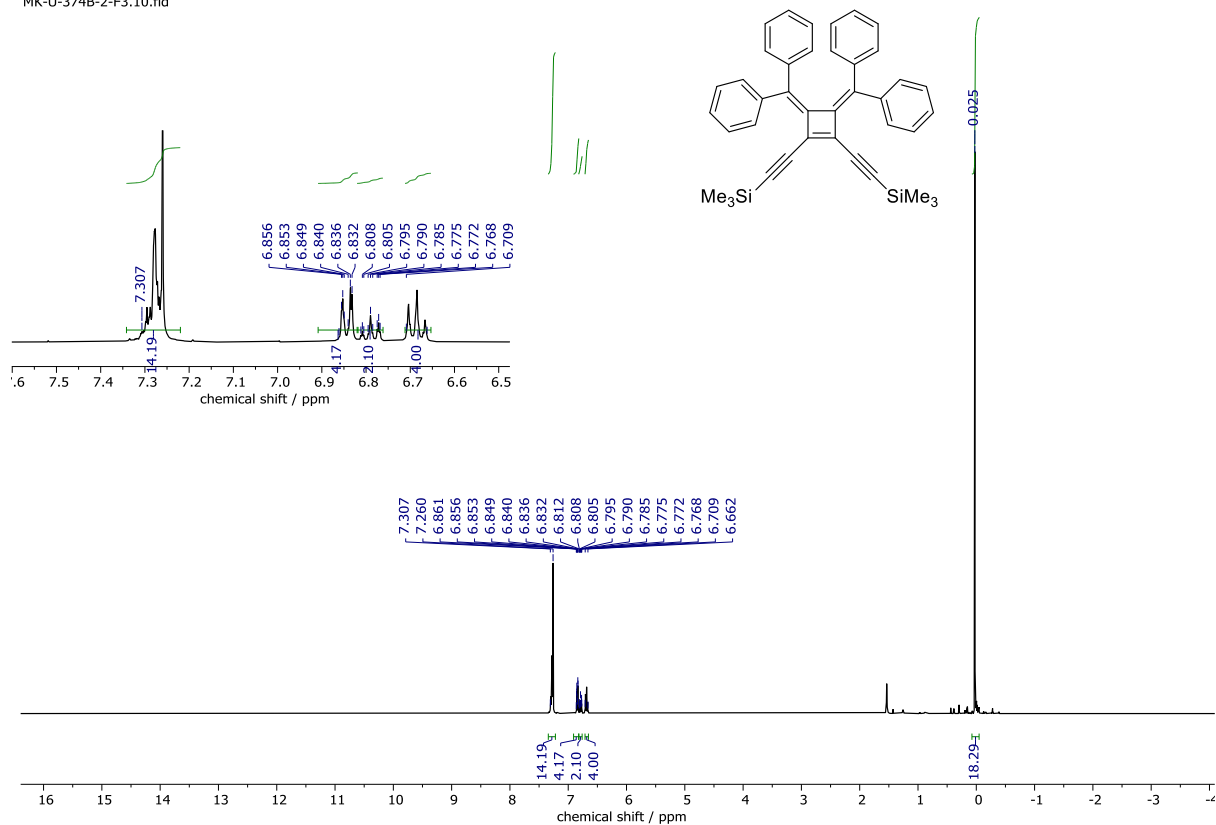
Nr	3m	[3m]²⁻
HOMO-29/31		
HOMO-3		
HOMO-2		
HOMO-1		
HOMO		

LUMO		
LUMO+1		
LUMO+2		
LUMO+3		

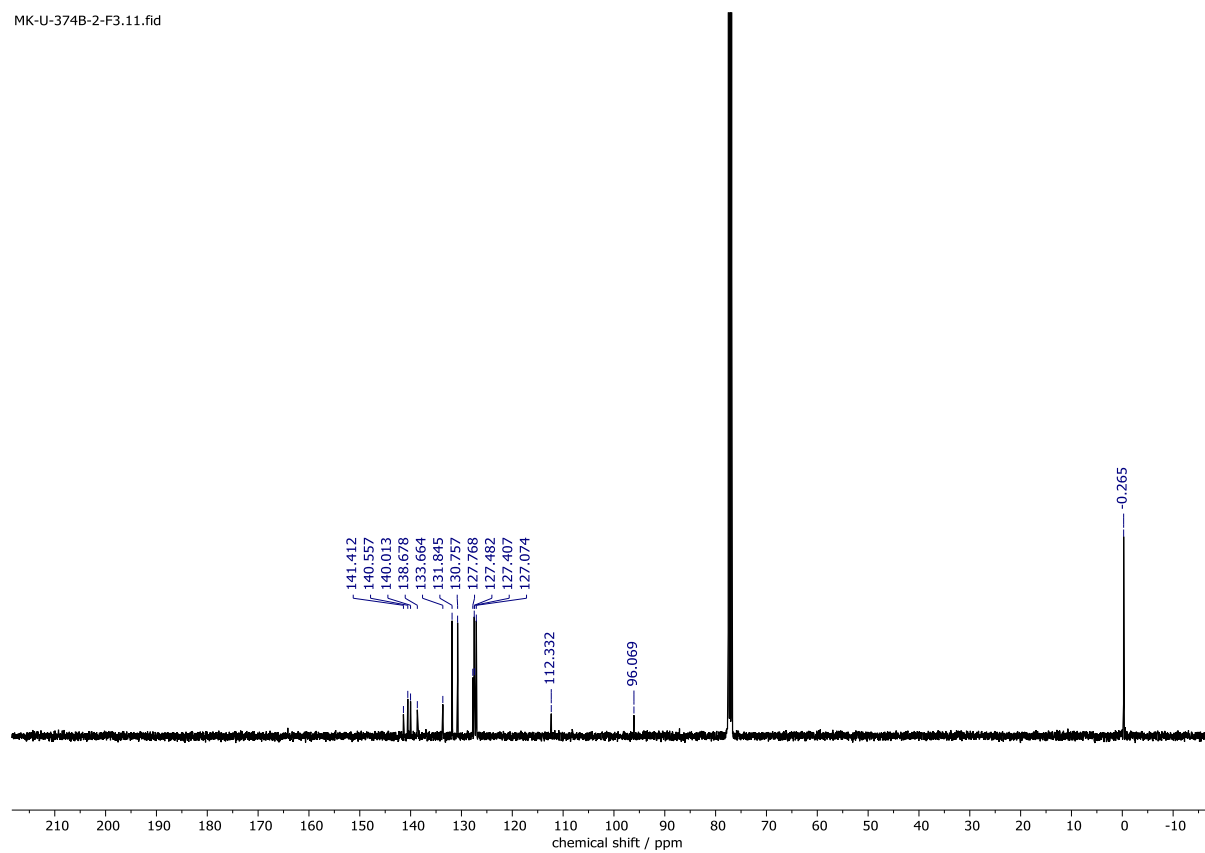
NMR spectra of new compounds

2a

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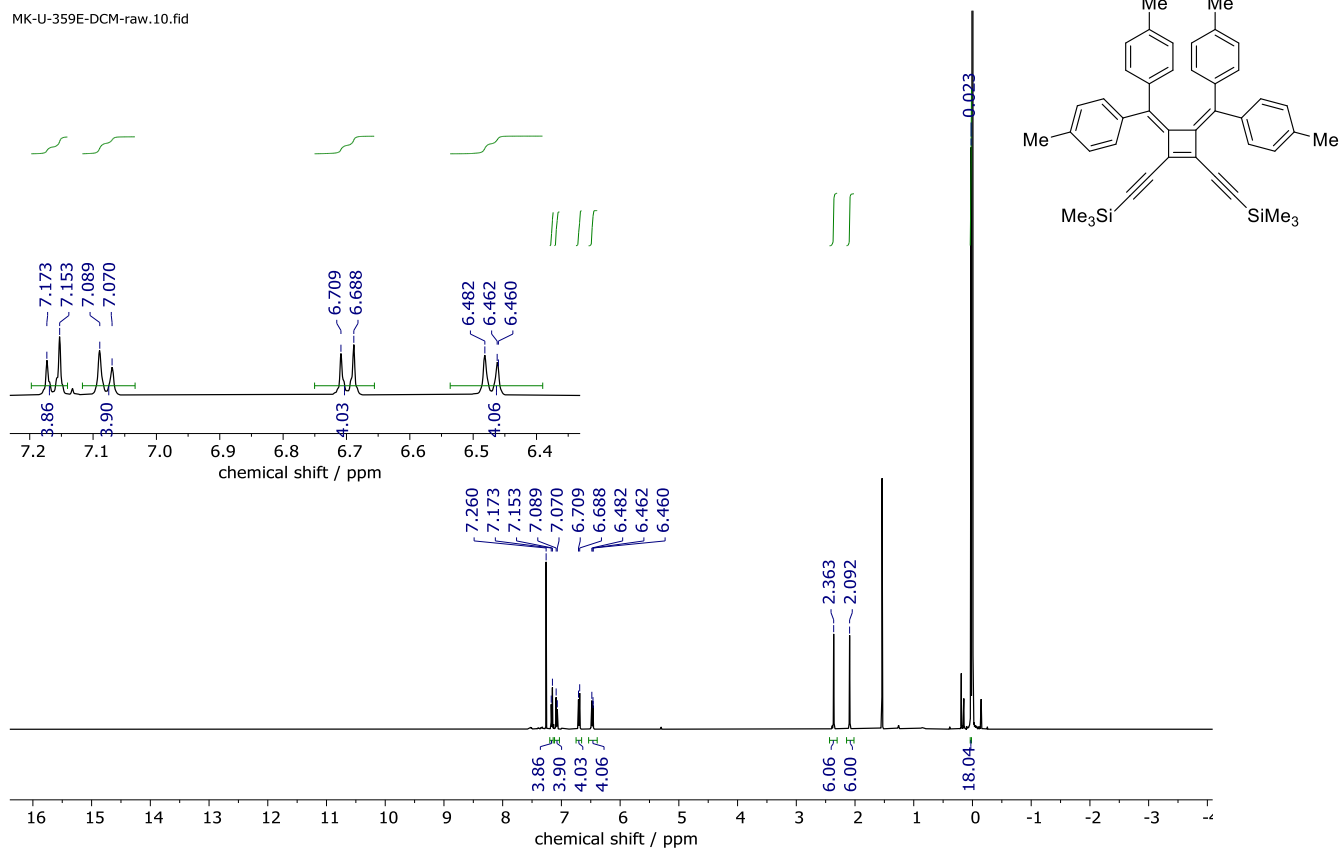


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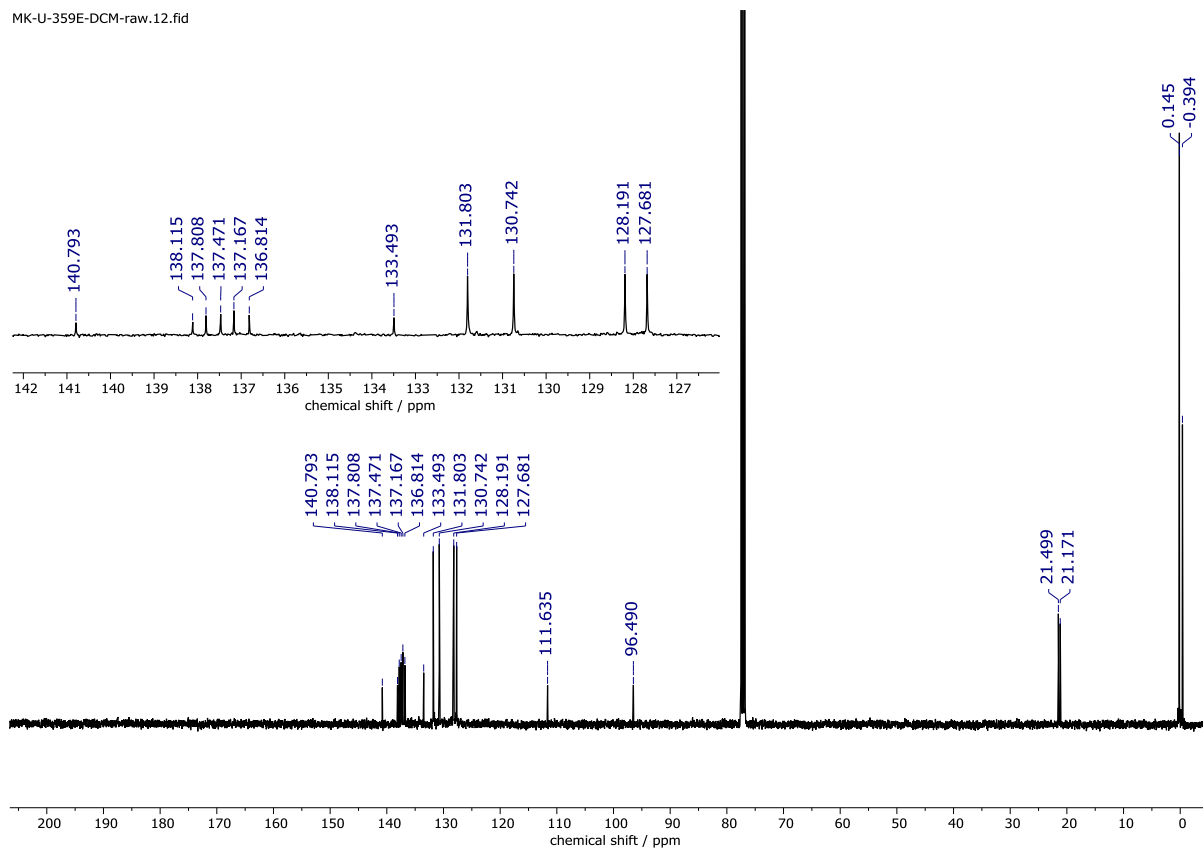


2b

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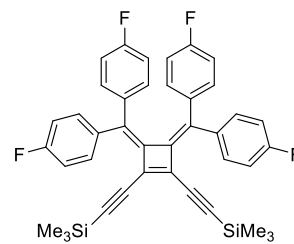
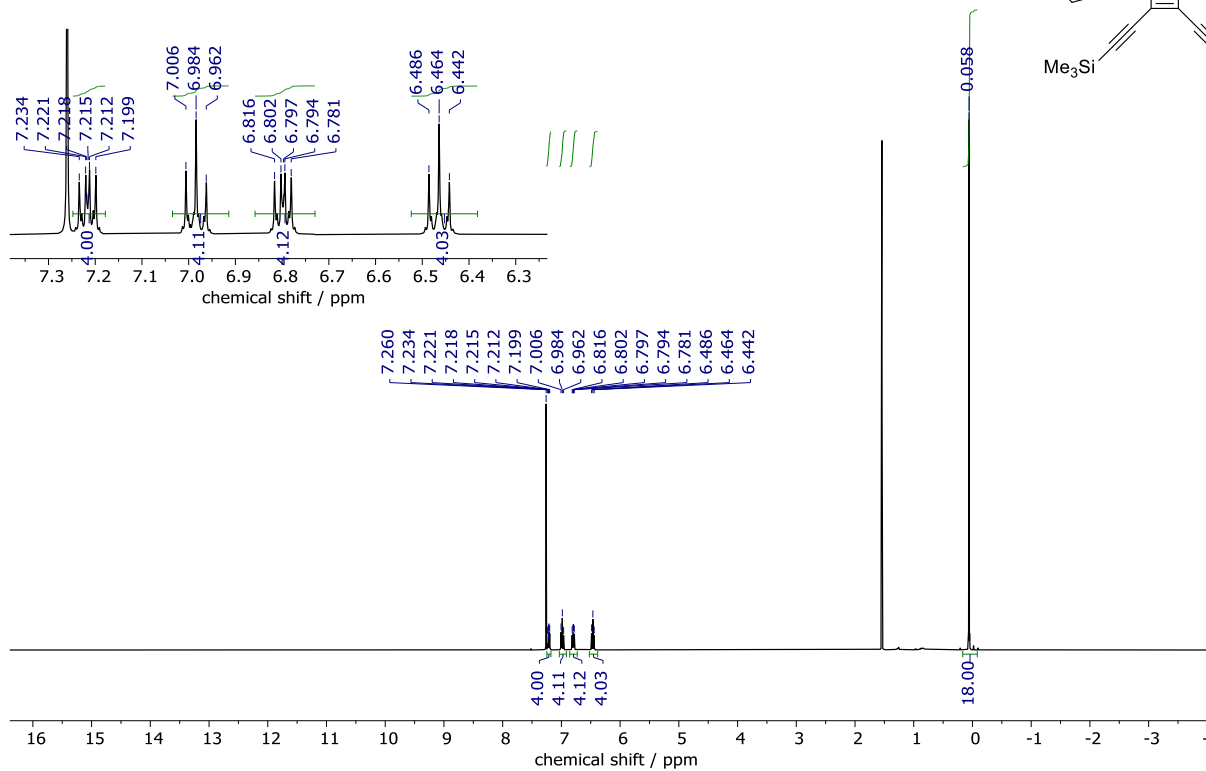


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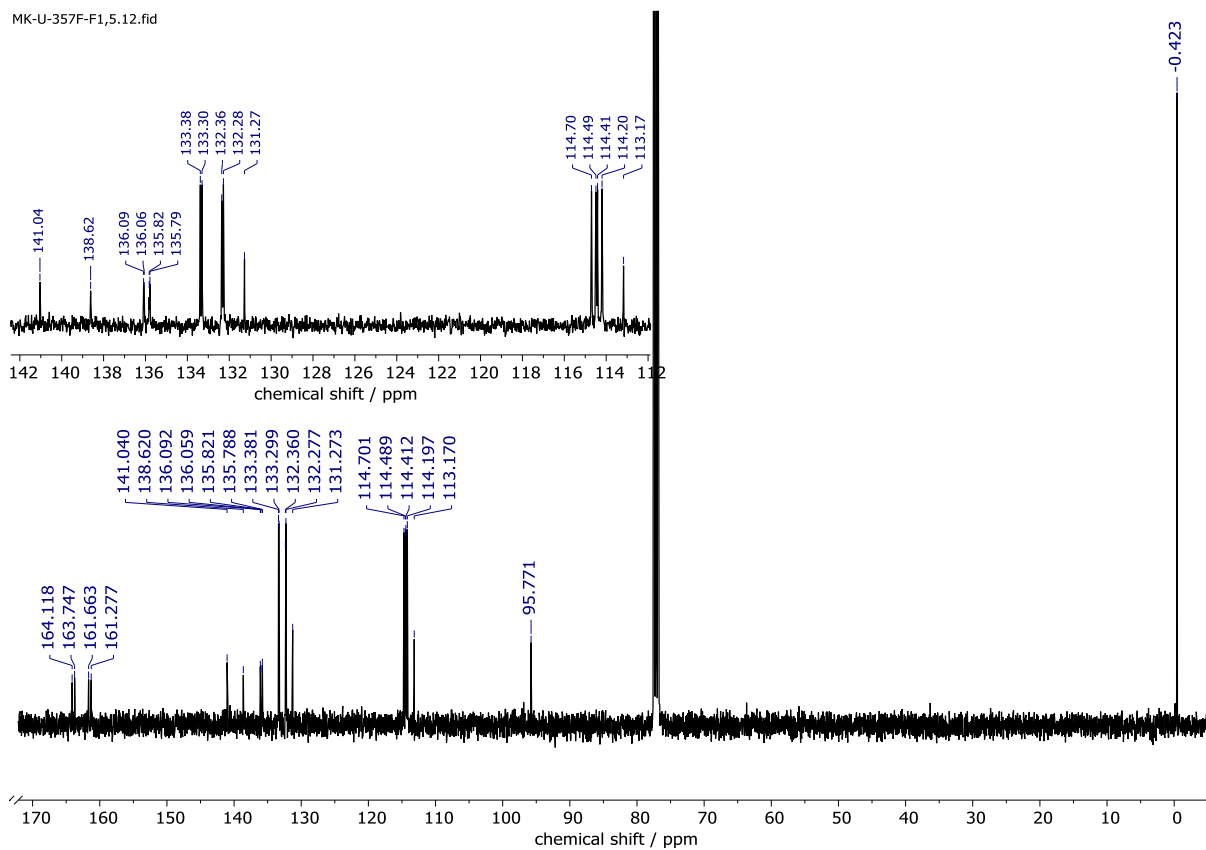


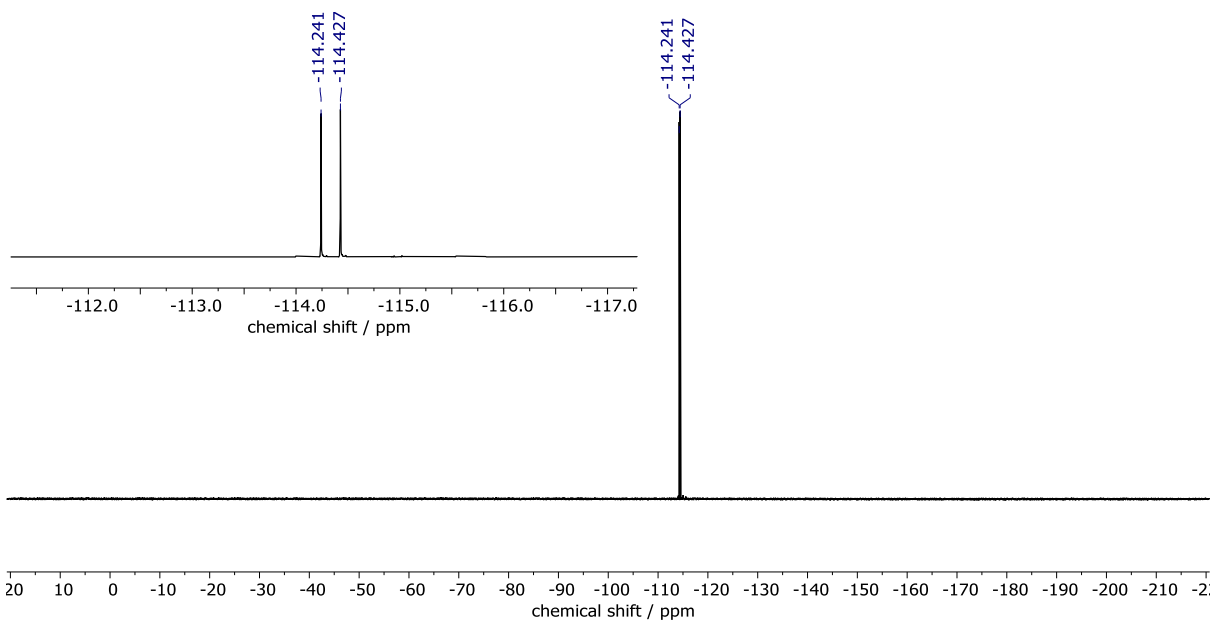
2c

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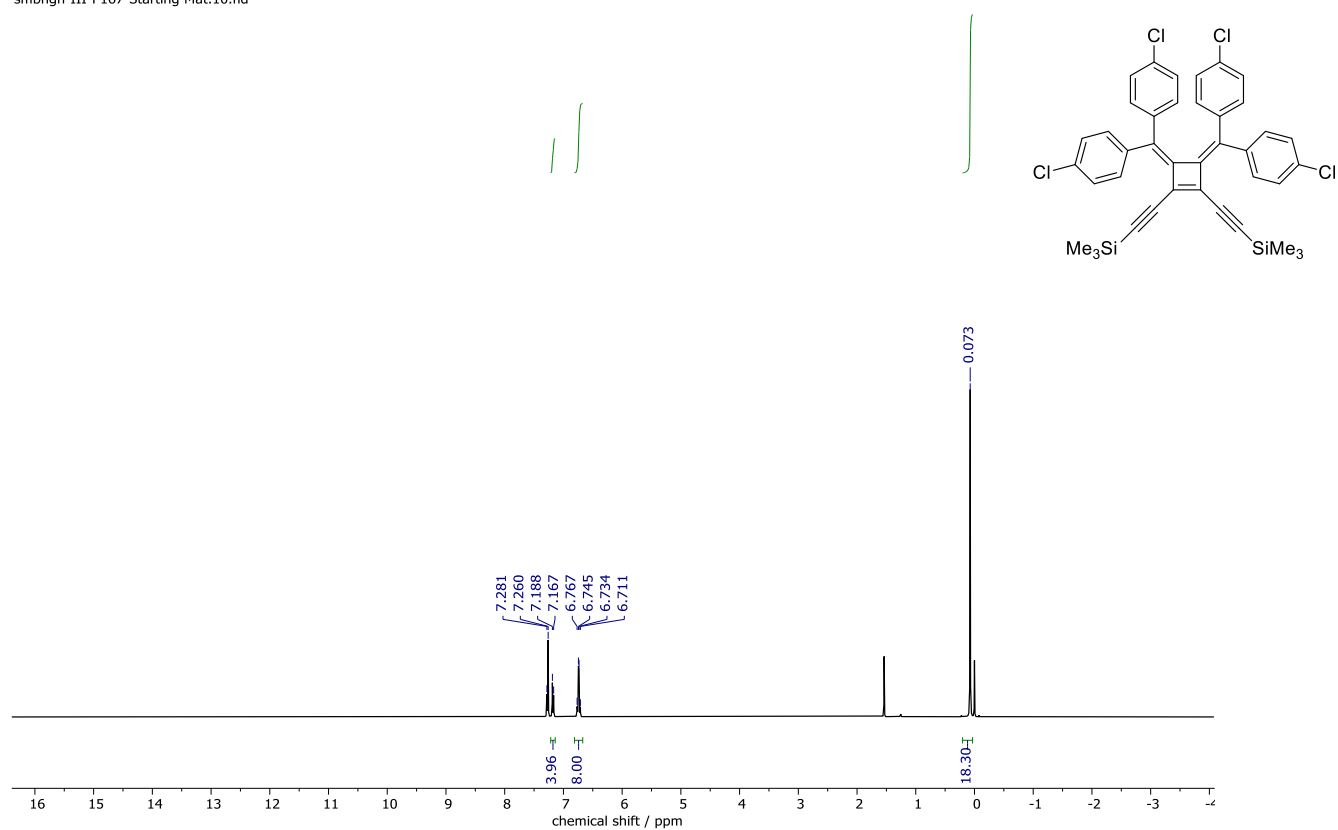
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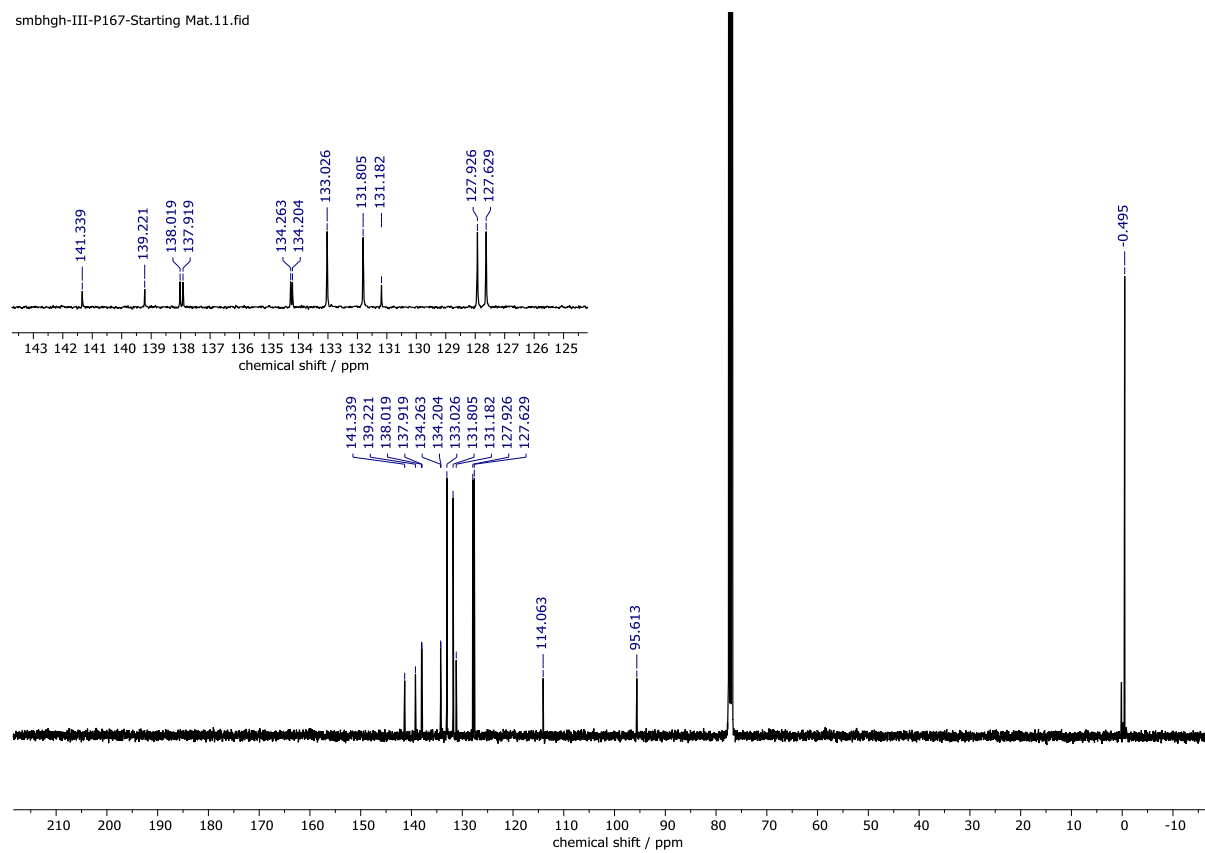


2d

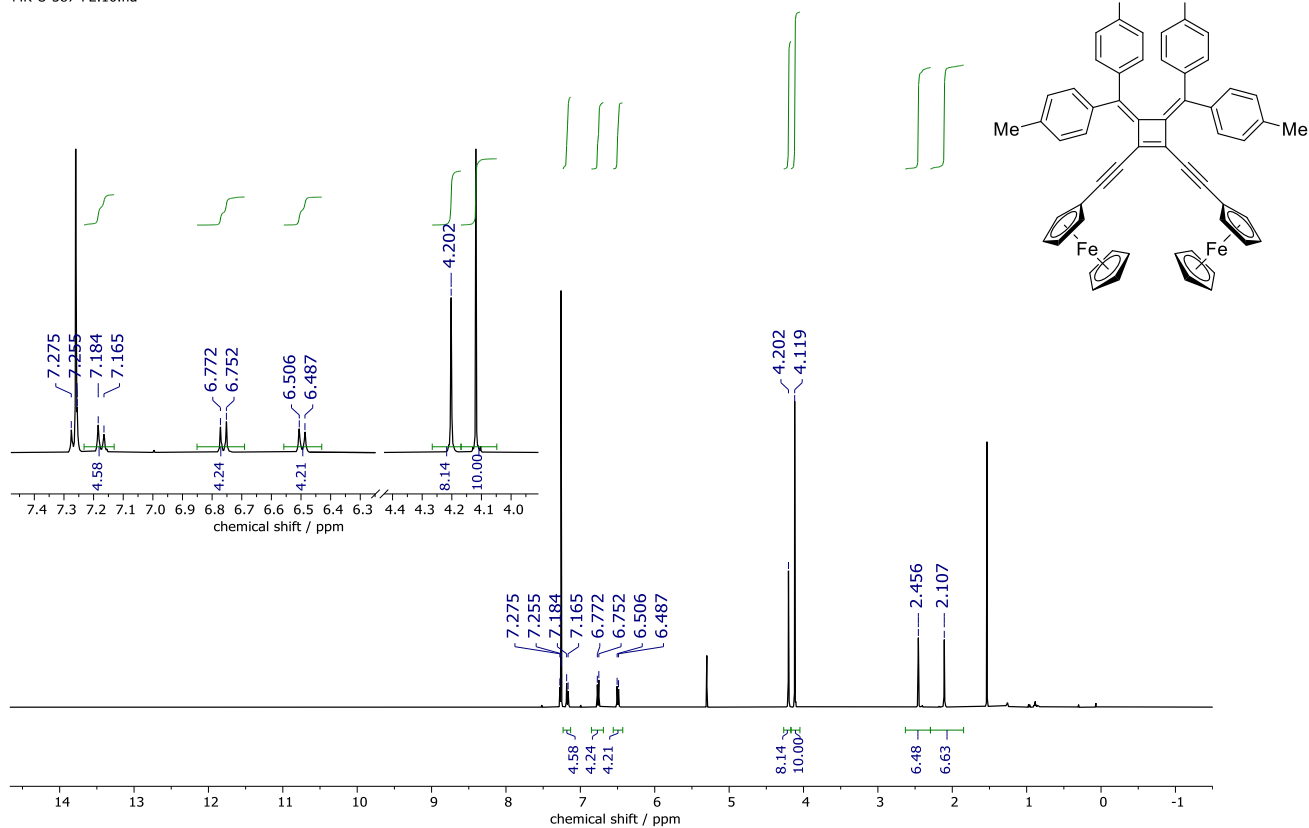
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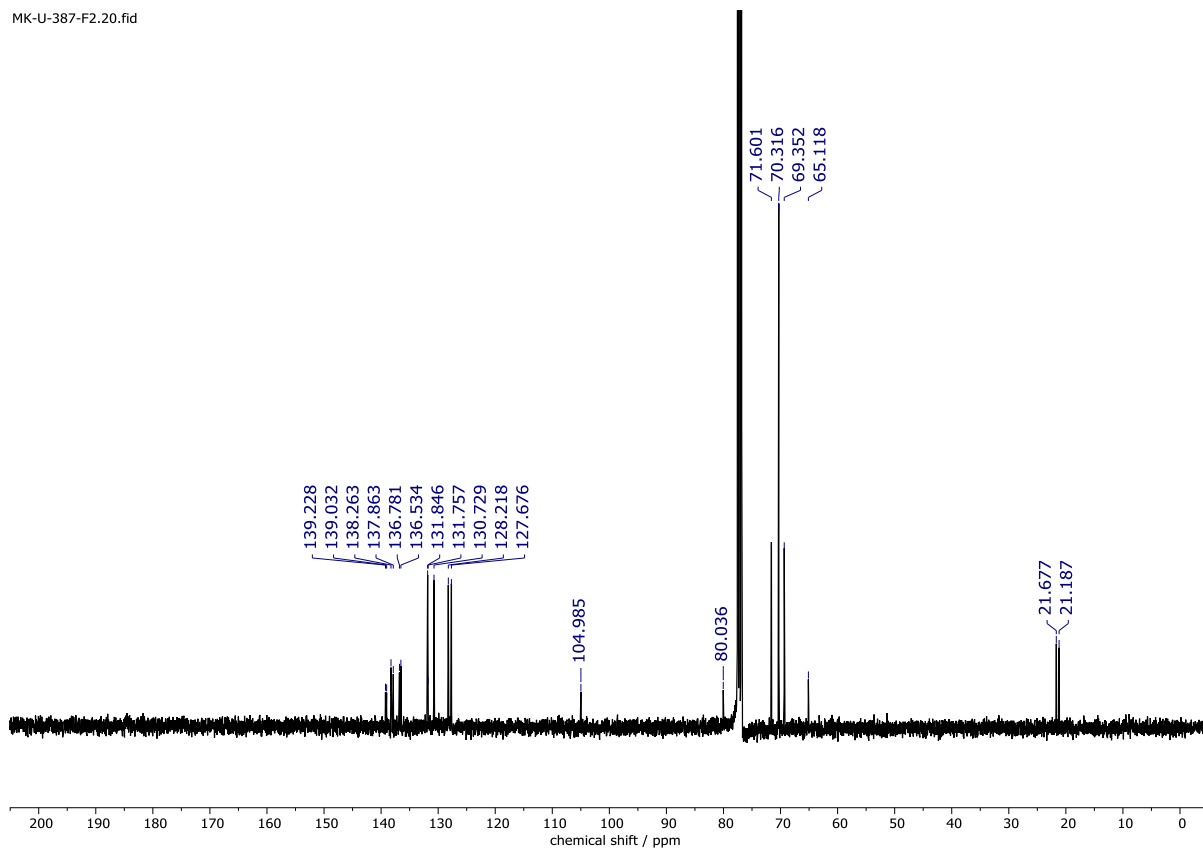
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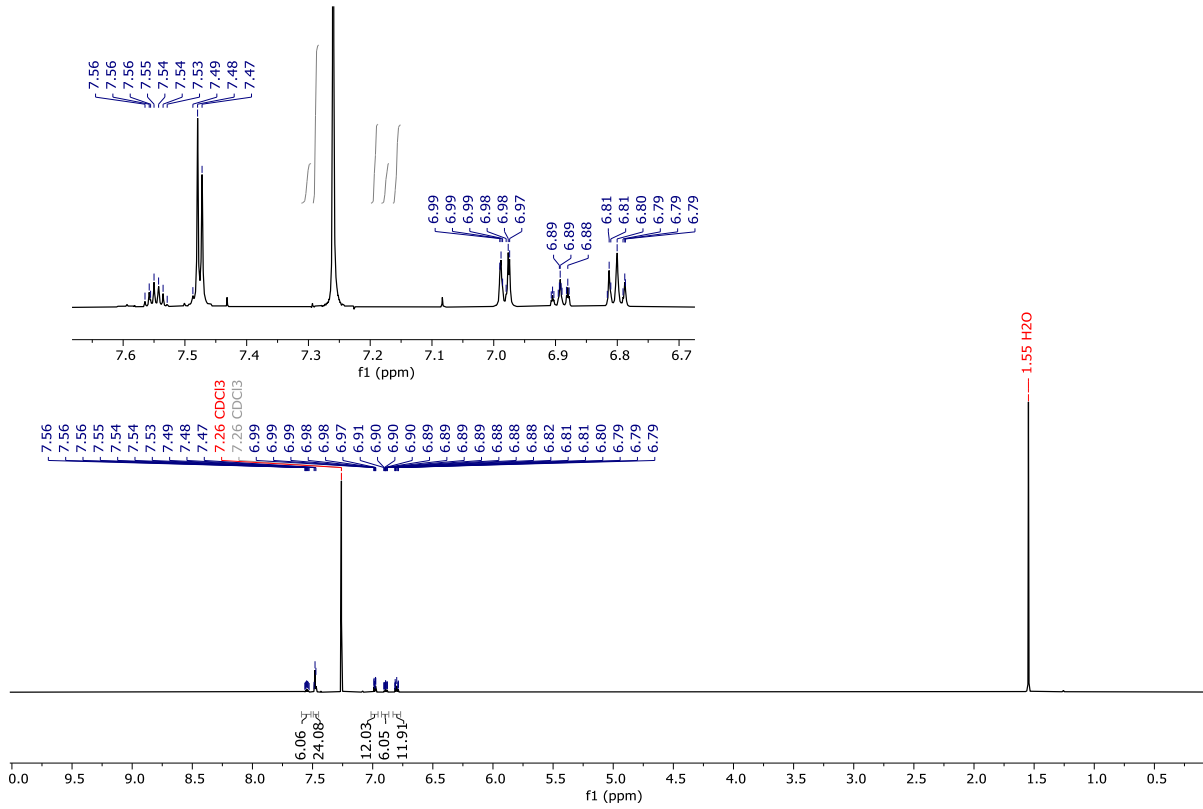


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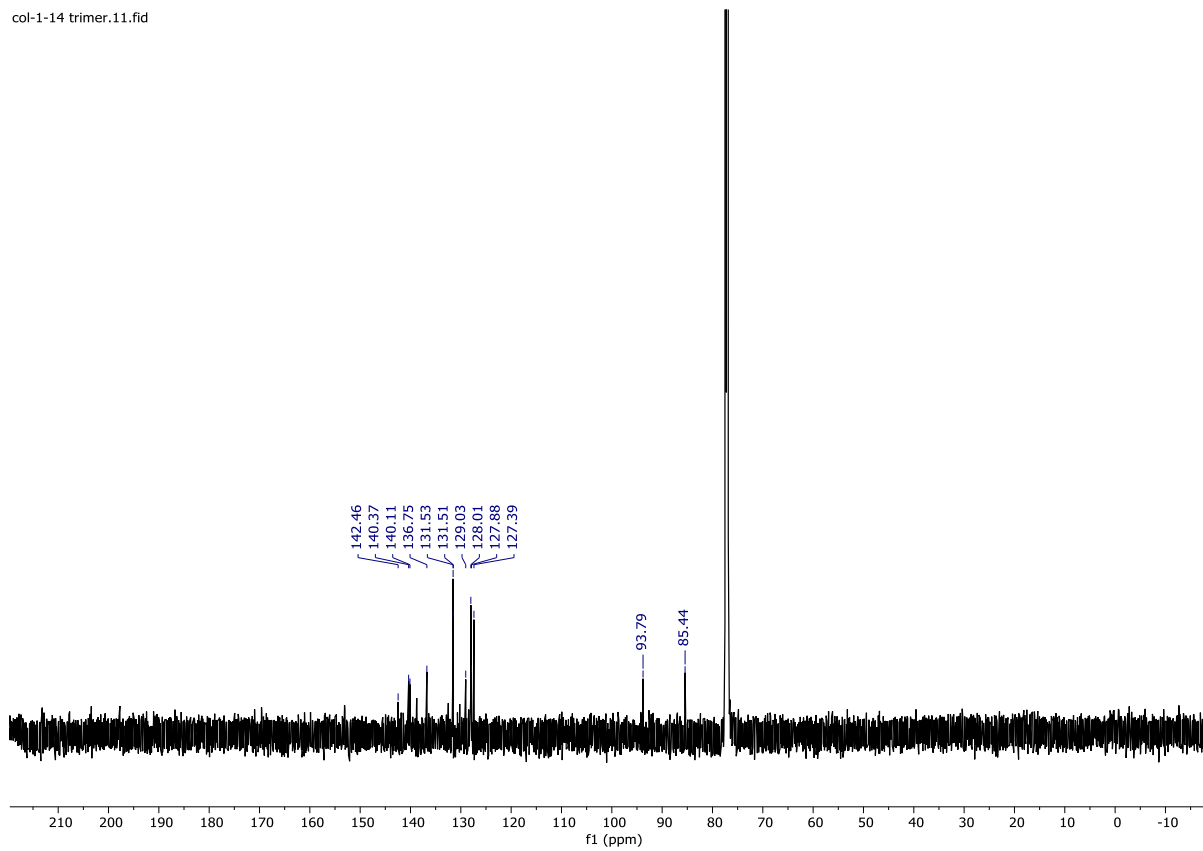


Compound 3a

col-1-14 trimer.10.fid

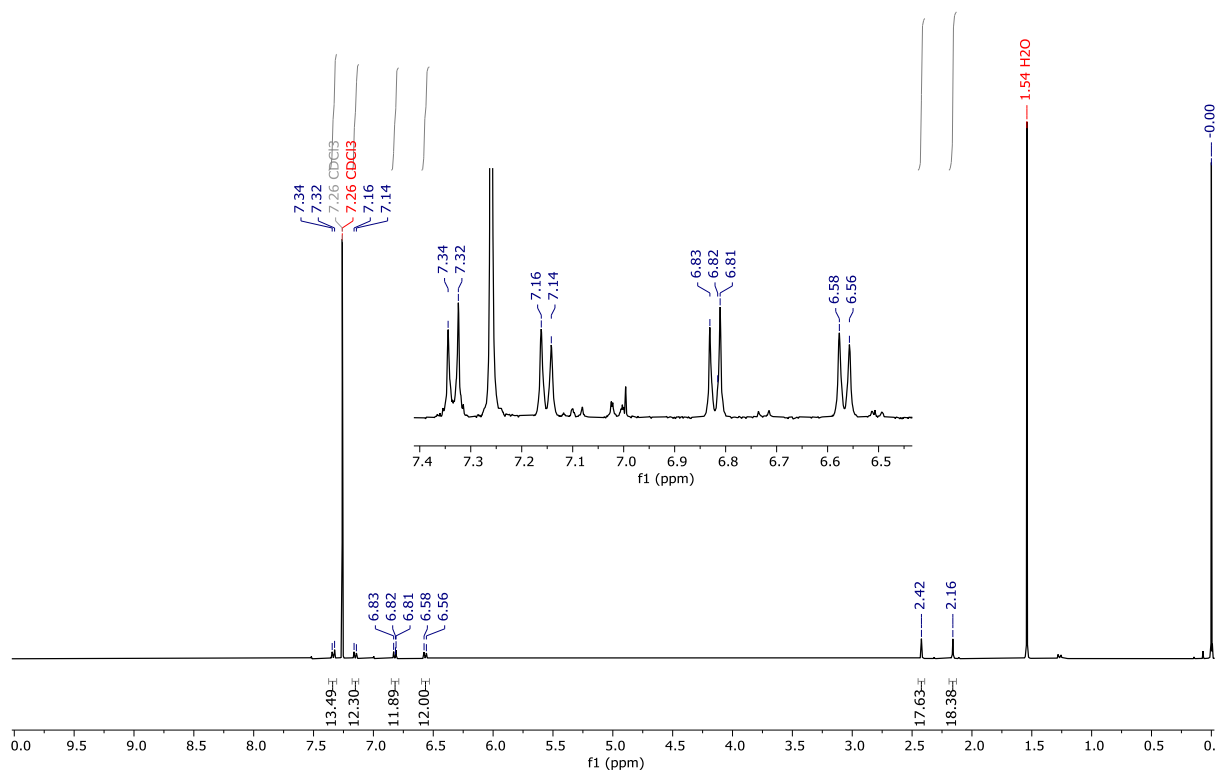


col-1-14 trimer.11.fid

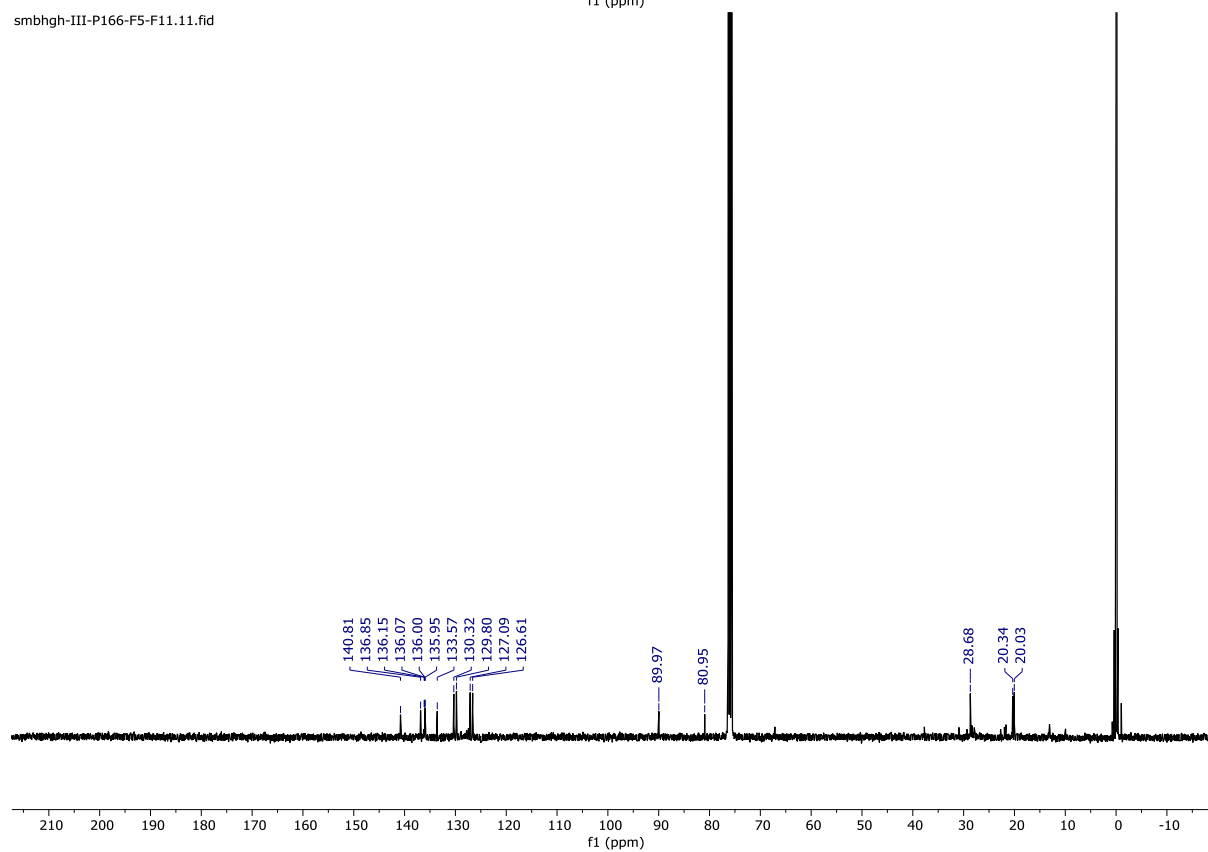


Compound 3b

IYD-1-131 f20-25 trimer.10.fid

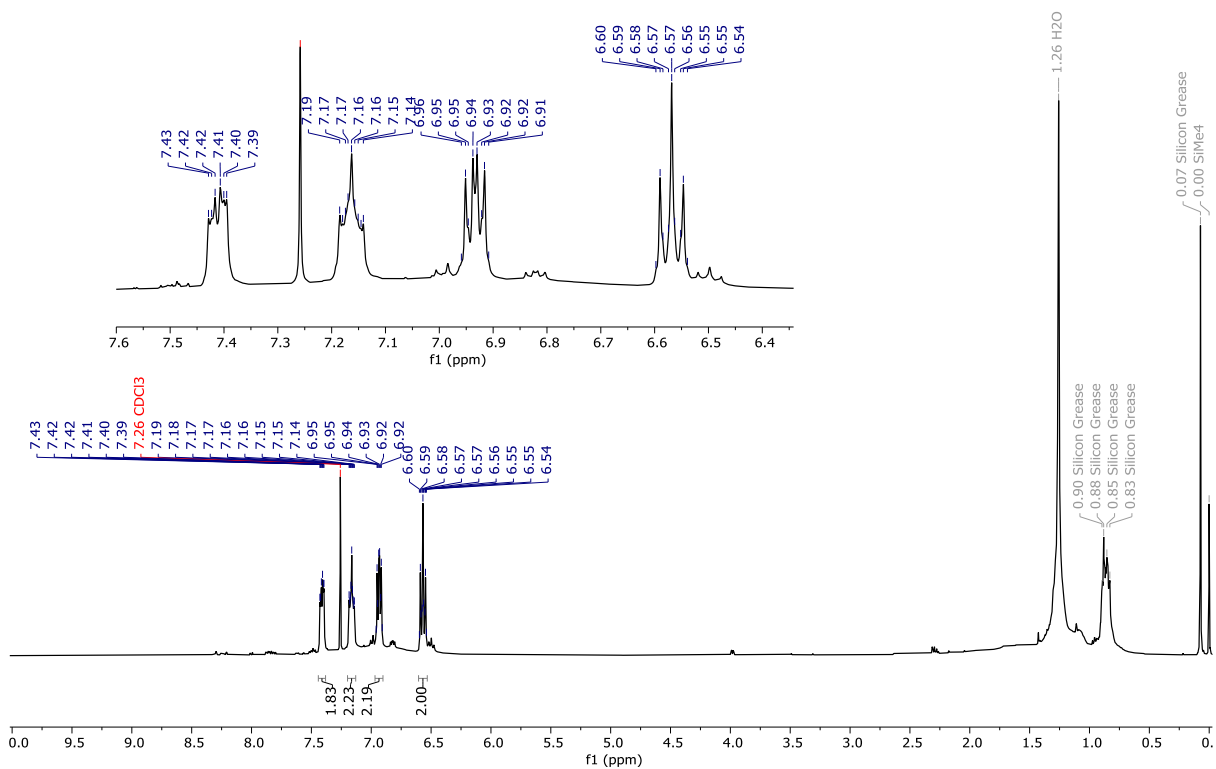


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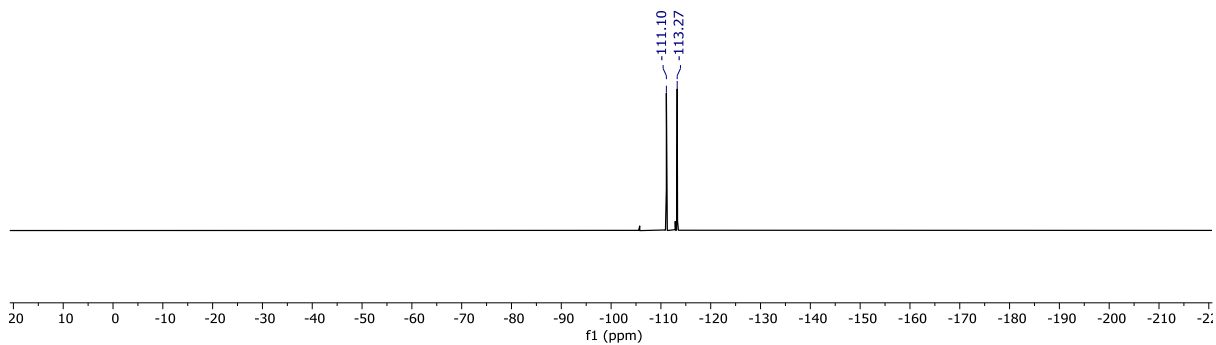


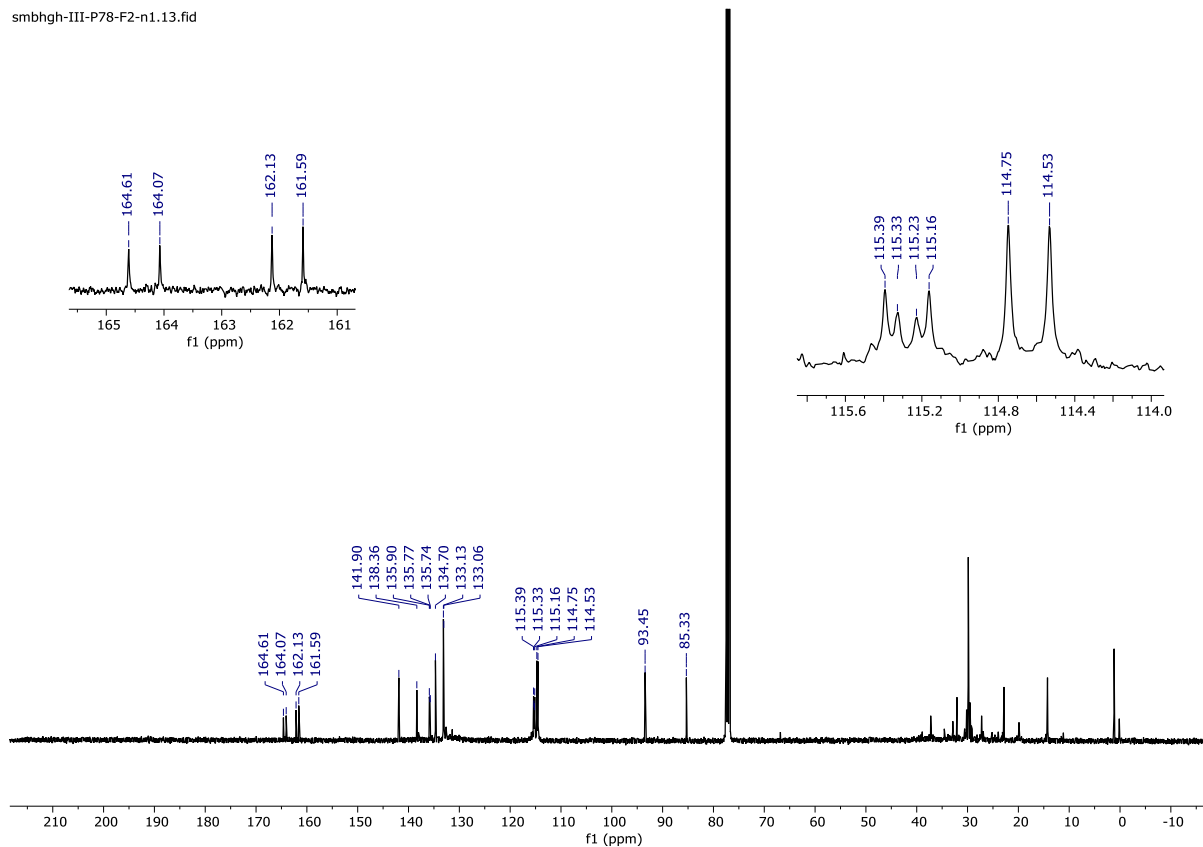
Compound 3d

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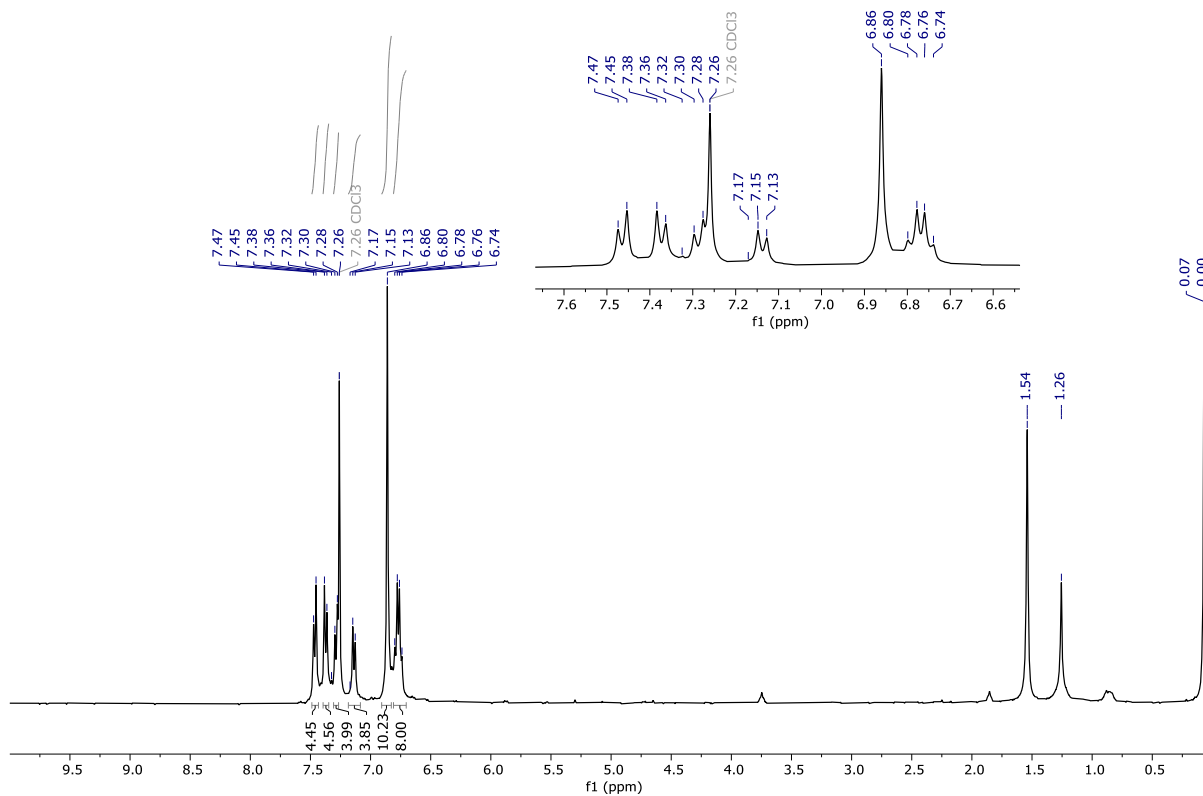
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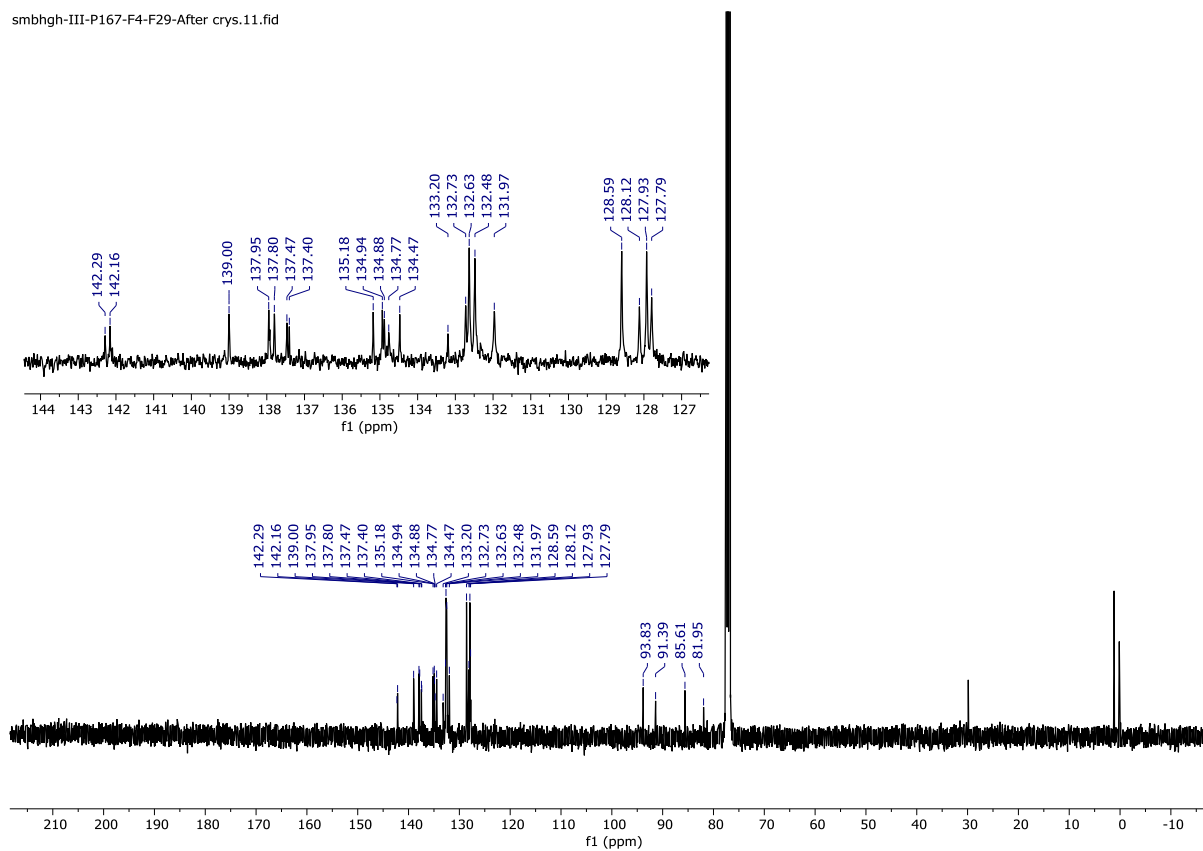


Compound 3c

smbhgh-III-P167-F4-F29-After crys.10.fid



smbhgh-III-P167-F4-F29-After crys.11.fid



Cartesian Coordinates of all the studied molecules (3a-3d, 3m)

3a				3a			
Cam-b3lyp/def2-SVP				Cam-b3lyp/def2-SVP			
0 1				0 3			
6	1.499110000	-3.971227000	-0.069101000	6	-0.613807000	-4.205842000	-0.009671000
6	0.144067000	-4.247369000	0.021864000	6	-1.939491000	-3.792920000	-0.010002000
6	0.390122000	-5.708410000	0.177412000	6	-2.431716000	-5.192178000	0.136653000
6	1.860420000	-5.415206000	-0.030661000	6	-0.987624000	-5.637946000	0.040940000
6	3.021564000	-6.066443000	-0.266883000	6	-0.256382000	-6.770172000	-0.108031000
6	3.113534000	-7.516964000	-0.566053000	6	-0.834686000	-8.098012000	-0.424768000
6	4.185771000	-8.277276000	-0.075614000	6	-0.283083000	-9.264023000	0.127830000
1	4.936826000	-7.798832000	0.555390000	1	0.557246000	-9.182624000	0.819443000
6	4.297551000	-9.629246000	-0.375749000	6	-0.798028000	-10.515505000	-0.186812000
1	5.134234000	-10.205866000	0.024894000	1	-0.360770000	-11.409884000	0.262599000
6	3.347873000	-10.247181000	-1.186762000	6	-1.866499000	-10.630196000	-1.073771000
6	2.288006000	-9.501070000	-1.694044000	6	-2.413262000	-9.483156000	-1.642112000
1	1.543978000	-9.974492000	-2.338094000	1	-3.244997000	-9.563583000	-2.345138000
6	2.172815000	-8.148889000	-1.388168000	6	-1.901560000	-8.229898000	-1.322368000
1	1.347773000	-7.565847000	-1.799885000	1	-2.324853000	-7.335612000	-1.781896000
6	-0.417711000	-6.716206000	0.575820000	6	-3.651127000	-5.686163000	0.445796000
6	0.055168000	-8.037656000	1.058088000	6	-3.904505000	-7.066890000	0.927799000
6	1.163870000	-8.152380000	1.904596000	6	-3.057028000	-7.683026000	1.855704000
1	1.707948000	-7.252817000	2.195794000	1	-2.178166000	-7.145347000	2.214278000
6	1.565457000	-9.394045000	2.387059000	6	-3.332326000	-8.960864000	2.332360000
1	2.432010000	-9.462022000	3.048080000	1	-2.659109000	-9.423563000	3.057047000
6	0.865760000	-10.544017000	2.033347000	6	-4.460996000	-9.645889000	1.891987000
6	-0.245838000	-10.443551000	1.199149000	6	-5.319230000	-9.040481000	0.976244000
1	-0.803641000	-11.339976000	0.919308000	1	-6.209623000	-9.568636000	0.627914000
6	-0.651994000	-9.202415000	0.724811000	6	-5.048374000	-7.761145000	0.506767000
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6	-3.981062000	-6.554495000	1.849294000	6	-6.808934000	-3.841953000	1.434285000
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6	-1.820156000	-2.520214000	-0.030295000	6	-2.813650000	-1.327568000	-0.110273000
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6	-3.756399000	1.945159000	0.002157000	6	-2.261943000	3.558611000	0.006125000
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6	-5.636302000	1.081155000	-0.174319000	6	-4.356380000	3.631708000	-0.153598000
6	-6.802089000	0.397490000	-0.126720000	6	-5.738545000	3.588642000	-0.111035000
6	-6.823874000	-1.064406000	-0.414357000	6	-6.440263000	2.362215000	-0.559693000
6	-6.231281000	-1.570468000	-1.577141000	6	-6.093343000	1.742810000	-1.769305000
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6	-10.514587000	1.145503000	-0.073512000	6	-8.647242000	5.957708000	0.370180000
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1	-7.028797000	2.542231000	-2.270228000	1	-4.989444000	5.617022000	-2.152671000
6	-8.788860000	3.783949000	-2.326827000	6	-6.005246000	7.515623000	-2.119057000
1	-9.253532000	3.208651000	-3.130334000	1	-6.696326000	7.237684000	-2.917635000
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1	-2.481007000	6.227897000	2.172399000	1	0.869776000	6.720759000	2.139567000
6	-2.864413000	7.061613000	0.221959000	6	0.822389000	7.720060000	0.229620000
6	-3.579042000	6.927881000	-0.967270000	6	0.078269000	7.966458000	-0.922581000
1	-3.445861000	7.655214000	-1.771085000	1	0.489740000	8.592511000	-1.717293000
6	-4.459445000	5.866856000	-1.135848000	6	-1.188053000	7.413490000	-1.065699000
1	-5.019579000	5.765822000	-2.067512000	1	-1.769605000	7.610434000	-1.968377000
6	-2.452604000	2.431237000	0.128007000	6	-0.948483000	3.371256000	0.122162000
6	-1.274527000	2.744256000	0.222956000	6	0.267834000	3.052896000	0.223138000
6	0.056079000	3.027171000	0.287935000	6	1.525654000	2.663002000	0.289120000
6	1.264656000	3.213306000	0.298037000	6	2.699394000	2.232606000	0.303441000
6	2.658036000	3.258344000	0.200547000	6	3.905330000	1.604763000	0.214296000
6	3.547136000	2.246001000	-0.125443000	6	4.207163000	0.245812000	-0.076845000
6	4.710147000	3.172523000	-0.112801000	6	5.647492000	0.503867000	-0.107391000
6	3.735820000	4.283799000	0.227910000	6	5.353482000	1.959505000	0.185967000
6	3.703366000	5.625008000	0.401168000	6	5.983782000	3.154165000	0.279308000
6	2.489058000	6.271137000	0.975298000	6	5.249196000	4.337077000	0.811652000
6	1.912194000	5.785902000	2.154961000	6	4.558847000	4.260674000	2.027069000
1	2.337357000	4.901460000	2.632797000	1	4.529983000	3.311814000	2.565590000
6	0.829392000	6.436242000	2.740505000	6	3.938191000	5.383565000	2.567100000
1	0.402951000	6.048133000	3.668043000	1	3.416475000	5.305416000	3.523449000
6	0.304272000	7.583866000	2.154929000	6	3.995160000	6.602394000	1.898212000
6	0.862500000	8.072613000	0.974425000	6	4.670087000	6.690376000	0.681587000
1	0.454899000	8.971622000	0.506488000	1	4.716277000	7.642320000	0.147838000

6	1.946755000	7.426323000	0.393993000	6	5.296278000	5.570825000	0.147369000
1	2.389551000	7.822683000	-0.521610000	1	5.836969000	5.649095000	-0.797712000
6	4.812994000	6.540649000	0.038077000	6	7.386749000	3.396216000	-0.137083000
6	5.127054000	7.639681000	0.851694000	6	8.213171000	4.253733000	0.604766000
1	4.572655000	7.795580000	1.778812000	1	7.826523000	4.714672000	1.515376000
6	6.136882000	8.524792000	0.495398000	6	9.515796000	4.516007000	0.199030000
1	6.372844000	9.368791000	1.147351000	1	10.146469000	5.178397000	0.796152000
6	6.844059000	8.339045000	-0.690848000	6	10.015295000	3.939325000	-0.966986000
6	6.532927000	7.261462000	-1.514895000	6	9.201213000	3.099385000	-1.721391000
1	7.076559000	7.112340000	-2.450075000	1	9.581150000	2.649776000	-2.641122000
6	5.526142000	6.371532000	-1.154583000	6	7.899341000	2.831248000	-1.311010000
1	5.275584000	5.536497000	-1.810610000	1	7.260416000	2.183659000	-1.913364000
6	6.035431000	2.944594000	-0.260190000	6	6.710345000	-0.346221000	-0.246505000
6	7.105360000	3.894082000	0.131037000	6	8.097661000	-0.018747000	0.147646000
6	7.024917000	4.622876000	1.323561000	6	8.367187000	0.721103000	1.306848000
1	6.145055000	4.508882000	1.958583000	1	7.535372000	1.081139000	1.914018000
6	8.057051000	5.471534000	1.710477000	6	9.675775000	0.983016000	1.697513000
1	7.975496000	6.030118000	2.645185000	1	9.863042000	1.559292000	2.605928000
6	9.190179000	5.606186000	0.913503000	6	10.742887000	0.510935000	0.938112000
6	9.287600000	4.880902000	-0.272308000	6	10.491543000	-0.231735000	-0.213894000
1	10.174142000	4.978401000	-0.902850000	1	11.322168000	-0.606819000	-0.815907000
6	8.259943000	4.027699000	-0.654758000	6	9.184476000	-0.500016000	-0.600165000
1	8.346449000	3.455864000	-1.580365000	1	8.995853000	-1.086375000	-1.500989000
6	6.492254000	1.642692000	-0.824772000	6	6.476624000	-1.713680000	-0.781870000
6	5.957546000	1.157929000	-2.023880000	6	5.725643000	-1.909987000	-1.947940000
1	5.186858000	1.736087000	-2.536971000	1	5.302408000	-1.045416000	-2.462284000
6	6.410098000	-0.037060000	-2.575943000	6	5.530445000	-3.186669000	-2.465899000
1	5.981347000	-0.397443000	-3.513282000	1	4.942869000	-3.317150000	-3.376946000
6	7.407331000	-0.766608000	-1.937677000	6	6.083543000	-4.291736000	-1.827030000
6	7.951782000	-0.293387000	-0.744600000	6	6.837995000	-4.111649000	-0.668515000
1	8.736566000	-0.859594000	-0.237572000	1	7.277492000	-4.973576000	-0.161170000
6	7.503716000	0.902306000	-0.196789000	6	7.037469000	-2.836622000	-0.154472000
1	7.939909000	1.273213000	0.732745000	1	7.632648000	-2.701803000	0.750554000
6	3.327979000	0.872362000	-0.255663000	6	3.350862000	-0.853418000	-0.157005000
6	3.014315000	-0.308999000	-0.283799000	6	2.499061000	-1.730280000	-0.165674000
6	2.592912000	-1.603620000	-0.259173000	6	1.496735000	-2.659195000	-0.140205000

6	2.151027000	-2.741499000	-0.190998000	6	0.559978000	-3.439065000	-0.088319000
6	4.306551000	-5.312019000	-0.272059000	6	1.227299000	-6.704482000	0.003307000
6	5.224417000	-5.469788000	-1.320167000	6	2.045461000	-7.298603000	-0.968644000
6	4.649389000	-4.473135000	0.794416000	6	1.837776000	-6.086901000	1.101123000
6	6.442196000	-4.800870000	-1.304485000	6	3.429320000	-7.261329000	-0.851472000
1	4.975357000	-6.128085000	-2.154704000	1	1.584518000	-7.792637000	-1.826130000
6	5.871128000	-3.806257000	0.813052000	6	3.224175000	-6.054004000	1.221748000
1	3.954182000	-4.357479000	1.627870000	1	1.214026000	-5.640360000	1.877550000
6	6.771220000	-3.970022000	-0.234648000	6	4.023583000	-6.640336000	0.246254000
1	7.143008000	-4.932595000	-2.132035000	1	4.050381000	-7.723574000	-1.622221000
1	6.121665000	-3.157260000	1.654633000	1	3.681396000	-5.567862000	2.085964000
1	7.633662000	9.037879000	-0.975307000	1	11.036952000	4.149844000	-1.290490000
1	10.000486000	6.271668000	1.219003000	1	11.770128000	0.717084000	1.246354000
1	7.761193000	-1.704336000	-2.370326000	1	5.927014000	-5.293648000	-2.231519000
1	7.731241000	-3.451078000	-0.216415000	1	5.110592000	-6.614231000	0.341605000
1	3.437805000	-11.308507000	-1.428155000	1	-2.268572000	-11.613749000	-1.326222000
1	1.182035000	-11.518011000	2.412961000	1	-4.676041000	-10.648792000	2.267138000
1	-5.737163000	-5.895269000	0.778428000	1	-7.943680000	-2.436795000	0.250208000
1	-7.106438000	-4.848793000	-1.314091000	1	-8.421818000	-0.736581000	-1.865041000
1	-11.562996000	2.529712000	1.211571000	1	-8.823166000	7.550221000	1.819505000
1	-10.419564000	5.190150000	-2.178281000	1	-6.831687000	9.495293000	-1.879187000
1	-2.166597000	7.890339000	0.352847000	1	1.819834000	8.148975000	0.340560000
1	-0.536090000	8.103451000	2.621005000	1	3.520110000	7.487293000	2.327954000

3a

Cam-b3lyp/def2-SVP

-2 1

6	-0.557939000	4.247077000	-0.183494000
6	0.829310000	4.178648000	-0.042275000
6	0.946679000	5.651637000	0.058989000
6	-0.529018000	5.726809000	-0.263343000
6	-1.441457000	6.648797000	-0.667668000
6	-1.089054000	8.034621000	-1.065338000
6	-1.947948000	9.105609000	-0.768187000
1	-2.865056000	8.909109000	-0.209678000
6	-1.647590000	10.402625000	-1.165560000

3a

Cam-b3lyp/def2-SVP

-2 3

6	-2.616577000	-3.322619000	-0.130007000
6	-3.588380000	-2.274323000	0.003653000
6	-4.684975000	-3.247633000	0.084128000
6	-3.688265000	-4.330810000	-0.248971000
6	-3.760766000	-5.606760000	-0.717696000
6	-5.033717000	-6.182055000	-1.229808000
6	-5.432429000	-7.487762000	-0.907205000
1	-4.820352000	-8.071596000	-0.216812000
6	-6.588035000	-8.042499000	-1.445346000

1	-2.329727000	11.217960000	-0.910880000	1	-6.881002000	-9.058026000	-1.166494000
6	-0.481062000	10.665693000	-1.881646000	6	-7.373849000	-7.308040000	-2.331742000
6	0.374937000	9.614150000	-2.195889000	6	-6.989987000	-6.013106000	-2.668548000
1	1.290421000	9.803571000	-2.761522000	1	-7.592422000	-5.426496000	-3.366883000
6	0.072166000	8.315393000	-1.798324000	6	-5.834312000	-5.459057000	-2.125454000
1	0.742365000	7.496156000	-2.061292000	1	-5.530090000	-4.449255000	-2.404719000
6	1.954415000	6.458659000	0.481926000	6	-5.979091000	-3.220257000	0.519017000
6	1.775176000	7.865555000	0.914843000	6	-6.666558000	-4.447468000	0.999705000
6	0.643961000	8.277475000	1.633243000	6	-6.028415000	-5.324746000	1.889025000
1	-0.135770000	7.548021000	1.855492000	1	-5.001291000	-5.112770000	2.189598000
6	0.509125000	9.591610000	2.070071000	6	-6.686640000	-6.438715000	2.401904000
1	-0.385953000	9.884466000	2.624176000	1	-6.163645000	-7.101333000	3.096360000
6	1.506334000	10.527551000	1.810598000	6	-8.004945000	-6.704251000	2.041974000
6	2.644134000	10.132314000	1.109372000	6	-8.656665000	-5.841271000	1.162470000
1	3.436505000	10.855272000	0.898483000	1	-9.689838000	-6.040167000	0.865729000
6	2.777435000	8.819789000	0.673238000	6	-7.997500000	-4.728065000	0.653758000
1	3.674282000	8.518171000	0.128961000	1	-8.517346000	-4.055531000	-0.031542000
6	3.324399000	5.890821000	0.635950000	6	-6.704214000	-1.937747000	0.680125000
6	4.035151000	6.053424000	1.835350000	6	-7.574708000	-1.723543000	1.763943000
1	3.576073000	6.613074000	2.653141000	1	-7.715801000	-2.519178000	2.497624000
6	5.295191000	5.491949000	2.003122000	6	-8.237935000	-0.513382000	1.929401000
1	5.818888000	5.611025000	2.955049000	1	-8.895480000	-0.372015000	2.791434000
6	5.880296000	4.758944000	0.971561000	6	-8.052851000	0.522186000	1.015267000
6	5.197480000	4.608030000	-0.230407000	6	-7.203908000	0.324586000	-0.070031000
1	5.642218000	4.022692000	-1.037048000	1	-7.038755000	1.130430000	-0.787794000
6	3.936302000	5.173044000	-0.397943000	6	-6.547082000	-0.889415000	-0.239665000
1	3.404381000	5.043840000	-1.341876000	1	-5.892579000	-1.031954000	-1.099763000
6	1.680632000	3.077339000	0.011440000	6	-3.415283000	-0.904977000	0.061137000
6	2.322253000	2.029515000	0.001876000	6	-3.112221000	0.291455000	0.059888000
6	2.976833000	0.843864000	-0.016683000	6	-2.702796000	1.579649000	0.046384000
6	3.497975000	-0.273890000	-0.026198000	6	-2.254037000	2.728953000	0.026741000
6	3.921819000	-1.587033000	-0.035692000	6	-1.592828000	3.942038000	-0.011462000
6	3.107744000	-2.810281000	-0.027350000	6	-0.184560000	4.229502000	-0.030362000
6	4.375760000	-3.603029000	-0.086657000	6	-0.461637000	5.676201000	-0.141226000
6	5.157159000	-2.323984000	0.072414000	6	-1.928786000	5.365411000	0.036398000
6	6.484778000	-2.034096000	0.326939000	6	-3.057913000	6.087199000	0.313290000

6	7.028436000	-0.686587000	0.078065000	6	-4.400288000	5.472660000	0.188919000
6	6.569911000	0.097091000	-0.999158000	6	-4.701042000	4.601480000	-0.870955000
1	5.783251000	-0.299616000	-1.641826000	1	-3.924293000	4.367848000	-1.599896000
6	7.108461000	1.348251000	-1.271764000	6	-5.967403000	4.045220000	-1.012540000
1	6.730220000	1.917134000	-2.125383000	1	-6.166157000	3.372069000	-1.850116000
6	8.127520000	1.873515000	-0.477991000	6	-6.976433000	4.343678000	-0.100084000
6	8.590037000	1.121013000	0.600960000	6	-6.697776000	5.204447000	0.960214000
1	9.379436000	1.517790000	1.245824000	1	-7.474740000	5.439841000	1.692468000
6	8.051904000	-0.131175000	0.873225000	6	-5.431780000	5.760802000	1.100614000
1	8.425138000	-0.698193000	1.727566000	1	-5.227357000	6.428550000	1.939448000
6	7.362821000	-3.038574000	0.967092000	6	-2.986742000	7.466378000	0.856265000
6	8.712790000	-3.197852000	0.602815000	6	-3.873027000	8.473605000	0.440647000
1	9.112711000	-2.592264000	-0.212641000	1	-4.597508000	8.248342000	-0.344375000
6	9.538742000	-4.110309000	1.247991000	6	-3.839118000	9.744156000	1.003209000
1	10.580180000	-4.212072000	0.930143000	1	-4.535169000	10.509716000	0.650146000
6	9.046181000	-4.902535000	2.284520000	6	-2.919797000	10.046745000	2.006489000
6	7.712932000	-4.762644000	2.662182000	6	-2.035660000	9.060436000	2.435341000
1	7.308614000	-5.366932000	3.478974000	1	-1.313194000	9.278105000	3.226309000
6	6.889769000	-3.843731000	2.019262000	6	-2.071303000	7.789315000	1.870427000
1	5.855503000	-3.723081000	2.345327000	1	-1.389124000	7.016142000	2.226869000
6	4.667872000	-4.866519000	-0.477967000	6	0.263340000	6.765646000	-0.514434000
6	6.023638000	-5.252097000	-0.965376000	6	-0.379726000	7.995461000	-1.051605000
6	6.638037000	-4.526318000	-1.993381000	6	-1.351813000	7.911865000	-2.058150000
1	6.136364000	-3.639784000	-2.384009000	1	-1.665091000	6.926214000	-2.405334000
6	7.862926000	-4.926433000	-2.519883000	6	-1.903828000	9.057683000	-2.623833000
1	8.320716000	-4.344627000	-3.323838000	1	-2.657711000	8.961763000	-3.409416000
6	8.501527000	-6.060945000	-2.026768000	6	-1.495198000	10.318349000	-2.198029000
6	7.903569000	-6.791679000	-1.002455000	6	-0.527452000	10.419991000	-1.200213000
1	8.399526000	-7.678743000	-0.600485000	1	-0.201831000	11.403544000	-0.851689000
6	6.675709000	-6.394161000	-0.483965000	6	0.025231000	9.273752000	-0.640252000
1	6.207686000	-6.974647000	0.313593000	1	0.787409000	9.361594000	0.136698000
6	3.618169000	-5.913106000	-0.574131000	6	1.746485000	6.724396000	-0.547036000
6	2.599760000	-6.014552000	0.383094000	6	2.480819000	6.068820000	0.451990000
1	2.586006000	-5.316028000	1.219688000	1	1.948614000	5.596046000	1.277679000
6	1.609378000	-6.985566000	0.276699000	6	3.869350000	6.005752000	0.401349000
1	0.813915000	-7.025875000	1.023028000	1	4.412349000	5.463494000	1.177839000

6	1.618831000	-7.888852000	-0.781837000	6	4.565210000	6.611512000	-0.640708000
6	2.633237000	-7.813120000	-1.734048000	6	3.854366000	7.285594000	-1.631779000
1	2.649857000	-8.512275000	-2.574226000	1	4.386256000	7.760761000	-2.460378000
6	3.620921000	-6.840778000	-1.628966000	6	2.466398000	7.342187000	-1.584365000
1	4.405487000	-6.784027000	-2.385539000	1	1.920712000	7.859732000	-2.375383000
6	1.789811000	-3.016343000	-0.013228000	6	0.903401000	3.393094000	-0.008780000
6	0.521867000	-3.039786000	0.034204000	6	1.792119000	2.530720000	0.041444000
6	-0.781531000	-2.987712000	0.078361000	6	2.700480000	1.539777000	0.087449000
6	-2.043456000	-2.859487000	0.109965000	6	3.478857000	0.578500000	0.118874000
6	-3.339585000	-2.544322000	0.143880000	6	4.199024000	-0.596719000	0.139233000
6	-4.057910000	-1.264429000	0.082861000	6	3.755777000	-1.955569000	0.076878000
6	-5.345282000	-1.901789000	0.256352000	6	5.139741000	-2.446661000	0.197412000
6	-4.662374000	-3.240684000	0.161789000	6	5.607401000	-1.016313000	0.126281000
6	-5.045765000	-4.513131000	-0.102004000	6	6.800171000	-0.377300000	-0.064032000
6	-4.081197000	-5.641018000	-0.025119000	6	6.923240000	1.083462000	0.154665000
6	-3.150701000	-5.720715000	1.020195000	6	6.273856000	1.709915000	1.230736000
1	-3.123574000	-4.925997000	1.766222000	1	5.658128000	1.108029000	1.899960000
6	-2.275604000	-6.797030000	1.121709000	6	6.412872000	3.073716000	1.463401000
1	-1.562694000	-6.832396000	1.948795000	1	5.893693000	3.528491000	2.310595000
6	-2.307483000	-7.821979000	0.180176000	6	7.209354000	3.854764000	0.629670000
6	-3.223916000	-7.757232000	-0.867593000	6	7.860242000	3.252288000	-0.445572000
1	-3.253041000	-8.550025000	-1.619498000	1	8.479354000	3.853317000	-1.116855000
6	-4.102144000	-6.683917000	-0.964857000	6	7.720644000	1.888969000	-0.677544000
1	-4.818040000	-6.643622000	-1.787888000	1	8.232315000	1.432028000	-1.526471000
6	-6.418478000	-4.848731000	-0.573595000	6	7.988613000	-1.088165000	-0.599383000
6	-7.138041000	-5.924369000	-0.036610000	6	9.281213000	-0.847172000	-0.106769000
1	-6.707433000	-6.488922000	0.792672000	1	9.407352000	-0.159496000	0.731731000
6	-8.386411000	-6.275329000	-0.539044000	6	10.393245000	-1.470210000	-0.660943000
1	-8.933868000	-7.109878000	-0.093699000	1	11.385693000	-1.271127000	-0.248009000
6	-8.939958000	-5.564875000	-1.601974000	6	10.247163000	-2.349727000	-1.732593000
6	-8.235012000	-4.496960000	-2.150395000	6	8.974026000	-2.597500000	-2.238257000
1	-8.656382000	-3.932241000	-2.985831000	1	8.842421000	-3.279002000	-3.082689000
6	-6.989071000	-4.143183000	-1.641053000	6	7.862045000	-1.973685000	-1.680807000
1	-6.434928000	-3.310624000	-2.076873000	1	6.869693000	-2.157728000	-2.094975000
6	-6.634418000	-1.507392000	0.551997000	6	5.712950000	-3.650840000	0.485792000
6	-7.571626000	-2.433419000	1.231742000	6	7.071152000	-3.744714000	1.083816000

6	-7.149286000	-3.220541000	2.317027000	6	7.430588000	-2.931680000	2.168565000
1	-6.107557000	-3.156214000	2.635330000	1	6.710960000	-2.199000000	2.536670000
6	-8.030661000	-4.052533000	3.000525000	6	8.672037000	-3.057996000	2.785155000
1	-7.666097000	-4.646525000	3.843097000	1	8.922163000	-2.412199000	3.630813000
6	-9.370961000	-4.118796000	2.628163000	6	9.587592000	-4.004694000	2.334584000
6	-9.813071000	-3.342097000	1.557946000	6	9.246275000	-4.823859000	1.259598000
1	-10.860072000	-3.387292000	1.245655000	1	9.957903000	-5.566959000	0.890362000
6	-8.929102000	-2.515687000	0.874210000	6	8.004494000	-4.697567000	0.647798000
1	-9.288584000	-1.916596000	0.035211000	1	7.744353000	-5.345923000	-0.191326000
6	-7.071735000	-0.114351000	0.348886000	6	4.953499000	-4.916347000	0.346510000
6	-6.574978000	0.663242000	-0.714540000	6	4.062571000	-5.120468000	-0.719159000
1	-5.855637000	0.219465000	-1.402900000	1	3.931763000	-4.331536000	-1.460123000
6	-6.985833000	1.976091000	-0.911712000	6	3.348438000	-6.307188000	-0.846696000
1	-6.566209000	2.548425000	-1.742493000	1	2.647281000	-6.427512000	-1.675463000
6	-7.918650000	2.563626000	-0.058889000	6	3.515896000	-7.333319000	0.079881000
6	-8.428526000	1.812075000	0.999300000	6	4.403104000	-7.154417000	1.140054000
1	-9.154094000	2.256734000	1.686504000	1	4.539214000	-7.947417000	1.880308000
6	-8.013056000	0.501546000	1.199558000	6	5.110283000	-5.965222000	1.270431000
1	-8.414426000	-0.062530000	2.042944000	1	5.792704000	-5.834580000	2.112034000
6	-3.539486000	0.008744000	-0.023416000	6	2.484530000	-2.477793000	0.002913000
6	-2.946160000	1.086367000	-0.122401000	6	1.292118000	-2.803187000	-0.068223000
6	-2.217752000	2.225684000	-0.187122000	6	-0.020885000	-3.083530000	-0.125371000
6	-1.505523000	3.226951000	-0.227192000	6	-1.245214000	-3.273486000	-0.159235000
6	-2.871661000	6.263242000	-0.826855000	6	-2.541975000	-6.438576000	-0.872113000
6	-3.580539000	6.618461000	-1.985921000	6	-2.381858000	-7.295899000	-1.974908000
6	-3.555018000	5.551512000	0.167283000	6	-1.512042000	-6.407118000	0.080193000
6	-4.914263000	6.264856000	-2.148372000	6	-1.239434000	-8.073202000	-2.124280000
1	-3.066882000	7.173045000	-2.773813000	1	-3.166101000	-7.339538000	-2.732750000
6	-4.889773000	5.190117000	0.004027000	6	-0.364786000	-7.179184000	-0.071143000
1	-3.027807000	5.273813000	1.080878000	1	-1.616192000	-5.763351000	0.953770000
6	-5.575460000	5.547249000	-1.152687000	6	-0.221914000	-8.018246000	-1.173129000
1	-5.440586000	6.542605000	-3.065216000	1	-1.138128000	-8.722068000	-2.998380000
1	-5.395434000	4.612079000	0.780267000	1	0.429857000	-7.116251000	0.675334000
1	-9.919259000	-5.842477000	-2.000148000	1	11.121595000	-2.837560000	-2.170625000
1	-10.065813000	-4.768206000	3.166812000	1	10.562694000	-4.105200000	2.817887000
1	-8.244634000	3.595145000	-0.215327000	1	2.956191000	-8.266372000	-0.021926000

1	-6.621501000	5.260068000	-1.279824000	1	0.679623000	-8.624486000	-1.291859000
1	-0.242440000	11.684954000	-2.195033000	1	-8.280860000	-7.744469000	-2.757655000
1	1.399701000	11.558792000	2.155957000	1	-8.523446000	-7.577969000	2.444877000
1	6.856773000	4.288968000	1.105866000	1	-8.556729000	1.481664000	1.152746000
1	8.553881000	2.855770000	-0.696897000	1	-7.971547000	3.906351000	-0.212487000
1	9.696036000	-5.619584000	2.792657000	1	-2.894596000	11.044830000	2.451124000
1	9.464792000	-6.374196000	-2.437455000	1	-1.927960000	11.218812000	-2.641232000
1	0.832734000	-8.642364000	-0.869242000	1	5.654704000	6.546801000	-0.685347000
1	-1.620238000	-8.667612000	0.261654000	1	7.320255000	4.925975000	0.814970000

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Cam-b3lyp/def2-SVP

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6	-1.402808000	4.012835000	-0.016433000
6	-0.045624000	4.217871000	0.176903000
6	-0.228990000	5.687447000	0.339818000
6	-1.690431000	5.472618000	0.006324000
6	-2.794198000	6.189535000	-0.308627000
6	-2.765094000	7.638019000	-0.626047000
6	-3.807011000	8.486002000	-0.227767000
1	-4.640295000	8.079019000	0.347516000
6	-3.790399000	9.839050000	-0.543085000
1	-4.612638000	10.477570000	-0.209545000
6	-2.742472000	10.397777000	-1.279501000
6	-1.715670000	9.546641000	-1.698273000
1	-0.890316000	9.951346000	-2.289820000
6	-1.724544000	8.195047000	-1.380094000
1	-0.916038000	7.551346000	-1.729844000
6	0.572242000	6.645680000	0.857543000
6	0.097353000	7.982138000	1.298033000
6	-1.076283000	8.139177000	2.043282000
1	-1.675537000	7.260758000	2.287321000
6	-1.477488000	9.393173000	2.487102000
1	-2.397324000	9.484642000	3.070560000
6	-0.728705000	10.538102000	2.202110000
6	0.452615000	10.378424000	1.472348000

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Cam-b3lyp/def2-SVP

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6	0.016144000	4.268943000	0.127622000
6	1.377827000	3.986917000	0.068790000
6	1.747716000	5.417977000	0.190112000
6	0.265158000	5.734085000	0.203631000
6	-0.569969000	6.800228000	0.173767000
6	-0.125311000	8.185977000	-0.109617000
6	-0.690533000	9.276022000	0.564619000
1	-1.452081000	9.099740000	1.326314000
6	-0.288113000	10.577027000	0.287082000
1	-0.738824000	11.407022000	0.837445000
6	0.680535000	10.842906000	-0.683938000
6	1.226322000	9.756221000	-1.374061000
1	1.976773000	9.933906000	-2.148698000
6	0.833321000	8.454436000	-1.094957000
1	1.267991000	7.625102000	-1.654968000
6	2.953978000	6.009795000	0.366849000
6	3.152838000	7.397100000	0.846756000
6	2.355197000	7.942327000	1.861025000
1	1.557268000	7.337577000	2.294334000
6	2.576694000	9.230176000	2.329038000
1	1.938588000	9.627821000	3.122461000
6	3.599789000	10.027118000	1.805861000
6	4.405153000	9.478310000	0.804968000

1	1.066241000	11.254072000	1.244866000	1	5.218667000	10.074190000	0.383028000
6	0.864314000	9.124868000	1.037480000	6	4.194016000	8.185465000	0.340226000
1	1.798153000	9.026819000	0.480537000	1	4.844477000	7.779326000	-0.436498000
6	2.010593000	6.359876000	1.119083000	6	4.191201000	5.216467000	0.119047000
6	2.553488000	6.637764000	2.381157000	6	5.203115000	5.144443000	1.083534000
1	1.915314000	7.069191000	3.154704000	1	5.077771000	5.670444000	2.032146000
6	3.882238000	6.355787000	2.665292000	6	6.356983000	4.404658000	0.853409000
1	4.273655000	6.565292000	3.664179000	1	7.124789000	4.352958000	1.629554000
6	4.727362000	5.802443000	1.698582000	6	6.554222000	3.725590000	-0.352284000
6	4.190109000	5.540601000	0.435851000	6	5.551540000	3.814369000	-1.321901000
1	4.824306000	5.099885000	-0.336680000	1	5.680403000	3.298557000	-2.277082000
6	2.856798000	5.816491000	0.148066000	6	4.391165000	4.543561000	-1.091985000
1	2.464759000	5.607503000	-0.848876000	1	3.625509000	4.601969000	-1.868108000
6	1.002394000	3.294672000	0.190937000	6	2.038864000	2.758337000	0.017808000
6	1.835616000	2.401673000	0.137669000	6	2.510025000	1.631005000	-0.008497000
6	2.714607000	1.364795000	0.058825000	6	2.967846000	0.347710000	-0.032411000
6	3.447616000	0.389586000	-0.022361000	6	3.308258000	-0.825029000	-0.051813000
6	4.143302000	-0.820190000	-0.089367000	6	3.533861000	-2.206229000	-0.087532000
6	3.672915000	-2.118139000	0.064768000	6	2.571698000	-3.323694000	-0.078847000
6	5.024929000	-2.694797000	-0.173313000	6	3.735813000	-4.262639000	-0.177988000
6	5.549095000	-1.282304000	-0.232356000	6	4.623606000	-3.063088000	-0.133190000
6	6.752776000	-0.664319000	-0.230569000	6	6.075396000	-2.858000000	-0.070784000
6	6.881743000	0.778618000	-0.557200000	6	6.714526000	-2.058179000	-1.091016000
6	6.144520000	1.348822000	-1.601372000	6	6.075794000	-1.811783000	-2.328926000
1	5.440058000	0.730255000	-2.159577000	1	5.089656000	-2.239650000	-2.515783000
6	6.323287000	2.680219000	-1.965741000	6	6.675804000	-1.045348000	-3.316651000
1	5.739808000	3.090433000	-2.793851000	1	6.150215000	-0.889528000	-4.262150000
6	7.250833000	3.491238000	-1.310385000	6	7.934808000	-0.465751000	-3.127913000
6	7.980779000	2.925095000	-0.257318000	6	8.566014000	-0.681730000	-1.894066000
1	8.711171000	3.536871000	0.279132000	1	9.539295000	-0.220957000	-1.703610000
6	7.804856000	1.598829000	0.110567000	6	7.980299000	-1.449792000	-0.902547000
1	8.396556000	1.183446000	0.928066000	1	8.489665000	-1.557027000	0.054455000
6	7.999155000	-1.385689000	0.137448000	6	6.773777000	-3.466581000	1.056615000
6	9.187448000	-1.223455000	-0.586682000	6	8.106139000	-3.918515000	0.974503000
1	9.190825000	-0.591349000	-1.476679000	1	8.643513000	-3.837765000	0.029858000
6	10.356758000	-1.859295000	-0.191770000	6	8.730999000	-4.518334000	2.059156000

1	11.267275000	-1.721481000	-0.781215000	1	9.760920000	-4.869313000	1.952957000
6	10.393432000	-2.668454000	0.949122000	6	8.067829000	-4.700149000	3.276793000
6	9.214175000	-2.813056000	1.682077000	6	6.737222000	-4.272449000	3.358620000
1	9.215700000	-3.424296000	2.588358000	1	6.186068000	-4.408319000	4.292957000
6	8.037661000	-2.187392000	1.283566000	6	6.102032000	-3.679981000	2.278713000
1	7.132370000	-2.303883000	1.881807000	1	5.065388000	-3.354424000	2.381364000
6	5.467249000	-3.927181000	-0.509012000	6	3.918018000	-5.588562000	-0.358326000
6	6.760995000	-4.140489000	-1.212822000	6	5.277252000	-6.131289000	-0.633316000
6	7.058144000	-3.432763000	-2.381580000	6	6.058645000	-5.643403000	-1.683192000
1	6.352790000	-2.683022000	-2.744356000	1	5.666474000	-4.850170000	-2.321564000
6	8.223406000	-3.689225000	-3.097100000	6	7.323354000	-6.168978000	-1.938114000
1	8.423596000	-3.128885000	-4.014150000	1	7.909285000	-5.771623000	-2.770847000
6	9.138311000	-4.651682000	-2.666828000	6	7.850763000	-7.194655000	-1.153378000
6	8.835805000	-5.364426000	-1.501441000	6	7.061090000	-7.689590000	-0.108324000
1	9.529339000	-6.131470000	-1.146316000	1	7.447079000	-8.496422000	0.520473000
6	7.666094000	-5.122931000	-0.793221000	6	5.796736000	-7.176313000	0.142808000
1	7.446055000	-5.705324000	0.103773000	1	5.197843000	-7.583751000	0.959944000
6	4.628829000	-5.133955000	-0.296979000	6	2.792560000	-6.554099000	-0.350683000
6	3.896340000	-5.326427000	0.881808000	6	1.718849000	-6.445133000	0.542687000
1	3.949136000	-4.577266000	1.673538000	1	1.721236000	-5.654359000	1.293163000
6	3.123940000	-6.466608000	1.065338000	6	0.655458000	-7.337494000	0.493551000
1	2.563094000	-6.588940000	1.995340000	1	-0.173923000	-7.217451000	1.194333000
6	3.054653000	-7.460580000	0.084187000	6	0.624645000	-8.379343000	-0.438834000
6	3.789056000	-7.270835000	-1.088684000	6	1.705472000	-8.500786000	-1.315234000
1	3.751796000	-8.030150000	-1.873940000	1	1.709742000	-9.305702000	-2.054708000
6	4.566975000	-6.135351000	-1.275188000	6	2.772464000	-7.611966000	-1.269719000
1	5.132312000	-6.016205000	-2.200941000	1	3.599984000	-7.727870000	-1.971814000
6	2.366142000	-2.572440000	0.257948000	6	1.227065000	-3.317388000	0.004766000
6	1.178742000	-2.831530000	0.393870000	6	-0.005532000	-3.137974000	0.102315000
6	-0.164812000	-3.040334000	0.473772000	6	-1.307822000	-2.863684000	0.182094000
6	-1.382170000	-3.156617000	0.471339000	6	-2.502609000	-2.532280000	0.216487000
6	-2.771187000	-3.148927000	0.316719000	6	-3.777051000	-2.025236000	0.148168000
6	-3.598004000	-2.137557000	-0.148145000	6	-4.223602000	-0.708565000	-0.116889000
6	-4.787623000	-3.027361000	-0.167309000	6	-5.633904000	-1.139338000	-0.181163000
6	-3.889629000	-4.127594000	0.369801000	6	-5.167421000	-2.549064000	0.117094000
6	-3.930662000	-5.433691000	0.724547000	6	-5.648218000	-3.811415000	0.245677000

6	-2.797077000	-6.033366000	1.481905000	6	-4.785526000	-4.871782000	0.838499000
6	-2.238155000	-5.377888000	2.584775000	6	-4.106023000	-4.651117000	2.042460000
1	-2.622715000	-4.399386000	2.877392000	1	-4.175956000	-3.674059000	2.523821000
6	-1.220327000	-5.964110000	3.330106000	6	-3.370456000	-5.663488000	2.648128000
1	-0.807588000	-5.426083000	4.187257000	1	-2.860972000	-5.462101000	3.594010000
6	-0.729312000	-7.231355000	3.011867000	6	-3.287891000	-6.936642000	2.079521000
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3b				3b			
Cam-b3lyp/def2-SVP				Cam-b3lyp/def2-SVP			
-2 1				-2 3			
6	-0.195256000	4.288366000	0.012017000	6	-2.262714000	3.585523000	-0.021895000

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Cam-b3lyp/def2-SVP				Cam-b3lyp/def2-SVP			
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6	-6.371763000	-2.196677000	-0.247822000	6	1.090457000	-6.599297000	-0.302043000
6	-5.758096000	-3.490382000	-0.660306000	6	2.397334000	-6.187984000	-0.871821000
6	-5.075630000	-3.580415000	-1.879227000	6	2.445393000	-5.552299000	-2.121130000
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6	-5.372639000	-5.864865000	-0.310505000	6	4.823844000	-6.062654000	-0.759070000
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6	-5.901349000	-4.651858000	0.111857000	6	3.606349000	-6.441027000	-0.206514000
1	-6.433521000	-4.601198000	1.063690000	1	3.589625000	-6.928229000	0.770104000
6	-7.810123000	-2.226956000	0.101560000	6	0.943048000	-7.981356000	0.163118000
6	-8.690784000	-3.097617000	-0.559327000	6	1.709496000	-9.019409000	-0.400442000
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6	-10.037499000	-3.152180000	-0.225600000	6	1.590096000	-10.328816000	0.042151000
1	-10.730805000	-3.818184000	-0.741200000	1	2.172327000	-11.139046000	-0.398944000
6	-10.508479000	-2.335917000	0.793460000	6	0.702386000	-10.610906000	1.072030000
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6	2.439724000	3.429433000	-0.133136000	6	-2.963591000	3.000712000	-0.071269000
6	3.157838000	4.731172000	-0.176275000	6	-4.117269000	3.900194000	-0.151693000
6	1.846116000	5.389356000	0.207086000	6	-5.004935000	2.729164000	0.212505000
6	1.290126000	6.604693000	0.418606000	6	-6.305817000	2.386666000	0.371312000
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6	6.670737000	8.088520000	-0.654225000	6	-6.831972000	7.948593000	-0.606995000

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6	5.011992000	3.263903000	-2.098464000	6	-2.322771000	5.473081000	-2.040446000
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1	8.393401000	-1.574294000	-1.889919000	1	2.909002000	7.987847000	-1.717684000
1	6.802744000	-0.615564000	1.969305000	1	1.739734000	6.498099000	2.123592000
9	8.512644000	0.013404000	0.141522000	9	1.359607000	8.306173000	0.321243000
3c Cam-b3lyp/def2-SVP				3c Cam-b3lyp/def2-SVP			
-2 1				-2 3			
6	-1.716436000	-3.872566000	0.070621000	6	2.935102000	-3.016910000	-0.011502000
6	-2.892525000	-3.120422000	0.095542000	6	1.768008000	-3.852955000	0.040120000
6	-3.728416000	-4.340267000	0.210840000	6	2.597275000	-5.057005000	0.207056000
6	-2.459399000	-5.148285000	0.050040000	6	3.824966000	-4.182121000	0.015910000
6	-2.052433000	-6.427708000	-0.167354000	6	5.167606000	-4.319344000	-0.188191000
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1	-6.033002000	1.735146000	-3.019719000	1	-3.961260000	-4.899637000	-3.268352000
6	-7.379638000	2.128367000	-1.395826000	6	-4.611156000	-5.991823000	-1.540768000
6	-7.638794000	2.838037000	-0.234119000	6	-5.249768000	-5.975824000	-0.310020000
1	-8.556128000	2.636068000	0.320450000	1	-5.283800000	-6.890334000	0.282727000
6	-6.702433000	3.768575000	0.206026000	6	-5.800120000	-4.780139000	0.139232000
1	-6.898215000	4.325060000	1.124586000	1	-6.306961000	-4.755107000	1.106000000
6	-4.987502000	6.285835000	0.482248000	6	-7.728696000	-2.369282000	0.284218000
6	-6.154710000	6.900575000	-0.012792000	6	-8.635824000	-3.310233000	-0.237383000
1	-6.688736000	6.431897000	-0.841054000	1	-8.301406000	-3.993688000	-1.019231000
6	-6.642718000	8.089707000	0.515972000	6	-9.949869000	-3.387159000	0.208743000
1	-7.543858000	8.562820000	0.120932000	1	-10.652469000	-4.113534000	-0.203859000
6	-5.960356000	8.694031000	1.561152000	6	-10.377099000	-2.512947000	1.196545000
6	-4.809760000	8.126975000	2.085086000	6	-9.516694000	-1.575014000	1.745540000
1	-4.301266000	8.618644000	2.916671000	1	-9.881340000	-0.907394000	2.528031000
6	-4.338726000	6.932168000	1.552009000	6	-8.203214000	-1.514905000	1.295115000
1	-3.449900000	6.470245000	1.983554000	1	-7.517661000	-0.792637000	1.739423000

6	-1.383703000	6.605494000	-0.354176000	6	-6.675681000	1.245051000	-0.300541000
6	-2.257921000	7.671734000	-0.915856000	6	-8.046662000	0.930392000	-0.774474000
6	-3.121535000	7.407021000	-1.986225000	6	-8.280690000	-0.011983000	-1.785703000
1	-3.186448000	6.389910000	-2.373695000	1	-7.433906000	-0.549157000	-2.213535000
6	-3.891779000	8.413358000	-2.560684000	6	-9.564973000	-0.273786000	-2.252409000
1	-4.566675000	8.211698000	-3.394031000	1	-9.748079000	-1.011398000	-3.035320000
6	-3.796073000	9.700888000	-2.058173000	6	-10.632947000	0.422846000	-1.711159000
6	-2.947678000	10.006617000	-1.004911000	6	-10.445577000	1.375130000	-0.720230000
1	-2.901434000	11.031935000	-0.634293000	1	-11.309843000	1.905631000	-0.316777000
6	-2.180416000	8.990252000	-0.446779000	6	-9.156684000	1.623758000	-0.264483000
1	-1.503499000	9.221546000	0.377950000	1	-9.001454000	2.373701000	0.513270000
6	0.065340000	6.935388000	-0.276044000	6	-6.371523000	2.694605000	-0.136989000
6	0.845123000	6.575344000	0.830691000	6	-5.736739000	3.196086000	1.006602000
1	0.379068000	6.037266000	1.656556000	1	-5.441864000	2.504311000	1.796729000
6	2.199311000	6.889417000	0.898912000	6	-5.476915000	4.555563000	1.158494000
1	2.813359000	6.615234000	1.756016000	1	-4.986660000	4.955746000	2.045329000
6	2.779228000	7.568682000	-0.159454000	6	-5.855439000	5.423440000	0.147614000
6	2.045004000	7.948132000	-1.273097000	6	-6.484474000	4.970589000	-1.002780000
1	2.540913000	8.476993000	-2.088809000	1	-6.758737000	5.685189000	-1.780747000
6	0.691926000	7.635442000	-1.319123000	6	-6.742316000	3.611865000	-1.133172000
1	0.105944000	7.928794000	-2.191905000	1	-7.237212000	3.246315000	-2.034910000
6	0.084617000	3.569604000	0.260677000	6	-3.278595000	1.390410000	0.135400000
6	1.178010000	2.938731000	0.385794000	6	-2.307235000	2.154144000	0.242919000
6	2.259062000	2.210444000	0.464100000	6	-1.200424000	2.909729000	0.310338000
6	3.257866000	1.430040000	0.472288000	6	-0.131319000	3.537527000	0.316686000
6	4.191659000	0.480051000	0.366688000	6	1.126199000	4.081504000	0.221001000
6	4.133269000	-0.948957000	0.082397000	6	2.386922000	3.481324000	-0.068516000
6	5.572100000	-1.074507000	0.007046000	6	3.061518000	4.782395000	-0.102609000
6	5.680369000	0.413953000	0.290002000	6	1.721232000	5.429674000	0.197730000
6	6.584607000	1.421394000	0.362627000	6	1.149601000	6.657397000	0.348820000
6	6.127517000	2.723587000	0.936192000	6	-0.209668000	6.723865000	0.959726000
6	5.621660000	2.765726000	2.240858000	6	-0.451337000	6.116386000	2.199094000
1	5.546451000	1.836972000	2.808350000	1	0.361428000	5.581551000	2.692686000
6	5.207762000	3.960717000	2.818402000	6	-1.699928000	6.177556000	2.807391000
1	4.807630000	4.001225000	3.832499000	1	-1.892176000	5.702062000	3.770361000
6	5.297534000	5.122657000	2.071878000	6	-2.720797000	6.854777000	2.163033000

6	5.780439000	5.126965000	0.771995000	6	-2.531422000	7.463989000	0.931470000
1	5.791181000	6.063415000	0.213188000	1	-3.376489000	7.951255000	0.444789000
6	6.205054000	3.923340000	0.217782000	6	-1.272093000	7.401300000	0.344227000
1	6.588020000	3.908856000	-0.804723000	1	-1.109948000	7.875024000	-0.626185000
6	7.990483000	1.363392000	-0.096412000	6	1.753391000	7.937092000	-0.076429000
6	8.990321000	2.110000000	0.546557000	6	1.497361000	9.129105000	0.622676000
1	8.727376000	2.714895000	1.415784000	1	0.865090000	9.098483000	1.511499000
6	10.309235000	2.090267000	0.107157000	6	2.036558000	10.344211000	0.216238000
1	11.090802000	2.661795000	0.610694000	1	1.844664000	11.268518000	0.764115000
6	10.633977000	1.321458000	-0.999739000	6	2.841733000	10.376979000	-0.912124000
6	9.674094000	0.581972000	-1.672951000	6	3.109120000	9.227915000	-1.639718000
1	9.965037000	-0.009484000	-2.542181000	1	3.741186000	9.290394000	-2.526856000
6	8.360291000	0.610909000	-1.221029000	6	2.559037000	8.021246000	-1.223477000
1	7.596231000	0.037692000	-1.746695000	1	2.752107000	7.115529000	-1.799141000
6	6.414827000	-2.146828000	-0.201959000	6	4.374964000	5.123289000	-0.274169000
6	7.842736000	-2.157573000	0.159468000	6	4.956662000	6.430579000	0.094965000
6	8.330840000	-1.469780000	1.285631000	6	4.523436000	7.135320000	1.229782000
1	7.628007000	-0.911178000	1.904685000	1	3.728302000	6.709158000	1.842287000
6	9.677189000	-1.488969000	1.633181000	6	5.085123000	8.355280000	1.589549000
1	10.047736000	-0.947119000	2.505163000	1	4.741740000	8.904277000	2.467773000
6	10.564110000	-2.222546000	0.861748000	6	6.108301000	8.880175000	0.816284000
6	10.128747000	-2.934531000	-0.246265000	6	6.581203000	8.210663000	-0.302549000
1	10.851589000	-3.503734000	-0.834123000	1	7.389927000	8.651662000	-0.888165000
6	8.782179000	-2.896705000	-0.587017000	6	6.006202000	6.994605000	-0.651857000
1	8.441971000	-3.450252000	-1.463847000	1	6.373558000	6.465599000	-1.532829000
6	5.841523000	-3.411498000	-0.733288000	6	5.315588000	4.097285000	-0.805160000
6	4.958043000	-3.409760000	-1.825018000	6	5.001240000	3.354716000	-1.952034000
1	4.683410000	-2.457357000	-2.280411000	1	4.049827000	3.533175000	-2.454735000
6	4.421150000	-4.586335000	-2.336351000	6	5.870088000	2.393819000	-2.458650000
1	3.727207000	-4.577492000	-3.178406000	1	5.619706000	1.806468000	-3.343225000
6	4.773454000	-5.793166000	-1.755208000	6	7.074440000	2.172728000	-1.812090000
6	5.642667000	-5.847781000	-0.676400000	6	7.429707000	2.886521000	-0.676265000
1	5.875601000	-6.814114000	-0.227846000	1	8.374600000	2.661884000	-0.181581000
6	6.167505000	-4.661126000	-0.176899000	6	6.550041000	3.844275000	-0.185801000
1	6.843669000	-4.699221000	0.679426000	1	6.818499000	4.404312000	0.712293000
6	3.028000000	-1.772412000	0.015674000	6	2.743752000	2.149805000	-0.163023000

6	1.962078000	-2.390608000	-0.004182000	6	2.920116000	0.928708000	-0.175959000
6	0.746630000	-2.989563000	0.004408000	6	3.034013000	-0.415192000	-0.155928000
6	-0.381389000	-3.473689000	0.029013000	6	3.061603000	-1.649433000	-0.103224000
9	-5.399383000	-10.648224000	-1.770737000	9	7.733392000	-9.094797000	-1.687131000
9	-7.285343000	-9.383634000	2.247449000	9	6.005545000	-10.047569000	2.639496000
9	-8.599391000	-0.185860000	0.723335000	9	-3.011730000	-8.147538000	0.721517000
9	-8.278187000	1.224722000	-1.836834000	9	-4.092453000	-7.146733000	-1.998368000
9	-6.430160000	9.844144000	2.081256000	9	-11.644977000	-2.584835000	1.637458000
9	-4.533447000	10.678103000	-2.609785000	9	-11.874358000	0.181687000	-2.162986000
9	4.088223000	7.876409000	-0.110810000	9	-5.617840000	6.739915000	0.279879000
9	4.895075000	6.281277000	2.625834000	9	-3.930391000	6.915541000	2.748433000
9	11.903116000	1.304484000	-1.436250000	9	3.360917000	11.548279000	-1.314981000
9	11.866439000	-2.257228000	1.199715000	9	6.663004000	10.053493000	1.163590000
9	4.262708000	-6.936806000	-2.249820000	9	7.920075000	1.250968000	-2.299533000
6	-0.602025000	-6.751294000	-0.043128000	6	6.040393000	-3.114550000	-0.102964000
6	0.089223000	-7.427962000	-1.059946000	6	6.987663000	-2.819556000	-1.096426000
6	0.109960000	-6.404451000	1.112202000	6	5.966317000	-2.251971000	0.999521000
6	1.436258000	-7.745463000	-0.935099000	6	7.831839000	-1.719681000	-0.995497000
1	-0.441683000	-7.700058000	-1.974590000	1	7.058730000	-3.467973000	-1.972004000
6	1.456829000	-6.721135000	1.258131000	6	6.805649000	-1.149139000	1.119649000
1	-0.405652000	-5.876045000	1.915446000	1	5.234141000	-2.454943000	1.782186000
6	2.099124000	-7.394591000	0.233167000	6	7.735438000	-0.905169000	0.123162000
1	1.992375000	-8.241297000	-1.730963000	1	8.554835000	-1.472019000	-1.773447000
1	2.016525000	-6.446190000	2.153085000	1	6.746100000	-0.475745000	1.975834000
9	3.388963000	-7.726291000	0.377450000	9	8.571356000	0.138665000	0.247910000

3d

Cam-b3lyp/def2-SVP

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6	-2.345843000	3.434019000	-0.080505000
6	-1.093098000	4.020902000	0.043011000
6	-1.691137000	5.358128000	0.315576000
6	-3.037570000	4.744165000	0.034851000
6	-4.288712000	5.181698000	-0.229235000
6	-4.557419000	6.612501000	-0.533219000
6	-5.611815000	7.306684000	0.073869000

3d

Cam-b3lyp/def2-SVP

0 3

6	-2.252602000	3.507969000	-0.033554000
6	-0.977571000	4.052473000	0.071214000
6	-1.518173000	5.405945000	0.348019000
6	-2.891744000	4.845160000	0.087166000
6	-4.126949000	5.327442000	-0.172672000
6	-4.349491000	6.766526000	-0.475196000
6	-5.378605000	7.493913000	0.136288000

1	-6.231826000	6.801550000	0.816720000	1	-6.011688000	7.008314000	0.881217000
6	-5.870918000	8.634996000	-0.237360000	6	-5.596529000	8.829948000	-0.173660000
1	-6.673396000	9.179931000	0.260774000	1	-6.379729000	9.399900000	0.327158000
6	-5.085164000	9.279699000	-1.189899000	6	-4.794397000	9.449545000	-1.129191000
6	-4.050697000	8.605820000	-1.829933000	6	-3.784516000	8.743166000	-1.773362000
1	-3.454250000	9.119521000	-2.584738000	1	-3.174853000	9.237844000	-2.530316000
6	-3.790698000	7.281604000	-1.494518000	6	-3.565720000	7.411124000	-1.439397000
1	-2.983335000	6.748613000	-1.999295000	1	-2.777715000	6.852824000	-1.947409000
6	-1.243126000	6.488268000	0.903690000	6	-1.015624000	6.530087000	0.910230000
6	-2.177975000	7.452697000	1.547019000	6	-1.900775000	7.530480000	1.566714000
6	-3.074771000	7.015431000	2.527873000	6	-2.805405000	7.129024000	2.556085000
1	-3.104698000	5.956791000	2.791205000	1	-2.876095000	6.072176000	2.818586000
6	-3.917003000	7.907833000	3.182718000	6	-3.603330000	8.053999000	3.220905000
1	-4.610042000	7.562873000	3.950900000	1	-4.302048000	7.736283000	3.995665000
6	-3.874083000	9.256226000	2.845686000	6	-3.507665000	9.400334000	2.886446000
6	-2.982923000	9.719727000	1.880803000	6	-2.607608000	9.828659000	1.913531000
1	-2.965866000	10.779498000	1.624541000	1	-2.548786000	10.887471000	1.659493000
6	-2.133060000	8.820107000	1.250214000	6	-1.802558000	8.896009000	1.272400000
1	-1.428380000	9.185023000	0.500511000	1	-1.091487000	9.233239000	0.515814000
6	0.204997000	6.782041000	1.039220000	6	0.444285000	6.777623000	0.997378000
6	0.711195000	7.309769000	2.236902000	6	1.005562000	7.307574000	2.169431000
1	0.035716000	7.484708000	3.075863000	1	0.363641000	7.515406000	3.027033000
6	2.059269000	7.606607000	2.379314000	6	2.365890000	7.565524000	2.263248000
1	2.447693000	8.007244000	3.316257000	1	2.796608000	7.968273000	3.180603000
6	2.920692000	7.397027000	1.305260000	6	3.185044000	7.313431000	1.165563000
6	2.446817000	6.887241000	0.101481000	6	2.657160000	6.799207000	-0.013661000
1	3.126766000	6.753261000	-0.739138000	1	3.304204000	6.630318000	-0.873965000
6	1.095763000	6.580110000	-0.021584000	6	1.294218000	6.531699000	-0.087909000
1	0.721678000	6.201059000	-0.973954000	1	0.878406000	6.149289000	-1.021433000
6	0.170869000	3.429217000	-0.020222000	6	0.267733000	3.408623000	-0.007153000
6	1.197528000	2.771145000	-0.110987000	6	1.263860000	2.711009000	-0.110361000
6	2.291767000	1.964422000	-0.199434000	6	2.330451000	1.861496000	-0.212542000
6	3.228975000	1.181999000	-0.261265000	6	3.241934000	1.049683000	-0.282818000
6	4.222028000	0.198133000	-0.271359000	6	4.205152000	0.038635000	-0.295905000
6	4.140032000	-1.171273000	-0.071540000	6	4.077503000	-1.362453000	-0.070895000
6	5.616708000	-1.337384000	-0.191230000	6	5.557364000	-1.534445000	-0.181231000

6	5.705180000	0.168198000	-0.335926000	6	5.661457000	-0.035182000	-0.346512000
6	6.608391000	1.173149000	-0.411575000	6	6.599206000	0.959973000	-0.432541000
6	6.152685000	2.511971000	-0.883864000	6	6.176943000	2.277503000	-0.977784000
6	5.511584000	2.626595000	-2.122719000	6	5.524953000	2.341569000	-2.216032000
1	5.308278000	1.726316000	-2.705451000	1	5.302942000	1.417366000	-2.752481000
6	5.158372000	3.867713000	-2.639890000	6	5.180964000	3.560017000	-2.788502000
1	4.676463000	3.951918000	-3.614430000	1	4.689239000	3.602979000	-3.760808000
6	5.441241000	5.012261000	-1.904376000	6	5.481608000	4.735581000	-2.110338000
6	6.054593000	4.928876000	-0.656318000	6	6.109126000	4.705046000	-0.866975000
1	6.238463000	5.836094000	-0.080704000	1	6.307093000	5.635967000	-0.335438000
6	6.416654000	3.682245000	-0.160977000	6	6.462269000	3.479676000	-0.315893000
1	6.915180000	3.616127000	0.808061000	1	6.965030000	3.454815000	0.652752000
6	8.043021000	1.045732000	-0.072552000	6	8.005389000	0.819746000	-0.013377000
6	9.014764000	1.780554000	-0.768635000	6	9.025519000	1.545810000	-0.650309000
1	8.711427000	2.438047000	-1.584786000	1	8.778513000	2.201642000	-1.486302000
6	10.362439000	1.674756000	-0.452748000	6	10.350017000	1.432599000	-0.251591000
1	11.113467000	2.236823000	-1.008803000	1	11.137123000	1.988798000	-0.761741000
6	10.757206000	0.835828000	0.586333000	6	10.675352000	0.593697000	0.811567000
6	9.812017000	0.116176000	1.311456000	6	9.682962000	-0.122732000	1.475288000
1	10.134385000	-0.524898000	2.132378000	1	9.950434000	-0.765092000	2.314767000
6	8.467470000	0.226325000	0.981365000	6	8.362675000	-0.005904000	1.063040000
1	7.726785000	-0.328353000	1.558972000	1	7.586071000	-0.556712000	1.595244000
6	6.405531000	-2.424266000	-0.339969000	6	6.339443000	-2.628120000	-0.327419000
6	7.823001000	-2.360732000	-0.780122000	6	7.757940000	-2.570868000	-0.766011000
6	8.221667000	-1.563599000	-1.857764000	6	8.159309000	-1.782725000	-1.849316000
1	7.478517000	-0.962431000	-2.383291000	1	7.418579000	-1.182297000	-2.379173000
6	9.547438000	-1.529093000	-2.274869000	6	9.484519000	-1.758036000	-2.269065000
1	9.852406000	-0.903746000	-3.114337000	1	9.790990000	-1.141554000	-3.114586000
6	10.495064000	-2.299306000	-1.609097000	6	10.429192000	-2.528940000	-1.599718000
6	10.121478000	-3.119445000	-0.546743000	6	10.053498000	-3.337650000	-0.529432000
1	10.874259000	-3.723776000	-0.039498000	1	10.804038000	-3.941806000	-0.018678000
6	8.792320000	-3.153344000	-0.148638000	6	8.724748000	-3.361844000	-0.128939000
1	8.500105000	-3.801545000	0.679608000	1	8.430500000	-4.002402000	0.704566000
6	5.873177000	-3.799740000	-0.128668000	6	5.795145000	-3.999339000	-0.123300000
6	5.191838000	-4.169118000	1.035369000	6	5.081049000	-4.360831000	1.023715000
1	5.015413000	-3.426243000	1.815211000	1	4.893427000	-3.615725000	1.798615000

6	4.761474000	-5.479022000	1.234329000	6	4.629502000	-5.665177000	1.211150000
1	4.247740000	-5.767366000	2.151762000	1	4.088886000	-5.946902000	2.115100000
6	5.010619000	-6.432011000	0.252791000	6	4.889897000	-6.620971000	0.235109000
6	5.672634000	-6.088447000	-0.923575000	6	5.586552000	-6.285949000	-0.923411000
1	5.854584000	-6.847825000	-1.684760000	1	5.777592000	-7.047241000	-1.680449000
6	6.106213000	-4.783298000	-1.101412000	6	6.040834000	-4.986238000	-1.089727000
1	6.641694000	-4.518875000	-2.014951000	1	6.601043000	-4.728553000	-1.990206000
6	3.012426000	-1.974434000	0.113751000	6	2.962037000	-2.120056000	0.111148000
6	1.937729000	-2.542560000	0.245229000	6	1.843598000	-2.662652000	0.246292000
6	0.695043000	-3.093539000	0.325685000	6	0.625876000	-3.158889000	0.335956000
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6	-1.801412000	-3.848371000	0.174427000	6	-1.870529000	-3.827640000	0.242032000
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6	-3.790772000	-4.230301000	-0.284037000	6	-3.896928000	-4.091935000	-0.249043000
6	-2.636002000	-5.077087000	0.217537000	6	-2.783346000	-4.995664000	0.239779000
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6	1.236587000	-7.102745000	2.813009000	6	1.025561000	-7.238601000	2.733094000
6	0.999025000	-7.830670000	1.649188000	6	0.790219000	-7.874986000	1.517015000
1	1.721496000	-8.576728000	1.320277000	1	1.512915000	-8.594447000	1.133290000
6	-0.154988000	-7.583226000	0.916574000	6	-0.361952000	-7.569007000	0.802092000
1	-0.346777000	-8.160310000	0.009888000	1	-0.552583000	-8.074102000	-0.146907000
6	-3.163209000	-7.528475000	0.240258000	6	-3.400160000	-7.430684000	0.174994000
6	-3.294225000	-8.585122000	1.153270000	6	-3.534854000	-8.531405000	1.035536000
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1	-4.185440000	-10.507250000	1.581454000	1	-4.477403000	-10.442272000	1.396449000
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6	-4.584121000	-8.752107000	-1.306104000	6	-4.911483000	-8.527125000	-1.382788000
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6	-3.808625000	-7.641809000	-0.997529000	6	-4.091496000	-7.459046000	-1.043858000
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1	-8.584113000	-7.245122000	-1.577841000	1	-8.908964000	-6.886071000	-1.367510000
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6	-5.736257000	-3.137154000	-1.278682000	6	-5.820306000	-2.966074000	-1.278025000
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6	-6.455297000	4.404436000	-1.240536000	6	-6.305139000	4.613556000	-1.204448000
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6	-6.731388000	2.437463000	0.708855000	6	-6.656723000	2.651516000	0.737605000
1	-4.847754000	3.130809000	1.466463000	1	-4.767593000	3.298338000	1.523007000
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17	-8.741167000	-8.905256000	0.733633000	17	-8.981264000	-8.592541000	0.913924000

17	-5.706734000	-11.152223000	-0.740448000	17	-6.099450000	-10.913387000	-0.898574000
17	-7.618172000	0.398247000	-3.403770000	17	-7.540659000	0.628602000	-3.441039000
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17	-4.949124000	10.373927000	3.629924000	17	-4.526205000	10.560028000	3.685059000
17	4.604443000	7.805609000	1.474664000	17	4.885088000	7.673934000	1.274099000
17	5.039083000	6.571460000	-2.567311000	17	5.078767000	6.265286000	-2.837658000
17	12.439929000	0.691258000	0.985462000	17	12.328217000	0.445729000	1.318509000
17	12.156378000	-2.240811000	-2.109070000	17	12.088978000	-2.488269000	-2.107290000
17	4.526720000	-8.085693000	0.494839000	17	4.374412000	-8.267669000	0.461817000
17	2.661622000	-7.424426000	3.758956000	17	2.446316000	-7.632844000	3.657164000

3d				3d			
Cam-b3lyp/def2-SVP				Cam-b3lyp/def2-SVP			
-2 1				-2 3			
6	-4.176976000	0.514648000	0.080654000	6	3.205056000	-2.694158000	-0.004298000
6	-3.774385000	1.855037000	0.121478000	6	2.103289000	-3.621875000	0.076317000
6	-5.177246000	2.311293000	0.287167000	6	3.035635000	-4.744473000	0.270185000
6	-5.604518000	0.883669000	0.076497000	6	4.178384000	-3.785604000	0.020053000
6	-6.764204000	0.224433000	-0.190522000	6	5.514564000	-3.904924000	-0.241483000
6	-7.971362000	0.950316000	-0.660494000	6	6.095954000	-5.196765000	-0.683936000
6	-9.252544000	0.656970000	-0.169992000	6	7.315654000	-5.677166000	-0.182359000
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6	-7.868325000	1.922016000	-1.666052000	6	5.461944000	-5.959125000	-1.676586000
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6	-5.767056000	3.446502000	0.735658000	6	2.938699000	-6.010023000	0.762853000
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6	-7.499351000	2.517590000	2.294594000	6	4.892893000	-6.089580000	2.336258000
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1	-7.862193000	5.088464000	0.113950000	1	3.855292000	-8.528616000	0.223719000
6	-5.033316000	4.732930000	0.837956000	6	1.635382000	-6.702940000	0.893824000
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6	3.589293000	4.304486000	-0.101507000	6	-5.413640000	-1.621061000	-0.174288000
6	3.568278000	5.686036000	-0.087388000	6	-6.135893000	-2.787486000	-0.136362000
6	2.375051000	6.412951000	-0.561918000	6	-5.514439000	-4.059850000	-0.564635000
6	1.631956000	5.936159000	-1.658393000	6	-4.661969000	-4.095592000	-1.681068000
1	1.936956000	5.006320000	-2.139427000	1	-4.445277000	-3.168688000	-2.212999000
6	0.532125000	6.620505000	-2.155198000	6	-4.103745000	-5.282222000	-2.137109000
1	-0.021461000	6.233173000	-3.011780000	1	-3.450075000	-5.289405000	-3.010219000
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6	1.940954000	7.619099000	0.020214000	6	-5.772744000	-5.279226000	0.085556000
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6	5.119465000	7.679490000	-0.065802000	6	-8.517233000	-3.628006000	-0.170157000

1	4.633976000	8.055169000	-0.968181000	1	-8.286769000	-4.214795000	-1.061098000
6	6.159641000	8.410828000	0.492616000	6	-9.800353000	-3.679295000	0.359162000
1	6.494568000	9.342559000	0.034270000	1	-10.574125000	-4.288263000	-0.110283000
6	6.796824000	7.933678000	1.634340000	6	-10.103561000	-2.926927000	1.490217000
6	6.391860000	6.738395000	2.217036000	6	-9.133085000	-2.133520000	2.090743000
1	6.887265000	6.379484000	3.120643000	1	-9.378530000	-1.558157000	2.984606000
6	5.348477000	6.018616000	1.646381000	6	-7.854700000	-2.089761000	1.546305000
1	5.017745000	5.093224000	2.120219000	1	-7.088485000	-1.480961000	2.028235000
6	5.975488000	3.221131000	-0.424632000	6	-6.794604000	0.621968000	-0.448660000
6	6.644536000	4.408333000	-1.031836000	6	-8.009056000	0.027597000	-1.073792000
6	6.129837000	4.991162000	-2.195540000	6	-7.901380000	-0.759328000	-2.227497000
1	5.207474000	4.594773000	-2.622467000	1	-6.911700000	-0.958120000	-2.640978000
6	6.771174000	6.059422000	-2.814597000	6	-9.025701000	-1.283689000	-2.857608000
1	6.362265000	6.507956000	-3.720858000	1	-8.928919000	-1.895731000	-3.755322000
6	7.943490000	6.560552000	-2.261314000	6	-10.284050000	-1.022455000	-2.329733000
6	8.483137000	6.000593000	-1.108353000	6	-10.427652000	-0.235908000	-1.190828000
1	9.395391000	6.415434000	-0.678213000	1	-11.421403000	-0.049785000	-0.781733000
6	7.835980000	4.925271000	-0.510282000	6	-9.294556000	0.287938000	-0.580414000
1	8.259086000	4.481813000	0.393083000	1	-9.406286000	0.906111000	0.312517000
6	6.789058000	1.981971000	-0.359614000	6	-6.780102000	2.097917000	-0.312835000
6	6.648392000	1.057311000	0.684420000	6	-6.140123000	2.739979000	0.757856000
1	5.921012000	1.248891000	1.473223000	1	-5.637300000	2.140137000	1.516780000
6	7.424332000	-0.095905000	0.745017000	6	-6.140763000	4.125405000	0.884189000
1	7.310246000	-0.801873000	1.567542000	1	-5.644950000	4.609245000	1.725841000
6	8.361462000	-0.337837000	-0.252823000	6	-6.794788000	4.895664000	-0.070960000
6	8.528335000	0.558427000	-1.303733000	6	-7.441603000	4.293486000	-1.145497000
1	9.264001000	0.351489000	-2.082183000	1	-7.944690000	4.910993000	-1.890993000
6	7.750610000	1.707849000	-1.346061000	6	-7.433637000	2.909554000	-1.255944000
1	7.885028000	2.407563000	-2.172320000	1	-7.939081000	2.444155000	-2.103535000
6	3.512315000	0.885963000	0.261125000	6	-3.413088000	1.164058000	0.179899000
6	3.217880000	-0.339798000	0.402455000	6	-2.513489000	2.010138000	0.305161000
6	2.821098000	-1.580742000	0.490074000	6	-1.475514000	2.853487000	0.380052000
6	2.347409000	-2.755727000	0.502665000	6	-0.459134000	3.565139000	0.381984000
6	1.690341000	-3.913236000	0.380542000	6	0.745967000	4.207906000	0.262665000
6	0.310355000	-4.242651000	0.053692000	6	2.041149000	3.719445000	-0.080307000
6	0.579238000	-5.657012000	-0.030167000	6	2.604037000	5.068135000	-0.124484000

6	2.028993000	-5.365708000	0.313110000	6	1.231689000	5.600990000	0.245040000
6	3.232965000	-5.975998000	0.436258000	6	0.575087000	6.776628000	0.447276000
6	4.352872000	-5.209845000	1.060165000	6	-0.756680000	6.734679000	1.116764000
6	4.201133000	-4.676478000	2.345260000	6	-0.904094000	6.079449000	2.346176000
1	3.245572000	-4.794203000	2.858339000	1	-0.041275000	5.576382000	2.785293000
6	5.241145000	-4.006444000	2.978639000	6	-2.119459000	6.062410000	3.019814000
1	5.115147000	-3.597739000	3.981779000	1	-2.220219000	5.552172000	3.978359000
6	6.452903000	-3.857278000	2.316071000	6	-3.215120000	6.705287000	2.457595000
6	6.631590000	-4.355886000	1.029147000	6	-3.111231000	7.350076000	1.228586000
1	7.577666000	-4.193756000	0.511881000	1	-3.992136000	7.815035000	0.785179000
6	5.584794000	-5.037146000	0.417277000	6	-1.884011000	7.367697000	0.575048000
1	5.722999000	-5.436040000	-0.589768000	1	-1.799648000	7.876414000	-0.387468000
6	3.550287000	-7.351565000	-0.009141000	6	1.071001000	8.105224000	0.033096000
6	4.476037000	-8.141810000	0.689415000	6	0.777582000	9.257356000	0.781649000
1	4.945226000	-7.744421000	1.590959000	1	0.194067000	9.163018000	1.699007000
6	4.801816000	-9.424694000	0.267122000	6	1.222891000	10.513815000	0.391027000
1	5.513371000	-10.034461000	0.825452000	1	0.997554000	11.398042000	0.988933000
6	4.207194000	-9.934542000	-0.882379000	6	1.970745000	10.641025000	-0.775384000
6	3.298410000	-9.170959000	-1.606656000	6	2.264667000	9.523828000	-1.549487000
1	2.841229000	-9.581189000	-2.507538000	1	2.845419000	9.636415000	-2.465622000
6	2.980772000	-7.890495000	-1.171002000	6	1.810533000	8.273872000	-1.147481000
1	2.271533000	-7.289309000	-1.740589000	1	2.030325000	7.400610000	-1.762493000
6	-0.223424000	-6.748838000	-0.303139000	6	3.877483000	5.510795000	-0.366100000
6	0.105960000	-8.128788000	0.077530000	6	4.387961000	6.842041000	0.009480000
6	0.847020000	-8.424076000	1.237330000	6	3.955843000	7.493626000	1.176355000
1	1.180613000	-7.602118000	1.871761000	1	3.220328000	7.001762000	1.813732000
6	1.155750000	-9.728437000	1.601927000	6	4.445717000	8.741820000	1.539638000
1	1.736534000	-9.930227000	2.503144000	1	4.093058000	9.235418000	2.446010000
6	0.709269000	-10.786370000	0.817510000	6	5.399736000	9.363164000	0.741015000
6	-0.044917000	-10.538726000	-0.326096000	6	5.866928000	8.739037000	-0.411855000
1	-0.391080000	-11.374096000	-0.937050000	1	6.616695000	9.235072000	-1.030016000
6	-0.338290000	-9.229746000	-0.683140000	6	5.365686000	7.492769000	-0.764323000
1	-0.921659000	-9.048029000	-1.587338000	1	5.733230000	7.010581000	-1.671691000
6	-1.542593000	-6.509192000	-0.942823000	6	4.839810000	4.571036000	-1.005689000
6	-1.665308000	-5.657823000	-2.053226000	6	4.493214000	3.880132000	-2.174943000
1	-0.774704000	-5.157001000	-2.435918000	1	3.502208000	4.030627000	-2.605828000

6	-2.886136000	-5.436374000	-2.677832000	6	5.380085000	3.009804000	-2.797539000
1	-2.958634000	-4.769846000	-3.538185000	1	5.094280000	2.476240000	-3.704654000
6	-4.025429000	-6.072558000	-2.197268000	6	6.642365000	2.815496000	-2.249390000
6	-3.947519000	-6.918405000	-1.095218000	6	7.018904000	3.479612000	-1.084909000
1	-4.853054000	-7.387617000	-0.709790000	1	8.000422000	3.289643000	-0.650142000
6	-2.717036000	-7.130094000	-0.483911000	6	6.122281000	4.352698000	-0.480009000
1	-2.664311000	-7.789355000	0.384856000	1	6.418284000	4.869899000	0.435110000
6	-0.791165000	-3.411122000	-0.026220000	6	2.514518000	2.424795000	-0.196415000
6	-1.693984000	-2.575290000	-0.046178000	6	2.813331000	1.229363000	-0.211358000
6	-2.626016000	-1.589783000	-0.024785000	6	3.062579000	-0.097468000	-0.183719000
6	-3.417393000	-0.653367000	0.015858000	6	3.209442000	-1.321432000	-0.116743000
6	-6.844775000	-1.253773000	-0.100714000	6	6.418906000	-2.733729000	-0.180646000
6	-7.601754000	-2.005729000	-1.014362000	6	7.509490000	-2.595012000	-1.057036000
6	-6.199707000	-1.950582000	0.932243000	6	6.249349000	-1.736322000	0.793838000
6	-7.720137000	-3.384833000	-0.900484000	6	8.395284000	-1.529240000	-0.959528000
1	-8.105781000	-1.497056000	-1.838052000	1	7.665918000	-3.341312000	-1.837698000
6	-6.308795000	-3.330608000	1.058706000	6	7.126489000	-0.664082000	0.903053000
1	-5.612175000	-1.396880000	1.665072000	1	5.417940000	-1.812681000	1.494746000
6	-7.081685000	-4.041135000	0.147947000	6	8.206329000	-0.572253000	0.032396000
1	-8.302265000	-3.958541000	-1.622213000	1	9.233574000	-1.434036000	-1.650801000
1	-5.802130000	-3.856253000	1.868651000	1	6.979217000	0.096855000	1.670261000
17	1.084760000	-12.432204000	1.274735000	17	6.024332000	10.930279000	1.192980000
17	4.615305000	-11.542055000	-1.425780000	17	2.533008000	12.216083000	-1.275886000
17	-5.561761000	-5.810537000	-2.988768000	17	7.764373000	1.734981000	-3.034426000
17	-7.280274000	-5.763035000	0.337154000	17	9.352599000	0.735357000	0.201899000
17	-11.650090000	3.135858000	-2.213112000	17	7.886982000	-9.117372000	-2.162065000
17	-11.317227000	3.428099000	3.108725000	17	7.636191000	-8.862826000	3.267644000
17	-2.849575000	8.706365000	1.210125000	17	-2.345062000	-8.874635000	1.340004000
17	-1.236792000	8.687158000	-2.191608000	17	-3.716221000	-7.970338000	-2.064302000
17	8.117535000	8.842471000	2.336583000	17	-11.718313000	-2.979732000	2.158474000
17	8.743595000	7.918447000	-3.015786000	17	-11.702055000	-1.693623000	-3.099007000
17	9.360044000	-1.771325000	-0.189839000	17	-6.827554000	6.637139000	0.076662000
17	7.770128000	-3.037633000	3.119822000	17	-4.738455000	6.706573000	3.313220000
3m Cam-b3lyp/def2-SVP				3m Cam-b3lyp/def2-SVP			

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6	0.235699000	4.225317000	0.000088000
6	1.587597000	3.922855000	0.000074000
6	1.970242000	5.359268000	-0.000211000
6	0.501722000	5.687851000	-0.000137000
6	-0.238467000	6.791428000	-0.000269000
6	3.110291000	6.042134000	-0.000302000
6	2.254830000	2.694789000	0.000153000
6	2.721957000	1.566246000	0.000153000
6	3.129273000	0.265894000	0.000149000
6	3.389379000	-0.927492000	0.000121000
6	3.541592000	-2.316794000	-0.000073000
6	2.603557000	-3.336206000	-0.000071000
6	3.656104000	-4.385924000	-0.000212000
6	4.675047000	-3.278577000	-0.000163000
6	6.000963000	-3.189534000	0.000088000
6	3.677322000	-5.714627000	-0.000433000
6	1.206420000	-3.299825000	0.000254000
6	-0.004470000	-3.139906000	0.000567000
6	-1.334263000	-2.842476000	0.000193000
6	-2.497826000	-2.471074000	0.000024000
6	-3.777211000	-1.908482000	0.000024000
6	-4.191256000	-0.586491000	0.000064000
6	-5.626557000	-0.973430000	-0.000026000
6	-5.176767000	-2.409464000	-0.000129000
6	-5.762232000	-3.602465000	-0.000439000
6	-6.787974000	-0.327730000	0.000062000
6	-3.461393000	0.605405000	0.000068000
6	-2.717546000	1.574181000	0.000183000
6	-1.794806000	2.576856000	0.000348000
6	-0.891250000	3.398699000	0.000349000
1	6.624192000	-4.086030000	0.000304000
1	6.500021000	-2.218381000	0.000363000
1	4.622400000	-6.261384000	-0.000303000
1	2.750868000	-6.292446000	-0.000316000
1	-5.170273000	-4.519965000	-0.000441000

0 3

6	-3.465317000	2.470856000	-0.000096000
6	-2.399150000	3.471981000	0.000061000
6	-3.450158000	4.534212000	0.000014000
6	-4.469084000	3.440279000	-0.000166000
6	-5.916744000	3.427477000	-0.000353000
6	-3.470483000	5.865130000	0.000244000
6	-1.048938000	3.374331000	0.000060000
6	0.174123000	3.149285000	0.000070000
6	1.466421000	2.794779000	0.000057000
6	2.625459000	2.367745000	0.000038000
6	3.859879000	1.750941000	0.000091000
6	4.220810000	0.391673000	-0.000104000
6	5.664640000	0.719050000	-0.000152000
6	5.285026000	2.173877000	0.000093000
6	5.931386000	3.336694000	0.000318000
6	6.800236000	0.021973000	-0.000314000
6	3.441855000	-0.759659000	-0.000122000
6	2.649728000	-1.694725000	-0.000136000
6	1.683333000	-2.650248000	-0.000107000
6	0.741383000	-3.431986000	-0.000097000
6	-0.419007000	-4.205556000	0.000033000
6	-1.762257000	-3.845126000	0.000114000
6	-2.203014000	-5.262604000	0.000124000
6	-0.750314000	-5.653915000	0.000035000
6	-0.058528000	-6.789371000	0.000071000
6	-3.371443000	-5.898094000	0.000103000
6	-2.378077000	-2.591135000	0.000104000
6	-2.800611000	-1.444558000	0.000074000
6	-3.159600000	-0.128952000	-0.000011000
6	-3.386184000	1.070670000	-0.000077000
1	7.022686000	3.373531000	0.000289000
1	5.386559000	4.282955000	0.000565000
1	7.769028000	0.525497000	-0.000297000
1	6.789871000	-1.069838000	-0.000384000
1	1.033353000	-6.782868000	0.000026000

1	-6.850169000	-3.694612000	-0.000693000	1	-0.565423000	-7.756446000	0.000152000
1	-7.733948000	-0.872931000	-0.000205000	1	-3.417900000	-6.988940000	-0.000039000
1	-6.825252000	0.763498000	-0.000124000	1	-4.312829000	-5.344913000	0.000096000
1	0.225946000	7.779568000	-0.000441000	1	-6.479100000	3.440453000	-0.938628000
1	-1.328994000	6.737640000	-0.000608000	1	-6.479377000	3.439601000	0.937761000
1	4.073842000	5.528512000	-0.000198000	1	-2.542704000	6.440312000	0.000407000
1	3.111508000	7.133971000	-0.000329000	1	-4.416393000	6.410499000	0.000241000

3m				3m			
Cam-b3lyp/def2-SVP				Cam-b3lyp/def2-SVP			
-2 1				-2 3			
6	-3.264694000	-2.734876000	0.000083000	6	-3.172416000	-2.804480000	0.000121000
6	-3.938905000	-1.482134000	0.000059000	6	-3.925741000	-1.586244000	-0.000078000
6	-5.250813000	-2.189746000	-0.000179000	6	-5.196899000	-2.329644000	-0.000204000
6	-4.511365000	-3.496737000	0.000191000	6	-4.405199000	-3.609721000	0.000007000
6	-4.904764000	-4.782072000	0.000464000	6	-4.730245000	-4.909020000	0.000075000
6	-6.530548000	-1.815527000	-0.000684000	6	-6.504513000	-2.039858000	-0.000412000
6	-3.541792000	-0.180641000	-0.000137000	6	-3.547839000	-0.258200000	-0.000008000
6	-3.032415000	0.964910000	-0.000345000	6	-3.068029000	0.882219000	-0.000059000
6	-2.391699000	2.121124000	-0.000370000	6	-2.428235000	2.072274000	-0.000194000
6	-1.670322000	3.155433000	-0.000295000	6	-1.741719000	3.101561000	-0.000317000
6	-0.766124000	4.147589000	-0.000163000	6	-0.842459000	4.149384000	-0.000079000
6	0.727365000	4.154245000	-0.000157000	6	0.589149000	4.192939000	0.000027000
6	0.727713000	5.629005000	0.000151000	6	0.580856000	5.665403000	0.000210000
6	-0.779688000	5.622261000	0.000208000	6	-0.923553000	5.619706000	0.000129000
6	-1.702177000	6.593892000	0.000386000	6	-1.886567000	6.550527000	0.000186000
6	1.641536000	6.608774000	0.000500000	6	1.485467000	6.653113000	0.000317000
6	1.640417000	3.170254000	0.000004000	6	1.550368000	3.201543000	-0.000178000
6	2.371513000	2.142752000	-0.000156000	6	2.298029000	2.215828000	-0.000302000
6	3.023520000	0.992911000	-0.000275000	6	3.009028000	1.066824000	-0.000156000
6	3.543707000	-0.147812000	-0.000257000	6	3.557291000	-0.042287000	-0.000048000
6	3.952643000	-1.445589000	-0.000099000	6	4.014958000	-1.345005000	-0.000060000
6	3.289902000	-2.704509000	0.000290000	6	3.336657000	-2.606662000	0.000081000
6	4.543486000	-3.454923000	0.000117000	6	4.615934000	-3.335774000	0.000016000
6	5.270956000	-2.141230000	-0.000272000	6	5.328710000	-2.010115000	-0.000223000
6	6.547216000	-1.755339000	-0.000594000	6	6.616441000	-1.641864000	-0.000510000

6	4.948562000	-4.736632000	0.000204000	6	5.019113000	-4.613030000	0.000151000
6	1.918992000	-3.007853000	0.000403000	6	1.997459000	-2.943234000	0.000297000
6	0.700828000	-3.128416000	0.000456000	6	0.769966000	-3.097786000	0.000473000
6	-0.671829000	-3.134973000	0.000319000	6	-0.580647000	-3.139036000	0.000467000
6	-1.891051000	-3.025717000	0.000175000	6	-1.815247000	-3.059343000	0.000364000
1	-1.408150000	7.647140000	0.000544000	1	-1.637229000	7.614848000	0.000256000
1	-2.769477000	6.359442000	0.000309000	1	-2.942387000	6.269580000	0.000143000
1	1.337902000	7.659289000	0.000803000	1	1.171833000	7.700287000	0.000360000
1	2.710901000	6.383897000	0.000346000	1	2.556430000	6.436969000	0.000441000
1	6.811376000	-0.695027000	-0.000835000	1	6.901373000	-0.587125000	-0.000630000
1	7.357384000	-2.489465000	-0.000711000	1	7.413315000	-2.390175000	-0.000516000
1	6.012603000	-4.985751000	0.000047000	1	6.082864000	-4.864811000	-0.000022000
1	4.228577000	-5.557929000	0.000316000	1	4.296573000	-5.432554000	0.000594000
1	-5.966528000	-5.040713000	0.000377000	1	-5.776789000	-5.224776000	-0.000414000
1	-4.177414000	-5.596865000	0.000524000	1	-3.959356000	-5.683217000	0.000197000
1	-6.804159000	-0.757617000	-0.001027000	1	-6.852546000	-1.004223000	-0.000554000
1	-7.334049000	-2.556953000	-0.000850000	1	-7.254773000	-2.834898000	-0.000426000

3m				3m			
Cam-b3lyp/def2-tzvpp				Cam-b3lyp/def2-tzvpp			
0 1				-2 3			
6	-2.499936000	3.375040000	-0.000045000	6	1.202928000	4.026006000	0.000107000
6	-1.275161000	4.001575000	0.000164000	6	2.478831000	3.392574000	0.000106000
6	-1.893254000	5.347030000	0.000051000	6	3.163963000	4.687841000	0.000089000
6	-3.229263000	4.663603000	0.000100000	6	1.820259000	5.354786000	-0.000056000
6	-4.495481000	5.035556000	0.000028000	6	1.411029000	6.621864000	-0.000135000
6	-1.453940000	6.591476000	0.000162000	6	4.420669000	5.127856000	0.000004000
6	0.016165000	3.487736000	0.000190000	6	2.860297000	2.074591000	0.000115000
6	1.087335000	2.926488000	0.000147000	6	3.056116000	0.864589000	0.000093000
6	2.224029000	2.191621000	-0.000146000	6	3.140512000	-0.474220000	-0.000069000
6	3.175174000	1.444808000	-0.000347000	6	3.098161000	-1.699230000	-0.000204000
6	4.172991000	0.477385000	-0.000149000	6	2.885091000	-3.054672000	-0.000176000
6	4.103313000	-0.896578000	-0.000015000	6	1.698738000	-3.843152000	0.000006000
6	5.577569000	-1.033896000	0.000006000	6	2.477889000	-5.083992000	-0.000035000
6	5.653580000	0.464848000	-0.000074000	6	3.727302000	-4.253753000	-0.000078000
6	6.608702000	1.375551000	-0.000092000	6	5.029289000	-4.532596000	-0.000145000

6	6.435739000	-2.036488000	0.000084000	6	2.230790000	-6.392414000	0.000073000
6	3.012731000	-1.758078000	-0.000043000	6	0.366483000	-3.514456000	0.000146000
6	1.991086000	-2.405108000	-0.000068000	6	-0.779224000	-3.078982000	0.000280000
6	0.786038000	-3.021518000	0.000142000	6	-1.980947000	-2.482635000	0.000202000
6	-0.336434000	-3.471476000	0.000301000	6	-3.020649000	-1.833498000	0.000105000
6	-1.673072000	-3.852201000	0.000127000	6	-4.088019000	-0.971289000	0.000001000
6	-2.828272000	-3.105113000	-0.000097000	6	-4.177620000	0.450532000	0.000057000
6	-3.684072000	-4.313380000	-0.000128000	6	-5.641801000	0.396110000	-0.000083000
6	-2.423959000	-5.128312000	0.000153000	6	-5.547475000	-1.101065000	-0.000075000
6	-2.112665000	-6.410789000	0.000398000	6	-6.440215000	-2.089004000	-0.000139000
6	-4.981405000	-4.555493000	-0.000392000	6	-6.651486000	1.264177000	-0.000122000
6	-3.029346000	-1.729935000	-0.000162000	6	-3.226870000	1.439887000	0.000122000
6	-3.079065000	-0.521657000	-0.000159000	6	-2.276908000	2.214417000	0.000068000
6	-3.010538000	0.830158000	-0.000111000	6	-1.159562000	2.956953000	-0.000015000
6	-2.838958000	2.027224000	-0.000087000	6	-0.077569000	3.532760000	-0.000017000
1	7.650889000	1.090164000	-0.000069000	1	5.376700000	-5.557146000	-0.000107000
1	6.375018000	2.430633000	-0.000147000	1	5.770553000	-3.745330000	-0.000261000
1	7.501465000	-1.858055000	0.000115000	1	3.040957000	-7.109359000	-0.000023000
1	6.096560000	-3.062527000	0.000147000	1	1.217920000	-6.771040000	0.000130000
1	-1.082054000	-6.735775000	0.000684000	1	-6.129353000	-3.124671000	-0.000127000
1	-2.880842000	-7.170752000	0.000372000	1	-7.501161000	-1.877309000	-0.000201000
1	-5.359387000	-5.567794000	-0.000591000	1	-7.677515000	0.921172000	-0.000271000
1	-5.700562000	-3.748872000	-0.000540000	1	-6.472992000	2.330661000	-0.000030000
1	-4.769243000	6.080864000	0.000086000	1	2.124560000	7.435048000	-0.000035000
1	-5.292483000	4.305762000	-0.000093000	1	0.358642000	6.870274000	-0.000346000
1	-0.395773000	6.810705000	0.000149000	1	5.254900000	4.439888000	0.000028000
1	-2.141373000	7.425186000	0.000260000	1	4.636787000	6.187909000	-0.000105000

3a
m06-2x/def2-SVP
0 1

6	1.786321000	-3.855768000	-0.103255000
6	0.451806000	-4.223276000	-0.004996000
6	0.798113000	-5.661277000	0.156621000

3a
m06-2x/def2-SVP
0 3

6	-0.762862000	4.187432000	-0.042730000
6	0.620527000	4.213453000	-0.004770000
6	0.649117000	5.692401000	0.144096000

6	2.244623000	-5.269429000	-0.038555000	6	-0.857148000	5.668020000	0.018303000
6	3.461362000	-5.835358000	-0.227536000	6	-1.907181000	6.512995000	-0.131627000
6	3.663270000	-7.286737000	-0.442996000	6	-1.761099000	7.966886000	-0.371752000
6	4.783921000	-7.932472000	0.104392000	6	-2.666717000	8.872107000	0.205173000
1	5.506049000	-7.351633000	0.681408000	1	-3.480800000	8.490942000	0.824732000
6	4.967843000	-9.301089000	-0.067266000	6	-2.522535000	10.242164000	0.008471000
1	5.836340000	-9.790844000	0.376121000	1	-3.226227000	10.933492000	0.475006000
6	4.043385000	-10.045214000	-0.801199000	6	-1.480092000	10.730458000	-0.780099000
6	2.939877000	-9.410256000	-1.370309000	6	-0.589278000	9.839566000	-1.378144000
1	2.216544000	-9.984665000	-1.951104000	1	0.224308000	10.213874000	-2.001430000
6	2.754092000	-8.041218000	-1.197704000	6	-0.731836000	8.468731000	-1.180739000
1	1.892146000	-7.542533000	-1.645032000	1	-0.037146000	7.770124000	-1.650963000
6	0.039076000	-6.718358000	0.533059000	6	1.662457000	6.536083000	0.456283000
6	0.578215000	-8.019453000	0.988718000	6	1.478522000	7.935192000	0.903677000
6	1.725212000	-8.094382000	1.790924000	6	0.426483000	8.296299000	1.756710000
1	2.226320000	-7.171636000	2.089544000	1	-0.265740000	7.526144000	2.102327000
6	2.223308000	-9.328507000	2.199879000	6	0.261203000	9.619864000	2.155966000
1	3.122429000	-9.370550000	2.816594000	1	-0.568668000	9.886343000	2.812360000
6	1.578875000	-10.505697000	1.820106000	6	1.149586000	10.601147000	1.716622000
6	0.423689000	-10.442515000	1.040173000	6	2.213890000	10.249829000	0.885567000
1	-0.089505000	-11.359592000	0.746441000	1	2.916820000	11.011590000	0.544485000
6	-0.078737000	-9.209072000	0.636326000	6	2.382954000	8.926204000	0.490162000
1	-0.984885000	-9.157651000	0.029408000	1	3.217090000	8.649379000	-0.157685000
6	-1.440649000	-6.562118000	0.557452000	6	3.059248000	6.024821000	0.411099000
6	-2.163498000	-6.914499000	1.708006000	6	3.915023000	6.223677000	1.506053000
1	-1.629712000	-7.327817000	2.566238000	1	3.549780000	6.777523000	2.373294000
6	-3.539166000	-6.718066000	1.764696000	6	5.204639000	5.703146000	1.497934000
1	-4.086588000	-6.974794000	2.672846000	1	5.852610000	5.846569000	2.363908000
6	-4.216376000	-6.183118000	0.666809000	6	5.665116000	4.989032000	0.389755000
6	-3.512404000	-5.861522000	-0.491206000	6	4.834349000	4.812809000	-0.714187000
1	-4.036585000	-5.444009000	-1.351785000	1	5.188505000	4.255979000	-1.582873000
6	-2.133097000	-6.053753000	-0.547303000	6	3.541073000	5.332509000	-0.705953000
1	-1.578795000	-5.799359000	-1.452995000	1	2.888640000	5.195876000	-1.570688000
6	-0.699477000	-3.428430000	-0.010003000	6	1.537440000	3.151586000	-0.032864000
6	-1.638167000	-2.640751000	-0.044414000	6	2.242526000	2.149469000	-0.075688000
6	-2.631831000	-1.707072000	-0.086674000	6	2.965252000	0.994958000	-0.120671000

6	-3.464760000	-0.807968000	-0.121244000	6	3.550983000	-0.087857000	-0.148678000
6	-4.267443000	0.338296000	-0.132550000	6	4.034591000	-1.385332000	-0.152282000
6	-3.895211000	1.670241000	-0.012700000	6	3.292395000	-2.640883000	-0.016530000
6	-5.305588000	2.135596000	-0.101710000	6	4.578123000	-3.395902000	-0.067843000
6	-5.713602000	0.681761000	-0.161727000	6	5.304259000	-2.073891000	-0.138801000
6	-6.825354000	-0.092856000	-0.137661000	6	6.596013000	-1.581696000	-0.116939000
6	-6.715259000	-1.545307000	-0.442714000	6	6.837429000	-0.179594000	-0.529695000
6	-6.006255000	-1.982843000	-1.569597000	6	6.237785000	0.338582000	-1.688544000
1	-5.504604000	-1.247718000	-2.202029000	1	5.562496000	-0.294188000	-2.267528000
6	-5.965951000	-3.335343000	-1.902885000	6	6.520375000	1.632355000	-2.118225000
1	-5.421502000	-3.655965000	-2.792881000	1	6.056644000	2.011492000	-3.030494000
6	-6.634576000	-4.269719000	-1.114025000	6	7.404423000	2.432736000	-1.395283000
6	-7.335702000	-3.846991000	0.017220000	6	7.996650000	1.935682000	-0.232681000
1	-7.857666000	-4.574534000	0.641320000	1	8.682960000	2.559772000	0.342438000
6	-7.381598000	-2.495862000	0.346340000	6	7.720626000	0.640687000	0.193500000
1	-7.944886000	-2.162101000	1.219940000	1	8.191696000	0.248552000	1.096682000
6	-8.178385000	0.423809000	0.169607000	6	7.757708000	-2.380759000	0.299404000
6	-9.303221000	-0.094632000	-0.492763000	6	9.022627000	-2.160061000	-0.278317000
1	-9.170495000	-0.886305000	-1.232592000	1	9.135539000	-1.384879000	-1.037998000
6	-10.574823000	0.404822000	-0.227968000	6	10.116374000	-2.937252000	0.086703000
1	-11.437169000	0.000926000	-0.760843000	1	11.085254000	-2.762409000	-0.383746000
6	-10.746302000	1.420804000	0.712859000	6	9.974511000	-3.942438000	1.044506000
6	-9.639518000	1.927157000	1.393834000	6	8.731765000	-4.158470000	1.641359000
1	-9.766914000	2.717149000	2.135547000	1	8.614325000	-4.938641000	2.394920000
6	-8.366868000	1.428847000	1.129125000	6	7.635632000	-3.384814000	1.275634000
1	-7.500128000	1.821437000	1.664307000	1	6.664963000	-3.553914000	1.745399000
6	-5.823486000	3.377546000	-0.258540000	6	4.808949000	-4.724631000	-0.212107000
6	-7.218318000	3.659102000	-0.667518000	6	6.120065000	-5.316630000	-0.558971000
6	-7.867386000	2.879539000	-1.634619000	6	6.972673000	-4.714480000	-1.494340000
1	-7.329504000	2.049574000	-2.096871000	1	6.657488000	-3.791423000	-1.984822000
6	-9.182170000	3.155744000	-2.000355000	6	8.207935000	-5.282256000	-1.795164000
1	-9.676740000	2.534204000	-2.748433000	1	8.863504000	-4.797115000	-2.520001000
6	-9.865468000	4.218968000	-1.410662000	6	8.608637000	-6.461865000	-1.168183000
6	-9.222348000	5.015246000	-0.462378000	6	7.758584000	-7.082995000	-0.252124000
1	-9.749103000	5.853317000	-0.003207000	1	8.062473000	-8.011128000	0.234569000
6	-7.905928000	4.744248000	-0.101348000	6	6.519707000	-6.521683000	0.041307000

1	-7.399287000	5.369249000	0.636766000	1	5.850812000	-7.008862000	0.753556000
6	-4.932798000	4.555670000	-0.075076000	6	3.669562000	-5.672508000	-0.079866000
6	-4.130003000	4.689614000	1.063582000	6	2.804338000	-5.627694000	1.019399000
1	-4.183615000	3.930149000	1.846236000	1	2.986183000	-4.899425000	1.812052000
6	-3.262229000	5.772659000	1.194771000	6	1.714465000	-6.493088000	1.097752000
1	-2.625103000	5.854093000	2.076788000	1	1.034377000	-6.433431000	1.948853000
6	-3.195192000	6.739248000	0.194105000	6	1.482543000	-7.418771000	0.082689000
6	-4.012685000	6.630264000	-0.932698000	6	2.354643000	-7.489960000	-1.005085000
1	-3.965798000	7.386589000	-1.717604000	1	2.178757000	-8.215090000	-1.801037000
6	-4.880771000	5.551741000	-1.062990000	6	3.444463000	-6.629350000	-1.082117000
1	-5.517988000	5.460429000	-1.944974000	1	4.126393000	-6.679098000	-1.933447000
6	-2.623997000	2.245249000	0.084827000	6	1.980555000	-2.876886000	0.068117000
6	-1.471393000	2.654611000	0.165156000	6	0.719868000	-2.979578000	0.155662000
6	-0.166460000	3.046718000	0.223364000	6	-0.583682000	-3.029387000	0.224237000
6	1.027575000	3.325250000	0.232743000	6	-1.850270000	-3.009356000	0.243293000
6	2.416874000	3.463993000	0.145237000	6	-3.171474000	-2.797178000	0.186530000
6	3.372928000	2.506517000	-0.165348000	6	-3.909701000	-1.572004000	-0.080650000
6	4.472025000	3.504936000	-0.145020000	6	-5.175883000	-2.271538000	-0.101953000
6	3.429846000	4.551196000	0.181130000	6	-4.449203000	-3.567001000	0.170604000
6	3.310131000	5.888986000	0.362429000	6	-4.679472000	-4.900132000	0.267864000
6	2.044106000	6.445363000	0.912363000	6	-3.597256000	-5.795334000	0.761491000
6	1.435377000	5.861939000	2.032103000	6	-2.880190000	-5.474994000	1.922443000
1	1.885921000	4.975313000	2.482424000	1	-3.100544000	-4.541819000	2.443964000
6	0.286043000	6.419852000	2.588781000	6	-1.914928000	-6.345328000	2.424062000
1	-0.167126000	5.958205000	3.467764000	1	-1.375755000	-6.085926000	3.336846000
6	-0.268941000	7.572818000	2.036580000	6	-1.653069000	-7.549756000	1.772600000
6	0.325387000	8.160500000	0.917790000	6	-2.355626000	-7.876381000	0.611294000
1	-0.105854000	9.062079000	0.478900000	1	-2.153178000	-8.816274000	0.094633000
6	1.474539000	7.605391000	0.363801000	6	-3.324375000	-7.009871000	0.113579000
1	1.947721000	8.073048000	-0.501721000	1	-3.885758000	-7.272071000	-0.785297000
6	4.381715000	6.859791000	0.043351000	6	-5.963054000	-5.544364000	-0.087944000
6	4.599189000	7.974327000	0.869569000	6	-6.451027000	-6.621955000	0.669579000
1	3.972314000	8.115676000	1.752156000	1	-5.871760000	-6.980880000	1.522496000
6	5.611605000	8.884170000	0.580335000	6	-7.667680000	-7.217923000	0.352106000
1	5.776934000	9.738417000	1.238863000	1	-8.040671000	-8.044644000	0.958841000
6	6.413364000	8.704252000	-0.547499000	6	-8.409029000	-6.759453000	-0.737758000

6	6.192508000	7.612919000	-1.387144000	6	-7.921852000	-5.707572000	-1.513179000
1	6.812332000	7.469078000	-2.273474000	1	-8.492480000	-5.349250000	-2.371337000
6	5.181985000	6.700151000	-1.096751000	6	-6.707411000	-5.107078000	-1.192954000
1	5.004253000	5.846941000	-1.754422000	1	-6.323172000	-4.285010000	-1.800163000
6	5.810649000	3.347929000	-0.287363000	6	-6.459098000	-1.781076000	-0.239975000
6	6.816967000	4.368446000	0.079510000	6	-7.668314000	-2.523030000	0.146910000
6	6.656916000	5.162392000	1.224131000	6	-7.664741000	-3.395062000	1.248643000
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m06-2x/def2-SVP				m06-2x/def2-SVP			
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1	5.277461000	0.251099000	-2.191162000	1	5.110466000	1.538194000	-2.288586000
6	6.167575000	-1.708955000	-2.231791000	6	6.359277000	-0.219437000	-2.255273000
1	5.554188000	-2.041212000	-3.071283000	1	5.868718000	-0.669510000	-3.119752000
6	7.102275000	-2.574357000	-1.663864000	6	7.405154000	-0.885709000	-1.619997000
6	7.865435000	-2.132548000	-0.581167000	6	8.011894000	-0.303465000	-0.505145000
1	8.595058000	-2.800952000	-0.116710000	1	8.827364000	-0.820132000	0.006664000
6	7.695554000	-0.846197000	-0.077138000	6	7.574405000	0.930392000	-0.032246000
1	8.291698000	-0.513671000	0.775245000	1	8.047771000	1.380273000	0.843169000
6	3.481190000	0.055366000	-0.105030000	6	3.363439000	0.881311000	-0.167414000
6	2.894660000	-1.029977000	-0.149752000	6	3.050116000	-0.317631000	-0.198888000
6	2.171464000	-2.180913000	-0.151389000	6	2.630161000	-1.600064000	-0.195787000
6	1.466699000	-3.189218000	-0.127106000	6	2.174690000	-2.752489000	-0.158310000
6	2.953879000	-6.166866000	-0.133035000	6	4.318910000	-5.308641000	-0.180679000
6	3.899371000	-6.614053000	-1.072436000	6	5.342468000	-5.558541000	-1.112011000
6	3.386553000	-5.291302000	0.874181000	6	4.558692000	-4.351446000	0.817670000
6	5.222585000	-6.188010000	-1.013389000	6	6.555733000	-4.879989000	-1.045375000
1	3.578859000	-7.298036000	-1.861279000	1	5.173180000	-6.299001000	-1.896634000
6	4.708082000	-4.852767000	0.925556000	6	5.766959000	-3.660691000	0.877018000
1	2.669146000	-4.946453000	1.620448000	1	3.779164000	-4.149095000	1.553587000
6	5.632591000	-5.302263000	-0.014444000	6	6.774599000	-3.928176000	-0.047706000
1	5.937893000	-6.538535000	-1.760617000	1	7.333929000	-5.089337000	-1.782867000
1	5.014571000	-4.146592000	1.698797000	1	5.919574000	-2.903972000	1.648355000
1	9.752311000	6.713594000	-0.990614000	1	7.899769000	8.807619000	-1.042095000
1	11.049858000	4.068764000	1.409264000	1	9.866150000	6.487317000	1.232727000
1	7.225506000	-3.585266000	-2.056764000	1	7.736174000	-1.858540000	-1.986756000
1	6.664723000	-4.952176000	0.026999000	1	7.722049000	-3.389628000	0.006385000
1	0.638043000	-11.840910000	-1.192088000	1	3.335514000	-11.353738000	-1.229437000
1	-1.570098000	-11.608726000	1.955988000	1	1.261552000	-11.626540000	2.003929000
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1	-7.935283000	-3.051368000	-1.564492000	1	-6.983380000	-4.853672000	-1.353219000
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1	1.290433000	8.220986000	1.897484000	1	-0.629263000	8.216740000	2.211353000
3b				3b			
m06-2x/def2-SVP				m06-2x/def2-SVP			
0 1				0 3			
6	-1.410805000	4.015285000	-0.047916000	6	0.994040000	-4.155365000	0.016530000
6	-0.051206000	4.204964000	0.155637000	6	-0.382504000	-4.216405000	0.150854000
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6	-2.697344000	10.436330000	-1.056302000	6	1.753991000	-10.657228000	-1.014882000
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6	0.622063000	6.641213000	0.743118000	6	-1.307495000	-6.586052000	0.680924000
6	0.187111000	8.009896000	1.106445000	6	-1.009720000	-7.990982000	1.046416000
6	-1.013273000	8.240580000	1.792181000	6	0.127950000	-8.329399000	1.791606000
1	-1.637808000	7.390302000	2.072949000	1	0.804829000	-7.537740000	2.118627000
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6	0.577890000	10.406895000	1.086641000	6	-1.596957000	-10.346626000	0.968968000
1	1.208586000	11.253737000	0.805907000	1	-2.279823000	-11.134399000	0.642012000
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1	4.696551000	4.567115000	-0.242457000	1	-5.135899000	-4.155362000	-0.472083000
6	2.834120000	5.587924000	0.111706000	6	-3.381856000	-5.326615000	-0.039400000
1	2.423405000	5.326646000	-0.865164000	1	-2.892159000	-5.069141000	-0.980048000
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6	1.844238000	2.394021000	0.160701000	6	-2.084419000	-2.217810000	0.086222000
6	2.768982000	1.395229000	0.085479000	6	-2.892217000	-1.124715000	-0.009565000
6	3.545207000	0.450093000	-0.004979000	6	-3.566159000	-0.098739000	-0.103063000
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6	6.833300000	-0.611756000	-0.158809000	6	-6.697243000	1.257518000	-0.165231000
6	6.906655000	0.853578000	-0.404322000	6	-6.906721000	-0.159510000	-0.536463000
6	6.168375000	1.452577000	-1.435660000	6	-6.223797000	-0.739175000	-1.619518000
1	5.492654000	0.839483000	-2.035023000	1	-5.493340000	-0.144568000	-2.170835000
6	6.321655000	2.804099000	-1.733524000	6	-6.498193000	-2.040906000	-2.025881000
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6	10.478565000	-1.627695000	-0.375577000	6	-10.234981000	2.596385000	-0.023233000
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6	10.541233000	-2.710016000	0.507971000	6	-10.121574000	3.642813000	0.898250000
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6	6.804998000	-4.320069000	-0.932380000	6	-6.387738000	4.957958000	-0.800870000

6	7.507405000	-3.552455000	-1.871316000	6	-7.205261000	4.273621000	-1.710326000
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6	8.688788000	-5.851087000	-0.849785000	6	-8.141341000	6.620557000	-0.553262000
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6	2.550300000	-6.136235000	0.623265000	6	-1.905885000	6.422956000	0.454666000
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6	-7.512506000	-0.712579000	-0.757567000	6	7.617203000	-0.012991000	-0.685682000
1	-8.111811000	-1.004960000	0.107011000	1	8.254017000	0.251441000	0.160469000
6	-3.340795000	-0.783714000	-0.351697000	6	3.454805000	0.417175000	-0.188119000
6	-3.018549000	0.398841000	-0.381529000	6	2.996268000	-0.723283000	-0.212914000
6	-2.579520000	1.689615000	-0.335914000	6	2.411915000	-1.956530000	-0.186328000

6	-2.111535000	2.818192000	-0.232688000	6	1.820457000	-3.027457000	-0.119262000
6	-4.122212000	5.510915000	-0.338584000	6	3.564660000	-5.881976000	-0.174621000
6	-5.078311000	5.805275000	-1.323546000	6	4.525144000	-6.247387000	-1.130901000
6	-4.478795000	4.618084000	0.680438000	6	3.958136000	-5.022785000	0.860042000
6	-6.344879000	5.233751000	-1.278357000	6	5.828390000	-5.769893000	-1.048261000
1	-4.822025000	6.501198000	-2.124783000	1	4.241051000	-6.920618000	-1.942079000
6	-5.746210000	4.042456000	0.717148000	6	5.262009000	-4.540329000	0.933264000
1	-3.758540000	4.392630000	1.469237000	1	3.233908000	-4.746302000	1.628675000
6	-6.707126000	4.353239000	-0.248899000	6	6.223391000	-4.915079000	-0.009653000
1	-7.076009000	5.484758000	-2.051162000	1	6.560916000	-6.073576000	-1.800570000
1	-6.000270000	3.353945000	1.525870000	1	5.542395000	-3.872216000	1.750440000
6	-10.497335000	-6.177319000	1.238914000	6	10.946559000	5.205075000	1.418805000
1	-11.053520000	-5.719643000	2.071434000	1	11.380967000	4.779109000	2.336164000
1	-11.207104000	-6.362519000	0.421559000	1	11.736672000	5.244459000	0.657181000
1	-10.116672000	-7.146733000	1.594271000	1	10.637838000	6.235562000	1.652124000
6	-8.570248000	-8.763182000	-0.469054000	6	9.431790000	7.805313000	-0.646254000
1	-8.381743000	-9.459324000	-1.300517000	1	9.353711000	8.432272000	-1.547400000
1	-8.872499000	-9.354982000	0.405261000	1	9.754138000	8.446224000	0.185181000
1	-9.415786000	-8.123087000	-0.763831000	1	10.219451000	7.059528000	-0.834387000
6	-7.404422000	2.105157000	-3.327953000	6	7.247291000	-2.872981000	-3.182590000
1	-8.481166000	2.323980000	-3.297741000	1	8.293883000	-3.201358000	-3.115413000
1	-6.871381000	2.959762000	-2.880147000	1	6.614245000	-3.661444000	-2.743783000
1	-7.095395000	2.037254000	-4.379653000	1	6.978621000	-2.787422000	-4.244235000
6	-8.107413000	3.809972000	-0.152061000	6	7.652654000	-4.462004000	0.121660000
1	-8.526386000	3.603982000	-1.146910000	1	8.132256000	-4.364217000	-0.862250000
1	-8.133413000	2.883628000	0.436684000	1	7.715711000	-3.494894000	0.638005000
1	-8.770730000	4.539333000	0.339072000	1	8.238049000	-5.192183000	0.702615000
6	-2.618110000	11.922068000	-1.282809000	6	1.558360000	-12.127808000	-1.268420000
1	-2.658917000	12.161032000	-2.356335000	1	1.627757000	-12.356572000	-2.342716000
1	-3.443038000	12.450203000	-0.786303000	1	2.311427000	-12.731035000	-0.744008000
1	-1.668248000	12.321375000	-0.895052000	1	0.561076000	-12.448577000	-0.929863000
6	-1.102348000	12.033038000	2.073279000	6	-0.110916000	-12.119230000	2.013808000
1	-1.113340000	12.198532000	3.161350000	1	-0.156367000	-12.296013000	3.099165000
1	-0.451800000	12.794121000	1.622087000	1	-0.805460000	-12.817405000	1.527788000
1	-2.128267000	12.193822000	1.708021000	1	0.911195000	-12.363218000	1.685556000
6	6.046169000	5.023753000	2.081753000	6	-6.670256000	-4.593561000	1.740367000

1	6.118610000	3.930249000	1.987711000	1	-6.638714000	-3.494401000	1.773302000
1	6.813325000	5.454875000	1.420012000	1	-7.399286000	-4.871885000	0.964109000
1	6.292456000	5.302159000	3.114872000	1	-7.042530000	-4.959440000	2.706325000
6	7.400471000	5.061428000	-1.366632000	6	-7.774643000	-4.217154000	-1.834685000
1	6.539667000	5.657975000	-1.022572000	1	-7.001384000	-4.924263000	-1.491971000
1	8.303565000	5.473958000	-0.897319000	1	-8.740132000	-4.562138000	-1.441077000
1	7.481497000	5.204300000	-2.453487000	1	-7.807363000	-4.277505000	-2.931534000
6	10.791684000	-5.441515000	-2.210468000	6	-10.357689000	6.401537000	-1.770733000
1	11.188116000	-6.286489000	-1.631756000	1	-10.637952000	7.275267000	-1.167388000
1	10.803803000	-5.724099000	-3.274157000	1	-10.434547000	6.682891000	-2.831894000
1	11.477068000	-4.588400000	-2.091372000	1	-11.096252000	5.605245000	-1.589845000
6	11.812735000	-3.485243000	0.724994000	6	-11.289374000	4.524673000	1.246717000
1	12.612174000	-3.145098000	0.053334000	1	-12.179249000	4.268154000	0.656743000
1	12.169668000	-3.377654000	1.760425000	1	-11.548738000	4.434575000	2.312362000
1	11.644610000	-4.558699000	0.547119000	1	-11.042529000	5.581340000	1.059090000
6	1.351777000	-8.065282000	-0.480159000	6	-0.654320000	8.271288000	-0.727159000
1	1.324335000	-8.646169000	0.453756000	1	-0.527473000	8.855765000	0.196252000
1	0.367915000	-7.583873000	-0.586831000	1	0.283005000	7.717668000	-0.887767000
1	1.487787000	-8.763184000	-1.316850000	1	-0.790845000	8.970919000	-1.562312000
6	0.515692000	-8.177578000	3.290872000	6	0.308666000	8.433243000	2.930282000
1	0.392327000	-9.267637000	3.237530000	1	0.474004000	9.492181000	2.690416000
1	1.488893000	-7.931918000	2.834895000	1	-0.705437000	8.167898000	2.589415000
1	0.569407000	-7.886915000	4.349041000	1	0.323714000	8.321060000	4.023490000

3b

m06-2x/def2-SVP

-2 1

6	0.211127000	-4.291822000	0.011757000
6	-1.162334000	-4.067413000	0.140669000
6	-1.439554000	-5.524686000	0.241329000
6	0.031472000	-5.756666000	-0.024485000
6	0.895093000	-6.779103000	-0.293954000
6	0.447580000	-8.140858000	-0.655250000
6	1.173364000	-9.279292000	-0.267674000
1	2.099642000	-9.151878000	0.295822000
6	0.712657000	-10.561354000	-0.558718000

3b

m06-2x/def2-SVP

-2 3

6	-0.574364000	4.242009000	-0.002867000
6	0.841922000	4.129138000	0.162614000
6	0.985060000	5.595328000	0.263132000
6	-0.499209000	5.708220000	-0.039306000
6	-1.430950000	6.670108000	-0.327540000
6	-1.078879000	8.057341000	-0.691019000
6	-1.893361000	9.144661000	-0.329965000
1	-2.819210000	8.955473000	0.216623000
6	-1.522192000	10.454874000	-0.622966000

1	1.287953000	-11.428747000	-0.222990000	1	-2.166838000	11.279907000	-0.306315000
6	-0.483455000	-10.759413000	-1.254725000	6	-0.328147000	10.736287000	-1.293241000
6	-1.188554000	-9.625251000	-1.675253000	6	0.466716000	9.653146000	-1.687821000
1	-2.124882000	-9.749637000	-2.225959000	1	1.404523000	9.841581000	-2.217672000
6	-0.730249000	-8.344834000	-1.394599000	6	0.097089000	8.344698000	-1.406781000
1	-1.299077000	-7.475235000	-1.728833000	1	0.736708000	7.517221000	-1.719254000
6	-2.540322000	-6.216179000	0.642183000	6	2.011936000	6.391760000	0.683789000
6	-2.527580000	-7.658221000	0.985138000	6	1.868845000	7.826371000	1.019820000
6	-1.463078000	-8.239977000	1.689418000	6	0.742481000	8.322270000	1.694746000
1	-0.627728000	-7.609256000	1.998925000	1	-0.046853000	7.625767000	1.983360000
6	-1.451190000	-9.601549000	1.967083000	6	0.611908000	9.678233000	1.968352000
1	-0.595093000	-10.033300000	2.492358000	1	-0.290857000	10.038235000	2.469319000
6	-2.502982000	-10.434086000	1.568300000	6	1.601796000	10.595122000	1.596262000
6	-3.585629000	-9.848605000	0.904716000	6	2.745764000	10.099084000	0.963627000
1	-4.425656000	-10.474533000	0.591311000	1	3.540052000	10.791393000	0.670392000
6	-3.603621000	-8.483722000	0.626897000	6	2.881749000	8.740334000	0.688711000
1	-4.455154000	-8.043514000	0.103550000	1	3.779642000	8.372552000	0.187311000
6	-3.820600000	-5.497021000	0.884274000	6	3.342229000	5.788097000	0.962347000
6	-4.526843000	-5.720988000	2.076791000	6	4.014048000	6.094933000	2.157451000
1	-4.153531000	-6.465885000	2.782917000	1	3.572137000	6.822578000	2.841567000
6	-5.663028000	-4.980943000	2.385422000	6	5.203204000	5.458870000	2.497383000
1	-6.177557000	-5.153582000	3.334250000	1	5.688849000	5.696415000	3.447673000
6	-6.137260000	-3.988900000	1.519903000	6	5.768243000	4.487542000	1.663365000
6	-5.457523000	-3.792539000	0.312215000	6	5.120759000	4.207103000	0.454823000
1	-5.790763000	-3.002675000	-0.366887000	1	5.521405000	3.428527000	-0.200270000
6	-4.331879000	-4.546956000	-0.009513000	6	3.943235000	4.860789000	0.100365000
1	-3.812990000	-4.369606000	-0.952481000	1	3.454073000	4.619272000	-0.843882000
6	-1.891815000	-2.883807000	0.161229000	6	1.654267000	3.016187000	0.191552000
6	-2.466499000	-1.793406000	0.096365000	6	2.315068000	1.968424000	0.137503000
6	-3.062133000	-0.582526000	0.009915000	6	2.998532000	0.807672000	0.053154000
6	-3.526380000	0.564052000	-0.068160000	6	3.560975000	-0.293164000	-0.034579000
6	-3.833576000	1.903559000	-0.147103000	6	3.968782000	-1.610427000	-0.130788000
6	-2.899768000	3.031458000	-0.109064000	6	3.174097000	-2.796600000	-0.118128000
6	-4.061884000	3.966046000	-0.199718000	6	4.374343000	-3.647231000	-0.247899000
6	-4.993732000	2.764285000	-0.134115000	6	5.214039000	-2.382482000	-0.175309000
6	-6.355202000	2.516398000	-0.070102000	6	6.533402000	-2.011232000	-0.109183000

6	-6.869519000	1.167243000	-0.400820000	6	6.921694000	-0.602984000	-0.377550000
6	-6.309554000	0.398102000	-1.439745000	6	6.316600000	0.137362000	-1.408180000
1	-5.445730000	0.789639000	-1.979007000	1	5.509500000	-0.318337000	-1.983670000
6	-6.845824000	-0.831528000	-1.805652000	6	6.743981000	1.424060000	-1.720871000
1	-6.383255000	-1.390503000	-2.624196000	1	6.251990000	1.965945000	-2.533147000
6	-7.973019000	-1.360059000	-1.162456000	6	7.800910000	2.029926000	-1.030270000
6	-8.527653000	-0.608265000	-0.121691000	6	8.397893000	1.301718000	0.004512000
1	-9.399836000	-0.996538000	0.412633000	1	9.217334000	1.751948000	0.571805000
6	-7.985931000	0.616857000	0.257708000	6	7.965619000	0.018895000	0.329206000
1	-8.443841000	1.174717000	1.076668000	1	8.454892000	-0.526096000	1.138839000
6	-7.331791000	3.539327000	0.337317000	6	7.617799000	-2.957011000	0.225150000
6	-8.642633000	3.574095000	-0.178669000	6	8.899768000	-2.848089000	-0.341785000
1	-8.950672000	2.809908000	-0.894729000	1	9.104320000	-2.033871000	-1.039635000
6	-9.538671000	4.580151000	0.172405000	6	9.897582000	-3.777426000	-0.058658000
1	-10.540835000	4.582813000	-0.267111000	1	10.877085000	-3.676640000	-0.535071000
6	-9.174472000	5.603655000	1.052819000	6	9.662187000	-4.852196000	0.803970000
6	-7.882804000	5.559488000	1.592262000	6	8.397372000	-4.944350000	1.397074000
1	-7.566424000	6.342055000	2.288011000	1	8.184197000	-5.772463000	2.078632000
6	-6.990607000	4.549697000	1.258576000	6	7.402219000	-4.014458000	1.126694000
1	-5.990955000	4.541234000	1.697334000	1	6.421973000	-4.110576000	1.597381000
6	-4.112014000	5.293458000	-0.495281000	6	4.526727000	-4.978939000	-0.512139000
6	-5.349819000	6.026254000	-0.857161000	6	5.802579000	-5.604039000	-0.928319000
6	-6.309392000	5.475541000	-1.717453000	6	6.681411000	-4.967579000	-1.818444000
1	-6.141839000	4.475970000	-2.122904000	1	6.413048000	-3.984124000	-2.208988000
6	-7.472694000	6.171300000	-2.023913000	6	7.885684000	-5.558809000	-2.180323000
1	-8.218520000	5.706445000	-2.674105000	1	8.562243000	-5.025595000	-2.853763000
6	-7.722891000	7.440975000	-1.491672000	6	8.259623000	-6.812889000	-1.684298000
6	-6.748496000	8.008700000	-0.665435000	6	7.368642000	-7.468155000	-0.828756000
1	-6.914961000	9.003719000	-0.243427000	1	7.631159000	-8.453015000	-0.432131000
6	-5.577344000	7.318637000	-0.362021000	6	6.159821000	-6.880053000	-0.464313000
1	-4.827210000	7.774809000	0.287581000	1	5.479380000	-7.405361000	0.209335000
6	-2.854689000	6.085043000	-0.585248000	6	3.336047000	-5.869757000	-0.514582000
6	-1.818022000	5.961799000	0.349073000	6	2.339954000	-5.795171000	0.469801000
1	-1.952486000	5.304633000	1.208363000	1	2.463454000	-5.097055000	1.298442000
6	-0.609724000	6.630987000	0.171997000	6	1.182964000	-6.564510000	0.382657000
1	0.209498000	6.454576000	0.874582000	1	0.390315000	-6.429444000	1.123962000

6	-0.407805000	7.481799000	-0.920482000	6	0.994398000	-7.471711000	-0.666200000
6	-1.460765000	7.646232000	-1.826615000	6	2.009816000	-7.586176000	-1.621474000
1	-1.327569000	8.304837000	-2.688877000	1	1.887011000	-8.286799000	-2.451708000
6	-2.659912000	6.960361000	-1.665743000	6	3.155022000	-6.799932000	-1.551671000
1	-3.457782000	7.081357000	-2.401309000	1	3.919367000	-6.885074000	-2.326872000
6	-1.563748000	3.078023000	-0.040912000	6	1.806147000	-2.943206000	-0.042892000
6	-0.302457000	2.987702000	0.070861000	6	0.569874000	-2.952873000	0.064419000
6	0.996474000	2.848735000	0.176409000	6	-0.773682000	-2.915444000	0.163121000
6	2.247232000	2.645868000	0.245263000	6	-2.009269000	-2.811703000	0.221121000
6	3.526385000	2.243692000	0.239832000	6	-3.356543000	-2.522690000	0.200994000
6	4.138821000	0.945745000	-0.003936000	6	-4.028391000	-1.289126000	-0.077611000
6	5.478790000	1.480875000	0.005122000	6	-5.340408000	-1.943588000	-0.054000000
6	4.889836000	2.854004000	0.285186000	6	-4.631635000	-3.250008000	0.270597000
6	5.282022000	4.147715000	0.440721000	6	-4.930167000	-4.567797000	0.499617000
6	4.329007000	5.182308000	0.932443000	6	-3.911482000	-5.481771000	1.078067000
6	3.427507000	4.917410000	1.974885000	6	-3.021996000	-5.058549000	2.080831000
1	3.383563000	3.912277000	2.395457000	1	-3.053461000	-4.020707000	2.414587000
6	2.606294000	5.918433000	2.487176000	6	-2.120291000	-5.941839000	2.667621000
1	1.916644000	5.677069000	3.300104000	1	-1.445607000	-5.573907000	3.445131000
6	2.661171000	7.228237000	1.996200000	6	-2.074757000	-7.291482000	2.298033000
6	3.558271000	7.493890000	0.955975000	6	-2.958603000	-7.717413000	1.300382000
1	3.622874000	8.506627000	0.549120000	1	-2.945342000	-8.764230000	0.984273000
6	4.369955000	6.493029000	0.430332000	6	-3.848871000	-6.834301000	0.697568000
1	5.067151000	6.730825000	-0.375305000	1	-4.524545000	-7.198587000	-0.078460000
6	6.652155000	4.626678000	0.136216000	6	-6.243686000	-5.163829000	0.170862000
6	7.292577000	5.575643000	0.947373000	6	-6.842297000	-6.134782000	0.991337000
1	6.768085000	5.968658000	1.820729000	1	-6.323972000	-6.455120000	1.897440000
6	8.590289000	5.998495000	0.670652000	6	-8.089507000	-6.671935000	0.683019000
1	9.076525000	6.719252000	1.333941000	1	-8.538818000	-7.410256000	1.353371000
6	9.290169000	5.499060000	-0.431674000	6	-8.787921000	-6.267665000	-0.459002000
6	8.637539000	4.580763000	-1.261496000	6	-8.180806000	-5.322449000	-1.293602000
1	9.164018000	4.172587000	-2.128144000	1	-8.704144000	-4.987071000	-2.193143000
6	7.343179000	4.155684000	-0.989553000	6	-6.933877000	-4.788766000	-0.993692000
1	6.856538000	3.422766000	-1.635916000	1	-6.480897000	-4.047468000	-1.655000000
6	6.721647000	0.895124000	-0.187556000	6	-6.605082000	-1.446938000	-0.245194000
6	7.980503000	1.492041000	0.280487000	6	-7.835662000	-2.140825000	0.184062000

6	8.031475000	2.265465000	1.457763000	6	-7.864872000	-2.894477000	1.370414000
1	7.111128000	2.407536000	2.028177000	1	-6.954999000	-2.960916000	1.970399000
6	9.211973000	2.854696000	1.889614000	6	-9.014824000	-3.562379000	1.770016000
1	9.201764000	3.467479000	2.795825000	1	-8.995013000	-4.160534000	2.685197000
6	10.413379000	2.687207000	1.189713000	6	-10.194435000	-3.496850000	1.018770000
6	10.380676000	1.895978000	0.036713000	6	-10.180497000	-2.724869000	-0.146843000
1	11.301114000	1.745322000	-0.535780000	1	-11.087201000	-2.654655000	-0.754670000
6	9.197346000	1.312454000	-0.407773000	6	-9.028248000	-2.057120000	-0.554956000
1	9.202387000	0.717292000	-1.323087000	1	-9.039881000	-1.471197000	-1.476149000
6	6.792512000	-0.433787000	-0.838560000	6	-6.771294000	-0.116401000	-0.885578000
6	5.938070000	-0.775272000	-1.905452000	6	-5.972224000	0.270183000	-1.975245000
1	5.197660000	-0.047473000	-2.240915000	1	-5.206837000	-0.416396000	-2.339617000
6	6.018493000	-2.008884000	-2.538386000	6	-6.141037000	1.502993000	-2.594437000
1	5.327610000	-2.235210000	-3.354741000	1	-5.490590000	1.775022000	-3.429263000
6	6.968381000	-2.964675000	-2.157417000	6	-7.129671000	2.399086000	-2.173065000
6	7.832008000	-2.629031000	-1.109315000	6	-7.943217000	2.010036000	-1.102793000
1	8.591602000	-3.349046000	-0.789686000	1	-8.734365000	2.682284000	-0.758601000
6	7.740830000	-1.401208000	-0.457803000	6	-7.763975000	0.784456000	-0.466264000
1	8.422761000	-1.178821000	0.365146000	1	-8.408623000	0.511826000	0.371659000
6	3.528712000	-0.295901000	-0.093895000	6	-3.533096000	-0.003928000	-0.180875000
6	2.869025000	-1.338438000	-0.134822000	6	-2.960956000	1.095331000	-0.207550000
6	2.053757000	-2.428982000	-0.122783000	6	-2.253449000	2.246640000	-0.185813000
6	1.256875000	-3.365766000	-0.084555000	6	-1.528878000	3.250817000	-0.128213000
6	2.359084000	-6.535071000	-0.226554000	6	-2.874889000	6.324854000	-0.279927000
6	3.240803000	-7.089178000	-1.167044000	6	-3.785265000	6.828534000	-1.222145000
6	2.915154000	-5.782502000	0.820654000	6	-3.392000000	5.529482000	0.756776000
6	4.616915000	-6.904574000	-1.058250000	6	-5.149553000	6.565335000	-1.119877000
1	2.835515000	-7.679272000	-1.991728000	1	-3.412508000	7.446795000	-2.041441000
6	4.288273000	-5.589168000	0.917744000	6	-4.751805000	5.258337000	0.848079000
1	2.253276000	-5.351743000	1.573708000	1	-2.708103000	5.128385000	1.506345000
6	5.167285000	-6.155769000	-0.011850000	6	-5.660139000	5.782780000	-0.078801000
1	5.281287000	-7.352044000	-1.802673000	1	-5.835490000	6.979024000	-1.864683000
1	4.688561000	-4.989099000	1.738330000	1	-5.119324000	4.631233000	1.664015000
6	11.678143000	3.346087000	1.675130000	6	-11.421783000	-4.246473000	1.466676000
1	11.983735000	2.960494000	2.661150000	1	-11.792952000	-3.870193000	2.433124000
1	12.510523000	3.177470000	0.976488000	1	-12.236469000	-4.156457000	0.734038000

1	11.538476000	4.434444000	1.781292000	1	-11.196830000	-5.317149000	1.598123000
6	10.710617000	5.904073000	-0.724804000	6	-10.154670000	-6.805520000	-0.792116000
1	10.797520000	6.376090000	-1.715793000	1	-10.153779000	-7.338053000	-1.756138000
1	11.089974000	6.612659000	0.024940000	1	-10.511176000	-7.502403000	-0.020306000
1	11.367392000	5.019273000	-0.723699000	1	-10.883513000	-5.982940000	-0.873681000
6	7.029574000	-4.305317000	-2.841969000	6	-7.286690000	3.739048000	-2.842813000
1	7.953191000	-4.843512000	-2.584173000	1	-8.254955000	4.198176000	-2.597482000
1	6.176029000	-4.937361000	-2.545792000	1	-6.491988000	4.430945000	-2.519023000
1	6.990236000	-4.196002000	-3.936432000	1	-7.215197000	3.646123000	-3.936595000
6	6.653250000	-5.956448000	0.125345000	6	-7.134329000	5.508680000	0.060565000
1	7.206062000	-6.541320000	-0.622909000	1	-7.712837000	6.025487000	-0.717967000
1	6.915391000	-4.895705000	-0.006848000	1	-7.338505000	4.430164000	-0.018824000
1	7.000457000	-6.259802000	1.124776000	1	-7.506251000	5.842353000	1.041675000
6	-1.020084000	-12.136472000	-1.544664000	6	0.115322000	12.147073000	-1.578489000
1	-1.092865000	-12.319664000	-2.628086000	1	0.220235000	12.326075000	-2.660106000
1	-0.378545000	-12.916738000	-1.111372000	1	-0.600637000	12.880703000	-1.181399000
1	-2.032310000	-12.253204000	-1.125110000	1	1.097230000	12.344233000	-1.118319000
6	-2.445168000	-11.912880000	1.848873000	6	1.414234000	12.064647000	1.869052000
1	-2.420599000	-12.115284000	2.930972000	1	1.328879000	12.266071000	2.948406000
1	-3.313920000	-12.436295000	1.425491000	1	2.255135000	12.655704000	1.479338000
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6	-7.325178000	-3.137842000	1.880684000	6	7.017784000	3.745756000	2.058434000
1	-7.075834000	-2.069436000	1.803369000	1	6.862676000	2.658785000	1.993195000
1	-8.169674000	-3.315631000	1.196216000	1	7.859419000	3.987872000	1.389662000
1	-7.665262000	-3.346206000	2.904688000	1	7.317983000	3.995236000	3.085860000
6	-8.543009000	-2.695636000	-1.565256000	6	8.259048000	3.421884000	-1.381167000
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1	-9.538826000	-2.851040000	-1.125831000	1	9.233964000	3.646062000	-0.925470000
1	-8.635438000	-2.777820000	-2.658742000	1	8.351798000	3.547725000	-2.470089000
6	-9.018438000	8.145836000	-1.796883000	6	9.588382000	-7.412122000	-2.064290000
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1	-9.873422000	7.542091000	-1.451921000	1	10.411834000	-6.734819000	-1.785669000
6	-10.111552000	6.728182000	1.407379000	6	10.710462000	-5.896194000	1.085458000
1	-11.078798000	6.619764000	0.895691000	1	11.639143000	-5.691422000	0.533997000
1	-10.304944000	6.768616000	2.491103000	1	10.955409000	-5.942975000	2.158125000

1	-9.680849000	7.700986000	1.117486000	1	10.350274000	-6.894883000	0.789014000
6	0.913815000	8.173446000	-1.123327000	6	-0.275799000	-8.272638000	-0.772029000
1	1.169003000	8.810235000	-0.261820000	1	-0.448833000	-8.872473000	0.135192000
1	1.725781000	7.438165000	-1.226086000	1	-1.146438000	-7.609024000	-0.883047000
1	0.898028000	8.803874000	-2.023421000	1	-0.245025000	-8.954037000	-1.633868000
6	1.771979000	8.308215000	2.556827000	6	-1.097460000	-8.243884000	2.937682000
1	2.170767000	9.307601000	2.331776000	1	-1.416024000	-9.287737000	2.805259000
1	0.757419000	8.249301000	2.128486000	1	-0.092791000	-8.143926000	2.493696000
1	1.670589000	8.214402000	3.647663000	1	-0.997016000	-8.048370000	4.015200000

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6	2.287774000	-3.559823000	-0.026597000
6	1.030672000	-4.144441000	0.034729000
6	1.609554000	-5.506616000	0.186568000
6	2.974745000	-4.874368000	0.037374000
6	4.281893000	-5.204689000	-0.106277000
6	4.758710000	-6.585348000	-0.335321000
6	5.965030000	-7.024065000	0.235372000
1	6.561291000	-6.328514000	0.828625000
6	6.396482000	-8.337062000	0.079796000
1	7.319304000	-8.699109000	0.533156000
6	5.616957000	-9.212443000	-0.667636000
6	4.438907000	-8.802380000	-1.281118000
1	3.868200000	-9.518881000	-1.872037000
6	4.018560000	-7.487944000	-1.114463000
1	3.094034000	-7.150279000	-1.586111000
6	1.037664000	-6.685277000	0.530107000
6	1.798213000	-7.877109000	0.966658000
6	2.921816000	-7.762178000	1.797914000
1	3.225189000	-6.774689000	2.150019000
6	3.656244000	-8.883940000	2.166640000
1	4.539039000	-8.810878000	2.801939000
6	3.256364000	-10.130228000	1.699490000
6	2.126128000	-10.287006000	0.905006000

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6	-4.016417000	-1.350823000	-0.004376000
6	-4.272138000	0.009259000	0.025884000
6	-5.732420000	-0.209946000	0.194301000
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6	-6.102860000	-2.878855000	-0.044017000
6	-7.560644000	-3.000093000	-0.260861000
6	-8.282224000	-4.045767000	0.338489000
1	-7.752801000	-4.782552000	0.945313000
6	-9.662226000	-4.140324000	0.193717000
1	-10.239833000	-4.932994000	0.669403000
6	-10.320588000	-3.184970000	-0.572125000
6	-9.634015000	-2.160917000	-1.213896000
1	-10.189558000	-1.443654000	-1.818208000
6	-8.255182000	-2.077105000	-1.057513000
1	-7.700725000	-1.276628000	-1.550568000
6	-6.733122000	0.646539000	0.511252000
6	-8.074072000	0.218917000	0.967652000
6	-8.237294000	-0.875760000	1.829215000
1	-7.354062000	-1.405431000	2.190500000
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1	-9.648986000	-2.155599000	2.874291000
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1	0.508364000	-9.261752000	-0.074681000	1	-9.101865000	1.782575000	-0.111316000
6	-0.444423000	-6.805226000	0.518770000	6	-6.486695000	2.111455000	0.439089000
6	-1.112938000	-7.327903000	1.637274000	6	-6.835114000	2.936462000	1.520368000
1	-0.533254000	-7.647600000	2.505281000	1	-7.285274000	2.490635000	2.409341000
6	-2.498617000	-7.428157000	1.657597000	6	-6.602930000	4.305795000	1.477293000
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6	-3.215522000	-7.024203000	0.536027000	6	-6.038707000	4.852902000	0.329727000
6	-2.586713000	-6.529349000	-0.598766000	6	-5.703153000	4.072502000	-0.768374000
1	-3.186558000	-6.256499000	-1.465237000	1	-5.291522000	4.549901000	-1.656223000
6	-1.198174000	-6.419056000	-0.596310000	6	-5.928408000	2.699319000	-0.702977000
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6	-1.259438000	-2.874007000	-0.035118000	6	-2.472162000	1.916502000	-0.061872000
6	-2.351843000	-2.057826000	-0.077858000	6	-1.414483000	2.774884000	-0.103963000
6	-3.280145000	-1.257469000	-0.106842000	6	-0.410500000	3.487334000	-0.127404000
6	-4.241344000	-0.240500000	-0.107026000	6	0.799414000	4.160064000	-0.129258000
6	-4.094383000	1.131478000	0.048798000	6	2.162398000	3.638885000	0.036834000
6	-5.561602000	1.359031000	-0.047858000	6	2.691537000	5.030582000	-0.044442000
6	-5.721964000	-0.140313000	-0.153017000	6	1.267246000	5.522336000	-0.150411000
6	-6.677669000	-1.101573000	-0.195866000	6	0.553486000	6.708869000	-0.197686000
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6	-6.443678000	-4.891685000	-0.299593000	6	-3.165192000	7.391198000	-0.503271000
1	-6.771639000	-5.773410000	0.249465000	1	-3.969014000	7.924525000	0.002246000
6	-6.746719000	-3.601236000	0.120045000	6	-1.861617000	7.385762000	-0.020989000
1	-7.347292000	-3.452585000	1.019446000	1	-1.620288000	7.940825000	0.887337000
6	-8.104659000	-0.857774000	0.101279000	6	1.113795000	8.006398000	0.193194000
6	-9.108086000	-1.547422000	-0.599727000	6	0.679614000	9.194507000	-0.427248000
1	-8.826102000	-2.283768000	-1.354274000	1	-0.096549000	9.147103000	-1.192427000
6	-10.454228000	-1.285664000	-0.368247000	6	1.250460000	10.421014000	-0.111060000

1	-11.244503000	-1.796955000	-0.918030000	1	0.940995000	11.344477000	-0.600567000
6	-10.795588000	-0.332876000	0.584691000	6	2.259167000	10.463461000	0.845620000
6	-9.830762000	0.340200000	1.325442000	6	2.689331000	9.318069000	1.507628000
1	-10.144832000	1.067497000	2.074236000	1	3.472194000	9.400614000	2.261621000
6	-8.489332000	0.069996000	1.081937000	6	2.114232000	8.098151000	1.179201000
1	-7.718405000	0.591588000	1.652021000	1	2.444653000	7.191022000	1.688024000
6	-6.285262000	2.495043000	-0.189967000	6	3.961803000	5.483657000	-0.187403000
6	-7.710404000	2.520743000	-0.591869000	6	4.309178000	6.876628000	-0.545830000
6	-8.204631000	1.670925000	-1.591326000	6	3.583269000	7.591704000	-1.509044000
1	-7.519699000	0.987197000	-2.096032000	1	2.756913000	7.101326000	-2.026896000
6	-9.551968000	1.681337000	-1.936653000	6	3.895180000	8.914813000	-1.803316000
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6	-10.407159000	2.553586000	-1.274348000	6	4.943495000	9.523372000	-1.123758000
6	-9.946126000	3.436248000	-0.303915000	6	5.710180000	8.834193000	-0.190338000
1	-10.650775000	4.112699000	0.179936000	1	6.533353000	9.347254000	0.307035000
6	-8.594874000	3.421186000	0.023826000	6	5.394276000	7.508471000	0.084172000
1	-8.216030000	4.106299000	0.784684000	1	5.984216000	6.952717000	0.815501000
6	-5.636028000	3.818693000	0.009172000	6	5.103558000	4.543626000	-0.029530000
6	-4.872040000	4.104727000	1.147646000	6	5.226411000	3.706915000	1.086883000
1	-4.752246000	3.340325000	1.917729000	1	4.468377000	3.746409000	1.871196000
6	-4.277064000	5.353486000	1.319219000	6	6.306384000	2.835992000	1.216513000
1	-3.696550000	5.603182000	2.206521000	1	6.431148000	2.192141000	2.086135000
6	-4.453559000	6.313909000	0.332094000	6	7.261531000	2.807593000	0.208616000
6	-5.210937000	6.068250000	-0.808183000	6	7.176756000	3.629234000	-0.910045000
1	-5.322888000	6.855043000	-1.554108000	1	7.952895000	3.573563000	-1.673232000
6	-5.808323000	4.823301000	-0.957072000	6	6.101824000	4.502740000	-1.016314000
1	-6.414761000	4.616036000	-1.840688000	1	6.023703000	5.161938000	-1.882855000
6	-2.933707000	1.900662000	0.174105000	6	2.607496000	2.386547000	0.153906000
6	-1.849790000	2.466257000	0.264303000	6	2.888725000	1.153972000	0.253894000
6	-0.605086000	3.020678000	0.315164000	6	3.109751000	-0.132463000	0.316838000
6	0.545868000	3.442764000	0.304629000	6	3.247854000	-1.390415000	0.315477000
6	1.899571000	3.772678000	0.184007000	6	3.227962000	-2.728326000	0.220715000
6	2.981009000	2.963049000	-0.133518000	6	2.136101000	-3.632992000	-0.082087000
6	3.911410000	4.119730000	-0.188552000	6	3.027222000	-4.774554000	-0.159301000
6	2.731019000	5.001518000	0.155416000	6	4.189484000	-3.864731000	0.162194000
6	2.392397000	6.302120000	0.337480000	6	5.539749000	-3.866073000	0.295926000

6	1.083592000	6.613899000	0.971382000	6	6.192066000	-2.670127000	0.895018000
6	0.690222000	5.942714000	2.137732000	6	5.707280000	-2.134673000	2.096507000
1	1.350654000	5.187803000	2.568153000	1	4.842340000	-2.596201000	2.575777000
6	-0.517174000	6.237481000	2.763491000	6	6.318666000	-1.035228000	2.690053000
1	-0.829227000	5.731558000	3.677308000	1	5.960068000	-0.616116000	3.630336000
6	-1.328658000	7.220213000	2.214335000	6	7.428493000	-0.475989000	2.071187000
6	-0.973261000	7.909992000	1.059671000	6	7.939055000	-0.977433000	0.878890000
1	-1.652405000	8.661463000	0.659504000	1	8.802336000	-0.492879000	0.424969000
6	0.239455000	7.607531000	0.450209000	6	7.320532000	-2.082707000	0.302851000
1	0.539298000	8.144160000	-0.451934000	1	7.712482000	-2.497042000	-0.628044000
6	3.251977000	7.439865000	-0.049412000	6	6.412423000	-4.987969000	-0.103491000
6	3.305478000	8.598597000	0.742438000	6	7.549717000	-5.313100000	0.654368000
1	2.695959000	8.658754000	1.645963000	1	7.795275000	-4.716110000	1.534535000
6	4.140871000	9.658449000	0.405706000	6	8.350039000	-6.398823000	0.315472000
1	4.209657000	10.556996000	1.019004000	1	9.223754000	-6.678412000	0.904271000
6	4.915768000	9.559509000	-0.744430000	6	8.015657000	-7.152199000	-0.804409000
6	4.859609000	8.444143000	-1.572259000	6	6.923125000	-6.833343000	-1.602783000
1	5.473921000	8.416545000	-2.472338000	1	6.709315000	-7.441427000	-2.481870000
6	4.024718000	7.390142000	-1.220092000	6	6.127622000	-5.750524000	-1.247223000
1	3.968905000	6.504819000	-1.856168000	1	5.263150000	-5.487363000	-1.859567000
6	5.251429000	4.178242000	-0.384522000	6	2.753205000	-6.110458000	-0.359711000
6	6.070599000	5.379417000	-0.111454000	6	3.705028000	-7.188472000	-0.049636000
6	5.832658000	6.177621000	1.017247000	6	4.564616000	-7.103240000	1.059127000
1	5.038172000	5.894976000	1.710401000	1	4.505813000	-6.230325000	1.711634000
6	6.586719000	7.321227000	1.256572000	6	5.485359000	-8.107273000	1.331622000
1	6.408280000	7.957918000	2.123201000	1	6.163899000	-8.050757000	2.182856000
6	7.588169000	7.663877000	0.355915000	6	5.548906000	-9.206939000	0.483131000
6	7.874095000	6.879439000	-0.756026000	6	4.694826000	-9.342769000	-0.606348000
1	8.676793000	7.181003000	-1.429065000	1	4.774433000	-10.226876000	-1.238976000
6	7.117622000	5.733725000	-0.977488000	6	3.770670000	-8.336358000	-0.860541000
1	7.327457000	5.107714000	-1.846854000	1	3.099842000	-8.424382000	-1.716952000
6	5.966606000	2.970543000	-0.877051000	6	1.417946000	-6.496796000	-0.870138000
6	5.470713000	2.224841000	-1.955047000	6	0.815966000	-5.802181000	-1.931077000
1	4.554136000	2.546847000	-2.452513000	1	1.353124000	-4.978940000	-2.404935000
6	6.132946000	1.085528000	-2.405199000	6	-0.449986000	-6.149723000	-2.391621000
1	5.757512000	0.494139000	-3.240172000	1	-0.929703000	-5.616737000	-3.212380000

6	7.308438000	0.704233000	-1.773744000	6	-1.113027000	-7.209392000	-1.786665000
6	7.842774000	1.429875000	-0.713456000	6	-0.542678000	-7.936022000	-0.745860000
1	8.764871000	1.087232000	-0.246302000	1	-1.105300000	-8.753752000	-0.298095000
6	7.169554000	2.564107000	-0.276214000	6	0.722785000	-7.578262000	-0.298800000
1	7.574656000	3.145311000	0.554330000	1	1.181036000	-8.133219000	0.521799000
6	3.052660000	1.570812000	-0.227403000	6	0.776024000	-3.370217000	-0.146391000
6	2.990814000	0.347027000	-0.242836000	6	-0.395948000	-3.000228000	-0.162424000
6	2.845383000	-1.007468000	-0.214733000	6	-1.672789000	-2.522383000	-0.149642000
6	2.647851000	-2.214825000	-0.146385000	6	-2.795054000	-2.034521000	-0.103257000
9	6.010877000	-10.475978000	-0.805919000	9	-11.643569000	-3.254480000	-0.699912000
9	3.971998000	-11.203083000	2.028374000	9	-11.830123000	-1.031259000	2.085362000
9	-4.545433000	-7.130243000	0.555237000	9	-5.829449000	6.170536000	0.285122000
9	-5.434075000	-6.288231000	-1.900044000	9	-4.685019000	6.708468000	-2.162179000
9	-12.080292000	-0.059891000	0.798233000	9	2.826084000	11.629702000	1.139054000
9	-11.701916000	2.546726000	-1.582466000	9	5.225163000	10.798585000	-1.380023000
9	-3.895446000	7.516987000	0.479242000	9	8.302532000	1.979567000	0.314188000
9	-2.480200000	7.513208000	2.822607000	9	8.022390000	0.571006000	2.648498000
9	5.730297000	10.561396000	-1.065880000	9	8.765119000	-8.203516000	-1.126195000
9	8.295402000	8.771201000	0.567512000	9	6.448480000	-10.156701000	0.723684000
9	7.952019000	-0.380340000	-2.208800000	9	-2.324997000	-7.548054000	-2.226646000
6	5.313957000	-4.135916000	-0.019928000	6	-5.323350000	-4.143555000	0.036284000
6	6.345312000	-4.051619000	-0.969415000	6	-5.517567000	-5.164320000	-0.909223000
6	5.305183000	-3.224214000	1.044250000	6	-4.411914000	-4.359280000	1.078513000
6	7.334820000	-3.080372000	-0.868486000	6	-4.815048000	-6.360689000	-0.827502000
1	6.367316000	-4.761376000	-1.798617000	1	-6.230843000	-5.010942000	-1.721280000
6	6.291031000	-2.247831000	1.162410000	6	-3.702756000	-5.554120000	1.177233000
1	4.520465000	-3.292201000	1.799954000	1	-4.267484000	-3.582892000	1.832005000
6	7.296557000	-2.199496000	0.207538000	6	-3.924033000	-6.539268000	0.225779000
1	8.135821000	-2.989247000	-1.601191000	1	-4.940939000	-7.158694000	-1.558429000
1	6.302171000	-1.537254000	1.988746000	1	-2.995556000	-5.738892000	1.985723000
9	8.267297000	-1.293554000	0.338364000	9	-3.277497000	-7.701648000	0.336483000
3c				3c			

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6	0.746671000	-4.165485000	0.006043000
6	-0.650193000	-4.222499000	0.038253000
6	-0.627644000	-5.700249000	0.178100000
6	0.876162000	-5.632306000	0.041148000
6	1.961032000	-6.448252000	-0.097672000
6	1.867165000	-7.895087000	-0.381261000
6	2.809477000	-8.795844000	0.147130000
1	3.628789000	-8.408864000	0.755640000
6	2.702785000	-10.166828000	-0.067254000
1	3.418068000	-10.872929000	0.355802000
6	1.642705000	-10.645901000	-0.826209000
6	0.710784000	-9.787723000	-1.394535000
1	-0.101864000	-10.201663000	-1.992245000
6	0.835531000	-8.418846000	-1.179252000
1	0.109835000	-7.732623000	-1.619214000
6	-1.608263000	-6.589167000	0.487176000
6	-1.355720000	-7.986898000	0.905779000
6	-0.271863000	-8.323301000	1.731475000
1	0.388242000	-7.529611000	2.085343000
6	-0.014235000	-9.646195000	2.079393000
1	0.839627000	-9.919478000	2.699858000
6	-0.861094000	-10.641234000	1.610870000
6	-1.968804000	-10.345499000	0.826291000
1	-2.614044000	-11.156211000	0.486635000
6	-2.211815000	-9.018641000	0.484714000
1	-3.073021000	-8.770337000	-0.138606000
6	-3.030139000	-6.150408000	0.471091000
6	-3.872431000	-6.449455000	1.554663000
1	-3.468091000	-7.002895000	2.404581000
6	-5.200693000	-6.039366000	1.568781000
1	-5.860050000	-6.248406000	2.411539000
6	-5.696381000	-5.333504000	0.477998000
6	-4.901690000	-5.033578000	-0.619417000
1	-5.335221000	-4.491027000	-1.457891000

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6	-2.255631000	3.567653000	-0.006465000
6	-0.955446000	4.159861000	0.049302000
6	-1.533438000	5.506842000	0.186960000
6	-2.907971000	4.882386000	0.030624000
6	-4.218833000	5.243948000	-0.110652000
6	-4.671644000	6.620794000	-0.389912000
6	-5.889214000	7.100842000	0.127129000
1	-6.510383000	6.432668000	0.726290000
6	-6.303019000	8.412652000	-0.085152000
1	-7.235708000	8.796119000	0.330017000
6	-5.491974000	9.259160000	-0.829693000
6	-4.299277000	8.816356000	-1.385968000
1	-3.693400000	9.508645000	-1.971376000
6	-3.903364000	7.499775000	-1.173537000
1	-2.966524000	7.139487000	-1.602029000
6	-0.971947000	6.710997000	0.500966000
6	-1.737270000	7.903151000	0.922760000
6	-2.876391000	7.800281000	1.738073000
1	-3.192076000	6.812775000	2.078772000
6	-3.616761000	8.924317000	2.092392000
1	-4.516296000	8.847595000	2.703885000
6	-3.203880000	10.171228000	1.643406000
6	-2.059550000	10.322585000	0.870585000
1	-1.763911000	11.320333000	0.544464000
6	-1.332502000	9.188771000	0.520617000
1	-0.437213000	9.291622000	-0.095695000
6	0.509081000	6.843380000	0.498159000
6	1.170378000	7.453588000	1.577610000
1	0.580611000	7.828458000	2.416549000
6	2.555819000	7.572041000	1.603325000
1	3.080036000	8.026742000	2.444409000
6	3.290578000	7.083952000	0.528974000
6	2.675494000	6.490998000	-0.564541000
1	3.286121000	6.134751000	-1.392269000

6	-3.570758000	-5.446000000	-0.613352000	6	1.287279000	6.374946000	-0.570184000
1	-2.933041000	-5.215309000	-1.468180000	1	0.790690000	5.905343000	-1.420676000
6	-1.590003000	-3.199681000	0.010964000	6	0.289343000	3.563898000	0.030478000
6	-2.281993000	-2.176510000	-0.037858000	6	1.321667000	2.879447000	-0.021470000
6	-2.969449000	-1.014694000	-0.082120000	6	2.392296000	2.056407000	-0.065279000
6	-3.513851000	0.100304000	-0.091217000	6	3.316493000	1.231757000	-0.090853000
6	-3.998121000	1.386121000	-0.089633000	6	4.241635000	0.204992000	-0.098300000
6	-3.284877000	2.661072000	0.044865000	6	4.075071000	-1.209880000	0.023918000
6	-4.592066000	3.375170000	-0.035737000	6	5.530280000	-1.426112000	-0.072607000
6	-5.294093000	2.030831000	-0.085320000	6	5.701853000	0.079379000	-0.127821000
6	-6.577711000	1.524286000	-0.114448000	6	6.689395000	1.027332000	-0.151228000
6	-6.769417000	0.117428000	-0.549687000	6	6.335663000	2.414985000	-0.553217000
6	-6.112663000	-0.372371000	-1.691922000	6	5.557471000	2.642940000	-1.698996000
1	-5.420043000	0.283469000	-2.222187000	1	5.173962000	1.786537000	-2.255910000
6	-6.328458000	-1.664681000	-2.158960000	6	5.276341000	3.932867000	-2.139320000
1	-5.825370000	-2.040702000	-3.050662000	1	4.679293000	4.114145000	-3.033631000
6	-7.217942000	-2.483657000	-1.477403000	6	5.784973000	5.008458000	-1.425771000
6	-7.871803000	-2.053844000	-0.330847000	6	6.537188000	4.830828000	-0.271553000
1	-8.534528000	-2.742665000	0.192605000	1	6.883837000	5.706858000	0.275828000
6	-7.643800000	-0.756279000	0.121284000	6	6.811659000	3.533355000	0.151768000
1	-8.155368000	-0.403151000	1.018958000	1	7.410269000	3.375800000	1.051251000
6	-7.773336000	2.285890000	0.270212000	6	8.099652000	0.763487000	0.188550000
6	-9.030051000	2.027668000	-0.316593000	6	9.144196000	1.469702000	-0.437473000
1	-9.113941000	1.232553000	-1.059421000	1	8.899108000	2.235274000	-1.175647000
6	-10.157049000	2.778401000	0.003672000	6	10.479509000	1.194037000	-0.158002000
1	-11.124005000	2.589146000	-0.464434000	1	11.292340000	1.724878000	-0.654903000
6	-10.039570000	3.810735000	0.925258000	6	10.780751000	0.199915000	0.763635000
6	-8.829410000	4.083321000	1.549574000	6	9.781076000	-0.499577000	1.426890000
1	-8.774764000	4.894824000	2.276319000	1	10.056578000	-1.268039000	2.149860000
6	-7.714634000	3.314675000	1.231976000	6	8.450951000	-0.205769000	1.145829000
1	-6.761190000	3.518956000	1.722389000	1	7.655676000	-0.748687000	1.659614000
6	-4.868991000	4.691877000	-0.224709000	6	6.274913000	-2.559495000	-0.220071000
6	-6.201577000	5.228255000	-0.589490000	6	7.700567000	-2.573163000	-0.615746000
6	-7.031732000	4.580277000	-1.515643000	6	8.211236000	-1.685063000	-1.575746000
1	-6.682604000	3.656862000	-1.980730000	1	7.532158000	-0.972655000	-2.047334000
6	-8.295517000	5.077828000	-1.820608000	6	9.562328000	-1.681589000	-1.911285000

1	-8.958428000	4.567165000	-2.519397000	1	9.970135000	-0.977588000	-2.637224000
6	-8.728298000	6.240695000	-1.198740000	6	10.411380000	-2.589231000	-1.293463000
6	-7.921975000	6.932415000	-0.303862000	6	9.939832000	-3.512629000	-0.368901000
1	-8.297389000	7.846638000	0.156801000	1	10.638152000	-4.214359000	0.088444000
6	-6.660002000	6.424085000	-0.011862000	6	8.587559000	-3.501122000	-0.041439000
1	-6.015158000	6.951638000	0.693722000	1	8.203826000	-4.214539000	0.690526000
6	-3.777267000	5.700840000	-0.129913000	6	5.632706000	-3.891468000	-0.054641000
6	-2.885891000	5.731044000	0.950607000	6	4.810782000	-4.190130000	1.041876000
1	-2.987419000	4.987782000	1.742504000	1	4.632838000	-3.421417000	1.795403000
6	-1.872467000	6.685089000	1.026691000	6	4.215987000	-5.442745000	1.184722000
1	-1.175939000	6.721849000	1.862961000	1	3.579426000	-5.687343000	2.034140000
6	-1.755371000	7.614925000	0.003504000	6	4.451489000	-6.406478000	0.214577000
6	-2.622580000	7.622259000	-1.082509000	6	5.265401000	-6.154357000	-0.883523000
1	-2.489909000	8.368683000	-1.866062000	1	5.418096000	-6.939168000	-1.624908000
6	-3.633024000	6.668755000	-1.137220000	6	5.854186000	-4.901014000	-1.007045000
1	-4.324581000	6.661749000	-1.982038000	1	6.494580000	-4.687974000	-1.865263000
6	-1.984472000	2.962282000	0.143412000	6	2.934535000	-1.975965000	0.121615000
6	-0.725409000	3.086970000	0.242211000	6	1.834506000	-2.542967000	0.208758000
6	0.583438000	3.123210000	0.307849000	6	0.598664000	-3.078912000	0.260292000
6	1.849759000	3.060452000	0.318558000	6	-0.572336000	-3.487414000	0.257518000
6	3.163819000	2.800958000	0.240342000	6	-1.918424000	-3.772922000	0.172371000
6	3.911087000	1.581517000	-0.010597000	6	-3.033240000	-2.917962000	-0.084767000
6	5.180684000	2.271491000	-0.072191000	6	-3.956150000	-4.060107000	-0.133521000
6	4.440906000	3.570325000	0.184142000	6	-2.770937000	-4.967354000	0.140545000
6	4.640004000	4.911495000	0.265794000	6	-2.460469000	-6.291462000	0.288052000
6	3.539185000	5.761731000	0.801469000	6	-1.146683000	-6.644171000	0.889819000
6	2.910024000	5.420073000	2.006969000	6	-0.699452000	-5.985897000	2.046479000
1	3.213641000	4.507234000	2.521125000	1	-1.318693000	-5.198618000	2.478898000
6	1.909190000	6.220393000	2.549753000	6	0.511779000	-6.315553000	2.646410000
1	1.414870000	5.963276000	3.486853000	1	0.862695000	-5.805949000	3.544234000
6	1.541708000	7.376801000	1.877483000	6	1.282342000	-7.324074000	2.086459000
6	2.130906000	7.746223000	0.674719000	6	0.883262000	-7.997926000	0.938916000
1	1.786244000	8.647649000	0.169610000	1	1.536369000	-8.761620000	0.518096000
6	3.135044000	6.936746000	0.150003000	6	-0.332648000	-7.655805000	0.353019000
1	3.615435000	7.213636000	-0.790641000	1	-0.660603000	-8.176051000	-0.549255000
6	5.881526000	5.606691000	-0.136601000	6	-3.339772000	-7.400608000	-0.125821000

6	6.336944000	6.732741000	0.568692000	6	-3.376849000	-8.609588000	0.592661000
1	5.755826000	7.098998000	1.417034000	1	-2.734605000	-8.725733000	1.467665000
6	7.524055000	7.371864000	0.221717000	6	-4.230046000	-9.646660000	0.226177000
1	7.898707000	8.233388000	0.775228000	1	-4.277958000	-10.579063000	0.789830000
6	8.255907000	6.883803000	-0.852758000	6	-5.055005000	-9.477993000	-0.878420000
6	7.821329000	5.794448000	-1.596216000	6	-5.027030000	-8.313047000	-1.633624000
1	8.424698000	5.443397000	-2.433603000	1	-5.684792000	-8.220727000	-2.498400000
6	6.633622000	5.165786000	-1.237395000	6	-4.164373000	-7.288091000	-1.259619000
1	6.282720000	4.299123000	-1.800442000	1	-4.131820000	-6.365459000	-1.841924000
6	6.476290000	1.832130000	-0.261658000	6	-5.311438000	-4.121597000	-0.302650000
6	7.665424000	2.633443000	0.065440000	6	-6.127156000	-5.317370000	-0.009063000
6	7.679409000	3.526194000	1.154968000	6	-5.835793000	-6.154253000	1.081759000
1	6.787762000	3.601982000	1.779995000	1	-4.992430000	-5.900819000	1.726662000
6	8.786837000	4.320655000	1.436243000	6	-6.582488000	-7.300999000	1.334937000
1	8.786640000	5.028444000	2.266161000	1	-6.345988000	-7.966506000	2.165702000
6	9.916969000	4.210244000	0.637871000	6	-7.647114000	-7.608645000	0.498763000
6	9.966186000	3.312719000	-0.421652000	6	-7.993107000	-6.789128000	-0.568163000
1	10.873251000	3.249000000	-1.024291000	1	-8.840298000	-7.062753000	-1.198048000
6	8.846568000	2.534433000	-0.698671000	6	-7.233966000	-5.648448000	-0.811524000
1	8.871545000	1.840017000	-1.540724000	1	-7.488235000	-5.001670000	-1.653419000
6	6.694656000	0.447148000	-0.747414000	6	-6.036902000	-2.909124000	-0.768188000
6	5.902296000	-0.103902000	-1.770207000	6	-5.543044000	-2.125247000	-1.822716000
1	5.114122000	0.505935000	-2.214114000	1	-4.608225000	-2.413548000	-2.305084000
6	6.090611000	-1.407839000	-2.220583000	6	-6.215741000	-0.985689000	-2.257061000
1	5.463478000	-1.838551000	-3.001583000	1	-5.826679000	-0.364059000	-3.063519000
6	7.099395000	-2.174119000	-1.655610000	6	-7.408043000	-0.636070000	-1.640965000
6	7.915707000	-1.670388000	-0.650370000	6	-7.938481000	-1.388030000	-0.598906000
1	8.682264000	-2.312845000	-0.217575000	1	-8.866634000	-1.063623000	-0.129679000
6	7.706537000	-0.368773000	-0.205226000	6	-7.249377000	-2.518757000	-0.172715000
1	8.334216000	0.030059000	0.594252000	1	-7.651068000	-3.114383000	0.649593000
6	3.446928000	0.279001000	-0.068720000	6	-3.108926000	-1.543226000	-0.149762000
6	2.915997000	-0.834038000	-0.095379000	6	-3.034607000	-0.306541000	-0.163661000
6	2.253752000	-2.020946000	-0.090792000	6	-2.870017000	1.031535000	-0.148697000
6	1.603680000	-3.063993000	-0.063347000	6	-2.643494000	2.248868000	-0.101938000
9	1.520438000	-11.965811000	-1.020601000	9	-5.873096000	10.529891000	-1.023155000
9	-0.609016000	-11.917042000	1.929831000	9	-3.920855000	11.255586000	1.970667000

9	-6.977627000	-4.949526000	0.491836000	9	4.625155000	7.202625000	0.555515000
9	-7.447556000	-3.723558000	-1.943945000	9	5.544603000	6.251569000	-1.869144000
9	-11.117867000	4.552988000	1.225312000	9	12.064607000	-0.085869000	1.024428000
9	-9.950563000	6.713657000	-1.475825000	9	11.715721000	-2.579939000	-1.601793000
9	-0.791222000	8.544045000	0.059191000	9	3.894810000	-7.619509000	0.335104000
9	0.594443000	8.160127000	2.413143000	9	2.440887000	-7.655590000	2.676040000
9	9.405981000	7.484297000	-1.185353000	9	-5.891822000	-10.465361000	-1.227890000
9	10.986117000	4.980399000	0.898780000	9	-8.361812000	-8.719022000	0.729979000
9	7.298462000	-3.427040000	-2.098131000	9	-8.073704000	0.443981000	-2.073262000
6	3.324841000	-5.866160000	0.024324000	6	-5.270663000	4.197325000	0.008296000
6	4.339757000	-6.196096000	-0.890890000	6	-6.335382000	4.124602000	-0.906199000
6	3.644449000	-4.992171000	1.074320000	6	-5.248907000	3.274012000	1.064956000
6	5.625055000	-5.679813000	-0.765842000	6	-7.344378000	3.175438000	-0.772926000
1	4.108270000	-6.869503000	-1.718770000	1	-6.366775000	4.830383000	-1.738862000
6	4.925021000	-4.461318000	1.211815000	6	-6.247716000	2.314788000	1.211954000
1	2.872239000	-4.725790000	1.797528000	1	-4.429255000	3.311909000	1.783932000
6	5.901150000	-4.826018000	0.296743000	6	-7.289671000	2.289755000	0.296875000
1	6.417010000	-5.911983000	-1.477188000	1	-8.166989000	3.098135000	-1.483357000
1	5.177517000	-3.772898000	2.018265000	1	-6.231654000	1.589961000	2.025905000
9	7.146932000	-4.365420000	0.454474000	9	-8.280962000	1.403281000	0.461785000

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6	-2.490813000	3.416042000	-0.020774000
6	-1.260277000	4.037522000	0.144178000
6	-1.894932000	5.373321000	0.313542000
6	-3.222626000	4.706717000	0.032233000
6	-4.519037000	5.019733000	-0.214362000
6	-4.986216000	6.404591000	-0.445889000
6	-6.232321000	6.832668000	0.041389000
1	-6.873005000	6.127244000	0.573700000
6	-6.648423000	8.150707000	-0.111741000
1	-7.602946000	8.490755000	0.289765000
6	-5.818643000	9.053303000	-0.776357000
6	-4.597873000	8.643119000	-1.309217000

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6	-2.981665000	-3.020814000	0.060091000
6	-3.815916000	-1.917267000	0.127832000
6	-5.021536000	-2.769228000	0.309617000
6	-4.117792000	-3.969638000	0.140242000
6	-4.177451000	-5.315504000	-0.023245000
6	-5.438102000	-6.053169000	-0.256837000
6	-5.636115000	-7.327232000	0.300512000
1	-4.840861000	-7.784510000	0.892153000
6	-6.841787000	-8.001483000	0.139695000
1	-7.006244000	-8.978590000	0.593737000
6	-7.860248000	-7.406146000	-0.603987000
6	-7.673418000	-6.162414000	-1.204730000

1	-3.972545000	9.361450000	-1.839272000	1	-8.477387000	-5.722734000	-1.794918000
6	-4.191543000	7.324103000	-1.145018000	6	-6.465736000	-5.496527000	-1.031532000
1	-3.233809000	6.998588000	-1.555141000	1	-6.315257000	-4.519881000	-1.495233000
6	-1.404912000	6.548897000	0.775805000	6	-6.288345000	-2.475321000	0.690201000
6	-2.254636000	7.684064000	1.203015000	6	-7.261750000	-3.494369000	1.145864000
6	-3.430430000	7.478866000	1.936239000	6	-6.870690000	-4.553966000	1.974637000
1	-3.714483000	6.463214000	2.217805000	1	-5.834258000	-4.614253000	2.311723000
6	-4.243488000	8.547792000	2.296683000	6	-7.779212000	-5.533966000	2.359234000
1	-5.165525000	8.388281000	2.855617000	1	-7.472374000	-6.366820000	2.991846000
6	-3.879547000	9.839713000	1.922465000	6	-9.097406000	-5.455450000	1.914881000
6	-2.694274000	10.076632000	1.226466000	6	-9.523907000	-4.389324000	1.123033000
1	-2.423079000	11.096615000	0.954507000	1	-10.562694000	-4.341778000	0.796575000
6	-1.883844000	8.999965000	0.883222000	6	-8.607587000	-3.410606000	0.754172000
1	-0.956028000	9.177171000	0.335615000	1	-8.933205000	-2.576271000	0.129711000
6	0.061534000	6.731697000	0.933321000	6	-6.756400000	-1.065031000	0.707066000
6	0.567749000	7.262068000	2.130834000	6	-7.462942000	-0.581112000	1.819827000
1	-0.123332000	7.531799000	2.931636000	1	-7.643334000	-1.242940000	2.668934000
6	1.932899000	7.439049000	2.313243000	6	-7.932613000	0.725235000	1.856198000
1	2.329616000	7.839402000	3.245958000	1	-8.475501000	1.105074000	2.721442000
6	2.806516000	7.101032000	1.279319000	6	-7.711483000	1.557310000	0.758712000
6	2.331635000	6.588545000	0.075164000	6	-7.019598000	1.103945000	-0.361039000
1	3.029364000	6.353358000	-0.727220000	1	-6.878134000	1.765014000	-1.215341000
6	0.959991000	6.407774000	-0.089627000	6	-6.546323000	-0.206525000	-0.378747000
1	0.578877000	6.020391000	-1.036324000	1	-6.022101000	-0.576282000	-1.261949000
6	0.023990000	3.481898000	0.150440000	6	-3.488378000	-0.553519000	0.081872000
6	1.090067000	2.878074000	0.101455000	6	-3.055452000	0.591876000	0.011929000
6	2.235465000	2.139294000	0.033219000	6	-2.496756000	1.833373000	-0.061753000
6	3.219124000	1.410547000	-0.035045000	6	-1.924151000	2.921886000	-0.117118000
6	4.237504000	0.451739000	-0.091894000	6	-1.148082000	4.069238000	-0.149505000
6	4.161655000	-0.929618000	0.031424000	6	0.305214000	4.222316000	0.021658000
6	5.631005000	-1.085440000	-0.137125000	6	0.148738000	5.700160000	-0.100289000
6	5.718781000	0.423273000	-0.199963000	6	-1.344615000	5.491602000	-0.205769000
6	6.642084000	1.416565000	-0.245488000	6	-2.514333000	6.238122000	-0.277871000
6	6.228000000	2.803669000	-0.584157000	6	-3.746155000	5.597797000	-0.784445000
6	5.364653000	3.045591000	-1.661371000	6	-3.705985000	4.755312000	-1.908205000
1	4.949659000	2.202330000	-2.216536000	1	-2.746628000	4.534577000	-2.379318000

6	5.064316000	4.344312000	-2.063938000	6	-4.871091000	4.230901000	-2.456008000
1	4.412552000	4.529251000	-2.917926000	1	-4.837446000	3.598111000	-3.342774000
6	5.641136000	5.415413000	-1.386583000	6	-6.098594000	4.550911000	-1.878594000
6	6.485539000	5.205525000	-0.296409000	6	-6.170438000	5.363797000	-0.747507000
1	6.914791000	6.059494000	0.226181000	1	-7.138928000	5.587153000	-0.302697000
6	6.776367000	3.904080000	0.093872000	6	-4.998381000	5.881696000	-0.210889000
1	7.453806000	3.733410000	0.932457000	1	-5.050512000	6.525290000	0.668832000
6	8.084629000	1.193256000	-0.004016000	6	-2.582197000	7.651426000	0.108881000
6	9.055904000	1.904000000	-0.728783000	6	-3.467205000	8.541583000	-0.531514000
1	8.742204000	2.643533000	-1.467710000	1	-4.127449000	8.171808000	-1.317384000
6	10.411957000	1.656632000	-0.545769000	6	-3.480665000	9.894535000	-0.216993000
1	11.165449000	2.189009000	-1.126119000	1	-4.143723000	10.586576000	-0.735986000
6	10.808983000	0.697332000	0.385404000	6	-2.611328000	10.375838000	0.762534000
6	9.867245000	0.008025000	1.147284000	6	-1.752732000	9.511700000	1.442354000
1	10.200366000	-0.726600000	1.880330000	1	-1.091382000	9.906244000	2.213660000
6	8.514796000	0.262142000	0.951979000	6	-1.742719000	8.163176000	1.114683000
1	7.772299000	-0.277375000	1.542917000	1	-1.066470000	7.486687000	1.640477000
6	6.399192000	-2.178893000	-0.360996000	6	1.066919000	6.681895000	-0.283318000
6	7.798710000	-2.115265000	-0.843281000	6	0.717427000	8.063862000	-0.685759000
6	8.181668000	-1.216803000	-1.846976000	6	-0.237784000	8.315969000	-1.678176000
1	7.431216000	-0.559951000	-2.290914000	1	-0.719533000	7.476305000	-2.183055000
6	9.503052000	-1.143778000	-2.274430000	6	-0.589233000	9.617928000	-2.017790000
1	9.804985000	-0.436349000	-3.046686000	1	-1.342518000	9.815522000	-2.780369000
6	10.456093000	-1.977831000	-1.693795000	6	0.016769000	10.683589000	-1.355868000
6	10.095376000	-2.907612000	-0.718540000	6	1.002752000	10.462293000	-0.393996000
1	10.855440000	-3.558044000	-0.285944000	1	1.473653000	11.311446000	0.101123000
6	8.768301000	-2.979445000	-0.309815000	6	1.356642000	9.155963000	-0.076305000
1	8.478290000	-3.704071000	0.453685000	1	2.125390000	8.973776000	0.677326000
6	5.839786000	-3.545346000	-0.183531000	6	2.519808000	6.404540000	-0.137235000
6	5.131972000	-3.918753000	0.965524000	6	3.047020000	5.714969000	0.961682000
1	4.971423000	-3.186453000	1.759106000	1	2.374948000	5.352135000	1.741363000
6	4.653166000	-5.218736000	1.124121000	6	4.420263000	5.509937000	1.089486000
1	4.121052000	-5.519778000	2.026936000	1	4.836581000	4.994829000	1.955430000
6	4.887846000	-6.152232000	0.117793000	6	5.271860000	6.000639000	0.102613000
6	5.583347000	-5.805786000	-1.040588000	6	4.773457000	6.682204000	-1.007315000
1	5.750606000	-6.554629000	-1.814423000	1	5.460834000	7.052913000	-1.767343000

6	6.062408000	-4.510384000	-1.179264000	6	3.404941000	6.887993000	-1.114893000
1	6.621302000	-4.235694000	-2.075696000	1	3.008905000	7.434769000	-1.972502000
6	3.042586000	-1.755090000	0.178102000	6	1.261773000	3.304789000	0.171217000
6	1.988235000	-2.370850000	0.286969000	6	2.055628000	2.323852000	0.297951000
6	0.771828000	-2.984347000	0.349510000	6	2.820967000	1.266993000	0.379035000
6	-0.356135000	-3.464363000	0.341475000	6	3.502874000	0.201670000	0.383599000
6	-1.689281000	-3.864098000	0.201935000	6	4.090892000	-0.999845000	0.271278000
6	-2.791321000	-3.122664000	-0.201806000	6	3.534083000	-2.286652000	-0.092897000
6	-3.667353000	-4.320330000	-0.229418000	6	4.847799000	-2.891311000	-0.195045000
6	-2.471030000	-5.125970000	0.228724000	6	5.464702000	-1.573580000	0.213378000
6	-2.110969000	-6.399460000	0.527206000	6	6.669242000	-0.983299000	0.422543000
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1	1.016359000	-5.477204000	3.872489000	1	5.481540000	1.906547000	3.893224000
6	1.527673000	-7.171634000	2.645605000	6	6.900023000	2.747576000	2.507870000
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1	1.811525000	-8.827051000	1.296638000	1	8.306772000	3.361694000	0.996526000
6	-0.003864000	-7.726995000	0.880638000	6	7.562581000	1.356999000	0.665259000
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1	-7.431183000	-3.432725000	0.122400000	1	4.840498000	-6.806578000	0.100378000
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17	12.493371000	0.349661000	0.601180000	17	-2.584365000	12.066084000	1.137222000
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17	4.343260000	-7.790890000	0.306465000	17	6.991123000	5.802540000	0.256487000
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3d				3d			
m06-2x/def2-SVP				m06-2x/def2-SVP			
-2 1				-2 3			
6	0.372311000	4.228735000	0.114309000	6	1.963552000	-3.741624000	0.048951000
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6	-4.280953000	-6.925629000	1.051916000	6	-0.031838000	8.145415000	1.333658000
1	-4.287859000	-7.929493000	0.629660000	1	-0.540528000	9.052042000	1.008116000
6	-4.971255000	-5.882508000	0.441827000	6	1.098036000	7.677506000	0.670516000
1	-5.541040000	-6.076891000	-0.468891000	1	1.484634000	8.235156000	-0.184644000
6	-7.145145000	-3.839787000	-0.033971000	6	3.980743000	7.075598000	0.022835000
6	-7.916916000	-4.745529000	0.712888000	6	4.187738000	8.225151000	0.807569000
1	-7.487525000	-5.201234000	1.607133000	1	3.606619000	8.356012000	1.722398000
6	-9.225639000	-5.050078000	0.351771000	6	5.135346000	9.182161000	0.459559000
1	-9.831432000	-5.732894000	0.947713000	1	5.306925000	10.058551000	1.085101000
6	-9.771527000	-4.454693000	-0.783186000	6	5.889744000	9.003042000	-0.698251000
6	-9.020311000	-3.579871000	-1.563367000	6	5.688340000	7.892932000	-1.514219000
1	-9.465551000	-3.125680000	-2.448486000	1	6.283688000	7.772260000	-2.419477000
6	-7.714511000	-3.282779000	-1.188653000	6	4.734517000	6.946738000	-1.155958000
1	-7.122087000	-2.586764000	-1.785454000	1	4.573578000	6.072897000	-1.790114000
6	-6.731314000	-0.074929000	-0.329402000	6	5.625294000	3.672308000	-0.390569000
6	-8.082799000	-0.536343000	0.017623000	6	6.544803000	4.772677000	-0.041513000
6	-8.319151000	-1.315914000	1.166042000	6	6.351578000	5.535037000	1.122392000
1	-7.477643000	-1.555710000	1.818865000	1	5.511962000	5.292539000	1.776508000
6	-9.585605000	-1.799489000	1.475247000	6	7.190088000	6.597681000	1.441239000
1	-9.746649000	-2.421202000	2.356581000	1	7.018290000	7.197741000	2.335064000
6	-10.659379000	-1.489245000	0.645256000	6	8.255535000	6.903215000	0.598898000
6	-10.475486000	-0.685038000	-0.478538000	6	8.500012000	6.145172000	-0.544695000
1	-11.326801000	-0.450155000	-1.118454000	1	9.341080000	6.398807000	-1.190480000
6	-9.201796000	-0.216637000	-0.780089000	6	7.650995000	5.087166000	-0.852167000
1	-9.056698000	0.395719000	-1.672235000	1	7.831876000	4.499134000	-1.754083000
6	-6.598639000	1.278501000	-0.914443000	6	6.226376000	2.450291000	-0.983471000
6	-5.640029000	1.563206000	-1.904887000	6	5.594409000	1.766017000	-2.034523000
1	-4.972204000	0.769048000	-2.241122000	1	4.640190000	2.135234000	-2.412307000
6	-5.524031000	2.828632000	-2.470934000	6	6.159049000	0.629543000	-2.605581000
1	-4.770272000	3.031725000	-3.231758000	1	5.654049000	0.100459000	-3.413504000
6	-6.388877000	3.840866000	-2.064343000	6	7.387704000	0.171685000	-2.139086000
6	-7.355315000	3.599001000	-1.090534000	6	8.048642000	0.830545000	-1.103838000
1	-8.015240000	4.406259000	-0.773382000	1	9.003410000	0.448657000	-0.744661000

6	-7.448414000	2.332782000	-0.524246000	6	7.464841000	1.957613000	-0.535762000
1	-8.198078000	2.151549000	0.248153000	1	7.977667000	2.470192000	0.280411000
6	-3.409853000	0.667008000	-0.051490000	6	3.229322000	1.274994000	-0.205377000
6	-2.608838000	1.605414000	-0.063139000	6	3.062236000	0.047545000	-0.208959000
6	-1.657504000	2.574813000	-0.031362000	6	2.794105000	-1.273540000	-0.165395000
6	-0.751171000	3.404500000	0.021108000	6	2.468945000	-2.466571000	-0.087500000
6	-1.634184000	6.584494000	0.043525000	6	4.909817000	-4.699842000	-0.074378000
6	-2.512480000	7.177619000	-0.879086000	6	5.964362000	-4.783834000	-0.999809000
6	-2.190445000	5.868793000	1.114136000	6	5.031162000	-3.772785000	0.972512000
6	-3.891689000	7.076262000	-0.735185000	6	7.106447000	-3.999959000	-0.874515000
1	-2.100801000	7.732020000	-1.724909000	1	5.887742000	-5.489410000	-1.829494000
6	-3.569049000	5.753683000	1.270265000	6	6.164880000	-2.976974000	1.109999000
1	-1.527945000	5.403717000	1.845839000	1	4.224377000	-3.686513000	1.701907000
6	-4.410758000	6.374349000	0.352458000	6	7.205130000	-3.112490000	0.195589000
1	-4.571448000	7.528394000	-1.456598000	1	7.921685000	-4.068980000	-1.594329000
1	-3.994100000	5.196171000	2.104536000	1	6.252982000	-2.265130000	1.930454000
17	-12.245205000	-2.118398000	1.017117000	17	9.291952000	8.252250000	0.982628000
17	-11.417299000	-4.805572000	-1.236448000	17	7.101601000	10.178603000	-1.134433000
17	-6.277293000	5.422651000	-2.798960000	17	8.121624000	-1.225867000	-2.881749000
17	-6.133672000	6.313656000	0.593478000	17	8.672761000	-2.198511000	0.423224000
17	2.010470000	12.250062000	-1.236499000	17	4.732569000	-11.456075000	-1.230691000
17	3.526864000	11.805198000	2.022365000	17	3.368277000	-11.807023000	2.108576000
17	8.435127000	2.869281000	1.134631000	17	-5.564145000	-6.846689000	1.386810000
17	8.530103000	1.832740000	-2.254194000	17	-6.285176000	-6.176062000	-2.008815000
17	9.629193000	-7.766228000	1.258533000	17	-12.358030000	1.464656000	0.972142000
17	8.283421000	-9.107175000	-1.822816000	17	-11.822560000	3.369228000	-2.060354000
17	-1.679939000	-8.924989000	-0.200739000	17	-3.278089000	8.413796000	0.064616000
17	-2.742738000	-7.977837000	3.032732000	17	-1.912050000	8.027649000	3.296917000
3m				3m			
m06-2x/def2-SVP				m06-2x/def2-SVP			
0 1				0 3			
6	3.727879000	2.024776000	-0.000077000	6	-3.432044000	2.533320000	-0.000039000
6	4.181741000	0.714723000	-0.000061000	6	-2.352420000	3.516197000	0.000213000
6	5.603834000	1.145052000	-0.000052000	6	-3.386361000	4.593467000	-0.000007000
6	5.111422000	2.566416000	-0.000023000	6	-4.420009000	3.514077000	-0.000216000

6	5.659975000	3.778970000	0.000048000	6	-5.868512000	3.524189000	-0.000429000
6	6.784997000	0.531767000	-0.000012000	6	-3.394434000	5.925642000	0.000039000
6	3.481013000	-0.497533000	-0.000069000	6	-0.999766000	3.390953000	0.000276000
6	2.760343000	-1.487280000	-0.000078000	6	0.217998000	3.140879000	0.000290000
6	1.866086000	-2.519551000	-0.000076000	6	1.511666000	2.763309000	0.000210000
6	0.989295000	-3.374073000	-0.000078000	6	2.663671000	2.322149000	0.000118000
6	-0.110414000	-4.240799000	0.000001000	6	3.900238000	1.688031000	0.000047000
6	-1.471880000	-3.978799000	-0.000081000	6	4.237951000	0.334922000	-0.000032000
6	-1.810265000	-5.425538000	0.000050000	6	5.689143000	0.635304000	-0.000212000
6	-0.333136000	-5.709794000	0.000117000	6	5.330420000	2.095677000	-0.000025000
6	0.442656000	-6.791184000	0.000294000	6	5.989490000	3.252044000	0.000060000
6	-2.931990000	-6.141769000	0.000078000	6	6.812687000	-0.081139000	-0.000449000
6	-2.171387000	-2.765844000	-0.000208000	6	3.429947000	-0.807030000	0.000005000
6	-2.668236000	-1.646867000	-0.000262000	6	2.620299000	-1.726140000	0.000048000
6	-3.115081000	-0.356287000	-0.000156000	6	1.633916000	-2.671755000	0.000111000
6	-3.416759000	0.830287000	-0.000067000	6	0.683258000	-3.442759000	0.000149000
6	-3.617496000	2.216028000	0.000018000	6	-0.490815000	-4.208813000	0.000044000
6	-2.709832000	3.264062000	0.000144000	6	-1.822808000	-3.830338000	-0.000009000
6	-3.793521000	4.280515000	0.000131000	6	-2.287075000	-5.240891000	-0.000016000
6	-4.778297000	3.143431000	-0.000023000	6	-0.840310000	-5.652925000	0.000014000
6	-6.102715000	3.012349000	-0.000187000	6	-0.161221000	-6.797441000	0.000084000
6	-3.852867000	5.610053000	0.000217000	6	-3.466806000	-5.857278000	-0.000107000
6	-1.309629000	3.263278000	0.000155000	6	-2.416037000	-2.558471000	0.000061000
6	-0.092149000	3.134009000	0.000110000	6	-2.816854000	-1.403277000	0.000098000
6	1.248961000	2.875762000	0.000026000	6	-3.156581000	-0.076542000	0.000020000
6	2.427420000	2.543794000	-0.000040000	6	-3.370284000	1.126390000	-0.000032000
1	0.006326000	-7.791091000	0.000336000	1	7.080302000	3.272899000	0.000012000
1	1.529727000	-6.698366000	0.000367000	1	5.451245000	4.201082000	0.000213000
1	-2.897846000	-7.232196000	0.000104000	1	7.787143000	0.409285000	-0.000566000
1	-3.906978000	-5.652131000	0.000126000	1	6.779462000	-1.171606000	-0.000542000
1	-6.565862000	2.024503000	-0.000314000	1	0.929820000	-6.798896000	0.000142000
1	-6.750448000	3.890223000	-0.000188000	1	-0.682511000	-7.755813000	0.000091000
1	-4.814294000	6.125638000	0.000164000	1	-3.527091000	-6.946553000	-0.000108000
1	-2.941351000	6.209624000	0.000167000	1	-4.395744000	-5.285093000	-0.000217000
1	6.744095000	3.900872000	0.000013000	1	-6.426100000	3.550170000	-0.938941000
1	5.036093000	4.674030000	0.000125000	1	-6.426337000	3.551181000	0.937920000

1	6.848507000	-0.557411000	-0.000043000	1	-2.461343000	6.490385000	0.000249000
1	7.712246000	1.106590000	0.000099000	1	-4.338924000	6.472437000	-0.000145000
3m				3m			
m06-2x/def2-SVP				m06-2x/def2-SVP			
-2 1				-2 3			
6	-3.296900000	-2.712258000	-0.000160000	6	-4.212348000	0.506416000	-0.000069000
6	-3.958312000	-1.452934000	-0.000205000	6	-3.803732000	1.879176000	-0.000056000
6	-5.276265000	-2.147889000	-0.000209000	6	-5.204154000	2.333670000	0.000009000
6	-4.550616000	-3.462131000	-0.000103000	6	-5.633352000	0.891731000	0.000117000
6	-4.957260000	-4.744825000	-0.000074000	6	-6.820667000	0.268604000	0.000288000
6	-6.553147000	-1.758145000	-0.000185000	6	-5.857519000	3.504627000	0.000025000
6	-3.544691000	-0.153105000	-0.000174000	6	-2.556947000	2.477047000	-0.000067000
6	-3.021161000	0.988132000	-0.000056000	6	-1.382128000	2.874824000	-0.000116000
6	-2.368575000	2.142521000	-0.000028000	6	-0.065508000	3.189102000	-0.000109000
6	-1.638836000	3.172796000	-0.000046000	6	1.162309000	3.364877000	-0.000072000
6	-0.727491000	4.163667000	0.000028000	6	2.544711000	3.394667000	0.000006000
6	0.762564000	4.157567000	-0.000102000	6	3.529350000	2.354475000	0.000110000
6	0.777011000	5.631760000	0.000129000	6	4.623071000	3.340109000	0.000124000
6	-0.730066000	5.637843000	0.000152000	6	3.588842000	4.432697000	-0.000070000
6	-1.646221000	6.617683000	0.000139000	6	3.642893000	5.772518000	-0.000264000
6	1.701190000	6.603991000	0.000392000	6	5.963839000	3.320611000	0.000254000
6	1.665859000	3.159450000	-0.000209000	6	3.423820000	0.975780000	0.000136000
6	2.386794000	2.122909000	-0.000351000	6	3.180960000	-0.240543000	0.000117000
6	3.029236000	0.962947000	-0.000390000	6	2.794864000	-1.537925000	0.000035000
6	3.543165000	-0.182736000	-0.000141000	6	2.333158000	-2.689118000	-0.000014000
6	3.945898000	-1.485861000	0.000023000	6	1.667613000	-3.901134000	0.000005000
6	3.274042000	-2.739808000	0.000390000	6	0.274447000	-4.233612000	-0.000039000
6	4.521491000	-3.499997000	0.000136000	6	0.581020000	-5.673659000	-0.000007000
6	5.258016000	-2.191821000	-0.000220000	6	2.044385000	-5.324423000	-0.000009000
6	6.538090000	-1.812696000	-0.000638000	6	3.177635000	-6.041205000	-0.000010000
6	4.917458000	-4.786048000	0.000207000	6	-0.106391000	-6.824949000	0.000002000
6	1.897159000	-3.026758000	0.000545000	6	-0.866713000	-3.452793000	-0.000125000
6	0.674853000	-3.132393000	0.000622000	6	-1.798638000	-2.634292000	-0.000137000
6	-0.701021000	-3.126456000	0.000401000	6	-2.729302000	-1.651370000	-0.000103000
6	-1.922387000	-3.010628000	0.000165000	6	-3.495464000	-0.675964000	-0.000088000

1	-1.339729000	7.666259000	0.000163000	1	4.604353000	6.290388000	-0.000195000
1	-2.713339000	6.387635000	0.000110000	1	2.729063000	6.369295000	-0.000429000
1	1.403429000	7.655080000	0.000563000	1	6.533649000	4.252229000	0.000166000
1	2.766355000	6.365062000	0.000248000	1	6.509600000	2.375430000	0.000345000
1	6.802157000	-0.753321000	-0.000857000	1	4.151445000	-5.548309000	-0.000068000
1	7.341265000	-2.553027000	-0.000799000	1	3.145276000	-7.132782000	-0.000009000
1	5.979612000	-5.038006000	-0.000134000	1	0.415552000	-7.784215000	0.000045000
1	4.189477000	-5.598599000	0.000533000	1	-1.197829000	-6.825045000	-0.000082000
1	-6.021501000	-4.987822000	0.000099000	1	-7.749884000	0.842326000	0.000504000
1	-4.236129000	-5.563470000	0.000097000	1	-6.880532000	-0.821185000	0.000310000
1	-6.808460000	-0.696627000	-0.000141000	1	-5.311812000	4.449857000	0.000082000
1	-7.362406000	-2.491820000	-0.000123000	1	-6.949221000	3.532345000	0.000093000

3m				3m			
m06-2x/def2-tzvpp				m06-2x/def2-tzvpp			
0 1				-2 3			
6	-1.838214000	3.789895000	-0.000173000	6	4.169755000	0.600101000	-0.000275000
6	-0.516564000	4.180314000	0.000010000	6	4.131083000	-0.825501000	0.000085000
6	-0.877058000	5.616818000	0.000130000	6	5.595111000	-0.902122000	0.000067000
6	-2.316211000	5.191637000	-0.000215000	6	5.635756000	0.597279000	-0.000050000
6	-3.494353000	5.792776000	-0.000331000	6	6.617685000	1.500454000	-0.000018000
6	-0.214713000	6.761640000	0.000454000	6	6.526573000	-1.857229000	0.000244000
6	0.657331000	3.430405000	0.000187000	6	3.090411000	-1.723734000	0.000241000
6	1.606442000	2.675442000	0.000322000	6	2.069716000	-2.409128000	0.000361000
6	2.590115000	1.740383000	0.000297000	6	0.887365000	-3.049253000	0.000186000
6	3.392465000	0.830983000	0.000251000	6	-0.244401000	-3.529547000	-0.000041000
6	4.201321000	-0.303112000	0.000190000	6	-1.565175000	-3.910855000	-0.000032000
6	3.878729000	-1.642923000	0.000128000	6	-2.780549000	-3.164722000	0.000120000
6	5.303012000	-2.048886000	-0.000035000	6	-3.578750000	-4.394380000	-0.000170000
6	5.654300000	-0.589932000	-0.000140000	6	-2.300479000	-5.179127000	-0.000122000
6	6.764004000	0.129700000	-0.000603000	6	-2.009084000	-6.481029000	-0.000234000
6	5.963560000	-3.194751000	0.000055000	6	-4.871570000	-4.723715000	-0.000298000
6	2.642323000	-2.284569000	0.000075000	6	-3.038291000	-1.814389000	0.000336000
6	1.513744000	-2.728485000	-0.000022000	6	-3.121792000	-0.587764000	0.000450000
6	0.212140000	-3.112849000	-0.000126000	6	-3.084916000	0.756236000	0.000301000
6	-0.976585000	-3.353003000	-0.000187000	6	-2.935010000	1.976528000	0.000192000

6	-2.363154000	-3.486601000	-0.000088000	6	-2.604601000	3.310937000	0.000125000
6	-3.362310000	-2.537491000	-0.000176000	6	-1.350627000	3.990161000	-0.000028000
6	-4.425864000	-3.568168000	0.000091000	6	-2.016161000	5.296392000	0.000111000
6	-3.337853000	-4.601677000	0.000030000	6	-3.335065000	4.582030000	-0.000099000
6	-3.269121000	-5.922498000	0.000361000	6	-4.608205000	4.980746000	-0.000198000
6	-5.748476000	-3.567632000	0.000046000	6	-1.654654000	6.580579000	0.000149000
6	-3.300010000	-1.145887000	-0.000217000	6	-0.052428000	3.537919000	-0.000089000
6	-3.120588000	0.053518000	-0.000172000	6	1.051492000	2.996679000	-0.000195000
6	-2.802658000	1.372939000	-0.000122000	6	2.197249000	2.293150000	-0.000422000
6	-2.416139000	2.522445000	-0.000128000	6	3.179277000	1.553425000	-0.000459000
1	7.734146000	-0.347706000	-0.000884000	1	-2.798116000	-7.222038000	-0.000259000
1	6.726868000	1.210315000	-0.000577000	1	-0.983105000	-6.823847000	-0.000292000
1	7.044679000	-3.211306000	0.000040000	1	-5.175315000	-5.762660000	-0.000410000
1	5.438659000	-4.140048000	0.000357000	1	-5.641565000	-3.963934000	-0.000286000
1	-2.314519000	-6.430277000	0.000351000	1	-5.418124000	4.263642000	-0.000235000
1	-4.167361000	-6.524391000	0.000641000	1	-4.855443000	6.034547000	-0.000280000
1	-6.303139000	-4.495770000	0.000214000	1	-2.402290000	7.363331000	0.000320000
1	-6.304980000	-2.640585000	-0.000079000	1	-0.611590000	6.867234000	0.000081000
1	-3.566436000	6.871599000	-0.000147000	1	7.653922000	1.187604000	-0.000060000
1	-4.411396000	5.219916000	-0.000465000	1	6.401689000	2.560396000	-0.000467000
1	0.866392000	6.779294000	0.000694000	1	6.253401000	-2.903932000	0.000210000
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3m (dianion)

CASSCF(12,12)/ma-def2-TZVPP

6	4.165653000	0.600275000	0.000726000
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6	6.518807000	-1.848152000	-0.000848000
6	3.078003000	-1.729336000	-0.000283000
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6	-0.231562000	-3.508015000	-0.000425000
6	-1.579388000	-3.891387000	-0.000311000

6	-2.767281000	-3.140931000	-0.000424000
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6	-2.002010000	-6.452466000	0.000405000
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6	3.166890000	1.559255000	0.000813000
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1	-0.981842000	-6.787313000	0.000506000
1	-5.187775000	-5.708090000	0.000415000
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1	-5.396591000	4.217602000	-0.000872000
1	-4.870393000	5.981597000	-0.000574000
1	-2.381718000	7.336847000	-0.000281000
1	-0.612051000	6.830329000	0.000379000
1	7.636241000	1.177050000	0.000072000
1	6.406985000	2.547130000	0.001055000
1	6.260045000	-2.890777000	-0.001514000
1	7.561492000	-1.589076000	-0.000969000

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