Supporting Information

Selective Terminal Heck Arylation of Vinyl Ethers with Aryl Chlorides: A Combined Experimental-Computational Approach Including Synthesis of Betaxolol

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EXPERIMENTAL

General Information and Materials

All microwave syntheses were carried out in a single-mode microwave cavity producing controlled irradiation at 2450 MHz. GC-MS analyses were performed with a CP-SIL 8 CB Low Bleed (30 m $\times$ 0.25 mm) or a CP-SIL 5 CB Low Bleed (30 m $\times$ 0.25 mm) capillary column using a 40-300 °C temperature gradient and EI ionization. RP-LC-MS analyses were performed using a Chromolith SpeedROD RP-18e column (50 $\times$ 4.6 mm) and a quadrupole mass spectrometer using a 4 mL/min CH₃CN/H₂O gradient (0.05% HCOOH) and detection by UV (DAD) and MS (ESI+). ¹H and ¹³C NMR spectra were recorded at 400 and 100 MHz, respectively using CDCl₃ as solvent. Chemical shifts for ¹H and ¹³C are referenced to TMS via the solvent signal. HRMS experiments were performed on a 7-tesla hybrid linear ion trap (LTQ) FT mass spectrometer modified with a nanoelectrospray ion source. Elemental analysis were performed for new compounds. Radial thin-layer chromatography were performed with a plate thickness of 2 mm, using Merck Silica gel 60 PF₂₅₄ containing gypsum and ethyl acetate/isohexane as eluent. Filtration of crude reaction mixtures were performed by pre-packed silica columns (Flash-Pack-Sil, 25 mL- 5 g). All reported yields were based on >95% pure products according to either GC-MS or LC-MS (TIC). The isolated yields of all Heck coupling products were calculated as an average of five separate reactions.

All Heck vinyl ether products were obtained as *E/Z* mixtures but enamide **5** was obtained as the pure *E*-product. The β/α ratios and conversions were determined from crude reaction mixtures by ¹H NMR and by GC-MS using adamantane or 2,3-dimethylnaphthalene as internal standard. Regioisomers were assumed to have the same GC-MS response factors. To obtain correct β/α ratios, GC-MS response factors were calculated also for the corresponding acetophenones (produced by hydrolysis of sensitive α -arylated vinyl ethers in the reaction mixture). In all cases, ¹H NMR analysis showed that the *Z*-isomer had shorter GC retention

time than the *E*-isomer. PEG 200 (methyl masked and unmasked) and PEG 2000 (methyl masked and unmasked) were commercially available from Acros and Aldrich respectively. Compounds **2b**¹, **3a**³, **3d**³, **3e**⁷, **3f**³, **3g**⁸, **3i**⁷, **3j**⁹, **5**¹⁰, **9**^{11,12} are known structures and spectroscopic data matched with referenced literatures. Products **3b**^{4,5}, **3c**^{4,6}, **3h**⁴, **8**^{11,12} are also known structures, although full characterization data were not provided in the referenced literature. All additional products, reactants and reagents used were commercially available.

General procedure for terminal arylation of electron-rich olefins (vinyl ethers **2a and **2b**) with aryl chlorides in DMF/Water (Method A):**

A thick wall glass vial (2-5 mL) with a Teflon coated stirring bar was charged with aryl chloride (**1a-i**) (1.00 mmol), butyl vinyl ether (**2a**) (300.0 mg, 388 μ L, 3.00 mmol) or (2-ethenyloxyethyl)dimethylamine (**2b**) (345.0 mg, 493 μ L, 3.00 mmol), Herrmann's palladacycle (trans-di-(μ -acetato)-bis[*o*-(di-*o*-tolylphosphino)benzyl]dipalladium(II)) (47.0 mg, 5.00 mol%), [(*t*-Bu)₃PH]BF₄ (29.0 mg, 10.00 mol%) and Cy₂NMe (645 μ L, 3.00 mmol). DMF/H₂O (2 mL/ 200 μ L) was thereafter added, followed by sealing of the vial under air. The vial was then heated to 160 °C by microwave irradiation for 60 min (ramp time approx. 40 s, hold time 3560 s). After cooling, the reaction mixture was filtered through a pre-packed silica column having glass wool and a celite bed on the top and the filtrate was concentrated *in vacuo*. The residue was taken in CH₂Cl₂ and partitioned between saturated NaHCO₃ solution and water respectively. Finally after separation, the organic phase was dried over K₂CO₃ and then evaporated to dryness. Chromatography of the crude product using radial thin-layer chromatography furnished pure **3a-i** and **3j** in good to moderate yield. All isolated products were >95% pure according to GC-MS.

General procedure for terminal arylation of electron-rich olefins (vinyl ethers **2a, **2b** and enamide **4**) with aryl chlorides in PEG (Method B):**

A thick wall glass vial (2-5 mL) with a Teflon coated stirring bar was charged with aryl chloride (**1a-i**) (1.00 mmol), butyl vinyl ether (**2a**) (300 mg, 388 μ L, 3.00 mmol) or (2-ethenyloxyethyl)dimethylamine (**2b**) (345.0 mg, 493 μ L, 3.00 mmol) or 1-vinyl-2-pyrrolidinone (**4**) (333.0 mg, 319 μ L, 3.00 mmol), Herrmann's palladacycle (trans-di-(μ -acetato)-bis[*o*-(di-*o*-tolylphosphino)benzyl]dipalladium(II)) (47.0 mg, 5.00 mol%), [(*t*-Bu)₃PH]BF₄ (29.0 mg, 10.00 mol%) and PMP (904 μ L, 5.00 mmol). PEG-200 (with free hydroxyl groups) (2 mL) was thereafter added, followed by sealing of the vial under air. The vial was then heated to 160 °C by microwave irradiation for 60 min (ramp time approx. 38 s, hold time 3562 s). After cooling, the reaction mixture was filtered through a pre-packed silica column having glass wool and a celite bed on the top and the filtrate was concentrated *in vacuo*. The residue was taken in CH₂Cl₂ and partitioned between saturated NaHCO₃ solution and water respectively. Finally after separation, the organic phase was dried over K₂CO₃ and then evaporated to dryness. Chromatography of this crude product using radial thin-layer chromatography furnished compound **3a-i**, **3j** and **5** in good to moderate yield. All isolated products were >95% pure according to GC-MS.

Synthesis of cyclopropylmethyl vinyl ether (2c**):**

Cyclopropylmethanol (7.54 g, 8.3 mL, 104.5 mmol), Pd(OAc)₂ (0.822 g, 3.66 mmol, 3.50 mol%) and 2,2'-bipyridyl (0.572 g, 3.66 mmol, 3.50 mol%) were placed in a 500 mL round bottomed flask and dissolved in ethyl vinyl ether (200 mL, 2090 mmol). The flask was pre-heated in a 50 °C oil-bath for 40 min, before refluxing the reaction for 72- 100 h. The cold reaction mixture was diluted with pentane (200 mL), washed with 0.1 M NaOH and water

and dried with K_2CO_3 overnight. The organic phase was thereafter distilled very slowly to obtain cyclopropylmethyl vinyl ether (**2c**). Product **2c** was obtained in 4.92 g (48%) as a colorless liquid with characteristic pungent smell, b.p. ~ 98 -100 $^{\circ}C$. 1H NMR (400 MHz, $CDCl_3$): δ 0.23-0.25 (m 2H), 0.53-0.55 (m, 2H) 1.08 - 1.11 (m, 1H) 3.51 (d, $J = 7.0$ Hz, 2H) 3.94 (dd, $J = 1.9, 6.7$ Hz, 1H) 4.12 (dd, $J = 1.9, 14.4$ Hz, 1H) 6.45 (dd, $J = 6.7, 14.3$ Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 2.9, 9.9, 72.7, 86.3, 151.8; EI-MS, m/z , (relative intensity, 70 eV) 99 ($M^+ + H$, 10), 81 (80), 55 (100). Elemental analysis: Calculated, C 73.43%; H 10.27%. Found, C 73.20%; H 10.39%.

Synthesis of *E/Z*-1-(2- cyclopropylmethoxyethenyl)-4-nitrobenzene (**6**):

A thick wall glass vial (2-5 mL) with a Teflon coated stirring bar was charged with 4-chloro nitrobenzene (**1a**) (157.0 mg, 1.00 mmol), cyclopropylmethyl vinyl ether (**2c**) (196.0 mg, 2.00 mmol), Herrmann's palladacycle (47.0 mg, 5.00 mol%), $[(t-Bu)_3PH]BF_4$ (29.0 mg, 10.00 mol%) and Cy_2NMe (645 μL , 3.00 mmol). DMF/ H_2O (2 mL/200 μL) was thereafter added, followed by rapid sealing of the vial under air. The vial was then heated to 160 $^{\circ}C$ by microwave irradiation for 60 min (ramp time approx. 40 s, hold time 3560 s). After cooling, the reaction mixture was filtered through a pre-packed silica column having glass wool and a celite bed on the top and the filtrate was concentrated *in vacuo*. The crude reaction mixture was taken in CH_2Cl_2 and partitioned between saturated $NaHCO_3$ solution and water respectively. Finally, the organic phase was dried over K_2CO_3 and then evaporated to dryness. Chromatography of the crude product was performed using radial thin-layer chromatography. The isolated yield of **6** was 60% (132.0 mg) and the product was obtained as an *E/Z*-mixture

(7:2) in the form of a yellow sticky liquid (R_f (TLC) = 0.32 (ethyl acetate/isohexane = 5/95)). ^1H NMR (400 MHz, CDCl_3): δ 0.31-0.35 (m, 2H) 0.62-0.67 (m, 2H) 1.18-1.25 (m, 1H) 3.74 (d, J = 7.4 Hz, 1.6H, *E*) 3.85 (d, J = 7.0 Hz, 0.4H, *Z*) 5.29 (d, J = 7.0 Hz, 0.2H, *Z*) 5.86 (d, J = 13.2 Hz, 0.8H, *E*) 6.45 (d, J = 7.0 Hz, 0.2H, *Z*) 7.21 (d, J = 13.2 Hz, 0.8H, *E*) 7.30-8.15 (m, 4H, aryl); ^{13}C NMR (100 MHz, CDCl_3): δ 3.1, 3.2, 10.2, 10.8, 75.5, 78.8, 103.8, 104.6, 123.6, 124.2, 124.9, 128.3, 143.1, 143.9, 145.3, 150.5, 151.6; EI-MS, m/z , (relative intensity, 70 eV) 219 (M^+ , 20), 165 (7), 148 (7.5), 118 (5), 89 (22), 55 (100). Elemental analysis: Calculated, C 65.74%; H 5.98%; N 6.39%. Found, C 65.74%; H 6.05%; N 6.49%.

Synthesis of *para*-[2-(cyclopropylmethoxy)ethyl] aniline (**7**):

A thick wall glass vial (2-5 mL) with a Teflon coated stirring bar was charged with *E*-/*Z*-1-(2-cyclopropylmethoxyethenyl)-4-nitrobenzene (**6**) (132.0 mg, 0.60 mmol), Pd/C (10%) (65.0 mg, 60 μmol) and ammonium formate (378.0 mg, 6.00 mmol). EtOH (2.5 mL) was thereafter added followed by sealing under air. The vial was then heated to 80 °C by microwave irradiation for 40 min (ramp time approx. 16 s, hold time 2384 s). (Occasionally, sublimation of ammonium formate inhibited full conversion. Extra ammonium formate addition and subsequent heating provided full conversion). Purification following the same procedure as for **6** furnished desired **7** in 79% (91.0 mg) yield as a sticky oil. ^1H NMR (400 MHz, CDCl_3): δ 0.18–0.21 (m, 2H) 0.50-0.54 (m, 2H) 1.01-1.13 (m, 1H) 1.56 (bs, 2H), 2.79 (t, J = 7.6 Hz, 2H) 3.28 (d, J = 6.9 Hz, 2H) 3.59 (t, J = 7.6 Hz, 2H) 6.61-6.64 (m, 2H) 7.0-7.02 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 2.9, 10.6, 35.5, 72.1, 75.6, 115.2, 128.9, 129.7, 144.5; EI-MS, m/z , (relative intensity, 70 eV) 191 (M^+ , 30), 120 (6), 106 (100), 77 (5). Elemental analysis: Calculated, C 75.35%; H 8.96%; N 7.32%. Found, C 75.12%; H 8.85%; N 7.15%.

Direct synthesis of 7 from 2c and 1a: A thick wall glass vial (2-5 mL) with a Teflon coated stirring bar was charged with 4-chloro nitrobenzene (**1a**) (157.0 mg, 1.00 mmol), cyclopropylmethyl vinyl ether (**2c**) (294.0 mg, 3.00 mmol), Herrmann's palladacycle (47.0 mg, 5.00 mol%), [(*t*-Bu)₃PH]BF₄ (29.0 mg, 10.00 mol%) and Cy₂NMe (645 μ L, 3.00 mmol). DMF/H₂O (2 mL/200 μ L) was thereafter added, followed by rapid sealing of the vial under air. The vial was then heated to 160 °C by microwave irradiation for 60 min (ramp time approx. 40 s, hold time 3560 s). The reaction mixture was concentrated *in vacuo*. The crude reaction mixture was dissolved in ethanol (2.5 mL) before Pd/C (10%) (65.0 mg, 60 μ mol) and ammonium formate (378.0 mg, 6.00 mmol) were added followed by sealing under air. The vial was then heated to 80 °C by microwave irradiation for 2400 s (ramp time approx. 16 s, hold time 2384 s). (Occasionally, sublimation of ammonium formate inhibited full conversion. Extra ammonium formate addition and subsequent heating provided full conversion). Purification following the same procedure as before furnished desired **7** in 55% (91.0 mg) direct yield from **1a** as a sticky oil.

Synthesis of *para*-[2-(cyclopropylmethoxy)ethyl] phenol (8**)^{11,12}:**

p-[2-(Cyclopropylmethoxy)ethyl] aniline (**7**) (91.0 mg, 0.48 mmol) was dissolved in 1 mL of 30% (aq) H₂SO₄ and transferred into a round bottomed flask. The solution was cooled below 0 °C and sodium nitrite (54.0 mg, 0.78 mmol) in 400 μ L of water was added slowly dropwise. The reaction temperature was not allowed to exceed +5 °C. After complete addition and stirring for another 15 min, a solution of urea (20.0 mg in 200 μ L of water) was added and the reaction mixture was stirred for another 5 min. Hot water (5 mL, 90-95 °C) was then poured into the reaction mixture under vigorous stirring. After reflux for 1 h, the reaction mixture was

allowed to cool and dichloromethane was added. Extraction of the aqueous phase and concentration of combined organic solutions provided the crude product. Chromatography of the crude product was performed using radial thin-layer chromatography and furnished 50% (46.0 mg) of pure **8** as a brownish liquid. R_f (TLC) = 0.53 (acetone/chloroform = 5/95). ^{13}C NMR (100 MHz, CDCl_3): 2.9, 10.6, 35.5, 71.8, 75.6, 115.2, 130.0, 131.2, 153.9; EI-MS, m/z , (relative intensity, 70 eV) 192 (M^+ , 42.5), 120 (20), 107 (100), 77 (15), 55 (25). High Resolution MS calculated for $\text{C}_{12}\text{H}_{16}\text{O}_2$: $[\text{M}+\text{H}]^+$ 193.1228, Found 193.1222.

Synthesis of (S)- (-)-3-[4-[2-(cyclopropylmethoxy)]ethyl]phenoxy-1-(N-isopropylamino)-propan-2-ol $\times$ HCl (Betaxolol) (9**):**

p-[2-(Cyclopropylmethoxy)ethyl] phenol (**8**) (46.0 mg, 0.24 mmol) and NaOH (19.0 mg, 0.48 mmol) was dissolved in 4.0 mL of ethanol. (*R*)-3-Isopropylamino-1,2-epoxypropane (prepared as described in literature²) (274.0 mg, 2.40 mmol in 2 mL of ethanol) was added to the reaction and the mixture was thereafter refluxed for 8 h. The reaction mixture was concentrated *in vacuo*, the residue was dissolved in minimum volume of chloroform, washed with water and the organic phase was dried over Na_2SO_4 (S). To this chloroform solution, double amount of Et_2O was added and dry HCl gas passed. The solid precipitated was filtered off and after recrystallisation (EtOH , EtOAc), pure (*S*)-**9** was obtained as an off white HCl salt. The isolated yield of **9** $\times$ HCl was 60 % (51.0 mg). R_f (TLC) = 0.25 (methanol), mp 95-96 $^\circ\text{C}$, $[\alpha]_D^{24} = -14.8^\circ$ (c 2.5, CH_3OH).

Spectroscopic and analytical data for compounds **3b^{4,5}, **3c**^{4,6} and **3h**⁴:**

3b (*E* + *Z*) (*E/Z* = 6/4): ¹³C NMR (100 MHz, CDCl₃): 13.8, 19.0, 19.1, 31.3, 31.9, 70.1, 73.9, 104.1, 104.6, 124.8, 124.8, 124.9, 125.0, 125.1, 125.4, 125.5, 125.6, 125.7, 128.0, 140.4, 140.5, 148.9, 150.0; EI-MS, *m/z*, (relative intensity, 70 eV) 244 (*M*⁺, 100), 188 (22.5), 159 (14), 119 (11), 91 (8); High Resolution MS calculated for C₁₃H₁₅OF₃ : [*M*+H]⁺ 245.1153, Found 245.1145.

3c (*E* + *Z*) (*E/Z* = 2/1): ¹³C NMR (100 MHz, CDCl₃): 12.7, 18.0, 18.1, 30.3, 30.9, 69.3, 73.1, 103.4, 104.1, 124.0, 127.3, 128.9, 129.3, 132.5, 132.7, 141.7, 142.5, 148.9, 150.1, 190.5, 190.8; EI-MS, *m/z*, (relative intensity, 70 eV) 204 (*M*⁺, 100), 148 (82.5), 119 (20), 91 (47.5), 65 (12.5); High Resolution MS calculated for C₁₃H₁₆O₂ : [*M*+H]⁺ 205.1229, Found 205.1232.

3h (*E* + *Z*) (*E/Z* = 4/3): ¹³C NMR (100 MHz, CDCl₃): 13.8, 13.9, 19.1, 19.2, 20.1, 20.2, 31.4, 31.9, 69.9, 73.3, 102.0, 103.9, 124.6, 125.6, 125.7, 125.8, 126.0, 128.8, 129.8, 130.1, 134.3, 134.6, 134.7, 135.3, 146.7, 148.6; EI-MS, *m/z*, (relative intensity, 70 eV) 190 (*M*⁺, 100), 134 (8), 106 (30); High Resolution MS calculated for C₁₃H₁₈O : [*M*+H]⁺ 191.1436, Found 191.1430.

Computational details:

Geometries and energies of all intermediates and transition states were fully optimized using the gradient-corrected hybrid density functional method B3LYP.¹³ We used a basis set of double- ζ valence quality labeled LANL2DZ in the Gaussian98 program.¹⁴ For Pd the core electrons were replaced by a relativistic electron core potential (ECP) developed by Hay and Wadt.¹⁵ For non-metal atoms the double- ζ basis sets of Huzinaga and Dunning were assigned.¹⁶ All relative energies were recalculated using a valence triple- ζ quality basis set at the B3LYP level. For all non metal atoms the 6-311G(d,p) basis set¹⁷ was employed and for Pd the primitive LANL2DZ basis set was recontracted to 4s4p3d and an f-function(1.472)

was added. The atomic charges were calculated using the Merz-Singh-Kollman scheme as implemented in Gaussian98.¹⁸

Appendix

GC-MS chromatogram compound 2c

GC-MS chromatogram compound 6

GC-MS chromatogram compound 7

GC-MS chromatogram compound 8

^{13}C NMR compound 8

**LC-UV-Chromatogram ($\lambda=254$)
Compound 9**

LC-MS (TIC) compound 9

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GC-MS chromatogram compound 3a

¹³C NMR compound 3a

GC-MS chromatogram compound 3b

¹³C NMR compound 3b

GC-MS chromatogram compound 3c

¹³C NMR compound 3c

GC-MS chromatogram compound 3d

GC-MS chromatogram compound 3e

GC-MS chromatogram compound 3f

¹³C NMR compound 3f

GC-MS chromatogram compound 3g

GC-MS chromatogram compound 3h

¹³C NMR compound 3h

GC-MS chromatogram compound 3i

GC-MS chromatogram compound 2b

GC-MS chromatogram compound 3j

GC-MS chromatogram compound (E)-5

^{13}C NMR compound (E)-5

Temperature and pressure profile of a microwave model reaction using Method A (Entry 4, Table 1)

Computational data for calculations:

Optimized structures

pd_clet_ph3_hx

46	-0.764818	-0.333398	-0.018017
6	1.218753	-0.061983	-0.001051
15	-1.200656	1.944304	0.086358
17	-3.115411	-0.951671	-0.038618
6	1.922705	-0.172023	1.218934
6	3.330805	-0.263152	1.209692
6	4.036721	-0.214049	-0.008655
6	1.926104	0.019022	-1.220776
6	3.334319	-0.072897	-1.221476
1	1.389835	-0.204921	2.16807
1	3.869684	-0.367722	2.149099
1	5.122148	-0.279144	-0.012344
1	1.396492	0.133938	-2.165234
1	3.875721	-0.030402	-2.164246
1	-1.914301	2.356373	1.248475
1	-0.147942	2.905518	0.052202
1	-2.054601	2.427012	-0.946117

pd_clet_ph3_h_pix

46	0.577359	-0.409463	-0.210561
6	0.597199	1.28762	-1.718302
6	1.273204	1.898672	-0.673322

6	-1.429748	-0.135138	-0.102759
15	0.422606	-2.437882	1.069164
17	3.043619	-0.826597	-0.230631
1	1.177677	0.75033	-2.463286
1	2.330989	1.6997	-0.495098
1	-0.415193	1.586931	-1.964744
8	0.676497	2.864006	0.09648
6	-1.980751	0.753717	0.846687
6	-3.378149	0.937824	0.927203
6	-4.238956	0.240854	0.057287
6	-2.298077	-0.832506	-0.973878
6	-3.694388	-0.641622	-0.896067
1	-1.332567	1.314692	1.516581
1	-3.788372	1.626056	1.664237
1	-5.315297	0.384911	0.119248
1	-1.897551	-1.518858	-1.718081
1	-4.349912	-1.181655	-1.576976
6	1.405428	3.27531	1.305515
1	0.844305	4.116203	1.715623
1	1.437546	2.448896	2.025336
1	2.425389	3.589889	1.050696
1	1.001127	-2.381832	2.372882
1	-0.833616	-3.045493	1.381418
1	1.129762	-3.55455	0.535229

pd_clet_ph3_h_tsax

Pd	-0.994883	-0.167619	0.044607
P	-1.692332	2.215906	-0.17819
Cl	-3.380922	-0.662707	-0.10034
C	1.112792	0.171202	0.162089
C	1.688801	0.465598	-1.098578
C	2.675726	1.46341	-1.218915
C	3.126006	2.154461	-0.07454
C	2.590153	1.839417	1.191947
C	1.595936	0.848459	1.309292
H	1.367612	-0.09078	-1.97648
H	3.094008	1.696865	-2.195624
H	3.892881	2.920215	-0.16641
H	2.943856	2.361057	2.078774
H	1.185822	0.614854	2.291069
C	0.875375	-1.908837	0.466945
C	-0.521316	-2.182396	0.264501
H	-1.115164	-2.437724	1.141984
H	1.252923	-1.840626	1.490229
O	1.759626	-2.448178	-0.455569
H	-0.802161	-2.69436	-0.654109
H	-0.822709	3.358586	-0.253252
H	-2.569517	2.688449	0.848583
H	-2.520121	2.50149	-1.308097
C	3.1929	-2.323427	-0.167802
H	3.691545	-2.972612	-0.889568

H	3.409794	-2.662275	0.854432
H	3.521246	-1.287112	-0.299901

pd_clet_ph3_h_tsbx

Pd	-0.519856	0.323498	-0.178694
P	0.182511	2.621851	0.499995
Cl	-2.821953	1.210699	-0.067529
C	1.428204	-0.516413	-0.249579
C	2.377603	0.017729	-1.154758
C	3.741639	0.073174	-0.802614
C	4.175578	-0.427725	0.443067
C	3.236454	-0.986594	1.334579
C	1.87397	-1.042558	0.988598
H	2.056212	0.399135	-2.122118
H	4.460962	0.499856	-1.499181
H	5.22973	-0.392763	0.708025
H	3.565935	-1.386749	2.290935
H	1.160132	-1.498577	1.670266
C	0.065801	-1.745953	-1.20235
C	-1.277438	-1.615211	-0.722395
O	-1.622027	-2.417771	0.364378
H	0.63604	-2.593219	-0.835263
H	0.24698	-1.482356	-2.241041
H	-2.091145	-1.294859	-1.375137
H	1.534642	3.033895	0.762475
H	-0.436022	3.142311	1.679319

H	-0.184526	3.666137	-0.40674
C	-2.980156	-2.240696	0.902116
H	-3.119083	-1.210112	1.243233
H	-3.05867	-2.950534	1.727867
H	-3.726004	-2.475044	0.130341

pd_clet_ph3_omex

46	1.446856	-0.337328	0.036417
6	-0.523796	0.011733	0.099414
15	1.952252	1.899177	-0.282857
17	3.773182	-1.038557	-0.005242
6	-1.302195	-0.175773	-1.060866
6	-2.711638	-0.213253	-0.984941
6	-3.344349	-0.025662	0.261369
6	-1.172191	0.238064	1.338217
6	-2.573037	0.204675	1.421518
1	-0.82658	-0.315771	-2.030479
1	-3.28783	-0.384479	-1.889143
8	-4.72692	-0.039116	0.455433
1	-0.594247	0.415613	2.243401
1	-3.086696	0.351252	2.367258
1	2.643593	2.183037	-1.495488
1	0.929269	2.892187	-0.306308
1	2.849305	2.443075	0.679878
6	-5.592338	-0.293364	-0.688162
1	-6.60837	-0.277214	-0.289261

1	-5.483594	0.488379	-1.453029
1	-5.385483	-1.276783	-1.132802

pd_clet_ph3_ome_pix

Pd	-1.203019	-0.371178	0.198677
C	-1.107306	1.275579	1.753213
C	-1.685471	1.967203	0.699869
C	0.827504	-0.313634	0.191534
P	-1.181732	-2.385732	-1.114585
Cl	-3.697595	-0.531868	0.0586
H	-1.760488	0.786233	2.470636
H	-2.752169	1.882476	0.488421
H	-0.079186	1.469323	2.036162
O	-0.97192	2.883099	-0.032817
C	1.521421	0.544543	-0.681968
C	2.934514	0.593595	-0.69209
C	3.664026	-0.22494	0.192057
C	1.578307	-1.130075	1.072016
C	2.982512	-1.085895	1.077246
H	0.977002	1.202426	-1.355881
H	3.437365	1.270509	-1.377151
O	5.062707	-0.259983	0.273442
H	1.075769	-1.797225	1.769915
H	3.56527	-1.702884	1.75578
C	-1.61528	3.371654	-1.261333
H	-0.969865	4.167366	-1.636131

H	-1.689708	2.560371	-1.995112
H	-2.614415	3.768199	-1.04071
H	-1.585475	-2.236829	-2.476527
H	0.005814	-3.161138	-1.297963
H	-2.095344	-3.401101	-0.704247
C	5.827833	0.6102	-0.605608
H	6.875159	0.416206	-0.364729
H	5.643451	0.374804	-1.663763
H	5.596135	1.668885	-0.419872

pd_clet_ph3_ome_tsax

Pd	-1.49972	-0.13472	-0.072567
P	-1.187119	-2.581267	0.266154
Cl	-3.889811	-0.643981	0.013731
C	0.558033	0.400525	-0.120385
C	1.166062	0.395884	1.163601
C	2.474859	-0.070093	1.343364
C	3.224324	-0.512087	0.227699
C	2.656929	-0.477337	-1.065928
C	1.334597	-0.016778	-1.224984
H	0.608586	0.765826	2.021101
H	2.940243	-0.097248	2.324657
O	4.51767	-0.946698	0.511248
H	3.221785	-0.798739	-1.935921
H	0.905302	-0.000643	-2.225681
C	-0.487103	2.226878	-0.500322

C	-1.875516	1.898313	-0.355616
H	-2.478007	1.86491	-1.262997
H	-0.06326	2.297502	-1.504263
O	0.061432	3.087234	0.4361
H	-2.388928	2.259522	0.53355
H	0.068336	-3.28172	0.317831
H	-1.859095	-3.421384	-0.675776
H	-1.767384	-3.104328	1.464384
C	1.433764	3.551365	0.199456
H	1.60718	4.334998	0.938987
H	1.527908	3.964306	-0.814158
H	2.144568	2.731151	0.342939
C	5.358812	-1.421127	-0.580848
H	6.301385	-1.709339	-0.111861
H	4.910784	-2.29245	-1.077914
H	5.539895	-0.6261	-1.317523

pd_clet_ph3_ome_tsbx

Pd	1.1187	0.308169	0.146135
P	0.536961	2.650832	-0.498826
Cl	3.456738	1.035761	-0.205233
C	-0.856511	-0.368704	0.47825
C	-1.653897	0.220884	1.486731
C	-3.038963	0.354373	1.319592
C	-3.653218	-0.117066	0.136023
C	-2.874761	-0.730201	-0.870268

C	-1.486328	-0.868569	-0.678755
H	-1.200113	0.586368	2.404929
H	-3.664475	0.811473	2.081696
O	-5.041598	0.075182	0.062071
H	-3.329644	-1.098015	-1.785665
H	-0.898746	-1.365692	-1.44623
C	0.538402	-1.66678	1.338652
C	1.81596	-1.648188	0.698626
O	1.974359	-2.50674	-0.393286
H	-0.131455	-2.478849	1.07988
H	0.498186	-1.340573	2.372739
H	2.72665	-1.358555	1.224331
H	-0.78718	3.179464	-0.687018
H	1.127671	3.116145	-1.714753
H	1.045467	3.66064	0.377683
C	3.295407	-2.485333	-1.042137
H	3.448493	-1.526201	-1.545135
H	3.28019	-3.314132	-1.751936
H	4.086579	-2.637969	-0.296544
C	-5.76297	-0.455691	-1.088069
H	-6.813861	-0.233448	-0.892506
H	-5.445634	0.038779	-2.017016
H	-5.62206	-1.541481	-1.177442

pd_clet_ph3_antx

46	-1.384221	0.132483	-0.33339
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6	0.506538	0.748943	-0.055716
15	-1.699416	-0.224163	1.934532
17	-3.648554	-0.508522	-0.926078
6	0.724427	2.124736	-0.012085
6	2.053835	2.649851	-0.051016
6	3.144381	1.792269	-0.088826
6	1.616561	-0.167265	-0.074273
6	2.95873	0.37347	-0.096976
1	-0.112974	2.819147	0.038488
1	2.199375	3.72748	-0.043013
1	4.157033	2.189881	-0.107893
6	1.455105	-1.590483	-0.085701
6	4.070951	-0.527255	-0.126312
1	-2.730571	0.567402	2.515983
1	-0.63547	-0.028097	2.86243
1	-2.132726	-1.537297	2.275436
6	2.555034	-2.438386	-0.107938
6	3.877388	-1.902029	-0.129158
1	5.077517	-0.1136	-0.148442
1	4.730146	-2.575943	-0.152813
1	2.412528	-3.516053	-0.118777
1	0.448224	-2.002948	-0.092104
pd_clet_ph3_ant_pix			
Pd	-0.975017	-0.462252	-0.026623
C	-1.172456	0.728401	-1.94355

C	-2.236117	1.258522	-1.228259
C	0.753022	0.557763	0.304347
P	-0.504845	-1.941648	1.809837
Cl	-3.08455	-1.776818	-0.297706
H	-1.359924	-0.132675	-2.579598
H	-3.1851	0.72501	-1.158807
H	-0.280994	1.319187	-2.121168
O	-2.18264	2.517495	-0.689983
C	0.712779	1.771825	0.9841
C	1.911324	2.500042	1.262082
C	3.144119	2.008394	0.857342
C	2.017813	0.030301	-0.137878
C	3.229119	0.768939	0.148524
H	-0.237214	2.193004	1.303649
H	1.845199	3.446104	1.795077
H	4.058397	2.559138	1.069575
C	2.132787	-1.202172	-0.86179
C	4.487589	0.242377	-0.287274
C	-3.278018	2.884183	0.220667
H	-3.126654	3.939008	0.453596
H	-3.227259	2.279245	1.133567
H	-4.248896	2.741206	-0.269948
H	-1.460873	-1.918301	2.868634
H	0.708867	-1.85628	2.560661
H	-0.519562	-3.333943	1.499941

C	3.368406	-1.688098	-1.27179
C	4.560605	-0.959021	-0.979703
H	5.392752	0.805468	-0.066232
H	5.52219	-1.347795	-1.306502
H	3.431849	-2.623122	-1.823427
H	1.223308	-1.749751	-1.101969

pd_clet_ph3_ant_tsax

Pd	-1.3106	-0.41599	-0.43945
P	-2.03036	1.96526	-0.60237
Cl	-3.68962	-0.94278	-0.61644
C	0.79214	-0.06968	-0.28764
C	1.36744	0.20128	-1.53392
C	2.3828	1.19083	-1.68019
C	2.86163	1.87115	-0.56592
C	2.33685	1.59834	0.73784
C	1.28025	0.6237	0.88169
H	1.04831	-0.36691	-2.40462
H	2.78702	1.40146	-2.6673
H	3.64736	2.61702	-0.67114
C	0.59084	-2.13733	-0.01547
C	-0.8051	-2.42238	-0.22915
H	-1.40079	-2.692	0.64318
H	0.96604	-2.07398	1.0092
O	1.47477	-2.68346	-0.93533
H	-1.06905	-2.94163	-1.14841

H	-1.16952	3.11568	-0.6489
H	-2.91382	2.40762	0.43193
H	-2.85608	2.27021	-1.72904
C	2.90835	-2.55457	-0.65403
H	3.40385	-3.22773	-1.35595
H	3.12745	-2.86039	0.37795
H	3.24063	-1.52434	-0.81956
C	0.74561	0.38991	2.187
C	2.82445	2.28017	1.89818
C	1.24133	1.06279	3.29813
C	2.29352	2.01651	3.15453
H	-0.0805	-0.3084	2.29836
H	0.82181	0.87121	4.28268
H	2.67089	2.53764	4.03095
H	3.6197	3.0141	1.78052

pd_clet_ph3_ant_tsbx

Pd	-0.85259	0.55984	-0.56861
P	-0.14536	2.78218	0.32452
Cl	-3.10753	1.56706	-0.68904
C	1.09524	-0.29946	-0.5923
C	1.97595	0.20591	-1.55479
C	3.36854	0.33215	-1.28184
C	3.88548	-0.07755	-0.05987
C	3.03011	-0.64112	0.93814
C	1.61415	-0.76975	0.67348

H	1.59686	0.52288	-2.52408
H	4.02245	0.74889	-2.04414
H	4.94924	0.01372	0.14827
C	-0.27675	-1.56908	-1.47771
C	-1.6576	-1.34428	-1.17167
O	-2.18168	-2.06234	-0.09649
H	0.20669	-2.40207	-0.97417
H	0.02626	-1.40328	-2.5068
H	-2.36501	-1.01754	-1.9348
H	1.19535	3.13844	0.69999
H	-0.82587	3.22231	1.50278
H	-0.43879	3.89943	-0.51891
C	-3.59947	-1.82659	0.22524
H	-3.75743	-0.77231	0.4719
H	-3.81274	-2.47647	1.07623
H	-4.22937	-2.10634	-0.62987
C	0.78151	-1.36191	1.67698
C	3.54719	-1.09004	2.19452
C	1.31804	-1.79822	2.8835
C	2.71274	-1.65642	3.14853
H	-0.28122	-1.47725	1.47924
H	0.67189	-2.25113	3.63141
H	3.11736	-1.99861	4.09796
H	4.61292	-0.98559	2.38808

pd_clet_ph3_no2x

46	-1.664595	-0.353282	-0.051153
6	0.316414	-0.050823	-0.016273
15	-2.171768	1.892988	0.24091
17	-4.009735	-0.936636	-0.105398
6	1.024476	-0.226903	1.198053
6	2.429575	-0.245548	1.207858
6	3.114606	-0.062882	-0.006854
6	1.033676	0.152645	-1.22015
6	2.438977	0.136287	-1.224097
1	0.488983	-0.363624	2.135167
1	2.990606	-0.393954	2.124177
7	4.589504	-0.072206	-0.003093
1	0.505692	0.306691	-2.158627
1	3.007042	0.273715	-2.137823
1	-2.820809	2.18559	1.472756
1	-1.140622	2.875646	0.21193
1	-3.09804	2.405012	-0.708961
8	5.190064	-0.249788	1.113882
8	5.198394	0.097121	-1.116014

pd_clet_ph3_no2_pix

Pd	1.359534	-0.411827	-0.196989
C	1.308353	1.23907	-1.751783
C	1.945857	1.929919	-0.730847
C	-0.655907	-0.246313	-0.120277

P	1.337911	-2.381935	1.184144
Cl	3.833491	-0.684214	-0.196856
H	1.925077	0.710135	-2.473672
H	3.011538	1.793062	-0.543002
H	0.287778	1.48263	-2.024293
O	1.294106	2.880353	0.006442
C	-1.268776	0.762547	0.66133
C	-2.667202	0.883053	0.718436
C	-3.455856	-0.016599	-0.020879
C	-1.480462	-1.135817	-0.854407
C	-2.880113	-1.02613	-0.813441
H	-0.659151	1.471383	1.214429
H	-3.147352	1.652957	1.312665
N	-4.919984	0.101758	0.03486
H	-1.035397	-1.9129	-1.471738
H	-3.520619	-1.697383	-1.375304
C	2.018403	3.42149	1.169839
H	1.391444	4.22543	1.557224
H	2.150742	2.638929	1.92595
H	2.993369	3.817433	0.86142
H	1.943431	-2.231289	2.466875
H	0.119367	-3.033735	1.551741
H	2.088816	-3.482098	0.676956
O	-5.429102	1.021234	0.767547
O	-5.623948	-0.740274	-0.627141

pd_clet_ph3_no2_tsax

Pd	1.638119	-0.187583	0.053297
P	1.114491	-2.613246	-0.258279
Cl	3.959625	-0.877311	-0.142523
C	-0.372278	0.544528	0.218332
C	-1.053195	0.55482	-1.026124
C	-2.378794	0.104783	-1.125214
C	-3.032112	-0.325261	0.0461
C	-2.403336	-0.30622	1.305395
C	-1.077281	0.144526	1.383155
H	-0.539819	0.920796	-1.911542
H	-2.905387	0.079414	-2.07379
N	-4.424401	-0.800885	-0.045203
H	-2.948701	-0.636057	2.182278
H	-0.579705	0.16455	2.350544
C	0.818688	2.218534	0.482564
C	2.189229	1.793115	0.324081
H	2.806092	1.73751	1.220755
H	0.441095	2.381962	1.496045
O	0.338868	3.10062	-0.476906
H	2.705332	2.119365	-0.576754
H	-0.187483	-3.222313	-0.25851
H	1.766981	-3.490857	0.662217
H	1.61149	-3.16829	-1.477329

C	-0.955349	3.746204	-0.22784
H	-1.012063	4.561767	-0.950395
H	-0.996507	4.146555	0.79386
H	-1.778876	3.042265	-0.39159
O	-4.99848	-0.760308	-1.190096
O	-4.99158	-1.232669	1.018668

pd_clet_ph3_no2_tsbx

Pd	1.286928	0.319396	0.183888
P	0.6186	2.592123	-0.591125
Cl	3.594938	1.152145	-0.022394
C	-0.662066	-0.480454	0.407036
C	-1.509848	0.060285	1.411778
C	-2.888586	0.188389	1.196209
C	-3.42944	-0.25274	-0.026897
C	-2.621485	-0.817415	-1.035079
C	-1.24473	-0.940549	-0.807952
H	-1.085358	0.392778	2.355826
H	-3.54397	0.614599	1.947378
N	-4.876755	-0.136886	-0.248464
H	-3.076986	-1.153568	-1.96081
H	-0.614654	-1.395739	-1.567898
C	0.697626	-1.761953	1.182781
C	2.039395	-1.638926	0.682644
O	2.347589	-2.404125	-0.431908
H	0.123045	-2.594066	0.784443

H	0.554415	-1.568301	2.242425
H	2.865609	-1.345753	1.33178
H	-0.730331	3.039344	-0.802721
H	1.181467	2.978099	-1.846306
H	1.093262	3.678809	0.206522
C	3.706705	-2.265778	-0.98513
H	3.869116	-1.237521	-1.321302
H	3.750564	-2.973794	-1.814488
H	4.451551	-2.527727	-0.222293
O	-5.600751	0.36817	0.682109
O	-5.349025	-0.545874	-1.369816

pd_clet_ph3_chox

46	1.367837	-0.358077	-0.037525
6	-0.608641	-0.062957	0.080253
15	1.901765	1.889928	0.148398
17	3.72627	-0.907219	-0.191303
6	-1.366975	0.125662	-1.103105
6	-2.769574	0.093159	-1.054759
6	-3.432908	-0.104355	0.180045
6	-1.270629	-0.233907	1.318429
6	-2.676707	-0.268612	1.362438
1	-0.868332	0.281905	-2.057854
1	-3.367543	0.220431	-1.953904
1	-0.70249	-0.354313	2.238816

1	-3.186682	-0.418194	2.313477
1	2.645996	2.402253	-0.950203
1	0.877286	2.871008	0.289536
1	2.752875	2.195875	1.245972
6	-4.912192	-0.131067	0.250422
8	-5.673556	0.017409	-0.729861
1	-5.330503	-0.300438	1.263049

pd_clet_ph3_cho_pix

Pd	1.1257	-0.384139	-0.199377
C	1.069318	1.289698	-1.723696
C	1.643294	1.978214	-0.66481
C	-0.896641	-0.297673	-0.17154
P	1.151952	-2.353248	1.184243
Cl	3.609202	-0.606244	-0.186655
H	1.729969	0.797922	-2.432679
H	2.705099	1.876024	-0.438303
H	0.050724	1.503364	-2.027488
O	0.929642	2.892427	0.063918
C	-1.574892	0.656663	0.629544
C	-2.977044	0.710107	0.64731
C	-3.733947	-0.186584	-0.14484
C	-1.658388	-1.192034	-0.962784
C	-3.064109	-1.132359	-0.952543
H	-1.006045	1.367299	1.223447
H	-3.503907	1.437441	1.260298

H	-1.162681	-1.927218	-1.59403
H	-3.64156	-1.819994	-1.569602
C	1.58422	3.429101	1.269465
H	0.918892	4.20986	1.640127
H	1.699396	2.636167	2.017508
H	2.562446	3.854549	1.015263
H	1.862387	-2.224086	2.414332
H	-0.048258	-2.979566	1.647183
H	1.830333	-3.475842	0.623706
C	-5.210838	-0.14523	-0.139983
O	-5.904517	0.637887	0.547598
H	-5.70154	-0.882572	-0.807786

pd_clet_ph3_cho_tsax

Pd	-1.436433	-0.134379	-0.092296
P	-1.108395	-2.575511	0.317746
Cl	-3.814498	-0.63966	0.013259
C	0.631919	0.431489	-0.15412
C	1.234731	0.368211	1.128388
C	2.528301	-0.156786	1.281607
C	3.260885	-0.586308	0.150133
C	2.683172	-0.484831	-1.139679
C	1.385916	0.025083	-1.287108
H	0.688531	0.737819	1.993231
H	2.974901	-0.22857	2.272618
C	4.628104	-1.126863	0.328592

H	3.265479	-0.809916	-1.998336
H	0.947071	0.096269	-2.280532
C	-0.419039	2.213428	-0.457431
C	-1.8184	1.892352	-0.343613
H	-2.40479	1.89046	-1.261664
H	-0.000999	2.338533	-1.459641
O	0.112584	3.051889	0.511272
H	-2.344107	2.240199	0.544036
H	0.149813	-3.270608	0.367604
H	-1.813462	-3.460518	-0.55298
H	-1.643093	-3.026642	1.565798
C	1.46923	3.564658	0.280782
H	1.61422	4.349566	1.024623
H	1.55234	3.986427	-0.729947
H	2.210237	2.77027	0.420147
O	5.370789	-1.499164	-0.605683
H	4.976266	-1.189339	1.379037

pd_clet_ph3_cho_tsbx

Pd	1.049876	0.319068	0.177102
P	0.405807	2.626065	-0.518862
Cl	3.371542	1.085903	-0.140649
C	-0.90661	-0.435337	0.47245
C	-1.728361	0.136528	1.477559
C	-3.109694	0.270484	1.26927
C	-3.702119	-0.18278	0.067641

C	-2.889142	-0.783278	-0.926011
C	-1.511833	-0.924283	-0.72045
H	-1.285997	0.483703	2.408585
H	-3.732163	0.725	2.039019
C	-5.158545	-0.031029	-0.131526
H	-3.359515	-1.135849	-1.840575
H	-0.895681	-1.409237	-1.473941
C	0.468241	-1.708569	1.273746
C	1.770918	-1.650151	0.674904
O	1.971958	-2.462633	-0.434282
H	-0.166242	-2.53417	0.964339
H	0.400581	-1.443424	2.325282
H	2.654358	-1.363611	1.246946
H	-0.939181	3.111422	-0.661138
H	0.926947	3.044514	-1.782212
H	0.934687	3.678098	0.292053
C	3.290597	-2.378317	-1.086326
H	3.461167	-1.362275	-1.454863
H	3.253215	-3.10148	-1.902938
H	4.080375	-2.650887	-0.373985
O	-5.780906	-0.399953	-1.152578
H	-5.699275	0.450794	0.708064

pd_clet_pph3_hx

6	5.144229	-0.329225	-0.109061
6	4.379928	-0.058098	-1.261274

6	3.000816	-0.351793	-1.28639
6	2.388913	-0.943424	-0.160913
6	3.14759	-1.193897	1.004871
6	4.526417	-0.895385	1.023268
1	6.206946	-0.098319	-0.092288
1	4.851207	0.383244	-2.137194
1	2.4197	-0.122557	-2.177225
1	2.681373	-1.629288	1.887771
1	5.110072	-1.103313	1.917934
6	2.178062	3.326096	0.826958
6	2.021289	4.196069	-0.271
6	1.090273	3.885822	-1.278043
6	0.311739	2.715329	-1.188522
6	0.462957	1.847593	-0.088144
6	1.408575	2.154651	0.915797
1	2.903478	3.551587	1.604299
1	1.556275	1.480966	1.755811
1	-0.406253	2.489935	-1.971711
1	0.966928	4.547344	-2.131809
1	2.622493	5.099192	-0.341878
6	-1.378619	0.308144	1.698411
6	-1.542955	1.514105	2.413832
6	-2.238407	1.514554	3.637323
6	-2.775709	0.317499	4.147025
6	-2.61469	-0.883838	3.429866

6	-1.916071	-0.894721	2.208176
1	-1.795902	-1.825818	1.656406
1	-3.02769	-1.812252	3.815741
1	-3.312633	0.320748	5.092546
1	-2.35987	2.445271	4.185948
1	-1.131123	2.444215	2.032142
6	-1.894491	0.441633	-1.235472
6	-1.937193	-0.411238	-2.35645
6	-2.961685	-0.264901	-3.311605
6	-3.947547	0.725121	-3.145212
6	-3.912401	1.568771	-2.017023
6	-2.889713	1.428649	-1.062958
1	-2.880008	2.074767	-0.18879
1	-4.679561	2.325969	-1.876501
1	-4.742834	0.83064	-3.879158
1	-2.995269	-0.933415	-4.167726
1	-1.202168	-1.203773	-2.465031
46	0.587871	-1.797946	-0.258798
15	-0.51907	0.253277	0.028186
17	-1.197	-3.450815	-0.366948

pd_clet_pph3_h_pix

6	3.374324	3.537317	-0.211354
6	2.51908	3.286068	-1.302316
6	1.861191	2.044541	-1.420303
6	2.057745	1.033495	-0.452268

6	2.922255	1.286488	0.634384
6	3.573135	2.533584	0.756015
1	3.88052	4.495586	-0.118775
1	2.357878	4.053461	-2.057388
1	1.198705	1.876481	-2.267253
1	3.115037	0.515675	1.376578
1	4.239823	2.711864	1.598312
6	-0.533653	3.99141	1.402124
6	-1.430169	4.720365	0.595959
6	-2.200761	4.046759	-0.368333
6	-2.083028	2.651413	-0.5237
6	-1.191197	1.917258	0.285528
6	-0.410214	2.601186	1.244314
1	0.078671	4.502559	2.140664
1	0.303225	2.057844	1.857382
1	-2.688904	2.146691	-1.270211
1	-2.892503	4.599224	-0.999862
1	-1.520931	5.797525	0.714734
6	3.17172	-1.410535	-1.683978
6	3.271396	-2.14141	-0.51425
8	4.143486	-1.787592	0.485594
6	3.980165	-2.489849	1.76613
1	3.804452	-0.545809	-1.847403
1	2.681678	-1.87181	-2.536108
1	4.006755	-3.576616	1.614888

1	3.032796	-2.199796	2.236309
1	4.822782	-2.176829	2.384527
1	2.727076	-3.078307	-0.39297
6	-1.472581	-0.656115	1.746039
6	-2.101748	0.123748	2.740132
6	-2.481072	-0.461601	3.964028
6	-2.240031	-1.827988	4.20044
6	-1.617048	-2.607407	3.206093
6	-1.230507	-2.02785	1.983597
1	-0.75988	-2.635883	1.214324
1	-1.433914	-3.665633	3.376383
1	-2.535777	-2.279186	5.144921
1	-2.96455	0.148263	4.72379
1	-2.296039	1.178949	2.571836
6	-2.386464	-0.416217	-1.072469
6	-2.111383	-0.70916	-2.42292
6	-3.159439	-1.035429	-3.302963
6	-4.486135	-1.081795	-2.836535
6	-4.763027	-0.80389	-1.483231
6	-3.71701	-0.470577	-0.602872
1	-3.938658	-0.268328	0.442051
1	-5.784293	-0.850797	-1.112623
1	-5.294796	-1.34373	-3.51485
1	-2.936338	-1.269865	-4.340429
1	-1.084646	-0.718749	-2.775447

46	1.192469	-0.77918	-0.698724
15	-0.973362	0.060234	0.071285
17	0.222795	-3.068597	-1.11411

pd_clet_pph3_h_tsa_1stx

Pd	-1.07072	-1.34793	-0.23807
P	1.06122	0.03527	-0.02085
Cl	0.20691	-3.43283	0.05955
C	-2.48916	0.2577	-0.21608
C	-2.73908	0.69035	1.11288
C	-2.95329	2.05143	1.39367
C	-2.96152	2.99619	0.34585
C	-2.75392	2.57365	-0.98168
C	-2.52294	1.21331	-1.26017
H	-2.78237	-0.04229	1.91585
H	-3.12055	2.37315	2.41928
H	-3.12953	4.04862	0.56158
H	-2.76055	3.29929	-1.79159
H	-2.36341	0.89741	-2.29032
C	2.43191	-0.34779	-1.27512
C	1.91191	-0.1881	1.65295
C	0.91719	1.91336	-0.17876
C	3.48285	0.56247	-1.53239
C	4.50499	0.23275	-2.43977
C	4.49209	-1.01213	-3.09871
C	2.42349	-1.59501	-1.93485

C	3.44992	-1.9215	-2.84323
H	3.50094	1.53561	-1.04957
H	5.30608	0.94367	-2.6291
H	5.28385	-1.26807	-3.7992
H	1.63999	-2.31555	-1.72004
H	3.43317	-2.88838	-3.34025
C	1.40161	-1.14908	2.54921
C	2.02153	-1.35245	3.7981
C	3.15638	-0.60345	4.15685
C	3.05637	0.55742	2.01396
C	3.67443	0.35222	3.25936
H	0.55109	-1.75845	2.26035
H	1.62387	-2.10262	4.47712
H	3.63723	-0.76531	5.11897
H	3.46885	1.2974	1.33354
H	4.55636	0.93021	3.52559
C	0.79251	2.74149	0.95599
C	0.6421	4.13403	0.81245
C	0.60555	4.7161	-0.46802
C	0.85907	2.50267	-1.46197
C	0.71159	3.89306	-1.60634
H	0.82454	2.30947	1.9522
H	0.55879	4.75873	1.69891
H	0.49985	5.79308	-0.57821
H	0.94772	1.88146	-2.3501

H	0.68455	4.33086	-2.6016
C	-3.63327	-1.41814	-0.68747
C	-2.76596	-2.5418	-0.46763
H	-2.46117	-3.1176	-1.3414
H	-2.9197	-3.12138	0.44018
H	-3.81925	-1.0936	-1.7147
O	-4.71968	-1.29389	0.17166
C	-5.6833	-0.22625	-0.11556
H	-6.54743	-0.43702	0.51719
H	-5.25844	0.75101	0.13655
H	-5.97825	-0.24942	-1.17409

pd_clet_pph3_h_tsb_1stx

Pd	1.48304	-0.66354	-0.41189
P	-0.95818	-0.11592	0.02343
Cl	1.01698	-3.11068	-0.50181
C	2.2041	1.3443	-0.3953
C	1.75564	2.29589	-1.34493
C	1.69678	3.66149	-1.01027
C	2.09418	4.0985	0.26804
C	2.54181	3.15988	1.21924
C	2.60908	1.7938	0.89029
H	1.45756	1.97245	-2.34041
H	1.34088	4.37898	-1.74603
H	2.05668	5.15564	0.51894
H	2.85452	3.48941	2.20781

H	3.0034	1.07909	1.60942
C	3.61725	0.12989	-1.23072
C	3.57881	-1.18225	-0.67285
O	4.26976	-1.36444	0.52454
H	4.36838	0.81161	-0.84566
H	3.41482	0.22097	-2.29467
H	3.42035	-2.06547	-1.2914
C	-1.62533	-0.76448	1.6722
C	-2.14075	-0.85801	-1.24874
C	-1.46003	1.70077	0.04818
C	4.20702	-2.70973	1.11555
H	3.16701	-2.98906	1.31058
H	4.78481	-2.64696	2.03976
H	4.66062	-3.44264	0.43518
C	-2.70039	-0.14687	2.34735
C	-3.1881	-0.68756	3.55149
C	-2.60936	-1.85431	4.08903
C	-1.04865	-1.93452	2.21004
C	-1.54095	-2.47488	3.41336
H	-3.15177	0.75899	1.95234
H	-4.01556	-0.20214	4.06437
H	-2.98703	-2.27334	5.01933
H	-0.23863	-2.43098	1.68256
H	-1.09256	-3.37987	3.81668
C	-1.60738	-1.54523	-2.35742

C	-2.46622	-2.10878	-3.32174
C	-3.86098	-1.99544	-3.18048
C	-3.54223	-0.75309	-1.10519
C	-4.3981	-1.31813	-2.06687
H	-0.53298	-1.67241	-2.44638
H	-2.04396	-2.64505	-4.16799
H	-4.52346	-2.43628	-3.92206
H	-3.97036	-0.2385	-0.24879
H	-5.47565	-1.23461	-1.94547
C	-2.07297	2.30649	-1.07035
C	-2.39181	3.67806	-1.05459
C	-2.09666	4.46121	0.07639
C	-1.14678	2.49863	1.17124
C	-1.46997	3.86603	1.1875
H	-2.31642	1.71269	-1.94718
H	-2.87246	4.12657	-1.92111
H	-2.34946	5.51878	0.09111
H	-0.65374	2.05718	2.03358
H	-1.22687	4.46365	2.0626

pd_clet_pph3_omex

6	6.846209	0.278813	-0.739037
8	6.062542	-0.237152	0.373319
6	4.696029	-0.466788	0.178522
6	4.006382	-0.200733	-1.022199
6	2.622893	-0.467639	-1.10342

6	1.932591	-1.024068	-0.010289
6	2.629737	-1.261954	1.199432
6	4.00522	-0.993868	1.290644
1	6.49189	1.271414	-1.051704
1	6.820058	-0.40776	-1.596934
1	7.867932	0.355954	-0.361579
1	4.518335	0.211757	-1.886455
1	2.099807	-0.240328	-2.029725
1	2.113724	-1.671305	2.066392
1	4.558624	-1.186808	2.205421
6	1.798032	3.239725	1.003958
6	1.720188	4.134193	-0.083052
6	0.831738	3.868792	-1.140627
6	0.018619	2.718595	-1.11257
6	0.091753	1.827396	-0.024287
6	0.993167	2.089343	1.030757
1	2.489247	3.429811	1.820934
1	1.080508	1.39765	1.864075
1	-0.665255	2.528713	-1.934193
1	0.767891	4.55015	-1.985502
1	2.34773	5.021997	-0.10575
6	-1.900551	0.331949	1.633061
6	-2.060062	1.535662	2.352434
6	-2.826694	1.551598	3.532968
6	-3.438581	0.370886	3.995296

6	-3.281387	-0.828287	3.273068
6	-2.512913	-0.853803	2.095034
1	-2.396986	-1.783194	1.540126
1	-3.751696	-1.743623	3.622808
1	-4.029578	0.385337	4.908101
1	-2.944951	2.480898	4.085039
1	-1.591	2.452705	2.007022
6	-2.234447	0.494955	-1.325547
6	-2.227577	-0.34337	-2.45687
6	-3.188794	-0.164086	-3.46982
6	-4.162189	0.844965	-3.350703
6	-4.177943	1.674376	-2.210923
6	-3.217086	1.5008	-1.199462
1	-3.24709	2.135263	-0.317385
1	-4.936959	2.445736	-2.10645
1	-4.909315	0.976406	-4.129882
1	-3.185115	-0.821636	-4.335008
1	-1.505419	-1.151027	-2.530951
46	0.114155	-1.824399	-0.205995
15	-0.941691	0.260396	0.017086
17	-1.729675	-3.40407	-0.443158

pd_clet_pph3_ome_pix

6	-6.304083	-2.160842	-0.590565
8	-5.709019	-1.231166	0.355817
6	-4.451703	-0.685801	0.052551

6	-3.70412	-0.992642	-1.101378
6	-2.4413	-0.388628	-1.29195
6	-1.91711	0.524136	-0.355763
6	-2.689853	0.830233	0.788202
6	-3.942394	0.228027	0.996759
1	-5.681035	-3.05803	-0.717065
1	-6.46574	-1.687159	-1.569516
1	-7.266217	-2.440599	-0.155625
1	-4.074047	-1.692844	-1.844856
1	-1.873606	-0.651725	-2.18259
1	-2.332201	1.550151	1.519833
1	-4.541458	0.459741	1.873348
6	-1.603848	-3.388623	1.467872
6	-1.347468	-4.514315	0.659752
6	-0.346732	-4.447747	-0.325966
6	0.40041	-3.266304	-0.500927
6	0.152175	-2.140507	0.309981
6	-0.862939	-2.208148	1.290894
1	-2.3851	-3.421772	2.223016
1	-1.089501	-1.341825	1.905704
1	1.172673	-3.233681	-1.263215
1	-0.14327	-5.308831	-0.958149
1	-1.923342	-5.426957	0.795029
6	-1.364798	3.085894	-1.716471
6	-0.98636	3.769697	-0.574773

8	-1.878398	4.038965	0.433508
6	-1.302196	4.540389	1.688931
1	-2.391447	2.764267	-1.849162
1	-0.716112	3.140936	-2.585904
1	-0.686966	5.429876	1.501385
1	-0.695899	3.759407	2.163743
1	-2.152154	4.799402	2.321988
1	0.009358	4.205854	-0.488895
6	1.962078	-0.244373	1.722478
6	2.000554	-1.224167	2.737874
6	2.684491	-0.968103	3.942219
6	3.33781	0.262667	4.138491
6	3.30428	1.238648	3.123431
6	2.61783	0.992472	1.919993
1	2.601144	1.746435	1.135644
1	3.812083	2.190047	3.262648
1	3.867426	0.457553	5.068217
1	2.707466	-1.729517	4.71832
1	1.50576	-2.181059	2.600469
6	2.494536	-1.015013	-1.091985
6	2.443858	-0.611575	-2.441268
6	3.46569	-0.993477	-3.331527
6	4.546788	-1.770676	-2.875505
6	4.60601	-2.162984	-1.52372
6	3.58327	-1.787667	-0.634523

1	3.642863	-2.085548	0.409031
1	5.44452	-2.753196	-1.162268
1	5.340598	-2.056803	-3.561634
1	3.423869	-0.668266	-4.36799
1	1.635448	0.026415	-2.785769
46	-0.141275	1.440112	-0.694652
15	1.096951	-0.530758	0.068309
17	1.999374	2.674006	-1.193508

pd_clet_pph3_ome_tsa_1stx

Pd	0.21408	-1.82123	0.15644
P	-1.21671	0.2737	-0.00666
Cl	-1.81397	-3.20771	0.02241
C	2.13712	-0.8888	0.31183
C	2.6056	-0.28059	-0.87601
C	3.3563	0.91004	-0.84859
C	3.68343	1.49222	0.39422
C	3.26167	0.88251	1.59787
C	2.49775	-0.28899	1.55084
H	2.39384	-0.75069	-1.834
H	3.67231	1.3649	-1.78216
O	4.428	2.66188	0.54614
H	3.53939	1.34426	2.5411
H	2.18077	-0.74896	2.48601
C	-2.28708	0.58159	1.52269
C	-2.46922	0.19914	-1.41718

C	-0.39971	1.95233	-0.30358
C	-2.68911	1.87263	1.92961
C	-3.50651	2.03852	3.0631
C	-3.93645	0.91611	3.79634
C	-2.7223	-0.54378	2.25794
C	-3.54447	-0.3732	3.38808
H	-2.36235	2.7497	1.37807
H	-3.80735	3.03837	3.36793
H	-4.56958	1.0446	4.67152
H	-2.43886	-1.54286	1.93559
H	-3.87798	-1.24752	3.94203
C	-2.28207	-0.74675	-2.44506
C	-3.18247	-0.80617	-3.52636
C	-4.28033	0.07203	-3.58179
C	-3.57645	1.07297	-1.47104
C	-4.47836	1.00939	-2.54832
H	-1.4629	-1.4562	-2.38201
H	-3.03427	-1.5468	-4.3083
H	-4.98069	0.01992	-4.41242
H	-3.74706	1.79222	-0.67457
H	-5.33208	1.68251	-2.57731
C	-0.41384	2.55602	-1.579
C	0.2354	3.7865	-1.79564
C	0.90907	4.42899	-0.73943
C	0.29314	2.59407	0.74668

C	0.9372	3.82571	0.53338
H	-0.94166	2.08162	-2.40101
H	0.20442	4.24311	-2.78246
H	1.39673	5.38789	-0.90206
H	0.32837	2.14078	1.73357
H	1.46253	4.30667	1.3548
C	2.57651	-2.96131	0.36561
C	1.29825	-3.60484	0.28837
H	0.89521	-4.03053	1.20672
H	1.06842	-4.15547	-0.62152
H	3.05503	-2.85803	1.34172
O	3.44682	-3.15745	-0.69693
C	4.82669	-2.6921	-0.51784
H	5.36785	-3.03477	-1.4016
H	4.85839	-1.59909	-0.45536
H	5.2658	-3.13805	0.38495
C	4.85177	3.38574	-0.64675
H	5.38073	4.26558	-0.27495
H	5.53234	2.77829	-1.25925
H	3.98541	3.6953	-1.24585

pd_clet_pph3_ome_tsb_1stx

Pd	0.14041	1.70696	-0.35417
P	0.94488	-0.6746	0.01452
Cl	2.47838	2.5759	-0.30508
C	-1.93422	1.27139	-0.40195

C	-2.50819	0.38501	-1.34205
C	-3.66409	-0.35729	-1.03358
C	-4.26487	-0.21299	0.23415
C	-3.71452	0.6782	1.18132
C	-2.57345	1.42321	0.86018
H	-2.0561	0.26599	-2.32472
H	-4.06864	-1.04071	-1.77353
O	-5.40327	-0.90653	0.64776
H	-4.20236	0.78093	2.14632
H	-2.18376	2.14007	1.57902
C	-1.59322	3.09774	-1.30793
C	-0.4735	3.76295	-0.72942
O	-0.72973	4.52186	0.4127
H	-2.57483	3.40449	-0.96084
H	-1.53649	2.82091	-2.35693
H	0.39662	4.042	-1.32383
C	1.80641	-0.98536	1.67482
C	2.21987	-1.26855	-1.24776
C	-0.36048	-2.03458	-0.03312
C	0.42713	5.17833	1.03785
H	1.15784	4.43185	1.36318
H	0.02031	5.73524	1.88436
H	0.90361	5.86656	0.32681
C	1.79146	-2.24606	2.30993
C	2.47599	-2.43796	3.52443

C	3.1874	-1.37372	4.11195
C	2.52096	0.07926	2.26356
C	3.20815	-0.11788	3.47646
H	1.2389	-3.07592	1.87812
H	2.45444	-3.41293	4.00649
H	3.71786	-1.52269	5.04997
H	2.55803	1.04646	1.77005
H	3.75966	0.70852	3.9184
C	2.63703	-0.39144	-2.26754
C	3.59096	-0.81177	-3.21571
C	4.13786	-2.10618	-3.1457
C	2.77757	-2.56397	-1.1728
C	3.73058	-2.98209	-2.11786
H	2.2508	0.6221	-2.29907
H	3.91314	-0.12413	-3.99378
H	4.87837	-2.42777	-3.87489
H	2.47927	-3.24709	-0.3819
H	4.15633	-3.98069	-2.05065
C	-0.53158	-2.86134	-1.16453
C	-1.54469	-3.83906	-1.18915
C	-2.4043	-3.99764	-0.08695
C	-1.2451	-2.18285	1.06016
C	-2.25373	-3.16166	1.03641
H	0.13035	-2.75898	-2.01968
H	-1.65263	-4.47619	-2.06401

H	-3.17611	-4.76405	-0.09957
H	-1.14833	-1.54013	1.93159
H	-2.92063	-3.26364	1.88886
C	-6.039	-1.81327	-0.29721
H	-6.89965	-2.22705	0.23216
H	-6.37909	-1.27684	-1.19427
H	-5.35593	-2.62268	-0.58859

pd_clet_pph3_chox

6	4.735484	-0.47266	0.108786
6	4.020097	-0.156826	-1.072002
6	2.647777	-0.432007	-1.160827
6	1.973338	-1.047107	-0.077446
6	2.681682	-1.346286	1.111011
6	4.058121	-1.068722	1.196679
6	6.180037	-0.181043	0.223148
8	6.87423	0.361338	-0.665518
1	4.555926	0.303622	-1.898528
1	2.106331	-0.172124	-2.067413
1	2.172345	-1.800249	1.959185
1	4.605537	-1.311417	2.107009
1	6.642818	-0.482431	1.18506
6	1.905062	3.177458	0.989439
6	1.84719	4.059911	-0.108166
6	0.947731	3.806753	-1.159174
6	0.104263	2.678915	-1.115136

6	0.157328	1.799117	-0.014956
6	1.070131	2.049637	1.033887
1	2.604599	3.360194	1.80084
1	1.13953	1.366708	1.876634
1	-0.587724	2.496773	-1.932162
1	0.900473	4.478563	-2.012555
1	2.500755	4.927845	-0.145516
6	-1.829193	0.321886	1.667302
6	-1.972418	1.530075	2.384656
6	-2.716977	1.55275	3.57886
6	-3.322332	0.37536	4.057989
6	-3.181367	-0.827056	3.338569
6	-2.43533	-0.859946	2.146154
1	-2.33497	-1.790889	1.591609
1	-3.648204	-1.739378	3.700427
1	-3.896411	0.39499	4.981243
1	-2.822887	2.484989	4.128271
1	-1.508698	2.445143	2.02701
6	-2.207434	0.516707	-1.292821
6	-2.19726	-0.27765	-2.455371
6	-3.164651	-0.069151	-3.456493
6	-4.147268	0.924699	-3.294727
6	-4.165975	1.710233	-2.124542
6	-3.199031	1.508064	-1.12393
1	-3.23063	2.110066	-0.219291

1	-4.931285	2.470289	-1.988143
1	-4.89885	1.078597	-4.0653
1	-3.157653	-0.692277	-4.34666
1	-1.466622	-1.073625	-2.564795
46	0.146456	-1.833254	-0.251063
15	-0.904848	0.253786	0.033033
17	-1.743322	-3.344815	-0.472043

pd_clet_pph3_cho_pix

6	-4.43743	-0.898486	0.019217
6	-3.63174	-1.206978	-1.103373
6	-2.408446	-0.549908	-1.295238
6	-1.960714	0.430645	-0.373367
6	-2.773727	0.746244	0.739236
6	-3.998302	0.084333	0.935342
6	-5.724645	-1.579819	0.248947
8	-6.211956	-2.470162	-0.485904
1	-3.980184	-1.961601	-1.804434
1	-1.799076	-0.804756	-2.159396
1	-2.468746	1.517538	1.441014
1	-4.620209	0.33408	1.794918
1	-6.277857	-1.239962	1.148808
6	-1.499536	-3.414168	1.517632
6	-1.330036	-4.480815	0.612707
6	-0.405586	-4.357726	-0.440011
6	0.346775	-3.176279	-0.589492

6	0.181193	-2.108595	0.315728
6	-0.753175	-2.233856	1.367487
1	-2.218803	-3.495554	2.328561
1	-0.908363	-1.413239	2.062943
1	1.058252	-3.098726	-1.406378
1	-0.269906	-5.173188	-1.146338
1	-1.916017	-5.389873	0.723281
6	-1.532871	2.987257	-1.74611
6	-1.171603	3.71219	-0.622317
8	-2.062988	3.957039	0.391973
6	-1.503786	4.536647	1.622552
1	-2.548711	2.626209	-1.86117
1	-0.905244	3.060431	-2.629699
1	-0.938089	5.448933	1.394561
1	-0.854438	3.80712	2.121338
1	-2.361848	4.775678	2.252388
1	-0.198615	4.200541	-0.559063
6	1.95286	-0.186998	1.734408
6	2.142529	-1.227633	2.670661
6	2.816984	-0.977119	3.880222
6	3.311696	0.310364	4.162226
6	3.129229	1.346541	3.226434
6	2.451684	1.103676	2.016499
1	2.335356	1.900843	1.286263
1	3.517482	2.341555	3.430441

1	3.834617	0.501997	5.096331
1	2.956184	-1.785157	4.594436
1	1.763265	-2.225697	2.471503
6	2.494954	-0.945652	-1.098143
6	2.474838	-0.475713	-2.425955
6	3.498818	-0.843516	-3.32006
6	4.550698	-1.672518	-2.889422
6	4.578103	-2.134346	-1.558326
6	3.553419	-1.774008	-0.665515
1	3.590374	-2.129051	0.360868
1	5.393121	-2.767269	-1.215896
1	5.345581	-1.948162	-3.578453
1	3.479833	-0.468742	-4.340202
1	1.690207	0.20034	-2.75029
46	-0.235666	1.433774	-0.693884
15	1.099867	-0.483642	0.076298
17	1.866525	2.73583	-1.128382

pd_clet_pph3_cho_tsa_1stx

Pd	0.21408	-1.82123	0.15644
C	2.13712	-0.8888	0.31183
C	2.49775	-0.28899	1.55084
C	3.26167	0.88251	1.59787
C	3.68343	1.49222	0.39422
C	3.3563	0.91004	-0.84859
C	2.6056	-0.28059	-0.87601

C	1.29825	-3.60484	0.28837
C	2.57651	-2.96131	0.36561
C	4.46106	2.74237	0.47373
O	4.88346	3.39412	-0.50963
C	0.90907	4.42899	-0.73943
C	0.2354	3.7865	-1.79564
C	-0.41384	2.55602	-1.579
C	-0.39971	1.95233	-0.30358
C	0.29314	2.59407	0.74668
P	-1.21671	0.2737	-0.00666
C	-2.28708	0.58159	1.52269
C	-2.7223	-0.54378	2.25794
C	-2.68911	1.87263	1.92961
C	-3.54447	-0.3732	3.38808
C	-3.50651	2.03852	3.0631
C	-3.93645	0.91611	3.79634
Cl	-1.81397	-3.20771	0.02241
C	-2.46922	0.19914	-1.41718
C	-2.28207	-0.74675	-2.44506
C	-3.18247	-0.80617	-3.52636
C	-4.28033	0.07203	-3.58179
C	-4.47836	1.00939	-2.54832
C	-3.57645	1.07297	-1.47104
O	3.44682	-3.15745	-0.69693
C	4.82669	-2.6921	-0.51784

H	2.39384	-0.75069	-1.834
H	3.67231	1.3649	-1.78216
H	3.53939	1.34426	2.5411
H	2.18077	-0.74896	2.48601
H	-2.36235	2.7497	1.37807
H	-3.80735	3.03837	3.36793
H	-4.56958	1.0446	4.67152
H	-2.43886	-1.54286	1.93559
H	-3.87798	-1.24752	3.94203
H	-1.4629	-1.4562	-2.38201
H	-3.03427	-1.5468	-4.3083
H	-4.98069	0.01992	-4.41242
H	-3.74706	1.79222	-0.67457
H	-5.33208	1.68251	-2.57731
C	0.9372	3.82571	0.53338
H	-0.94166	2.08162	-2.40101
H	0.20442	4.24311	-2.78246
H	1.39673	5.38789	-0.90206
H	0.32837	2.14078	1.73357
H	1.46253	4.30667	1.3548
H	0.89521	-4.03053	1.20672
H	1.06842	-4.15547	-0.62152
H	3.05503	-2.85803	1.34172
H	5.36785	-3.03477	-1.4016
H	4.85839	-1.59909	-0.45536

H	5.2658	-3.13805	0.38495
H	4.67582	3.09299	1.50438

pd_clet_pph3_cho_tsb_1stx

Pd	0.14041	1.70696	-0.35417
C	-1.93422	1.27139	-0.40195
C	-2.50819	0.38501	-1.34205
C	-3.66409	-0.35729	-1.03358
C	-4.26487	-0.21299	0.23415
C	-3.71452	0.6782	1.18132
C	-2.57345	1.42321	0.86018
C	-1.59322	3.09774	-1.30793
C	-0.4735	3.76295	-0.72942
Cl	2.47838	2.5759	-0.30508
P	0.94488	-0.6746	0.01452
C	1.80641	-0.98536	1.67482
C	2.47599	-2.43796	3.52443
C	2.21987	-1.26855	-1.24776
C	-0.36048	-2.03458	-0.03312
C	-1.2451	-2.18285	1.06016
C	-0.53158	-2.86134	-1.16453
C	-1.54469	-3.83906	-1.18915
C	-2.4043	-3.99764	-0.08695
C	-2.25373	-3.16166	1.03641
H	-2.0561	0.26599	-2.32472
H	-4.06864	-1.04071	-1.77353

H	-4.20236	0.78093	2.14632
H	-2.18376	2.14007	1.57902
O	-0.72973	4.52186	0.4127
H	-2.57483	3.40449	-0.96084
H	-1.53649	2.82091	-2.35693
H	0.39662	4.042	-1.32383
C	0.42713	5.17833	1.03785
H	1.15784	4.43185	1.36318
H	0.02031	5.73524	1.88436
H	0.90361	5.86656	0.32681
C	1.79146	-2.24606	2.30993
C	3.1874	-1.37372	4.11195
C	2.52096	0.07926	2.26356
C	3.20815	-0.11788	3.47646
H	1.2389	-3.07592	1.87812
H	2.45444	-3.41293	4.00649
H	3.71786	-1.52269	5.04997
H	2.55803	1.04646	1.77005
H	3.75966	0.70852	3.9184
C	2.63703	-0.39144	-2.26754
C	3.59096	-0.81177	-3.21571
C	4.13786	-2.10618	-3.1457
C	2.77757	-2.56397	-1.1728
C	3.73058	-2.98209	-2.11786
H	2.2508	0.6221	-2.29907

H	3.91314	-0.12413	-3.99378
H	4.87837	-2.42777	-3.87489
H	2.47927	-3.24709	-0.3819
H	4.15633	-3.98069	-2.05065
H	0.13035	-2.75898	-2.01968
H	-1.65263	-4.47619	-2.06401
H	-3.17611	-4.76405	-0.09957
H	-1.14833	-1.54013	1.93159
H	-2.92063	-3.26364	1.88886
C	-5.47157	-0.9764	0.60155
O	-6.05573	-1.80346	-0.13664
H	-5.86652	-0.76392	1.61652

pd_clet_ptbu3_omex

6	-6.741406	0.571185	0.71453
8	-5.896985	0.4214	-0.461231
6	-4.539211	0.134657	-0.279979
6	-3.906374	0.020481	0.974766
6	-2.524337	-0.264159	1.034907
6	-1.774719	-0.456038	-0.143023
6	-2.419597	-0.325651	-1.397343
6	-3.793875	-0.041905	-1.465601
1	-6.416198	1.418294	1.335189
1	-6.749898	-0.34692	1.318771
1	-7.743647	0.764615	0.32677
1	-4.463068	0.145547	1.898605

1	-2.05245	-0.35669	2.010416
1	-1.866046	-0.471592	-2.321939
1	-4.30638	0.041874	-2.419921
6	1.955738	0.764783	1.913525
6	3.301834	1.520081	2.069268
6	0.865308	1.524399	2.714265
6	2.080802	-0.651046	2.538866
1	3.522334	1.605718	3.143267
1	4.136858	0.9849	1.609603
1	3.269681	2.533115	1.658453
1	1.119169	1.455925	3.781378
1	0.816062	2.587021	2.457847
1	-0.127354	1.081201	2.580263
1	2.360071	-0.533958	3.596317
1	1.13221	-1.196487	2.49174
1	2.835803	-1.273452	2.057364
6	0.706497	2.330622	-0.651116
6	1.663601	3.501478	-0.297744
6	0.529163	2.24151	-2.190567
6	-0.690066	2.667467	-0.062239
1	1.313968	4.397365	-0.830974
1	1.640689	3.735158	0.772
1	2.699523	3.326901	-0.59222
1	0.012389	3.151028	-2.527804
1	1.478379	2.184102	-2.729321

1	-0.091269	1.385008	-2.474837
1	-0.951941	3.683189	-0.394676
1	-1.458031	1.986399	-0.426232
1	-0.718585	2.66144	1.027782
6	2.951197	0.023959	-1.110752
6	3.887799	1.203944	-1.48253
6	3.799585	-1.052818	-0.383011
6	2.390881	-0.633327	-2.402087
1	4.734754	0.7892	-2.047497
1	3.408354	1.949753	-2.122608
1	4.300388	1.707958	-0.602315
1	4.546785	-1.42115	-1.100874
1	4.347658	-0.653516	0.476166
1	3.201221	-1.913111	-0.070644
1	3.241688	-0.937926	-3.028509
1	1.813719	-1.532259	-2.16241
1	1.765453	0.039808	-2.993205
46	-0.025952	-1.387472	-0.044046
15	1.377831	0.566222	0.017006
17	1.20547	-3.499823	0.070595

pd_clet_ptbu3_ome_pix

6	-6.173598	-2.461676	-0.681105
8	-5.487969	-1.766726	0.395293
6	-4.247303	-1.170957	0.127845
6	-3.592458	-1.202011	-1.122193

6	-2.340692	-0.565779	-1.266993
6	-1.722089	0.095352	-0.18404
6	-2.406546	0.131526	1.050297
6	-3.652685	-0.498084	1.212075
1	-5.58068	-3.310184	-1.052453
1	-6.402966	-1.78289	-1.515177
1	-7.103682	-2.829102	-0.241929
1	-4.040415	-1.70269	-1.976193
1	-1.856387	-0.593845	-2.241571
1	-1.97582	0.655267	1.899931
1	-4.175112	-0.472521	2.164012
6	-1.4347	2.720611	-1.37183
6	-1.206464	3.329259	-0.149815
8	-2.177705	3.382834	0.815561
6	-1.764263	3.890035	2.128712
1	-2.405302	2.289957	-1.590582
1	-0.753037	2.942785	-2.187504
1	-1.316097	4.887438	2.033754
1	-1.049151	3.202468	2.596071
1	-2.676087	3.945861	2.72472
1	-0.278637	3.870722	0.033725
6	2.324348	-1.541232	-1.582963
6	3.638543	-2.348464	-1.420266
6	1.25475	-2.464415	-2.225805
6	2.561319	-0.361873	-2.562944

1	3.912509	-2.761844	-2.402848
1	4.473038	-1.725458	-1.088258
1	3.537803	-3.18875	-0.72791
1	1.548892	-2.657473	-3.267672
1	1.182922	-3.432773	-1.721459
1	0.261609	-2.001607	-2.238445
1	2.915764	-0.775615	-3.519318
1	1.637964	0.198158	-2.748916
1	3.300945	0.355726	-2.206145
6	0.875515	-2.33424	1.20667
6	1.832712	-3.547584	1.35319
6	0.512556	-1.77353	2.609801
6	-0.440616	-2.884413	0.589045
1	1.347741	-4.275256	2.02157
1	1.990772	-4.052737	0.394322
1	2.805265	-3.305932	1.781692
1	-0.006129	-2.560792	3.175127
1	1.386471	-1.47451	3.193254
1	-0.168157	-0.919625	2.531608
1	-0.921911	-3.532235	1.335938
1	-1.132769	-2.088288	0.331636
1	-0.263436	-3.490758	-0.301901
6	3.126504	-0.013296	1.185292
6	3.938442	-1.042861	2.014477
6	4.142027	0.721956	0.268007

6	2.50268	1.052341	2.131141
1	4.76756	-0.500436	2.491949
1	3.362299	-1.515733	2.813767
1	4.38068	-1.823966	1.386701
1	4.838315	1.269463	0.921344
1	4.741534	0.030001	-0.332018
1	3.660923	1.453882	-0.3827
1	3.305518	1.485147	2.745984
1	2.05254	1.859188	1.544674
1	1.74911	0.638008	2.80689
46	-0.013929	1.133895	-0.481682
15	1.603356	-0.798314	0.11976
17	1.793734	2.834918	-1.080183

pd_clet_ptbu3_ome_tsa_1stx

Pd	0.21274	-1.82093	0.15632
C	2.13712	-0.8888	0.31183
C	2.49775	-0.28899	1.55084
C	3.26167	0.88251	1.59787
C	3.68343	1.49222	0.39422
C	3.3563	0.91004	-0.84859
C	2.6056	-0.28059	-0.87601
P	-1.2392	0.30663	-0.00922
C	-0.45182	2.03414	0.67558
C	-0.25302	1.86719	2.20682
C	-1.30554	3.29905	0.38775

C	0.95103	2.30274	0.0637
C	-2.91595	-0.02953	1.06656
C	-2.48221	-0.81918	2.33382
C	-3.68745	1.24886	1.48874
C	-3.91849	-0.92433	0.28777
C	-1.72811	0.56521	-1.92137
C	-2.0052	-0.82902	-2.54365
C	-0.51127	1.16835	-2.67334
C	-2.95766	1.48333	-2.14597
Cl	-1.81397	-3.20771	0.02241
C	1.29825	-3.60484	0.28837
C	2.57493	-2.98207	0.09788
O	3.26299	-3.29645	-1.06515
C	4.65557	-2.84321	-1.15429
O	4.41891	2.67461	0.46942
H	-4.34293	-0.3608	-0.57305
H	3.53939	1.34426	2.5411
H	3.67231	1.3649	-1.78216
H	2.39384	-0.75069	-1.834
H	2.18077	-0.74896	2.48601
H	4.70124	-1.75009	-1.20506
H	5.04679	-3.27977	-2.07498
H	5.23186	-3.20888	-0.29353
H	3.20406	-2.79489	0.97058
H	0.92342	-4.23574	-0.51499

H	1.04584	-3.93232	1.29637
H	-0.80707	4.16421	0.85004
H	-1.38813	3.45314	-0.69898
H	-2.31401	3.17033	0.81557
H	0.4191	2.66427	2.55558
H	-1.19081	1.96546	2.76146
H	0.20632	0.90592	2.4621
H	1.34107	3.23571	0.4979
H	1.65309	1.49484	0.29635
H	0.93702	2.41125	-1.02101
H	-3.08326	1.61274	-3.23168
H	-0.7511	1.21065	-3.74544
H	-2.02745	-0.71209	-3.63686
H	-1.19855	-1.53936	-2.25476
H	-3.8675	1.01201	-1.71151
H	-2.98272	-1.21504	-2.17734
H	-0.3054	2.19394	-2.2932
H	-2.78522	2.46759	-1.65584
H	0.38396	0.52786	-2.50892
H	-4.65081	0.9251	1.91095
H	-4.71998	-1.20379	0.98823
H	-3.37618	-1.00774	2.94656
H	-2.01973	-1.78628	2.03456
H	-3.10496	1.81039	2.253
H	-1.74294	-0.22083	2.9119

H	-3.39674	-1.83164	-0.09076
H	-3.84936	1.90037	0.60102
C	4.79225	3.35051	-0.76764
H	5.32352	4.25096	-0.45283
H	5.45287	2.70038	-1.38378
H	3.8804	3.59814	-1.3558

pd_clet_ptbu3_h_tsax

C	1.29825	-3.60484	0.28837
C	2.57754	-2.97797	0.13188
C	2.13712	-0.8888	0.31183
P	-1.2392	0.30663	-0.00922
Cl	-1.81397	-3.20771	0.02241
C	-2.91595	-0.02953	1.06656
C	-0.45182	2.03414	0.67558
C	2.49775	-0.28899	1.55084
C	2.6056	-0.28059	-0.87601
Pd	0.21274	-1.82093	0.15632
C	3.26167	0.88251	1.59787
C	3.68343	1.49222	0.39422
C	3.3563	0.91004	-0.84859
H	4.25462	2.41049	0.45262
C	0.95103	2.30274	0.0637
C	-1.30554	3.29905	0.38775
C	-2.48221	-0.81918	2.33382

C	-3.68745	1.24886	1.48874
H	-4.34293	-0.3608	-0.57305
C	-1.72811	0.56521	-1.92137
C	-2.0052	-0.82902	-2.54365
C	-0.51127	1.16835	-2.67334
C	-2.95766	1.48333	-2.14597
O	3.2898	-3.27684	-1.02063
C	4.68317	-2.82059	-1.07553
C	-3.91849	-0.92433	0.28777
C	-0.25302	1.86719	2.20682
H	3.53939	1.34426	2.5411
H	3.67231	1.3649	-1.78216
H	2.39384	-0.75069	-1.834
H	2.18077	-0.74896	2.48601
H	4.72807	-1.72686	-1.11173
H	5.09389	-3.24507	-1.99337
H	5.2423	-3.19618	-0.20776
H	3.18835	-2.80082	1.01956
H	0.941	-4.22618	-0.5303
H	1.02578	-3.94524	1.28682
H	-0.80707	4.16421	0.85004
H	-1.38813	3.45314	-0.69898
H	-2.31401	3.17033	0.81557
H	0.4191	2.66427	2.55557
H	-1.19081	1.96546	2.76146

H	0.20632	0.90592	2.4621
H	1.34107	3.23571	0.4979
H	1.65309	1.49484	0.29635
H	0.93702	2.41125	-1.02101
H	-3.08326	1.61274	-3.23168
H	-0.7511	1.21065	-3.74544
H	-2.02745	-0.71209	-3.63686
H	-1.19855	-1.53936	-2.25476
H	-3.8675	1.01201	-1.71151
H	-2.98272	-1.21504	-2.17734
H	-0.3054	2.19394	-2.2932
H	-2.78522	2.46759	-1.65584
H	0.38396	0.52786	-2.50892
H	-4.65081	0.9251	1.91095
H	-4.71998	-1.20379	0.98823
H	-3.37618	-1.00774	2.94656
H	-2.01973	-1.78628	2.03456
H	-3.10496	1.81039	2.253
H	-1.74294	-0.22083	2.9119
H	-3.39674	-1.83164	-0.09076
H	-3.84936	1.90037	0.60102

pd_clet_ptbu3_ome_tsbx

Cl	-2.82195	1.2107	-0.06753
P	0.20606	2.69891	0.52275
C	1.4282	-0.51641	-0.24958

C	0.0658	-1.74595	-1.20235
C	-1.32518	-1.51685	-0.94855
O	-1.86444	-2.17527	0.15581
C	-3.27632	-1.89294	0.45898
C	1.87397	-1.04256	0.9886
C	2.3776	0.01773	-1.15476
C	3.74164	0.07317	-0.80261
C	4.17558	-0.42773	0.44307
C	3.23645	-0.98659	1.33458
C	2.02927	2.90573	1.35918
Pd	-0.51942	0.32335	-0.1787
C	0.13524	3.86321	-1.09357
C	1.38213	3.58685	-1.97591
C	-1.11342	3.46467	-1.92432
C	0.08045	5.38107	-0.77895
C	-1.12609	3.37286	1.88219
C	-1.483	2.16423	2.79355
C	-0.62312	4.55558	2.75092
C	-2.43992	3.84507	1.20205
C	2.00318	2.14675	2.71469
C	3.12623	2.23278	0.4879
C	2.48615	4.37272	1.58303
H	2.05621	0.39914	-2.12212
H	4.46096	0.49986	-1.49918
O	5.58412	-0.38101	0.7971

H	3.56594	-1.38675	2.29093
H	1.16013	-1.49858	1.67027
H	0.51582	-2.58239	-0.67734
H	0.37659	-1.62895	-2.2372
H	-2.01766	-1.24907	-1.74829
H	-3.41279	-0.8256	0.65878
H	-3.50988	-2.49841	1.33691
H	-3.91164	-2.19186	-0.38592
H	0.12058	5.9301	-1.73167
H	1.34563	4.26463	-2.84203
H	-1.12975	4.08174	-2.83527
H	2.30878	3.77407	-1.38855
H	1.37109	2.52768	-2.3176
H	-0.86556	5.6214	-0.24415
H	-1.05582	2.38758	-2.19868
H	0.94639	5.66166	-0.13853
H	-2.03394	3.6426	-1.32456
H	3.44832	4.34418	2.11636
H	3.02211	2.13622	3.1268
H	4.04473	2.16416	1.0882
H	2.79551	1.21404	0.1854
H	1.31673	2.664	3.42177
H	2.6097	4.88543	0.60294
H	1.72428	4.91483	2.18667
H	1.64788	1.10461	2.55216

H	3.30854	2.84569	-0.42305
H	-1.45663	4.86407	3.39864
H	-3.1765	4.0248	1.99949
H	-2.18845	2.50663	3.5651
H	-1.95305	1.36014	2.18427
H	0.24239	4.23144	3.37104
H	-2.25757	4.78374	0.63253
H	-0.30763	5.39672	2.0939
H	-0.55793	1.77123	3.27158
H	-2.80512	3.05881	0.5041
C	6.5239	0.1833	-0.15686
H	6.29877	1.23945	-0.36488
H	6.52733	-0.3825	-1.09967
H	7.50305	0.1047	0.32066

pd_clet_ptbu3_hx

6	-5.018293	0.784841	-0.015428
6	-4.34442	0.552129	1.19913
6	-2.995096	0.142497	1.197862
6	-2.315896	-0.059407	-0.027062
6	-2.988399	0.19454	-1.245846
6	-4.338389	0.604173	-1.235308
1	-4.862733	0.688061	2.146318
1	-2.488986	-0.030109	2.145561
1	-2.479384	0.05678	-2.19807
1	-4.852968	0.778459	-2.178347

1	-6.05813	1.10277	-0.011795
6	1.742917	0.474492	1.864934
6	3.182585	1.047897	1.94805
6	0.810895	1.320236	2.770782
6	1.725543	-0.976956	2.413445
1	3.473677	1.089147	3.00783
1	3.914308	0.416542	1.436795
1	3.258962	2.062531	1.54707
1	1.082905	1.12744	3.817715
1	0.918973	2.39551	2.597074
1	-0.242363	1.045301	2.643774
1	2.106094	-0.95418	3.445015
1	0.71063	-1.388804	2.429751
1	2.343327	-1.667846	1.839806
6	0.547277	2.338255	-0.529818
6	1.697439	3.351265	-0.27524
6	0.188749	2.314789	-2.038902
6	-0.703266	2.85425	0.228656
1	1.386828	4.322782	-0.687035
1	1.87812	3.499385	0.794585
1	2.639695	3.077791	-0.752884
1	-0.186082	3.30887	-2.320454
1	1.04827	2.095425	-2.677465
1	-0.603675	1.587937	-2.249812
1	-0.970392	3.832458	-0.198107

1	-1.559431	2.192248	0.108222
1	-0.525469	3.002201	1.295094
6	2.391095	-0.2476	-1.265067
6	3.441074	0.815452	-1.682531
6	3.140655	-1.453704	-0.643306
6	1.643365	-0.772327	-2.521551
1	4.186849	0.316113	-2.317389
1	3.011306	1.6307	-2.271501
1	3.974654	1.240224	-0.826123
1	3.773166	-1.887403	-1.431471
1	3.801665	-1.164471	0.178631
1	2.455961	-2.23797	-0.308999
1	2.393885	-1.141517	-3.235698
1	0.987016	-1.609888	-2.263057
1	1.050835	-0.005508	-3.027323
46	-0.701648	-1.223393	-0.025977
15	1.01003	0.463364	0.01419
17	0.27711	-3.480253	-0.020729

pd_clet_ptbu3_h_pix

6	3.392258	3.432621	-0.178866
6	2.752117	3.06941	-1.381452
6	1.959332	1.905354	-1.442314
6	1.789776	1.084374	-0.300046
6	2.448712	1.448352	0.894032
6	3.239787	2.61533	0.956023

1	2.877663	3.684085	-2.271188
1	1.48402	1.638342	-2.384692
1	2.356444	0.825865	1.781112
1	3.736219	2.876865	1.888843
1	4.004954	4.329678	-0.133981
6	2.861531	-1.396188	-1.318085
6	2.931127	-1.996508	-0.073625
8	3.781648	-1.536358	0.89861
6	3.637954	-2.137548	2.229404
1	3.504163	-0.554661	-1.551086
1	2.395661	-1.950987	-2.126392
1	3.735919	-3.229251	2.171675
1	2.667302	-1.8716	2.665223
1	4.447596	-1.721479	2.830907
1	2.381796	-2.91579	0.129066
6	-2.551223	0.46696	-1.557917
6	-4.088345	0.529236	-1.361522
6	-2.082004	1.779997	-2.240348
6	-2.201193	-0.699054	-2.520081
1	-4.553523	0.723148	-2.339628
1	-4.497622	-0.412744	-0.987995
1	-4.396886	1.331775	-0.686225
1	-2.437342	1.773208	-3.280726
1	-2.497558	2.670467	-1.759595
1	-0.990265	1.869068	-2.259667

1	-2.745368	-0.539821	-3.463268
1	-1.129053	-0.729715	-2.742105
1	-2.474767	-1.679634	-2.129975
6	-1.618574	1.929425	1.18474
6	-3.051484	2.496308	1.377387
6	-0.970802	1.647404	2.567838
6	-0.785872	3.058576	0.516791
1	-2.975593	3.3802	2.028737
1	-3.479751	2.836241	0.428362
1	-3.750642	1.802519	1.843631
1	-0.916032	2.593271	3.125557
1	-1.543966	0.941546	3.173405
1	0.050726	1.268972	2.456264
1	-0.671551	3.871375	1.248624
1	0.205491	2.725157	0.224497
1	-1.281808	3.47934	-0.360376
6	-2.418901	-1.207294	1.247746
6	-3.607492	-0.704368	2.109169
6	-2.959727	-2.366199	0.366424
6	-1.321228	-1.805535	2.172323
1	-4.032092	-1.577996	2.625645
1	-3.315994	0.014084	2.880024
1	-4.407697	-0.266522	1.502503
1	-3.277533	-3.172282	1.044922
1	-3.837587	-2.076989	-0.22006

1	-2.192924	-2.777259	-0.291747
1	-1.78464	-2.577306	2.804628
1	-0.54064	-2.282598	1.572096
1	-0.863724	-1.061758	2.831671
46	0.819408	-0.675077	-0.501992
15	-1.521335	0.213635	0.126529
17	0.087423	-3.058874	-1.044094

pd_clet_ptbu3_h_tsax

C	1.29825	-3.60484	0.28837
C	2.57754	-2.97797	0.13188
C	2.13712	-0.8888	0.31183
P	-1.2392	0.30663	-0.00922
Cl	-1.81397	-3.20771	0.02241
C	-2.91595	-0.02953	1.06656
C	-0.45182	2.03414	0.67558
C	2.49775	-0.28899	1.55084
C	2.6056	-0.28059	-0.87601
Pd	0.21274	-1.82093	0.15632
C	3.26167	0.88251	1.59787
C	3.68343	1.49222	0.39422
C	3.3563	0.91004	-0.84859
H	4.25462	2.41049	0.45262
C	0.95103	2.30274	0.0637
C	-1.30554	3.29905	0.38775
C	-2.48221	-0.81918	2.33382

C	-3.68745	1.24886	1.48874
H	-4.34293	-0.3608	-0.57305
C	-1.72811	0.56521	-1.92137
C	-2.0052	-0.82902	-2.54365
C	-0.51127	1.16835	-2.67334
C	-2.95766	1.48333	-2.14597
O	3.2898	-3.27684	-1.02063
C	4.68317	-2.82059	-1.07553
C	-3.91849	-0.92433	0.28777
C	-0.25302	1.86719	2.20682
H	3.53939	1.34426	2.5411
H	3.67231	1.3649	-1.78216
H	2.39384	-0.75069	-1.834
H	2.18077	-0.74896	2.48601
H	4.72807	-1.72686	-1.11173
H	5.09389	-3.24507	-1.99337
H	5.2423	-3.19618	-0.20776
H	3.18835	-2.80082	1.01956
H	0.941	-4.22618	-0.5303
H	1.02578	-3.94524	1.28682
H	-0.80707	4.16421	0.85004
H	-1.38813	3.45314	-0.69898
H	-2.31401	3.17033	0.81557
H	0.4191	2.66427	2.55557
H	-1.19081	1.96546	2.76146

H	0.20632	0.90592	2.4621
H	1.34107	3.23571	0.4979
H	1.65309	1.49484	0.29635
H	0.93702	2.41125	-1.02101
H	-3.08326	1.61274	-3.23168
H	-0.7511	1.21065	-3.74544
H	-2.02745	-0.71209	-3.63686
H	-1.19855	-1.53936	-2.25476
H	-3.8675	1.01201	-1.71151
H	-2.98272	-1.21504	-2.17734
H	-0.3054	2.19394	-2.2932
H	-2.78522	2.46759	-1.65584
H	0.38396	0.52786	-2.50892
H	-4.65081	0.9251	1.91095
H	-4.71998	-1.20379	0.98823
H	-3.37618	-1.00774	2.94656
H	-2.01973	-1.78628	2.03456
H	-3.10496	1.81039	2.253
H	-1.74294	-0.22083	2.9119
H	-3.39674	-1.83164	-0.09076
H	-3.84936	1.90037	0.60102

pd_clet_ptbu3_h_tsbx

Pd	-0.51986	0.3235	-0.17869
C	1.4282	-0.51641	-0.24958
C	1.87397	-1.04256	0.9886

C	3.23645	-0.98659	1.33458
C	4.17558	-0.42773	0.44307
C	3.74164	0.07317	-0.80261
C	2.3776	0.01773	-1.15476
P	0.20606	2.69891	0.52275
Cl	-2.82195	1.2107	-0.06753
C	0.13524	3.86321	-1.09357
C	1.38213	3.58685	-1.97591
C	-1.11342	3.46467	-1.92432
C	0.08045	5.38107	-0.77895
C	-1.12609	3.37286	1.88219
C	-1.483	2.16423	2.79355
C	-0.62312	4.55558	2.75092
C	-2.43992	3.84507	1.20205
C	2.02927	2.90573	1.35918
C	2.00318	2.14675	2.71469
C	3.12623	2.23278	0.4879
C	2.48615	4.37272	1.58303
C	0.0658	-1.74595	-1.20235
C	-1.31872	-1.5398	-0.89845
O	-1.8153	-2.23381	0.20413
C	-3.21969	-1.97602	0.55947
H	2.05621	0.39914	-2.12212
H	4.46096	0.49986	-1.49918
H	5.22973	-0.39276	0.70802

H	3.56594	-1.38675	2.29094
H	1.16013	-1.49858	1.67027
H	0.54465	-2.58743	-0.71205
H	0.34819	-1.59462	-2.24088
H	-2.03925	-1.25864	-1.66825
H	-3.36108	-0.91607	0.79246
H	-3.41857	-2.6075	1.42756
H	-3.87849	-2.25946	-0.27269
H	0.12058	5.9301	-1.73167
H	1.34563	4.26463	-2.84203
H	-1.12975	4.08174	-2.83527
H	2.30878	3.77407	-1.38855
H	1.37109	2.52768	-2.3176
H	-0.86556	5.6214	-0.24415
H	-1.05582	2.38758	-2.19868
H	0.94639	5.66166	-0.13853
H	-2.03394	3.6426	-1.32456
H	3.44832	4.34418	2.11636
H	3.02211	2.13622	3.1268
H	4.04473	2.16416	1.0882
H	2.79551	1.21404	0.1854
H	1.31673	2.664	3.42177
H	2.6097	4.88543	0.60294
H	1.72428	4.91483	2.18667
H	1.64788	1.10461	2.55216

H	3.30854	2.84569	-0.42305
H	-1.45663	4.86407	3.39864
H	-3.1765	4.0248	1.99949
H	-2.18845	2.50663	3.5651
H	-1.95305	1.36014	2.18427
H	0.24239	4.23144	3.37104
H	-2.25757	4.78374	0.63253
H	-0.30763	5.39672	2.0939
H	-0.55793	1.77123	3.27158
H	-2.80512	3.05881	0.5041

pd_clet_ptbu3_chox

6	-4.58163	0.136993	-0.213794
6	-3.921423	0.038078	1.03569
6	-2.551756	-0.259992	1.08982
6	-1.822042	-0.47656	-0.107897
6	-2.477819	-0.371109	-1.357547
6	-3.852035	-0.077668	-1.404866
6	-6.021723	0.459699	-0.288022
8	-6.754013	0.689266	0.70051
1	-4.497922	0.197605	1.944023
1	-2.059309	-0.34405	2.055672
1	-1.93186	-0.53763	-2.282749
1	-4.358289	-0.011688	-2.367104
1	-6.445471	0.482897	-1.312182
6	1.893806	0.7894	1.90509

6	3.236491	1.55173	2.05348
6	0.799194	1.549622	2.699432
6	2.024381	-0.622859	2.53788
1	3.445999	1.66236	3.127145
1	4.077231	1.007949	1.614698
1	3.206402	2.555124	1.619846
1	1.050522	1.486092	3.767316
1	0.746627	2.611161	2.439378
1	-0.192113	1.10255	2.566549
1	2.313411	-0.499435	3.591784
1	1.074107	-1.167256	2.505096
1	2.774662	-1.249186	2.053947
6	0.637391	2.326424	-0.678433
6	1.587435	3.505162	-0.334773
6	0.458294	2.221903	-2.21689
6	-0.760857	2.655098	-0.089454
1	1.221581	4.39748	-0.862472
1	1.576191	3.738099	0.735024
1	2.620987	3.341547	-0.643297
1	-0.056077	3.129493	-2.5624
1	1.406609	2.157231	-2.755724
1	-0.164667	1.364362	-2.493739
1	-1.044355	3.655308	-0.448665
1	-1.518774	1.95132	-0.430931
1	-0.784529	2.680182	1.000387

6	2.894714	0.021519	-1.114036
6	3.822939	1.204288	-1.497125
6	3.749292	-1.040687	-0.372586
6	2.339569	-0.654166	-2.398981
1	4.671325	0.788953	-2.058796
1	3.337352	1.9399	-2.143843
1	4.233618	1.719829	-0.622744
1	4.497246	-1.414474	-1.086425
1	4.296844	-0.627256	0.480223
1	3.157476	-1.900533	-0.047276
1	3.19349	-0.9514	-3.024109
1	1.777205	-1.56062	-2.152785
1	1.704179	0.004351	-2.99546
46	-0.073052	-1.394135	-0.032364
15	1.32052	0.574736	0.008527
17	1.148804	-3.49744	0.062616

pd_clet_ptbu3_cho_pix

6	-4.256563	-1.345849	0.063826
6	-3.565917	-1.361913	-1.17393
6	-2.334721	-0.70398	-1.301392
6	-1.759437	-0.014034	-0.201318
6	-2.462569	0.011585	1.02334
6	-3.695145	-0.64997	1.156827
6	-5.55322	-2.035836	0.218755
8	-6.136214	-2.683723	-0.681012

1	-4.015102	-1.887443	-2.013685
1	-1.825161	-0.718998	-2.262137
1	-2.058476	0.553737	1.874183
1	-4.224644	-0.623962	2.109011
1	-6.006737	-1.946948	1.22802
6	-1.608186	2.623809	-1.354953
6	-1.384922	3.248832	-0.141063
8	-2.337835	3.26008	0.844402
6	-1.93428	3.825577	2.138537
1	-2.566202	2.160195	-1.557899
1	-0.952879	2.872737	-2.183144
1	-1.573988	4.854202	2.011865
1	-1.152898	3.207321	2.596855
1	-2.833416	3.818013	2.756266
1	-0.477481	3.829135	0.025817
6	2.358761	-1.47443	-1.569011
6	3.701592	-2.229413	-1.3882
6	1.331085	-2.442883	-2.213683
6	2.560921	-0.294545	-2.556505
1	3.991244	-2.65137	-2.36224
1	4.512238	-1.569499	-1.069202
1	3.630495	-3.059317	-0.680432
1	1.644216	-2.632719	-3.250193
1	1.291093	-3.409725	-1.703419
1	0.320808	-2.020304	-2.243663

1	2.943667	-0.702847	-3.503962
1	1.61957	0.226624	-2.761076
1	3.267851	0.45408	-2.197678
6	0.933714	-2.299517	1.225367
6	1.948743	-3.460918	1.403578
6	0.52364	-1.737073	2.614479
6	-0.343334	-2.92537	0.598656
1	1.496732	-4.196516	2.085937
1	2.13696	-3.97883	0.457359
1	2.905742	-3.162083	1.830726
1	0.037855	-2.541009	3.185338
1	1.373414	-1.385546	3.204597
1	-0.197011	-0.918665	2.515329
1	-0.795292	-3.5965	1.343002
1	-1.07669	-2.171533	0.330987
1	-0.125356	-3.523585	-0.287821
6	3.077392	0.119495	1.193148
6	3.930343	-0.865006	2.035622
6	4.063184	0.891573	0.274541
6	2.399555	1.161833	2.1274
1	4.729393	-0.279896	2.513747
1	3.370235	-1.357675	2.834657
1	4.413585	-1.629875	1.41859
1	4.726545	1.480297	0.925774
1	4.699391	0.220084	-0.309728

1	3.555244	1.589441	-0.391896
1	3.178024	1.633326	2.745351
1	1.917942	1.944345	1.533057
1	1.66073	0.71816	2.801053
46	-0.103435	1.090565	-0.495403
15	1.599573	-0.746843	0.124317
17	1.613609	2.85748	-1.116283

pd_clet_ptbu3_cho_tsax

P	-1.2392	0.30663	-0.00922
C	-0.45182	2.03414	0.67558
C	2.13712	-0.8888	0.31183
C	2.57851	-2.97623	0.14753
C	1.29825	-3.60484	0.28837
Cl	-1.81397	-3.20771	0.02241
C	-2.91595	-0.02953	1.06656
Pd	0.21353	-1.8204	0.15638
C	-3.91849	-0.92433	0.28777
C	2.49775	-0.28899	1.55084
C	3.26167	0.88251	1.59787
C	3.68343	1.49222	0.39422
C	3.3563	0.91004	-0.84859
C	2.6056	-0.28059	-0.87601
C	4.46106	2.74237	0.47373
O	4.88346	3.39412	-0.50963
C	-0.25302	1.86719	2.20682

C	-1.30554	3.29905	0.38775
C	0.95103	2.30274	0.0637
C	-1.72811	0.56521	-1.92137
C	-2.95766	1.48333	-2.14597
C	-2.0052	-0.82902	-2.54365
C	-0.51127	1.16835	-2.67334
C	-2.48221	-0.81918	2.33382
C	-3.68745	1.24886	1.48874
O	3.30181	-3.26801	-0.9999
C	4.6953	-2.81052	-1.03905
H	4.67582	3.09299	1.50438
H	3.53939	1.34426	2.5411
H	3.67231	1.3649	-1.78216
H	2.39384	-0.75069	-1.834
H	2.18077	-0.74896	2.48601
H	4.73975	-1.71656	-1.06856
H	5.11495	-3.22946	-1.9554
H	5.2465	-3.1907	-0.16821
H	3.18079	-2.80376	1.04193
H	0.94918	-4.22171	-0.53718
H	1.01663	-3.95114	1.28225
H	-0.80707	4.16421	0.85004
H	-1.38813	3.45314	-0.69898
H	-2.31401	3.17033	0.81557
H	0.4191	2.66426	2.55558

H	-1.19081	1.96546	2.76146
H	0.20632	0.90592	2.4621
H	1.34107	3.23571	0.4979
H	1.65309	1.49484	0.29635
H	0.93702	2.41125	-1.02101
H	-3.08326	1.61274	-3.23168
H	-0.7511	1.21065	-3.74544
H	-2.02745	-0.71209	-3.63686
H	-1.19855	-1.53935	-2.25476
H	-3.8675	1.01201	-1.71151
H	-2.98272	-1.21504	-2.17734
H	-0.3054	2.19394	-2.2932
H	-2.78522	2.46759	-1.65584
H	0.38396	0.52786	-2.50892
H	-4.65081	0.9251	1.91095
H	-4.71998	-1.20379	0.98823
H	-3.37618	-1.00774	2.94656
H	-2.01973	-1.78628	2.03456
H	-4.34293	-0.3608	-0.57305
H	-3.10496	1.81039	2.253
H	-1.74294	-0.22083	2.9119
H	-3.39674	-1.83164	-0.09076
H	-3.84936	1.90037	0.60103

pd_clet_ptbu3_cho_tsbx

Pd	-0.51915	0.32419	-0.17846
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C	-1.32694	-1.50844	-0.96654
C	0.0658	-1.74595	-1.20235
C	1.4282	-0.51641	-0.24958
P	0.20606	2.69891	0.52275
Cl	-2.82195	1.2107	-0.06753
C	2.02927	2.90573	1.35918
C	3.12623	2.23278	0.4879
C	2.00318	2.14675	2.71469
C	2.48615	4.37272	1.58303
C	-1.12609	3.37286	1.88219
C	-1.483	2.16423	2.79355
C	-0.62312	4.55558	2.75092
C	-2.43992	3.84507	1.20205
C	0.08045	5.38107	-0.77895
C	0.13524	3.86321	-1.09357
C	1.38213	3.58685	-1.97591
C	-1.11342	3.46467	-1.92432
C	-3.29539	-1.86225	0.42253
O	-1.88144	-2.15356	0.13812
C	1.87397	-1.04256	0.9886
C	3.23645	-0.98659	1.33458
C	4.17558	-0.42773	0.44307
C	3.74164	0.07317	-0.80261
C	2.3776	0.01773	-1.15476
C	5.60738	-0.38024	0.80295

O	6.51559	0.09455	0.08257
H	2.05621	0.39914	-2.12212
H	4.46096	0.49986	-1.49918
H	3.56594	-1.38675	2.29094
H	1.16013	-1.49858	1.67027
H	0.50516	-2.58018	-0.66494
H	0.38672	-1.64153	-2.23545
H	-2.00921	-1.24569	-1.77665
H	-3.42946	-0.7924	0.61021
H	-3.54144	-2.45797	1.30371
H	-3.92247	-2.16686	-0.42648
H	0.12058	5.9301	-1.73167
H	1.34563	4.26463	-2.84203
H	-1.12975	4.08174	-2.83527
H	2.30878	3.77407	-1.38855
H	1.3711	2.52768	-2.3176
H	-0.86556	5.6214	-0.24415
H	-1.05582	2.38758	-2.19868
H	0.94639	5.66166	-0.13853
H	-2.03394	3.6426	-1.32456
H	3.44832	4.34418	2.11636
H	3.02211	2.13622	3.1268
H	4.04473	2.16416	1.0882
H	2.79551	1.21404	0.1854
H	1.31673	2.664	3.42177

H	2.6097	4.88543	0.60294
H	1.72428	4.91483	2.18667
H	1.64788	1.10461	2.55216
H	3.30854	2.84569	-0.42305
H	-1.45663	4.86407	3.39864
H	-3.1765	4.0248	1.99949
H	-2.18845	2.50663	3.5651
H	-1.95305	1.36014	2.18427
H	0.24239	4.23144	3.37104
H	-2.25757	4.78374	0.63253
H	-0.30763	5.39672	2.0939
H	-0.55793	1.77123	3.27158
H	-2.80512	3.05881	0.5041
H	5.8485	-0.80817	1.7984

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