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Quantitative DFT modeling of product concentration in organometallic reactions: Cu-mediated pentafluoroethylation of benzoic acid chlorides as a case study

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Supporting Information

Extended Computational Details

All the structures have been fully optimized in tetrahydrofuran (in PCM, see below) using the Gaussian09[1] suite of programs with 14 different functionals: BP86,[2] B3LYP,[3] CAM-B3LYP,[4] B3PW91,[3c, 5] PBE,[6] LC-wPBE,[7] PBE0,[6, 8] TPSS,[9] B97D,[10] wB97xD,[11] M06-L,[12] MN12SX,[13] M06,[14] and M06-2X.[14] In the optimization process the standard 6-31G*[15] basis set is used for all H, C, N, O, F, P and Cl atoms while the Stuttgart triple zeta basis set (SDD),[16] along with the associated ECP to describe the core electrons, has been employed for Cu, Br and I. Tight convergence criteria as well as ultrafine integration grids have been used in order to ensure satisfactory convergence. This is necessary because some of the species under study present a number of low frequency vibrational modes (<100 cm^{-1}) that contribute significantly to the entropy and have to be properly computed. In all cases the solvation energies are computed with the (IEF-PCM)[17] continuum dielectric solvation model using the SMD[18] radii and non-electrostatic terms. The dispersion correction terms have been included in the optimization process, except for B97D, wB97xD and MN12SX, by using the D3 method of Grimme[19] with the Becke-Jonhson damping parameter set to zero. These computational settings are named BS1. In all cases frequency calculations are carried out to ensure the nature of stationary points and transition states. Additional single point calculations, including solvation and dispersion corrections, on the optimized geometries for each functional are employed to obtain improved Gibss energy values with larger basis sets (BS2). The aug-cc-pVTZ-PP[20] basis set including polarization and the associated electron core potential has been employed for Cu, Br and I while the 6-311+G**[15c, 21] all-electron basis set is used for all the other atoms. Single point calculations with the DLNPO-CCSD(T)[22] method were carried out for the B3LYP optimized structures using the ORCA[23] software. Two different basis sets: def2-TZVPP[24] and aug-cc-pPVTZ,[25] and their corresponding auxiliary counterparts, were employed for this purpose. The computed Gibss energies were corrected to use a standard state corresponding to species in solution with a standard concentration of 1 M. The final Gibbs energies at a given temperature, computed on the basis of the rigid rotor/harmonic oscillator approach to statistical mechanics, are obtained with the following formula:

$$G_T^\circ = E_{BS2} + H_{corr,BS1} - TS_{BS1} + RT \ln (C^\circ/C^{1atm})$$

where E_{BS2} is the electronic energy, including the solvent and dispersion terms, obtained with the large basis sets (BS2). $H_{corr,BS1}$ is the thermal correction to the enthalpy and contains the zero-point energy plus the vibrational, rotational and translational energies; $T\Delta S_{BS1}$ accounts for the entropic correction. Both these terms are obtained with the small basis sets (BS1). Gibbs energies as output by Gaussian, which refer to an ideal gas (p = 1 atm) standard state, were corrected to use a standard state corresponding to species in solution with a standard concentration of 1 M. This was performed by adding an extra term to the Gaussian computed Gibss energy of each species; this correction is computed as RT ln(C°/C^{1atm}), where C° is the standard

reference state concentration (1 M), and C^{1atm} is the concentration of an ideal gas under the standard p = 1 atm conditions ($C^{1atm} = 1/V_m = P/RT = 0.0360$ M for an ideal gas at 338.15 K and 1 atm). Numerically, this corrective term equals to 2.3 kcal mol^{-1} per molecule at 338.15 K.
In the case of DLPNO-CCSD(T) calculations the formula for computing the Gibbs energy values takes the form:

$$G_T^\circ = E_{CCSD(T)} + H_{corr,BS1} - TS_{BS1} + RT \ln (C^\circ/C^{1atm}) + E_{solv,BS2}$$

where $E_{CCSD(T)}$ is the computed DLPNO-CCSD(T) energy. The energy of solvation in tetrahydrofuran $E_{solv,BS2}$ was computed as the energy difference between the species in solvent and in gas phase with BS2 ($E_{THF,BS2} - E_{gas,BS2}$).

Kinetics

The kinetics model, which allows the calculation of the transient concentrations of all the species during the reaction course, was built using the COPASI[26] software using the simple mass action law. The forward and backward rate constants for each step were calculated from the Gibbs energy differences along the reaction pathway. In the model all the steps were considered to be reversible although the energy difference between some of them would point to a non-reversible behavior; nevertheless, this assumption did not produce significant differences in the kinetics profiles. In all cases the reaction time and the initial concentrations of copper catalyst and substrate in the model were identical to those used in the experiments.

Rate constant calculations

For reactions proceeding without a barrier on the potential energy surface, *i.e.* the association/dissociation reactions, the rate constants are estimated, as in previous reports.[27] They are assumed to be diffusion controlled, with rate constants in solution given by the approximate expression:

$$k_{diff} = 8k_B T N_A / 3\eta$$

where k_B is the Boltzmann constant, T is the temperature, N_A is Avogadro's number and η is the solvent viscosity at that temperature.[28] For tetrahydrofuran at 65ºC and 1 atm, η has been estimated to be 0.308 mPa s, yielding a diffusion-controlled rate constant of 2.433 x 10^{10} M^{-1} s^{-1}. It has to be noted that this expression is employed for the association reaction, corresponding either to the forward (k_f) or backward (k_b) rate constant. Thus, once k_f or k_b is known the other one is easily computed through the formulation of the thermodynamic equilibrium constant K and the computed Gibbs energy difference between the intermediates involved (ΔG°):

$$\Delta G^\circ = -RTlnK$$

$$K = exp(-\Delta G°/RT)$$
$$K = k_f/k_b$$

For example, in the barrierless reaction $A + B \leftrightharpoons C$, the forward rate constant k_1 is equal to k_{diff}. The equilibrium constant K is computed placing the Gibbs energy in the expression above and, consequently, $k_b = k_f/K$.

In contrast, the rate constants of all the steps governed by a transition state are computed with the Eyring-Polanyi equation:

$$k = \frac{k_B T}{h} exp(-\Delta G^{\ddagger}/RT)$$

where k_B is the Boltzmann constant, T is the temperature, h is the Planck constant, $\Delta G^{\ddagger}$ is the activation Gibbs energy and R is the gas constant. The forward (k_f) and backward (k_b) rate constants are computed independently using their corresponding activation energies. For instance, in a reaction such as $A \leftrightharpoons B$ with a transition state TS_{AB} connecting both species, $\Delta G^{\ddagger}_{forward} = G°_{TSAB} - G°_A$ while $\Delta G^{\ddagger}_{backward} = G°_{TSAB} - G°_B$.

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Table S1. Energy terms (in Hartrees) and relative Gibbs energies (in kcal mol^{-1}) for the pentafluoroethylation of benzoic acid chloride using B3LYP without dispersion

Species	E_{BS2}	$H_{corr,BS1}$	TS_{BS1}	$G^{\circ}_{338.15K}$	Rel. $G^{\circ}_{338.15K}$
I	-2381.32193	0.51120	0.12520	-2380.93237	0.0
II	-1344.79926	0.21791	0.07876	-1344.65655	-11.1
III	-2150.11959	0.32945	0.11020	-2149.89678	-2.6
OATS	-2150.09624	0.32765	0.10081	-2149.86584	16.8
IV	-2150.11348	0.32944	0.09931	-2149.87979	8.0
RETS	-2150.09160	0.32838	0.09857	-2149.85824	21.6
V	-2150.15685	0.33135	0.10705	-2149.92899	-22.8
VI	-1229.48173	0.18829	0.06286	-1229.35274	-33.2
VII	-2266.00803	0.48049	0.10993	-2265.63390	-25.5
C_6H_5COCl	-805.31995	0.10966	0.04700	-805.25373	-
$C_6H_5COC_2F_5$	-920.67601	0.14128	0.06159	-920.59277	-
PPh_3	-1036.51688	0.29125	0.07143	-1036.29350	-

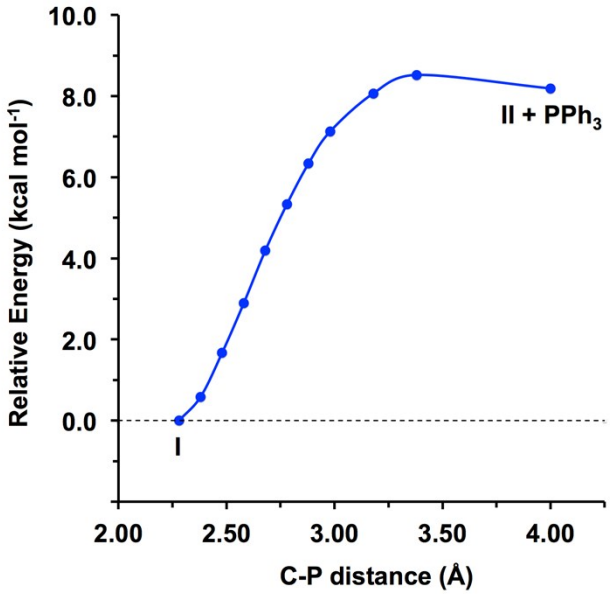


Figure S1. C-P bond elongation analysis describing the PPh_3 dissociation from complex **I** (energy values, in kcal mol^{-1}, correspond to electronic energies obtained with the large basis sets).

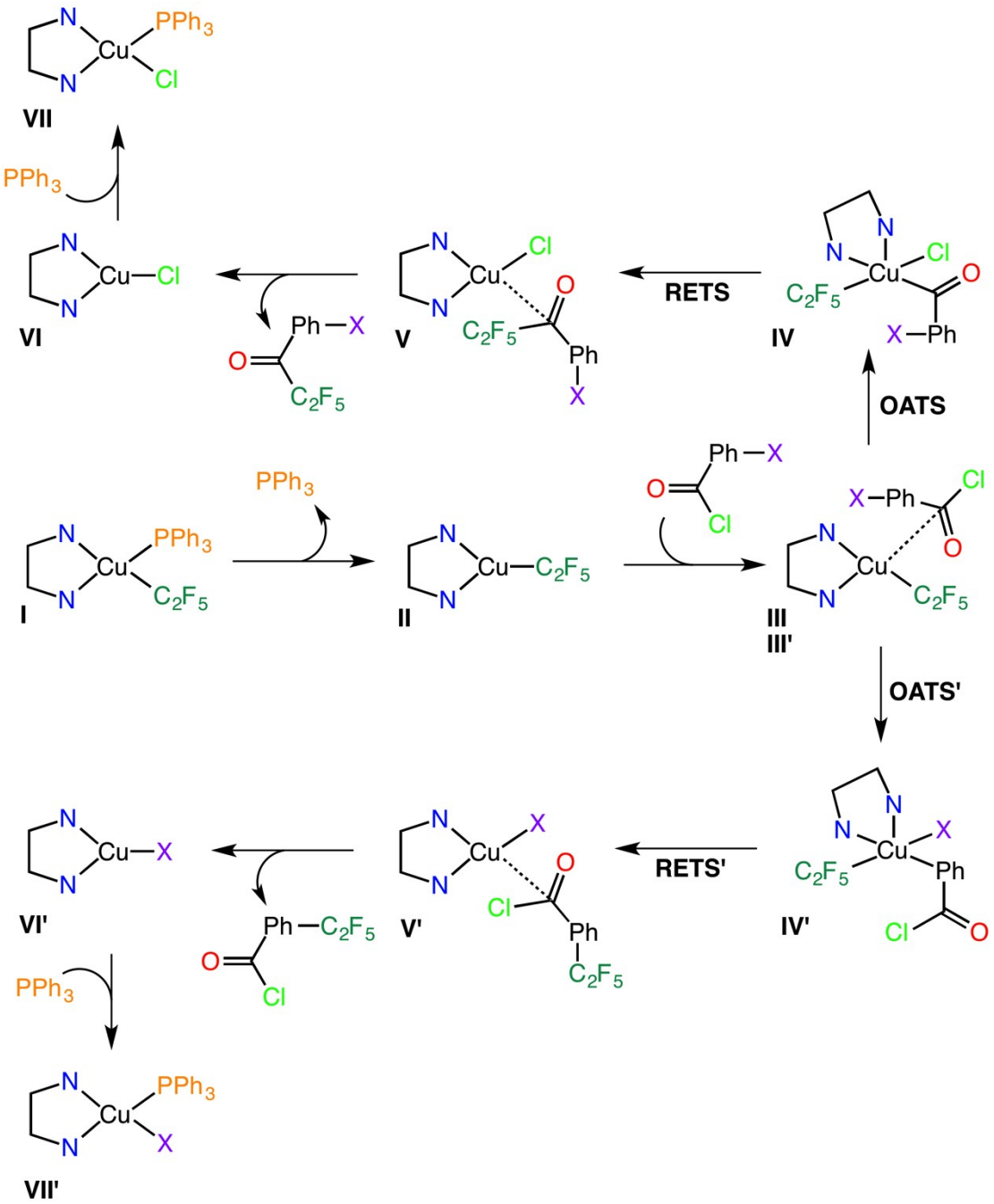
Table S2. Computed Gibbs energy profiles (in kcal mol^{-1}) and calculated concentrations in solution for the Cu-mediated pentafluoroethylation of benzoic acid chloride with B3LYP and DLPNO-CCSD(T) with different basis sets.

Functional	I	II	III	OATS	IV	RETS	V	VI	VII	Yield (%)
B3LYP	0.0	4.8	6.0	22.4	11.0	25.8	-10.8	-18.1	-24.6	92
CCSD(T)/ def2-TZVPP	0.0	2.4	5.6	24.2	12.1	25.2	-15.6	-24.1	-28.5	96
CCSD(T)/ aug-cc-pVTZ	0.0	5.5	6.0	25.1	11.9	25.4	-15.7	-23.1	-29.0	93

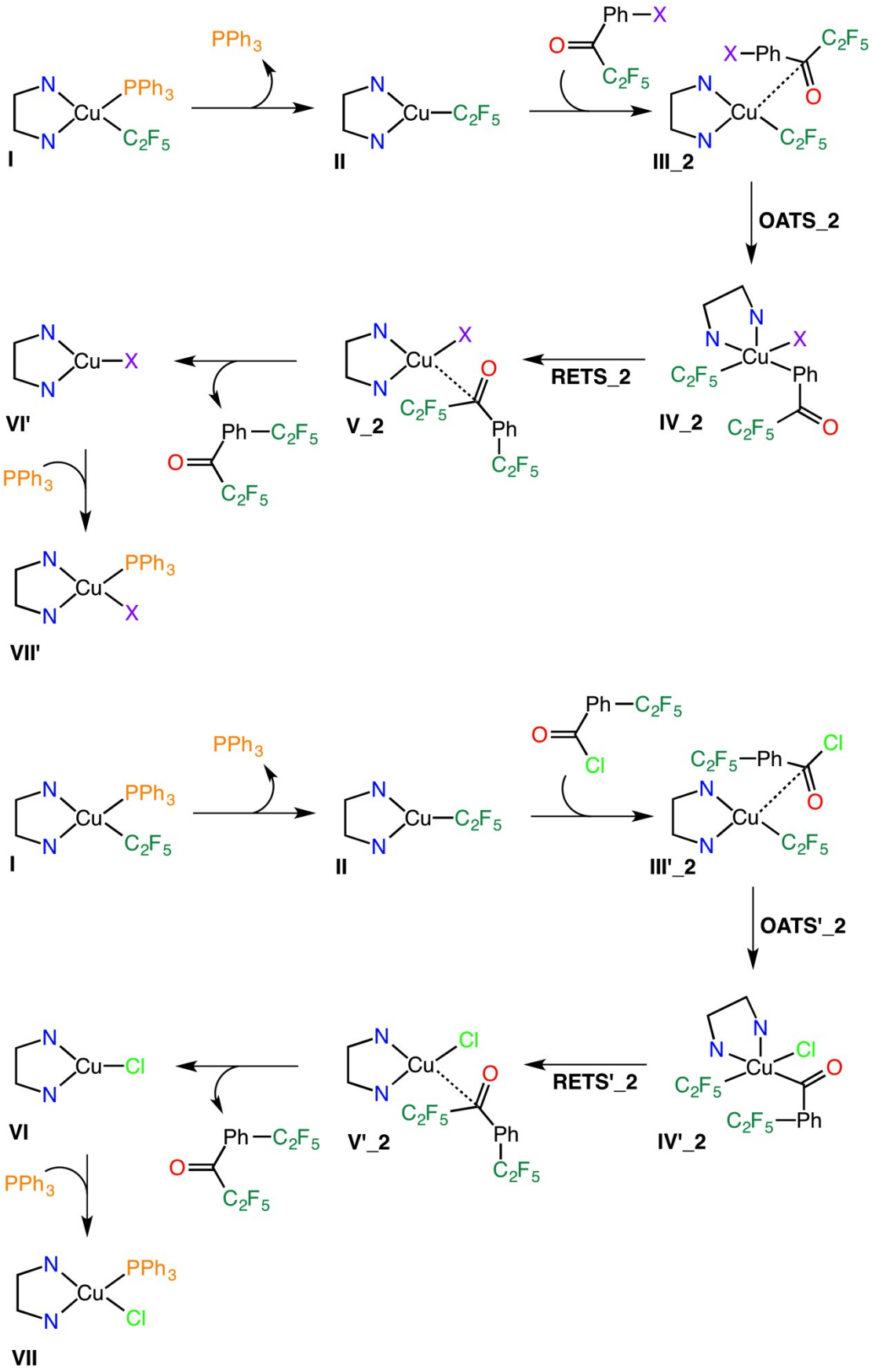
Table S3. Computed Gibbs energy profiles (in kcal mol^{-1}) for the Cu-mediated pentafluoroethylation of monosubstituted benzoic acid chlorides.

Substrate	I	II	III	OATS	IV	RETS	V	VI	VII
C_6H_5COCl	0.0	4.8	6.0	22.4	11.0	25.8	-10.8	-18.1	-24.6
C_6F_5COCl*	0.0	6.4	7.5	19.4	8.4	21.1	-15.2	-17.1	-24.9
o-F-C_6H_4COCl	0.0	4.8	6.7	21.6	10.2	24.4	-10.4	-17.7	-24.1
p-F-C_6H_4COCl	0.0	4.8	7.0	22.3	10.6	24.8	-10.6	-18.3	-24.7
o-Cl-C_6H_4COCl	0.0	4.8	7.0	22.2	10.1	25.5	-12.4	-18.1	-24.5
p-Cl-C_6H_4COCl	0.0	4.8	6.3	22.1	10.6	25.2	-11.9	-18.2	-24.6
o-Me-C_6H_4COCl	0.0	4.8	7.1	21.4	10.2	25.1	-11.9	-17.0	-23.4
p-Me-C_6H_4COCl	0.0	4.8	8.5	22.5	11.1	26.4	-11.3	-18.4	-24.9
m-CF_3-C_6H_4COCl	0.0	4.8	5.3	22.1	9.7	24.3	-10.7	-18.4	-24.9
p-MeO-C_6H_4COCl	0.0	4.8	7.9	22.3	10.8	26.4	-9.9	-18.1	-24.6

* Reaction carried out at room temperature.



Scheme S1. Proposed mechanism for the first pentafluroethylation of benzoic acid chlorides with more than one reactive position, X-$C_6H_4COC_2F_5$ (X = *o*-Br, *p*-I) and C_2F_5-C_6H_4COCl products are obtained.



Scheme S2. Catalytic cycles for the obtention of the doubly pentafluoroethylated product using X-$C_6H_4COC_2F_5$ (X = *o*-Br, *p*-I) and C_2F_5-C_6H_4COCl as substrates.

Table S4. Computed Gibbs energy profiles for *p*-I-C_6H_4COCl and *o*-Br-C_6H_4COCl (in kcal mol^{-1}).

Species	*p*-I-C_6H_4COCl	*o*-Br-C_6H_4COCl
I	0.00	0.00
II	4.84	4.84
III	6.61	6.84
OATS	22.47	22.08
IV	10.64	10.02
RETS	25.35	25.51
V	-10.50	-13.10
VI	-16.91	-17.06
VII	-23.38	-23.53
III’	4.01	5.67
OATS’	23.60	25.82
IV’	14.19	13.66
RETS’	25.59	26.30
V’	-35.33	-24.76
VI’	-35.59	-29.55
VII’	-44.46	-36.79
II	-18.53	-18.69
III_2	-18.06	-18.24
OATS_2	-0.11	1.42
IV_2	-8.84	-10.48
RETS_2	1.93	3.32
V_2	-59.18	-46.20
VI’	-60.58	-53.70
VII’	-69.45	-60.94
II	-39.62	-31.95
III’_2	-38.13	-29.29
OATS’_2	-22.80	-12.14
IV’_2	-34.13	-25.48
RETS’_2	-20.30	-10.41
V’_2	-60.55	-46.50
VI	-62.98	-54.47
VII	-69.45	-60.94

Computed energy terms (in Hartrees) for all the species. The final G_T° values are computed with the formula shown above. The value of the term $RT \ln(C^\circ/C^{1atm})$ is equal to 0.00356 and 0.00302 Hartrees at 338.15 K and 298.15 K, respectively.

Substrate: C_6H_5COCl

Functional: B3LYP

Species	E_{BS2}	$H_{corr,BS1}$	TS_{BS1}	$G^\circ_{338.15K}$
I	-2381.40937	0.51109	0.12367	-2381.01839
II	-1344.82847	0.21795	0.07911	-1344.68608
III	-2150.17686	0.32957	0.10419	-2149.94792
OATS	-2150.15227	0.32774	0.10073	-2149.92170
IV	-2150.17454	0.32981	0.09875	-2149.93991
RETS	-2150.15205	0.32863	0.09643	-2149.91629
V	-2150.20530	0.33150	0.10441	-2149.97465
VI	-1229.50446	0.18837	0.06320	-1229.37572
VII	-2266.08419	0.48169	0.11169	-2265.71064
C_6H_5COCl	-805.32988	0.10971	0.04698	-805.26360
$C_6H_5COC_2F_5$	-920.69411	0.14140	0.06135	-920.61049
PPh_3	-1036.54803	0.29135	0.07148	-1036.32460
$I^{+\cdot}$	-2381.24786	0.51271	0.11828	-2380.84987
$II^{+\cdot}$	-1344.66101	0.21954	0.07514	-1344.51305
$C_6H_5COCl^{-\cdot}$	-805.42326	0.10658	0.04888	-805.36199
IV_triplet	-2149.64306	0.32900	0.10547	-2149.90647
IV_cationic	-1689.74608	0.32830	0.09105	-1689.50527
Cl^-	-460.39750	0.00249	0.01972	-460.41117

Substrate: C_6H_5COCl				
Functional: BP86				
Species	E_{BS2}	$H_{corr,BS1}$	TS_{BS1}	$G^{\circ}_{338.15K}$
I	-2381.53692	0.49751	0.12388	-2381.15973
II	-1344.93815	0.21213	0.07901	-1344.80147
III	-2150.32213	0.32073	0.10387	-2150.10171
OATS	-2150.30258	0.31917	0.10339	-2150.08325
IV	-2150.32806	0.32111	0.10036	-2150.10376
RETS	-2150.30492	0.32003	0.09712	-2150.07845
V	-2150.33809	0.32269	0.10167	-2150.11351
VI	-1229.63635	0.18340	0.06366	-1229.51305
VII	-2266.23385	0.46872	0.11060	-2265.87218
C_6H_5COCl	-805.35941	0.10685	0.04750	-805.29651
$C_6H_5COC_2F_5$	-920.69497	0.13747	0.06245	-920.61639
PPh_3	-1036.55100	0.28351	0.07367	-1036.33760

Substrate: C_6H_5COCl				
Functional: CAM-B3LYP				
Species	E_{BS2}	$H_{corr,BS1}$	TS_{BS1}	$G^{\circ}_{338.15K}$
I	-2380.44503	0.51746	0.12316	-2380.04717
II	-1344.30070	0.22092	0.07855	-1344.15477
III	-2149.45984	0.33383	0.10314	-2149.22559
OATS	-2149.43543	0.33192	0.10020	-2149.20014
IV	-2149.45548	0.33411	0.09725	-2149.21506
RETS	-2149.43437	0.33291	0.09477	-2149.19267
V	-2149.49439	0.33574	0.10260	-2149.25769
VI	-1229.11465	0.19067	0.06238	-1228.98279
VII	-2265.25835	0.48745	0.11082	-2264.87816
C_6H_5COCl	-805.14295	0.11100	0.04667	-805.07507
$C_6H_5COC_2F_5$	-920.37311	0.14333	0.06141	-920.28762
PPh_3	-1036.11377	0.29475	0.07082	-1035.88628

Substrate: C_6H_5COCl				
Functional: B3PW91				
Species	E_{BS2}	$H_{corr,BS1}$	TS_{BS1}	$G^{\circ}_{338.15K}$
I	-2380.68333	0.51258	0.12168	-2380.28887
II	-1344.41582	0.21867	0.07957	-1344.27316
III	-2149.57485	0.33059	0.10251	-2149.34321
OATS	-2149.55103	0.32889	0.10055	-2149.31913
IV	-2149.57323	0.33090	0.09854	-2149.33731
RETS	-2149.55249	0.32970	0.09596	-2149.31518
V	-2149.59952	0.33257	0.10313	-2149.36652
VI	-1229.25647	0.18889	0.06298	-1229.12700
VII	-2265.52317	0.48263	0.10955	-2265.14653
C_6H_5COCl	-805.13581	0.11000	0.04694	-805.06920
$C_6H_5COC_2F_5$	-920.33703	0.14188	0.06146	-920.25305
PPh_3	-1036.22395	0.29194	0.07223	-1036.00068

Substrate: C_6H_5COCl				
Functional: PBE				
Species	E_{BS2}	$H_{corr,BS1}$	TS_{BS1}	$G^{\circ}_{338.15K}$
I	-2379.04911	0.49866	0.12672	-2378.67361
II	-1343.56123	0.21278	0.07907	-1343.42397
III	-2148.28161	0.32163	0.10546	-2148.06188
OATS	-2148.26916	0.32011	0.10202	-2148.04751
IV	-2148.28842	0.32191	0.10074	-2148.06369
RETS	-2148.26594	0.32086	0.09753	-2148.03906
V	-2148.30509	0.32345	0.10630	-2148.08439
VI	-1228.57698	0.18390	0.06388	-1228.45339
VII	-2264.06302	0.47029	0.11310	-2263.70227
C_6H_5COCl	-804.70300	0.10716	0.04741	-804.63969
$C_6H_5COC_2F_5$	-919.72106	0.13787	0.06239	-919.64203
PPh_3	-1035.44966	0.28435	0.07331	-1035.23507

Substrate: C_6H_5COCl				
Functional: LC-wPBE				
Species	E_{BS2}	$H_{corr,BS1}$	TS_{BS1}	$G^{\circ}_{338.15K}$
I	-2379.99686	0.52155	0.12010	-2379.59186
II	-1344.08174	0.22265	0.07781	-1343.93335
III	-2149.02551	0.33630	0.10193	-2148.78758
OATS	-2148.99797	0.33458	0.09903	-2148.75887
IV	-2149.01871	0.33664	0.09740	-2148.77591
RETS	-2148.99959	0.33554	0.09431	-2148.75480
V	-2149.05679	0.33828	0.10353	-2148.81847
VI	-1228.93201	0.19218	0.06235	-1228.79863
VII	-2264.84468	0.49111	0.10807	-2264.45808
C_6H_5COCl	-804.92308	0.11187	0.04659	-804.85425
$C_6H_5COC_2F_5$	-920.11759	0.14440	0.06100	-920.03063
PPh_3	-1035.87271	0.29696	0.07117	-1035.64336

Substrate: C_6H_5COCl				
Functional: PBE0				
Species	E_{BS2}	$H_{corr,BS1}$	TS_{BS1}	$G^{\circ}_{338.15K}$
I	-2379.08977	0.51482	0.12399	-2378.69538
II	-1343.50705	0.21992	0.07883	-1343.36241
III	-2148.27763	0.33210	0.10443	-2148.04640
OATS	-2148.25831	0.33052	0.09981	-2148.02405
IV	-2148.27613	0.33251	0.09855	-2148.03861
RETS	-2148.25732	0.33136	0.09549	-2148.01789
V	-2148.31112	0.33418	0.10550	-2148.07887
VI	-1228.57350	0.18977	0.06269	-1228.44286
VII	-2264.15466	0.48488	0.11195	-2263.77818
C_6H_5COCl	-804.75271	0.11052	0.04680	-804.68543
$C_6H_5COC_2F_5$	-919.73037	0.14272	0.06156	-919.64565
PPh_3	-1035.54713	0.29327	0.07171	-1035.32201

Substrate: C_6H_5COCl

Functional: TPSS

Species	E_{BS2}	$H_{corr,BS1}$	TS_{BS1}	$G^{\circ}_{338.15K}$
I	-2381.61584	0.50375	0.12454	-2381.23307
II	-1344.90252	0.21441	0.08041	-1344.76495
III	-2150.31397	0.32433	0.10453	-2150.09061
OATS	-2150.29821	0.32303	0.10131	-2150.07293
IV	-2150.32506	0.32479	0.10044	-2150.09716
RETS	-2150.30005	0.32368	0.09726	-2150.07007
V	-2150.33503	0.32635	0.10543	-2150.11055
VI	-1229.53444	0.18567	0.06401	-1229.40922
VII	-2266.24558	0.47526	0.11216	-2265.87892
C_6H_5COCl	-805.39194	0.10822	0.04738	-805.32754
$C_6H_5COC_2F_5$	-920.79323	0.13894	0.06235	-920.71308
PPh_3	-1036.67219	0.28756	0.07321	-1036.45428

Substrate: C_6H_5COCl

Functional: B97D

Species	E_{BS2}	$H_{corr,BS1}$	TS_{BS1}	$G^{\circ}_{338.15K}$
I	-2380.56452	0.49848	0.12573	-2380.18821
II	-1344.56102	0.21230	0.08042	-1344.42558
III	-2149.66480	0.32110	0.10860	-2149.44875
OATS	-2149.64561	0.31998	0.10220	-2149.42426
IV	-2149.66405	0.32170	0.10002	-2149.43880
RETS	-2149.64326	0.32063	0.09834	-2149.41742
V	-2149.68564	0.32317	0.10513	-2149.46405
VI	-1229.54530	0.18367	0.06385	-1229.42192
VII	-2265.54922	0.46993	0.11359	-2265.18932
C_6H_5COCl	-805.08629	0.10714	0.04756	-805.02315
$C_6H_5COC_2F_5$	-920.13553	0.13783	0.06154	-920.05568
PPh_3	-1035.97033	0.28444	0.07342	-1035.75575

Substrate: C_6H_5COCl				
Functional: wB97xD				
Species	E_{BS2}	$H_{corr,BS1}$	TS_{BS1}	$G^{\circ}_{338.15K}$
I	-2380.70222	0.51645	0.12279	-2380.30499
II	-1344.41886	0.22049	0.07903	-1344.27385
III	-2149.61433	0.33316	0.10218	-2149.37979
OATS	-2149.58551	0.33131	0.10153	-2149.35217
IV	-2149.60218	0.33320	0.09853	-2149.36395
RETS	-2149.58477	0.33226	0.09581	-2149.34475
V	-2149.64609	0.33527	0.10304	-2149.41030
VI	-1229.24492	0.19044	0.06243	-1229.11335
VII	-2265.52582	0.48660	0.10948	-2265.14514
C_6H_5COCl	-805.17537	0.11074	0.04682	-805.10789
$C_6H_5COC_2F_5$	-920.39384	0.14297	0.06225	-920.30956
PPh_3	-1036.24888	0.29440	0.07106	-1036.02199

Substrate: C_6H_5COCl				
Functional: M06-L				
Species	E_{BS2}	$H_{corr,BS1}$	TS_{BS1}	$G^{\circ}_{338.15K}$
I	-2381.08617	0.50910	0.12634	-2380.69986
II	-1344.65789	0.21748	0.07767	-1344.51452
III	-2149.92980	0.32888	0.10179	-2149.69916
OATS	-2149.91534	0.32701	0.09918	-2149.68395
IV	-2149.94188	0.32899	0.09920	-2149.70852
RETS	-2149.91731	0.32774	0.09720	-2149.68321
V	-2149.96151	0.33096	0.09965	-2149.72664
VI	-1229.39971	0.18795	0.06293	-1229.27113
VII	-2265.82581	0.48025	0.11083	-2265.45283
C_6H_5COCl	-805.25062	0.10965	0.04685	-805.18427
$C_6H_5COC_2F_5$	-920.55146	0.14122	0.06137	-920.46804
PPh_3	-1036.39136	0.29053	0.07226	-1036.16953

Substrate: C_6H_5COCl				
Functional: MN12SX				
Species	E_{BS2}	$H_{corr,BS1}$	TS_{BS1}	$G^{\circ}_{338.15K}$
I	-2378.07714	0.51356	0.12249	-2377.68251
II	-1342.17149	0.21957	0.07834	-1342.02670
III	-2147.18311	0.33129	0.10235	-2146.95060
OATS	-2147.15781	0.32975	0.10049	-2146.92498
IV	-2147.18967	0.33208	0.09825	-2146.95228
RETS	-2147.15938	0.33065	0.09530	-2146.92047
V	-2147.21049	0.33353	0.10341	-2146.97681
VI	-1227.14100	0.18913	0.06238	-1227.01069
VII	-2263.04687	0.48345	0.10884	-2262.66870
C_6H_5COCl	-804.99465	0.11024	0.04682	-804.92767
$C_6H_5COC_2F_5$	-920.06397	0.14267	0.06152	-919.97926
PPh_3	-1035.87917	0.29257	0.07224	-1035.65529

Substrate: C_6H_5COCl				
Functional: M06				
Species	E_{BS2}	$H_{corr,BS1}$	TS_{BS1}	$G^{\circ}_{338.15K}$
I	-2380.15503	0.50957	0.12128	-2379.76318
II	-1344.18855	0.21824	0.07760	-1344.04436
III	-2149.24894	0.32944	0.10073	-2149.01667
OATS	-2149.22561	0.32750	0.09778	-2148.99233
IV	-2149.24095	0.32915	0.09835	-2149.00660
RETS	-2149.22307	0.32848	0.09556	-2148.98659
V	-2149.27630	0.33166	0.09967	-2149.04075
VI	-1229.04432	0.18777	0.06232	-1228.91531
VII	-2265.00803	0.47908	0.10856	-2264.63395
C_6H_5COCl	-805.03608	0.10932	0.04695	-804.97016
$C_6H_5COC_2F_5$	-920.22188	0.14189	0.06068	-920.13711
PPh_3	-1035.92637	0.28971	0.07177	-1035.70488

Substrate: C_6H_5COCl				
Functional: M06-2X				
Species	E_{BS2}	$H_{corr,BS1}$	TS_{BS1}	$G^{\circ}_{338.15K}$
I	-2380.63228	0.51562	0.12611	-2380.23921
II	-1344.41927	0.22051	0.07995	-1344.27515
III	-2149.58470	0.33294	0.10260	-2149.35080
OATS	-2149.55178	0.33131	0.10077	-2149.31768
IV	-2149.55969	0.33306	0.09895	-2149.32202
RETS	-2149.55641	0.33180	0.09873	-2149.31978
V	-2149.62398	0.33522	0.10142	-2149.38662
VI	-1229.25837	0.19002	0.06274	-1229.12753
VII	-2265.46852	0.48536	0.10981	-2265.08942
C_6H_5COCl	-805.14429	0.11069	0.04678	-805.07682
$C_6H_5COC_2F_5$	-920.35794	0.14341	0.06133	-920.27230
PPh_3	-1036.18598	0.29365	0.07200	-1035.96078

Substrate: C_6F_5COCl				
Functional: B3LYP				
Species	E_{BS2}	$H_{corr,BS1}$	TS_{BS1}	$G^{\circ}_{338.15K}$
I	-2381.40937	0.51096	0.10904	-2381.00443
II	-1344.82847	0.21782	0.06976	-1344.67739
III	-2646.46613	0.29265	0.09846	-2646.26893
OATS	-2646.44569	0.29083	0.09825	-2646.25009
IV	-2646.46633	0.29275	0.09701	-2646.26758
RETS	-2646.44512	0.29161	0.09683	-2646.24732
V	-2646.50530	0.29434	0.09775	-2646.30569
VI	-1229.50446	0.18825	0.05572	-1229.36892
VII	-2266.08419	0.48156	0.09848	-2265.69809
C_6H_5COCl	-1301.61648	0.07242	0.05229	-1301.59333
$C_6H_5COC_2F_5$	-1416.98206	0.10391	0.06423	-1416.93936
PPh_3	-1036.54803	0.29122	0.06302	-1036.31681

Substrate: *o*-F-C_6H_4COCl				
Functional: B3LYP				
Species	E_{BS2}	$H_{corr,BS1}$	TS_{BS1}	$G^{\circ}_{338.15K}$
III	-2249.43604	0.32202	0.10522	-2249.21568
OATS	-2249.41635	0.32042	0.10264	-2249.19501
IV	-2249.43827	0.32245	0.10098	-2249.21324
RETS	-2249.41570	0.32127	0.09980	-2249.19067
V	-2249.46839	0.32388	0.10501	-2249.24596
C_6H_5COCl	-904.59188	0.10216	0.04950	-904.53567
$C_6H_5COC_2F_5$	-1019.95597	0.13380	0.06324	-1019.88186

Substrate: *p*-F-C_6H_4COCl				
Functional: B3LYP				
Species	E_{BS2}	$H_{corr,BS1}$	TS_{BS1}	$G^{\circ}_{338.15K}$
III	-2249.44489	0.32226	0.10595	-2249.22503
OATS	-2249.42154	0.32027	0.10286	-2249.20057
IV	-2249.44386	0.32234	0.10127	-2249.21922
RETS	-2249.42137	0.32116	0.09989	-2249.19654
V	-2249.47487	0.32411	0.10584	-2249.25304
C_6H_5COCl	-904.59876	0.10219	0.04930	-904.54231
$C_6H_5COC_2F_5$	-1019.96328	0.13387	0.06365	-1019.88950

Substrate: *o*-Cl-C_6H_4COCl				
Functional: B3LYP				
Species	E_{BS2}	$H_{corr,BS1}$	TS_{BS1}	$G^{\circ}_{338.15K}$
III	-2609.79157	0.32078	0.10731	-2609.57455
OATS	-2609.76984	0.31923	0.10335	-2609.55040
IV	-2609.79247	0.32140	0.10219	-2609.56970
RETS	-2609.77014	0.32013	0.09867	-2609.54512
V	-2609.82423	0.32266	0.10744	-2609.60545
C_6H_5COCl	-1264.94579	0.10104	0.05074	-1264.89193
$C_6H_5COC_2F_5$	-1380.30970	0.13259	0.06522	-1380.23876

Substrate: *p*-Cl-C_6H_4COCl				
Functional: B3LYP				
Species	E_{BS2}	$H_{corr,BS1}$	TS_{BS1}	$G^{\circ}_{338.15K}$
III	-2609.80221	0.32114	0.10679	-2609.58430
OATS	-2609.77774	0.31928	0.10432	-2609.55923
IV	-2609.79988	0.32138	0.10261	-2609.57754
RETS	-2609.77760	0.32020	0.10038	-2609.55422
V	-2609.83071	0.32304	0.10915	-2609.61327
C_6H_5COCl	-1264.95461	0.10122	0.05076	-1264.90059
$C_6H_5COC_2F_5$	-1380.31912	0.13293	0.06499	-1380.24762

Substrate: *o*-Me-C_6H_4COCl				
Functional: B3LYP				
Species	E_{BS2}	$H_{corr,BS1}$	TS_{BS1}	$G^{\circ}_{338.15K}$
III	-2189.50792	0.35929	0.10399	-2189.24907
OATS	-2189.48338	0.35746	0.10383	-2189.22619
IV	-2189.50432	0.35927	0.10252	-2189.24402
RETS	-2189.48183	0.35809	0.10011	-2189.22029
V	-2189.54040	0.36114	0.10353	-2189.27923
C_6H_5COCl	-844.65837	0.13913	0.05086	-844.56655
$C_6H_5COC_2F_5$	-960.02183	0.17081	0.06417	-959.91163

Substrate: *p*-Me-C_6H_4COCl				
Functional: B3LYP				
Species	E_{BS2}	$H_{corr,BS1}$	TS_{BS1}	$G^{\circ}_{338.15K}$
III	-2189.50762	0.35886	0.10689	-2189.25209
OATS	-2189.48471	0.35706	0.10577	-2189.22986
IV	-2189.50686	0.35913	0.10381	-2189.24799
RETS	-2189.48420	0.35799	0.10096	-2189.22361
V	-2189.53865	0.36080	0.10940	-2189.28369
C_6H_5COCl	-844.66263	0.13905	0.05187	-844.57190
$C_6H_5COC_2F_5$	-960.02708	0.17068	0.06643	-959.91927

Substrate: *m*-CF_3-C_6H_4COCl

Functional: B3LYP

Species	E_{BS2}	$H_{corr,BS1}$	TS_{BS1}	$G^{\circ}_{338.15K}$
III	-2487.33105	0.33763	0.11294	-2487.10281
OATS	-2487.30669	0.33621	0.10919	-2487.07611
IV	-2487.32775	0.33812	0.10981	-2487.09589
RETS	-2487.30596	0.33685	0.10704	-2487.07259
V	-2487.35724	0.33978	0.11441	-2487.12831
C_6H_5COCl	-1142.48097	0.11787	0.05796	-1142.41751
$C_6H_5COC_2F_5$	-1257.84549	0.14954	0.07249	-1257.76487

Substrate: *p*-MeO-C_6H_4COCl

Functional: B3LYP

Species	E_{BS2}	$H_{corr,BS1}$	TS_{BS1}	$G^{\circ}_{338.15K}$
III	-2264.74194	0.36509	0.10944	-2264.48273
OATS	-2264.71815	0.36308	0.10821	-2264.45973
IV	-2264.74039	0.36519	0.10639	-2264.47803
RETS	-2264.71744	0.36403	0.10341	-2264.45326
V	-2264.77272	0.36715	0.10911	-2264.51111
C_6H_5COCl	-919.89653	0.14513	0.05366	-919.80150
$C_6H_5COC_2F_5$	-1035.26117	0.17692	0.06773	-1035.14842

Substrate: *p*-I-C_6H_4COCl				
Functional: B3LYP				
Species	E_{BS2}	$H_{corr,BS1}$	TS_{BS1}	$G^{\circ}_{338.15K}$
III	-2445.37758	0.32057	0.10848	-2445.16192
OATS	-2445.35242	0.31872	0.10650	-2445.13664
IV	-2445.37449	0.32079	0.10536	-2445.15550
RETS	-2445.35221	0.31961	0.10301	-2445.13205
V	-2445.40570	0.32246	0.10950	-2445.18918
III’	-2445.37860	0.32026	0.11128	-2445.16607
OATS’	-2445.34902	0.31862	0.10801	-2445.13485
IV’	-2445.36912	0.32145	0.10574	-2445.14985
RETS’	-2445.35066	0.32041	0.10498	-2445.13167
V’	-2445.44836	0.32316	0.10711	-2445.22875
VI’	-1065.08376	0.18824	0.06505	-1064.95702
VII’	-2101.66792	0.48182	0.11321	-2101.29575
III_2	-2560.74255	0.35203	0.12203	-2560.50899
OATS_2	-2560.71427	0.35047	0.12013	-2560.48038
IV_2	-2560.73286	0.35379	0.11879	-2560.49430
RETS_2	-2560.71520	0.35216	0.11765	-2560.47714
V_2	-2560.81351	0.35485	0.11943	-2560.57452
III’_2	-2725.19118	0.35289	0.12113	-2724.95586
OATS’_2	-2725.16769	0.35114	0.11843	-2724.93142
IV’_2	-2725.18950	0.35319	0.11674	-2724.94949
RETS’_2	-2725.16775	0.35200	0.11526	-2724.92745
V’_2	-2725.23215	0.35497	0.11796	-2724.99159
p-I-C_6H_4COCl	-1100.52949	0.10067	0.05340	-1100.47866
p-I-$C_6H_4COC_2F_5$	-1215.89386	0.13244	0.06580	-1215.82367
p-C_2F_5-C_6H_4COCl	-1380.34337	0.13299	0.06533	-1380.27215
p-C_2F_5-$C_6H_4COC_2F_5$	-1495.70762	0.16455	0.08021	-1495.61973

Substrate: *o*-Br-C_6H_4COCl				
Functional: B3LYP				
Species	E_{BS2}	$H_{corr,BS1}$	TS_{BS1}	$G^{\circ}_{338.15K}$
III	-2566.48753	0.32045	0.10756	-2566.27108
OATS	-2566.46368	0.31883	0.10550	-2566.24679
IV	-2566.48627	0.32090	0.10420	-2566.26601
RETS	-2566.46385	0.31969	0.10072	-2566.24133
V	-2566.52223	0.32237	0.10656	-2566.30286
III’	-2566.48856	0.32061	0.10856	-2566.27295
OATS’	-2566.45740	0.31873	0.10572	-2566.24083
IV’	-2566.48210	0.32126	0.10293	-2566.26021
RETS’	-2566.46160	0.32002	0.10206	-2566.24007
V’	-2566.53654	0.32266	0.11111	-2566.32143
VI’	-1186.19548	0.18828	0.06520	-1186.06884
VII’	-2222.77651	0.48166	0.11369	-2222.40498
III_2	-2681.85196	0.35198	0.12237	-2681.61880
OATS_2	-2681.82366	0.35051	0.11787	-2681.58747
IV_2	-2681.84792	0.35293	0.11501	-2681.60644
RETS_2	-2681.82462	0.35172	0.11510	-2681.58444
V_2	-2681.90047	0.35433	0.12078	-2681.66336
III’_2	-2725.17910	0.35271	0.11924	-2724.94207
OATS’_2	-2725.15331	0.35112	0.11611	-2724.91473
IV’_2	-2725.17661	0.35289	0.11584	-2724.93600
RETS’_2	-2725.15455	0.35200	0.11300	-2724.91198
V’_2	-2725.20999	0.35460	0.11767	-2724.96950
o-Br-C_6H_4COCl	-1221.63981	0.10059	0.05252	-1221.58818
o-Br-$C_6H_4COC_2F_5$	-1337.00373	0.13217	0.06544	-1336.93344
o-C_2F_5-C_6H_4COCl	-1380.33216	0.13276	0.06439	-1380.26023
o-C_2F_5-$C_6H_4COC_2F_5$	-1495.69579	0.16424	0.07848	-1495.60647

Substrate: C_6H_5COCl

Method/basis set: DLPNO-CCSD(T)/def2-TZVPP

($H_{corr,BS1}$ and $T\Delta S_{BS1}$ are the same used above for the B3LYP functional)

Species	$E_{CCSD(T)}$	$E_{solv,BS2}$	$G^{\circ}_{338.15K}$
I	-3819.37062	-0.04212	-3819.02176
II	-2784.78707	-0.03316	-2784.67783
III	-3588.91823	-0.03754	-3588.72682
OATS	-3588.89177	-0.03605	-3588.69724
IV	-3588.91287	-0.03822	-3588.71647
RETS	-3588.89054	-0.04089	-3588.69567
V	-3588.94322	-0.04804	-3588.76062
VI	-2669.79427	-0.03845	-2669.70399
VII	-3704.37258	-0.05209	-3704.05111
C_6H_5COCl	-804.10774	-0.01261	-804.05407
$C_6H_5COC_2F_5$	-919.14323	-0.01058	-919.07020
PPh_3	-1034.54500	-0.01850	-1034.34007

Substrate: C_6H_5COCl

Method/basis set: DLPNO-CCSD(T)/aug-cc-PVTZ

($H_{corr,BS1}$ and $T\Delta S_{BS1}$ are the same used above for the B3LYP functional)

Species	$E_{CCSD(T)}$	$E_{solv,BS2}$	$G^{\circ}_{338.15K}$
I	-3819.53595	-0.04212	-3819.18708
II	-2784.90712	-0.03316	-2784.79789
III	-3589.07057	-0.03754	-3588.87916
OATS	-3589.04333	-0.03605	-3588.84880
IV	-3589.06630	-0.03822	-3588.86990
RETS	-3589.04322	-0.04089	-3588.84835
V	-3589.09648	-0.04804	-3588.91388
VI	-2669.90161	-0.03845	-2669.81133
VII	-3704.52265	-0.05209	-3704.20118
C_6H_5COCl	-804.13580	-0.01261	-804.08213
$C_6H_5COC_2F_5$	-919.18723	-0.01058	-919.11420
PPh_3	-1034.58535	-0.01850	-1034.38042

Computed forward(k_f), backward (k_b) and equilibrium (K) constants. Note that all the bimolecular reactions, where the rate constants are given in M^{-1} s^{-1}, produce a Gibbs energy of activation that implicitly contains a reference to a standard state for the translational degrees of freedom of 1 M, so is consistent with the Gibbs energies as computed in this work. All the other rate constants are given in s^{-1}.

Substrate: C_6H_5COCl, Functional: B3LYP			
Step	k_f	k_b	K
$I \leftrightharpoons II + PPh_3$	1.804E+07	2.433E+10	7.415E-04
$II + C_6H_5COCl \leftrightharpoons III$	2.433E+10	1.257E+11	1.936E-01
$III \leftrightharpoons IV\ (OATS)$	1.639E+02	2.900E+05	-
$IV \leftrightharpoons V\ (RETS)$	1.855E+03	1.505E-11	-
$V \leftrightharpoons VI + C_6H_5COC_2F_5$	1.195E+15	2.433E+10	4.910E+04
$VI + PPh_3 \leftrightharpoons VII$	2.433E+10	1.599E+06	1.522E+04

Substrate: C_6H_5COCl, Functional: BP86			
Step	k_f	k_b	K
$I \leftrightharpoons II + PPh_3$	1.018E+02	2.433E+10	4.182E-09
$II + C_6H_5COCl \leftrightharpoons III$	2.433E+10	7.463E+08	3.260E+01
$III \leftrightharpoons IV\ (OATS)$	2.295E+05	3.371E+04	-
$IV \leftrightharpoons V\ (RETS)$	3.813E+02	4.256E-02	-
$V \leftrightharpoons VI + C_6H_5COC_2F_5$	7.063E+16	2.433E+10	2.903E+06
$VI + PPh_3 \leftrightharpoons VII$	2.433E+10	4.539E+01	5.360E+08

Substrate: C_6H_5COCl, Functional: CAM-B3LYP			
Step	k_f	k_b	K
$I \leftrightharpoons II + PPh_3$	8.050E+07	2.433E+10	3.309E-03
$II + C_6H_5COCl \leftrightharpoons III$	2.433E+10	1.290E+12	1.886E-02
$III \leftrightharpoons IV\ (OATS)$	3.373E+02	6.289E+06	-
$IV \leftrightharpoons V\ (RETS)$	5.886E+03	3.011E-14	-
$V \leftrightharpoons VI + C_6H_5COC_2F_5$	3.523E+15	2.433E+10	1.448E+05
$VI + PPh_3 \leftrightharpoons VII$	2.433E+10	5.031E+06	4.836E+03

Substrate: C_6H_5COCl, Functional: B3PW91			
Step	k_f	k_b	K
$I \leftrightharpoons II + PPh_3$	1.962E+04	2.433E+10	8.065E-07
$II + C_6H_5COCl \leftrightharpoons III$	2.433E+10	1.101E+10	2.210E+00
$III \leftrightharpoons IV\ (OATS)$	1.202E+03	2.974E+05	-
$IV \leftrightharpoons V\ (RETS)$	7.461E+03	1.060E-08	-
$V \leftrightharpoons VI + C_6H_5COC_2F_5$	7.467E+15	2.433E+10	3.069E+05
$VI + PPh_3 \leftrightharpoons VII$	2.433E+10	5.545E+02	4.388E+07

Substrate: C_6H_5COCl, Functional: PBE			
Step	k_f	k_b	K
$I \leftrightharpoons II + PPh_3$	2.986E+04	2.433E+10	1.227E-06
$II + C_6H_5COCl \leftrightharpoons III$	2.433E+10	1.279E+11	1.902E-01
$III \leftrightharpoons IV\ (OATS)$	1.043E+07	1.932E+06	-
$IV \leftrightharpoons V\ (RETS)$	7.197E+02	2.902E-06	-
$V \leftrightharpoons VI + C_6H_5COC_2F_5$	7.274E+14	2.433E+10	2.990E+04
$VI + PPh_3 \leftrightharpoons VII$	2.433E+10	6.092E+04	3.994E+05

Substrate: C_6H_5COCl, Functional: LC-wPBE			
Step	k_f	k_b	K
$I \leftrightharpoons II + PPh_3$	1.735E+04	2.433E+10	7.131E-07
$II + C_6H_5COCl \leftrightharpoons III$	2.433E+10	2.480E+10	9.811E-01
$III \leftrightharpoons IV\ (OATS)$	1.606E+01	8.664E+05	-
$IV \leftrightharpoons V\ (RETS)$	1.937E+04	1.057E-13	-
$V \leftrightharpoons VI + C_6H_5COC_2F_5$	5.742E+14	2.433E+10	2.360E+04
$VI + PPh_3 \leftrightharpoons VII$	2.433E+10	7.257E+03	3.353E+06

Substrate: C_6H_5COCl, Functional: PBE0			
Step	k_f	k_b	K
$I \leftrightharpoons II + PPh_3$	8.702E+05	2.433E+10	3.577E-05
$II + C_6H_5COCl \leftrightharpoons III$	2.433E+10	9.356E+10	2.601E-01
$III \leftrightharpoons IV\ (OATS)$	6.092E+03	8.773E+06	-
$IV \leftrightharpoons V\ (RETS)$	2.792E+04	1.302E-12	-
$V \leftrightharpoons VI + C_6H_5COC_2F_5$	1.978E+14	2.433E+10	8.132E+03
$VI + PPh_3 \leftrightharpoons VII$	2.433E+10	9.730E+04	2.500E+05

Substrate: C_6H_5COCl, Functional: TPSS			
Step	k_f	k_b	K
$I \leftrightharpoons II + PPh_3$	5.938E+04	2.433E+10	2.441E-06
$II + C_6H_5COCl \leftrightharpoons III$	2.433E+10	1.422E+11	1.711E-01
$III \leftrightharpoons IV\ (OATS)$	4.772E+05	1.048E+03	-
$IV \leftrightharpoons V\ (RETS)$	7.275E+01	2.703E-04	-
$V \leftrightharpoons VI + C_6H_5COC_2F_5$	1.419E+15	2.433E+10	5.832E+04
$VI + PPh_3 \leftrightharpoons VII$	2.433E+10	1.345E+04	1.809E+06

Substrate: C_6H_5COCl, Functional: B97D			
Step	k_f	k_b	K
$I \leftrightharpoons II + PPh_3$	3.937E+07	2.433E+10	1.618E-03
$II + C_6H_5COCl \leftrightharpoons III$	2.433E+10	2.398E+10	1.014E+00
$III \leftrightharpoons IV\ (OATS)$	8.288E+02	8.920E+06	-
$IV \leftrightharpoons V\ (RETS)$	1.495E+04	8.658E-07	-
$V \leftrightharpoons VI + C_6H_5COC_2F_5$	7.654E+15	2.433E+10	3.146E+05
$VI + PPh_3 \leftrightharpoons VII$	2.433E+10	4.582E+05	5.310E+04

Substrate: C_6H_5COCl, Functional: wB97xD			
Step	k_f	k_b	K
$I \leftrightharpoons II + PPh_3$	4.707E+06	2.433E+10	1.935E-04
$II + C_6H_5COCl \leftrightharpoons III$	2.433E+10	1.497E+11	1.625E-01
$III \leftrightharpoons IV\ (OATS)$	4.418E+01	1.172E+08	-
$IV \leftrightharpoons V\ (RETS)$	1.146E+05	1.825E-14	-
$V \leftrightharpoons VI + C_6H_5COC_2F_5$	3.168E+15	2.433E+10	1.302E+05
$VI + PPh_3 \leftrightharpoons VII$	2.433E+10	2.592E+06	9.386E+03

Substrate: C_6H_5COCl, Functional: M06-L			
Step	k_f	k_b	K
$I \leftrightharpoons II + PPh_3$	9.471E+03	2.433E+10	3.893E-07
$II + C_6H_5COCl \leftrightharpoons III$	2.433E+10	1.720E+10	1.415E+00
$III \leftrightharpoons IV\ (OATS)$	4.790E+06	7.617E+02	-
$IV \leftrightharpoons V\ (RETS)$	3.817E+02	1.709E-05	-

$V \leftrightharpoons VI + C_6H_5COC_2F_5$	2.925E+15	2.433E+10	1.202E+05
$VI + PPh_3 \leftrightharpoons VII$	2.433E+10	2.817E+05	8.636E+04

Substrate: C_6H_5COCl, Functional: MN12SX			
Step	k_f	k_b	K
$I \leftrightharpoons II + PPh_3$	1.485E+10	2.433E+10	6.104E-01
$II + C_6H_5COCl \leftrightharpoons III$	2.433E+10	8.205E+11	2.965E-02
$III \leftrightharpoons IV\ (OATS)$	2.865E+02	6.006E+01	-
$IV \leftrightharpoons V\ (RETS)$	8.886E-01	9.969E-11	-
$V \leftrightharpoons VI + C_6H_5COC_2F_5$	5.234E+15	2.433E+10	2.151E+05
$VI + PPh_3 \leftrightharpoons VII$	2.433E+10	1.917E+09	1.269E+01

Substrate: C_6H_5COCl, Functional: M06			
Step	k_f	k_b	K
$I \leftrightharpoons II + PPh_3$	5.352E+04	2.433E+10	2.200E-06
$II + C_6H_5COCl \leftrightharpoons III$	2.433E+10	3.252E+09	7.482E+00
$III \leftrightharpoons IV\ (OATS)$	9.458E+02	1.152E+07	-
$IV \leftrightharpoons V\ (RETS)$	1.482E+05	2.078E-09	-
$V \leftrightharpoons VI + C_6H_5COC_2F_5$	1.310E+15	2.433E+10	5.384E+04
$VI + PPh_3 \leftrightharpoons VII$	2.433E+10	6.371E+04	3.819E+05

Substrate: C_6H_5COCl, Functional: M06-2X			
Step	k_f	k_b	K
$I \leftrightharpoons II + PPh_3$	1.129E+09	2.433E+10	4.640E-02
$II + C_6H_5COCl \leftrightharpoons III$	2.433E+10	7.311E+10	3.328E-01
$III \leftrightharpoons IV\ (OATS)$	2.607E-01	1.226E+11	-
$IV \leftrightharpoons V\ (RETS)$	8.708E+11	5.505E-15	-
$V \leftrightharpoons VI + C_6H_5COC_2F_5$	5.564E+15	2.433E+10	2.287E+05
$VI + PPh_3 \leftrightharpoons VII$	2.433E+10	8.601E+09	2.829E+00
Substrate: C_6F_5COCl, Functional: B3LYP, at room temperature (298.15 K)			
Step	k_f	k_b	K
$I \leftrightharpoons II + PPh_3$	2.836E+05	1.448E+17	1.958E-05
$II + C_6F_5COCl \leftrightharpoons III$	1.448E+17	9.625E+17	1.505E-01
$III \leftrightharpoons IV\ (OATS)$	1.342E+04	5.619E+04	-
$IV \leftrightharpoons V\ (RETS)$	2.978E+03	8.797E-15	-
$V \leftrightharpoons VI + C_6F_5COC_2F_5$	2.241E+11	1.448E+10	1.547E+01
$VI + PPh_3 \leftrightharpoons VII$	1.448E+17	2.974E+04	4.870E+05

Substrate: *o*-F-C_6H_4COCl, Functional: B3LYP			
Step	k_f	k_b	K
$I \leftrightharpoons II + PPh_3$	1.804E+07	2.433E+10	7.415E-04
$II + oFC_6H_4COCl \leftrightharpoons III$	2.433E+10	3.861E+11	6.301E-02
$III \leftrightharpoons IV\ (OATS)$	1.600E+03	2.844E+05	-
$IV \leftrightharpoons V\ (RETS)$	4.914E+03	2.664E-10	-
$V \leftrightharpoons VI + oFC_6H_4COC_2F_5$	1.268E+15	2.433E+10	5.212E+04
$VI + PPh_3 \leftrightharpoons VII$	2.433E+10	1.599E+06	1.522E+04

Substrate: *p*-F-C_6H_4COCl, Functional: B3LYP			
Step	k_f	k_b	K
$I \leftrightharpoons II + PPh_3$	1.804E+07	2.433E+10	7.415E-04
$II + pFC_6H_4COCl \leftrightharpoons III$	2.433E+10	5.462E+11	4.312E-02
$III \leftrightharpoons IV\ (OATS)$	8.519E+02	1.920E+05	-

$IV \leftrightharpoons V\ (RETS)$	4.422E+03	8.538E-11	-
$V \leftrightharpoons VI + pFC_6H_4COC_2F_5$	2.141E+15	2.433E+10	8.799E+04
$VI + PPh_3 \leftrightharpoons VII$	2.433E+10	1.599E+06	1.522E+04

Substrate: *o*-Cl-C_6H_4COCl, Functional: B3LYP

Step	k_f	k_b	K
$I \leftrightharpoons II + PPh_3$	1.804E+07	2.433E+10	7.415E-04
$II + oClC_6H_4COCl \leftrightharpoons III$	2.433E+10	6.163E+11	3.948E-02
$III \leftrightharpoons IV\ (OATS)$	1.132E+03	1.045E+05	-
$IV \leftrightharpoons V\ (RETS)$	7.551E+02	2.393E-12	-
$V \leftrightharpoons VI + oClC_6H_4COC_2F_5$	1.125E+14	2.433E+10	4.623E+03
$VI + PPh_3 \leftrightharpoons VII$	2.433E+10	1.599E+06	1.522E+04

Substrate: *p*-Cl-C_6H_4COCl, Functional: B3LYP

Step	k_f	k_b	K
$I \leftrightharpoons II + PPh_3$	1.804E+07	2.433E+10	7.415E-04
$II + pClC_6H_4COCl \leftrightharpoons III$	2.433E+10	2.219E+11	1.097E-01
$III \leftrightharpoons IV\ (OATS)$	4.767E+02	2.634E+05	-
$IV \leftrightharpoons V\ (RETS)$	2.450E+03	7.952E-12	-
$V \leftrightharpoons VI + pClC_6H_4COC_2F_5$	2.967E+14	2.433E+10	1.220E+04
$VI + PPh_3 \leftrightharpoons VII$	2.433E+10	1.599E+06	1.522E+04

Substrate: *o*-Me-C_6H_4COCl, Functional: B3LYP

Step	k_f	k_b	K
$I \leftrightharpoons II + PPh_3$	1.804E+07	2.433E+10	7.415E-04
$II + oMeC_6H_4COCl \leftrightharpoons III$	2.433E+10	6.749E+11	3.605E-02
$III \leftrightharpoons IV\ (OATS)$	3.699E+03	4.127E+05	-
$IV \leftrightharpoons V\ (RETS)$	1.676E+03	8.743E-12	-
$V \leftrightharpoons VI + oMeC_6H_4COC_2F_5$	4.791E+13	2.433E+10	1.969E+03
$VI + PPh_3 \leftrightharpoons VII$	2.433E+10	1.599E+06	1.522E+04

Substrate: *p*-Me-C_6H_4COCl, Functional: B3LYP

Step	k_f	k_b	K
$I \leftrightharpoons II + PPh_3$	1.804E+07	2.433E+10	7.415E-04
$II + pMeC_6H_4COCl \leftrightharpoons III$	2.433E+10	5.931E+12	4.102E-03
$III \leftrightharpoons IV\ (OATS)$	6.779E+03	3.139E+05	-
$IV \leftrightharpoons V\ (RETS)$	9.137E+02	3.022E-12	-
$V \leftrightharpoons VI + pMeC_6H_4COC_2F_5$	9.356E+14	2.433E+10	3.845E+04
$VI + PPh_3 \leftrightharpoons VII$	2.433E+10	1.599E+06	1.522E+04

Substrate: *m*-CF_3-C_6H_4COCl, Functional: B3LYP

Step	k_f	k_b	K
$I \leftrightharpoons II + PPh_3$	1.804E+07	2.433E+10	7.415E-04
$II + mCF_3OC_6H_4COCl \leftrightharpoons III$	2.433E+10	5.030E+10	4.837E-01
$III \leftrightharpoons IV\ (OATS)$	1.047E+02	6.717E+04	-
$IV \leftrightharpoons V\ (RETS)$	2.501E+03	1.769E-10	-
$V \leftrightharpoons VI + mCF_3C_6H_4COC_2F_5$	2.347E+15	2.433E+10	9.644E+04
$VI + PPh_3 \leftrightharpoons VII$	2.433E+10	1.599E+06	1.522E+04

Substrate: *p*-MeO-C_6H_4COCl, Functional: B3LYP

Step	k_f	k_b	K
$I \leftrightharpoons II + PPh_3$	1.804E+07	2.433E+10	7.415E-04
$II + pMeOC_6H_4COCl \leftrightharpoons III$	2.433E+10	2.257E+12	1.078E-02

$III \leftrightharpoons IV\ (OATS)$	3.291E+03	2.646E+05	-
$IV \leftrightharpoons V\ (RETS)$	6.316E+02	2.423E-11	-
$V \leftrightharpoons VI + pMeOC_6H_4COC_2F_5$	4.690E+15	2.433E+10	1.927E+05
$VI + PPh_3 \leftrightharpoons VII$	2.433E+10	1.599E+06	1.522E+04

Substrate: *p*-I-C_6H_4COCl, Functional: B3LYP			
Step	k_f	k_b	K
$I \leftrightharpoons II + PPh_3$	1.804E+07	2.433E+10	7.415E-04
$II + pIC_6H_4COCl \leftrightharpoons III$	2.433E+10	3.369E+11	7.222E-02
$III \leftrightharpoons IV\ (OATS)$	3.941E+02	1.588E+05	-
$IV \leftrightharpoons V\ (RETS)$	2.179E+03	4.746E-11	-
$V \leftrightharpoons VI + pIC_6H_4COC_2F_5$	3.370E+14	2.433E+10	1.385E+04
$VI + PPh_3 \leftrightharpoons VII$	2.433E+10	1.599E+06	1.522E+04
$II + pIC_6H_4COCl \leftrightharpoons III'$	2.433E+10	7.027E+09	3.462E+00
$III' \leftrightharpoons IV'\ (OATS')$	1.534E+00	5.808E+06	-
$IV' \leftrightharpoons V'\ (RETS')$	2.987E+05	2.968E-27	-
$V' \leftrightharpoons VI' + pC_2F_5C_6H_4COCl$	3.582E+10	2.433E+10	1.472E+00
$VI' + PPh_3 \leftrightharpoons VII'$	2.433E+10	4.489E+04	5.420E+05
$II + pIC_6H_4COC_2F_5 \leftrightharpoons III\_2$	2.433E+10	4.925E+10	4.940E-01
$III\_2 \leftrightharpoons IV\_2\ (OATS\_2)$	1.756E+01	1.603E+07	-
$IV\_2 \leftrightharpoons V\_2\ (RETS\_2)$	7.732E+05	2.234E-27	-
$V\_2 \leftrightharpoons VI' + pC_2F_5C_6H_4COC_2F_5$	1.933E+11	2.433E+10	7.947E+00
$II + pC_2F_5C_6H_4COCl \leftrightharpoons III'\_2$	2.433E+10	2.222E+11	1.095E-01
$III'\_2 \leftrightharpoons IV'\_2\ (OATS'\_2)$	8.646E+02	3.319E+05	-
$IV'\_2 \leftrightharpoons V'\_2\ (RETS'\_2)$	8.090E+03	6.818E-14	-
$V'\_2 \leftrightharpoons VI + pC_2F_5C_6H_4COC_2F_5$	9.001E+11	2.433E+10	3.699E+01

Substrate: *o*-Br-C_6H_4COCl, Functional: B3LYP			
Step	k_f	k_b	K
$I \leftrightharpoons II + PPh_3$	1.804E+07	2.433E+10	7.415E-04
$II + oBrC_6H_4COCl \leftrightharpoons III$	2.433E+10	4.752E+11	5.120E-02
$III \leftrightharpoons IV\ (OATS)$	9.885E+02	1.120E+05	-
$IV \leftrightharpoons V\ (RETS)$	6.834E+02	7.799E-13	-
$V \leftrightharpoons VI + oBrC_6H_4COC_2F_5$	8.780E+12	2.433E+10	3.609E+02
$VI + PPh_3 \leftrightharpoons VII$	2.433E+10	1.599E+06	1.522E+04
$II + oBrC_6H_4COCl \leftrightharpoons III'$	2.433E+10	8.307E+10	2.929E-01
$III' \leftrightharpoons IV'\ (OATS')$	6.653E-01	9.737E+04	-
$IV' \leftrightharpoons V'\ (RETS')$	4.792E+04	7.094E-21	-
$V' \leftrightharpoons VI' + oC_2F_5C_6H_4COCl$	3.066E+13	2.433E+10	1.260E+03
$VI' + PPh_3 \leftrightharpoons VII'$	2.433E+10	5.083E+05	4.786E+04
$II + oBrC_6H_4COC_2F_5 \leftrightharpoons III\_2$	2.433E+10	4.761E+10	5.111E-01
$III\_2 \leftrightharpoons IV\_2\ (OATS\_2)$	1.387E+00	1.421E+05	-
$IV\_2 \leftrightharpoons V\_2\ (RETS\_2)$	8.408E+03	6.915E-20	-
$V\_2 \leftrightharpoons VI' + oC_2F_5C_6H_4COC_2F_5$	1.720E+15	2.433E+10	7.069E+04
$II + oC_2F_5C_6H_4COCl \leftrightharpoons III'\_2$	2.433E+10	1.277E+12	1.905E-02
$III'\_2 \leftrightharpoons IV'\_2\ (OATS'\_2)$	5.770E+01	1.671E+04	-
$IV'\_2 \leftrightharpoons V'\_2\ (RETS'\_2)$	1.281E+03	3.321E-11	-
$V'\_2 \leftrightharpoons VI + oC_2F_5C_6H_4COC_2F_5$	3.450E+15	2.433E+10	1.418E+05

Substrate: C_6H_5COCl, Functional: DLPNO-CCSD(T)/def2-TZVPP			
Step	k_f	k_b	K
$I \leftrightharpoons II + PPh_3$	6.596E+08	2.433E+10	2.711E-02
$II + C_6H_5COCl \leftrightharpoons III$	2.433E+10	2.792E+12	8.715E-03
$III \leftrightharpoons IV\ (OATS)$	7.088E+00	1.121E+05	-
$IV \leftrightharpoons V\ (RETS)$	2.588E+04	3.228E-14	-
$V \leftrightharpoons VI + C_6H_5COC_2F_5$	7.748E+15	2.433E+10	3.185E+05
$VI + PPh_3 \leftrightharpoons VII$	2.433E+10	3.361E+07	7.238E+02

Substrate: C_6H_5COCl, Functional: DLPNO-CCSD(T)/aug-cc-PVTZ			
Step	k_f	k_b	K
$I \leftrightharpoons II + PPh_3$	6.702E+06	2.433E+10	2.755E-04
$II + C_6H_5COCl \leftrightharpoons III$	2.433E+10	5.373E+10	4.528E-01
$III \leftrightharpoons IV\ (OATS)$	3.411E+00	1.958E+04	-
$IV \leftrightharpoons V\ (RETS)$	1.280E+04	1.858E-14	-
$V \leftrightharpoons VI + C_6H_5COC_2F_5$	1.289E+15	2.433E+10	5.297E+04
$VI + PPh_3 \leftrightharpoons VII$	2.433E+10	3.629E+06	6.704E+03

Cartesian Coordinates (in multi-xyz format)

64
I_B3LYP
Cu 2.169970 17.884766 1.137232
C 0.317086 16.273249 3.089735
H -0.346970 16.250938 2.230202
C -0.104541 15.795665 4.343435
H -1.106881 15.395448 4.456084
C 0.772516 15.850340 5.410564
H 0.480509 15.494206 6.394800
C 2.066222 16.382666 5.218106
C 2.398108 16.842229 3.917972
C 3.032788 16.493422 6.274322
H 2.759587 16.133580 7.262573
C 4.259806 17.043364 6.049380
H 4.983996 17.130127 6.854902
C 4.620942 17.539441 4.751148
C 5.855066 18.170672 4.482715
H 6.590228 18.270664 5.276773
C 6.105262 18.661807 3.214216
H 7.040262 19.158232 2.975360
C 5.121031 18.514516 2.220027
H 5.279227 18.898244 1.216457
C 3.692885 17.437633 3.682425
C 2.576031 21.294396 1.279770
C 3.438027 21.039715 0.200595
H 3.403742 20.073535 -0.297535
C 4.329353 22.022432 -0.237594
H 4.990443 21.815260 -1.075106
C 4.373290 23.262944 0.402851
H 5.070558 24.025695 0.066157
C 3.518338 23.522938 1.479111
H 3.549363 24.487654 1.978967
C 2.621828 22.545961 1.914376
H 1.966939 22.753956 2.755703
C -0.205626 20.486703 1.091746
C -0.735574 19.756668 0.017005
H -0.189784 18.900929 -0.373204
C -1.952718 20.134725 -0.557546
H -2.355070 19.565128 -1.391205
C -2.649124 21.237689 -0.059631
H -3.597251 21.529339 -0.503879
C -2.125894 21.969066 1.012888
H -2.666040 22.828499 1.401562
C -0.909274 21.598042 1.584938
H -0.510886 22.166547 2.420728
C 1.249715 20.091628 3.584910
C 0.047512 19.730166 4.217716
H -0.839170 19.526638 3.624300
C -0.018855 19.623019 5.607996
H -0.956672 19.341379 6.079776
C 1.112779 19.871367 6.389292
H 1.060834 19.783509 7.471155
C 2.313735 20.226350 5.769944
H 3.202240 20.413730 6.366956
C 2.385031 20.329093 4.379965
H 3.331165 20.585869 3.912350
N 1.527816 16.781442 2.877099
N 3.951284 17.921616 2.440919
P 1.419060 19.947058 1.762592
F 1.017594 17.122923 -1.385166
F 3.059098 17.991585 -1.579132
F 2.103004 14.899000 -0.188917
F 2.896578 15.365200 -2.162348
F 4.105293 15.748612 -0.392934
C 2.262517 17.204041 -0.710369
C 2.840679 15.803436 -0.879011

30
II_B3LYP
Cu 2.559516 18.222819 0.854201
C -0.097721 16.709013 2.274861
H -0.566792 16.797506 1.298253
C -0.775284 16.104798 3.353641
H -1.780297 15.720922 3.211826
C -0.138460 16.015853 4.576249
H -0.628584 15.557176 5.430790
C 1.171791 16.528719 4.718713
C 1.764936 17.115771 3.572449
C 1.907661 16.478566 5.950170
H 1.435252 16.023826 6.816501
C 3.169337 16.988918 6.032892
H 3.723689 16.950168 6.966396
C 3.801329 17.590717 4.892061
C 5.106207 18.131700 4.933796
H 5.668129 18.099908 5.863184
C 5.647561 18.692353 3.793617
H 6.645986 19.116143 3.790213
C 4.883431 18.711007 2.613854
H 5.275650 19.142119 1.699110
C 3.103396 17.654570 3.660353
N 1.130247 17.198549 2.379576
N 3.650104 18.210396 2.543264
F 0.651630 18.082375 -1.191800
F 2.023977 19.813276 -1.431674
F 2.727159 16.380498 -1.772135
F 2.318581 17.888731 -3.288986
F 4.075482 18.080200 -2.018271
C 1.988296 18.483980 -0.969208
C 2.772324 17.710519 -2.025662

44
III_B3LYP
Cu 2.625711 18.125468 0.843247
C -0.019597 16.546200 2.236781
H -0.454039 16.561989 1.240870
C -0.747979 16.053292 3.338940
H -1.755825 15.677761 3.194778
C -0.155919 16.061050 4.586891
H -0.684821 15.688400 5.460076
C 1.158492 16.562230 4.731622
C 1.801726 17.039141 3.561150
C 1.849606 16.607490 5.988905
H 1.338816 16.237762 6.873763
C 3.118474 17.099450 6.072111
H 3.640586 17.130713 7.024231
C 3.797509 17.597716 4.908810
C 5.105170 18.130921 4.954747
H 5.636143 18.162327 5.902010
C 5.685780 18.611332 3.797713
H 6.685822 19.031018 3.797931
C 4.953384 18.568802 2.599033
H 5.368127 18.955383 1.674899
C 3.139542 17.579064 3.654455
N 1.213139 17.021248 2.342567
N 3.718711 18.072378 2.523877
F 0.635747 18.030912 -1.121519
F 1.895185 19.849613 -1.294475
F 2.767719 16.497148 -1.930408
F 2.198873 18.086918 -3.306069
F 4.007926 18.285558 -2.111502
C 1.962084 18.487056 -0.933331
C 2.728443 17.842757 -2.083872
O 3.434097 21.477083 2.581608
C 2.558871 21.138147 3.320777
C 1.215821 20.654924 2.957363
Cl 2.902239 21.236910 5.144697
C 0.257185 20.213863 3.884721
C 0.928624 20.615520 1.578900
C -0.978321 19.756768 3.434253
H 0.475721 20.221301 4.945725
C -0.309037 20.155379 1.137998
H 1.676864 20.927163 0.861210
C -1.263915 19.730426 2.064445
H -1.715880 19.410463 4.151661
H -0.503116 20.095385 0.072992
H -2.227211 19.364175 1.720310

44
OATS_B3LYP
C 1.115899 15.949533 2.920561
H 1.406884 15.369781 2.049885
C 0.586681 15.326118 4.065576
H 0.480918 14.246591 4.089072
C 0.207149 16.109324 5.138991
H -0.208266 15.661907 6.037901
C 0.357658 17.512800 5.065696
C 0.902599 18.047718 3.871036
C -0.012440 18.399895 6.132664
H -0.429015 17.970501 7.039576
C 0.154778 19.748173 6.015024
H -0.125275 20.413777 6.826853
C 0.702345 20.323879 4.818774
C 0.897542 21.713452 4.647350
H 0.626740 22.394463 5.449620
C 1.431809 22.185146 3.463676
H 1.597567 23.245119 3.301682
C 1.766243 21.265085 2.451815
H 2.197315 21.592811 1.510621

C	1.072860	19.477719	3.743484	Cl	4.389278	18.096586	1.922219	H	6.204329	18.370536	-3.756606
N	1.273874	17.265006	2.826328	C	3.229191	19.031566	-0.497553	H	5.763043	15.924916	-3.847865
N	1.590641	19.955944	2.584660	C	3.929080	18.143199	-1.455324	O	2.787200	20.337344	-0.801264
F	-0.163099	19.147042	-0.475696	C	3.947257	16.751495	-1.298812				
F	1.463007	18.404671	-1.775500	C	4.567518	18.740730	-2.555063	44			
F	-0.644611	16.662962	0.421230	C	4.603179	15.958285	-2.235689	V_B3LYP			
F	-0.561923	16.731489	-1.752209	H	3.455832	16.300818	-0.442064	Cu	2.873262	16.126411	0.741172
F	1.085224	15.849654	-0.632338	C	5.222222	17.941852	-3.489362	C	0.376332	16.806785	2.793735
C	0.892912	18.214557	-0.518696	H	4.542525	19.820246	-2.664477	H	-0.256631	16.312743	2.062218
C	0.182583	16.863368	-0.630602	C	5.240101	16.552338	-3.330879	C	-0.175858	17.404810	3.944510
Cu	1.952357	18.391371	1.121521	H	4.619512	14.879181	-2.114092	H	-1.248011	17.369221	4.108394
Cl	4.414603	18.446348	1.860432	H	5.717205	18.401461	-4.340115	C	0.668114	18.026218	4.844914
C	3.920910	19.106963	0.010179	H	5.750523	15.931003	-4.061743	H	0.279601	18.498134	5.743455
C	4.220934	18.082654	-1.012426	O	3.182705	20.227402	-0.524788	C	2.058983	18.050445	4.592750
C	4.206695	16.704177	-0.760353					C	2.512860	17.426254	3.403605
C	4.472686	18.561827	-2.308939	44				C	3.007542	18.674693	5.470810
C	4.448003	15.810684	-1.799276	RETS_B3LYP				H	2.639936	19.143970	6.379217
H	3.987952	16.340385	0.236658	C	1.803480	15.927441	2.812753	C	4.338325	18.680012	5.174450
C	4.721504	17.660809	-3.341154	H	2.254077	15.365215	2.000961	H	5.052680	19.152749	5.842494
H	4.467669	19.630301	-2.495220	C	1.350639	15.284837	3.979222	C	4.831240	18.078345	3.967294
C	4.706505	16.285880	-3.089700	H	1.449698	14.208508	4.071647	C	6.194674	18.101271	3.599390
H	4.429533	14.742541	-1.603890	C	0.786228	16.044804	4.985653	H	6.919199	18.570522	4.259341
H	4.920956	18.031594	-4.342422	H	0.424383	15.581746	5.899595	C	6.585277	17.534159	2.401823
H	4.893584	15.584504	-3.898070	C	0.678938	17.445030	4.825758	H	7.622804	17.538412	2.085395
O	3.844833	20.293396	-0.104680	C	1.163184	18.001674	3.615897	C	5.611889	16.949639	1.573699
				C	0.108032	18.308139	5.821333	H	5.880010	16.505606	0.621005
44				H	-0.257454	17.861952	6.742011	C	3.921365	17.455800	3.077113
IV_B3LYP				C	0.024083	19.653988	5.618868	N	1.676050	16.815949	2.532535
C	1.467005	15.892553	2.772743	H	-0.409230	20.302123	6.375564	N	4.319189	16.908705	1.896085
H	1.839274	15.327856	1.924553	C	0.505859	20.250420	4.404694	Cl	1.984158	15.035590	-0.934863
C	1.021289	15.244173	3.936759	C	0.444642	21.638993	4.146292	O	0.536325	19.130596	0.765025
H	1.049377	14.161209	3.991054	H	0.015702	22.303097	4.891742	C	1.081382	20.214104	0.848043
C	0.552434	16.007548	4.988274	C	0.931572	22.131356	2.951075	C	0.461102	21.391774	1.496413
H	0.195189	15.540214	5.901793	H	0.899697	23.191464	2.722361	C	2.531987	20.318842	0.269700
C	0.538578	17.415836	4.876577	C	1.478458	21.233617	2.014329	C	0.897594	22.713502	1.295181
C	1.014098	17.982802	3.667305	H	1.866820	21.573592	1.060224	C	-0.626430	21.141548	2.355324
C	0.070482	18.278435	5.925057	C	1.075819	19.427779	3.401159	C	3.607019	20.665964	1.348347
H	-0.292083	17.823082	6.842336	N	1.708851	17.239572	2.634976	F	2.586886	21.262763	-0.714129
C	0.079307	19.633694	5.776651	N	1.548902	19.926716	2.232109	F	2.871147	19.131041	-0.276473
H	-0.276595	20.280589	6.573812	F	0.227012	19.774749	-0.469049	C	0.252215	23.763098	1.947643
C	0.562027	20.240144	4.568283	F	0.788208	18.345635	-2.044412	H	1.718274	22.932039	0.624906
C	0.601369	21.638779	4.364556	F	-0.595797	17.860610	1.109007	C	-1.256592	22.192393	3.011892
H	0.251210	22.303301	5.149894	F	-1.225737	17.374959	-0.905677	H	-0.949957	20.117011	2.507134
C	1.086039	22.139054	3.171704	F	0.436740	16.297252	-0.015102	F	3.168006	20.280186	2.562700
H	1.130156	23.206959	2.984114	C	0.818905	18.573515	-0.690281	F	3.842663	21.984599	1.389968
C	1.533329	21.237015	2.185254	C	-0.150717	17.509382	-0.107004	F	4.762801	20.037989	1.099217
H	1.928374	21.587430	1.236528	Cu	2.479456	18.355671	1.024527	C	-0.818623	23.506192	2.807329
C	1.030954	19.418843	3.511842	Cl	4.704413	18.159280	1.489346	H	0.585736	24.783285	1.781898
N	1.457469	17.214131	2.639657	C	2.747875	19.131756	-0.788326	H	-2.087310	21.991960	3.682404
N	1.508249	19.922484	2.350280	C	3.539262	18.212897	-1.646005	H	-1.312736	24.328194	3.317891
F	0.388690	19.514213	-0.537037	C	3.290123	16.834887	-1.697957				
F	1.038939	17.662866	-1.548369	C	4.591315	18.767044	-2.391810	24			
F	-0.947752	18.016044	1.319948	C	4.088477	16.015238	-2.491196	VI_B3LYP			
F	-1.463159	17.574171	-0.742226	H	2.472570	16.410306	-1.127342	Cu	-0.949467	-0.230463	0.081115
F	-0.223946	16.180001	0.376334	C	5.388274	17.942147	-3.181564	N	0.709552	1.371123	0.035894
C	0.789405	18.217227	-0.306480	H	4.777418	19.834632	-2.337575	N	0.698678	-1.357176	0.043165
C	-0.476966	17.489750	0.174776	C	5.139429	16.566535	-3.231404	C	0.693175	2.697187	0.038568
Cu	2.295999	18.190619	1.005746	H	3.891339	14.947931	-2.533291	C	1.866412	3.477708	0.007349

C 3.090976 2.839781 -0.028930
C 4.369290 0.684750 -0.069042
C 4.363283 -0.678427 -0.070200
C 3.081677 -2.825930 -0.031534
C 1.857886 -3.464731 0.007683
C 0.685640 -2.690746 0.044844
C 1.903873 0.733642 0.001946
C 3.140996 1.426636 -0.032643
C 3.130159 -1.413852 -0.033326
C 1.898564 -0.712549 0.003673
H -0.287609 3.165076 0.066637
H 1.793869 4.560366 0.011909
H 4.017427 3.407124 -0.054150
H 5.305661 1.235113 -0.096690
H 5.294283 -1.237523 -0.099059
H 4.008296 -3.392508 -0.060523
H 1.783530 -4.546851 0.010348
H -0.292474 -3.158234 0.076589
Cl -3.037970 0.403351 0.129789

58
VII_B3LYP
Cu 11.356316 3.598940 1.183039
C 11.185477 0.565903 2.130391
H 12.268067 0.644039 2.172518
C 10.523697 -0.576323 2.618544
H 11.100466 -1.391003 3.043765
C 9.145169 -0.632533 2.544700
H 8.599504 -1.498805 2.908933
C 8.434317 0.455715 1.990747
C 9.190869 1.568047 1.539876
C 7.002857 0.482523 1.882512
H 6.442615 -0.381878 2.228616
C 6.358797 1.563931 1.358157
H 5.275376 1.578120 1.276568
C 7.091159 2.714683 0.909101
C 8.506886 2.724483 1.005054
C 6.465822 3.864309 0.375970
H 5.383314 3.890932 0.284396
C 7.241159 4.936627 -0.020682
H 6.794695 5.833533 -0.437438
C 8.638408 4.858613 0.128842
H 9.276063 5.687626 -0.162325
C 10.595561 5.883068 3.631347
C 10.302192 6.773091 2.585734
H 10.697146 6.576170 1.592063
C 9.509647 7.899298 2.814531
H 9.290493 8.580774 1.996747
C 8.992715 8.141720 4.090090
H 8.369794 9.014148 4.268973
C 9.275063 7.257495 5.135502
H 8.874069 7.441959 6.128803
C 10.073754 6.134369 4.910052
H 10.281358 5.450194 5.727496
C 13.361287 5.020135 3.672853
C 14.385894 4.836812 2.733109
H 14.154549 4.379683 1.773066
C 15.688790 5.252090 3.024911
H 16.477266 5.109502 2.290644
C 15.972892 5.852284 4.253013
H 16.985354 6.176576 4.479268
C 14.953018 6.040818 5.193280
H 15.172214 6.511355 6.148289
C 13.652608 5.628073 4.905411
H 12.864064 5.779141 5.637652
C 11.253571 3.190227 4.503468
C 9.910042 2.792969 4.631299
H 9.138278 3.304796 4.062864
C 9.558762 1.739695 5.473709
H 8.516370 1.443932 5.557882
C 10.544534 1.059758 6.197227
H 10.271186 0.234810 6.849674
C 11.880727 1.443220 6.072023
H 12.653550 0.919942 6.629164
C 12.235797 2.501321 5.229390
H 13.280082 2.784724 5.139411
Cl 12.777791 3.665532 -0.629211
N 10.545153 1.604983 1.606902
N 9.256201 3.793745 0.629268
P 11.673313 4.446700 3.225999

14
C6H5COCl_B3LYP
C -1.428183 -0.635289 0.292760
C -0.043109 -0.638992 0.145004
C 0.635068 0.567582 -0.088651
C -0.087365 1.774345 -0.169777
C -1.469402 1.768269 -0.018900
C -2.141633 0.563644 0.212124
H -1.950920 -1.570196 0.471236
H 0.502980 -1.572457 0.209240
H 0.444646 2.702301 -0.349735
H -2.022783 2.700594 -0.081141
H -3.221750 0.559937 0.329294
C 2.096396 0.677911 -0.262945
O 2.722477 1.669906 -0.487178
Cl 3.040623 -0.911306 -0.112123

20
C6H5COC2F5_B3LYP
C -1.468314 -0.585701 0.409231
C -0.085021 -0.624631 0.245298
C 0.617356 0.550859 -0.081889
C -0.095943 1.755860 -0.241790
C -1.475682 1.785851 -0.082613
C -2.165607 0.612971 0.243946
H -2.002475 -1.496260 0.664434
H 0.430712 -1.564938 0.380046
H 0.450708 2.659086 -0.491035
H -2.015332 2.719669 -0.211078
H -3.244547 0.634925 0.370472
C 2.085578 0.625604 -0.262514
C 2.974855 -0.658267 -0.179747
C 3.368850 -1.049330 1.263094
F 4.131859 -0.423646 -0.844705
F 2.374154 -1.738167 -0.758128
F 2.284259 -1.392540 1.978770
F 3.965858 -0.009544 1.864276
F 4.215088 -2.088123 1.251298
O 2.686680 1.663518 -0.473531

34
PPh3_B3LYP
C 2.568164 21.637412 1.233001
C 3.211303 21.628424 -0.016347
H 3.172227 20.735839 -0.637024
C 3.901464 22.752863 -0.471657
H 4.390553 22.730310 -1.442093
C 3.971896 23.899731 0.323531
H 4.516054 24.773426 -0.025616
C 3.344924 23.916568 1.571842
H 3.396950 24.805329 2.195744
C 2.645026 22.795144 2.023249
H 2.157000 22.824437 2.992876
C -0.031366 20.396602 1.063366
C -0.905953 19.296889 1.027378
H -0.565027 18.323889 1.374999
C -2.210539 19.438195 0.552706
H -2.875673 18.578622 0.536567
C -2.656086 20.679308 0.089741
H -3.669272 20.789024 -0.288049
C -1.792005 21.776522 0.110438
H -2.131781 22.744609 -0.249045
C -0.489516 21.638362 0.596611
H 0.168377 22.501960 0.613849
C 1.426441 20.357166 3.547273
C 2.460839 19.930890 4.397792
H 3.348253 19.463286 3.976386
C 2.364574 20.101858 5.779393
H 3.175948 19.770800 6.422567
C 1.223253 20.687308 6.334107
H 1.143153 20.813970 7.410612
C 0.183861 21.104181 5.499287
H -0.707309 21.559104 5.924479
C 0.284681 20.943798 4.115061
H -0.528052 21.279217 3.477779
P 1.669374 20.097298 1.730255

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I^{+}_B3LYP
Cu 2.313872 17.904090 0.894519
C 2.877772 18.107031 3.949467
H 2.532681 19.128028 3.839590
C 3.281431 17.606816 5.200164
H 3.248445 18.256667 6.067720
C 3.703844 16.294927 5.297544
H 4.011633 15.877266 6.251845
C 3.741487 15.485741 4.138571
C 3.330137 16.078022 2.921757
C 4.171450 14.115708 4.141363
H 4.481136 13.675609 5.084640
C 4.192163 13.381850 2.991103
H 4.517181 12.345729 3.000943
C 3.790431 13.958791 1.739098

C	3.791309	13.254074	0.512830	C	0.036159	15.962520	4.086759	H	-0.600862	20.576068	6.303184
H	4.109299	12.215577	0.493645	H	-0.519855	15.412188	4.840228	C	0.524747	20.158270	4.492643
C	3.391821	13.894914	-0.644895	C	1.305326	16.496347	4.410767	C	0.768991	21.502837	4.131691
H	3.384485	13.381058	-1.599842	C	1.984548	17.202382	3.393241	H	0.385525	22.301790	4.760372
C	2.992779	15.242547	-0.580926	C	1.927097	16.361624	5.698478	C	1.488493	21.782737	2.986696
H	2.685270	15.786732	-1.467585	H	1.395953	15.815538	6.472193	H	1.691881	22.803615	2.681472
C	3.365194	15.307685	1.706937	C	3.153566	16.905621	5.949384	C	1.968089	20.716965	2.203667
C	0.284134	20.007265	2.711275	H	3.616705	16.799803	6.925637	H	2.539721	20.896115	1.299446
C	1.061642	21.156674	2.475056	C	3.862937	17.630913	4.933258	C	1.041053	19.149250	3.641572
H	1.504727	21.325138	1.498425	C	5.133231	18.223033	5.125138	N	1.295182	16.813613	3.124088
C	1.265762	22.086314	3.494131	H	5.623667	18.135528	6.090184	N	1.752073	19.446385	2.525097
H	1.861229	22.973950	3.299789	C	5.736673	18.905130	4.084705	F	1.070880	19.000900	-0.569365
C	0.710117	21.873924	4.760247	H	6.709352	19.369234	4.203675	F	1.524506	16.868627	-0.967650
H	0.874508	22.596775	5.554418	C	5.074850	18.999922	2.847953	F	-0.825293	18.188285	1.299370
C	-0.054549	20.730854	5.001439	H	5.515687	19.527484	2.008482	F	-1.123439	17.495788	-0.742012
H	-0.487861	20.560932	5.983180	C	3.273401	17.775432	3.658021	F	-0.406473	16.109403	0.773794
C	-0.268567	19.798169	3.983290	N	1.459184	17.373808	2.149822	C	1.126553	17.753277	0.025264
H	-0.858461	18.910804	4.186992	N	3.879661	18.450419	2.644769	C	-0.323843	17.383097	0.340421
C	-0.824702	19.536735	0.034920	F	0.479826	18.724643	-0.670532	C	3.926798	19.617286	-0.726562
C	-1.474375	20.769858	0.183015	F	2.355339	19.568489	-1.492697	C	4.315251	18.712681	-1.819967
H	-1.389103	21.329645	1.108804	F	1.495554	16.191868	-0.968364	C	4.613498	17.373047	-1.530109
C	-2.235816	21.286354	-0.868169	F	1.499124	17.337364	-2.823528	C	4.366673	19.184710	-3.145772
H	-2.736615	22.243076	-0.747713	F	3.364204	17.016491	-1.739012	C	4.970870	16.506996	-2.562462
C	-2.355089	20.577424	-2.065322	C	1.839337	18.516579	-0.760510	H	4.572193	17.032135	-0.499999
H	-2.946454	20.983457	-2.881391	C	2.042767	17.253830	-1.598846	C	4.715509	18.311518	-4.171225
C	-1.711634	19.344671	-2.213511					H	4.128813	20.223950	-3.352335
H	-1.800252	18.790534	-3.143854	14				C	5.018378	16.974798	-3.879003
C	-0.946620	18.826229	-1.170158	$C_6H_5COCl^-$				H	5.208517	15.470178	-2.342520
H	-0.439140	17.874594	-1.295180	C	-1.418732	-0.629916	0.294579	H	4.754087	18.666132	-5.197474
C	-0.911585	17.418319	1.981580	C	-0.042617	-0.633172	0.145999	H	5.292084	16.297360	-4.683483
C	-2.273165	17.645800	2.247021	C	0.674706	0.587166	-0.096053	O	3.747817	20.802321	-0.753582
H	-2.699796	18.633316	2.095097	C	-0.111953	1.797950	-0.174157				
C	-3.078394	16.603564	2.704331	C	-1.484927	1.768950	-0.021389	43			
H	-4.129196	16.786103	2.911040	C	-2.171828	0.559743	0.217188	IV_cationic			
C	-2.537283	15.326601	2.890833	H	-1.927556	-1.575664	0.475910	Cu	-1.367453	0.124826	0.108114
H	-3.169529	14.516162	3.242889	H	0.508632	-1.563867	0.209787	C	0.601878	0.098303	-0.036100
C	-1.188890	15.091928	2.615845	H	0.402810	2.736777	-0.356901	C	1.092295	0.321015	-1.406330
H	-0.766567	14.099648	2.748166	H	-2.042653	2.702305	-0.086881	C	0.232920	0.331955	-2.517106
C	-0.378016	16.134406	2.161382	H	-3.251687	0.545375	0.336091	C	2.474447	0.541633	-1.570184
H	0.665496	15.945569	1.935272	C	2.062473	0.742649	-0.263219	C	0.753067	0.561346	-3.786958
N	2.890123	17.363617	2.845647	O	2.806564	1.680974	-0.471702	H	-0.829891	0.146057	-2.388851
N	2.977694	15.922756	0.560266	Cl	3.073815	-1.063021	-0.120045	C	2.983876	0.766678	-2.843968
P	0.162969	18.770215	1.368770					H	3.125546	0.531510	-0.702079
F	4.050538	18.139129	-1.196299	44				C	2.125564	0.776835	-3.950061
F	1.972383	18.247211	-1.935051	IV_triplet				H	0.092727	0.565144	-4.648548
F	3.688565	20.587166	0.071512	Cu	2.446941	17.724986	1.480553	H	4.048599	0.933036	-2.977326
F	3.517983	20.574135	-2.103058	Cl	4.534702	17.306381	2.240410	H	2.529329	0.950375	-4.943390
F	1.730801	20.760048	-0.876422	C	1.092784	15.532275	3.401767	O	1.222918	0.065715	0.983595
C	2.787980	18.633878	-0.893369	H	1.506757	14.816478	2.698043	C	-1.195112	-1.840059	0.202790
C	2.932615	20.155584	-0.966339	C	0.380970	15.105817	4.538077	C	-1.340991	-2.576087	-1.137988
				H	0.244316	14.045071	4.719918	F	-2.279322	-2.211569	0.972916
30				C	-0.132439	16.055698	5.399933	F	-0.103198	-2.368937	0.826343
$II^{+\cdot}$_B3LYP				H	-0.690764	15.763986	6.285307	F	-1.665244	-3.867384	-0.962531
Cu	2.749989	18.439424	0.967797	C	0.069873	17.427754	5.128039	F	-2.313813	-2.002877	-1.880670
C	0.263343	16.866896	1.865883	C	0.805442	17.758586	3.961830	F	-0.192554	-2.520495	-1.829975
H	-0.108881	17.035414	0.863768	C	-0.432529	18.475416	5.970933	N	-1.399375	2.138511	0.260002
C	-0.481684	16.149345	2.819170	H	-0.993216	18.198706	6.859343	C	-0.393398	2.987145	0.474174
H	-1.452528	15.753827	2.542409	C	-0.216238	19.785900	5.664565	C	-2.651951	2.640174	0.057627

H 0.585692 2.557523 0.644698
C -0.569036 4.380084 0.481454
C -2.914899 4.029996 0.033031
C -3.727191 1.706301 -0.123205
H 0.287674 5.019450 0.662154
C -1.825608 4.903820 0.249935
C -4.254934 4.486386 -0.203524
C -5.039724 2.185018 -0.345036
N -3.427947 0.379369 -0.062112
H -1.990641 5.977142 0.237250
H -4.437258 5.556476 -0.229298
C -5.274669 3.600082 -0.388042
C -6.060528 1.221389 -0.511988
C -4.410113 -0.505038 -0.220595
H -6.287603 3.948624 -0.565995
H -7.082000 1.547799 -0.685333
C -5.743583 -0.120757 -0.448492
H -4.136535 -1.549322 -0.164585
H -6.501767 -0.886751 -0.568386

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I_BP86

Cu 2.193105 17.870765 1.170376
C 0.289667 16.344609 3.092828
H -0.381417 16.326389 2.227645
C -0.133396 15.889460 4.359933
H -1.151822 15.508494 4.482841
C 0.754638 15.935012 5.432636
H 0.456477 15.591206 6.429235
C 2.062307 16.445475 5.228188
C 2.396508 16.890476 3.913457
C 3.040935 16.563708 6.277484
H 2.773166 16.213450 7.280708
C 4.276148 17.118724 6.037812
H 5.008436 17.217202 6.847147
C 4.629088 17.611172 4.731690
C 5.851939 18.271011 4.448818
H 6.599044 18.392424 5.241088
C 6.077034 18.768054 3.165684
H 7.005231 19.290874 2.915306
C 5.088978 18.592245 2.173439
H 5.230089 18.973875 1.157388
C 3.687021 17.486836 3.664732
C 2.599693 21.260629 1.279876
C 3.452621 21.015326 0.181570
H 3.392960 20.051565 -0.340032
C 4.362547 21.999018 -0.239781
H 5.019714 21.801254 -1.094252
C 4.433212 23.228052 0.437903
H 5.148016 23.993146 0.114232
C 3.585737 23.476767 1.533080
H 3.638327 24.435348 2.061919
C 2.668705 22.499926 1.951917
H 2.015725 22.696221 2.809619
C -0.196127 20.470850 1.073956
C -0.734018 19.753964 -0.014949
H -0.187093 18.891896 -0.416366
C -1.957586 20.150662 -0.581984
H -2.370808 19.591873 -1.429418
C -2.649319 21.256615 -0.060790
H -3.605352 21.563161 -0.500348
C -2.116167 21.972640 1.027631
H -2.655096 22.835657 1.435143
C -0.892594 21.584360 1.593101
H -0.481880 22.138879 2.444456
C 1.248729 20.027615 3.563847
C 0.039816 19.626220 4.179119
H -0.845162 19.425619 3.565176
C -0.032285 19.472366 5.571878
H -0.975104 19.155712 6.032070
C 1.098046 19.713716 6.372410
H 1.041331 19.586683 7.459161
C 2.304973 20.106372 5.769259
H 3.196053 20.283067 6.381647
C 2.385403 20.251741 4.375750
H 3.340154 20.529695 3.915145
N 1.520948 16.831009 2.862544
N 3.921689 17.967413 2.404523
P 1.428899 19.912676 1.739854
F 0.947029 17.079671 -1.290064
F 2.974809 18.003694 -1.576845
F 2.129024 14.881137 -0.108227
F 2.864180 15.344573 -2.126502
F 4.124547 15.777004 -0.380451
C 2.227044 17.201148 -0.663172
C 2.834493 15.800287 -0.835823

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II_BP86

Cu 2.568194 18.275246 0.891101
C -0.024536 16.686493 2.178020
H -0.468125 16.777400 1.180180
C -0.721648 16.061896 3.240943
H -1.724862 15.660110 3.069184
C -0.113186 15.971465 4.488925
H -0.623748 15.493989 5.332681
C 1.191085 16.506092 4.671289
C 1.805391 17.117530 3.537250
C 1.905687 16.458856 5.920081
H 1.421743 15.985564 6.781642
C 3.167937 16.993360 6.033205
H 3.707597 16.952830 6.985740
C 3.814899 17.619505 4.908957
C 5.115912 18.185799 4.973714
H 5.672324 18.154791 5.916935
C 5.663694 18.770656 3.836602
H 6.663400 19.214117 3.850683
C 4.912713 18.793598 2.640687
H 5.308448 19.246983 1.727470
C 3.130846 17.684296 3.658986
N 1.202584 17.200834 2.317578
N 3.678135 18.268819 2.545581
F 0.602851 18.412564 -1.088378
F 2.287813 19.840776 -1.470526
F 2.321877 16.288756 -1.571208
F 2.156203 17.743952 -3.209838
F 3.970282 17.694086 -1.972242
C 2.012224 18.563565 -0.915043
C 2.608798 17.577168 -1.931965

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III_BP86

Cu 2.492423 18.056440 0.770785
C -0.037630 16.342113 2.014858
H -0.400031 16.261682 0.984248
C -0.830281 15.918719 3.108452
H -1.820722 15.490586 2.926303
C -0.329753 16.053861 4.400017
H -0.916858 15.737114 5.269349
C 0.959110 16.618131 4.593095
C 1.676934 17.013973 3.424131
C 1.554318 16.822338 5.887771
H 0.986046 16.527001 6.776876
C 2.807137 17.376670 6.011323
H 3.255434 17.527547 6.999503
C 3.560763 17.779061 4.852058
C 4.852244 18.365567 4.925624
H 5.322126 18.515435 5.903578
C 5.497873 18.748452 3.755105
H 6.491043 19.205351 3.776757
C 4.840175 18.577855 2.517340
H 5.297734 18.901084 1.578694
C 2.986060 17.615410 3.558459
N 1.182628 16.870855 2.162520
N 3.613061 18.039222 2.415227
F 0.540121 18.001998 -1.235728
F 1.774164 19.867567 -1.288178
F 2.754322 16.533042 -2.030897
F 2.190008 18.171211 -3.384076
F 3.966992 18.371680 -2.108393
C 1.862872 18.481523 -0.986181
C 2.686601 17.894813 -2.142328
O 3.690748 21.513672 2.543544
C 2.856666 21.200269 3.357269
C 1.532561 20.608300 3.110398
Cl 3.259194 21.514799 5.167777
C 0.658462 20.163999 4.128489
C 1.166402 20.453595 1.747120
C -0.575945 19.600803 3.786586
H 0.950240 20.245984 5.178283
C -0.079602 19.901892 1.419179
H 1.840580 20.792624 0.957073
C -0.950270 19.476602 2.434918
H -1.245023 19.246238 4.576898
H -0.336592 19.763589 0.365873
H -1.915858 19.029936 2.175191

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OATS_BP86

C 1.057736 15.957476 2.779057
H 1.278030 15.394908 1.866660
C 0.628938 15.308887 3.960043
H 0.532729 14.219124 3.973238
C 0.332284 16.073106 5.084735

H	-0.006480	15.601154	6.013786	H	1.131173	23.227352	2.970702	C	0.785364	18.576858	-0.726155
C	0.468374	17.485989	5.025332	C	1.536450	21.245324	2.167633	C	-0.173306	17.499681	-0.125554
C	0.913746	18.046371	3.790349	H	1.935464	21.593552	1.209425	Cu	2.471189	18.369365	1.044459
C	0.185725	18.360901	6.133367	C	1.033335	19.417223	3.502330	Cl	4.678275	18.123128	1.482568
H	-0.159256	17.917003	7.073747	N	1.458757	17.215258	2.611736	C	2.704190	19.150747	-0.760406
C	0.346455	19.722259	6.020252	N	1.512779	19.919853	2.332008	C	3.517889	18.233991	-1.612863
H	0.132600	20.380306	6.869792	F	0.360494	19.539365	-0.540334	C	3.282610	16.844658	-1.654901
C	0.798470	20.318109	4.789498	F	1.025038	17.675464	-1.559930	C	4.575400	18.792655	-2.363020
C	0.992117	21.714996	4.619788	F	-0.975891	18.016700	1.336160	C	4.096770	16.019650	-2.440081
H	0.792755	22.393850	5.456379	F	-1.506930	17.583613	-0.744491	H	2.457040	16.417344	-1.079783
C	1.437656	22.198805	3.393527	F	-0.247189	16.172339	0.367364	C	5.389058	17.962902	-3.144827
H	1.603700	23.267880	3.231399	C	0.765958	18.232174	-0.309761	H	4.751731	19.871730	-2.315953
C	1.679469	21.290002	2.338447	C	-0.506156	17.494568	0.174449	C	5.152858	16.576381	-3.184293
H	2.044786	21.625993	1.363724	Cu	2.264507	18.220582	1.000135	H	3.906892	14.941379	-2.474041
C	1.074639	19.478587	3.669125	Cl	4.360894	18.115931	1.920678	H	6.211067	18.397467	-3.724267
N	1.202117	17.286348	2.693655	C	3.223280	19.057180	-0.485263	H	5.790774	15.929794	-3.797086
N	1.500747	19.968008	2.465789	C	3.928412	18.158447	-1.437713	O	2.738308	20.374646	-0.806156
F	-0.315843	19.008090	-0.847706	C	3.935540	16.759385	-1.268717				
F	1.496521	18.275837	-1.922989	C	4.580515	18.743725	-2.546852	44			
F	-0.727210	16.553680	0.220770	C	4.593750	15.947597	-2.199340	V_BP86			
F	-0.459335	16.468687	-1.957405	H	3.429721	16.321757	-0.400662	Cu	2.949060	16.124727	0.829566
F	1.145965	15.769196	-0.630588	C	5.237270	17.926187	-3.475255	C	0.363215	16.967635	2.667417
C	0.806595	18.140090	-0.711827	H	4.563149	19.831700	-2.666694	H	-0.244429	16.414059	1.944132
C	0.182420	16.731710	-0.782715	C	5.244668	16.529944	-3.303152	C	-0.232881	17.677326	3.737291
Cu	1.646818	18.509873	0.993010	H	4.601589	14.860549	-2.066285	H	-1.321111	17.672171	3.851055
Cl	4.351221	18.664397	1.993007	H	5.743888	18.378064	-4.335014	C	0.581255	18.373922	4.625057
C	3.877136	19.241157	0.169948	H	5.758578	15.892981	-4.031700	H	0.152738	18.939609	5.459749
C	4.165618	18.179556	-0.822463	O	3.189639	20.268175	-0.533632	C	1.989839	18.352040	4.443790
C	4.152961	16.802697	-0.516181					C	2.491114	17.609831	3.332132
C	4.415824	18.609243	-2.145959	44				C	2.914253	19.034244	5.310266
C	4.389911	15.864297	-1.526298	RETS_BP86				H	2.514298	19.600700	6.158693
H	3.929727	16.478030	0.503605	C	1.812449	15.909830	2.790280	C	4.269201	18.978271	5.082665
C	4.664165	17.663589	-3.147803	H	2.273126	15.350304	1.970531	H	4.967622	19.498323	5.747506
H	4.409612	19.679036	-2.373729	C	1.348743	15.262604	3.957883	C	4.807293	18.252349	3.961457
C	4.647589	16.291243	-2.842371	H	1.442368	14.176298	4.045898	C	6.194308	18.198092	3.664072
H	4.366978	14.795542	-1.288765	C	0.783200	16.023655	4.976402	H	6.908872	18.709340	4.318495
H	4.864583	17.998106	-4.171407	H	0.416930	15.552255	5.895118	C	6.623453	17.499083	2.539888
H	4.832243	15.553025	-3.630563	C	0.682278	17.432329	4.824043	H	7.683996	17.438534	2.278739
O	3.776486	20.434776	-0.013563	C	1.167763	17.993286	3.605279	C	5.671366	16.866055	1.713245
				C	0.123757	18.303511	5.825084	H	5.970570	16.320654	0.813905
44				H	-0.243442	17.858721	6.756541	C	3.915712	17.572934	3.079435
IV_BP86				C	0.052964	19.662058	5.622591	N	1.685262	16.933651	2.466566
C	1.479421	15.882781	2.741117	H	-0.369709	20.318395	6.391350	N	4.349279	16.900025	1.965519
H	1.852709	15.323485	1.878628	C	0.529619	20.257247	4.400965	Cl	2.081643	15.000774	-0.810236
C	1.046430	15.225812	3.913221	C	0.483616	21.652512	4.137357	O	0.421185	19.032849	0.583109
H	1.083625	14.133893	3.963921	H	0.070870	22.331249	4.891976	C	1.017681	20.087843	0.783713
C	0.575592	15.985034	4.979351	C	0.964874	22.136134	2.925060	C	0.461074	21.200602	1.590891
H	0.225344	15.506258	5.900487	H	0.944601	23.204841	2.692141	C	2.429874	20.241943	0.100071
C	0.551236	17.400746	4.873938	C	1.487132	21.226397	1.976532	C	1.043053	22.488471	1.655026
C	1.018466	17.978496	3.654694	H	1.868090	21.552307	1.004162	C	-0.711929	20.927238	2.335779
C	0.084809	18.263082	5.928564	C	1.082570	19.420051	3.386269	C	3.636881	20.533411	1.077109
H	-0.273857	17.802697	6.855725	N	1.719835	17.233542	2.615539	F	2.359191	21.265700	-0.817784
C	0.087294	19.630165	5.780957	N	1.546566	19.908416	2.198691	F	2.710927	19.090420	-0.568853
H	-0.270303	20.278406	6.588815	F	0.176309	19.781329	-0.507306	C	0.464060	23.477182	2.461425
C	0.564051	20.243046	4.568869	F	0.762856	18.335897	-2.087648	H	1.933612	22.731951	1.072079
C	0.602320	21.648422	4.362930	F	-0.615984	17.858389	1.102605	C	-1.279314	21.915252	3.145603
H	0.251372	22.319410	5.155041	F	-1.263069	17.343979	-0.921655	H	-1.151888	19.927915	2.272157
C	1.087681	22.150460	3.159891	F	0.431100	16.281374	-0.025955	F	3.235444	20.391902	2.367644

F	4.099787	21.796088	0.919198
F	4.660873	19.681686	0.857691
C	-0.690902	23.192708	3.210809
H	0.915340	24.474018	2.503424
H	-2.180883	21.694009	3.726898
H	-1.135511	23.967985	3.844563

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VI_BP86

Cu	-0.913646	-0.230379	0.085180
N	0.694605	1.363672	0.037374
N	0.684196	-1.357642	0.045136
C	0.674324	2.701075	0.040784
C	1.849951	3.489378	0.008946
C	3.087374	2.854627	-0.028867
C	4.376995	0.691349	-0.070469
C	4.371484	-0.683463	-0.071849
C	3.085604	-2.842737	-0.032288
C	1.850085	-3.480762	0.008663
C	0.672383	-2.704911	0.047282
C	1.902007	0.732235	0.001878
C	3.145327	1.434840	-0.033357
C	3.136558	-1.423697	-0.034396
C	1.897891	-0.715469	0.003583
H	-0.318788	3.164141	0.070079
H	1.772240	4.580830	0.014224
H	4.018034	3.432447	-0.054606
H	5.321969	1.245231	-0.098688
H	5.311709	-1.245025	-0.101521
H	4.018021	-3.417023	-0.062147
H	1.772888	-4.571790	0.011802
H	-0.315429	-3.172358	0.080862
Cl	-2.970076	0.448298	0.115807

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VII_BP86

Cu	11.296900	3.755851	0.967284
C	11.921774	0.774432	1.703006
H	12.956234	1.031774	1.451063
C	11.601065	-0.450243	2.329326
H	12.399106	-1.159540	2.568888
C	10.271205	-0.729403	2.633126
H	9.987388	-1.666341	3.125218
C	9.269454	0.222143	2.308171
C	9.691197	1.432642	1.679052
C	7.875245	0.036358	2.612001
H	7.567378	-0.898284	3.094007
C	6.950785	1.013594	2.327188
H	5.893728	0.870289	2.578209
C	7.346882	2.256673	1.718948
C	8.720132	2.462252	1.381243
C	6.444997	3.323609	1.470644
H	5.385108	3.206550	1.723014
C	6.926101	4.508318	0.917766
H	6.259622	5.352429	0.715976
C	8.298639	4.615412	0.604958
H	8.710024	5.529790	0.166184
C	10.637198	6.225552	3.247453
C	10.414112	7.021145	2.103721
H	10.744113	6.652702	1.124027
C	9.774306	8.266321	2.219497
H	9.604555	8.876662	1.325402
C	9.346874	8.720222	3.478656
H	8.841200	9.688102	3.570653
C	9.564879	7.930577	4.622751
H	9.231089	8.282930	5.605402
C	10.208406	6.688531	4.510462
H	10.364031	6.071868	5.402385
C	13.189537	4.855172	3.665587
C	14.259046	4.780790	2.749298
H	14.043711	4.572174	1.692468
C	15.579161	4.974293	3.190979
H	16.406466	4.917560	2.474523
C	15.834322	5.235980	4.547389
H	16.863776	5.384055	4.893027
C	14.769325	5.306637	5.465398
H	14.969133	5.508710	6.523933
C	13.449641	5.118366	5.028382
H	12.623111	5.165837	5.746516
C	10.676878	3.469038	4.187711
C	9.271593	3.501045	4.344389
H	8.686640	4.298847	3.873049
C	8.618348	2.510490	5.093605
H	7.529475	2.549129	5.206738
C	9.353020	1.463373	5.675846
H	8.839827	0.683602	6.249422
C	10.747829	1.414844	5.508520
H	11.327041	0.596833	5.951509
C	11.407831	2.408979	4.769801
H	12.494502	2.358892	4.640933
Cl	12.589982	4.232641	-0.836395
N	11.000401	1.696096	1.382643
N	9.181314	3.626070	0.824974
P	11.490477	4.610217	2.997261

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C6H5COCl_BP86

C	-1.432798	-0.642232	0.295107
C	-0.040297	-0.645093	0.146975
C	0.641189	0.569252	-0.088733
C	-0.086630	1.783164	-0.171181
C	-1.476292	1.775010	-0.020023
C	-2.151594	0.563075	0.212829
H	-1.959065	-1.585231	0.475590
H	0.513945	-1.584814	0.212047
H	0.450220	2.718797	-0.353137
H	-2.034845	2.714662	-0.083773
H	-3.240719	0.558507	0.330418
C	2.104590	0.681414	-0.263295
O	2.741162	1.680650	-0.485525
Cl	3.048179	-0.930914	-0.118093

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C6H5COC2F5_BP86

C	-1.475885	-0.592266	0.406242
C	-0.086551	-0.633974	0.230463
C	0.621136	0.549816	-0.093278
C	-0.094960	1.765220	-0.238756
C	-1.480658	1.797634	-0.067476
C	-2.175385	0.616819	0.256139
H	-2.015395	-1.511194	0.658938
H	0.433868	-1.584193	0.352466
H	0.460101	2.675145	-0.486744
H	-2.023319	2.741737	-0.184473
H	-3.262199	0.640748	0.392552
C	2.091202	0.623744	-0.289509
C	2.986440	-0.666512	-0.184184
C	3.366122	-1.047949	1.276379
F	4.159681	-0.430201	-0.842357
F	2.389154	-1.760821	-0.769023
F	2.266934	-1.410718	1.983166
F	3.938795	0.015808	1.887311
F	4.239741	-2.080248	1.286052
O	2.694213	1.668602	-0.530072

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PPh3_BP86

C	2.578997	21.616619	1.235382
C	3.179605	21.632976	-0.043811
H	3.110799	20.747772	-0.688398
C	3.861170	22.772406	-0.498583
H	4.318427	22.771840	-1.494651
C	3.966182	23.905805	0.326204
H	4.506228	24.792772	-0.024074
C	3.380565	23.895497	1.603419
H	3.458916	24.776508	2.251019
C	2.687389	22.760327	2.055485
H	2.226381	22.765582	3.049250
C	-0.018626	20.379819	1.055813
C	-0.909795	19.283119	1.027633
H	-0.574858	18.300320	1.382485
C	-2.221473	19.440598	0.554144
H	-2.903231	18.582450	0.543136
C	-2.655151	20.692909	0.085413
H	-3.676481	20.814620	-0.292886
C	-1.773122	21.786481	0.099914
H	-2.105708	22.765624	-0.263861
C	-0.463665	21.633827	0.585251
H	0.213183	22.494995	0.601314
C	1.427762	20.341378	3.546362
C	2.479335	19.954678	4.407978
H	3.388108	19.504166	3.989464
C	2.374144	20.145832	5.794216
H	3.200219	19.846079	6.449270
C	1.208283	20.709995	6.340676
H	1.121580	20.851947	7.423896
C	0.153070	21.087047	5.493179
H	-0.758551	21.527543	5.913451
C	0.261746	20.908418	4.103870
H	-0.562789	21.215142	3.451046
P	1.683096	20.067248	1.728048

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I_CAM-B3LYP

Cu	2.186296	17.897930	1.165712
C	0.324849	16.272854	3.080550
H	-0.339934	16.259912	2.222199
C	-0.092803	15.772595	4.322402
H	-1.091528	15.364246	4.427717
C	0.780225	15.815917	5.384273
H	0.491940	15.442036	6.362147
C	2.066384	16.357105	5.199972
C	2.392354	16.834787	3.917337
C	3.033170	16.452590	6.257435
H	2.760286	16.075846	7.238412
C	4.251679	17.002144	6.040043
H	4.978989	17.076227	6.842743
C	4.610042	17.515180	4.747678
C	5.843555	18.139899	4.485863
H	6.579732	18.225482	5.279581
C	6.094491	18.640338	3.228908
H	7.031415	19.132180	2.992925
C	5.109481	18.511341	2.238671
H	5.269455	18.904639	1.239683
C	3.687122	17.431822	3.688198
C	2.565599	21.296896	1.277051
C	3.421550	21.046067	0.200176
H	3.394651	20.077623	-0.293126
C	4.297336	22.031602	-0.246496
H	4.955691	21.826959	-1.085459
C	4.330897	23.270962	0.383829
H	5.017763	24.038354	0.039507
C	3.481891	23.527518	1.458394
H	3.505239	24.494479	1.951970
C	2.601704	22.547321	1.901384
H	1.948776	22.753419	2.743911
C	-0.194546	20.482355	1.098391
C	-0.721280	19.753850	0.029124
H	-0.175348	18.898404	-0.360313
C	-1.933374	20.129369	-0.545264
H	-2.334495	19.559072	-1.377688
C	-2.626976	21.228656	-0.052185
H	-3.573757	21.519290	-0.497582
C	-2.106704	21.959580	1.014932
H	-2.646426	22.819216	1.400744
C	-0.895722	21.590387	1.585997
H	-0.497614	22.160697	2.419935
C	1.259035	20.104058	3.580359
C	0.062069	19.756265	4.215939
H	-0.825788	19.549232	3.626603
C	-0.003503	19.667407	5.602448
H	-0.940998	19.396254	6.078664
C	1.125400	19.921110	6.375647
H	1.074160	19.848993	7.457769
C	2.322069	20.262798	5.753125
H	3.210606	20.456316	6.346543
C	2.390856	20.347636	4.366976
H	3.336266	20.597506	3.894985
N	1.525843	16.788404	2.880127
N	3.943423	17.927102	2.456811
P	1.424213	19.950067	1.765002
F	1.045169	17.151816	-1.349501
F	3.084430	17.989128	-1.530636
F	2.089949	14.922165	-0.169764
F	2.887051	15.396080	-2.125874
F	4.091757	15.742707	-0.361693
C	2.278779	17.216613	-0.670897
C	2.836167	15.817890	-0.846100

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II_CAM-B3LYP

Cu	2.477559	18.254972	0.895551
C	-0.053492	16.700980	2.242118
H	-0.518880	16.794137	1.265357
C	-0.724603	16.073543	3.305295
H	-1.721364	15.676188	3.151132
C	-0.096850	15.978258	4.524683
H	-0.583969	15.500071	5.369124
C	1.199297	16.509255	4.680955
C	1.782936	17.118030	3.556806
C	1.931941	16.453358	5.914287
H	1.463445	15.977730	6.770272
C	3.176783	16.979900	6.008348
H	3.730056	16.936337	6.941237
C	3.800042	17.610739	4.878684
C	5.090457	18.173600	4.926454
H	5.655209	18.136865	5.853060
C	5.615314	18.760171	3.799468
H	6.605030	19.201680	3.799858
C	4.848175	18.785804	2.625923
H	5.229721	19.241071	1.718895
C	3.107077	17.682104	3.658685
N	1.159522	17.206915	2.362893
N	3.632226	18.265752	2.553899
F	0.652414	18.372682	-1.216328
F	2.304406	19.813156	-1.468781
F	2.412130	16.319882	-1.615941
F	2.305495	17.786247	-3.205217
F	4.026253	17.744609	-1.893674
C	2.020214	18.546014	-0.946276
C	2.687989	17.601046	-1.928530

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III_CAM-B3LYP

Cu	2.586587	18.119681	0.906732
C	-0.001286	16.624720	2.280273
H	-0.452762	16.683414	1.294566
C	-0.709613	16.091312	3.370945
H	-1.720749	15.727046	3.228737
C	-0.098602	16.045297	4.601418
H	-0.613309	15.639908	5.467429
C	1.216831	16.532046	4.741867
C	1.836096	17.048073	3.590284
C	1.932147	16.523600	5.986362
H	1.435974	16.119511	6.863302
C	3.195836	17.005738	6.064710
H	3.736866	16.998573	7.005700
C	3.853516	17.547009	4.908646
C	5.158808	18.074659	4.946053
H	5.708968	18.072440	5.882003
C	5.714033	18.589904	3.799260
H	6.713979	19.007380	3.792332
C	4.961353	18.582076	2.616653
H	5.362487	18.990896	1.696586
C	3.177534	17.573614	3.677484
N	1.229584	17.086238	2.385634
N	3.732197	18.091804	2.553159
F	0.642930	18.028846	-1.085170
F	1.907871	19.825378	-1.252143
F	2.762028	16.484415	-1.845119
F	2.216631	18.059963	-3.226711
F	4.006954	18.254010	-2.026255
C	1.960964	18.475016	-0.876434
C	2.732429	17.821344	-2.006656
O	3.363419	21.472509	2.569809
C	2.486482	21.135653	3.301560
C	1.140051	20.678122	2.913175
Cl	2.816644	21.186981	5.093931
C	0.156014	20.277160	3.821405
C	0.886432	20.625983	1.537276
C	-1.073712	19.839613	3.350604
H	0.347550	20.302487	4.886872
C	-0.342863	20.180509	1.073798
H	1.658487	20.910165	0.834208
C	-1.324176	19.792598	1.980186
H	-1.837026	19.526463	4.055078
H	-0.511491	20.106267	0.006070
H	-2.285618	19.440181	1.619272

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OATS_CAM-B3LYP

C	1.274457	15.813795	3.001536
H	1.640459	15.220563	2.169518
C	0.725217	15.203119	4.138446
H	0.667176	14.122056	4.191458
C	0.269387	15.997055	5.164609
H	-0.163019	15.559810	6.059537
C	0.363062	17.398050	5.053302
C	0.927568	17.916716	3.874525
C	-0.087505	18.298951	6.076547
H	-0.519702	17.877712	6.978828
C	0.023291	19.640136	5.921240
H	-0.318125	20.319018	6.696525
C	0.591574	20.201206	4.727949
C	0.725376	21.587706	4.516658
H	0.388279	22.280051	5.282213
C	1.281016	22.042646	3.344513
H	1.400103	23.102311	3.149305
C	1.703442	21.108985	2.385077
H	2.158752	21.425480	1.452839
C	1.041883	19.346455	3.706611
N	1.374660	17.124902	2.874158
N	1.586712	19.805388	2.558147
F	1.278333	18.804329	-1.470448
F	1.468507	16.640111	-1.106370
F	-0.809852	18.878047	0.318411

F	-1.038940	17.550307	-1.375817
F	-0.637932	16.730902	0.586039
C	1.160507	17.840937	-0.473876
C	-0.341771	17.748230	-0.243231
Cu	2.106843	18.192532	1.200067
Cl	4.466656	18.369245	1.868476
C	3.837160	19.010503	0.060532
C	4.205574	18.049955	-1.003039
C	4.464163	16.698026	-0.780429
C	4.215907	18.564755	-2.302321
C	4.753210	15.869003	-1.854098
H	4.426745	16.297106	0.224828
C	4.505134	17.729077	-3.371394
H	3.993480	19.612975	-2.463030
C	4.773967	16.381471	-3.149034
H	4.955888	14.817247	-1.680261
H	4.516427	18.129953	-4.379744
H	4.997373	15.728128	-3.986746
O	3.679266	20.187341	-0.025032

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IV_CAM-B3LYP

C	1.465251	15.891798	2.764750
H	1.833379	15.321825	1.918869
C	1.019793	15.249323	3.926978
H	1.044110	14.167348	3.983127
C	0.557208	16.013480	4.972017
H	0.199438	15.550646	5.886692
C	0.548286	17.416694	4.856316
C	1.020847	17.973622	3.655045
C	0.082774	18.283453	5.902265
H	-0.279607	17.831069	6.820000
C	0.093946	19.629129	5.748905
H	-0.259678	20.281518	6.541311
C	0.576666	20.228157	4.537044
C	0.616214	21.620943	4.326727
H	0.267290	22.289277	5.108238
C	1.097152	22.111839	3.136265
H	1.141639	23.177455	2.941736
C	1.541486	21.206896	2.157785
H	1.935101	21.551242	1.207195
C	1.040181	19.407440	3.493707
N	1.460168	17.206434	2.630818
N	1.515471	19.900343	2.332108
F	0.408918	19.522419	-0.494410
F	1.049101	17.696896	-1.530891
F	-0.908751	18.011951	1.333758
F	-1.420756	17.593781	-0.721386
F	-0.187012	16.196519	0.375588
C	0.814045	18.231854	-0.286844
C	-0.441543	17.500271	0.189264
Cu	2.292559	18.189480	1.022508
Cl	4.370310	18.101642	1.904391
C	3.182477	19.018246	-0.479417
C	3.893136	18.138296	-1.434513
C	3.913389	16.752788	-1.286741
C	4.539257	18.744550	-2.514645
C	4.580491	15.971499	-2.218092
H	3.414673	16.294774	-0.438829
C	5.206615	17.958483	-3.443946
H	4.511642	19.824248	-2.614505
C	5.226397	16.574001	-3.296152
H	4.599123	14.892476	-2.104848
H	5.710750	18.425635	-4.283825
H	5.747712	15.960234	-4.024375
O	3.125220	20.207209	-0.506013

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RETS_CAM-B3LYP

C	1.798786	15.938553	2.794918
H	2.241033	15.375776	1.979616
C	1.368380	15.297441	3.965448
H	1.478582	14.223343	4.059589
C	0.811295	16.052505	4.970364
H	0.462935	15.590488	5.889148
C	0.691927	17.446483	4.807205
C	1.158306	17.999529	3.602038
C	0.119981	18.306030	5.805038
H	-0.235367	17.857186	6.727327
C	0.022539	19.641486	5.600656
H	-0.413165	20.288860	6.355340
C	0.495865	20.237983	4.383544
C	0.422534	21.620871	4.124096
H	-0.012645	22.281566	4.867820
C	0.903584	22.113078	2.934186
H	0.862610	23.171258	2.702573
C	1.458385	21.220428	2.003941
H	1.846017	21.562710	1.050971
C	1.065703	19.424581	3.388521
N	1.692949	17.242750	2.617540
N	1.536724	19.921419	2.223990
F	0.287750	19.791221	-0.421071
F	0.839307	18.369127	-1.987075
F	-0.573310	17.890828	1.127322
F	-1.180155	17.444807	-0.889852
F	0.437567	16.327700	0.004174
C	0.867526	18.591713	-0.638027
C	-0.121835	17.544225	-0.078891
Cu	2.446282	18.348011	1.011753
Cl	4.653256	18.155163	1.484015
C	2.761383	19.119214	-0.771648
C	3.541479	18.200408	-1.635329
C	3.285521	16.830912	-1.687057
C	4.583060	18.752118	-2.382655
C	4.073955	16.013086	-2.483079
H	2.469097	16.408818	-1.113000
C	5.370093	17.929629	-3.176685
H	4.771294	19.818603	-2.327248
C	5.117731	16.560940	-3.225631
H	3.874620	14.947204	-2.525369
H	6.183026	18.355933	-3.755725
H	5.735475	15.918662	-3.845684
O	2.815435	20.316636	-0.769736

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V_CAM-B3LYP

Cu	2.837980	16.121457	0.763152
C	0.429539	16.745093	2.844378
H	-0.218839	16.272793	2.113094
C	-0.094271	17.289806	4.028595
H	-1.160106	17.235819	4.219559
C	0.764417	17.882784	4.923781
H	0.397609	18.315674	5.849712
C	2.142297	17.933087	4.633876
C	2.566072	17.361521	3.421643
C	3.106719	18.543012	5.504485
H	2.757921	18.974659	6.437516
C	4.418673	18.581785	5.170106
H	5.146777	19.044892	5.828605
C	4.882502	18.024496	3.930937
C	6.229175	18.078692	3.524060
H	6.965909	18.540626	4.174330
C	6.589681	17.552824	2.306291
H	7.615654	17.581603	1.958367
C	5.602301	16.974084	1.497235
H	5.849338	16.556461	0.527582
C	3.963287	17.417586	3.058114
N	1.715507	16.777942	2.552367
N	4.329766	16.905450	1.858280
Cl	1.963229	15.028750	-0.900998
O	0.507506	19.193018	0.864930
C	1.055160	20.270648	0.916969
C	0.415215	21.483554	1.471633
C	2.523136	20.332913	0.410126
C	0.904120	22.779958	1.273975
C	-0.746329	21.288279	2.230142
C	3.540266	20.642105	1.539444
F	2.659451	21.271378	-0.558646
F	2.852679	19.142694	-0.117580
C	0.236914	23.861229	1.835758
H	1.788777	22.957554	0.678317
C	-1.402152	22.370293	2.793938
H	-1.113679	20.278613	2.376236
F	3.041641	20.234992	2.714953
F	3.783265	21.949560	1.620178
F	4.693224	20.010096	1.329393
C	-0.910327	23.659433	2.596213
H	0.614971	24.865650	1.675737
H	-2.296723	22.212107	3.387526
H	-1.423771	24.508555	3.036646

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VI_CAM-B3LYP

Cu	-0.904293	-0.118790	0.094588
N	0.718567	1.362555	0.030278
N	0.708251	-1.342746	0.039904
C	0.698148	2.682700	0.031432
C	1.866809	3.461226	0.002789
C	3.086599	2.828275	-0.028854
C	4.366275	0.678013	-0.064090
C	4.360606	-0.676573	-0.065751
C	3.070603	-2.817686	-0.032422

C 1.848859 -3.446492 0.002750
C 0.684068 -2.666822 0.039414
C 1.912421 0.731487 0.000015
C 3.137668 1.420041 -0.031496
C 3.126607 -1.410293 -0.032648
C 1.907160 -0.712323 0.002229
H -0.281818 3.149606 0.056413
H 1.791495 4.542591 0.006165
H 4.011673 3.396394 -0.051411
H 5.300800 1.229784 -0.088433
H 5.290105 -1.236591 -0.091778
H 3.993459 -3.389037 -0.059801
H 1.768124 -4.527240 0.003476
H -0.296156 -3.129485 0.069332
Cl -3.040322 0.284270 0.151310

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VII_CAM-B3LYP
Cu 11.308666 3.582076 1.235500
C 11.127670 0.576901 2.195313
H 12.206027 0.662855 2.286507
C 10.458720 -0.575601 2.635331
H 11.024170 -1.390814 3.072058
C 9.092130 -0.641704 2.500381
H 8.538676 -1.517510 2.825588
C 8.399152 0.444753 1.932237
C 9.157950 1.561051 1.533803
C 6.974405 0.456598 1.756318
H 6.410236 -0.417796 2.066040
C 6.349171 1.528837 1.214372
H 5.272176 1.534145 1.077863
C 7.091029 2.690204 0.811356
C 8.488675 2.714588 0.975965
C 6.481352 3.831387 0.255343
H 5.405337 3.845490 0.109800
C 7.259002 4.908782 -0.096380
H 6.825039 5.802346 -0.530450
C 8.643698 4.844377 0.121265
H 9.284562 5.681415 -0.135753
C 10.602272 5.880759 3.678563
C 10.283033 6.764241 2.643230
H 10.648814 6.563831 1.639894
C 9.504426 7.890054 2.888985
H 9.265062 8.569093 2.076192
C 9.027323 8.137947 4.172559
H 8.413925 9.012838 4.365874
C 9.334851 7.260050 5.208525
H 8.963263 7.449290 6.211137
C 10.119328 6.137623 4.964778
H 10.346642 5.455855 5.778100
C 13.351775 5.024427 3.664880
C 14.356989 4.834722 2.714842
H 14.111285 4.369082 1.763458
C 15.659319 5.252523 2.980126
H 16.435084 5.104139 2.235052
C 15.961316 5.861944 4.192393
H 16.976015 6.189261 4.398734
C 14.960701 6.057332 5.143825
H 15.194557 6.536647 6.089724
C 13.662064 5.641779 4.881573
H 12.886016 5.798821 5.624866
C 11.274217 3.205868 4.542128
C 9.940727 2.804523 4.693752
H 9.158088 3.306132 4.131733
C 9.607679 1.765433 5.552002
H 8.569064 1.466445 5.656863
C 10.604016 1.103525 6.267420
H 10.344921 0.287196 6.934753
C 11.930335 1.491284 6.119207
H 12.713149 0.980457 6.671837
C 12.265558 2.536495 5.260818
H 13.306012 2.824645 5.152661
Cl 12.721553 3.617479 -0.568943
N 10.502085 1.610357 1.661911
N 9.242167 3.788550 0.643810
P 11.664643 4.449566 3.253468

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C6H5COCl_CAM-B3LYP
C -1.424484 -0.631087 0.291418
C -0.044261 -0.635850 0.144181
C 0.630117 0.564728 -0.087939
C -0.085258 1.766207 -0.168708
C -1.462599 1.762972 -0.018514
C -2.133035 0.563985 0.211254
H -1.948107 -1.564511 0.469559
H 0.500660 -1.569399 0.208336
H 0.449403 2.691937 -0.348400
H -2.014525 2.695090 -0.080486
H -3.212301 0.561442 0.328307
C 2.091998 0.671098 -0.261830
O 2.706705 1.665402 -0.487149
Cl 3.022733 -0.885767 -0.110822

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C6H5COC2F5_CAM-B3LYP
C -1.458799 -0.582705 0.411210
C -0.080201 -0.621742 0.249891
C 0.616345 0.548051 -0.077544
C -0.090139 1.747215 -0.240867
C -1.465504 1.778363 -0.084158
C -2.152276 0.611060 0.242844
H -1.993164 -1.491703 0.667470
H 0.436498 -1.560819 0.386259
H 0.458388 2.648137 -0.491301
H -2.004414 2.711098 -0.215377
H -3.230500 0.633199 0.367814
C 2.083267 0.621634 -0.256484
C 2.966034 -0.653644 -0.176960
C 3.357466 -1.045025 1.255957
F 4.116376 -0.418953 -0.836954
F 2.364957 -1.724288 -0.751857
F 2.279245 -1.393296 1.964294
F 3.946634 -0.010268 1.856591
F 4.202918 -2.074034 1.237996
O 2.679906 1.654915 -0.464990
C 4.217227 17.092897 6.022608
H 4.937178 17.178550 6.832584
C 4.587601 17.579529 4.726447
C 5.820282 18.209624 4.461409
H 6.552964 18.314378 5.257708
C 6.073984 18.695531 3.192999

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PPh3_CAM-B3LYP
P 1.665523 20.105372 1.731585
C 2.559895 21.636925 1.237077
C 3.209572 21.623691 -0.001738
H 3.178513 20.727734 -0.616463
C 3.897608 22.742964 -0.456327
H 4.393889 22.716736 -1.421827
C 3.958234 23.889219 0.330323
H 4.501837 24.762029 -0.018844
C 3.324619 23.910586 1.568827
H 3.369977 24.801530 2.188234
C 2.627643 22.793570 2.018613
H 2.134128 22.825750 2.984578
C -0.026437 20.401967 1.068733
C -0.894854 19.305427 1.029860
H -0.550797 18.332847 1.372943
C -2.194867 19.443996 0.558003
H -2.857307 18.583736 0.539205
C -2.641349 20.680545 0.101063
H -3.654051 20.789213 -0.275493
C -1.783269 21.775111 0.124435
H -2.124730 22.742400 -0.232331
C -0.485368 21.638404 0.607660
H 0.170736 22.502438 0.625564
C 1.424905 20.362128 3.539159
C 2.451420 19.928570 4.385190
H 3.333349 19.453684 3.962608
C 2.357785 20.097311 5.761711
H 3.165689 19.758925 6.403655
C 1.225948 20.688802 6.314940
H 1.147127 20.814713 7.390634
C 0.193834 21.113268 5.484467
H -0.693010 21.573582 5.910139
C 0.292973 20.954124 4.105509
H -0.517429 21.295043 3.469367

64
I_B3PW91
Cu 2.189250 17.904359 1.130655
C 0.291097 16.353401 3.049083
H -0.365840 16.336208 2.183740
C -0.146851 15.895294 4.301774
H -1.157484 15.514386 4.410783
C 0.722429 15.941742 5.373794
H 0.416590 15.597677 6.358535
C 2.023850 16.450705 5.186333
C 2.368856 16.894640 3.887687
C 2.984677 16.556914 6.244548
H 2.703309 16.207488 7.234678
C 4.217227 17.092897 6.022608
H 4.937178 17.178550 6.832584
C 4.587601 17.579529 4.726447
C 5.820282 18.209624 4.461409
H 6.552964 18.314378 5.257708
C 6.073984 18.695531 3.192999

H	7.009545	19.192585	2.955973	C	1.785680	17.119910	3.556744	Cl	3.074802	21.316188	4.684545
C	5.096923	18.541684	2.196484	C	1.933138	16.439013	5.915036	C	0.353808	20.096023	3.903044
H	5.259640	18.915662	1.189869	H	1.466496	15.961793	6.772880	C	0.616354	20.483394	1.517070
C	3.666302	17.476090	3.656193	C	3.188614	16.960601	6.008406	C	-0.893102	19.529967	3.664357
C	2.582536	21.291403	1.278258	H	3.742730	16.907081	6.941838	H	0.735549	20.149993	4.916274
C	3.447962	21.047244	0.203124	C	3.811978	17.592898	4.882747	C	-0.631830	19.914234	1.288411
H	3.420297	20.080523	-0.296412	C	5.108262	18.149032	4.928758	H	1.213480	20.843864	0.687202
C	4.334555	22.035799	-0.224653	H	5.677994	18.104706	5.853383	C	-1.388778	19.443649	2.360825
H	5.001016	21.837855	-1.060554	C	5.633213	18.740515	3.798163	H	-1.475444	19.144921	4.496078
C	4.368078	23.270436	0.423658	H	6.626841	19.176531	3.797691	H	-0.991397	19.813969	0.269629
H	5.062749	24.039566	0.094951	C	4.861083	18.777322	2.625798	H	-2.361031	18.992034	2.181760
C	3.508806	23.518997	1.496929	H	5.240335	19.235233	1.717851				
H	3.533332	24.480966	2.003167	C	3.111462	17.675578	3.657710	44			
C	2.617080	22.536126	1.921890	N	1.160129	17.218505	2.363789	OATS_B3PW91			
H	1.956561	22.733339	2.762324	N	3.637193	18.263313	2.553321	C	1.153056	15.951661	2.909908
C	-0.189974	20.473788	1.104557	F	0.638978	18.421205	-1.195709	H	1.447134	15.374832	2.038184
C	-0.727452	19.748917	0.033690	F	2.315375	19.839037	-1.469595	C	0.640364	15.324179	4.057451
H	-0.175416	18.901769	-0.369080	F	2.367995	16.329714	-1.616158	H	0.549234	14.242992	4.083523
C	-1.955430	20.119346	-0.517096	F	2.276899	17.792626	-3.217450	C	0.257073	16.102828	5.130782
H	-2.366368	19.553941	-1.349853	F	4.008213	17.730507	-1.910945	H	-0.147410	15.650780	6.032850
C	-2.652948	21.209033	0.003101	C	2.016850	18.571562	-0.946233	C	0.389394	17.505837	5.053751
H	-3.611558	21.495541	-0.422583	C	2.663807	17.608307	-1.936797	C	0.919628	18.042721	3.856823
C	-2.121196	21.934441	1.073136					C	0.016430	18.390038	6.118464
H	-2.664530	22.784263	1.479148	44				H	-0.390548	17.959601	7.029742
C	-0.893662	21.571154	1.621441	III_B3PW91				C	0.168581	19.738552	5.996006
H	-0.486414	22.133663	2.457846	Cu	2.459167	18.239568	0.885168	H	-0.114076	20.403133	6.808355
C	1.284156	20.051942	3.562482	C	0.045259	16.547928	2.271751	C	0.702620	20.314786	4.797179
C	0.095036	19.655228	4.193577	H	-0.412746	16.570191	1.286837	C	0.883852	21.703300	4.619271
H	-0.789709	19.440371	3.599957	C	-0.618872	15.966504	3.368281	H	0.611816	22.386371	5.419949
C	0.040587	19.523784	5.579835	H	-1.601640	15.526691	3.230491	C	1.406148	22.173083	3.431370
H	-0.887192	19.211614	6.052841	C	-0.001966	15.969933	4.602379	H	1.561413	23.234115	3.263402
C	1.171137	19.781376	6.356501	H	-0.484701	15.529334	5.471159	C	1.741293	21.252714	2.423079
H	1.129028	19.671737	7.437132	C	1.277273	16.551911	4.736378	H	2.162210	21.579193	1.476737
C	2.359642	20.168370	5.736933	C	1.854898	17.110778	3.572968	C	1.073866	19.470581	3.724453
H	3.249804	20.358276	6.331046	C	2.002068	16.593928	5.972037	N	1.292081	17.266411	2.812683
C	2.419936	20.295275	4.350506	H	1.541920	16.162974	6.857510	N	1.578203	19.945447	2.562965
H	3.359353	20.572318	3.878707	C	3.243745	17.152180	6.037125	F	-0.141343	19.189380	-0.488785
N	1.510220	16.836561	2.841957	H	3.792712	17.174432	6.974878	F	1.474397	18.422783	-1.772323
N	3.928541	17.950605	2.415750	C	3.857435	17.726516	4.875685	F	-0.665831	16.712913	0.404181
P	1.439280	19.938259	1.745441	C	5.138662	18.317179	4.889085	F	-0.591235	16.796593	-1.762297
F	1.130598	17.178298	-1.439721	H	5.708576	18.340224	5.814277	F	1.038284	15.877984	-0.660640
F	3.225208	17.900988	-1.518354	C	5.646007	18.863331	3.728148	C	0.893522	18.240797	-0.525937
F	1.982865	14.915636	-0.144665	H	6.625517	19.329276	3.703750	C	0.158840	16.904929	-0.645761
F	2.923462	15.284989	-2.065580	C	4.867214	18.829806	2.560528	Cu	1.929330	18.384618	1.120346
F	4.040686	15.622185	-0.236044	H	5.222978	19.268414	1.634235	Cl	4.355917	18.438404	1.854555
C	2.327577	17.190358	-0.693753	C	3.157383	17.721101	3.648529	C	3.934639	19.093460	0.058299
C	2.819240	15.751066	-0.799203	N	1.242518	17.102619	2.369513	C	4.215274	18.072374	-0.971736
				N	3.658791	18.277643	2.517886	C	4.172360	16.694838	-0.730108
30				F	0.627057	18.241911	-1.239584	C	4.487722	18.553950	-2.259903
II_B3PW91				F	2.069332	19.912802	-1.368211	C	4.404935	15.804704	-1.771281
Cu	2.496098	18.273096	0.892111	F	2.664302	16.472873	-1.765802	H	3.933154	16.327194	0.262118
C	-0.059957	16.718360	2.243498	F	2.364074	18.018751	-3.259957	C	4.728480	17.656782	-3.295055
H	-0.524503	16.820625	1.266097	F	4.070607	18.127580	-1.923514	H	4.504813	19.624221	-2.438497
C	-0.734577	16.088441	3.306078	C	1.964035	18.576754	-0.944210	C	4.684947	16.282750	-3.053931
H	-1.735378	15.697352	3.152077	C	2.762079	17.802069	-1.987406	H	4.362234	14.735434	-1.583710
C	-0.103999	15.981902	4.528912	O	3.123741	21.646694	2.095646	H	4.944470	18.030635	-4.292214
H	-0.594493	15.501312	5.371606	C	2.437127	21.208695	2.969775	H	4.865960	15.583075	-3.865733
C	1.198075	16.505019	4.686626	C	1.109514	20.589785	2.830359	O	3.864093	20.280946	-0.068824

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IV_B3PW91
C 1.475909 15.902193 2.739092
H 1.841133 15.345488 1.882271
C 1.055023 15.245979 3.905456
H 1.094073 14.162749 3.954986
C 0.595935 15.999340 4.966410
H 0.257004 15.524066 5.883318
C 0.568828 17.405859 4.860844
C 1.020825 17.978406 3.648910
C 0.111531 18.261355 5.916180
H -0.234577 17.802729 6.838684
C 0.108959 19.615893 5.770274
H -0.240035 20.258407 6.574587
C 0.569721 20.226482 4.558552
C 0.598013 21.623246 4.354901
H 0.254548 22.286937 5.144466
C 1.063605 22.124667 3.156717
H 1.098925 23.193074 2.968030
C 1.502955 21.226235 2.166693
H 1.883720 21.577184 1.212212
C 1.028160 19.411171 3.497003
N 1.451224 17.221327 2.612950
N 1.487120 19.914342 2.332472
F 0.392162 19.549907 -0.538103
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F -0.944568 18.045466 1.308217
F -1.464180 17.624123 -0.749760
F -0.230568 16.220981 0.349882
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C 3.206309 19.039081 -0.488532
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C 3.918337 16.752954 -1.262469
C 4.565301 18.724705 -2.524804
C 4.579844 15.948611 -2.182827
H 3.412468 16.312460 -0.407570
C 5.225870 17.915084 -3.443099
H 4.548472 19.804012 -2.643807
C 5.233341 16.528941 -3.273085
H 4.588062 14.870084 -2.051928
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H 5.749453 15.898219 -3.992462
O 3.168638 20.233788 -0.527868

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RETS_B3PW91
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H 2.274689 15.379815 1.971626
C 1.406576 15.289265 3.964361
H 1.530700 14.215491 4.060439
C 0.842239 16.040646 4.975155
H 0.503828 15.573353 5.896415
C 0.705817 17.435770 4.811650
C 1.163931 17.994508 3.596043
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H -0.217136 17.844390 6.734806
C 0.022087 19.633649 5.599689
H -0.416760 20.277155 6.357777
C 0.485833 20.231833 4.382566
C 0.404005 21.616307 4.119618
H -0.034124 22.278116 4.862380
C 0.883489 22.109401 2.923602
H 0.836550 23.168329 2.690207
C 1.443284 21.217035 1.992811
H 1.830042 21.558059 1.038132
C 1.061356 19.416019 3.380725
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F 0.824087 18.383373 -2.036275
F -0.597307 17.936942 1.096876
F -1.230541 17.496289 -0.918579
F 0.384907 16.357463 -0.036712
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Cl 4.649750 18.127524 1.483021
C 2.752197 19.135221 -0.769297
C 3.537992 18.207761 -1.619467
C 3.287231 16.832094 -1.650612
C 4.586965 18.749121 -2.373358
C 4.083705 15.999749 -2.428588
H 2.468942 16.418894 -1.070652
C 5.381626 17.912433 -3.150031
H 4.774101 19.817836 -2.335169
C 5.133099 16.538283 -3.176917
H 3.887072 14.931384 -2.452567
H 6.197667 18.331304 -3.732878
H 5.757043 15.886341 -3.782883
O 2.817993 20.339552 -0.780781

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V_B3PW91
Cu 2.873262 16.126411 0.741172
C 0.376332 16.806785 2.793735
H -0.256631 16.312743 2.062218
C -0.175858 17.404810 3.944510
H -1.248011 17.369221 4.108394
C 0.668114 18.026218 4.844914
H 0.279601 18.498134 5.743455
C 2.058983 18.050445 4.592750
C 2.512860 17.426254 3.403605
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H 2.639936 19.143970 6.379217
C 4.338325 18.680012 5.174450
H 5.052680 19.152749 5.842494
C 4.831240 18.078345 3.967294
C 6.194674 18.101271 3.599390
H 6.919199 18.570522 4.259341
C 6.585277 17.534159 2.401823
H 7.622804 17.538412 2.085395
C 5.611889 16.949639 1.573699
H 5.880010 16.505606 0.621005
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N 1.676050 16.815949 2.532535
N 4.319189 16.908705 1.896085
Cl 1.984158 15.035590 -0.934863
O 0.536325 19.130596 0.765025
C 1.081382 20.214104 0.848043
C 0.461102 21.391774 1.496413
C 2.531987 20.318842 0.269700
C 0.897594 22.713502 1.295181
C -0.626430 21.141548 2.355324
C 3.607019 20.665964 1.348347
F 2.586886 21.262763 -0.714129
F 2.871147 19.131041 -0.276473
C 0.252215 23.763098 1.947643
H 1.718274 22.932039 0.624906
C -1.256592 22.192393 3.011892
H -0.949957 20.117011 2.507134
F 3.168006 20.280186 2.562700
F 3.842663 21.984599 1.389968
F 4.762801 20.037989 1.099217
C -0.818623 23.506192 2.807329
H 0.585736 24.783285 1.781898
H -2.087310 21.991960 3.682404
H -1.312736 24.328194 3.317891

24
VI_B3PW91
Cu -0.906835 -0.139299 0.096390
N 0.714596 1.360663 0.024146
N 0.705210 -1.341295 0.041513
C 0.692978 2.685159 0.023750
C 1.861984 3.467376 -0.003321
C 3.088418 2.835613 -0.032265
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C 3.075695 -2.822643 -0.028339
C 1.848156 -3.451588 0.007226
C 0.681963 -2.670680 0.042868
C 1.910458 0.731287 -0.002707
C 3.142966 1.424839 -0.033309
C 3.132786 -1.412627 -0.030521
C 1.905899 -0.710357 0.002609
H -0.290348 3.147813 0.046161
H 1.785315 4.550069 -0.001097
H 4.012478 3.407753 -0.053751
H 5.306624 1.233409 -0.086785
H 5.296368 -1.236367 -0.087540
H 3.998255 -3.396769 -0.054391
H 1.766984 -4.533673 0.009293
H -0.300503 -3.130864 0.073669
Cl -3.036838 0.290023 0.156083

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VII_B3PW91
Cu 11.289647 3.879392 0.960074
C 11.913135 0.859476 1.581785
H 12.936653 1.134997 1.341872
C 11.612400 -0.391096 2.146204

H 12.411955 -1.097725 2.345422
C 10.297715 -0.692680 2.439586
H 10.026557 -1.647911 2.882025
C 9.292221 0.258354 2.168008
C 9.696497 1.490605 1.601168
C 7.907395 0.036378 2.460708
H 7.617138 -0.917590 2.893350
C 6.975799 0.999648 2.216839
H 5.928199 0.828900 2.451505
C 7.353220 2.267682 1.666483
C 8.711464 2.514014 1.349733
C 6.435694 3.316973 1.453885
H 5.385190 3.167671 1.690806
C 6.888460 4.522747 0.955411
H 6.210722 5.352960 0.783153
C 8.254819 4.668744 0.666454
H 8.647155 5.603402 0.276492
C 10.673288 6.237991 3.354300
C 10.462667 7.070697 2.247618
H 10.774716 6.732846 1.261037
C 9.857393 8.317377 2.407179
H 9.698721 8.955852 1.541717
C 9.451416 8.736193 3.674128
H 8.973385 9.704531 3.800249
C 9.655089 7.909286 4.781871
H 9.337362 8.233941 5.769710
C 10.264582 6.666193 4.625208
H 10.409040 6.023404 5.489531
C 13.178162 4.807032 3.717632
C 14.239432 4.737619 2.806904
H 14.024028 4.572969 1.751799
C 15.554933 4.882763 3.250302
H 16.374216 4.829777 2.537633
C 15.813851 5.092384 4.604381
H 16.838253 5.203057 4.951626
C 14.757720 5.159163 5.517898
H 14.960391 5.321105 6.573798
C 13.443874 5.018026 5.078212
H 12.625732 5.062548 5.792701
C 10.651157 3.461731 4.179849
C 9.257369 3.517484 4.336066
H 8.693230 4.335754 3.895756
C 8.585925 2.522409 5.043617
H 7.506391 2.579506 5.155251
C 9.292111 1.450103 5.589720
H 8.765534 0.669093 6.132196
C 10.676016 1.379801 5.426054
H 11.232979 0.543340 5.840721
C 11.352766 2.376894 4.725494
H 12.429711 2.306573 4.598490
Cl 12.485204 4.482475 -0.868522
N 10.989003 1.772986 1.314717
N 9.141831 3.698763 0.854074
P 11.486603 4.625984 3.043305

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C6H5COCl_B3PW91
C -1.426368 -0.634264 0.291873
C -0.043133 -0.638713 0.144494
C 0.634659 0.565530 -0.088446
C -0.085050 1.770702 -0.169121
C -1.465402 1.765988 -0.018375
C -2.137718 0.563641 0.211776
H -1.950064 -1.569183 0.469911
H 0.501664 -1.574086 0.208620
H 0.448050 2.698891 -0.348777
H -2.018097 2.699201 -0.080166
H -3.218240 0.560759 0.328921
C 2.094907 0.673430 -0.262795
O 2.714962 1.668545 -0.490159
Cl 3.026876 -0.894192 -0.108549

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C6H5COC2F5_B3PW91
C -1.469574 -0.584930 0.406385
C -0.087737 -0.625551 0.246593
C 0.615662 0.546975 -0.077871
C -0.093822 1.751150 -0.239609
C -1.472260 1.783249 -0.085001
C -2.163694 0.613021 0.239081
H -2.005913 -1.495021 0.660326
H 0.425598 -1.567830 0.383253
H 0.455171 2.654251 -0.487505
H -2.010305 2.718172 -0.215311
H -3.243378 0.636364 0.362326
C 2.082099 0.621890 -0.253719
C 2.970700 -0.658180 -0.179444
C 3.373183 -1.045912 1.260914
F 4.119052 -0.419874 -0.848263
F 2.371172 -1.734178 -0.752734
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F 3.980295 -0.011354 1.851107
F 4.210014 -2.087215 1.244734
O 2.681065 1.660536 -0.455164

34
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H 4.290130 22.765490 -1.472356
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H 4.486154 24.770242 -0.012456
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H 3.455314 24.754613 2.249503
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H 2.230242 22.763370 3.044642
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H -0.562764 18.325101 1.394075
C -2.198208 19.449537 0.566053
H -2.872854 18.596852 0.558629
C -2.630932 20.689948 0.094769
H -3.644289 20.807191 -0.281338
C -1.757089 21.777224 0.104415
H -2.088459 22.746143 -0.261616
C -0.456897 21.630071 0.588010
H 0.211596 22.486638 0.599037
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H 3.362997 19.504688 3.978946
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H 3.178498 19.838001 6.420761
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H 1.122281 20.847826 7.390670
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H -0.739342 21.534166 5.893287
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64
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30
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H 3.710737 16.938581 6.979151
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F 2.152359 17.762751 -3.207744
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H 3.479282 17.022606 7.024617
C 3.683811 17.574704 4.924326
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44
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44
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44
V_PBE
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H -0.965140 20.190779 2.528386
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VII_PBE
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C 9.803526 8.175954 2.767772
H 9.715390 8.904734 1.954992

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C	10.033619	6.297670	4.845691
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N	10.619857	1.626128	1.508472
N	9.131698	3.783831	0.822014
P	11.617098	4.517748	3.228976

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C	0.640860	0.568715	-0.088630
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C	-1.474071	1.773144	-0.019940
C	-2.148786	0.562906	0.212540
H	-1.957253	-1.583299	0.475019
H	0.514717	-1.582566	0.211687
H	0.451793	2.715237	-0.352748
H	-2.032175	2.712295	-0.083584
H	-3.237256	0.558530	0.329987
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C	-1.476294	1.798091	-0.063049
C	-2.173867	0.620053	0.256474
H	-2.021347	-1.507836	0.650753
H	0.425079	-1.588816	0.342412
H	0.466844	2.668665	-0.480532
H	-2.015487	2.743889	-0.176025
H	-3.259830	0.647059	0.393634
C	2.087722	0.617283	-0.293129
C	2.983985	-0.667373	-0.179484
C	3.368847	-1.043134	1.278479
F	4.153354	-0.429452	-0.838839
F	2.390060	-1.763750	-0.758051
F	2.278445	-1.421909	1.985785
F	3.927504	0.025566	1.888566
F	4.255401	-2.061254	1.283908
O	2.686935	1.660351	-0.544002

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PPh3_PBE

C	2.568408	21.637430	1.235080
C	3.177887	21.638987	-0.038472
H	3.106031	20.749550	-0.675559
C	3.873502	22.766684	-0.495861
H	4.337456	22.754194	-1.487924
C	3.985369	23.902909	0.321048
H	4.537319	24.780878	-0.031010
C	3.392646	23.907109	1.593015
H	3.477214	24.790447	2.235370
C	2.684990	22.783878	2.047508
H	2.220252	22.800344	3.038760
C	-0.031909	20.394891	1.063831
C	-0.911578	19.290734	1.034511
H	-0.569018	18.313743	1.395769
C	-2.219190	19.432371	0.550126
H	-2.891747	18.567950	0.538694
C	-2.660358	20.675684	0.069838
H	-3.678755	20.784909	-0.317890
C	-1.789714	21.776011	0.083527
H	-2.127796	22.748595	-0.290362
C	-0.484409	21.639438	0.580222
H	0.184031	22.506453	0.593545
C	1.424271	20.360245	3.553442
C	2.473788	19.953960	4.406147
H	3.376257	19.501014	3.978628
C	2.373866	20.126089	5.793539
H	3.198821	19.810967	6.441517
C	1.214738	20.689346	6.350570
H	1.131724	20.815778	7.435249
C	0.160868	21.084257	5.512579
H	-0.746566	21.523422	5.941285
C	0.264398	20.924929	4.122153
H	-0.560735	21.244061	3.477063
P	1.669673	20.095083	1.735116

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I_LC-wPBE

Cu	2.195853	17.920660	1.142887
C	0.304236	16.348419	3.042941
H	-0.352147	16.328265	2.177362
C	-0.132410	15.881462	4.289868
H	-1.138850	15.490621	4.394239
C	0.729636	15.934093	5.355888
H	0.426668	15.584630	6.339111
C	2.023787	16.452382	5.171808
C	2.364556	16.896952	3.889976
C	2.985441	16.555061	6.236698
H	2.699504	16.201531	7.223301
C	4.209000	17.080263	6.017731
H	4.932835	17.160182	6.823856
C	4.581965	17.565740	4.716117
C	5.820487	18.175993	4.452368
H	6.553367	18.269671	5.249155
C	6.082033	18.652469	3.191884
H	7.024498	19.133319	2.952709
C	5.102420	18.514361	2.199594
H	5.272327	18.884971	1.192879
C	3.669591	17.474710	3.658765
C	2.568259	21.293855	1.278269
C	3.437633	21.058081	0.213778
H	3.427970	20.088027	-0.280465
C	4.304668	22.055274	-0.216940
H	4.977046	21.863898	-1.048614
C	4.312252	23.289451	0.418656
H	4.993089	24.068334	0.086243
C	3.448065	23.530342	1.482210
H	3.453136	24.496011	1.980088
C	2.577610	22.538397	1.909284
H	1.909929	22.729969	2.745255
C	-0.177625	20.472718	1.109341
C	-0.710528	19.763339	0.035188
H	-0.159702	18.918859	-0.374883
C	-1.931338	20.140220	-0.513826
H	-2.340691	19.584658	-1.352939
C	-2.624225	21.221298	0.012386
H	-3.580169	21.514030	-0.413309
C	-2.096603	21.932588	1.086548
H	-2.639038	22.778998	1.498590
C	-0.877351	21.561885	1.632032
H	-0.470978	22.115631	2.474656
C	1.291902	20.048265	3.555107
C	0.111141	19.649783	4.184190
H	-0.770878	19.421756	3.591233
C	0.054491	19.532699	5.566219
H	-0.870996	19.219198	6.041243
C	1.177230	19.806552	6.337755
H	1.133840	19.709628	7.418973
C	2.358374	20.196137	5.719435
H	3.243946	20.402932	6.313872
C	2.418160	20.310631	4.337063
H	3.355077	20.594840	3.863722
N	1.511528	16.839193	2.845848
N	3.934077	17.945732	2.422530
P	1.443778	19.936592	1.743014
F	1.140695	17.167360	-1.411074
F	3.229801	17.880179	-1.494292
F	1.979611	14.921381	-0.108820
F	2.919150	15.287399	-2.024171
F	4.033391	15.619318	-0.198909

C 2.331737 17.185397 -0.664681
C 2.816747 15.750097 -0.762721

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II_LC-wPBE
Cu 2.335179 18.201641 0.908461
C -0.061262 16.668151 2.267824
H -0.537058 16.753175 1.295162
C -0.713406 16.034588 3.336633
H -1.706438 15.623544 3.190737
C -0.076047 15.950053 4.547931
H -0.550430 15.466804 5.397586
C 1.213053 16.497703 4.690673
C 1.775665 17.107031 3.566885
C 1.959654 16.454803 5.919269
H 1.504369 15.975888 6.781325
C 3.194372 16.995360 5.999386
H 3.757559 16.962297 6.927568
C 3.798689 17.629807 4.858534
C 5.081304 18.209245 4.885221
H 5.660475 18.186174 5.804162
C 5.580677 18.793699 3.749589
H 6.564914 19.248659 3.733080
C 4.795974 18.801188 2.587769
H 5.158421 19.255605 1.671010
C 3.094878 17.686825 3.653675
N 1.143692 17.188544 2.377597
N 3.591178 18.266730 2.539061
F 0.750512 18.722747 -1.357376
F 2.678184 19.788553 -1.411862
F 2.075511 16.351493 -1.644732
F 2.443687 17.819962 -3.191968
F 3.970551 17.406966 -1.714503
C 2.087699 18.605425 -0.950508
C 2.642978 17.548435 -1.889955

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III_LC-wPBE
Cu 2.409862 18.170032 0.975277
C 0.041909 16.557400 2.308735
H -0.395963 16.569954 1.315003
C -0.636562 15.971870 3.389384
H -1.610486 15.521528 3.230681
C -0.047453 15.982351 4.627439
H -0.542068 15.537545 5.486602
C 1.220777 16.573435 4.784862
C 1.809793 17.131293 3.647803
C 1.923199 16.618144 6.039010
H 1.447024 16.181111 6.912031
C 3.147599 17.180840 6.127598
H 3.681049 17.208119 7.073352
C 3.779314 17.761635 4.973095
C 5.053071 18.359181 5.008136
H 5.605493 18.388392 5.943178
C 5.576552 18.898584 3.861179
H 6.553394 19.369157 3.851233
C 4.821740 18.850324 2.681260
H 5.196710 19.280943 1.758474
C 3.110557 17.749250 3.747230
N 1.224194 17.121061 2.433244
N 3.626125 18.294857 2.623250
F 0.862800 18.069369 -1.361559
F 2.240279 19.787373 -1.350461
F 3.006828 16.381692 -1.571373
F 2.836611 17.882225 -3.122639
F 4.353262 18.084541 -1.591673
C 2.130272 18.464378 -0.901382
C 3.080211 17.705535 -1.811305
O 3.109550 21.599855 2.011188
C 2.386479 21.202647 2.871027
C 1.049332 20.600511 2.675961
Cl 2.936149 21.345077 4.565727
C 0.241327 20.146582 3.717580
C 0.619437 20.482713 1.352571
C -0.998300 19.597259 3.433276
H 0.573354 20.218663 4.747334
C -0.620831 19.928206 1.075297
H 1.265126 20.810629 0.545464
C -1.430928 19.492308 2.115159
H -1.627964 19.244001 4.244117
H -0.940259 19.822238 0.043668
H -2.402086 19.055799 1.898856

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OATS_LC-wPBE
C 1.169887 15.956755 2.944411
H 1.480925 15.373499 2.082758
C 0.644129 15.334686 4.084384
H 0.557156 14.254085 4.114773
C 0.245314 16.115072 5.139587
H -0.170238 15.668833 6.038870
C 0.372661 17.513852 5.054355
C 0.911869 18.040775 3.876570
C -0.024958 18.403440 6.112289
H -0.441504 17.972248 7.018034
C 0.115246 19.739561 5.983063
H -0.185527 20.410620 6.782539
C 0.665002 20.311546 4.783448
C 0.830930 21.697168 4.599136
H 0.535122 22.381588 5.389449
C 1.363974 22.162280 3.424506
H 1.506836 23.222954 3.248355
C 1.730666 21.238664 2.434726
H 2.163161 21.564556 1.493583
C 1.060021 19.472861 3.736969
N 1.303279 17.263467 2.845028
N 1.582564 19.939749 2.584831
F -0.128276 19.235194 -0.224564
F 1.396522 18.565958 -1.654096
F -0.629912 16.736601 0.511248
F -0.651650 16.956885 -1.641034
F 1.006785 15.952925 -0.676793
C 0.895885 18.296867 -0.392137
C 0.145960 16.983072 -0.559753
Cu 2.030446 18.344165 1.185618
Cl 4.326363 18.366803 1.803922
C 3.808686 18.997793 0.045209
C 4.115194 17.982610 -0.995807
C 4.101012 16.612596 -0.757667
C 4.394527 18.474428 -2.267606
C 4.370854 15.734362 -1.794141
H 3.864382 16.235032 0.231841
C 4.671129 17.591515 -3.299733
H 4.389270 19.545715 -2.439943
C 4.657713 16.222294 -3.064286
H 4.354049 14.664263 -1.610695
H 4.892620 17.973584 -4.291798
H 4.869657 15.530717 -3.874747
O 3.732977 20.180656 -0.087676

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IV_LC-wPBE
C 1.493641 15.910765 2.717711
H 1.861587 15.355562 1.860816
C 1.074732 15.249671 3.878001
H 1.117978 14.167144 3.923164
C 0.614404 15.994228 4.933735
H 0.275566 15.516185 5.848617
C 0.583591 17.396955 4.832032
C 1.030405 17.968203 3.637326
C 0.118791 18.249116 5.893487
H -0.226722 17.783571 6.811946
C 0.110524 19.591255 5.751648
H -0.242379 20.233556 6.553439
C 0.573168 20.206912 4.537267
C 0.593491 21.600373 4.338130
H 0.244046 22.259353 5.128248
C 1.055766 22.104300 3.149653
H 1.085598 23.172182 2.961674
C 1.501198 21.212313 2.161922
H 1.880746 21.569753 1.209622
C 1.032661 19.404863 3.488694
N 1.463771 17.222424 2.598713
N 1.491448 19.908163 2.327357
F 0.421567 19.611308 -0.484826
F 1.052989 17.811176 -1.566865
F -0.886661 18.067702 1.312092
F -1.404890 17.679925 -0.747009
F -0.162488 16.269510 0.322500
C 0.827581 18.318763 -0.312576
C -0.423818 17.574006 0.158987
Cu 2.273320 18.243608 1.012237
Cl 4.337387 18.166584 1.875700
C 3.147658 19.033707 -0.494207
C 3.864648 18.123427 -1.420332
C 3.888842 16.747064 -1.225800
C 4.512421 18.695586 -2.511986
C 4.563271 15.939005 -2.125095
H 3.387887 16.314877 -0.363717
C 5.187484 17.883168 -3.410433
H 4.481713 19.772208 -2.648696
C 5.211914 16.507439 -3.216957
H 4.586573 14.863839 -1.975156
H 5.694862 18.324843 -4.262932

H 5.740720 15.871629 -3.921528
O 3.107878 20.220961 -0.542630

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RETS_LC-wPBE
C 1.803434 15.952618 2.761632
H 2.244518 15.397407 1.939510
C 1.390581 15.303041 3.932263
H 1.512095 14.229098 4.021182
C 0.836601 16.047503 4.941983
H 0.499744 15.578393 5.862284
C 0.706191 17.439945 4.785421
C 1.154862 17.997676 3.585012
C 0.137923 18.292850 5.794391
H -0.207785 17.837492 6.717924
C 0.034597 19.623997 5.597536
H -0.396860 20.267672 6.358736
C 0.498072 20.227835 4.377391
C 0.422781 21.611101 4.128010
H -0.007187 22.268054 4.879049
C 0.895624 22.108865 2.941257
H 0.855181 23.168992 2.715723
C 1.442786 21.221405 2.003643
H 1.826153 21.571415 1.050837
C 1.057159 19.425121 3.378856
N 1.682332 17.252380 2.591628
N 1.519713 19.924625 2.214432
F 0.303094 19.810681 -0.434654
F 0.862553 18.373706 -1.982846
F -0.568297 17.933346 1.126108
F -1.176345 17.496877 -0.891900
F 0.416294 16.349686 0.007316
C 0.883529 18.610477 -0.637314
C -0.120904 17.574507 -0.076830
Cu 2.407512 18.367659 0.988877
Cl 4.596496 18.174104 1.462607
C 2.739797 19.121091 -0.777754
C 3.530381 18.194066 -1.627936
C 3.282829 16.826086 -1.654551
C 4.567266 18.738473 -2.378512
C 4.077330 15.999121 -2.430692
H 2.467085 16.410986 -1.071657
C 5.361144 17.907734 -3.154330
H 4.749928 19.807740 -2.340842
C 5.117905 16.539674 -3.178805
H 3.885828 14.930499 -2.453065
H 6.174360 18.328471 -3.738308
H 5.742469 15.889627 -3.785051
O 2.806749 20.317190 -0.781187

44
V_LC-wPBE
Cu 2.830430 16.117889 0.779271
C 0.428659 16.731723 2.823710
H -0.210291 16.248983 2.089862
C -0.107504 17.278486 3.999694
H -1.174723 17.216574 4.183752
C 0.738253 17.883377 4.894022
H 0.361065 18.319894 5.814855
C 2.116420 17.941169 4.613301
C 2.549785 17.368541 3.414316
C 3.072654 18.561954 5.489389
H 2.714070 18.998117 6.417339
C 4.382356 18.602280 5.166220
H 5.104964 19.071289 5.827672
C 4.857354 18.036364 3.932321
C 6.206430 18.086698 3.537507
H 6.938780 18.553288 4.190564
C 6.575896 17.550969 2.330619
H 7.605418 17.575013 1.990971
C 5.594628 16.967824 1.519136
H 5.849159 16.541356 0.554272
C 3.951113 17.426622 3.060679
N 1.712820 16.774784 2.542011
N 4.323328 16.904701 1.869827
Cl 1.963494 15.032244 -0.882242
O 0.513109 19.200624 0.829027
C 1.069735 20.269894 0.892997
C 0.436940 21.479758 1.471364
C 2.533433 20.334715 0.386117
C 0.885160 22.778808 1.230296
C -0.671124 21.268790 2.294840
C 3.539916 20.669210 1.515912
F 2.659743 21.258937 -0.594721
F 2.871190 19.139815 -0.120756
C 0.228219 23.851840 1.815005
H 1.730569 22.967350 0.580854
C -1.316142 22.342199 2.883283
H -1.008663 20.252642 2.473285
F 3.038954 20.266643 2.690991
F 3.764018 21.980216 1.582838
F 4.700998 20.050337 1.316541
C -0.865898 23.636103 2.642333
H 0.573376 24.862660 1.619817
H -2.171589 22.172363 3.530199
H -1.372021 24.480481 3.101666

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VI_LC-wPBE
Cu -0.889717 -0.099296 0.093042
N 0.721579 1.356177 0.032527
N 0.712530 -1.339820 0.039959
C 0.697003 2.672462 0.033402
C 1.862583 3.452987 0.003050
C 3.080395 2.823767 -0.029593
C 4.364786 0.675428 -0.065270
C 4.359909 -0.674298 -0.066319
C 3.067237 -2.814940 -0.031427
C 1.847902 -3.440823 0.003976
C 0.685471 -2.659425 0.040007
C 1.915834 0.730645 0.000788
C 3.133041 1.416879 -0.031774
C 3.123616 -1.408770 -0.032240
C 1.911172 -0.714766 0.002604
H -0.284889 3.136801 0.059545
H 1.784693 4.534765 0.006041
H 4.004826 3.394168 -0.053404
H 5.299053 1.228861 -0.090673
H 5.289907 -1.234764 -0.092801
H 3.989966 -3.387818 -0.058668
H 1.765554 -4.522087 0.005311
H -0.296354 -3.120878 0.069885
Cl -3.020389 0.287612 0.145444

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VII_LC-wPBE
Cu 11.330002 3.582201 1.216561
C 11.154418 0.615775 2.230542
H 12.236204 0.692956 2.293358
C 10.483422 -0.510359 2.727825
H 11.049540 -1.315234 3.183805
C 9.116869 -0.564546 2.624952
H 8.560891 -1.421422 2.995413
C 8.425217 0.509038 2.034702
C 9.184050 1.594519 1.583508
C 6.994390 0.534771 1.892070
H 6.426161 -0.321643 2.244029
C 6.373385 1.594081 1.332156
H 5.292992 1.611524 1.220529
C 7.123589 2.732973 0.874945
C 8.516645 2.741620 1.006621
C 6.517915 3.865191 0.299929
H 5.438425 3.892496 0.179187
C 7.301412 4.916075 -0.102046
H 6.871280 5.803305 -0.554009
C 8.688199 4.836191 0.087106
H 9.337167 5.653746 -0.212173
C 10.591500 5.850277 3.640046
C 10.288485 6.738852 2.608569
H 10.674971 6.546916 1.609903
C 9.502912 7.857745 2.850316
H 9.274596 8.543990 2.039603
C 9.004894 8.091375 4.125969
H 8.384530 8.962710 4.316919
C 9.298538 7.207982 5.158294
H 8.909521 7.387993 6.156642
C 10.090021 6.092716 4.918625
H 10.309482 5.404680 5.730662
C 13.330702 5.016292 3.658071
C 14.338388 4.886885 2.706093
H 14.101280 4.455545 1.734799
C 15.630308 5.314429 2.994815
H 16.412146 5.213050 2.247323
C 15.915659 5.871052 4.233157
H 16.924460 6.205742 4.459259
C 14.910562 6.004551 5.187859
H 15.134259 6.442433 6.156721
C 13.622917 5.579768 4.901929
H 12.840215 5.684380 5.649275
C 11.267736 3.178100 4.479975
C 9.932007 2.799387 4.642553
H 9.149496 3.331312 4.105963
C 9.595895 1.744725 5.476157
H 8.553601 1.460642 5.591682

C 10.591496 1.046306 6.152741
H 10.329015 0.215491 6.801732
C 11.919822 1.411961 5.991014
H 12.702900 0.869623 6.513627
C 12.258619 2.472825 5.157274
H 13.303589 2.743083 5.033310
Cl 12.719576 3.618804 -0.576782
N 10.528838 1.632413 1.674785
N 9.278859 3.790806 0.628770
P 11.662149 4.434490 3.216523

14
C6H5COCl_LC-wPBE
C -1.423957 -0.629647 0.290422
C -0.045547 -0.635713 0.143400
C 0.628082 0.561371 -0.087484
C -0.082683 1.760405 -0.167662
C -1.458413 1.760014 -0.017718
C -2.129371 0.564291 0.211028
H -1.949206 -1.563053 0.468139
H 0.496570 -1.572581 0.207469
H 0.453508 2.686617 -0.347108
H -2.009104 2.693669 -0.079268
H -3.209314 0.563202 0.328151
C 2.095234 0.663788 -0.261795
O 2.699254 1.664723 -0.491528
Cl 3.011992 -0.860836 -0.106840

20
C6H5COC2F5_LC-wPBE
C -1.464175 -0.578811 0.413057
C -0.086279 -0.618905 0.262716
C 0.610312 0.545436 -0.066252
C -0.091299 1.740640 -0.242778
C -1.466429 1.774026 -0.097796
C -2.154762 0.611711 0.231247
H -2.000932 -1.486461 0.672001
H 0.428374 -1.558849 0.410389
H 0.459158 2.641279 -0.495139
H -2.003804 2.706797 -0.240023
H -3.234598 0.634851 0.347601
C 2.082392 0.621057 -0.233065
C 2.964055 -0.652183 -0.178308
C 3.371335 -1.048442 1.249139
F 4.105114 -0.408407 -0.848486
F 2.356304 -1.715367 -0.753284
F 2.299051 -1.384420 1.971078
F 3.979471 -0.019553 1.839639
F 4.204978 -2.086068 1.216626
O 2.674770 1.658865 -0.414528

34
PPh3_LC-wPBE
C 2.562954 21.618825 1.249470
C 3.155380 21.633319 -0.014837
H 3.087873 20.754164 -0.652063
C 3.830009 22.757945 -0.468426
H 4.282575 22.755209 -1.456135
C 3.934241 23.879819 0.344522
H 4.468737 24.758787 -0.005173
C 3.356797 23.872235 1.607529
H 3.436297 24.746302 2.248112
C 2.671639 22.750365 2.056768
H 2.218593 22.760341 3.044124
C -0.005680 20.394262 1.064798
C -0.884774 19.309428 1.043407
H -0.550583 18.336874 1.398785
C -2.182386 19.458484 0.575043
H -2.856397 18.606358 0.568999
C -2.613712 20.693192 0.105855
H -3.627041 20.810214 -0.268296
C -1.744068 21.775774 0.113385
H -2.075598 22.743434 -0.253222
C -0.448547 21.629140 0.593222
H 0.219281 22.485902 0.600331
C 1.419697 20.352837 3.531295
C 2.455491 19.959577 4.381201
H 3.351605 19.504378 3.964635
C 2.355307 20.144301 5.752767
H 3.171727 19.837565 6.400715
C 1.208554 20.711333 6.295037
H 1.124848 20.850538 7.369346
C 0.168225 21.095786 5.459449
H -0.731510 21.538373 5.878152
C 0.273687 20.921577 4.085127
H -0.544509 21.233718 3.442214
P 1.673023 20.091985 1.734925

64
I_PBE0
Cu 2.197383 17.918006 1.154639
C 0.309465 16.322917 3.060230
H -0.355136 16.318878 2.200153
C -0.115782 15.825595 4.301223
H -1.120921 15.429501 4.404990
C 0.758489 15.853315 5.367233
H 0.463847 15.479187 6.344377
C 2.052594 16.378484 5.184702
C 2.384336 16.858720 3.897650
C 3.019859 16.457746 6.238081
H 2.744854 16.082119 7.220280
C 4.251053 16.993131 6.019501
H 4.980101 17.053454 6.823481
C 4.613298 17.505153 4.731925
C 5.856031 18.112372 4.467253
H 6.598096 18.184172 5.258453
C 6.109058 18.613570 3.207128
H 7.054032 19.091182 2.968438
C 5.117874 18.503407 2.220165
H 5.281917 18.895163 1.219911
C 3.682323 17.439937 3.669723
C 2.563527 21.315675 1.276671
C 3.421633 21.074288 0.196747
H 3.400035 20.105202 -0.298990
C 4.292956 22.068429 -0.244830
H 4.953439 21.871983 -1.085560
C 4.319554 23.306014 0.394181
H 5.002979 24.080011 0.054249
C 3.468563 23.552013 1.472278
H 3.487349 24.517138 1.972208
C 2.591959 22.563773 1.910988
H 1.936884 22.760931 2.755846
C -0.195729 20.482628 1.101827
C -0.725330 19.749385 0.034542
H -0.171786 18.898557 -0.358544
C -1.947076 20.115206 -0.529335
H -2.351115 19.542016 -1.359857
C -2.646899 21.209278 -0.026886
H -3.601307 21.492464 -0.463485
C -2.123250 21.944188 1.038352
H -2.668071 22.799137 1.430718
C -0.902101 21.585370 1.599751
H -0.501112 22.158266 2.432329
C 1.266238 20.103483 3.571523
C 0.070944 19.736233 4.205465
H -0.814823 19.521230 3.613138
C 0.008105 19.637266 5.593096
H -0.926699 19.350795 6.068346
C 1.136338 19.898906 6.368649
H 1.086788 19.817653 7.451333
C 2.330523 20.259144 5.747058
H 3.218354 20.458471 6.341783
C 2.398567 20.354618 4.359677
H 3.341327 20.619972 3.887305
N 1.519332 16.824703 2.859216
N 3.940253 17.936622 2.439559
P 1.430919 19.959403 1.757672
F 1.142566 17.189875 -1.414446
F 3.228198 17.913274 -1.492863
F 1.995263 14.931450 -0.135721
F 2.930516 15.314461 -2.048689
F 4.045577 15.639074 -0.223796
C 2.335345 17.202932 -0.671748
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30
II_PBE0
Cu 2.468224 18.259259 0.892672
C -0.062424 16.712454 2.249344
H -0.530567 16.810688 1.273082
C -0.734010 16.083265 3.312219
H -1.733815 15.689769 3.159333
C -0.102802 15.980376 4.532902
H -0.590573 15.500226 5.377346
C 1.196638 16.506261 4.687762
C 1.780442 17.119449 3.557975
C 1.931557 16.443531 5.915176
H 1.465463 15.966457 6.773248
C 3.184057 16.967319 6.006794
H 3.739785 16.917304 6.939339
C 3.804015 17.598345 4.880002
C 5.097553 18.156927 4.924243
H 5.667402 18.115305 5.848867
C 5.619378 18.746683 3.793596

H	6.611706	19.185235	3.790995	H	-0.832003	19.977869	0.195933	C	0.572688	17.406174	4.860157
C	4.846241	18.778883	2.623052	H	-2.304631	19.264575	2.071648	C	1.022940	17.976563	3.649011
H	5.226163	19.236675	1.715090					C	0.116824	18.259989	5.915828
C	3.104290	17.677550	3.656909	44				H	-0.227743	17.799880	6.838033
N	1.154705	17.214904	2.367197	OATS_PBE0				C	0.113681	19.612384	5.770194
N	3.626060	18.262790	2.552811	C	1.870903	16.081965	2.354008	H	-0.234198	20.255934	6.573993
F	0.651117	18.376359	-1.227732	H	2.298202	15.707522	1.427674	C	0.572375	20.221662	4.558451
F	2.294620	19.826374	-1.464875	C	1.503342	15.201653	3.384294	C	0.598654	21.616943	4.356593
F	2.427455	16.332791	-1.623154	H	1.649904	14.133962	3.256735	H	0.255228	22.278723	5.147686
F	2.325381	17.796903	-3.213367	C	0.961966	15.718967	4.541010	C	1.061513	22.119136	3.159977
F	4.033754	17.768112	-1.887023	H	0.667263	15.069620	5.361488	H	1.095713	23.187409	2.971475
C	2.014998	18.556009	-0.952803	C	0.782814	17.112146	4.659071	C	1.499758	21.222475	2.170130
C	2.697721	17.614893	-1.932764	C	1.182887	17.912241	3.565265	H	1.878685	21.578116	1.216208
				C	0.219032	17.731739	5.820749	C	1.029368	19.408831	3.497365
44				H	-0.078510	17.097586	6.651744	N	1.451636	17.220520	2.613915
III_PBE0				C	0.056844	19.080868	5.884284	N	1.485510	19.912155	2.333974
Cu	2.506458	18.137558	0.901272	H	-0.372736	19.547359	6.766919	F	0.400952	19.554588	-0.537002
C	-0.005587	16.540866	2.202865	C	0.442074	19.920606	4.790150	F	1.038134	17.724115	-1.561427
H	-0.429246	16.575636	1.202578	C	0.285427	21.321393	4.802413	F	-0.936626	18.050570	1.290590
C	-0.727399	15.984865	3.273755	H	-0.143341	21.804542	5.676670	F	-1.443723	17.631633	-0.764223
H	-1.720102	15.581391	3.101566	C	0.675647	22.056925	3.704269	F	-0.218250	16.232935	0.337182
C	-0.153364	15.964460	4.526457	H	0.568026	23.136422	3.679799	C	0.794485	18.264138	-0.324771
H	-0.680596	15.541376	5.377775	C	1.218642	21.386931	2.596578	C	-0.467616	17.536100	0.150206
C	1.139254	16.499174	4.705008	H	1.531942	21.933283	1.711116	Cu	2.270285	18.219936	1.000977
C	1.774642	17.037626	3.564820	C	1.003840	19.341368	3.630497	Cl	4.348569	18.143634	1.891684
C	1.818330	16.517383	5.965639	N	1.724096	17.394176	2.441320	C	3.192212	19.036240	-0.494888
H	1.312736	16.099591	6.832268	N	1.378262	20.073880	2.559938	C	3.900793	18.137190	-1.430807
C	3.070018	17.039621	6.077081	F	1.481051	19.453925	-1.832116	C	3.911681	16.751732	-1.258249
H	3.585031	17.047510	7.033947	F	1.125297	17.382664	-1.183367	C	4.555113	18.719807	-2.523119
C	3.741279	17.595658	4.940162	F	-0.498047	20.307359	-0.159084	C	4.577738	15.947788	-2.173583
C	5.035033	18.151547	5.003682	F	-1.097668	18.808216	-1.598548	H	3.405705	16.313061	-0.402117
H	5.567056	18.163710	5.951313	F	-0.853896	18.263235	0.479711	C	5.220469	17.910690	-3.436135
C	5.603939	18.674588	3.862971	C	1.134456	18.696846	-0.727504	H	4.534517	19.798835	-2.644021
H	6.596671	19.111855	3.875244	C	-0.340522	19.019062	-0.507200	C	5.231689	16.526834	-3.262132
C	4.874155	18.651539	2.664780	Cu	2.150697	18.907363	0.928008	H	4.589599	14.869868	-2.039702
H	5.285739	19.068559	1.751296	Cl	4.468214	19.311299	1.618683	H	5.730239	18.359295	-4.284287
C	3.092313	17.605157	3.687395	C	4.016778	19.247564	-0.309300	H	5.752063	15.895854	-3.977912
N	1.205859	17.050647	2.342311	C	4.233052	17.903992	-0.886421	O	3.148823	20.227986	-0.539199
N	3.654552	18.136697	2.576271	C	4.462913	16.746711	-0.135234				
F	0.750929	18.240480	-1.276935	C	4.148550	17.828680	-2.283420	44			
F	2.238888	19.864496	-1.328688	C	4.612120	15.525113	-0.780467	RETS_PBE0			
F	2.752219	16.429752	-1.771281	H	4.522316	16.802994	0.946071	C	1.805901	15.939355	2.792025
F	2.526228	18.002939	-3.239622	C	4.297829	16.602604	-2.918970	H	2.248679	15.378249	1.974340
F	4.195701	18.047775	-1.864491	H	3.952315	18.729510	-2.854279	C	1.389360	15.295449	3.966890
C	2.081950	18.529691	-0.935226	C	4.527831	15.449011	-2.170855	H	1.509640	14.221300	4.061599
C	2.886598	17.755251	-1.966332	H	4.796748	14.628848	-0.194602	C	0.831780	16.047843	4.977837
O	3.295954	21.640592	2.126926	H	4.231366	16.547968	-4.002031	H	0.493450	15.582939	5.900272
C	2.550987	21.287942	2.989370	H	4.642887	14.490924	-2.670572	C	0.701379	17.441771	4.814521
C	1.201835	20.728107	2.813986	O	4.016509	20.302874	-0.864803	C	1.157882	17.998302	3.599605
Cl	3.103612	21.464004	4.712870					C	0.133594	18.296558	5.813456
C	0.385265	20.301759	3.868527	44				H	-0.214515	17.847406	6.739785
C	0.756018	20.608697	1.487724	IV_PBE0				C	0.029240	19.637335	5.609056
C	-0.873316	19.780075	3.595834	C	1.473593	15.903315	2.741321	H	-0.404791	20.282185	6.368624
H	0.729940	20.372648	4.894332	H	1.835550	15.341285	1.885988	C	0.492935	20.234534	4.392933
C	-0.504430	20.087023	1.224993	C	1.054422	15.248127	3.907382	C	0.417376	21.618686	4.135680
H	1.403453	20.913977	0.673063	H	1.092494	14.165028	3.956638	H	-0.015807	22.279168	4.882445
C	-1.320562	19.677205	2.277773	C	0.598671	16.001484	4.967186	C	0.896280	22.113088	2.942198
H	-1.504929	19.446733	4.414032	H	0.260656	15.528225	5.885405	H	0.854970	23.172864	2.712418

C	1.448363	21.221095	2.008470	C	0.849545	22.856460	1.201232	H	5.274141	1.548846	1.155320
H	1.835346	21.567273	1.055056	C	-0.787936	21.366732	2.192695	C	7.090519	2.698633	0.855562
C	1.061006	19.420496	3.388246	C	3.510473	20.705740	1.565446	C	8.497330	2.718106	0.993464
N	1.687849	17.244513	2.611938	F	2.665051	21.307321	-0.554845	C	6.475615	3.845379	0.314190
N	1.526098	19.918947	2.223320	F	2.834736	19.186558	-0.075139	H	5.395986	3.866216	0.189114
F	0.287543	19.808560	-0.464114	C	0.164218	23.944498	1.731150	C	7.254913	4.921975	-0.049724
F	0.841935	18.372700	-2.013682	H	1.733468	23.031531	0.600913	H	6.816547	5.819727	-0.473618
F	-0.597474	17.918888	1.095178	C	-1.460213	22.455813	2.726277	C	8.643905	4.849943	0.140921
F	-1.210731	17.485352	-0.921837	H	-1.142317	20.354918	2.365038	H	9.284880	5.684786	-0.128139
F	0.389860	16.344823	-0.030424	F	3.030710	20.247682	2.727697	C	10.596413	5.877406	3.657542
C	0.855029	18.603186	-0.668085	F	3.702343	22.018684	1.680560	C	10.326616	6.785106	2.625707
C	-0.151145	17.568039	-0.110044	F	4.686711	20.127010	1.336125	H	10.730719	6.599716	1.632381
Cu	2.430665	18.347082	0.998432	C	-0.984396	23.747758	2.494848	C	9.550318	7.915874	2.865222
Cl	4.631213	18.140705	1.480438	H	0.528498	24.950501	1.543548	H	9.349499	8.614509	2.057056
C	2.764048	19.124153	-0.771575	H	-2.355077	22.301588	3.322600	C	9.025638	8.143698	4.136453
C	3.543692	18.201619	-1.628911	H	-1.511096	24.602431	2.911063	H	8.413196	9.021980	4.323692
C	3.292465	16.827964	-1.667441					C	9.284199	7.241119	5.167151
C	4.584670	18.748994	-2.386160	24				H	8.875964	7.415106	6.159539
C	4.082991	16.003005	-2.456932	VI_PBE0				C	10.068079	6.113735	4.932052
H	2.476842	16.408771	-1.086720	Cu	-0.905485	-0.113940	0.094617	H	10.260867	5.413720	5.740836
C	5.373788	17.919196	-3.173174	N	0.717206	1.359069	0.030270	C	13.342762	5.018145	3.662316
H	4.770016	19.817849	-2.342086	N	0.706820	-1.339653	0.041033	C	14.358186	4.810713	2.723537
C	5.125793	16.546973	-3.207501	C	0.696840	2.681516	0.031290	H	14.117773	4.334267	1.773873
H	3.886618	14.934997	-2.487992	C	1.864902	3.462243	0.002304	C	15.660429	5.227377	2.999029
H	6.185434	18.342328	-3.758630	C	3.088957	2.830249	-0.029780	H	16.445107	5.066495	2.264249
H	5.745679	15.899612	-3.822122	C	4.367245	0.680998	-0.065060	C	15.950813	5.853381	4.208529
O	2.820570	20.325135	-0.779960	C	4.361492	-0.679427	-0.066310	H	16.965342	6.180387	4.422090
				C	3.073646	-2.819922	-0.031685	C	14.939039	6.066559	5.146977
44				C	1.847662	-3.447631	0.004386	H	15.164394	6.559445	6.089342
V_PBE0				C	0.683097	-2.666093	0.041189	C	13.639339	5.652197	4.875972
Cu	2.838303	16.114563	0.767869	C	1.910675	0.729820	-0.000137	H	12.853038	5.823687	5.607371
C	0.454951	16.723451	2.875369	C	3.141722	1.421102	-0.032279	C	11.263604	3.201357	4.527662
H	-0.202575	16.271207	2.137835	C	3.130744	-1.411512	-0.032553	C	9.927659	2.799543	4.677742
C	-0.056567	17.241057	4.077852	C	1.905448	-0.711020	0.002616	H	9.144235	3.303245	4.115988
H	-1.122208	17.187945	4.276814	H	-0.284901	3.147495	0.056409	C	9.595941	1.757013	5.535956
C	0.814225	17.806980	4.983745	H	1.788477	4.544741	0.005623	H	8.556318	1.457056	5.640269
H	0.456905	18.217069	5.925003	H	4.013925	3.400732	-0.052738	C	10.594199	1.093093	6.250468
C	2.190882	17.856875	4.683285	H	5.303836	1.231672	-0.090057	H	10.335365	0.274414	6.916864
C	2.600927	17.313252	3.446296	H	5.293058	-1.238385	-0.092719	C	11.922893	1.481426	6.101725
C	3.164920	18.434566	5.559111	H	3.996520	-3.393404	-0.059171	H	12.706818	0.968783	6.653458
H	2.829193	18.843926	6.508292	H	1.765698	-4.529491	0.005694	C	12.258622	2.529392	5.244530
C	4.479669	18.474073	5.212125	H	-0.298456	-3.128827	0.071837	H	13.300064	2.819485	5.134346
H	5.216299	18.915184	5.878270	Cl	-3.043421	0.282535	0.148633	Cl	12.733493	3.646560	-0.565714
C	4.927527	17.947556	3.957880					N	10.517811	1.612622	1.637371
C	6.272667	17.998026	3.540879	58				N	9.249431	3.788434	0.650330
H	7.020709	18.437025	4.196026	VII_PBE0				P	11.657856	4.443379	3.241576
C	6.617193	17.495516	2.305027	Cu	11.312602	3.577202	1.224520				
H	7.641744	17.521667	1.949060	C	11.151484	0.575563	2.161026	14			
C	5.616613	16.944876	1.490835	H	12.232829	0.659152	2.229916	C6H5COCl_PBE0			
H	5.852657	16.545921	0.509244	C	10.488913	-0.575703	2.615758	C	-1.424452	-0.633374	0.291725
C	3.992483	17.367875	3.073203	H	11.061954	-1.391905	3.043620	C	-0.042594	-0.637966	0.144585
N	1.740323	16.757620	2.570096	C	9.116550	-0.641736	2.506716	C	0.633409	0.564886	-0.088137
N	4.343720	16.879787	1.859902	H	8.568395	-1.517678	2.844155	C	-0.083990	1.768648	-0.169066
Cl	1.975690	15.017074	-0.901089	C	8.414091	0.445687	1.949692	C	-1.462935	1.764496	-0.018655
O	0.482363	19.255203	0.877631	C	9.172028	1.564667	1.535513	C	-2.134369	0.563482	0.211365
C	1.028490	20.336468	0.912864	C	6.989918	0.462188	1.800937	H	-1.948579	-1.567819	0.469902
C	0.376852	21.556274	1.431800	H	6.426550	-0.410611	2.120852	H	0.503800	-1.572551	0.208702
C	2.505809	20.387262	0.426523	C	6.354930	1.541732	1.269907	H	0.451408	2.695502	-0.348895

H	-2.015731	2.697434	-0.080581	H	3.176853	19.817343	6.413419	C	1.111677	19.814904	6.370550
H	-3.214749	0.560790	0.328385	C	1.211979	20.699507	6.316956	H	1.057715	19.712251	7.453626
C	2.092510	0.671223	-0.261944	H	1.128723	20.829620	7.392946	C	2.316064	20.188757	5.756774
O	2.709339	1.666771	-0.487918	C	0.168699	21.094043	5.482033	H	3.203839	20.376037	6.359691
Cl	3.013977	-0.885272	-0.110259	H	-0.730450	21.535505	5.904831	C	2.391339	20.308651	4.362992
				C	0.273127	20.930275	4.101999	H	3.338674	20.578582	3.897502
20				H	-0.544271	21.248321	3.460272	N	1.519731	16.843645	2.857684
C6H5COC2F5_PBE0								N	3.932247	17.954240	2.419827
C	-1.467721	-0.584728	0.404238	64				P	1.429225	19.945387	1.735869
C	-0.087463	-0.627412	0.243562	I_TPSS				F	1.041200	17.123116	-1.341208
C	0.615367	0.543732	-0.078695	Cu	2.213582	17.897645	1.182910	F	3.118573	17.946577	-1.537637
C	-0.090092	1.747912	-0.237172	C	0.290941	16.349730	3.074151	F	2.063529	14.891297	-0.077686
C	-1.466892	1.782267	-0.081260	H	-0.375654	16.348173	2.214066	F	2.896804	15.298008	-2.065712
C	-2.158772	0.613612	0.240433	C	-0.131903	15.866059	4.327839	F	4.104134	15.688999	-0.277720
H	-2.005651	-1.494193	0.656199	H	-1.143238	15.481178	4.439126	C	2.290333	17.195159	-0.646309
H	0.425309	-1.571020	0.376179	C	0.751452	15.890009	5.401106	C	2.836661	15.770517	-0.784138
H	0.462583	2.649202	-0.483484	H	0.452671	15.525079	6.382693				
H	-2.003656	2.718093	-0.208748	C	2.057652	16.403839	5.210456	30			
H	-3.238140	0.638404	0.364691	C	2.393865	16.876075	3.909546	II_TPSS			
C	2.080304	0.617760	-0.257023	C	3.037197	16.491028	6.260478	Cu	2.465120	18.268230	0.909465
C	2.966941	-0.657064	-0.175859	H	2.768228	16.125319	7.250638	C	-0.073888	16.741275	2.229138
C	3.368695	-1.041047	1.260790	C	4.277905	17.029350	6.029853	H	-0.537503	16.855416	1.250876
F	4.112294	-0.419433	-0.841236	H	5.009586	17.097050	6.834006	C	-0.749657	16.099763	3.291354
F	2.369933	-1.731789	-0.743840	C	4.637762	17.537218	4.732871	H	-1.753066	15.711166	3.132648
F	2.296834	-1.381528	1.980109	C	5.878624	18.159986	4.454089	C	-0.118505	15.978155	4.522085
F	3.966942	-0.006358	1.850091	H	6.628854	18.244943	5.239048	H	-0.613243	15.489083	5.359932
F	4.210234	-2.072973	1.241764	C	6.115278	18.663259	3.179070	C	1.190769	16.499373	4.688106
O	2.675988	1.653758	-0.466903	H	7.055336	19.151810	2.932067	C	1.785048	17.127625	3.557974
				C	5.118442	18.539278	2.191430	C	1.931664	16.423131	5.918703
34				H	5.269114	18.927384	1.186622	H	1.465887	15.938970	6.775848
PPh3_PBE0				C	3.690666	17.456883	3.670983	C	3.196700	16.946376	6.015179
P	1.668601	20.100164	1.736773	C	2.580483	21.307283	1.271771	H	3.752025	16.884184	6.949856
C	2.560959	21.630989	1.242056	C	3.442934	21.069401	0.182359	C	3.823553	17.588986	4.890520
C	3.163449	21.636862	-0.023388	H	3.405460	20.106787	-0.329273	C	5.126480	18.147532	4.934566
H	3.094691	20.754955	-0.657330	C	4.336514	22.063080	-0.242061	H	5.702229	18.098324	5.857490
C	3.849229	22.759706	-0.477843	H	4.997920	21.870429	-1.086117	C	5.647817	18.749123	3.797160
H	4.307836	22.750601	-1.463390	C	4.381642	23.296670	0.423277	H	6.643365	19.186243	3.795799
C	3.957222	23.887261	0.334674	H	5.080334	24.066938	0.098573	C	4.871844	18.794921	2.620764
H	4.500496	24.761528	-0.014833	C	3.525762	23.539259	1.509698	H	5.248628	19.258430	1.712730
C	3.371458	23.887374	1.598960	H	3.558449	24.497438	2.027397	C	3.113714	17.680062	3.661218
H	3.453755	24.763344	2.237681	C	2.625766	22.552071	1.931783	N	1.158886	17.243898	2.353068
C	2.674057	22.768366	2.049881	H	1.968878	22.745062	2.779054	N	3.635435	18.277220	2.544917
H	2.215992	22.782353	3.035314	C	-0.205015	20.481011	1.075660	F	0.612462	18.383626	-1.202361
C	-0.019308	20.397208	1.068481	C	-0.742144	19.749391	-0.001117	F	2.286295	19.846196	-1.465161
C	-0.894646	19.302780	1.040131	H	-0.190923	18.896696	-0.398587	F	2.405331	16.303169	-1.595027
H	-0.555846	18.331521	1.395830	C	-1.972100	20.123615	-0.562745	F	2.283314	17.770093	-3.221992
C	-2.194404	19.445947	0.563158	H	-2.381008	19.554430	-1.396884	F	4.032372	17.750793	-1.900163
H	-2.863521	18.589255	0.552205	C	-2.672933	21.223608	-0.049092	C	2.006998	18.557143	-0.930873
C	-2.631715	20.682253	0.090071	H	-3.630162	21.511800	-0.482259	C	2.674458	17.602593	-1.925585
H	-3.643661	20.793239	-0.291048	C	-2.141800	21.955998	1.025645				
C	-1.765357	21.773353	0.102792	H	-2.685218	22.811568	1.425475	44			
H	-2.100390	22.739671	-0.266050	C	-0.911955	21.589779	1.585659	III_TPSS			
C	-0.467857	21.634241	0.591905	H	-0.506319	22.157361	2.422473	Cu	2.209369	18.249877	0.957052
H	0.196684	22.494024	0.603263	C	1.253778	20.073074	3.559591	C	-0.144104	16.664493	2.272621
C	1.422460	20.361835	3.541112	C	0.047672	19.690405	4.186702	H	-0.618376	16.769162	1.299590
C	2.460905	19.956323	4.390655	H	-0.836246	19.484124	3.584617	C	-0.810927	16.039163	3.348826
H	3.355144	19.500479	3.969772	C	-0.020318	19.564995	5.580260	H	-1.815633	15.649608	3.201700
C	2.360843	20.132095	5.767770	H	-0.958550	19.267000	6.047207	C	-0.171426	15.933207	4.576713

H	-0.660739	15.456187	5.424628	C	1.736568	21.191399	2.276225	C	-0.514857	17.530504	0.152920
C	1.141068	16.450399	4.723464	H	2.110239	21.473496	1.295741	Cu	2.259664	18.242225	0.995988
C	1.727273	17.064701	3.582002	C	1.067757	19.468675	3.686130	Cl	4.356508	18.150293	1.911955
C	1.897430	16.379632	5.945372	N	1.084480	17.234612	2.809923	C	3.223084	19.066380	-0.499833
H	1.436101	15.911104	6.813539	N	1.531359	19.881943	2.468144	C	3.928461	18.157999	-1.439389
C	3.173449	16.880243	6.018252	F	-0.250814	18.843768	-0.810612	C	3.929212	16.764094	-1.252756
H	3.741419	16.814782	6.945126	F	1.566678	18.095228	-1.859714	C	4.586902	18.728116	-2.549427
C	3.793264	17.503084	4.878721	F	-0.721916	16.420232	0.237830	C	4.589036	15.940503	-2.167832
C	5.107111	18.037230	4.890090	F	-0.372929	16.306094	-1.923853	H	3.419236	16.341372	-0.387515
H	5.703503	17.980790	5.799362	F	1.164254	15.595580	-0.530969	C	5.245021	17.898332	-3.461622
C	5.611218	18.628998	3.739783	C	0.868882	17.970257	-0.646584	H	4.573940	19.808044	-2.682286
H	6.613613	19.049435	3.715164	C	0.227965	16.575299	-0.730159	C	5.246907	16.506964	-3.272183
C	4.802433	18.699797	2.585833	Cu	1.695207	18.350429	1.074243	H	4.592974	14.861553	-2.022827
H	5.157810	19.172766	1.674035	Cl	4.206241	18.010185	2.053834	H	5.755242	18.334870	-4.318876
C	3.060262	17.606880	3.664915	C	4.049792	18.983480	0.347189	H	5.760325	15.863622	-3.985476
N	1.090618	17.168772	2.379443	C	4.264452	18.110532	-0.820836	O	3.188937	20.274356	-0.556210
N	3.556466	18.208028	2.543031	C	4.175090	16.705732	-0.781506				
F	0.758984	18.591090	-1.466509	C	4.528707	18.770990	-2.041487	44			
F	2.487348	19.995813	-1.280283	C	4.349180	15.969855	-1.954996	RETS_TPSS			
F	2.536275	16.469112	-1.674723	H	3.949268	16.203022	0.154568	C	1.804895	15.901510	2.807384
F	2.786753	18.059489	-3.165030	C	4.706910	18.024788	-3.208238	H	2.255326	15.339498	1.992698
F	4.230777	17.863169	-1.525826	H	4.585265	19.856743	-2.060942	C	1.356968	15.262135	3.981871
C	2.075643	18.679249	-0.915006	C	4.612987	16.625040	-3.168942	H	1.455894	14.183314	4.075453
C	2.902586	17.776878	-1.835413	H	4.270289	14.884564	-1.925419	C	0.800024	16.025665	4.999081
O	3.356032	21.635442	2.203117	H	4.912568	18.534929	-4.147874	H	0.447936	15.561111	5.918889
C	2.576649	21.245656	3.033929	H	4.743952	16.045835	-4.081838	C	0.691758	17.430557	4.838449
C	1.232726	20.689861	2.825596	O	4.107572	20.187208	0.415049	C	1.162421	17.985339	3.614956
Cl	3.109803	21.365863	4.833040					C	0.140159	18.304362	5.838817
C	0.377259	20.264952	3.864770	44				H	-0.214573	17.866413	6.770600
C	0.814526	20.580526	1.474138	IV_TPSS				C	0.063289	19.658085	5.629634
C	-0.896758	19.783219	3.558212	C	1.481039	15.886662	2.730852	H	-0.352107	20.313570	6.393671
H	0.705600	20.318114	4.898959	H	1.843034	15.331686	1.869325	C	0.527879	20.247384	4.402202
C	-0.471985	20.106489	1.182857	C	1.061346	15.227138	3.903081	C	0.476060	21.639201	4.134230
H	1.471479	20.918488	0.677051	H	1.100613	14.141585	3.949166	H	0.068658	22.316127	4.883689
C	-1.326881	19.714791	2.220580	C	0.601174	15.979800	4.974556	C	0.947904	22.117771	2.919924
H	-1.555609	19.457768	4.360992	H	0.263816	15.499468	5.891763	H	0.923711	23.179091	2.684097
H	-0.781978	20.022216	0.144280	C	0.571976	17.393459	4.873609	C	1.466681	21.208592	1.973473
H	-2.323955	19.342079	1.990898	C	1.024729	17.975057	3.655025	H	1.840145	21.534576	1.006210
				C	0.112829	18.250803	5.933558	C	1.073722	19.408384	3.390031
44				H	-0.232613	17.789948	6.857728	N	1.706750	17.222391	2.624693
OATS_TPSS				C	0.107084	19.614834	5.788500	N	1.529860	19.892264	2.197884
C	0.891289	15.919868	2.960932	H	-0.244038	20.256088	6.595811	F	0.200812	19.803843	-0.541843
H	1.087730	15.307160	2.084412	C	0.567712	20.231445	4.573701	F	0.781904	18.354633	-2.116485
C	0.448724	15.347224	4.172441	C	0.593224	21.634868	4.368698	F	-0.628969	17.908139	1.055160
H	0.312746	14.270161	4.238467	H	0.247512	22.299585	5.159181	F	-1.252054	17.385378	-0.971450
C	0.188202	16.173374	5.257666	C	1.060810	22.139343	3.163197	F	0.410912	16.310873	-0.041863
H	-0.161455	15.762649	6.203733	H	1.093039	23.210096	2.974584	C	0.804464	18.593878	-0.753039
C	0.378954	17.572871	5.129848	C	1.505941	21.241035	2.167579	C	-0.173048	17.535432	-0.162792
C	0.841314	18.055053	3.871993	H	1.887341	21.594151	1.212155	Cu	2.457066	18.357495	1.047340
C	0.132599	18.508259	6.194223	C	1.030975	19.411142	3.505327	Cl	4.667672	18.105578	1.483015
H	-0.222916	18.125454	7.149752	N	1.457892	17.218177	2.605531	C	2.705740	19.146572	-0.764094
C	0.337555	19.852758	6.014104	N	1.495476	19.916506	2.331025	C	3.520352	18.231856	-1.611764
H	0.146862	20.555573	6.823839	F	0.363296	19.564348	-0.553696	C	3.284264	16.845243	-1.651459
C	0.811243	20.370030	4.758158	F	1.017638	17.698943	-1.571347	C	4.575676	18.789703	-2.360966
C	1.042811	21.748607	4.521325	F	-0.988549	18.052442	1.311911	C	4.096547	16.021087	-2.434828
H	0.858414	22.469653	5.316300	F	-1.509227	17.629197	-0.769940	H	2.462559	16.419951	-1.080371
C	1.503132	22.157058	3.277014	F	-0.273117	16.206062	0.345864	C	5.386016	17.960463	-3.141556
H	1.690114	23.206253	3.060577	C	0.763323	18.254091	-0.317400	H	4.750876	19.862461	-2.316424

C 5.149658 16.576592 -3.178916
H 3.908114 14.949180 -2.467861
H 6.201884 18.391419 -3.720044
H 5.782668 15.933438 -3.788728
O 2.749041 20.368733 -0.791597

44
V_TPSS
Cu 2.864231 16.104405 0.810114
C 0.394605 16.772273 2.824668
H -0.240087 16.275822 2.093265
C -0.150549 17.369551 3.982917
H -1.224439 17.333176 4.152718
C 0.699546 17.992042 4.887602
H 0.311849 18.460835 5.791089
C 2.093986 18.018068 4.628663
C 2.543794 17.395885 3.429420
C 3.053485 18.639414 5.500979
H 2.695919 19.109049 6.416292
C 4.389862 18.643442 5.190691
H 5.111131 19.115025 5.856427
C 4.874008 18.043152 3.976111
C 6.238549 18.058782 3.592948
H 6.976054 18.524336 4.244999
C 6.611617 17.484315 2.385018
H 7.648399 17.481578 2.057306
C 5.627482 16.903400 1.561925
H 5.883712 16.456064 0.605275
C 3.947704 17.423582 3.091353
N 1.702599 16.781961 2.551573
N 4.325297 16.869580 1.895400
Cl 1.933915 14.996702 -0.819371
O 0.523255 19.175807 0.719007
C 1.066904 20.271026 0.819285
C 0.429787 21.442042 1.464667
C 2.528390 20.382174 0.255599
C 0.895845 22.768140 1.322597
C -0.711009 21.184557 2.260264
C 3.608560 20.696808 1.345015
F 2.599916 21.352191 -0.718102
F 2.862091 19.193520 -0.318511
C 0.229048 23.812408 1.972211
H 1.754514 22.993218 0.698561
C -1.363031 22.230229 2.913567
H -1.056593 20.158099 2.363185
F 3.147991 20.316954 2.565490
F 3.884277 22.018720 1.395073
F 4.758678 20.034976 1.102118
C -0.894083 23.547335 2.769468
H 0.585364 24.834079 1.852917
H -2.233806 22.024318 3.533860
H -1.404290 24.364485 3.277302

24
VI_TPSS
Cu -0.899016 -0.182726 0.102003
N 0.697626 1.355005 0.022794
N 0.689213 -1.352837 0.039897
C 0.675116 2.691488 0.024545
C 1.847612 3.478721 -0.000167
C 3.084503 2.848681 -0.029694
C 4.376454 0.688973 -0.062962
C 4.372187 -0.682816 -0.064809
C 3.085388 -2.840219 -0.032173
C 1.850486 -3.473708 0.003230
C 0.675603 -2.697663 0.039933
C 1.907085 0.727698 -0.004118
C 3.145213 1.431289 -0.033118
C 3.138803 -1.423389 -0.033474
C 1.903914 -0.716226 0.000118
H -0.312016 3.150545 0.046470
H 1.767787 4.563474 0.003797
H 4.007668 3.426104 -0.049684
H 5.315562 1.240052 -0.085091
H 5.307625 -1.239820 -0.089097
H 4.010500 -3.413852 -0.058367
H 1.771714 -4.558165 0.004738
H -0.306188 -3.162236 0.070889
Cl -2.987132 0.434496 0.167752

58
VII_TPSS
Cu 11.253727 3.651384 1.187993
C 11.393944 0.620513 1.945510
H 12.470450 0.778837 1.944490
C 10.834870 -0.598164 2.381222
H 11.489787 -1.395791 2.724705
C 9.455043 -0.757976 2.361165
H 8.992582 -1.687641 2.689725
C 8.639373 0.311406 1.913896
C 9.294456 1.508587 1.504490
C 7.202740 0.251058 1.880611
H 6.715076 -0.672269 2.190676
C 6.458239 1.331398 1.479157
H 5.370306 1.279655 1.464152
C 7.089458 2.562228 1.083749
C 8.511420 2.649275 1.094178
C 6.366684 3.719162 0.697923
H 5.278083 3.692384 0.677127
C 7.062074 4.871846 0.355476
H 6.539493 5.777224 0.054723
C 8.471280 4.866800 0.401490
H 9.044964 5.753902 0.143872
C 10.620693 6.009702 3.566707
C 10.467995 6.949878 2.526372
H 10.931683 6.755080 1.558436
C 9.727087 8.120759 2.731723
H 9.617782 8.841217 1.921833
C 9.119267 8.357371 3.974304
H 8.535414 9.263354 4.132725
C 9.261267 7.423530 5.011709
H 8.790227 7.603878 5.977569
C 10.010657 6.255236 4.812809
H 10.113577 5.533804 5.622179
C 13.338150 4.980931 3.662056
C 14.380238 4.618783 2.787238
H 14.138460 4.108171 1.853589
C 15.709265 4.933099 3.107913
H 16.511306 4.652974 2.425938
C 16.001202 5.613455 4.298492
H 17.032841 5.861485 4.545853
C 14.963976 5.983389 5.170748
H 15.190121 6.517016 6.093400
C 13.636251 5.669436 4.856008
H 12.833971 5.959399 5.533932
C 11.112456 3.286394 4.469153
C 9.748783 2.920934 4.524991
H 9.024398 3.444593 3.901462
C 9.324117 1.887333 5.366697
H 8.269439 1.615500 5.395520
C 10.255701 1.194959 6.157476
H 9.926494 0.384936 6.807173
C 11.610869 1.548661 6.104493
H 12.339354 1.016649 6.715724
C 12.040483 2.588105 5.265214
H 13.096771 2.850565 5.228967
Cl 12.628297 3.935725 -0.619897
N 10.653388 1.650946 1.515176
N 9.187358 3.792444 0.762969
P 11.622734 4.509082 3.190204

14
C6H5COCl_TPSS
C -1.430033 -0.640152 0.294486
C -0.040242 -0.642900 0.146585
C 0.638128 0.569966 -0.088594
C -0.087539 1.781856 -0.170961
C -1.474398 1.773118 -0.019908
C -2.147430 0.562866 0.212476
H -1.953371 -1.577439 0.473861
H 0.511812 -1.576464 0.210978
H 0.446622 2.711697 -0.351833
H -2.030504 2.706667 -0.083039
H -3.230027 0.557900 0.329466
C 2.098249 0.681795 -0.262737
O 2.736626 1.677202 -0.484786
Cl 3.039151 -0.929862 -0.116788

20
C6H5COC2F5_TPSS
C -1.479671 -0.588815 0.403021
C -0.092684 -0.633102 0.230944
C 0.615472 0.547637 -0.091440
C -0.096171 1.762238 -0.238728
C -1.479422 1.796812 -0.070656
C -2.175089 0.619243 0.251203
H -2.018388 -1.501113 0.653259
H 0.422783 -1.579191 0.352951
H 0.457840 2.665621 -0.484428
H -2.017472 2.735949 -0.188120
H -3.255669 0.644802 0.384328
C 2.082821 0.619992 -0.283565
C 2.980095 -0.662496 -0.175363
C 3.375346 -1.047383 1.274284

F	4.148488	-0.423727	-0.841002
F	2.387676	-1.761480	-0.755889
F	2.288103	-1.417169	1.992914
F	3.952162	0.012041	1.885519
F	4.251099	-2.075702	1.269788
O	2.685717	1.663040	-0.525185

34
PPh3_TPSS

C	2.571046	21.626295	1.233721
C	3.180372	21.634084	-0.039055
H	3.112468	20.751255	-0.675675
C	3.869634	22.765556	-0.493719
H	4.331191	22.757823	-1.480668
C	3.975018	23.899973	0.324830
H	4.519071	24.777156	-0.023770
C	3.382592	23.898536	1.595852
H	3.461735	24.776586	2.236434
C	2.681668	22.771384	2.047787
H	2.219103	22.783851	3.033651
C	-0.026461	20.388120	1.062812
C	-0.911004	19.288945	1.029363
H	-0.574594	18.313576	1.382905
C	-2.218643	19.439426	0.550522
H	-2.891816	18.582769	0.536112
C	-2.655549	20.686938	0.080312
H	-3.669580	20.802688	-0.300843
C	-1.780659	21.782580	0.098132
H	-2.114103	22.753959	-0.266294
C	-0.475259	21.637020	0.588917
H	0.193145	22.496605	0.605397
C	1.427212	20.353131	3.548689
C	2.477649	19.960564	4.405542
H	3.380035	19.515031	3.985179
C	2.374681	20.141493	5.790556
H	3.196733	19.838651	6.438467
C	1.211787	20.700306	6.341726
H	1.127080	20.833448	7.419704
C	0.157112	21.081740	5.500257
H	-0.749078	21.515485	5.922518
C	0.263493	20.913434	4.112140
H	-0.558720	21.221054	3.467663
P	1.674379	20.082878	1.731893

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I_B97D

Cu	2.173435	17.896119	1.109153
C	0.313613	16.290727	3.091605
H	-0.356003	16.247630	2.230319
C	-0.105441	15.832849	4.360133
H	-1.111239	15.429857	4.482653
C	0.779485	15.906228	5.431374
H	0.492397	15.562968	6.427150
C	2.076063	16.441225	5.225014
C	2.403599	16.885714	3.907614
C	3.048723	16.568002	6.277834
H	2.778725	16.218599	7.276327
C	4.281985	17.123041	6.038247
H	5.013742	17.223873	6.842256
C	4.633957	17.607987	4.729920
C	5.866215	18.249455	4.448680
H	6.607136	18.362561	5.242549
C	6.105411	18.733749	3.165440
H	7.039457	19.237978	2.915479
C	5.114333	18.566729	2.173002
H	5.268381	18.940834	1.159889
C	3.694360	17.488394	3.659401
C	2.583083	21.265465	1.274356
C	3.459382	21.019463	0.196107
H	3.418830	20.059527	-0.323211
C	4.375620	22.004460	-0.208163
H	5.049230	21.806521	-1.044762
C	4.428537	23.235541	0.466170
H	5.145049	23.999113	0.155896
C	3.557608	23.484890	1.542246
H	3.595841	24.441822	2.067388
C	2.635615	22.506243	1.943571
H	1.966239	22.700128	2.783087
C	-0.225846	20.489342	1.072809
C	-0.767136	19.800029	-0.031670
H	-0.225627	18.952907	-0.458078
C	-1.993094	20.208853	-0.584148
H	-2.406980	19.672587	-1.440812
C	-2.684529	21.300200	-0.033743
H	-3.639201	21.614963	-0.460720
C	-2.148044	21.989379	1.069582
H	-2.684048	22.838773	1.498779
C	-0.922344	21.588197	1.620281
H	-0.509958	22.119926	2.479391
C	1.232563	20.037395	3.551628
C	0.024866	19.653243	4.176295
H	-0.859656	19.450442	3.570505
C	-0.044705	19.526677	5.571588
H	-0.985342	19.227537	6.039030
C	1.088023	19.779867	6.363941
H	1.032946	19.678168	7.449717
C	2.293660	20.157947	5.750379
H	3.181617	20.350368	6.355699
C	2.369920	20.277065	4.354827
H	3.315989	20.552887	3.887632
N	1.530053	16.801319	2.861651
N	3.941948	17.962392	2.403520
P	1.402336	19.923320	1.727085
F	1.043361	17.091077	-1.434315
F	3.128809	17.908092	-1.607826
F	2.045716	14.873159	-0.109353
F	2.921229	15.220891	-2.091501
F	4.090742	15.666999	-0.289571
C	2.283651	17.165239	-0.728466
C	2.834719	15.729760	-0.824641

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II_B97D

Cu	2.495396	18.298582	0.861376
C	-0.064886	16.697791	2.232393
H	-0.531097	16.794565	1.249548
C	-0.743242	16.061698	3.300908
H	-1.745640	15.662386	3.144141
C	-0.111334	15.960183	4.535028
H	-0.601394	15.476385	5.382097
C	1.194559	16.494432	4.697382
C	1.788473	17.118174	3.558227
C	1.926735	16.431667	5.934763
H	1.454945	15.949607	6.792995
C	3.189496	16.963987	6.034146
H	3.744395	16.913855	6.972689
C	3.816874	17.602876	4.906467
C	5.117977	18.167042	4.963247
H	5.681794	18.120549	5.896718
C	5.651474	18.768186	3.829254
H	6.647818	19.209791	3.836428
C	4.882756	18.807350	2.644543
H	5.269620	19.273293	1.738014
C	3.116164	17.685662	3.665563
N	1.161090	17.210708	2.354353
N	3.649664	18.285308	2.556307
F	0.612674	18.465118	-1.240062
F	2.338535	19.862515	-1.536648
F	2.326566	16.309470	-1.611681
F	2.273844	17.742038	-3.273664
F	4.010506	17.687459	-1.934565
C	2.011555	18.592681	-0.990581
C	2.649213	17.587739	-1.971153

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III_B97D

Cu	2.465986	18.157678	0.830386
C	-0.063643	16.475820	2.132360
H	-0.472170	16.481693	1.120038
C	-0.809021	15.952209	3.216654
H	-1.804871	15.543732	3.042279
C	-0.247855	15.966254	4.488598
H	-0.788940	15.567125	5.348782
C	1.050858	16.509111	4.673025
C	1.712291	17.019869	3.514965
C	1.710110	16.566375	5.950788
H	1.186406	16.173153	6.824150
C	2.971235	17.098853	6.068809
H	3.472884	17.137278	7.037324
C	3.664832	17.626657	4.922495
C	4.963697	18.193031	4.999073
H	5.476022	18.230933	5.961970
C	5.559023	18.694400	3.848003
H	6.554214	19.137710	3.870348
C	4.848395	18.644818	2.628573
H	5.276405	19.047968	1.711304
C	3.031621	17.601823	3.644717
N	1.159057	16.989456	2.273673
N	3.617347	18.122302	2.522334
F	0.539006	18.111085	-1.234611
F	1.901179	19.879193	-1.394214
F	2.663232	16.439722	-1.854823
F	2.261091	17.996405	-3.349703
F	4.003877	18.175746	-2.029285

C	1.885480	18.518785	-0.985028
C	2.695441	17.788280	-2.073029
O	3.562521	21.667943	2.397148
C	2.742191	21.319450	3.202444
C	1.416968	20.727683	2.953115
Cl	3.170872	21.590412	5.028971
C	0.566302	20.215607	3.959767
C	1.018078	20.657414	1.592964
C	-0.671469	19.666901	3.610180
H	0.871999	20.238707	5.003897
C	-0.227231	20.113776	1.256554
H	1.676984	21.032371	0.813462
C	-1.073327	19.621685	2.262311
H	-1.321183	19.266375	4.389104
H	-0.509668	20.043557	0.207415
H	-2.039750	19.189257	1.997603

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OATS_B97D

C	1.918558	16.136104	2.255533
H	2.314948	15.774294	1.306265
C	1.616869	15.237781	3.304523
H	1.782991	14.169578	3.163480
C	1.114481	15.740741	4.498961
H	0.873367	15.079920	5.333785
C	0.905105	17.137956	4.633499
C	1.237373	17.963544	3.515192
C	0.375571	17.738566	5.829751
H	0.132901	17.087790	6.671861
C	0.177244	19.095354	5.910966
H	-0.225957	19.547173	6.819133
C	0.488056	19.955805	4.800046
C	0.288379	21.360861	4.828229
H	-0.114315	21.826823	5.729638
C	0.604647	22.119345	3.706839
H	0.461810	23.200035	3.695127
C	1.115749	21.467646	2.560099
H	1.368064	22.029772	1.659124
C	1.016895	19.393430	3.597914
N	1.748079	17.458822	2.354444
N	1.316443	20.148347	2.504887
F	0.924983	20.328847	-1.486042
F	1.315140	18.180327	-1.941882
F	-1.068531	19.567453	0.285994
F	-1.325339	18.783577	-1.745591
F	-0.655518	17.449572	-0.136994
C	0.950296	19.050466	-0.898889
C	-0.537536	18.713936	-0.635953
Cu	1.956980	18.961467	0.780190
Cl	4.505171	19.663992	1.470651
C	3.965190	19.283097	-0.504471
C	4.224345	17.873880	-0.880756
C	4.433307	16.829840	0.045459
C	4.212577	17.593735	-2.268876
C	4.633116	15.522770	-0.412726
H	4.434223	17.042209	1.111589
C	4.414100	16.282829	-2.715314
H	4.038369	18.401431	-2.977936
C	4.621543	15.243974	-1.791645
H	4.797723	14.720632	0.308742
H	4.405834	16.072657	-3.786261
H	4.775403	14.222193	-2.143672
O	3.918687	20.263350	-1.195223

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IV_B97D

C	1.500461	15.882073	2.778662
H	1.882037	15.319128	1.926805
C	1.052715	15.222769	3.944189
H	1.091270	14.134795	3.995522
C	0.566213	15.982140	5.001409
H	0.204774	15.508893	5.916236
C	0.539166	17.396354	4.892122
C	1.021862	17.974789	3.678008
C	0.051959	18.251132	5.942683
H	-0.313854	17.785032	6.859330
C	0.045812	19.616757	5.797077
H	-0.325469	20.261674	6.595801
C	0.532657	20.232328	4.591027
C	0.555437	21.638058	4.393128
H	0.188159	22.295719	5.183457
C	1.046402	22.152058	3.199033
H	1.078293	23.226321	3.015095
C	1.515724	21.255023	2.208768
H	1.914078	21.620318	1.261242
C	1.024658	19.415348	3.526795
N	1.479992	17.211486	2.645218
N	1.507699	19.931648	2.366211
F	0.381442	19.563433	-0.581348
F	1.033530	17.683856	-1.573184
F	-0.956391	18.070457	1.323679
F	-1.504021	17.606388	-0.741121
F	-0.237898	16.213692	0.379624
C	0.780904	18.258886	-0.331912
C	-0.496266	17.530772	0.169742
Cu	2.309450	18.244309	0.993475
Cl	4.438895	18.154960	1.925785
C	3.292847	19.080269	-0.526314
C	3.967276	18.160237	-1.477070
C	3.959998	16.763763	-1.289731
C	4.604580	18.722939	-2.607490
C	4.589874	15.932441	-2.221911
H	3.466880	16.341825	-0.413226
C	5.231449	17.884822	-3.536898
H	4.599430	19.804662	-2.743900
C	5.225209	16.491412	-3.345947
H	4.586658	14.851194	-2.074837
H	5.723975	18.317507	-4.409561
H	5.714474	15.840783	-4.073400
O	3.272530	20.284732	-0.568293

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RETS_B97D

C	1.869949	15.917816	2.853136
H	2.353838	15.355064	2.053734
C	1.376158	15.266884	4.006666
H	1.474341	14.185230	4.098758
C	0.773332	16.025964	5.002961
H	0.380090	15.558939	5.907869
C	0.666929	17.432251	4.842435
C	1.189728	17.996686	3.639599
C	0.059909	18.291473	5.824602
H	-0.332327	17.838173	6.736778
C	-0.024993	19.647188	5.620262
H	-0.484735	20.296397	6.367677
C	0.487196	20.247921	4.416677
C	0.421615	21.642161	4.157526
H	-0.031478	22.303821	4.898176
C	0.935333	22.140812	2.966510
H	0.901767	23.205908	2.736704
C	1.508630	21.242944	2.035543
H	1.911738	21.591609	1.085110
C	1.092823	19.424695	3.419235
N	1.777200	17.237872	2.671879
N	1.585891	19.928100	2.252161
F	0.193064	19.798334	-0.511683
F	0.745313	18.342239	-2.088348
F	-0.589215	17.876359	1.127615
F	-1.312283	17.391935	-0.873568
F	0.391953	16.296711	-0.044160
C	0.776181	18.582380	-0.729816
C	-0.194097	17.521658	-0.115152
Cu	2.535459	18.375961	1.037348
Cl	4.782069	18.190258	1.490499
C	2.777044	19.163209	-0.801915
C	3.559243	18.233097	-1.663992
C	3.294725	16.849772	-1.696883
C	4.616843	18.769308	-2.431555
C	4.077897	16.006740	-2.493531
H	2.473139	16.443283	-1.111779
C	5.399565	17.920703	-3.223026
H	4.817981	19.839934	-2.392518
C	5.133250	16.539669	-3.255026
H	3.865931	14.936506	-2.521849
H	6.218600	18.334813	-3.814026
H	5.745995	15.880965	-3.873521
O	2.813927	20.377541	-0.839742

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V_B97D

Cu	2.918775	16.036399	0.706320
C	0.601221	16.297357	2.990760
H	-0.061204	15.844164	2.250672
C	0.115836	16.677516	4.264880
H	-0.933428	16.516045	4.513472
C	0.993165	17.253486	5.176495
H	0.656509	17.561040	6.168504
C	2.350419	17.449813	4.809591
C	2.739133	17.034142	3.500339
C	3.324518	18.050679	5.681766
H	3.007097	18.360677	6.679237
C	4.621365	18.236206	5.268842
H	5.357610	18.696457	5.930340
C	5.045167	17.837998	3.952406

C	6.366567	18.035033	3.475881
H	7.108907	18.496863	4.129430
C	6.690619	17.639799	2.183194
H	7.694498	17.778409	1.781769
C	5.694908	17.051356	1.373413
H	5.915086	16.734748	0.353618
C	4.105619	17.233650	3.064843
N	1.871514	16.467962	2.616948
N	4.436093	16.849718	1.793520
Cl	2.079362	14.983804	-1.037976
O	0.180643	19.483753	1.371245
C	0.790820	20.527901	1.175097
C	0.208379	21.873728	1.413717
C	2.292556	20.373502	0.697482
C	0.846153	23.093840	1.080060
C	-1.071197	21.910659	2.026136
C	3.331338	20.651230	1.837092
F	2.589601	21.190865	-0.364746
F	2.487588	19.087899	0.288588
C	0.216352	24.313713	1.358798
H	1.820419	23.105666	0.602451
C	-1.691239	23.130750	2.303595
H	-1.559193	20.970384	2.282870
F	2.908755	20.065531	2.982960
F	3.466341	21.976154	2.065376
F	4.544586	20.152163	1.519105
C	-1.047808	24.337568	1.970398
H	0.715742	25.247426	1.095284
H	-2.672807	23.145631	2.780205
H	-1.531907	25.291840	2.186978

24
VI_B97D

Cu	-0.956165	-0.184616	0.104221
N	0.700299	1.370977	0.003004
N	0.687775	-1.358970	0.022709
C	0.684882	2.705672	0.004860
C	1.863381	3.490498	-0.009371
C	3.097566	2.851094	-0.028087
C	4.381677	0.689320	-0.050558
C	4.375611	-0.684196	-0.053017
C	3.090473	-2.839592	-0.032233
C	1.856923	-3.479721	-0.007574
C	0.678794	-2.702728	0.021013
C	1.903079	0.733228	-0.012968
C	3.149352	1.432083	-0.031306
C	3.138995	-1.421459	-0.032386
C	1.897707	-0.715476	-0.008235
H	-0.300901	3.175799	0.018298
H	1.789505	4.578290	-0.005903
H	4.028731	3.420802	-0.039821
H	5.322073	1.243397	-0.063753
H	5.310680	-1.246915	-0.068966
H	4.022143	-3.407839	-0.051079
H	1.781032	-4.566946	-0.007693
H	-0.303856	-3.173732	0.044598
Cl	-3.074050	0.383894	0.267660

58
VII_B97D

Cu	11.282733	3.895538	0.920090
C	11.863121	0.812264	1.517138
H	12.890762	1.066723	1.249737
C	11.554658	-0.442709	2.088773
H	12.350978	-1.166415	2.265189
C	10.233264	-0.727076	2.415578
H	9.953286	-1.683029	2.862511
C	9.231443	0.245729	2.168371
C	9.643585	1.485509	1.589538
C	7.845989	0.038237	2.494723
H	7.555628	-0.918273	2.933594
C	6.912878	1.021088	2.273358
H	5.863951	0.864061	2.532463
C	7.295193	2.290774	1.715548
C	8.660894	2.525501	1.363274
C	6.377658	3.355164	1.526093
H	5.327573	3.211041	1.788200
C	6.833963	4.567474	1.018100
H	6.156957	5.408021	0.862830
C	8.202880	4.702289	0.695042
H	8.593342	5.640184	0.296738
C	10.663460	6.245167	3.316742
C	10.516346	7.133882	2.230708
H	10.895710	6.848020	1.246835
C	9.881305	8.373354	2.409893
H	9.773156	9.054441	1.563185
C	9.380271	8.730053	3.673015
H	8.879807	9.690715	3.811633
C	9.517090	7.845947	4.757781
H	9.126067	8.119366	5.740192
C	10.156436	6.609026	4.582570
H	10.247948	5.920168	5.423310
C	13.223470	4.844463	3.658498
C	14.297187	4.391686	2.865809
H	14.094626	3.968952	1.878658
C	15.616588	4.493080	3.338770
H	16.443784	4.141450	2.718660
C	15.867950	5.052381	4.601971
H	16.893323	5.135831	4.968357
C	14.799398	5.510661	5.394650
H	14.993972	5.949745	6.375557
C	13.481427	5.405589	4.927267
H	12.655199	5.762919	5.544095
C	10.721975	3.462042	4.163236
C	9.316541	3.453765	4.307619
H	8.715729	4.226203	3.826510
C	8.687545	2.457870	5.068657
H	7.601198	2.466801	5.174320
C	9.448995	1.446556	5.678240
H	8.956871	0.666405	6.262640
C	10.845981	1.442469	5.529830
H	11.445381	0.660015	6.000271
C	11.480807	2.443998	4.778876
H	12.566583	2.433424	4.670546
Cl	12.329744	4.461696	-1.053409
N	10.943557	1.752320	1.270197
N	9.094769	3.716746	0.856585
P	11.515184	4.643288	2.994025

14
C6H5COCl_B97D

C	-1.434298	-0.641040	0.294403
C	-0.042396	-0.644450	0.146074
C	0.641439	0.569333	-0.089257
C	-0.088509	1.782929	-0.170722
C	-1.477443	1.774826	-0.019104
C	-2.153143	0.563639	0.213242
H	-1.958198	-1.580941	0.473695
H	0.505225	-1.582711	0.210774
H	0.442965	2.716772	-0.351462
H	-2.033210	2.711548	-0.081974
H	-3.238259	0.559214	0.330821
C	2.105125	0.683898	-0.264582
O	2.741750	1.676401	-0.489556
Cl	3.065996	-0.933169	-0.113146

20
C6H5COC2F5_B97D

C	-1.480988	-0.588407	0.410882
C	-0.090907	-0.625645	0.245439
C	0.616541	0.556571	-0.084933
C	-0.105712	1.766921	-0.246502
C	-1.492319	1.794684	-0.086455
C	-2.184888	0.615080	0.243500
H	-2.015242	-1.504124	0.668993
H	0.425842	-1.569769	0.384414
H	0.440232	2.675975	-0.498129
H	-2.035522	2.732130	-0.216750
H	-3.268860	0.635591	0.370950
C	2.089650	0.634487	-0.265291
C	2.989222	-0.664943	-0.187327
C	3.385934	-1.061113	1.270770
F	4.154679	-0.423915	-0.854602
F	2.392425	-1.752079	-0.778194
F	2.291838	-1.387211	1.998217
F	4.002246	-0.018500	1.869793
F	4.224169	-2.119495	1.266379
O	2.694694	1.680959	-0.467321

34
PPh3_B97D

C	2.579823	21.614785	1.227211
C	3.203071	21.624274	-0.040285
H	3.151168	20.737808	-0.677786
C	3.888962	22.762655	-0.490596
H	4.363340	22.756112	-1.474319
C	3.973609	23.902672	0.326530
H	4.514630	24.786029	-0.019324
C	3.364079	23.899780	1.592120
H	3.425887	24.783025	2.231888
C	2.667786	22.765103	2.039300
H	2.190603	22.775115	3.020297
C	-0.028833	20.379281	1.056141
C	-0.923032	19.286001	1.024782

H	-0.593676	18.304067	1.374697	H	-0.190173	18.969305	-0.422029	F	2.710689	16.384247	-1.766044
C	-2.233801	19.448655	0.551386	C	-1.951903	20.203124	-0.548925	F	2.420796	17.911294	-3.271669
H	-2.915355	18.595319	0.537622	H	-2.364000	19.654690	-1.390995	F	4.105500	18.038929	-1.920901
C	-2.664188	20.703301	0.087191	C	-2.641515	21.287143	-0.013923	C	1.985486	18.490563	-0.971825
H	-3.681606	20.828608	-0.289334	H	-3.595978	21.587750	-0.436653	C	2.802277	17.708206	-1.996389
C	-1.779353	21.793952	0.105850	C	-2.107185	21.988817	1.067712				
H	-2.107811	22.771992	-0.253016	H	-2.643866	22.834905	1.487237	44			
C	-0.470809	21.635410	0.590790	C	-0.885658	21.606703	1.611014	III_wB97xD			
H	0.205842	22.490836	0.609677	H	-0.479437	22.154096	2.457330	Cu	2.470934	18.160732	0.873669
C	1.431506	20.339732	3.548445	C	1.276461	20.064572	3.537558	C	0.026772	16.502474	2.190262
C	2.490545	19.969401	4.407139	C	0.093401	19.642639	4.156687	H	-0.402259	16.525282	1.192919
H	3.402084	19.533647	3.989601	H	-0.782076	19.409343	3.556781	C	-0.674682	15.925190	3.263231
C	2.386138	20.158765	5.793293	C	0.028606	19.506174	5.540485	H	-1.654335	15.492272	3.093830
H	3.215551	19.872138	6.443556	H	-0.895914	19.173863	6.003894	C	-0.096560	15.922175	4.512319
C	1.214305	20.706185	6.343045	C	1.144820	19.785938	6.326125	H	-0.608331	15.483643	5.364367
H	1.128972	20.846647	7.422672	H	1.095207	19.674321	7.405374	C	1.181041	16.494190	4.685859
C	0.152146	21.067808	5.498411	C	2.327155	20.202249	5.719223	C	1.796880	17.047435	3.548914
H	-0.761358	21.494205	5.919092	H	3.205322	20.415425	6.321915	C	1.864034	16.530660	5.949705
C	0.260136	20.890313	4.109123	C	2.395597	20.334078	4.334819	H	1.371167	16.099880	6.816385
H	-0.567102	21.183492	3.461233	H	3.332226	20.638647	3.875001	C	3.098497	17.082758	6.057771
P	1.678476	20.065230	1.724626	N	1.527299	16.812870	2.856275	H	3.615950	17.104011	7.012332
				N	3.962045	17.920788	2.414401	C	3.754827	17.656036	4.914344
64				P	1.441679	19.968362	1.716218	C	5.036739	18.240394	4.974771
I_wB97xD				F	1.088813	17.032391	-1.410737	H	5.571471	18.263961	5.919890
Cu	2.198582	17.916666	1.091265	F	3.179639	17.729848	-1.580516	C	5.590378	18.775766	3.834230
C	0.319786	16.314113	3.066231	F	1.954158	14.832118	-0.031694	H	6.572432	19.234406	3.843535
H	-0.344129	16.286680	2.206751	F	2.862227	15.104216	-1.975890	C	4.857144	18.737399	2.638192
C	-0.107893	15.847294	4.318868	F	4.006952	15.517714	-0.187437	H	5.258775	19.164714	1.725623
H	-1.111227	15.451435	4.431031	C	2.301026	17.077440	-0.693869	C	3.104233	17.650341	3.668336
C	0.763383	15.907778	5.382997	C	2.780793	15.629825	-0.735818	N	1.223139	17.046280	2.326537
H	0.467713	15.560324	6.368988					N	3.649844	18.195376	2.553730
C	2.056973	16.431495	5.188686	30				F	0.760919	18.261801	-1.350974
C	2.391027	16.875492	3.894757	II_wB97xD				F	2.218558	19.915770	-1.339031
C	3.020694	16.542013	6.248926	Cu	2.441167	18.187315	0.877364	F	2.805995	16.495485	-1.846249
H	2.740947	16.192031	7.238494	C	-0.100930	16.708229	2.291879	F	2.591376	18.099505	-3.282560
C	4.247181	17.073388	6.022761	H	-0.577041	16.795175	1.319571	F	4.226950	18.135128	-1.867451
H	4.972160	17.158621	6.827198	C	-0.770194	16.104202	3.370716	C	2.080361	18.568925	-0.971905
C	4.614970	17.552122	4.718613	H	-1.774733	15.720040	3.232630	C	2.923298	17.828322	-2.005908
C	5.857210	18.159722	4.450067	C	-0.129964	16.014547	4.585871	O	3.188085	21.685520	2.107982
H	6.591119	18.256354	5.245303	H	-0.615966	15.554257	5.441427	C	2.484159	21.292624	2.984916
C	6.120000	18.629078	3.182186	C	1.177319	16.527846	4.720360	C	1.148196	20.680160	2.842522
H	7.063593	19.105395	2.939785	C	1.758413	17.112523	3.580588	Cl	3.079652	21.478469	4.696371
C	5.137449	18.486796	2.190049	C	1.921588	16.476568	5.948528	C	0.414818	20.151784	3.910433
H	5.311054	18.851655	1.181872	H	1.454815	16.020271	6.816534	C	0.632272	20.623576	1.539528
C	3.695199	17.455032	3.655906	C	3.176875	16.985046	6.023020	C	-0.831460	19.585013	3.674620
C	2.569988	21.344536	1.277256	H	3.738062	16.945609	6.951984	H	0.811755	20.175313	4.918726
C	3.473634	21.127026	0.231899	C	3.798920	17.589610	4.876624	C	-0.616074	20.057988	1.313532
H	3.493255	20.162739	-0.270312	C	5.100404	18.131830	4.905166	H	1.213269	21.013481	0.711821
C	4.341068	22.139823	-0.173614	H	5.673798	18.100725	5.827181	C	-1.348702	19.542005	2.380309
H	5.036796	21.959978	-0.988044	C	5.624731	18.692667	3.763069	H	-1.397514	19.170487	4.502533
C	4.315690	23.375452	0.467122	H	6.621576	19.118201	3.747951	H	-1.005275	20.007251	0.302304
H	4.993730	24.164698	0.155162	C	4.847107	18.711485	2.595005	H	-2.322252	19.094623	2.202620
C	3.417999	23.600201	1.511064	H	5.231910	19.146661	1.678724				
H	3.395557	24.563496	2.012462	C	3.095771	17.654286	3.660445	44			
C	2.548137	22.591746	1.913116	N	1.123000	17.197404	2.391591	OATS_wB97xD			
H	1.857887	22.773935	2.732144	N	3.620549	18.210159	2.540459	C	1.644022	16.182169	2.162734
C	-0.187152	20.514924	1.079962	F	0.659446	18.145669	-1.284141	H	2.041335	15.816694	1.220732
C	-0.729091	19.815300	-0.002299	F	2.093161	19.817530	-1.407487	C	1.182622	15.284811	3.138822

H	1.225555	14.217926	2.950192	H	0.211453	22.267282	5.170849	F	-1.212339	17.540791	-0.953133
C	0.684305	15.786612	4.319085	C	1.033646	22.127772	3.191009	F	0.358053	16.361900	-0.058127
H	0.321960	15.124653	5.100549	H	1.059811	23.196469	3.009274	C	0.873515	18.621226	-0.661395
C	0.634892	17.182531	4.511219	C	1.486685	21.241206	2.199004	C	-0.161356	17.594863	-0.127640
C	1.115980	17.999324	3.469775	H	1.866487	21.609113	1.250986	Cu	2.435084	18.360583	0.994818
C	0.112149	17.785599	5.706394	C	1.022484	19.415662	3.513861	Cl	4.647985	18.157285	1.497309
H	-0.246521	17.134295	6.498119	N	1.473853	17.230047	2.622487	C	2.804772	19.120845	-0.782861
C	0.062829	19.133678	5.842115	N	1.482787	19.930091	2.354506	C	3.575087	18.187686	-1.645481
H	-0.335332	19.586853	6.745287	F	0.405923	19.592779	-0.530607	C	3.317224	16.816259	-1.683574
C	0.527065	19.997387	4.791748	F	1.046922	17.778159	-1.578514	C	4.613346	18.731103	-2.406997
C	0.477355	21.404206	4.877730	F	-0.930547	18.058748	1.282617	C	4.098443	15.989520	-2.480126
H	0.078912	21.872812	5.773106	F	-1.432607	17.659105	-0.776402	H	2.505365	16.394021	-1.100933
C	0.931395	22.163570	3.823631	F	-0.202657	16.254772	0.311952	C	5.393140	17.899112	-3.201471
H	0.906653	23.247076	3.855009	C	0.808373	18.300887	-0.331106	H	4.808045	19.797644	-2.365400
C	1.433319	21.511906	2.685547	C	-0.455569	17.559640	0.137001	C	5.137983	16.529357	-3.237036
H	1.797689	22.079773	1.834705	Cu	2.292132	18.253744	1.000623	H	3.896833	14.923364	-2.510981
C	1.052174	19.438271	3.611318	Cl	4.383604	18.186787	1.888044	H	6.202188	18.319705	-3.790641
N	1.625409	17.495113	2.322117	C	3.212243	19.047410	-0.518486	H	5.749646	15.880410	-3.856745
N	1.492447	20.195006	2.581730	C	3.908587	18.126389	-1.449829	O	2.871620	20.316707	-0.783687
F	0.809721	20.659473	-0.814180	C	3.910997	16.744152	-1.259279				
F	1.606964	18.960327	-1.955376	C	4.559162	18.690984	-2.552074	44			
F	-0.828946	18.941388	0.553600	C	4.566101	15.924587	-2.168236	V_wB97xD			
F	-1.025803	18.854304	-1.597276	H	3.406009	16.316194	-0.398270	Cu	2.838208	16.136540	0.764508
F	-0.009505	17.259380	-0.547232	C	5.213448	17.865750	-3.459161	C	0.397569	16.791745	2.793466
C	1.154185	19.313207	-0.694296	H	4.547080	19.767183	-2.691011	H	-0.234841	16.310651	2.053637
C	-0.189389	18.591868	-0.576718	C	5.216841	16.485163	-3.267628	C	-0.154703	17.360509	3.954297
Cu	2.280189	19.062991	0.895011	H	4.571114	14.849279	-2.020664	H	-1.225777	17.315843	4.117941
Cl	4.560425	19.295711	1.619739	H	5.719758	18.300322	-4.315462	C	0.684534	17.964169	4.863334
C	4.086330	19.137591	-0.356703	H	5.728069	15.842053	-3.977931	H	0.294652	18.414521	5.771894
C	4.241019	17.739843	-0.835895	O	3.179417	20.235802	-0.567256	C	2.071779	17.997451	4.610658
C	4.355436	16.627684	0.001597					C	2.523733	17.404380	3.417570
C	4.239406	17.575675	-2.226592	44				C	3.018368	18.605426	5.504338
C	4.461441	15.357097	-0.551831	RETS_wB97xD				H	2.648355	19.054325	6.421509
H	4.367479	16.751563	1.077796	C	1.775763	15.941935	2.778162	C	4.342295	18.617632	5.211286
C	4.343629	16.301647	-2.770615	H	2.221394	15.384335	1.960515	H	5.056401	19.075876	5.889019
H	4.147905	18.443306	-2.869368	C	1.340393	15.287590	3.940346	C	4.835563	18.036818	3.992708
C	4.450955	15.190956	-1.935792	H	1.449570	14.212206	4.023065	C	6.197885	18.057840	3.632193
H	4.554603	14.495371	0.101883	C	0.779328	16.032816	4.952260	H	6.922733	18.512521	4.301407
H	4.339749	16.176798	-3.848866	H	0.426168	15.560135	5.864310	C	6.588663	17.506009	2.433561
H	4.530696	14.196085	-2.363516	C	0.665155	17.430289	4.803958	H	7.626809	17.506954	2.121561
O	4.214618	20.149393	-0.967341	C	1.138542	17.996986	3.606088	C	5.616055	16.938946	1.596835
				C	0.092347	18.278090	5.813194	H	5.890606	16.504878	0.641211
44				H	-0.269778	17.818128	6.727959	C	3.933887	17.436813	3.095179
IV_wB97xD				C	0.003161	19.618304	5.628019	N	1.692665	16.812377	2.533953
C	1.505448	15.912881	2.746303	H	-0.432657	20.256556	6.391118	N	4.328596	16.903008	1.913253
H	1.879923	15.354087	1.894934	C	0.487662	20.229839	4.421318	Cl	2.013760	15.093930	-0.966045
C	1.080324	15.249773	3.905814	C	0.427140	21.619276	4.186762	O	0.526513	19.173685	0.766071
H	1.126789	14.167762	3.951523	H	-0.007142	22.271288	4.939333	C	1.072064	20.250478	0.836747
C	0.609305	15.995116	4.962469	C	0.921859	22.128905	3.008120	C	0.450013	21.433334	1.478278
H	0.266893	15.515812	5.875085	H	0.892836	23.191684	2.795391	C	2.516416	20.347287	0.255050
C	0.573673	17.400290	4.859422	C	1.474758	21.246489	2.065766	C	0.837891	22.752604	1.213096
C	1.028268	17.977626	3.659262	H	1.872862	21.608258	1.123237	C	-0.584567	21.181430	2.390317
C	0.099603	18.247362	5.919337	C	1.056546	19.428410	3.413971	C	3.590376	20.717089	1.320356
H	-0.248801	17.779436	6.835338	N	1.671929	17.249957	2.612215	F	2.565910	21.264342	-0.741602
C	0.086449	19.596047	5.780623	N	1.538474	19.940902	2.260093	F	2.852933	19.156683	-0.263061
H	-0.273144	20.233219	6.583357	F	0.321871	19.835477	-0.459180	C	0.194470	23.803555	1.858141
C	0.551796	20.216478	4.571136	F	0.871103	18.402928	-2.011239	H	1.618970	22.971767	0.496058
C	0.566734	21.613765	4.379076	F	-0.618405	17.936118	1.076690	C	-1.212986	22.234064	3.039899

H	-0.874702	20.154821	2.589852
F	3.178389	20.320233	2.530610
F	3.793306	22.033004	1.360359
F	4.749768	20.121502	1.053952
C	-0.824025	23.547082	2.772847
H	0.489585	24.825590	1.642621
H	-2.005992	22.034050	3.753741
H	-1.317647	24.371763	3.278347

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VI_wB97xD

Cu	-0.921958	-0.112197	0.091172
N	0.718300	1.363836	0.041577
N	0.707074	-1.344452	0.031462
C	0.699332	2.685854	0.052525
C	1.868938	3.464694	0.028769
C	3.089912	2.830682	-0.008687
C	4.369565	0.678973	-0.060945
C	4.363587	-0.677105	-0.072333
C	3.073564	-2.820029	-0.052719
C	1.850572	-3.449987	-0.020633
C	0.684683	-2.670294	0.022170
C	1.912634	0.732363	0.005818
C	3.139483	1.420901	-0.021884
C	3.127997	-1.411058	-0.043099
C	1.906805	-0.713702	-0.002688
H	-0.280344	3.153914	0.081662
H	1.794456	4.546315	0.040268
H	4.015110	3.399598	-0.027881
H	5.305131	1.230109	-0.082474
H	5.293977	-1.236408	-0.103284
H	3.996474	-3.391901	-0.084885
H	1.770344	-4.531013	-0.027130
H	-0.294326	-3.137069	0.049700
Cl	-3.065601	0.280843	0.146933

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VII_wB97xD

Cu	11.368387	3.575195	1.163760
C	11.157601	0.568183	2.171208
H	12.241397	0.631280	2.205570
C	10.488449	-0.552505	2.689034
H	11.058323	-1.361983	3.131257
C	9.114528	-0.595106	2.620750
H	8.561187	-1.446750	3.006419
C	8.416411	0.486023	2.045482
C	9.177536	1.572246	1.571617
C	6.983624	0.521917	1.941544
H	6.417863	-0.330254	2.307255
C	6.351559	1.591579	1.398640
H	5.268603	1.615067	1.318318
C	7.095831	2.725806	0.924280
C	8.501636	2.725820	1.015596
C	6.478693	3.866357	0.371269
H	5.396490	3.900529	0.282401
C	7.258448	4.919626	-0.048483
H	6.819372	5.811178	-0.482202
C	8.652061	4.831167	0.099122
H	9.294081	5.648835	-0.214686
C	10.600877	5.873825	3.605798
C	10.317786	6.772959	2.571370
H	10.723231	6.594214	1.578278
C	9.525746	7.894038	2.805152
H	9.315278	8.584867	1.993879
C	9.000495	8.122253	4.075074
H	8.377179	8.992729	4.258326
C	9.274464	7.230272	5.110462
H	8.867059	7.404411	6.102197
C	10.072487	6.112853	4.879265
H	10.275544	5.422559	5.693106
C	13.354221	5.033616	3.677411
C	14.394325	4.886181	2.755930
H	14.193219	4.442422	1.783176
C	15.682855	5.312818	3.077215
H	16.484634	5.196253	2.353929
C	15.936570	5.888436	4.318383
H	16.939689	6.221871	4.568728
C	14.901475	6.040099	5.242677
H	15.097320	6.491253	6.211183
C	13.616566	5.615739	4.924252
H	12.815878	5.736573	5.649188
C	11.271002	3.184405	4.460958
C	9.930456	2.811606	4.631802
H	9.144515	3.355916	4.114319
C	9.593150	1.742260	5.453660
H	8.549694	1.465492	5.573939
C	10.590999	1.022595	6.111017
H	10.327890	0.183569	6.748608
C	11.924559	1.382428	5.942705
H	12.708292	0.827004	6.449821
C	12.264637	2.456777	5.121178
H	13.310844	2.719695	4.994289
Cl	12.751020	3.603286	-0.669597
N	10.527774	1.596812	1.628991
N	9.257824	3.775585	0.617815
P	11.684489	4.450709	3.200550

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C6H5COCl_wB97xD

C	-1.424812	-0.632445	0.291087
C	-0.042942	-0.636339	0.143462
C	0.631574	0.566260	-0.088555
C	-0.085259	1.768883	-0.168771
C	-1.464444	1.764276	-0.017854
C	-2.134891	0.563593	0.211701
H	-1.947819	-1.566625	0.468814
H	0.500961	-1.571571	0.207261
H	0.446062	2.697321	-0.348118
H	-2.016895	2.696428	-0.079152
H	-3.214392	0.560352	0.329103
C	2.095811	0.670759	-0.262832
O	2.713694	1.663064	-0.491450
Cl	3.020397	-0.887707	-0.105490

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C6H5COC2F5_wB97xD

C	-1.470330	-0.584599	0.394858
C	-0.091774	-0.630475	0.221431
C	0.612170	0.540511	-0.092318
C	-0.088299	1.748482	-0.230039
C	-1.463744	1.786858	-0.059908
C	-2.157231	0.618173	0.253485
H	-2.009116	-1.494709	0.638824
H	0.415478	-1.578877	0.334279
H	0.462245	2.651594	-0.470483
H	-1.996542	2.726096	-0.170217
H	-3.234406	0.646004	0.388469
C	2.080607	0.608850	-0.287529
C	2.975502	-0.664987	-0.174903
C	3.363487	-1.033530	1.275288
F	4.126844	-0.429973	-0.830944
F	2.389755	-1.747551	-0.741225
F	2.289915	-1.394375	1.982172
F	3.929245	0.017884	1.869352
F	4.229173	-2.045948	1.277348
O	2.670056	1.637767	-0.534104

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PPh3_wB97xD

C	2.563622	21.630654	1.241754
C	3.184446	21.629690	-0.013729
H	3.132231	20.742570	-0.640845
C	3.868684	22.752818	-0.469573
H	4.341606	22.737357	-1.447297
C	3.955046	23.888813	0.332420
H	4.495511	24.763620	-0.017675
C	3.350602	23.896770	1.587299
H	3.416084	24.778967	2.217863
C	2.656324	22.776552	2.038735
H	2.184462	22.799114	3.016722
C	-0.020720	20.397865	1.065144
C	-0.895324	19.304038	1.034268
H	-0.556805	18.331749	1.385470
C	-2.196282	19.447395	0.561195
H	-2.864019	18.590751	0.548510
C	-2.635769	20.684874	0.095226
H	-3.648255	20.796840	-0.281926
C	-1.770664	21.776186	0.110617
H	-2.107000	22.743099	-0.252845
C	-0.471999	21.635434	0.595295
H	0.189716	22.496494	0.607955
C	1.421944	20.357551	3.540733
C	2.457742	19.945471	4.388866
H	3.348678	19.484414	3.968282
C	2.361402	20.121147	5.766064
H	3.175608	19.800750	6.409784
C	1.218207	20.696840	6.316682
H	1.137663	20.827970	7.391964
C	0.177183	21.099006	5.483521
H	-0.717488	21.546641	5.907086
C	0.278674	20.933893	4.103757
H	-0.538025	21.258715	3.465712

P	1.668652	20.098292	1.734027	N	1.547764	16.926338	2.888206	H	3.631047	17.055392	7.031495
				N	3.984206	17.988613	2.465701	C	3.753255	17.623642	4.942865
64				P	1.447445	20.036111	1.747809	C	5.043434	18.186918	4.997490
I_M06-L				F	1.224505	17.222040	-1.429974	H	5.588196	18.188146	5.940279
Cu	2.241885	18.011521	1.163155	F	3.360534	17.827035	-1.462958	C	5.593224	18.731908	3.856447
C	0.324373	16.446437	3.097394	F	1.903406	14.982985	-0.010099	H	6.585049	19.175213	3.862391
H	-0.341362	16.448197	2.233359	F	2.922710	15.228720	-1.910936	C	4.849042	18.725997	2.669785
C	-0.110533	15.965620	4.339394	F	4.000305	15.572620	-0.058134	H	5.247109	19.164819	1.757553
H	-1.124379	15.587858	4.444927	C	2.393282	17.209577	-0.633256	C	3.082410	17.644273	3.696712
C	0.764139	15.978869	5.407876	C	2.805158	15.748079	-0.666359	N	1.188780	17.073364	2.366116
H	0.461104	15.611742	6.387439					N	3.624972	18.204729	2.581956
C	2.068139	16.477946	5.225583	30				F	0.654324	17.953149	-1.191689
C	2.412384	16.950153	3.934279	II_M06-L				F	1.855500	19.799587	-1.396178
C	3.037606	16.540889	6.274352	Cu	2.529891	18.196409	0.870337	F	2.887657	16.460658	-1.710102
H	2.756465	16.174335	7.260651	C	-0.086236	16.724974	2.275505	F	2.359575	17.918947	-3.229998
C	4.283151	17.048202	6.051856	H	-0.557850	16.815880	1.297261	F	4.068747	18.275938	-1.941954
H	5.014996	17.093425	6.857152	C	-0.764353	16.121820	3.347262	C	1.943426	18.475612	-0.924114
C	4.657581	17.546461	4.765402	H	-1.771555	15.739733	3.202398	C	2.810228	17.786485	-1.962930
C	5.915500	18.116314	4.493533	C	-0.132976	16.028265	4.569518	O	3.374700	21.617665	2.192362
H	6.663131	18.170693	5.283646	H	-0.627242	15.568113	5.423879	C	2.588641	21.261379	3.020044
C	6.180385	18.600691	3.227274	C	1.173985	16.535817	4.715131	C	1.256220	20.699424	2.808460
H	7.141772	19.045507	2.983337	C	1.770334	17.122039	3.572068	Cl	3.074024	21.441342	4.792114
C	5.185718	18.516231	2.244260	C	1.905888	16.483922	5.940943	C	0.413207	20.250498	3.835581
H	5.362627	18.892547	1.236255	H	1.431419	16.029265	6.809079	C	0.841654	20.597919	1.467163
C	3.718474	17.500913	3.703926	C	3.168325	16.990967	6.024803	C	-0.839129	19.738921	3.523488
C	2.519060	21.426497	1.232841	H	3.722266	16.950531	6.961156	H	0.738825	20.301933	4.871889
C	3.349695	21.222689	0.123104	C	3.800828	17.587608	4.890198	C	-0.415974	20.088200	1.166063
H	3.343799	20.252038	-0.377395	C	5.103140	18.123590	4.929050	H	1.502517	20.938136	0.674961
C	4.174306	22.245950	-0.339060	H	5.667759	18.092603	5.859541	C	-1.257449	19.665156	2.192579
H	4.814055	22.075968	-1.203337	C	5.640894	18.678819	3.787141	H	-1.492622	19.391974	4.321405
C	4.183490	23.479231	0.308736	H	6.641856	19.101132	3.781146	H	-0.724336	20.007397	0.126189
H	4.832292	24.277765	-0.047229	C	4.878945	18.696295	2.612125	H	-2.241505	19.263219	1.956398
C	3.363435	23.689749	1.417282	H	5.275582	19.125874	1.694912				
H	3.370050	24.652073	1.926564	C	3.102970	17.651366	3.660326	44			
C	2.533478	22.671113	1.876551	N	1.142667	17.212788	2.377329	OATS_M06-L			
H	1.901519	22.839847	2.748727	N	3.643852	18.199766	2.539091	C	1.778131	16.206380	2.387342
C	-0.214498	20.479704	1.125988	F	0.653768	18.020494	-1.200405	H	2.174422	15.807036	1.453405
C	-0.794706	19.653523	0.156994	F	1.967712	19.790272	-1.416815	C	1.394262	15.346380	3.425799
H	-0.245061	18.779086	-0.196832	F	2.799940	16.397939	-1.752039	H	1.499382	14.271940	3.301063
C	-2.053081	19.953956	-0.362259	F	2.310932	17.876417	-3.265309	C	0.889834	15.887740	4.589345
H	-2.495373	19.306534	-1.117456	F	4.064121	18.151702	-2.016706	H	0.584580	15.252470	5.419568
C	-2.740308	21.078861	0.085963	C	1.975522	18.461455	-0.953018	C	0.759569	17.285656	4.701862
H	-3.724034	21.313687	-0.317078	C	2.782148	17.725239	-2.007675	C	1.169994	18.070905	3.595429
C	-2.168547	21.907942	1.052590					C	0.233103	17.927929	5.865043
H	-2.704717	22.788380	1.402957	44				H	-0.071613	17.305971	6.705184
C	-0.911926	21.611654	1.569917	III_M06-L				C	0.111597	19.283999	5.924844
H	-0.470069	22.258728	2.328635	Cu	2.482557	18.227994	0.913908	H	-0.291238	19.766988	6.813625
C	1.306882	20.213692	3.558023	C	-0.018186	16.538282	2.243716	C	0.501739	20.105813	4.823153
C	0.122591	19.860851	4.222893	H	-0.457071	16.570153	1.246239	C	0.386254	21.509968	4.828770
H	-0.776116	19.635911	3.647955	C	-0.715834	15.962254	3.318145	H	-0.012691	22.010757	5.709659
C	0.083106	19.789081	5.613112	H	-1.704104	15.539394	3.156005	C	0.777111	22.228371	3.718158
H	-0.845994	19.514022	6.110518	C	-0.124955	15.942446	4.564174	H	0.701006	23.312078	3.690890
C	1.224538	20.063219	6.364554	H	-0.633657	15.501948	5.420530	C	1.276388	21.538310	2.604296
H	1.193281	20.003222	7.451160	C	1.159720	16.497787	4.731089	H	1.587398	22.072063	1.706506
C	2.409130	20.408040	5.715203	C	1.774591	17.059632	3.584997	C	1.028542	19.501030	3.655169
H	3.309605	20.617450	6.291612	C	1.853028	16.515428	5.980041	N	1.684156	17.529835	2.462701
C	2.453240	20.475334	4.325624	H	1.363166	16.083914	6.851461	N	1.400635	20.216811	2.568408
H	3.390835	20.730688	3.829540	C	3.102474	17.051435	6.079767	F	-0.071983	19.993109	-0.602875

F 1.531347 19.347232 -1.975408
F -0.537124 17.418639 0.089976
F -0.601633 17.772702 -2.049545
F 1.093867 16.729171 -1.179788
C 0.963151 19.048455 -0.740306
C 0.222066 17.741594 -0.979401
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C 4.065120 19.332613 -0.386215
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C 4.295033 16.833553 -0.017436
C 4.125740 17.770608 -2.250598
C 4.345780 15.558368 -0.564038
H 4.339302 16.969973 1.060187
C 4.176861 16.490495 -2.786093
H 4.031286 18.640711 -2.894290
C 4.280745 15.381944 -1.947054
H 4.435888 14.696351 0.094296
H 4.132612 16.357847 -3.865025
H 4.315251 14.379937 -2.370050
O 4.079268 20.355260 -1.003301

44
IV_M06-L
C 1.434664 15.905711 2.728709
H 1.770817 15.342396 1.859758
C 1.053071 15.250468 3.905987
H 1.093333 14.165909 3.954040
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H 0.322249 15.528998 5.910999
C 0.601474 17.407619 4.877193
C 1.013540 17.984168 3.650110
C 0.182202 18.257266 5.946800
H -0.132806 17.793865 6.880161
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H 0.298518 22.279158 5.199332
C 1.043276 22.131516 3.184062
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H 4.609483 19.797406 -2.649459
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H 5.846968 18.330679 -4.237002
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O 3.137721 20.252509 -0.594082

44
RETS_M06-L
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H 1.519207 14.191950 4.093982
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C 0.729783 17.421591 4.836464
C 1.161815 17.970343 3.604438
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C 0.433241 21.595000 4.126222
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C 0.881570 22.079774 2.916257
H 0.833376 23.139241 2.679491
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H 1.772318 21.522767 1.007077
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F -0.578074 18.012075 1.042012
F -1.277264 17.600902 -0.960527
F 0.326161 16.408567 -0.123462
C 0.831086 18.657134 -0.769801
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C 3.269056 16.852037 -1.650326
C 4.586251 18.760408 -2.353295
C 4.078120 16.014312 -2.405861
H 2.434568 16.444608 -1.081215
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C 5.141883 16.547013 -3.134916
H 3.880084 14.944778 -2.428583
H 6.221784 18.333680 -3.679186
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O 2.803515 20.359238 -0.778958

44
V_M06-L
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C 0.743753 16.139484 3.001706
H 0.067723 15.715948 2.258721
C 0.297948 16.418398 4.303631
H -0.734332 16.215197 4.576841
C 1.187769 16.948676 5.213441
H 0.881268 17.175723 6.233566
C 2.516437 17.202211 4.817195
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C 3.505056 17.746114 5.693222
H 3.221567 17.971281 6.720233
C 4.773869 17.981862 5.255601
H 5.524553 18.398118 5.925432
C 5.154457 17.699703 3.906980
C 6.447210 17.953905 3.409318
H 7.201991 18.376384 4.070712
C 6.733596 17.664490 2.091527
H 7.719104 17.848738 1.672685
C 5.731173 17.125163 1.277576
H 5.926357 16.888486 0.234299
C 4.199715 17.153574 3.014531
N 1.985515 16.363509 2.596745
N 4.494937 16.873122 1.713878
Cl 1.922633 15.318644 -1.065838
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C 0.698940 20.773495 1.874769
C 0.093539 22.086354 1.599291
C 2.064167 20.373742 1.253894
C 0.759131 23.153942 0.973037
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F 2.078165 19.029682 1.099045
C 0.102972 24.364348 0.782824
H 1.787551 23.057717 0.643099
C -1.886076 23.468565 1.823702
H -1.737566 21.431808 2.515413
F 3.078348 20.240354 3.377920
F 3.425047 22.050374 2.223306
F 4.388423 20.190445 1.643698
C -1.217041 24.523111 1.199609
H 0.626370 25.188154 0.302579
H -2.916877 23.590812 2.149455
H -1.727139 25.471146 1.038951

24
VI_M06-L
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N 0.696556 -1.350934 0.041973
C 0.690249 2.680770 0.028257
C 1.856359 3.462243 0.003606
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C 4.355049 -0.677558 -0.066215
C 3.082034 -2.819969 -0.033641

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C 1.902522 0.725798 -0.001254
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C 1.899190 -0.711662 0.002151
H -0.294554 3.147658 0.050499
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H 4.008562 3.401937 -0.047595
H 5.298018 1.237111 -0.086930
H 5.289041 -1.236276 -0.092851
H 4.010734 -3.387514 -0.062178
H 1.783647 -4.539169 0.003504
H -0.288672 -3.158566 0.073178
Cl -2.984211 0.456906 0.154804

58
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Cu 11.282588 3.550563 1.301653
C 11.059273 0.540565 2.219885
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H 10.918211 -1.431422 3.084722
C 9.001097 -0.663375 2.469580
H 8.432594 -1.539936 2.776879
C 8.329793 0.431194 1.890042
C 9.112842 1.550321 1.511393
C 6.917014 0.460179 1.677720
H 6.331745 -0.410212 1.970642
C 6.312791 1.547359 1.120026
H 5.236175 1.560968 0.957583
C 7.070642 2.698206 0.740626
C 8.473265 2.705783 0.943998
C 6.490474 3.849145 0.172666
H 5.415656 3.878719 -0.000305
C 7.295680 4.919128 -0.158936
H 6.882326 5.819770 -0.605383
C 8.672519 4.837846 0.091205
H 9.333567 5.667206 -0.158610
C 10.609510 5.860154 3.696259
C 10.284992 6.742447 2.657098
H 10.664978 6.545193 1.653036
C 9.488910 7.858962 2.896769
H 9.244820 8.535456 2.079287
C 8.999760 8.102221 4.179037
H 8.370756 8.970437 4.367822
C 9.315199 7.229901 5.219669
H 8.936259 7.417122 6.223078
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H 10.354076 5.436968 5.801437
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H 16.430347 5.218885 2.193255
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H 16.975569 6.271578 4.377095
C 14.971505 6.072679 5.147321
H 15.208058 6.536368 6.103635
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H 12.904651 5.749123 5.653714
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H 12.823579 0.960671 6.661560
C 12.335993 2.523806 5.266936
H 13.378851 2.796396 5.107500
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N 10.458958 1.591420 1.670339
N 9.254310 3.772500 0.634008
P 11.680298 4.433332 3.278734

14
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C -1.421442 -0.633372 0.292141
C -0.040228 -0.635457 0.144726
C 0.635495 0.569170 -0.088809
C -0.086715 1.772418 -0.170019
C -1.465097 1.764894 -0.019242
C -2.133970 0.562306 0.211443
H -1.944661 -1.569964 0.471081
H 0.512094 -1.568889 0.208479
H 0.448722 2.701253 -0.350973
H -2.020738 2.697907 -0.081510
H -3.215922 0.557444 0.328977
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Cl 3.003087 -0.908265 -0.111796

20
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C 0.609849 0.545787 -0.062976
C -0.098896 1.748683 -0.233044
C -1.477507 1.780335 -0.099638
C -2.172335 0.610702 0.213713
H -2.021513 -1.496414 0.641213
H 0.414684 -1.569041 0.401752
H 0.459053 2.650814 -0.473050
H -2.015385 2.715807 -0.238344
H -3.255414 0.633140 0.319441
C 2.072911 0.623056 -0.218288
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C 3.405429 -1.042082 1.250898
F 4.087633 -0.419016 -0.871860
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F 2.346378 -1.323782 2.023897
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F 4.196883 -2.117842 1.208489
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34
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C 3.042705 21.686943 -0.065532
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C 3.725557 22.809779 -0.522008
H 4.078120 22.846667 -1.551544
C 3.967212 23.878743 0.340329
H 4.509907 24.754143 -0.012409
C 3.514626 23.818828 1.656216
H 3.698760 24.650012 2.335294
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H -0.545482 18.324127 1.411851
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H -2.852318 18.583168 0.557728
C -2.609238 20.671608 0.074624
H -3.621569 20.783784 -0.309928
C -1.737936 21.758924 0.079264
H -2.069103 22.725420 -0.297735
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H 0.226219 22.479281 0.580941
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H 3.171751 19.948821 6.439468
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H 1.067135 20.873618 7.392082
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H -0.813954 21.467035 5.879345
C 0.232573 20.884231 4.092280
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P 1.680554 20.091095 1.748448

64
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C 4.246808 17.110761 6.022247
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C 4.613110 17.587603 4.721211
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H 6.591109 18.301993 5.243162
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H	7.051742	19.149030	2.926308	C	1.746073	17.107843	3.569819	Cl	3.200259	21.210826	4.638720
C	5.121582	18.520474	2.185321	C	1.906815	16.487668	5.947363	C	0.417419	20.184795	3.844033
H	5.295024	18.881614	1.168990	H	1.436291	16.036581	6.822443	C	0.696818	20.638291	1.471600
C	3.689148	17.483068	3.655555	C	3.165555	16.994781	6.016865	C	-0.862929	19.707423	3.591422
C	2.570331	21.277187	1.282431	H	3.732147	16.962147	6.948593	H	0.802193	20.188825	4.863280
C	3.456386	21.043612	0.223224	C	3.786255	17.587623	4.869207	C	-0.582077	20.154484	1.229008
H	3.451514	20.071037	-0.278000	C	5.089495	18.124114	4.903374	H	1.319773	20.996749	0.652241
C	4.329801	22.044133	-0.200015	H	5.657378	18.093072	5.835054	C	-1.363196	19.695183	2.289063
H	5.013471	21.852290	-1.028137	C	5.624090	18.677935	3.762255	H	-1.474258	19.340871	4.416541
C	4.329167	23.282732	0.435944	H	6.626932	19.101446	3.749267	H	-0.964836	20.130350	0.208719
H	5.014940	24.065496	0.108717	C	4.854153	18.693734	2.590736	H	-2.368936	19.316760	2.098749
C	3.450044	23.524090	1.492158	H	5.247284	19.124695	1.669577				
H	3.447369	24.494662	1.990156	C	3.082617	17.646233	3.645416	44			
C	2.573187	22.529001	1.912403	N	1.105390	17.180914	2.385824	OATS_MN12SX			
H	1.892329	22.724601	2.743956	N	3.623190	18.196329	2.528540	C	1.041423	15.956584	2.935432
C	-0.187811	20.485546	1.098774	F	0.714661	18.067850	-1.164019	H	1.293114	15.365233	2.052399
C	-0.733103	19.804377	0.004757	F	2.037850	19.801993	-1.409607	C	0.571505	15.338544	4.105477
H	-0.195774	18.953506	-0.423243	F	2.809198	16.417183	-1.765694	H	0.464390	14.255289	4.135963
C	-1.948886	20.212638	-0.542733	F	2.328577	17.900601	-3.255463	C	0.251474	16.122677	5.191955
H	-2.365801	19.677264	-1.396815	F	4.092363	18.135725	-2.037919	H	-0.119767	15.677559	6.116924
C	-2.628689	21.297950	0.002661	C	2.028361	18.489051	-0.944584	C	0.403141	17.522105	5.106776
H	-3.581936	21.615475	-0.422354	C	2.812722	17.734869	-2.015792	C	0.885490	18.048710	3.887930
C	-2.092152	21.981199	1.095080					C	0.094594	18.411629	6.187206
H	-2.624343	22.831731	1.523362	44				H	-0.276817	17.983763	7.119530
C	-0.877475	21.579493	1.639824	III_MN12SX				C	0.260903	19.754619	6.056268
H	-0.466215	22.114110	2.499392	Cu	2.685496	18.258185	0.888316	H	0.026702	20.428595	6.881788
C	1.261047	20.045100	3.545414	C	-0.035760	16.647288	2.210150	C	0.746824	20.321368	4.833167
C	0.075682	19.622158	4.166133	H	-0.467209	16.698439	1.207487	C	0.937754	21.706177	4.645830
H	-0.802272	19.384743	3.560651	C	-0.766876	16.096000	3.279440	H	0.712147	22.395004	5.462011
C	0.006570	19.493682	5.550519	H	-1.772643	15.714482	3.107229	C	1.406587	22.166799	3.435763
H	-0.923874	19.163401	6.015142	C	-0.185161	16.047068	4.526355	H	1.566929	23.228953	3.256191
C	1.120017	19.780084	6.339014	H	-0.715860	15.621506	5.380234	C	1.682200	21.241392	2.414376
H	1.065730	19.677107	7.423607	C	1.122088	16.548897	4.702265	H	2.059398	21.570495	1.444184
C	2.304901	20.193215	5.733322	C	1.762257	17.091517	3.564661	C	1.056136	19.473268	3.746693
H	3.184014	20.413890	6.341230	C	1.810403	16.519353	5.958194	N	1.197042	17.266813	2.829484
C	2.378584	20.318172	4.348144	H	1.296502	16.094636	6.822046	N	1.513069	19.938224	2.563510
H	3.321960	20.622650	3.886656	C	3.078595	16.995985	6.068699	F	-0.246974	19.142771	-0.437154
N	1.537488	16.821459	2.850006	H	3.607978	16.962308	7.021997	F	1.396599	18.567149	-1.758300
N	3.947898	17.948541	2.412779	C	3.756487	17.558512	4.938311	F	-0.621904	16.591619	0.280564
P	1.429120	19.925835	1.735458	C	5.071575	18.060877	5.010720	F	-0.637437	16.886763	-1.856472
F	1.119047	17.105684	-1.420970	H	5.610641	18.018501	5.958899	F	1.053832	15.934504	-0.914436
F	3.195693	17.821078	-1.534631	C	5.653701	18.599925	3.885627	C	0.829727	18.260990	-0.540813
F	1.981723	14.883826	-0.090128	H	6.666519	18.998914	3.902789	C	0.146805	16.911959	-0.770875
F	2.894286	15.223991	-2.013836	C	4.915608	18.647095	2.694319	Cu	1.833692	18.340075	1.094853
F	4.022213	15.589112	-0.212813	H	5.340336	19.082301	1.789106	Cl	4.237734	18.362334	1.887499
C	2.309104	17.148451	-0.682264	C	3.096135	17.625752	3.691537	C	3.752928	19.014725	0.087798
C	2.803022	15.705304	-0.762780	N	1.185312	17.130208	2.346368	C	4.094079	18.004818	-0.938893
				N	3.676131	18.176482	2.594599	C	4.096093	16.628797	-0.699959
30				F	0.796088	18.185232	-1.128242	C	4.386745	18.504317	-2.213354
II_MN12SX				F	2.178942	19.872527	-1.360949	C	4.396589	15.754654	-1.736197
Cu	2.619617	18.240002	0.836238	F	2.843559	16.464522	-1.719185	H	3.850976	16.243570	0.290109
C	-0.118767	16.693171	2.297869	F	2.413251	17.962939	-3.209189	C	4.692959	17.622602	-3.242028
H	-0.601883	16.772149	1.321358	F	4.179335	18.143631	-1.985146	H	4.369115	19.580356	-2.385584
C	-0.788117	16.099712	3.383985	C	2.124231	18.558483	-0.897387	C	4.696081	16.248910	-3.005896
H	-1.798572	15.715036	3.251923	C	2.888357	17.782289	-1.967800	H	4.394480	14.680020	-1.553002
C	-0.143334	16.019967	4.597692	O	3.269042	21.617084	2.077319	H	4.926287	18.009557	-4.234286
H	-0.627204	15.566855	5.465027	C	2.563038	21.193474	2.939468	H	4.931524	15.557964	-3.816314
C	1.165397	16.531820	4.722886	C	1.198148	20.659634	2.783280	O	3.676539	20.200039	-0.029091

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IV_MN12SX

C	1.444320	15.901253	2.728381
H	1.799166	15.330342	1.868557
C	1.034927	15.252560	3.901747
H	1.069535	14.165657	3.953247
C	0.596822	16.011740	4.963842
H	0.267571	15.541734	5.892363
C	0.576542	17.416776	4.852732
C	1.011575	17.982719	3.634069
C	0.142152	18.276520	5.913743
H	-0.191449	17.817177	6.845280
C	0.145668	19.627620	5.765423
H	-0.185896	20.278479	6.576017
C	0.587638	20.232031	4.544192
C	0.618748	21.627152	4.337419
H	0.292756	22.295891	5.136237
C	1.061415	22.121889	3.131271
H	1.098808	23.193060	2.937458
C	1.476002	21.220147	2.134079
H	1.838283	21.575210	1.167371
C	1.021784	19.414388	3.477355
N	1.424797	17.218785	2.595802
N	1.458610	19.910229	2.301935
F	0.408657	19.506119	-0.508474
F	1.013883	17.659121	-1.506248
F	-0.958064	18.059570	1.331567
F	-1.471556	17.647157	-0.717026
F	-0.300213	16.219732	0.392694
C	0.783135	18.214638	-0.275441
C	-0.505638	17.525127	0.197646
Cu	2.262284	18.157447	0.985717
Cl	4.303403	18.070461	1.919140
C	3.174758	18.999112	-0.474774
C	3.906415	18.129891	-1.430583
C	3.915954	16.741238	-1.291622
C	4.580877	18.740956	-2.494260
C	4.600457	15.960079	-2.213501
H	3.392539	16.277693	-0.452125
C	5.265394	17.955241	-3.413059
H	4.560932	19.827339	-2.587560
C	5.274592	16.567498	-3.273226
H	4.611504	14.875152	-2.107263
H	5.794104	18.425780	-4.242539
H	5.812059	15.952904	-3.996758
O	3.129619	20.193571	-0.506850

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RETS_MN12SX

C	1.813450	15.934495	2.772931
H	2.252078	15.371869	1.946339
C	1.421325	15.290227	3.956909
H	1.552676	14.213430	4.051096
C	0.877309	16.040071	4.976186
H	0.559924	15.572701	5.910204
C	0.731854	17.433217	4.812814
C	1.158293	17.990197	3.587504
C	0.179938	18.288424	5.821329
H	-0.145181	17.837713	6.760151
C	0.062881	19.626894	5.614559
H	-0.358832	20.275392	6.384039
C	0.493626	20.223862	4.385160
C	0.402218	21.607012	4.124526
H	-0.018516	22.270186	4.882616
C	0.847715	22.098584	2.918189
H	0.793873	23.160695	2.683551
C	1.383276	21.207465	1.972525
H	1.745588	21.558489	1.005027
C	1.043928	19.410146	3.370702
N	1.679891	17.238345	2.592518
N	1.477198	19.906138	2.190139
F	0.307051	19.846126	-0.505639
F	0.831213	18.394572	-2.042508
F	-0.560686	18.010540	1.087958
F	-1.217977	17.561523	-0.906156
F	0.360306	16.396722	-0.021817
C	0.874004	18.640592	-0.702700
C	-0.147798	17.627862	-0.115521
Cu	2.418754	18.336108	0.987768
Cl	4.615123	18.138635	1.474794
C	2.733425	19.120146	-0.770950
C	3.524140	18.194601	-1.622273
C	3.255053	16.825513	-1.677562
C	4.598212	18.732786	-2.337876
C	4.059282	15.994304	-2.446538
H	2.411749	16.409457	-1.124850
C	5.399830	17.896865	-3.105069
H	4.799290	19.802577	-2.276884
C	5.132902	16.528993	-3.158398
H	3.848285	14.925715	-2.493027
H	6.240027	18.312769	-3.661979
H	5.765268	15.874723	-3.759918
O	2.813550	20.322605	-0.772493

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V_MN12SX

Cu	3.058741	16.233954	0.521065
C	0.687861	16.237279	2.949923
H	0.012780	15.812165	2.203351
C	0.233334	16.522964	4.250351
H	-0.803618	16.322844	4.517020
C	1.118801	17.050805	5.162217
H	0.807674	17.282224	6.182694
C	2.451142	17.300091	4.770678
C	2.801974	16.984918	3.438251
C	3.435802	17.848693	5.654233
H	3.142698	18.079274	6.679812
C	4.705010	18.077646	5.226042
H	5.456019	18.495247	5.898322
C	5.092708	17.786165	3.877846
C	6.391094	18.036287	3.390563
H	7.143674	18.456094	4.060582
C	6.687237	17.749545	2.077045
H	7.677729	17.930818	1.662732
C	5.685338	17.213899	1.255520
H	5.887601	16.978142	0.210360
C	4.146011	17.242606	2.980208
N	1.929242	16.454554	2.558680
N	4.453439	16.965058	1.687340
Cl	1.959953	15.409903	-1.149121
O	0.232336	19.751313	2.490090
C	0.758263	20.634374	1.848237
C	0.149772	21.961697	1.624149
C	2.153269	20.278782	1.256131
C	0.824643	23.053781	1.057699
C	-1.184628	22.110332	2.037337
C	3.325933	20.633185	2.193269
F	2.386360	20.867365	0.066486
F	2.208785	18.948524	1.077908
C	0.166428	24.269505	0.909751
H	1.860571	22.976593	0.736420
C	-1.836434	23.322680	1.876967
H	-1.698042	21.256087	2.478701
F	3.097299	20.143167	3.407091
F	3.472408	21.951710	2.285141
F	4.457172	20.112673	1.728961
C	-1.160177	24.405254	1.311935
H	0.694967	25.116669	0.472578
H	-2.874906	23.428348	2.191536
H	-1.671783	25.360311	1.184853

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VI_MN12SX

Cu	-0.951813	-0.305373	0.072204
N	0.713032	1.371760	0.047583
N	0.698381	-1.349562	0.046564
C	0.698361	2.692131	0.050160
C	1.869073	3.471236	0.011928
C	3.088893	2.834078	-0.030491
C	4.361681	0.683881	-0.075471
C	4.353236	-0.674838	-0.074965
C	3.075268	-2.814488	-0.029611
C	1.855633	-3.451421	0.013114
C	0.686528	-2.679074	0.050103
C	1.901370	0.736692	0.006357
C	3.136232	1.424049	-0.033878
C	3.121128	-1.405763	-0.033046
C	1.893792	-0.706498	0.006410
H	-0.286219	3.164812	0.084278
H	1.796653	4.558015	0.016364
H	4.020785	3.401764	-0.061052
H	5.301726	1.236862	-0.108188
H	5.285544	-1.240466	-0.107216
H	4.007310	-3.381686	-0.060287
H	1.779087	-4.537424	0.017837
H	-0.294632	-3.153219	0.083114
Cl	-2.985341	0.417400	0.091600

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VII_MN12SX

Cu	11.332445	3.603789	1.258121
C	11.117410	0.606826	2.265957
H	12.205472	0.675585	2.337620
C	10.433136	-0.510150	2.774201

H 10.992792 -1.314369 3.250148
C 9.061531 -0.563516 2.653307
H 8.495435 -1.418248 3.028293
C 8.379320 0.504150 2.034608
C 9.157469 1.591294 1.574994
C 6.956982 0.530541 1.861328
H 6.376244 -0.322398 2.216441
C 6.344762 1.587577 1.264567
H 5.262270 1.601384 1.127945
C 7.100897 2.715945 0.807133
C 8.504808 2.727599 0.971610
C 6.509557 3.842518 0.199777
H 5.428310 3.868795 0.052106
C 7.307999 4.890956 -0.200481
H 6.887428 5.774624 -0.678441
C 8.692837 4.815210 0.023183
H 9.351441 5.632884 -0.277985
C 10.596223 5.859558 3.666411
C 10.248624 6.732341 2.627028
H 10.613165 6.533481 1.615453
C 9.454826 7.849295 2.874851
H 9.194206 8.522486 2.057037
C 8.990247 8.099446 4.164234
H 8.362760 8.970001 4.360048
C 9.326146 7.234346 5.204545
H 8.963700 7.427711 6.215151
C 10.125484 6.120791 4.959792
H 10.376660 5.446483 5.781145
C 13.348111 5.030050 3.668446
C 14.353887 4.926961 2.701899
H 14.114890 4.508178 1.719725
C 15.648289 5.361100 2.987765
H 16.426958 5.279582 2.228192
C 15.942636 5.898200 4.237396
H 16.954816 6.238331 4.461059
C 14.943113 6.005042 5.206344
H 15.173712 6.427146 6.185488
C 13.651850 5.574368 4.924002
H 12.874147 5.658297 5.687216
C 11.291894 3.191371 4.508298
C 9.951253 2.825108 4.708261
H 9.154634 3.384291 4.209550
C 9.624812 1.752584 5.530448
H 8.577720 1.482226 5.676096
C 10.633086 1.021171 6.160227
H 10.377636 0.177099 6.802113
C 11.965278 1.371792 5.962369
H 12.759338 0.804839 6.450426
C 12.295537 2.449479 5.140382
H 13.345742 2.705839 4.988136
Cl 12.693040 3.597893 -0.599126
N 10.503614 1.624102 1.683047
N 9.276221 3.773881 0.595598
P 11.673320 4.446728 3.239703

14
C6H5COCl_MN12SX
C -1.423737 -0.633300 0.292325
C -0.041942 -0.639151 0.145512
C 0.631768 0.564222 -0.087598
C -0.083389 1.768830 -0.169567
C -1.461986 1.764578 -0.019582
C -2.132843 0.563538 0.211038
H -1.950486 -1.570530 0.471794
H 0.504760 -1.578633 0.210834
H 0.455388 2.698734 -0.350667
H -2.017289 2.700528 -0.082450
H -3.217362 0.560875 0.328238
C 2.092882 0.670614 -0.260928
O 2.708522 1.666848 -0.482788
Cl 3.012761 -0.880904 -0.116954

20
C6H5COC2F5_MN12SX
C -1.471593 -0.581729 0.408682
C -0.090304 -0.623089 0.257908
C 0.609768 0.547920 -0.069828
C -0.095852 1.750265 -0.242573
C -1.473350 1.781452 -0.096739
C -2.163780 0.613263 0.229360
H -2.011345 -1.493208 0.665998
H 0.423490 -1.569825 0.404703
H 0.457896 2.654870 -0.493841
H -2.014372 2.717624 -0.236188
H -3.248216 0.636117 0.345581
C 2.076523 0.623948 -0.237431
C 2.965023 -0.653623 -0.176888
C 3.383527 -1.050660 1.254445
F 4.104958 -0.412198 -0.844115
F 2.370603 -1.724566 -0.743590
F 2.320887 -1.377670 1.985588
F 4.003202 -0.030134 1.835891
F 4.207551 -2.090768 1.218008
O 2.678419 1.659208 -0.421135

34
PPh3_MN12SX
C 2.563530 21.625658 1.259406
C 3.060742 21.673859 -0.051437
H 2.907415 20.821902 -0.718620
C 3.743214 22.794110 -0.513823
H 4.117343 22.816776 -1.538315
C 3.958458 23.878738 0.334992
H 4.502776 24.754044 -0.021957
C 3.480311 23.837451 1.642040
H 3.645950 24.683029 2.311421
C 2.782676 22.721671 2.101703
H 2.406783 22.710521 3.126262
C 0.000410 20.392062 1.066824
C -0.875350 19.297326 1.038302
H -0.536081 18.324783 1.403735
C -2.171765 19.435288 0.552088
H -2.842019 18.574588 0.541365
C -2.607111 20.667791 0.068814
H -3.619782 20.775696 -0.321996
C -1.742702 21.759896 0.082325
H -2.078529 22.727307 -0.294274
C -0.448675 21.625976 0.581285
H 0.214014 22.493316 0.594012
C 1.410383 20.367769 3.545868
C 2.454994 19.997014 4.404985
H 3.366691 19.560629 3.989217
C 2.345917 20.181491 5.779669
H 3.170597 19.893321 6.433086
C 1.180155 20.721780 6.319682
H 1.088441 20.858503 7.398009
C 0.130753 21.081241 5.477601
H -0.784562 21.503569 5.895118
C 0.244755 20.910392 4.099283
H -0.583225 21.205637 3.452252
P 1.675228 20.099209 1.752138

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I_M06
Cu 2.347815 18.045783 1.058831
C 0.293670 16.470773 2.915235
H -0.350287 16.513489 2.034691
C -0.197864 15.981048 4.134325
H -1.228431 15.641901 4.204483
C 0.646711 15.942523 5.221181
H 0.305628 15.571517 6.187316
C 1.973330 16.393126 5.084973
C 2.371132 16.874949 3.818274
C 2.903870 16.402385 6.172584
H 2.570847 16.025790 7.139252
C 4.167286 16.873192 6.005970
H 4.874028 16.883539 6.835224
C 4.600361 17.381675 4.740275
C 5.884021 17.919677 4.532763
H 6.595221 17.937498 5.358358
C 6.220626 18.416761 3.292779
H 7.203513 18.839401 3.099385
C 5.265387 18.373616 2.266379
H 5.498255 18.760554 1.272862
C 3.708913 17.383570 3.644265
C 2.559320 21.492566 1.255903
C 3.394863 21.336183 0.144681
H 3.421101 20.375274 -0.375088
C 4.188282 22.392029 -0.295079
H 4.833804 22.259750 -1.161960
C 4.159871 23.609379 0.379004
H 4.784742 24.434516 0.040313
C 3.336583 23.771484 1.491851
H 3.316743 24.722206 2.022663
C 2.539143 22.719546 1.929199
H 1.907588 22.850784 2.808517
C -0.144285 20.417911 1.112743
C -0.789617 19.421757 0.375434
H -0.264781 18.484891 0.171864
C -2.081382 19.624097 -0.104549
H -2.575381 18.842018 -0.679013

C	-2.732432	20.827345	0.147028	C	1.981482	18.476552	-0.947802	C	0.684888	17.226689	4.568293
H	-3.741432	20.989827	-0.229331	C	2.779602	17.717478	-1.988796	C	1.151310	18.028193	3.503410
C	-2.093801	21.828808	0.878461					C	0.126894	17.842609	5.733223
H	-2.603399	22.771401	1.073144	44				H	-0.218279	17.198368	6.541135
C	-0.806694	21.625394	1.361137	III_M06				C	0.026938	19.194034	5.827881
H	-0.314394	22.409847	1.937193	Cu	2.602584	18.122979	0.811480	H	-0.399216	19.663333	6.713892
C	1.379987	20.174125	3.550414	C	-0.011344	16.351821	2.036736	C	0.474337	20.037446	4.762581
C	0.175152	19.870065	4.193319	H	-0.386095	16.307255	1.013171	C	0.380222	21.441871	4.809101
H	-0.728408	19.699983	3.606252	C	-0.787234	15.864848	3.102635	H	-0.047905	21.917936	5.690748
C	0.119128	19.776586	5.581684	H	-1.766361	15.434178	2.907513	C	0.827257	22.190706	3.744195
H	-0.826938	19.540083	6.067169	C	-0.280638	15.944978	4.379877	H	0.768988	23.276086	3.749646
C	1.264890	19.980631	6.345488	H	-0.847695	15.579022	5.235466	C	1.366005	21.526793	2.632018
H	1.220583	19.904000	7.430875	C	0.992005	16.511785	4.588328	H	1.729019	22.085645	1.768543
C	2.471499	20.275681	5.713954	C	1.687913	16.974250	3.450016	C	1.034960	19.462031	3.602027
H	3.376595	20.426266	6.301814	C	1.583434	16.639329	5.884755	N	1.695315	17.504611	2.381174
C	2.531103	20.364137	4.327533	H	1.021765	16.281225	6.746839	N	1.465613	20.209455	2.562967
H	3.484784	20.583399	3.843069	C	2.817484	17.187498	6.035576	F	0.416595	20.468597	-0.558538
N	1.534198	16.905241	2.756325	H	3.273016	17.279903	7.020703	F	1.653491	19.291914	-1.925480
N	4.049050	17.877552	2.432842	C	3.553578	17.664075	4.904367	F	-0.639861	18.216321	0.454867
P	1.539929	20.048123	1.730530	C	4.830555	18.246507	5.018967	F	-0.776448	18.313029	-1.692365
F	1.892649	17.646482	-1.773242	H	5.292259	18.327717	6.002416	F	0.662935	16.995080	-0.773584
F	3.988468	17.420959	-1.139408	C	5.471780	18.709918	3.892934	C	1.138764	19.289475	-0.650735
F	1.253302	15.374451	-0.425162	H	6.455780	19.167674	3.946622	C	0.083535	18.199038	-0.671458
F	2.819595	15.143985	-1.889602	C	4.822963	18.607024	2.655465	Cu	2.300795	19.110969	0.921147
F	3.311694	15.152345	0.209767	H	5.287599	18.987782	1.747456	Cl	4.577133	19.305127	1.652646
C	2.674436	17.224179	-0.697451	C	2.987273	17.577636	3.615553	C	4.102533	19.193745	-0.328900
C	2.518836	15.718637	-0.713471	N	1.185646	16.886201	2.201029	C	4.212593	17.811566	-0.833148
				N	3.619016	18.063133	2.517118	C	4.337724	16.676124	-0.027797
30				F	0.664520	18.063363	-1.174467	C	4.127623	17.677491	-2.225779
II_M06				F	1.968308	19.819942	-1.362219	C	4.362417	15.417063	-0.612877
Cu	2.568977	18.219159	0.862669	F	2.754854	16.461430	-1.872505	H	4.421838	16.779073	1.051600
C	-0.092820	16.713377	2.271928	F	2.258187	18.001000	-3.298816	C	4.146508	16.414305	-2.799879
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C	-0.768010	16.113570	3.348520	C	1.979403	18.484859	-0.971776	C	4.257079	15.282544	-1.995884
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C	-0.129887	16.027327	4.564580	O	3.548296	21.627265	2.133925	H	4.075073	16.313794	-3.881207
H	-0.616954	15.570170	5.425475	C	2.812065	21.337732	3.024679	H	4.268799	14.292516	-2.448347
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C	3.793985	17.588761	4.874346	C	-0.292944	20.048010	1.428529	C	1.084898	15.260121	3.885126
C	5.095470	18.124586	4.916750	H	1.560546	20.924234	0.772590	H	1.136358	14.175574	3.930661
H	5.654977	18.089896	5.850956	C	-1.045382	19.632911	2.524900	C	0.652739	16.006289	4.957900
C	5.639298	18.681905	3.782099	H	-1.125458	19.433878	4.672067	H	0.345460	15.528072	5.887400
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C	4.877645	18.701365	2.606082	H	-2.028033	19.188681	2.372140	C	1.019083	17.992086	3.640835
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44
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44
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H 10.201302 -1.714166 2.694822
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14
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C -1.463002 1.763741 -0.019456
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H -2.018077 2.697351 -0.081957
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20
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34
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64
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H 6.556610 18.407640 5.288115
C 6.105492 18.670900 3.202355
H 7.049797 19.135118 2.941550
C 5.129094 18.469810 2.210259
H 5.313523 18.775538 1.183424
C 3.674183 17.518955 3.717207
C 2.530047 21.313621 1.326079
C 3.414499 21.062391 0.271308
H 3.396174 20.095439 -0.228921
C 4.307246 22.047939 -0.149737
H 4.987084 21.844516 -0.971555
C 4.325653 23.286363 0.485944
H 5.022812 24.053348 0.162329
C 3.446761 23.543732 1.539439
H 3.459094 24.509991 2.034612
C 2.551284 22.563870 1.956824
H 1.873333 22.768188 2.781845
C -0.247948 20.567705 1.146813
C -0.765243 19.939326 0.009185
H -0.220402 19.114942 -0.447793
C -1.970646 20.371117 -0.544528
H -2.364682 19.880031 -1.429042
C -2.667039 21.425124 0.040261
H -3.607864 21.758723 -0.387127
C -2.157793 22.053654 1.178063
H -2.700603 22.875538 1.635116
C -0.952803 21.629281 1.728253
H -0.562848 22.117861 2.617780
C 1.215288 20.079267 3.593531
C 0.032067 19.664667 4.220173
H -0.842513 19.420605 3.621699
C -0.035209 19.562625 5.607695
H -0.960397 19.242496 6.078008
C 1.079765 19.864488 6.388422
H 1.027311 19.783003 7.469983
C 2.265061 20.263420 5.773434
H 3.141768 20.491303 6.372921
C 2.336014 20.363712 4.385428
H 3.272142 20.661052 3.917194
N 1.512327 16.802872 2.943537
N 3.954449 17.913067 2.455063

P	1.367261	19.966983	1.773269
F	1.082593	17.140279	-1.597975
F	3.115990	17.986324	-1.678315
F	2.098725	14.851043	-0.533235
F	2.971019	15.443688	-2.418897
F	4.095664	15.692828	-0.590375
C	2.290830	17.170759	-0.887388
C	2.863004	15.788463	-1.121431

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II_M06-2X

Cu	2.078775	18.026284	0.827295
C	-0.217597	16.627541	2.432525
H	-0.737016	16.685838	1.480538
C	-0.839175	16.051577	3.555496
H	-1.847311	15.662924	3.469357
C	-0.145878	15.996676	4.743010
H	-0.589983	15.559190	5.632798
C	1.164368	16.516451	4.806065
C	1.698120	17.073018	3.627800
C	1.955830	16.495536	6.006026
H	1.520047	16.059968	6.900315
C	3.213237	17.005045	6.019869
H	3.811731	16.988676	6.925963
C	3.787933	17.581707	4.834978
C	5.090243	18.124203	4.799138
H	5.698030	18.111709	5.699579
C	5.568791	18.658951	3.624877
H	6.564201	19.082945	3.560090
C	4.739195	18.651115	2.487982
H	5.086405	19.065772	1.545747
C	3.038645	17.620146	3.643249
N	1.008934	17.121768	2.465088
N	3.516049	18.150224	2.495331
F	0.783542	18.324381	-1.765677
F	2.277651	19.891414	-1.372526
F	2.780274	16.490414	-1.957221
F	2.958371	18.184843	-3.286487
F	4.253745	18.030325	-1.564340
C	2.000437	18.545884	-1.114873
C	2.996939	17.816570	-1.993759

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III_M06-2X

Cu	2.372953	18.190853	0.930379
C	0.076221	16.446380	2.287828
H	-0.351790	16.447574	1.288847
C	-0.607455	15.844292	3.361613
H	-1.568727	15.373267	3.190050
C	-0.030577	15.866419	4.610835
H	-0.523424	15.410503	5.465100
C	1.225612	16.485647	4.784699
C	1.824252	17.063675	3.648120
C	1.902572	16.537765	6.051772
H	1.418037	16.086637	6.912690
C	3.120572	17.125149	6.165869
H	3.637794	17.156801	7.120233
C	3.759898	17.725435	5.026501
C	5.026084	18.344236	5.095947
H	5.556862	18.368273	6.043571
C	5.566145	18.910325	3.963703
H	6.534820	19.396275	3.979241
C	4.829599	18.867916	2.766014
H	5.217630	19.323327	1.859352
C	3.111644	17.714626	3.776269
N	1.250003	17.036540	2.424973
N	3.643082	18.289109	2.672301
F	0.902084	18.328512	-1.552608
F	2.276052	20.029931	-1.332181
F	3.039526	16.667051	-1.860868
F	2.935309	18.314207	-3.255453
F	4.389909	18.350270	-1.658018
C	2.148823	18.673162	-1.014743
C	3.126271	18.005481	-1.960409
O	3.072215	21.590151	1.996440
C	2.358795	21.179597	2.854392
C	1.026096	20.561181	2.681157
Cl	2.925743	21.327664	4.572784
C	0.264295	20.049623	3.737328
C	0.552277	20.487375	1.363343
C	-0.973169	19.474006	3.472362
H	0.631711	20.097890	4.756403
C	-0.686266	19.907915	1.108450
H	1.160787	20.870008	0.550302
C	-1.448839	19.405553	2.161944
H	-1.565857	19.075508	4.289564
H	-1.046279	19.841344	0.086972
H	-2.414811	18.951156	1.961821

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OATS_M06-2X

C	1.743509	16.130541	2.324164
H	2.186005	15.744337	1.409586
C	1.231496	15.249113	3.293192
H	1.283192	14.179312	3.126477
C	0.673928	15.774273	4.435945
H	0.269236	15.130049	5.211590
C	0.619894	17.174149	4.600174
C	1.155380	17.972169	3.568658
C	0.041915	17.795578	5.760422
H	-0.357792	17.154433	6.540571
C	-0.005564	19.146038	5.875863
H	-0.443497	19.616530	6.751303
C	0.516446	19.991841	4.837746
C	0.474232	21.400327	4.907922
H	0.036085	21.877670	5.779974
C	0.986168	22.146534	3.871294
H	0.970545	23.230214	3.890677
C	1.537824	21.476743	2.764301
H	1.949681	22.033559	1.926695
C	1.093530	19.415262	3.688520
N	1.717208	17.445483	2.456427
N	1.588966	20.159340	2.676039
F	0.731300	20.491786	-0.661228
F	1.492664	18.823249	-1.862317
F	-0.644360	18.719858	0.888680
F	-1.067312	18.574845	-1.224314
F	0.154888	17.069291	-0.269749
C	1.153107	19.175625	-0.570352
C	-0.114621	18.383948	-0.297801
Cu	2.433163	19.014109	1.000876
Cl	4.740902	19.318687	1.506425
C	3.909833	19.220534	-0.578182
C	4.135942	17.850915	-1.089065
C	4.254700	16.724267	-0.272683
C	4.164448	17.734650	-2.483592
C	4.410448	15.474286	-0.859126
H	4.235881	16.830577	0.806542
C	4.323101	16.478903	-3.057884
H	4.053064	18.619536	-3.100731
C	4.443933	15.350601	-2.248551
H	4.510125	14.595820	-0.229855
H	4.347339	16.382462	-4.138292
H	4.564919	14.371447	-2.701153
O	3.955470	20.273028	-1.095493

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IV_M06-2X

C	1.598339	15.906146	2.781243
H	1.975289	15.351450	1.926433
C	1.221905	15.236203	3.957923
H	1.307144	14.157115	4.011184
C	0.752609	15.975799	5.019089
H	0.450830	15.497067	5.946440
C	0.663647	17.378702	4.903167
C	1.067561	17.959384	3.684583
C	0.184490	18.216459	5.968494
H	-0.119452	17.742089	6.896889
C	0.113711	19.562553	5.817408
H	-0.249172	20.195737	6.621735
C	0.519844	20.188181	4.588851
C	0.466543	21.583717	4.386564
H	0.103690	22.224524	5.185417
C	0.875574	22.109804	3.182666
H	0.848077	23.176508	2.991887
C	1.341030	21.234335	2.183780
H	1.673839	21.612621	1.221271
C	0.997896	19.397721	3.524925
N	1.520831	17.218755	2.646892
N	1.401818	19.926030	2.349581
F	0.398885	19.769191	-0.463122
F	0.993919	18.134871	-1.786152
F	-0.742085	18.040756	1.212897
F	-1.320186	17.665259	-0.828671
F	0.092185	16.347048	0.137644
C	0.864150	18.492606	-0.472189
C	-0.293977	17.624134	0.028217
Cu	2.328927	18.331847	1.005727
Cl	4.513965	18.315464	1.762997
C	3.055051	19.103228	-0.677372
C	3.771368	18.121821	-1.522070
C	3.525926	16.751625	-1.426510
C	4.718345	18.623956	-2.418879
C	4.235055	15.873947	-2.234696

H	2.776006	16.386919	-0.727591
C	5.427646	17.737418	-3.221855
H	4.894058	19.693475	-2.474961
C	5.186401	16.367508	-3.129373
H	4.047808	14.807339	-2.169983
H	6.168454	18.115784	-3.918539
H	5.741506	15.678665	-3.758511
O	3.045420	20.283424	-0.719456

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RETS_M06-2X

C	1.799321	15.879689	2.864060
H	2.260856	15.312171	2.060299
C	1.340292	15.234737	4.026234
H	1.447016	14.160437	4.122592
C	0.760152	15.992964	5.016978
H	0.387404	15.534765	5.928801
C	0.647669	17.389282	4.848556
C	1.144655	17.943977	3.652048
C	0.050419	18.242179	5.839249
H	-0.325755	17.786214	6.750296
C	-0.043218	19.579979	5.638335
H	-0.496909	20.226127	6.384088
C	0.458629	20.180915	4.433014
C	0.382883	21.568428	4.188042
H	-0.071884	22.216747	4.931807
C	0.886305	22.077028	3.013312
H	0.845928	23.137060	2.790462
C	1.464741	21.191846	2.085446
H	1.868778	21.556582	1.145650
C	1.054847	19.376348	3.441018
N	1.700376	17.184369	2.680879
N	1.545865	19.889075	2.289621
F	0.341686	19.929540	-0.472546
F	0.738493	18.456691	-2.040096
F	-0.490636	18.091257	1.167427
F	-1.270776	17.644149	-0.788834
F	0.357882	16.470554	-0.000350
C	0.833347	18.695881	-0.703639
C	-0.152165	17.706666	-0.060858
Cu	2.517313	18.327250	1.038666
Cl	4.810392	18.203585	1.375966
C	2.875786	19.216277	-0.899787
C	3.586395	18.244082	-1.741380
C	3.216114	16.899168	-1.780747
C	4.672891	18.719293	-2.483970
C	3.944046	16.018361	-2.569992
H	2.367363	16.549851	-1.201323
C	5.392937	17.830308	-3.271504
H	4.945741	19.768262	-2.430471
C	5.030324	16.483582	-3.311954
H	3.665985	14.970523	-2.607460
H	6.239431	18.185387	-3.849860
H	5.598108	15.791585	-3.926085
O	2.970600	20.386288	-0.780288

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V_M06-2X

Cu	2.539401	16.325305	0.685228
C	0.445571	16.746475	2.973267
H	-0.248775	16.338643	2.244756
C	-0.007992	17.191728	4.227886
H	-1.061401	17.121067	4.473697
C	0.905153	17.711645	5.116978
H	0.596043	18.069322	6.095252
C	2.265509	17.784427	4.751349
C	2.620187	17.311119	3.472614
C	3.276795	18.327870	5.616302
H	2.975647	18.686461	6.596280
C	4.572015	18.393833	5.218341
H	5.335245	18.806615	5.871464
C	4.968891	17.925091	3.918746
C	6.298748	17.996253	3.453252
H	7.069409	18.405888	4.100429
C	6.597368	17.551259	2.185771
H	7.606769	17.594403	1.793152
C	5.560414	17.036354	1.386489
H	5.760066	16.682861	0.378815
C	4.003668	17.387040	3.044739
N	1.714999	16.803348	2.608143
N	4.307917	16.953953	1.801100
Cl	1.987806	15.465641	-1.319230
O	0.512922	19.198981	1.100565
C	1.047737	20.282101	1.062110
C	0.362111	21.543225	1.433154
C	2.543056	20.301076	0.639439
C	0.882107	22.818635	1.177025
C	-0.877621	21.410455	2.075270
C	3.498982	20.654481	1.801947
F	2.762826	21.175893	-0.366778
F	2.884377	19.076229	0.207119
C	0.162050	23.944652	1.564939
H	1.828545	22.948626	0.667836
C	-1.586505	22.537389	2.463929
H	-1.264500	20.414904	2.267054
F	2.995061	20.203413	2.954058
F	3.659273	21.971161	1.900766
F	4.690466	20.096098	1.613410
C	-1.065723	23.807046	2.208005
H	0.562240	24.932159	1.360334
H	-2.542395	22.429953	2.966151
H	-1.619983	24.690445	2.509799

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VI_M06-2X

Cu	-0.966592	0.029219	0.075913
N	0.728596	1.381025	0.046044
N	0.710191	-1.338153	0.044390
C	0.720144	2.703377	0.048322
C	1.895958	3.474928	0.011014
C	3.111039	2.830533	-0.029996
C	4.377854	0.674540	-0.073370
C	4.368584	-0.681967	-0.073535
C	3.072037	-2.820416	-0.030970
C	1.848159	-3.448015	0.009296
C	0.683232	-2.660250	0.046103
C	1.917576	0.737660	0.006220
C	3.149342	1.420072	-0.032786
C	3.129937	-1.410551	-0.033279
C	1.907784	-0.711058	0.005637
H	-0.254953	3.180691	0.080774
H	1.827979	4.556664	0.014784
H	4.042215	3.389322	-0.060065
H	5.312781	1.226098	-0.104813
H	5.295893	-1.246271	-0.105070
H	3.995447	-3.391945	-0.060801
H	1.764962	-4.528667	0.012661
H	-0.298478	-3.123865	0.077541
Cl	-3.213981	0.049895	0.109398

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VII_M06-2X

Cu	11.419291	3.565924	0.990250
C	11.139366	0.588360	2.171997
H	12.225667	0.631266	2.183781
C	10.460250	-0.499705	2.750189
H	11.023843	-1.299129	3.217789
C	9.084763	-0.519037	2.704344
H	8.519779	-1.341943	3.133589
C	8.395687	0.550847	2.095937
C	9.167777	1.602924	1.560174
C	6.961331	0.603743	2.019690
H	6.393294	-0.223334	2.435723
C	6.334309	1.658687	1.442411
H	5.250675	1.699210	1.381849
C	7.087035	2.757511	0.902025
C	8.496218	2.742965	0.963071
C	6.470471	3.879573	0.310041
H	5.386663	3.920139	0.245772
C	7.251204	4.902836	-0.175924
H	6.813526	5.779150	-0.640276
C	8.649047	4.801017	-0.055312
H	9.293804	5.594486	-0.424244
C	10.599045	5.839584	3.624273
C	10.257436	6.704904	2.578656
H	10.639363	6.512810	1.577719
C	9.439737	7.808697	2.812459
H	9.183254	8.474321	1.993881
C	8.948407	8.049670	4.093562
H	8.306105	8.905505	4.277643
C	9.279157	7.188971	5.140012
H	8.896194	7.374266	6.139012
C	10.100831	6.088637	4.908777
H	10.346036	5.417369	5.727617
C	13.370778	5.028427	3.700836
C	14.399016	4.939210	2.758238
H	14.189714	4.537488	1.768000
C	15.686030	5.371031	3.082300
H	16.479513	5.300298	2.344637
C	15.947442	5.891902	4.345860
H	16.948487	6.228350	4.598577
C	14.923026	5.985001	5.290855

H	15.126832	6.392972	6.276265
C	13.639964	5.555471	4.970735
H	12.845330	5.627384	5.709664
C	11.298520	3.164858	4.460906
C	9.955579	2.803334	4.644576
H	9.169294	3.359724	4.137968
C	9.617998	1.738254	5.473463
H	8.573510	1.472422	5.608393
C	10.617422	1.011647	6.122627
H	10.353908	0.178717	6.767335
C	11.952855	1.357187	5.936528
H	12.736516	0.796022	6.436589
C	12.294113	2.427522	5.108968
H	13.340756	2.683922	4.969691
Cl	12.940208	3.738098	-0.763730
N	10.518602	1.601065	1.592515
N	9.253219	3.763090	0.497149
P	11.707923	4.438974	3.207756

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C6H5COCl_M06-2X

C	-1.424756	-0.633391	0.291260
C	-0.041923	-0.638082	0.143606
C	0.628851	0.565586	-0.088171
C	-0.084324	1.769433	-0.169062
C	-1.464048	1.765124	-0.018075
C	-2.134385	0.563499	0.211713
H	-1.948375	-1.566986	0.468942
H	0.505360	-1.571484	0.206900
H	0.452169	2.695132	-0.348669
H	-2.016872	2.696861	-0.079413
H	-3.213756	0.560393	0.329164
C	2.095093	0.671151	-0.262697
O	2.709951	1.662862	-0.490423
Cl	3.014062	-0.883851	-0.105868

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C6H5COC2F5_M06-2X

C	-1.463304	-0.586112	0.408123
C	-0.081323	-0.624612	0.252541
C	0.613435	0.548412	-0.072533
C	-0.091371	1.749616	-0.239160
C	-1.469774	1.779167	-0.088319
C	-2.157574	0.609003	0.236192
H	-1.998220	-1.495464	0.662207
H	0.435101	-1.565606	0.390215
H	0.459258	2.650857	-0.487738
H	-2.009482	2.711195	-0.221880
H	-3.236535	0.630004	0.356066
C	2.085028	0.623916	-0.244780
C	2.964645	-0.654246	-0.176822
C	3.366639	-1.043019	1.252516
F	4.108950	-0.421562	-0.842964
F	2.358868	-1.722150	-0.742237
F	2.291828	-1.358265	1.975876
F	3.988364	-0.020247	1.834110
F	4.184889	-2.090796	1.229050
O	2.683615	1.657104	-0.436628

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PPh3_M06-2X

C	2.569114	21.616683	1.246626
C	3.148032	21.638219	-0.029016
H	3.068417	20.763265	-0.670612
C	3.824021	22.767237	-0.483396
H	4.264353	22.770472	-1.476088
C	3.944094	23.885420	0.340285
H	4.478719	24.764046	-0.008249
C	3.380271	23.870318	1.614305
H	3.471876	24.738519	2.260414
C	2.693011	22.744265	2.065083
H	2.251697	22.747240	3.058076
C	-0.006849	20.388622	1.060878
C	-0.889975	19.301179	1.038010
H	-0.554983	18.328112	1.391200
C	-2.192104	19.453729	0.569588
H	-2.867205	18.603090	0.562261
C	-2.622961	20.694119	0.101393
H	-3.635761	20.813391	-0.271797
C	-1.748845	21.779026	0.110051
H	-2.079413	22.747296	-0.254432
C	-0.448492	21.629485	0.589839
H	0.221842	22.484629	0.598312
C	1.420309	20.349790	3.535824
C	2.463340	19.969812	4.390586
H	3.363951	19.522864	3.974778
C	2.359643	20.159581	5.765789
H	3.178495	19.864714	6.415343
C	1.201878	20.716980	6.306529
H	1.115428	20.858835	7.379684
C	0.154448	21.087327	5.466025
H	-0.750269	21.520654	5.882425
C	0.262846	20.908663	4.087569
H	-0.558146	21.208486	3.441983
P	1.680956	20.076270	1.731792

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III_C6F5COCl_B3LYP

Cu	2.447239	17.106318	1.198594
C	0.553584	14.785561	2.934916
H	0.181677	14.469516	1.964981
C	0.092037	14.179599	4.120946
H	-0.642996	13.382972	4.068534
C	0.585616	14.623268	5.331717
H	0.250650	14.184392	6.267669
C	1.538075	15.668329	5.356053
C	1.941604	16.207883	4.107408
C	2.089399	16.196745	6.570720
H	1.767082	15.768013	7.515467
C	2.992224	17.217531	6.542016
H	3.405025	17.619886	7.462707
C	3.417424	17.795143	5.298413
C	4.326368	18.874430	5.232565
H	4.739054	19.281762	6.151332
C	4.671960	19.400533	4.003651
H	5.363052	20.231886	3.916391
C	4.107907	18.845114	2.843619
H	4.350198	19.235222	1.861390
C	2.898269	17.293037	4.078547
N	1.446310	15.765907	2.927288
N	3.249345	17.823992	2.872938
F	1.352740	17.719295	-1.367167
F	3.133445	16.395449	-1.426174
F	-0.093116	15.678090	-0.204100
F	0.825796	15.197569	-2.118028
F	1.661372	14.384911	-0.278845
C	2.007571	16.704869	-0.638706
C	1.098876	15.488725	-0.827175
O	1.970505	20.642423	-0.365052
C	0.828597	20.299459	-0.319721
C	0.199673	19.549003	0.791806
Cl	-0.308962	20.801905	-1.644765
C	-0.754516	18.533449	0.622484
C	0.679314	19.777384	2.093037
C	-1.193561	17.771869	1.699397
C	0.209828	19.052865	3.179110
C	-0.715227	18.034628	2.977981
F	-1.231478	18.218050	-0.579024
F	-2.042099	16.758117	1.506153
F	-1.111654	17.285117	4.005349
F	0.691172	19.286275	4.405503
F	1.606850	20.708706	2.328783

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OATS_C6F5COCl_B3LYP

C	1.380419	15.814269	2.982275
H	1.722708	15.239466	2.126646
C	0.947327	15.180406	4.161978
H	0.956010	14.097291	4.223445
C	0.515864	15.957313	5.220429
H	0.171255	15.500445	6.144105
C	0.523306	17.366056	5.101102
C	0.984785	17.910393	3.877115
C	0.094095	18.250465	6.147962
H	-0.260112	17.815528	7.078368
C	0.129058	19.603871	5.982041
H	-0.197832	20.267530	6.777725
C	0.600540	20.188004	4.757531
C	0.665932	21.582895	4.537094
H	0.343119	22.263892	5.319841
C	1.142305	22.059980	3.331087
H	1.207400	23.124284	3.130884
C	1.553730	21.141443	2.346982
H	1.950356	21.473984	1.393141
C	1.029740	19.343732	3.704098
N	1.398622	17.134899	2.844141
N	1.497268	19.826680	2.525064
F	1.396958	18.747785	-1.679660
F	1.425952	16.600839	-1.142769
F	-0.825875	19.090311	-0.082308
F	-1.024452	17.606210	-1.663281
F	-0.802520	16.961836	0.404118
C	1.134787	17.869904	-0.626561
C	-0.391814	17.879571	-0.501255
Cu	1.947854	18.281244	1.111167

Cl	4.499718	18.530730	1.877768
C	3.815022	19.067361	0.099581
C	4.206274	18.085732	-0.946273
C	4.233777	16.690495	-0.779818
C	4.492487	18.575947	-2.234345
C	4.547996	15.834790	-1.826206
C	4.814781	17.726094	-3.286215
C	4.843064	16.350950	-3.083730
O	3.639343	20.245731	-0.052750
F	3.908134	16.112499	0.381740
F	4.546084	14.510773	-1.632424
F	5.145731	15.530895	-4.089607
F	5.099437	18.228554	-4.493049
F	4.483023	19.883156	-2.499755

44
IV_C6F5COCl_B3LYP

C	1.541354	15.924428	2.749115
H	1.922044	15.377096	1.893838
C	1.123812	15.260807	3.914510
H	1.181261	14.178854	3.963640
C	0.644658	16.007149	4.973946
H	0.308307	15.525965	5.888171
C	0.593028	17.415236	4.870420
C	1.043561	18.000304	3.660925
C	0.111116	18.261739	5.925726
H	-0.232490	17.793848	6.843944
C	0.083055	19.617423	5.781949
H	-0.284356	20.251822	6.583840
C	0.541367	20.241158	4.572672
C	0.542544	21.640789	4.371883
H	0.179011	22.294088	5.160508
C	1.007706	22.156491	3.177636
H	1.022043	23.225572	2.992561
C	1.474341	21.269525	2.186364
H	1.854408	21.633567	1.236516
C	1.024995	19.436190	3.510958
N	1.495006	17.247010	2.625693
N	1.483872	19.954325	2.348100
F	0.333142	19.545230	-0.498852
F	0.984020	17.707291	-1.533436
F	-0.959573	18.020748	1.370278
F	-1.505768	17.587777	-0.686472
F	-0.232982	16.199536	0.401356
C	0.742625	18.253381	-0.285653
C	-0.505419	17.505656	0.214032
Cu	2.276544	18.229471	1.001523
Cl	4.407176	18.168082	1.829771
C	3.159741	19.032321	-0.520438
C	3.878167	18.137801	-1.464341
C	3.799732	16.737353	-1.405256
C	4.681325	18.690659	-2.477970
C	4.479015	15.925858	-2.301840
C	5.371743	17.888361	-3.380177
C	5.268686	16.503735	-3.293231
O	3.115484	20.227848	-0.591561
F	3.056305	16.117804	-0.476594
F	4.379407	14.595134	-2.220714
F	5.924057	15.730211	-4.155823
F	6.132606	18.441621	-4.330182
F	4.820286	20.010144	-2.605547

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RETS_C6F5COCl_B3LYP

C	1.730797	15.893159	2.890398
H	2.184122	15.316500	2.090416
C	1.244196	15.271966	4.054657
H	1.319089	14.194842	4.158953
C	0.679273	16.053392	5.044582
H	0.293122	15.606548	5.956600
C	0.602506	17.453955	4.870272
C	1.119469	17.988665	3.664590
C	0.031326	18.339075	5.845866
H	-0.358926	17.910873	6.764850
C	-0.023061	19.683760	5.625880
H	-0.457653	20.349195	6.366576
C	0.492529	20.256846	4.414207
C	0.460289	21.643020	4.138465
H	0.027568	22.323464	4.866737
C	0.979771	22.111693	2.947874
H	0.970326	23.169011	2.704960
C	1.532728	21.194111	2.034155
H	1.948752	21.518621	1.087089
C	1.067601	19.412837	3.432043
N	1.665829	17.205914	2.701602
N	1.576964	19.888224	2.267106
F	0.329050	19.751074	-0.624433
F	0.892376	18.120999	-1.999970
F	-0.624302	18.076969	1.140582
F	-1.277435	17.509384	-0.846755
F	0.242733	16.331880	0.158226
C	0.863010	18.506740	-0.685726
C	-0.203783	17.581956	-0.034908
Cu	2.495250	18.271533	1.100536
Cl	4.694795	17.889104	1.448706
C	2.807045	19.045477	-0.691377
C	3.605612	18.199462	-1.629649
C	3.484141	16.805792	-1.712248
C	4.549470	18.802996	-2.477770
C	4.250435	16.044876	-2.581397
C	5.326291	18.053090	-3.356138
C	5.176549	16.672277	-3.411079
O	2.862165	20.251622	-0.664527
F	2.614305	16.146827	-0.932449
F	4.104339	14.715926	-2.627980
F	5.916523	15.950318	-4.251561
F	6.216505	18.658940	-4.149878
F	4.749690	20.121861	-2.476461

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V_C6F5COCl_B3LYP

Cu	3.386090	17.143327	1.218528
C	0.474278	16.937583	2.691410
H	0.138424	16.438935	1.787576
C	-0.390902	17.108194	3.790959
H	-1.409289	16.738630	3.734826
C	0.078091	17.751815	4.919883
H	-0.562077	17.907085	5.783757
C	1.407674	18.233802	4.943770
C	2.194292	18.023070	3.783934
C	1.963514	18.955138	6.053435
H	1.343854	19.109539	6.932236
C	3.230516	19.457791	5.999072
H	3.640565	20.018420	6.834131
C	4.048764	19.278679	4.832908
C	5.345699	19.826400	4.710099
H	5.765731	20.395510	5.534659
C	6.055608	19.636776	3.540636
H	7.051256	20.047224	3.410800
C	5.470219	18.897116	2.497848
H	5.999690	18.725128	1.566532
C	3.537135	18.553901	3.728458
N	1.725625	17.380158	2.686294
N	4.250509	18.369184	2.584008
Cl	3.541461	15.608992	-0.335152
O	0.425636	18.788031	-0.103033
C	1.027257	19.813433	0.129228
C	1.090541	20.434033	1.480235
C	1.645262	20.559617	-1.092442
C	2.222874	21.076859	1.999428
C	-0.031499	20.332593	2.320319
C	2.851513	19.826134	-1.725359
F	2.024731	21.823755	-0.781843
F	0.680657	20.630351	-2.046139
C	2.236640	21.614811	3.279717
C	-0.034975	20.875058	3.598535
F	2.454658	18.663602	-2.249862
F	3.795474	19.583115	-0.798022
F	3.388584	20.582922	-2.691241
C	1.103198	21.515396	4.080595
F	-1.141203	19.717494	1.908199
F	-1.106989	20.742957	4.386126
F	1.120141	21.996118	5.321532
F	3.349278	22.173341	3.766525
F	3.363086	21.124517	1.301897

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C6F5COCl_B3LYP

C	-1.424310	-0.619948	0.367407
C	-0.039028	-0.615190	0.256497
C	0.663368	0.561969	-0.042043
C	-0.081723	1.742016	-0.209375
C	-1.467695	1.743041	-0.118297
C	-2.139027	0.559317	0.175966
C	2.139292	0.651481	-0.144023
O	2.809299	1.559213	0.242243
Cl	2.927166	-0.734399	-1.021627
F	0.524353	2.891830	-0.508763
F	-2.156822	2.871407	-0.309219
F	-3.465965	0.555160	0.277175
F	-2.071079	-1.748934	0.670788
F	0.600066	-1.765071	0.480966

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C6F5COCl_B3LYP
C -1.592312 -0.518375 0.492363
C -0.208122 -0.509810 0.605789
C 0.555477 0.596502 0.209610
C -0.133916 1.712544 -0.292120
C -1.516460 1.711919 -0.427123
C -2.246791 0.594951 -0.028616
C 2.038402 0.663430 0.325553
C 2.899887 -0.552469 -0.131010
C 3.697198 -1.200633 1.026115
F 3.801946 -0.088556 -1.035143
F 2.154329 -1.511645 -0.732410
F 2.879688 -1.474750 2.056623
F 4.651090 -0.363057 1.449799
F 4.268010 -2.339512 0.613420
O 2.634100 1.655326 0.682749
F 0.531469 2.793678 -0.704256
F -2.148041 2.775583 -0.932725
F -3.573036 0.592605 -0.142879
F -2.297826 -1.579615 0.894795
F 0.377506 -1.583319 1.147401

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III_oF_B3LYP
Cu 3.021831 17.418299 0.933537
C 0.336636 16.151445 2.653777
H 0.070518 15.661024 1.722697
C -0.449593 15.986630 3.812605
H -1.337975 15.364401 3.776821
C -0.065395 16.624418 4.976005
H -0.644303 16.519951 5.889766
C 1.099437 17.426104 4.978445
C 1.814860 17.533448 3.758349
C 1.563045 18.131991 6.138345
H 1.002205 18.032757 7.063701
C 2.678786 18.913696 6.081964
H 3.025028 19.450588 6.960669
C 3.420132 19.057635 4.860834
C 4.555822 19.890486 4.750599
H 4.905310 20.436238 5.622848
C 5.200216 20.005908 3.534181
H 6.071630 20.640163 3.412312
C 4.713499 19.279625 2.434056
H 5.194419 19.342023 1.464191
C 2.994734 18.367043 3.698248
N 1.428018 16.903260 2.625436
N 3.647137 18.482677 2.508078
F 2.535116 17.160312 -1.862278
F 4.318773 16.050760 -1.141872
F 0.909737 15.413715 -0.527767
F 2.307712 14.468955 -1.902518
F 2.647913 14.343632 0.244831
C 3.026548 16.468489 -0.746527
C 2.225214 15.166472 -0.745294
O 0.900951 19.735930 -1.015373
C 0.304512 19.418575 -0.033202
C 0.456104 19.962463 1.329995
Cl -1.005187 18.118094 -0.202489
C -0.484013 19.765306 2.358394
C 1.576397 20.766260 1.618651
C -0.313924 20.355670 3.605242
H -1.351751 19.145636 2.171568
C 1.756281 21.365359 2.856374
C 0.803007 21.160233 3.852784
H -1.049669 20.186738 4.384415
H 2.647624 21.958872 3.025748
H 0.942216 21.617407 4.827490
F 2.538580 20.940811 0.696481

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OATS_oF_B3LYP
C 1.824519 16.132819 2.332484
H 2.228886 15.752905 1.399318
C 1.472969 15.257680 3.376750
H 1.609566 14.188753 3.250289
C 0.958524 15.784355 4.545648
H 0.677085 15.140008 5.374183
C 0.790950 17.182577 4.663679
C 1.173852 17.981950 3.556343
C 0.253736 17.809949 5.838586
H -0.030217 17.178892 6.676228
C 0.100761 19.163228 5.904261
H -0.307592 19.632538 6.795050
C 0.470472 20.002665 4.799694
C 0.325231 21.408617 4.814911
H -0.081824 21.894684 5.697453
C 0.700627 22.144011 3.707226
H 0.601624 23.224247 3.686199
C 1.218524 21.469341 2.585308
H 1.520102 22.012518 1.694256
C 1.006602 19.416416 3.625252
N 1.688867 17.452047 2.416917
N 1.367140 20.150728 2.544430
F 0.830011 20.415614 -1.142416
F 1.525770 18.475844 -1.950746
F -0.975228 19.063070 0.448638
F -1.134917 18.651365 -1.681952
F -0.262736 17.161858 -0.354468
C 1.061895 19.082716 -0.779879
C -0.338327 18.490894 -0.600355
Cu 2.090155 18.947097 0.879569
Cl 4.491883 19.371687 1.623858
C 4.058550 19.247370 -0.387614
C 4.258130 17.877916 -0.894258
C 4.413847 16.743453 -0.077766
C 4.235274 17.684713 -2.288142
C 4.544124 15.476936 -0.633856
H 4.423387 16.870303 0.996684
C 4.363311 16.423560 -2.855613
C 4.516085 15.315558 -2.024519
H 4.668230 14.615860 0.015138
H 4.336400 16.333831 -3.936399
H 4.614549 14.327162 -2.463306
O 4.081343 20.293943 -0.951279
F 4.083954 18.731690 -3.111669

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IV_oF_B3LYP
C 1.475889 15.894981 2.767948
H 1.851579 15.333325 1.919248
C 1.028721 15.242403 3.929001
H 1.059366 14.159374 3.980541
C 0.555026 16.001850 4.981209
H 0.196402 15.531232 5.892495
C 0.537744 17.410341 4.873122
C 1.015433 17.981745 3.666748
C 0.063889 18.268846 5.922323
H -0.300186 17.810136 6.837325
C 0.068913 19.624446 5.777083
H -0.291586 20.268412 6.574541
C 0.553580 20.235301 4.571723
C 0.588542 21.634552 4.371643
H 0.233363 22.295842 5.157455
C 1.075349 22.139357 3.181649
H 1.116197 23.207812 2.996544
C 1.529566 21.241405 2.194668
H 1.926694 21.596066 1.248546
C 1.028895 19.418199 3.514878
N 1.463517 17.216892 2.638378
N 1.508876 19.926255 2.356220
F 0.405198 19.522034 -0.544146
F 1.056871 17.666792 -1.547581
F -0.938509 18.028235 1.313768
F -1.449204 17.585794 -0.749466
F -0.215224 16.190372 0.373239
C 0.803213 18.225303 -0.308177
C -0.465688 17.500440 0.170245
Cu 2.305325 18.200188 1.009764
Cl 4.397432 18.098699 1.930579
C 3.242276 19.056351 -0.486641
C 3.931359 18.170497 -1.447890
C 3.957674 16.775584 -1.285694
C 4.564689 18.713484 -2.578825
C 4.595765 15.960442 -2.211751
H 3.476046 16.342651 -0.415041
C 5.205847 17.913165 -3.515967
C 5.219739 16.531585 -3.327764
H 4.609276 14.884788 -2.068190
H 5.679787 18.382698 -4.371519
H 5.719131 15.899609 -4.056320
O 3.194646 20.251313 -0.488723
F 4.557359 20.041631 -2.779892

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RETS_oF_B3LYP
C 1.831875 15.943400 2.781429
H 2.284189 15.388588 1.965555
C 1.379706 15.290796 3.942542
H 1.480944 14.213999 4.026645
C 0.813025 16.041722 4.954445
H 0.451933 15.570740 5.864633
C 0.701968 17.442830 4.805149
C 1.183072 18.009608 3.598768
C 0.129793 18.297032 5.807645

H	-0.232665	17.843286	6.725814	C	3.581463	17.322469	3.205457	F	2.251005	-1.624263	-0.775901
C	0.041517	19.644007	5.614699	N	1.194283	17.158074	3.044358	F	2.453292	-1.433413	2.006605
H	-0.391765	20.285640	6.376918	N	3.620197	17.267147	1.851259	F	4.256980	-0.235855	1.757509
C	0.516685	20.250099	4.402716	Cl	0.756177	17.251041	-1.000377	F	4.186745	-2.273164	0.985364
C	0.448250	21.639981	4.153176	O	2.322882	20.120690	2.620733	O	2.739552	1.719906	0.038978
H	0.021199	22.297750	4.905297	C	2.133043	20.878486	1.689960	F	0.460136	2.879031	-0.710378
C	0.925515	22.141466	2.957883	C	0.871206	21.611562	1.456092				
H	0.888269	23.202773	2.735718	C	3.307433	21.027916	0.675552	44			
C	1.468891	21.251499	2.011708	C	0.843308	22.957940	1.046350	III_pF_B3LYP			
H	1.847724	21.599277	1.056555	C	-0.354210	20.979940	1.721515	Cu	2.896952	16.719798	0.928414
C	1.085797	19.436115	3.391742	C	4.595002	21.559187	1.339976	C	0.592775	14.736854	2.558909
N	1.732850	17.256486	2.613169	F	3.014089	21.853251	-0.361813	H	0.446043	14.246299	1.601397
N	1.547540	19.943793	2.221756	F	3.583460	19.799373	0.162240	C	-0.191907	14.389543	3.677372
F	0.169618	19.756509	-0.457773	C	-0.366788	23.633577	0.918367	H	-0.953652	13.622173	3.584621
F	0.726962	18.343546	-2.048812	H	1.776694	23.476334	0.860264	C	0.028762	15.041396	4.874660
F	-0.599262	17.828498	1.125312	C	-1.569825	21.629381	1.570122	H	-0.557301	14.804488	5.758310
F	-1.255412	17.331629	-0.879208	F	5.085921	20.670699	2.211824	C	1.028940	16.037420	4.950084
F	0.438963	16.281185	-0.015370	F	4.315011	22.703052	1.994380	C	1.750651	16.324976	3.762731
C	0.772677	18.564584	-0.693904	F	5.529640	21.813490	0.414164	C	1.310502	16.772277	6.149604
C	-0.170158	17.484446	-0.098174	C	-1.570396	22.967604	1.172165	H	0.745381	16.535011	7.046728
Cu	2.477642	18.387692	1.001205	H	-0.372484	24.676467	0.617835	C	2.259896	17.750666	6.162797
Cl	4.715255	18.229735	1.426912	H	-2.488306	21.085412	1.764015	H	2.470521	18.307487	7.071614
C	2.705257	19.168391	-0.815146	H	-2.516376	23.488680	1.057876	C	2.995253	18.084343	4.975525
C	3.508532	18.246113	-1.652003	F	-0.363861	19.684645	2.092880	C	3.951651	19.123859	4.938505
C	3.228607	16.872371	-1.738166					H	4.166035	19.684984	5.844057
C	4.634936	18.728416	-2.337036	14				C	4.594298	19.416269	3.752029
C	4.031574	16.023760	-2.490876	C6H5COCl_oF_B3LYP				H	5.330811	20.209826	3.686077
H	2.371867	16.475663	-1.208557	C	-1.420516	-0.633442	0.281981	C	4.274731	18.671623	2.603999
C	5.451262	17.894425	-3.089396	C	-0.039725	-0.621194	0.130145	H	4.749158	18.880810	1.652055
C	5.144675	16.536015	-3.166884	C	0.654622	0.582803	-0.098361	C	2.741529	17.378510	3.772936
H	3.793167	14.966521	-2.550466	C	-0.105851	1.769605	-0.163182	N	1.530621	15.672863	2.597700
H	6.312142	18.319595	-3.594593	C	-1.484635	1.770645	-0.007366	N	3.377777	17.685046	2.607621
H	5.778435	15.878068	-3.754127	C	-2.142889	0.562592	0.214994	F	3.111206	17.042690	-1.887448
O	2.705444	20.372168	-0.836971	H	-1.934209	-1.573819	0.453347	F	3.889819	15.110164	-1.121370
F	4.962466	20.029761	-2.259314	H	0.513052	-1.550617	0.183523	F	0.532693	16.180132	-1.239068
				H	-2.015475	2.714983	-0.062641	F	1.653390	14.945253	-2.636180
44				H	-3.221981	0.557020	0.336606	F	1.373346	14.274635	-0.585025
V_oF_B3LYP				C	2.113777	0.668614	-0.276071	C	2.885680	16.078327	-0.891717
Cu	1.672540	17.248616	0.998129	O	2.769032	1.624979	-0.552949	C	1.611609	15.369406	-1.352417
C	-0.007295	17.111989	3.610395	Cl	3.025270	-0.938107	-0.021478	O	2.354476	20.610881	0.905913
H	-0.852323	17.037261	2.933473	F	0.496709	2.949175	-0.373360	C	1.414842	19.909077	0.664776
C	-0.196355	17.164110	5.004091					C	0.501809	19.295234	1.646725
H	-1.201636	17.123721	5.410143	20				Cl	1.001095	19.589402	-1.095069
C	0.908044	17.269964	5.827534	C6H5COC2F5_oF_B3LYP				C	-0.381955	18.246843	1.342723
H	0.798619	17.316702	6.907634	C	-1.474302	-0.551089	0.482319	C	0.580274	19.788207	2.963770
C	2.199223	17.321298	5.254890	C	-0.085919	-0.543596	0.412622	C	-1.179500	17.696043	2.340376
C	2.287061	17.258265	3.842806	C	0.618047	0.614571	0.019351	C	-0.220446	19.251395	3.962300
C	3.401272	17.443681	6.031654	C	-0.148404	1.751673	-0.305871	C	-1.079566	18.206608	3.629954
H	3.314138	17.488580	7.113700	C	-1.534699	1.753626	-0.257422	F	-1.829238	17.655911	4.604380
C	4.622837	17.511634	5.429438	C	-2.199291	0.595344	0.143627	H	-0.422301	17.836154	0.341822
H	5.528083	17.611918	6.021902	H	-1.991239	-1.451385	0.798837	H	-1.850288	16.869014	2.138177
C	4.746425	17.456638	3.999600	H	0.456185	-1.438502	0.684823	H	-0.174277	19.606498	4.985307
C	5.985087	17.540691	3.324145	H	-2.067743	2.657735	-0.532034	H	1.275346	20.587530	3.194718
H	6.901729	17.651972	3.897145	H	-3.284333	0.590337	0.189820				
C	6.011532	17.481967	1.944143	C	2.094065	0.691477	-0.022123	44			
H	6.944566	17.545494	1.394029	C	2.939676	-0.617617	-0.170498	OATS_pF_B3LYP			
C	4.799131	17.341237	1.243456	C	3.475752	-1.154046	1.175517	C	1.107663	15.947225	2.922974
H	4.782599	17.295445	0.159041	F	4.021176	-0.332751	-0.938247	H	1.397721	15.365000	2.053680

C	0.575841	15.327353	4.068669	C	0.606572	21.639277	4.361961	F	-0.595982	17.855951	1.108088
H	0.467085	14.248176	4.094032	H	0.257882	22.304647	5.147224	F	-1.224232	17.368265	-0.906521
C	0.197457	16.113591	5.140240	C	1.091270	22.138305	3.168618	F	0.441134	16.294906	-0.015760
H	-0.220057	15.668999	6.039576	H	1.136899	23.206059	2.980552	C	0.817615	18.571459	-0.691177
C	0.351891	17.516503	5.064550	C	1.536663	21.235259	2.182261	C	-0.150066	17.505596	-0.107603
C	0.899494	18.047827	3.869500	H	1.931787	21.584706	1.233246	Cu	2.476685	18.355639	1.022837
C	-0.017055	18.406400	6.129564	C	1.032435	19.418365	3.509977	Cl	4.701517	18.149954	1.484873
H	-0.435745	17.979692	7.036753	N	1.455983	17.212640	2.638823	C	2.746708	19.131952	-0.788242
C	0.153625	19.754027	6.009631	N	1.509752	19.920783	2.347830	C	3.536341	18.215619	-1.645462
H	-0.125821	20.421874	6.819816	F	0.387821	19.505735	-0.543610	C	3.290923	16.835937	-1.695200
C	0.704291	20.326102	4.813103	F	1.039078	17.649975	-1.546398	C	4.589245	18.768936	-2.392376
C	0.903284	21.714879	4.639587	F	-0.949287	18.013863	1.319605	C	4.084229	16.010366	-2.483224
H	0.632731	22.397956	5.440169	F	-1.464837	17.568124	-0.741746	C	5.391585	17.952715	-3.181900
C	1.440929	22.183137	3.456113	F	-0.227150	16.175096	0.379865	C	5.122437	16.586925	-3.210073
H	1.609572	23.242399	3.292479	C	0.787873	18.209990	-0.307312	O	2.786958	20.337953	-0.801234
C	1.775512	21.260411	2.446750	C	-0.479159	17.484586	0.175683	F	5.895503	15.790466	-3.975299
H	2.210010	21.585206	1.506197	Cu	2.293908	18.187593	1.005702	H	4.776336	19.836163	-2.341912
C	1.074440	19.477065	3.739970	Cl	4.387366	18.089780	1.920695	H	6.213085	18.352501	-3.766925
N	1.269274	17.262096	2.826430	C	3.225120	19.030718	-0.496806	H	3.912014	14.941139	-2.543373
N	1.596405	19.951944	2.581593	C	3.925735	18.146687	-1.453050	H	2.475526	16.407700	-1.124960
F	-0.155431	19.132129	-0.476001	C	3.943796	16.753405	-1.300353				
F	1.474793	18.397075	-1.774762	C	4.568297	18.744722	-2.551316	44			
F	-0.630717	16.645660	0.415523	C	4.598630	15.955760	-2.230548	V_pF_B3LYP			
F	-0.540192	16.714410	-1.757501	C	5.226650	17.956637	-3.488659	Cu	2.809836	16.262240	0.650510
F	1.106893	15.840118	-0.631531	C	5.227271	16.575905	-3.308008	C	0.552139	16.505279	3.053184
C	0.903440	18.203784	-0.518738	O	3.177685	20.227107	-0.524132	H	-0.152118	16.112058	2.325178
C	0.199164	16.849648	-0.633165	F	5.861823	15.806471	-4.213882	C	0.130605	16.867377	4.348153
Cu	1.960287	18.383606	1.123800	H	4.545820	19.823859	-2.661466	H	-0.911638	16.751372	4.627255
Cl	4.416280	18.426773	1.873174	H	5.731523	18.389302	-4.345860	C	1.061774	17.365342	5.238994
C	3.925498	19.100404	0.026712	H	3.450934	16.298335	-0.447324	H	0.774688	17.654629	6.246446
C	4.224331	18.084959	-1.001082	H	4.630669	14.875668	-2.136820	C	2.408210	17.506631	4.831863
C	4.218516	16.703678	-0.757746					C	2.728825	17.117160	3.507178
C	4.455685	18.570509	-2.300063	44				C	3.437254	18.031287	5.684135
C	4.450007	15.811178	-1.796698	RETS_pF_B3LYP				H	3.172231	18.320596	6.697400
C	4.695081	17.684941	-3.344526	C	1.801241	15.927303	2.811037	C	4.716826	18.169166	5.234261
C	4.684230	16.320457	-3.071895	H	2.251213	15.364782	1.999125	H	5.492011	18.570514	5.881100
O	3.854815	20.288452	-0.082337	C	1.348423	15.284845	3.977559	C	5.074435	17.800253	3.893425
F	4.908878	15.456903	-4.081421	H	1.446822	14.208444	4.069792	C	6.379170	17.959465	3.376287
H	4.442819	19.638878	-2.484176	C	0.784885	16.045041	4.984306	H	7.161867	18.361848	4.013549
H	4.880817	18.032189	-4.355187	H	0.423091	15.582077	5.898308	C	6.638710	17.606832	2.066260
H	4.445013	14.738498	-1.636397	C	0.678530	17.445365	4.824694	H	7.627380	17.719865	1.634477
H	4.014067	16.330094	0.238265	C	1.162479	18.001842	3.614649	C	5.593374	17.097774	1.276840
				C	0.108999	18.308762	5.820790	H	5.758358	16.817061	0.242133
44				H	-0.256317	17.862706	6.741590	C	4.084116	17.273526	3.027859
IV_pF_B3LYP				C	0.026267	19.654742	5.618705	N	1.808987	16.622402	2.646981
C	1.464498	15.891100	2.772919	H	-0.405845	20.303142	6.375850	N	4.353599	16.933197	1.737746
H	1.835803	15.325287	1.925087	C	0.507808	20.250979	4.404345	Cl	1.723213	15.435190	-1.057019
C	1.018737	15.243986	3.937549	C	0.448055	21.639708	4.146451	O	0.391871	19.364691	1.192765
H	1.045871	14.161043	3.992549	H	0.020547	22.304078	4.892481	C	0.919664	20.461823	1.175984
C	0.551044	16.008526	4.988731	C	0.934666	22.131900	2.951041	C	0.216406	21.709252	1.544434
H	0.193777	15.542139	5.902715	H	0.903988	23.192130	2.722756	C	2.430074	20.493377	0.767325
C	0.538536	17.416738	4.876106	C	1.479723	21.233864	2.013546	C	0.770810	22.999379	1.429310
C	1.013917	17.982509	3.666232	H	1.867877	21.573765	1.059346	C	-1.094789	21.566810	2.044899
C	0.072057	18.280443	5.924377	C	1.076088	19.427990	3.400169	C	3.391493	20.710287	1.969007
H	-0.290491	17.825997	6.842099	N	1.707196	17.239498	2.633372	F	2.682029	21.464910	-0.156428
C	0.082524	19.635603	5.775263	N	1.548808	19.926773	2.230838	F	2.753584	19.304316	0.210753
H	-0.272040	20.283366	6.572304	F	0.225034	19.771987	-0.470990	C	0.035473	24.117165	1.810724
C	0.565315	20.240790	4.566306	F	0.787949	18.341842	-2.045067	C	-1.835418	22.674676	2.429372

F	2.923108	20.060490	3.050102
F	3.493306	22.012685	2.273695
F	4.615709	20.244043	1.689284
C	-1.251799	23.934102	2.304608
F	-1.962017	25.014457	2.677365
H	-2.843238	22.583531	2.820049
H	-1.518662	20.572308	2.130337
H	0.442643	25.119040	1.727795
H	1.767491	23.148126	1.039429

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pF-C6H4COCl_B3LYP

C	-1.426447	-0.645052	0.294221
C	-0.044262	-0.639453	0.145669
C	0.635953	0.567352	-0.088561
C	-0.088739	1.774207	-0.169554
C	-1.468298	1.777777	-0.020561
C	-2.111025	0.563506	0.208456
C	2.094335	0.677775	-0.262512
O	2.719791	1.671095	-0.485205
Cl	3.036472	-0.911359	-0.114729
F	-3.448272	0.559200	0.352832
H	0.440521	2.703377	-0.349342
H	-2.046907	2.693353	-0.078094
H	-1.974974	-1.563207	0.474005
H	0.498744	-1.574285	0.210949

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pF-C6H4COC2F5_B3LYP

C	-1.465038	-0.597323	0.408937
C	-0.084800	-0.627722	0.240227
C	0.619670	0.548502	-0.084879
C	-0.094684	1.755025	-0.238759
C	-1.471535	1.795213	-0.078464
C	-2.132077	0.611694	0.243898
C	2.084655	0.624154	-0.269478
C	2.974043	-0.658676	-0.179998
C	3.363741	-1.045326	1.265237
F	4.131929	-0.426645	-0.843281
F	2.373355	-1.740530	-0.755653
F	2.276341	-1.389461	1.976716
F	3.955436	-0.002769	1.866542
F	4.212145	-2.082080	1.259333
O	2.683628	1.662092	-0.488590
F	-3.468036	0.640567	0.402854
H	0.449725	2.659740	-0.485988
H	-2.035903	2.714081	-0.196301
H	-2.025267	-1.491078	0.661562
H	0.427401	-1.570194	0.370769

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III_oCl_B3LYP

Cu	2.938383	17.401298	1.022534
C	0.361919	16.025291	2.734965
H	0.127889	15.513032	1.807055
C	-0.440667	15.856814	3.881947
H	-1.308632	15.206749	3.840765
C	-0.098938	16.526581	5.040781
H	-0.692436	16.420341	5.944949
C	1.041052	17.363512	5.050768
C	1.776903	17.469116	3.843511
C	1.463592	18.104320	6.205220
H	0.886696	18.009721	7.121104
C	2.563759	18.908626	6.156973
H	2.880726	19.467519	7.033032
C	3.328700	19.045056	4.949173
C	4.458005	19.887691	4.847870
H	4.784434	20.451548	5.717511
C	5.127237	19.986412	3.643457
H	5.997129	20.624224	3.529318
C	4.665308	19.242934	2.543643
H	5.161304	19.298950	1.581344
C	2.936019	18.330612	3.789920
N	1.432173	16.807655	2.714724
N	3.601962	18.441880	2.608039
F	2.269362	17.319730	-1.736070
F	4.205590	16.347218	-1.251045
F	0.940919	15.287118	-0.457610
F	2.309643	14.632872	-2.017026
F	2.840955	14.356532	0.076651
C	2.913482	16.588152	-0.727419
C	2.251904	15.211340	-0.794588
O	0.556154	19.823586	-1.192322
C	0.191221	19.440385	-0.125856
C	0.524598	20.002488	1.206128
Cl	-0.973124	17.999365	-0.089095
C	-0.312130	19.781996	2.316037
C	1.651697	20.841477	1.385062
C	-0.060092	20.377506	3.546014
H	-1.176938	19.140988	2.204665
C	1.908590	21.431748	2.621351
C	1.051965	21.205863	3.697884
H	-0.725885	20.188765	4.381374
H	2.788011	22.053924	2.740847
H	1.265900	21.670164	4.655529
Cl	2.821506	21.152406	0.117680

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OATS_oCl_B3LYP

C	1.137814	15.946470	2.902762
H	1.425760	15.374788	2.025721
C	0.617324	15.311494	4.045360
H	0.516723	14.231336	4.060696
C	0.239058	16.084306	5.126760
H	-0.170047	15.627720	6.023934
C	0.381500	17.489112	5.063533
C	0.918972	18.036001	3.870992
C	0.009225	18.366307	6.137835
H	-0.401428	17.927870	7.043112
C	0.166261	19.716495	6.028480
H	-0.116104	20.374697	6.845515
C	0.704998	20.304133	4.833991
C	0.886244	21.696471	4.669839
H	0.612371	22.370323	5.477103
C	1.409996	22.179815	3.486259
H	1.564175	23.242226	3.329024
C	1.748416	21.269037	2.467448
H	2.170713	21.606818	1.526132
C	1.078508	19.467806	3.752203
N	1.289908	17.263476	2.818566
N	1.586591	19.957299	2.593563
F	-0.143506	19.187971	-0.516205
F	1.491966	18.420899	-1.790389
F	-0.657087	16.705839	0.390452
F	-0.566936	16.778286	-1.782839
F	1.066923	15.876102	-0.659780
C	0.899958	18.242354	-0.540950
C	0.175037	16.899527	-0.658729
Cu	1.931208	18.409731	1.116825
Cl	4.444514	18.493808	1.844458
C	3.904217	19.172153	0.006700
C	4.215221	18.160451	-1.030500
C	4.153775	16.786043	-0.741269
C	4.511547	18.547207	-2.356619
C	4.378055	15.827732	-1.718763
H	3.899955	16.480244	0.265884
C	4.746335	17.583374	-3.339017
C	4.675919	16.228483	-3.023464
H	4.313993	14.774332	-1.465520
H	4.978619	17.901097	-4.349658
H	4.852534	15.490429	-3.800220
O	3.787621	20.355153	-0.067914
Cl	4.617354	20.222062	-2.867617

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IV_oCl_B3LYP

C	1.488295	15.897316	2.761447
H	1.871972	15.341257	1.912659
C	1.033960	15.237519	3.915550
H	1.067307	14.154335	3.961764
C	0.549545	15.990159	4.967819
H	0.184822	15.513770	5.873663
C	0.528883	17.399100	4.866947
C	1.015032	17.978168	3.667648
C	0.043005	18.250731	5.916223
H	-0.327508	17.786253	6.825714
C	0.044140	19.607003	5.777345
H	-0.325935	20.245919	6.574465
C	0.537307	20.225422	4.579304
C	0.568171	21.625707	4.386163
H	0.202870	22.281780	5.171709
C	1.063858	22.138016	3.203109
H	1.101793	23.207448	3.023169
C	1.531509	21.246705	2.216412
H	1.936329	21.608001	1.276218
C	1.025658	19.415342	3.523010
N	1.473140	17.219900	2.638946
N	1.514925	19.930625	2.371375
F	0.435201	19.542065	-0.539917
F	1.088289	17.687177	-1.542977
F	-0.923197	18.046378	1.307261
F	-1.423458	17.610857	-0.759966
F	-0.199011	16.209419	0.365651
C	0.827811	18.243724	-0.304519

C	-0.445465	17.520534	0.164961
Cu	2.322527	18.211370	1.021154
Cl	4.412420	18.095146	1.946738
C	3.269449	19.078137	-0.465350
C	3.947908	18.210105	-1.462412
C	3.990068	16.820547	-1.256770
C	4.541000	18.724482	-2.637024
C	4.603382	15.968484	-2.164929
H	3.539286	16.414118	-0.358116
C	5.155639	17.870932	-3.554564
C	5.188350	16.497653	-3.317699
H	4.624816	14.899935	-1.975941
H	5.605288	18.286256	-4.450064
H	5.670643	15.844803	-4.039291
O	3.229285	20.271575	-0.426489
Cl	4.540024	20.434063	-3.034434

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RETS_oCl_B3LYP

C	1.863864	15.951570	2.795552
H	2.340346	15.404748	1.988071
C	1.384414	15.288304	3.939534
H	1.488556	14.211403	4.018556
C	0.786751	16.029132	4.940996
H	0.403157	15.549728	5.837494
C	0.672484	17.430731	4.798734
C	1.182234	18.008368	3.609463
C	0.067885	18.274628	5.790810
H	-0.317027	17.812553	6.695600
C	-0.022668	19.622337	5.604164
H	-0.480276	20.256549	6.358327
C	0.481285	20.239092	4.409282
C	0.411496	21.630266	4.167511
H	-0.038312	22.280477	4.912896
C	0.916306	22.142263	2.988182
H	0.879229	23.204833	2.772197
C	1.487281	21.261643	2.049523
H	1.886188	21.618456	1.106115
C	1.081420	19.435374	3.408114
N	1.761899	17.265258	2.633798
N	1.568327	19.952829	2.252327
F	0.203829	19.762684	-0.458054
F	0.774951	18.349062	-2.043639
F	-0.565165	17.842409	1.126005
F	-1.210376	17.333811	-0.879479
F	0.480484	16.290673	-0.000637
C	0.812396	18.573102	-0.690275
C	-0.129459	17.492373	-0.093575
Cu	2.519056	18.408189	1.034800
Cl	4.752969	18.231674	1.432887
C	2.743453	19.195079	-0.788755
C	3.552499	18.292488	-1.655227
C	3.279306	16.913804	-1.662048
C	4.626606	18.755181	-2.444197
C	4.030465	16.023641	-2.417050
H	2.458975	16.543764	-1.061084
C	5.389180	17.863477	-3.200758
C	5.092503	16.501679	-3.187785
H	3.790415	14.965172	-2.403243
H	6.213983	18.240907	-3.795738
H	5.693468	15.819456	-3.781778
O	2.725689	20.397874	-0.780158
Cl	5.091219	20.446344	-2.526348

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V_oCl_B3LYP

Cu	2.818511	16.324638	0.766550
C	0.385327	16.238389	3.046993
H	-0.222270	15.775030	2.274263
C	-0.139416	16.478572	4.333575
H	-1.162790	16.197083	4.558992
C	0.667368	17.074967	5.283281
H	0.297682	17.278033	6.284761
C	1.992568	17.434440	4.944372
C	2.424646	17.147855	3.624658
C	2.890191	18.077898	5.860568
H	2.539920	18.287819	6.867514
C	4.150806	18.426950	5.475983
H	4.826086	18.920439	6.169339
C	4.620243	18.158433	4.145981
C	5.908879	18.527855	3.699162
H	6.587582	19.031123	4.382337
C	6.284357	18.247570	2.400187
H	7.263381	18.521560	2.021875
C	5.373609	17.593396	1.552794
H	5.634204	17.356834	0.526941
C	3.765010	17.509070	3.221403
N	1.625081	16.558454	2.704089
N	4.151802	17.233460	1.944996
Cl	2.015917	15.231810	-0.951949
O	0.300020	19.189867	0.653699
C	0.891608	20.246214	0.650287
C	0.414153	21.475793	1.343251
C	2.267260	20.302083	-0.096684
C	0.503583	22.729436	0.709716
C	-0.174742	21.417733	2.624407
C	3.435640	20.733377	0.825516
F	2.220154	21.166220	-1.152504
F	2.557763	19.075664	-0.579499
C	-0.002876	23.876882	1.312810
H	0.953403	22.799522	-0.272278
C	-0.659862	22.569528	3.240538
F	3.287677	20.152353	2.032172
F	3.441564	22.062682	0.993863
F	4.614863	20.360758	0.313072
C	-0.583848	23.795970	2.578660
H	-1.092053	22.505156	4.233366
H	-0.974275	24.686577	3.062182
H	0.061337	24.829176	0.795971
Cl	-0.250461	19.919479	3.540385

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C6H5COCl_oCl_B3LYP

C	-1.416819	-0.635700	0.217343
C	-0.035549	-0.609705	0.065938
C	0.654812	0.602144	-0.115788
C	-0.092204	1.802397	-0.124582
C	-1.474467	1.777226	0.051553
C	-2.135579	0.560220	0.214041
H	-1.927080	-1.585353	0.341935
H	0.520874	-1.539336	0.067728
H	-2.027772	2.709904	0.062777
H	-3.213806	0.554165	0.342943
C	2.116428	0.608363	-0.354672
O	2.755703	1.375632	-1.002255
Cl	3.026067	-0.767930	0.497980
Cl	0.657668	3.381973	-0.287775

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C6H5COC2F5_oCl_B3LYP

C	-1.471801	-0.518050	0.542078
C	-0.082188	-0.476861	0.519556
C	0.609793	0.667925	0.077561
C	-0.154029	1.771563	-0.360650
C	-1.546252	1.723804	-0.363237
C	-2.203933	0.582189	0.095818
H	-1.978204	-1.407682	0.902839
H	0.474770	-1.334217	0.874031
H	-2.110374	2.577483	-0.723169
H	-3.289708	0.558290	0.097980
C	2.092884	0.711946	0.154073
C	2.916123	-0.580979	-0.159282
C	3.529698	-1.230116	1.102099
F	3.947300	-0.227952	-0.969112
F	2.182427	-1.529455	-0.800089
F	2.560438	-1.484395	2.004527
F	4.424452	-0.408169	1.660273
F	4.132499	-2.384411	0.790175
O	2.748938	1.693140	0.434710
Cl	0.590458	3.235343	-0.991482

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III_pCl_B3LYP

Cu	2.858839	16.812012	0.862473
C	0.781838	14.672300	2.517772
H	0.630328	14.193837	1.554980
C	0.085885	14.231987	3.661733
H	-0.609278	13.402411	3.583694
C	0.305281	14.874083	4.864551
H	-0.215250	14.566793	5.767081
C	1.213428	15.955780	4.919727
C	1.859585	16.322880	3.712161
C	1.481643	16.691867	6.121622
H	0.968841	16.398046	7.033165
C	2.353110	17.740504	6.119522
H	2.553404	18.297266	7.030650
C	3.022839	18.143300	4.915027
C	3.911627	19.240718	4.864103
H	4.121526	19.801049	5.771209
C	4.497026	19.587636	3.662617
H	5.182424	20.424815	3.586418
C	4.186186	18.841250	2.512986
H	4.615407	19.092508	1.549919
C	2.774404	17.441627	3.709319

N	1.641450	15.681781	2.539864	C	4.216450	18.084325	-0.996492	Cl 6.085543 15.566974 -4.480137
N	3.350673	17.802905	2.529234	C	4.214396	16.706199	-0.746163	
F	2.919758	17.224182	-1.953763	C	4.446035	18.560660	-2.296911	44
F	3.874645	15.337338	-1.281462	C	4.445402	15.806879	-1.780250	RETS_pCl_B3LYP
F	0.443937	16.146551	-1.189557	C	4.685435	17.668909	-3.337335	C 1.797714 15.926876 2.813383
F	1.575030	15.060577	-2.697782	C	4.679509	16.299831	-3.066431	H 2.247153 15.363627 2.001716
F	1.468412	14.291599	-0.664981	O	3.850759	20.294407	-0.092741	C 1.345243 15.285650 3.980672
C	2.814716	16.221572	-0.976214	H	4.431916	19.627449	-2.490094	H 1.443240 14.209297 4.073701
C	1.575322	15.430505	-1.396962	H	4.867184	18.031055	-4.343280	C 0.782827 16.046912 4.987259
O	2.133438	20.628400	0.932566	H	4.437984	14.738967	-1.592461	H 0.421592 15.584803 5.901903
C	1.211271	19.893588	0.726728	H	4.012822	16.335375	0.251590	C 0.677056 17.447184 4.826765
C	0.366373	19.239195	1.747900	Cl	4.973012	15.165347	-4.377145	C 1.160247 18.002487 3.615957
Cl	0.713623	19.582682	-1.007731					C 0.109257 18.311775 5.822808
C	-0.475023	18.149258	1.481593	44				H -0.255478 17.866690 6.744292
C	0.454356	19.753341	3.053702	IV_pCl_B3LYP				C 0.027656 19.657720 5.619956
C	-1.236541	17.589080	2.503538	C	1.460752	15.891751	2.767737	H -0.402926 20.307053 6.377159
C	-0.312120	19.209234	4.076598	H	1.829362	15.326162	1.918638	C 0.508525 20.252698 4.404722
C	-1.154532	18.132751	3.786186	C	1.017941	15.244403	3.933282	C 0.450271 21.641348 4.146014
H	-0.517760	17.716937	0.489540	H	1.044608	14.161429	3.987587	H 0.024415 22.306742 4.892061
H	-1.878012	16.737916	2.306482	C	0.553848	16.008664	4.986261	C 0.936332 22.132218 2.949847
H	-0.254196	19.607609	5.082968	H	0.199074	15.541940	5.901030	H 0.906868 23.192342 2.720970
H	1.120911	20.583490	3.259058	C	0.541991	17.416959	4.874605	C 1.479293 21.232978 2.012326
Cl	-2.132371	17.446240	5.072190	C	1.013926	17.983228	3.663675	H 1.867063 21.572045 1.057696
				C	0.079862	18.280343	5.925049	C 1.074760 19.428422 3.400518
44				H	-0.280099	17.825560	6.843607	N 1.704012 17.239038 2.634915
OATS_pCl_B3LYP				C	0.091520	19.635615	5.777044	N 1.546893 19.925914 2.230343
C	1.115517	15.949181	2.914688	H	-0.259489	20.283145	6.575832	F 0.224956 19.768617 -0.472971
H	1.406505	15.369230	2.044200	C	0.570999	20.241215	4.566998	F 0.794967 18.337990 -2.043975
C	0.583951	15.326218	4.058786	C	0.613720	21.639827	4.363758	F -0.598975 17.852329 1.105540
H	0.476478	14.246872	4.081675	H	0.268768	22.305012	5.150812	F -1.221820 17.363702 -0.910737
C	0.203946	16.109624	5.131873	C	1.095183	22.139196	3.169253	F 0.442416 16.292036 -0.015525
H	-0.213577	15.662465	6.029919	H	1.141939	23.207037	2.982024	C 0.817917 18.568383 -0.690440
C	0.356553	17.512928	5.059406	C	1.535742	21.236432	2.180510	C -0.150216 17.501790 -0.108978
C	0.904089	18.047542	3.865896	H	1.928162	21.586310	1.230537	Cu 2.472367 18.351803 1.024731
C	-0.014313	18.400164	6.125968	C	1.033342	19.419078	3.508413	Cl 4.695725 18.141752 1.477027
H	-0.433078	17.971010	7.031957	N	1.452468	17.213472	2.634497	C 2.746878 19.128172 -0.779886
C	0.154574	19.748285	6.008918	N	1.507354	19.921824	2.345001	C 3.539393 18.212339 -1.641598
H	-0.126385	20.414051	6.820276	F	0.376389	19.505446	-0.541294	C 3.295326 16.834458 -1.697479
C	0.705117	20.323602	4.813872	F	1.032722	17.654313	-1.548997	C 4.589148 18.767860 -2.387411
C	0.902158	21.713002	4.642952	F	-0.956444	18.005959	1.318347	C 4.087699 16.012069 -2.491061
H	0.630278	22.394223	5.444657	F	-1.471657	17.562867	-0.743771	C 5.391604 17.955486 -3.182108
C	1.439508	22.184310	3.460539	F	-0.229459	16.171133	0.374573	C 5.130110 16.584356 -3.223478
H	1.606599	23.244121	3.298987	C	0.778752	18.210382	-0.309013	O 2.787665 20.333950 -0.799141
C	1.775663	21.264116	2.449425	C	-0.485840	17.480066	0.173205	H 4.777744 19.834772 -2.334583
H	2.209712	21.591347	1.509491	Cu	2.285065	18.188556	1.003281	H 6.207182 18.378394 -3.758663
C	1.076930	19.477215	3.739340	Cl	4.381857	18.096032	1.909928	H 3.899927 14.945138 -2.541925
N	1.275481	17.264552	2.821274	C	3.212081	19.030968	-0.497901	H 2.481559 16.400945 -1.128597
N	1.598372	19.955120	2.581925	C	3.919105	18.145357	-1.454119	Cl 6.137659 15.550243 -4.228237
F	-0.155862	19.139922	-0.477418	C	3.937995	16.753972	-1.301915	
F	1.475210	18.412631	-1.778950	C	4.567198	18.742324	-2.546929	44
F	-0.626196	16.649751	0.406150	C	4.600553	15.955822	-2.227517	V_pCl_B3LYP
F	-0.536916	16.725383	-1.766790	C	5.234367	17.954639	-3.479650	Cu 2.797836 16.197912 0.704150
F	1.112385	15.850807	-0.644202	C	5.242625	16.568859	-3.306605	C 0.513844 16.567691 3.068477
C	0.903882	18.213612	-0.524464	O	3.164911	20.226858	-0.533741	H -0.188603 16.160532 2.346458
C	0.202503	16.858147	-0.642598	H	4.545527	19.821243	-2.659983	C 0.082705 16.987151 4.342853
Cu	1.956048	18.391908	1.120692	H	5.739044	18.407068	-4.326326	H -0.965088 16.901633 4.612009
Cl	4.423661	18.449914	1.864962	H	3.440508	16.296301	-0.452827	C 1.011884 17.500753 5.226865
C	3.921926	19.107067	0.030738	H	4.620899	14.877479	-2.115230	H 0.717485 17.833531 6.218678

C	2.366050	17.600658	4.833152
C	2.695942	17.155366	3.528382
C	3.393833	18.138816	5.678509
H	3.121375	18.470876	6.676591
C	4.681052	18.237660	5.240264
H	5.455220	18.649692	5.881542
C	5.048247	17.812169	3.918916
C	6.361559	17.930417	3.412567
H	7.143138	18.344019	4.044020
C	6.630971	17.524997	2.119977
H	7.626505	17.606179	1.696926
C	5.586971	17.003352	1.337041
H	5.759801	16.681749	0.315615
C	4.059577	17.269958	3.060961
N	1.777655	16.645865	2.674991
N	4.339099	16.876357	1.787996
Cl	1.698550	15.359902	-0.989380
O	0.407265	19.326317	1.198425
C	0.942444	20.418174	1.161780
C	0.248283	21.674557	1.528313
C	2.447413	20.439239	0.733464
C	0.792216	22.960702	1.359394
C	-1.039378	21.542004	2.083498
C	3.423565	20.694722	1.916394
F	2.682274	21.382979	-0.222759
F	2.764977	19.234495	0.209812
C	0.068458	24.086995	1.741820
C	-1.768030	22.657779	2.471198
F	2.958796	20.092814	3.026674
F	3.540500	22.006914	2.167636
F	4.639709	20.204591	1.644248
C	-1.201580	23.923826	2.295457
H	-2.756812	22.552216	2.904104
H	-1.458160	20.549871	2.212154
H	0.487178	25.078376	1.608616
H	1.771937	23.103894	0.926161
Cl	-2.111168	25.343171	2.786660

14
pCl-C6H4COCl_B3LYP

C	-1.428533	-0.643351	0.294374
C	-0.045214	-0.637688	0.145612
C	0.634873	0.566753	-0.088338
C	-0.088776	1.771570	-0.168755
C	-1.469251	1.775421	-0.019715
C	-2.124877	0.563359	0.209954
C	2.096659	0.676086	-0.263076
O	2.717413	1.671831	-0.486969
Cl	3.036348	-0.907964	-0.114167
H	0.438095	2.702250	-0.348154
H	-2.029041	2.702130	-0.080226
H	-1.957494	-1.572803	0.473781
H	0.495070	-1.574203	0.211279
Cl	-3.870955	0.559567	0.396518

20
pCl-C6H4COC2F5_B3LYP

C	-1.466473	-0.594895	0.410313
C	-0.085204	-0.624754	0.241643
C	0.618350	0.549119	-0.084248
C	-0.095870	1.752905	-0.240349
C	-1.473670	1.792756	-0.080653
C	-2.146017	0.611770	0.245047
C	2.086581	0.624801	-0.267143
C	2.975411	-0.658069	-0.180080
C	3.364579	-1.047489	1.264782
F	4.132633	-0.424706	-0.843262
F	2.372269	-1.737009	-0.757731
F	2.276141	-1.390349	1.975227
F	3.957836	-0.006570	1.867086
F	4.210795	-2.085575	1.256896
O	2.682374	1.664127	-0.483039
H	0.445521	2.659224	-0.488772
H	-2.020010	2.721346	-0.204589
H	-2.006961	-1.499826	0.665173
H	0.425055	-1.568091	0.374235
Cl	-3.889923	0.649442	0.453086

47
III_oMe_B3LYP

Cu	2.399116	16.752468	0.725251
C	0.490483	15.084724	3.002026
H	0.014188	14.618317	2.145112
C	0.043999	14.820548	4.313274
H	-0.784878	14.138527	4.472681
C	0.676981	15.441773	5.371688
H	0.362530	15.263748	6.396592
C	1.753154	16.323330	5.118375
C	2.120908	16.525075	3.763313
C	2.469106	17.006523	6.157649
H	2.169774	16.839887	7.188730
C	3.502392	17.845306	5.860504
H	4.043788	18.360056	6.649170
C	3.900244	18.076439	4.499998
C	4.959039	18.943527	4.149179
H	5.506255	19.461909	4.931694
C	5.280918	19.121078	2.818439
H	6.086618	19.779761	2.513094
C	4.535116	18.441651	1.840736
H	4.748042	18.568761	0.785494
C	3.207706	17.424953	3.449195
N	1.493495	15.908704	2.734093
N	3.525862	17.622933	2.139221
F	0.828589	17.108054	-1.625222
F	2.718746	15.993063	-1.972572
F	-0.176455	14.989649	-0.235046
F	0.532491	14.489736	-2.231209
F	1.690789	13.888597	-0.488493
C	1.717702	16.205202	-1.001877
C	0.939253	14.889179	-1.004208
O	2.155588	20.672171	2.991779
C	1.569054	20.199813	2.064532
C	0.405019	19.298451	2.071880
Cl	2.194874	20.688302	0.367406
C	-0.045267	18.681923	0.889852
C	-0.233014	19.014840	3.314190

C	-1.122009	17.803297	0.907025
C	-1.321373	18.135491	3.293704
C	-1.766092	17.535496	2.114281
H	0.462843	18.865621	-0.045686
H	-1.425124	17.313899	-0.011215
H	-1.823578	17.909129	4.230016
C	0.203206	19.598509	4.633083
H	1.223694	19.295690	4.884293
H	0.197751	20.693737	4.615062
H	-0.462852	19.260707	5.432558
H	-2.607721	16.848692	2.144891

47
OATS_oMe_B3LYP

C	1.885110	16.201702	2.211806
H	2.312430	15.896633	1.261545
C	1.544064	15.247404	3.189117
H	1.707723	14.193343	2.990046
C	1.008779	15.679179	4.387072
H	0.738482	14.972988	5.167436
C	0.804186	17.061508	4.598262
C	1.173892	17.943202	3.550395
C	0.244291	17.593885	5.808700
H	-0.026004	16.900530	6.600339
C	0.052451	18.934869	5.963668
H	-0.372463	19.331536	6.881538
C	0.400866	19.855957	4.918809
C	0.210118	21.252333	5.024844
H	-0.216374	21.666436	5.934496
C	0.565965	22.070501	3.969835
H	0.431757	23.146042	4.018512
C	1.109782	21.487563	2.810182
H	1.397672	22.096292	1.958008
C	0.960035	19.363990	3.711935
N	1.717323	17.507753	2.385345
N	1.301227	20.179526	2.684216
F	1.407379	20.317082	-1.570446
F	1.329413	18.101716	-1.562697
F	-0.702212	20.395504	0.165763
F	-1.073196	19.263566	-1.655426
F	-0.770194	18.214244	0.227346
C	1.157029	19.220296	-0.734053
C	-0.357117	19.273972	-0.506925
Cu	2.128956	19.167167	0.968127
Cl	4.470880	19.581183	1.778598
C	4.140977	19.399216	-0.295175
C	4.354904	18.019628	-0.772876
C	4.574404	16.950261	0.112034
C	4.295583	17.794255	-2.176309
C	4.751024	15.657838	-0.365560
C	4.473056	16.477702	-2.621687
C	4.697501	15.420349	-1.741101
O	4.189380	20.447467	-0.848857
H	4.429282	16.282978	-3.689831
H	4.925997	14.844246	0.331974
H	4.599242	17.140374	1.176323
C	4.042393	18.884354	-3.184664
H	3.113024	19.415981	-2.965313

H 4.846246 19.628691 -3.180801
H 3.973632 18.459965 -4.190537
H 4.829144 14.413990 -2.129028

47
IV_oMe_B3LYP
C 1.440667 15.901695 2.816624
H 1.814694 15.335051 1.970417
C 0.988092 15.255331 3.979246
H 1.012747 14.172309 4.034602
C 0.517073 16.020941 5.028143
H 0.154605 15.555557 5.940621
C 0.507457 17.429125 4.914820
C 0.990130 17.993475 3.707005
C 0.036067 18.293835 5.960055
H -0.331703 17.840347 6.876209
C 0.047628 19.648814 5.809702
H -0.311270 20.297458 6.604117
C 0.537031 20.252786 4.602773
C 0.578003 21.651087 4.397497
H 0.224128 22.316843 5.180140
C 1.068700 22.149339 3.206334
H 1.113974 23.216949 3.017199
C 1.520925 21.245541 2.223756
H 1.921198 21.594803 1.276930
C 1.010696 19.429532 3.549731
N 1.436100 17.223048 2.682237
N 1.494758 19.931165 2.390100
F 0.403100 19.525476 -0.518797
F 1.038843 17.660878 -1.514884
F -0.955306 18.052272 1.342991
F -1.466613 17.602925 -0.718511
F -0.246582 16.203135 0.413917
C 0.791915 18.225263 -0.276201
C -0.484300 17.514488 0.202944
Cu 2.290876 18.194479 1.045004
Cl 4.378665 18.084896 1.979661
C 3.242832 19.038250 -0.458859
C 3.927733 18.160802 -1.433447
C 3.933051 16.771306 -1.231521
C 4.553945 18.725995 -2.575775
C 4.553787 15.921409 -2.137130
C 5.169674 17.843346 -3.473750
C 5.174603 16.464318 -3.265353
O 3.191358 20.233828 -0.435715
H 5.655535 18.252292 -4.355588
H 4.554133 14.849065 -1.966664
H 3.453397 16.361130 -0.348985
H 5.663216 15.813542 -3.985564
C 4.582183 20.205852 -2.857617
H 3.570807 20.622491 -2.920443
H 5.098131 20.755101 -2.062382
H 5.095982 20.403664 -3.803259

47
RETS_oMe_B3LYP
C 1.812935 15.946425 2.810511
H 2.265090 15.391715 1.994295
C 1.363437 15.293416 3.972554
H 1.466268 14.216768 4.056931
C 0.797358 16.044025 4.984984
H 0.438086 15.573029 5.895906
C 0.684364 17.444936 4.835183
C 1.164694 18.012169 3.628552
C 0.110341 18.298169 5.837455
H -0.251393 17.843885 6.755669
C 0.018483 19.644758 5.643797
H -0.417397 20.285546 6.405274
C 0.493719 20.251663 4.432248
C 0.420895 21.641212 4.182359
H -0.010790 22.297504 4.933147
C 0.899461 22.144092 2.988169
H 0.858225 23.205161 2.765391
C 1.449492 21.255828 2.044252
H 1.830184 21.604525 1.090249
C 1.067317 19.439173 3.422374
N 1.713389 17.259435 2.642185
N 1.531971 19.948348 2.254244
F 0.170983 19.797546 -0.432438
F 0.693655 18.379945 -2.030477
F -0.621708 17.881630 1.150955
F -1.303417 17.412887 -0.851397
F 0.369622 16.316580 -0.004798
C 0.755294 18.595651 -0.674712
C -0.208295 17.534883 -0.077512
Cu 2.468516 18.394087 1.031724
Cl 4.706794 18.235951 1.464772
C 2.696749 19.172477 -0.803596
C 3.491424 18.254939 -1.656101
C 3.171293 16.888233 -1.692789
C 4.596523 18.752591 -2.393556
C 3.914788 15.998944 -2.458083
C 5.328939 17.832898 -3.155554
C 5.000812 16.477359 -3.194631
O 2.703399 20.377473 -0.793182
H 6.180839 18.192632 -3.726580
H 3.650401 14.945941 -2.479659
H 2.329592 16.524253 -1.117772
C 5.022042 20.198016 -2.371575
H 4.238020 20.857270 -2.758747
H 5.237092 20.530344 -1.349904
H 5.922172 20.337391 -2.977987
H 5.594854 15.796542 -3.798336

47
V_oMe_B3LYP
Cu 2.944942 16.858698 1.013299
C 0.620802 15.914483 3.261448
H 0.256808 15.237030 2.493284
C -0.008364 15.986327 4.520700
H -0.869343 15.359911 4.729970
C 0.492306 16.858925 5.467241
H 0.036965 16.940276 6.450600
C 1.615477 17.658653 5.153511
C 2.166592 17.521871 3.853563
C 2.202017 18.584437 6.079341
H 1.765966 18.671913 7.070574
C 3.279127 19.340251 5.723381
H 3.719803 20.043494 6.424239
C 3.856422 19.236903 4.413292
C 4.962419 20.014514 4.003327
H 5.403312 20.723499 4.698358
C 5.464188 19.862552 2.726192
H 6.310745 20.443195 2.376074
C 4.856020 18.937877 1.860749
H 5.218694 18.797623 0.850078
C 3.302364 18.332417 3.473752
N 1.670185 16.657939 2.936855
N 3.805102 18.197505 2.214002
Cl 2.591070 15.484386 -0.647427
O 0.748526 19.355410 0.107809
C 1.337427 20.378694 0.408900
C 1.395750 20.951488 1.769884
C 2.023441 21.104087 -0.804674
C 2.355163 21.930897 2.101592
C 0.486758 20.492444 2.769009
C 3.476424 20.654819 -1.090406
F 2.030762 22.460806 -0.672272
F 1.311798 20.803566 -1.918401
C 2.435379 22.455552 3.386469
C 0.583332 21.053954 4.046846
F 3.552154 19.314856 -1.120796
F 4.316123 21.103746 -0.137681
F 3.887980 21.136502 -2.269324
C 1.540382 22.018257 4.362472
H -0.106510 20.717624 4.815453
H 3.190301 23.200307 3.619486
H 3.056118 22.283989 1.360103
H 1.587075 22.421656 5.370207
C -0.578257 19.453844 2.521581
H -1.217291 19.721475 1.673081
H -0.140013 18.482885 2.279653
H -1.207433 19.342520 3.410049

17
oMe-C6H4COCl_B3LYP
C -1.414909 -0.568418 0.244228
C -0.032147 -0.609420 0.121889
C 0.710034 0.565890 -0.099664
C 0.046420 1.823376 -0.194027
C -1.347158 1.829023 -0.056758
C -2.074346 0.658643 0.155845
C 2.175662 0.529091 -0.255452
O 2.911799 1.402097 -0.601334
Cl 2.988322 -1.110475 0.159933
H -1.871650 2.778477 -0.119870
H -1.971169 -1.486125 0.408761
H 0.477742 -1.561850 0.190350
C 0.755927 3.133358 -0.422980
H 1.539420 3.307665 0.321826
H 1.247439 3.157803 -1.401253
H 0.042061 3.960606 -0.374851
H -3.155503 0.706885 0.253255

23
oMe-C6H4COC2F5_B3LYP
C -1.425416 -0.473910 0.433242
C -0.036777 -0.490126 0.383487
C 0.692212 0.662785 0.023923
C -0.001112 1.863076 -0.301866
C -1.399961 1.839287 -0.264681
C -2.109834 0.695609 0.100953
C 2.170329 0.649161 0.027311
C 2.960966 -0.693856 -0.141387
C 3.458863 -1.280589 1.198461
F 4.065955 -0.436764 -0.888211
F 2.247776 -1.661103 -0.781863
F 2.420542 -1.504019 2.026998
F 4.297807 -0.422683 1.792535
F 4.096722 -2.441482 0.995644
O 2.878874 1.634435 0.138129
H -1.943973 2.743282 -0.525475
H -1.967018 -1.368872 0.724509
H 0.478665 -1.402852 0.647828
H -3.196016 0.719839 0.124761
C 0.689433 3.145703 -0.694783
H 1.194966 3.602663 0.162221
H 1.459812 2.982505 -1.455265
H -0.039467 3.861245 -1.087710

47
III_pMe_B3LYP
Cu 2.924750 16.973012 0.833516
C 0.523096 14.737395 1.651487
H 0.536666 14.454018 0.603210
C -0.295248 14.059770 2.578057
H -0.926279 13.243070 2.242896
C -0.273179 14.453605 3.902165
H -0.889661 13.954985 4.645363
C 0.560282 15.525671 4.296006
C 1.338582 16.145364 3.285861
C 0.629636 16.014211 5.643723
H 0.029668 15.522297 6.404413
C 1.421316 17.077532 5.962788
H 1.465034 17.450041 6.982134
C 2.210778 17.739248 4.962581
C 3.017159 18.864464 5.243594
H 3.058198 19.252540 6.257654
C 3.735216 19.458532 4.224013
H 4.358885 20.327834 4.402807
C 3.658889 18.915357 2.929896
H 4.218752 19.346383 2.106927
C 2.181688 17.268861 3.626264
N 1.310997 15.748202 1.992574
N 2.910863 17.852045 2.635152
F 3.316933 17.278312 -1.972320
F 4.941245 16.159691 -0.951065
F 1.606024 15.162767 -1.501029
F 3.423883 14.667352 -2.591620
F 3.217038 14.080808 -0.504581
C 3.549119 16.396957 -0.903354
C 2.955023 15.074042 -1.388777
O 1.119617 19.895917 -0.307461
C 0.317463 19.150527 0.174760
C -0.147116 19.133789 1.571935
Cl -0.467463 17.897782 -0.936137
C -1.060631 18.206376 2.094110
C 0.391814 20.122431 2.419290
C -1.426692 18.271795 3.435047
C 0.018085 20.176141 3.753822
C -0.899497 19.253685 4.286047
H -1.473317 17.428114 1.464066
H -2.127064 17.541632 3.830236
H 0.447378 20.937124 4.399722
H 1.104667 20.834766 2.018983
C -1.314317 19.333478 5.731390
H -1.699649 18.375282 6.092927
H -0.477274 19.634426 6.370554
H -2.107735 20.082068 5.861961

47
OATS_pMe_B3LYP
C 1.163301 15.960506 2.971380
H 1.472400 15.376304 2.109958
C 0.631943 15.340865 4.117459
H 0.543394 14.260059 4.151711
C 0.228376 16.129379 5.178110
H -0.189791 15.685078 6.077294
C 0.357614 17.534208 5.091251
C 0.907684 18.064917 3.896965
C -0.039714 18.426633 6.143907
H -0.459917 18.000403 7.050651
C 0.105628 19.776166 6.012656
H -0.196223 20.446090 6.813053
C 0.658154 20.347700 4.816683
C 0.830350 21.738557 4.631585
H 0.535666 22.423699 5.421846
C 1.372205 22.206309 3.449808
H 1.520172 23.267266 3.277256
C 1.737971 21.280807 2.453893
H 2.176548 21.605386 1.515017
C 1.057386 19.496126 3.756022
N 1.301777 17.277096 2.864590
N 1.583759 19.970323 2.599372
F -0.156913 19.114416 -0.440226
F 1.469983 18.374129 -1.740815
F -0.610048 16.637258 0.484735
F -0.532738 16.679432 -1.689381
F 1.125809 15.828707 -0.562706
C 0.909677 18.193122 -0.477925
C 0.213001 16.833406 -0.571089
Cu 1.980879 18.398189 1.153365
Cl 4.430824 18.466781 1.896305
C 3.936981 19.125558 0.030493
C 4.238728 18.100330 -0.982764
C 4.242563 16.720971 -0.726974
C 4.459003 18.565252 -2.289110
C 4.465891 15.826783 -1.764251
C 4.690577 17.657601 -3.318192
C 4.692499 16.276373 -3.077511
O 3.853912 20.311529 -0.080376
H 4.440208 19.631113 -2.489666
H 4.862092 18.026784 -4.325883
H 4.456611 14.759111 -1.560060
H 4.047658 16.357534 0.275131
C 4.929872 15.285816 -4.188067
H 4.975994 15.776429 -5.165126
H 5.873506 14.745461 -4.036266
H 4.132492 14.533259 -4.218377

47
IV_pMe_B3LYP
C 1.444909 15.904795 2.812294
H 1.815044 15.333806 1.967356
C 0.995835 15.264562 3.979582
H 1.019092 14.181782 4.039715
C 0.529865 16.035656 5.026702
H 0.170058 15.574933 5.942581
C 0.522461 17.443369 4.907303
C 1.000813 18.001653 3.695042
C 0.057889 18.313593 5.951039
H -0.307072 17.864719 6.870567
C 0.073025 19.667982 5.795561
H -0.280145 20.320654 6.589236
C 0.558832 20.265812 4.584143
C 0.604789 21.663189 4.373341
H 0.257711 22.333375 5.155228
C 1.091847 22.155110 3.178012
H 1.141132 23.221853 2.985076
C 1.534604 21.245891 2.196090
H 1.931234 21.589444 1.245501
C 1.023999 19.436865 3.531923
N 1.441184 17.225583 2.671746
N 1.503263 19.932357 2.367699
F 0.372828 19.507815 -0.519409
F 1.014605 17.646892 -1.519013
F -0.963096 18.027080 1.351761
F -1.485272 17.574083 -0.706252
F -0.248890 16.182186 0.418087
C 0.771237 18.211101 -0.280020
C -0.496777 17.491801 0.208769
Cu 2.281969 18.189216 1.028256
Cl 4.374915 18.092655 1.946554
C 3.212938 19.023668 -0.483917
C 3.904220 18.131480 -1.436552
C 3.928613 16.741402 -1.275820
C 4.532938 18.715172 -2.550951
C 4.575724 15.944222 -2.213871
C 5.175238 17.909330 -3.482468
C 5.209001 16.512200 -3.330520
O 3.165724 20.219930 -0.511810
H 4.506919 19.793311 -2.674258
H 5.658208 18.365148 -4.343429
H 4.590721 14.865645 -2.081840
H 3.445954 16.291274 -0.413661
C 5.923845 15.654023 -4.342617
H 5.630369 15.920517 -5.364970
H 7.010438 15.796710 -4.274519

H 5.715044 14.590544 -4.190240
47
RETS_pMe_B3LYP
C 1.785439 15.926664 2.822822
H 2.226339 15.362918 2.006633
C 1.353747 15.287309 3.999027
H 1.460235 14.212027 4.095338
C 0.800006 16.049272 5.009882
H 0.453552 15.588835 5.931100
C 0.683799 17.448178 4.845197
C 1.152261 18.002462 3.627899
C 0.118538 18.312120 5.843307
H -0.235685 17.867525 6.769152
C 0.024255 19.656508 5.636139
H -0.407202 20.304956 6.393660
C 0.494888 20.251362 4.416871
C 0.424436 21.638754 4.154711
H -0.007232 22.302320 4.899086
C 0.906092 22.130537 2.957158
H 0.866659 23.189689 2.725054
C 1.458248 21.233497 2.022823
H 1.844878 21.573274 1.068050
C 1.063726 19.428677 3.412531
N 1.684316 17.237876 2.641334
N 1.534073 19.927210 2.242520
F 0.246274 19.858680 -0.444206
F 0.757620 18.422681 -2.030097
F -0.625323 17.952577 1.126352
F -1.281956 17.517212 -0.890318
F 0.347658 16.372204 -0.025389
C 0.803621 18.642556 -0.673561
C -0.197941 17.604498 -0.096602
Cu 2.456844 18.343083 1.024594
Cl 4.680705 18.126267 1.504156
C 2.739337 19.141635 -0.779661
C 3.504121 18.209727 -1.639147
C 3.224719 16.839319 -1.706934
C 4.579387 18.734909 -2.375606
C 4.011132 16.006295 -2.497256
C 5.358128 17.894729 -3.160369
C 5.090932 16.516101 -3.233349
O 2.814958 20.346180 -0.775040
H 4.796532 19.796443 -2.316342
H 6.190394 18.307946 -3.725285
H 3.784418 14.944444 -2.545264
H 2.391596 16.426970 -1.149527
C 5.951762 15.620593 -4.086898
H 5.926497 15.935819 -5.137774
H 7.000137 15.664427 -3.765700
H 5.624902 14.577297 -4.037297
47
V_pMe_B3LYP
Cu 2.740658 16.092044 0.718814
C 0.592347 16.361161 3.242530
H -0.142989 15.940414 2.562038
C 0.231198 16.753507 4.547089
H -0.794494 16.634301 4.880771
C 1.198938 17.286433 5.376134
H 0.958404 17.599833 6.388523
C 2.521794 17.430887 4.898626
C 2.780897 17.009093 3.570285
C 3.585463 17.987952 5.685121
H 3.367073 18.302643 6.701912
C 4.840126 18.124733 5.169741
H 5.641630 18.550805 5.766705
C 5.135869 17.721709 3.823726
C 6.413138 17.875993 3.240505
H 7.222028 18.302212 3.827529
C 6.612935 17.488889 1.929883
H 7.578597 17.597564 1.447801
C 5.535634 16.950363 1.205805
H 5.654024 16.642428 0.172493
C 4.109437 17.164285 3.021241
N 1.825284 16.480987 2.770490
N 4.320378 16.789669 1.729505
Cl 1.574179 15.239055 -0.923244
O 0.277079 19.422281 1.693639
C 0.844807 20.477135 1.470311
C 0.235632 21.799939 1.715652
C 2.310027 20.362454 0.932980
C 0.846176 23.030334 1.411486
C -1.044525 21.808345 2.309694
C 3.382850 20.616112 2.023408
F 2.549243 21.219227 -0.100745
F 2.508717 19.104092 0.475118
C 0.191554 24.225856 1.698586
C -1.685351 23.004197 2.591010
F 3.010907 20.022557 3.171520
F 3.532086 21.929029 2.256495
F 4.568073 20.115758 1.647490
C -1.077891 24.237979 2.291611
H -1.517602 20.861204 2.547332
H -2.669957 22.992595 3.052026
H 0.677333 25.167278 1.455964
H 1.823361 23.071061 0.951442
C -1.787486 25.529040 2.604892
H -2.736650 25.594873 2.057834
H -2.030016 25.592551 3.673077
H -1.180794 26.400286 2.339980
17
pMe-C6H4COCl_B3LYP
C -1.409339 -0.583487 0.259591
C -0.026777 -0.628924 0.134740
C 0.695964 0.555184 -0.089212
C 0.003322 1.777290 -0.181731
C -1.379532 1.807954 -0.052196
C -2.110398 0.631035 0.170797
C 2.157783 0.624175 -0.240115
O 2.820215 1.593840 -0.459739
Cl 3.053603 -0.996154 -0.062211
H 0.558425 2.693233 -0.354310
H -1.902237 2.757893 -0.124543
H -1.959161 -1.505589 0.429894
H 0.487181 -1.579893 0.208150
C -3.609599 0.655770 0.311000
H -4.082433 0.009970 -0.439278
H -3.916884 0.279476 1.294922
H -4.010341 1.666862 0.192785
23
pMe-C6H4COC2F5_B3LYP
C -1.436129 -0.547869 0.290350
C -0.051493 -0.602175 0.157885
C 0.682189 0.574144 -0.084497
C -0.015796 1.795352 -0.189590
C -1.395032 1.835958 -0.061170
C -2.132485 0.663712 0.183936
C 2.150815 0.635287 -0.228869
C 3.018507 -0.664391 -0.167994
C 3.348728 -1.125779 1.269600
F 4.204721 -0.421205 -0.776144
F 2.426173 -1.709749 -0.815889
F 2.231580 -1.481805 1.926290
F 3.937945 -0.125018 1.940961
F 4.178587 -2.177908 1.243886
O 2.773271 1.671177 -0.388714
H 0.545572 2.704899 -0.375812
H -1.916374 2.785847 -0.150297
H -1.987344 -1.465617 0.477799
H 0.440781 -1.560381 0.248345
C -3.628127 0.723310 0.345740
H -4.083941 -0.268249 0.263364
H -3.893677 1.132992 1.329565
H -4.082048 1.378194 -0.406814
47
III_mCF3_B3LYP
Cu 2.667062 18.089105 0.765862
C 0.030435 16.340007 2.004229
H -0.321275 16.274448 0.977895
C -0.769651 15.893916 3.075009
H -1.750981 15.475166 2.877907
C -0.285842 16.012217 4.363367
H -0.878826 15.692461 5.215338
C 0.992634 16.574557 4.577858
C 1.715928 16.996556 3.433670
C 1.563798 16.750765 5.882894
H 0.985364 16.436514 6.746952
C 2.802684 17.298311 6.036088
H 3.235497 17.425105 7.024399
C 3.566553 17.732965 4.899635
C 4.847352 18.317954 5.015487
H 5.294574 18.434132 5.998717
C 5.509131 18.741183 3.879659
H 6.491453 19.197561 3.933316
C 4.878288 18.600873 2.632214
H 5.351559 18.951372 1.721951
C 3.018120 17.603992 3.599805
N 1.232640 16.872707 2.175590
N 3.669184 18.056528 2.491292
F 0.672252 18.057369 -1.194605
F 1.936813 19.876222 -1.315231

F	2.796461	16.542801	-2.057284
F	2.231260	18.177631	-3.381121
F	4.043281	18.331362	-2.184067
C	2.000759	18.503328	-0.997438
C	2.762492	17.892502	-2.169016
O	3.479506	21.529081	2.360233
C	2.671031	21.246196	3.192986
C	1.334855	20.661040	2.965747
Cl	3.098986	21.583445	4.957566
C	0.491603	20.220925	3.993064
C	0.944389	20.509634	1.621565
C	-0.736121	19.647459	3.670021
H	0.790390	20.304065	5.030426
C	-0.288066	19.940413	1.313843
H	1.608435	20.824055	0.826505
C	-1.133430	19.509824	2.335581
H	-0.561484	19.793158	0.275388
H	-2.087993	19.051685	2.100468
C	-1.652311	19.216216	4.781406
F	-2.529830	18.267968	4.383072
F	-2.384523	20.252282	5.257945
F	-0.967528	18.712545	5.836824

47
OATS_mCF3_B3LYP

C	1.495936	16.234823	1.917514
H	1.706710	15.922887	0.902250
C	1.271910	15.282149	2.928877
H	1.343006	14.226107	2.691075
C	0.973983	15.722173	4.203832
H	0.797466	15.018644	5.012987
C	0.887073	17.110588	4.458046
C	1.144857	17.989160	3.374413
C	0.553982	17.653502	5.744924
H	0.367577	16.963776	6.563489
C	0.467657	19.000618	5.937703
H	0.211367	19.405265	6.912882
C	0.708649	19.918912	4.860210
C	0.620372	21.322009	5.007714
H	0.359236	21.742617	5.975019
C	0.865625	22.138306	3.920595
H	0.804538	23.218584	3.999431
C	1.202505	21.547674	2.688462
H	1.408094	22.155832	1.812460
C	1.051719	19.417638	3.579203
N	1.462043	17.543556	2.134115
N	1.294810	20.232991	2.521564
F	0.018951	20.268192	-0.864109
F	1.691214	19.576055	-2.133917
F	-0.587710	17.709048	-0.221735
F	-0.450529	18.032241	-2.369115
F	1.132109	16.953500	-1.334099
C	1.028594	19.294715	-0.941171
C	0.270715	17.995512	-1.225367
Cu	2.013419	19.239567	0.754194
Cl	4.356898	19.424436	1.623149
C	4.025997	19.346308	-0.402834
C	4.142494	17.964574	-0.925634
C	4.147872	16.823398	-0.116913
C	4.175915	17.838396	-2.324366
C	4.177504	15.565939	-0.710501
H	4.113237	16.918927	0.959129
C	4.211928	16.572265	-2.904375
H	4.160368	18.728733	-2.941448
C	4.205672	15.430803	-2.103363
H	4.239296	16.475719	-3.985171
H	4.225475	14.443432	-2.553456
O	4.188241	20.380092	-0.971222
C	4.085776	14.335421	0.147757
F	4.444490	14.568298	1.428809
F	4.858851	13.329974	-0.317789
F	2.811498	13.853286	0.184966

47
IV_mCF3_B3LYP

C	1.511291	15.898238	2.771969
H	1.889656	15.336761	1.924395
C	1.076649	15.246851	3.938367
H	1.119638	14.164539	3.994825
C	0.599438	16.006097	4.989186
H	0.250079	15.535784	5.904202
C	0.567033	17.413930	4.875297
C	1.033444	17.984832	3.664617
C	0.089631	18.272681	5.922761
H	-0.266219	17.814596	6.841274
C	0.081544	19.627729	5.771925
H	-0.281564	20.271640	6.568217
C	0.556221	20.238018	4.562304
C	0.579433	21.636632	4.355948
H	0.221520	22.298543	5.139964
C	1.058806	22.140419	3.162384
H	1.090602	23.208406	2.972932
C	1.517222	21.242140	2.177737
H	1.908861	21.595671	1.228771
C	1.034248	19.420477	3.507266
N	1.483560	17.219592	2.637096
N	1.506812	19.927629	2.345122
F	0.380730	19.508547	-0.529912
F	1.051652	17.667442	-1.545393
F	-0.936525	17.990302	1.325791
F	-1.449015	17.544804	-0.736516
F	-0.189716	16.165389	0.378337
C	0.794257	18.216466	-0.303163
C	-0.461603	17.471286	0.179320
Cu	2.301090	18.203916	1.008372
Cl	4.403725	18.123620	1.903254
C	3.223984	19.047502	-0.493010
C	3.931086	18.156045	-1.448982
C	3.928270	16.768366	-1.287876
C	4.592099	18.740458	-2.539912
C	4.587362	15.969401	-2.215760
H	3.425988	16.321522	-0.437593
C	5.252342	17.931391	-3.463089
H	4.583976	19.819710	-2.652423
C	5.250253	16.545078	-3.306173
H	5.769193	18.380639	-4.305422
H	5.763867	15.911620	-4.022231
O	3.177734	20.242678	-0.537577
C	4.529894	14.473229	-2.083909
F	3.513934	13.946691	-2.812374
F	4.333561	14.080206	-0.804253
F	5.664973	13.881707	-2.519920

47
RETS_mCF3_B3LYP

C	1.831938	15.934183	2.774222
H	2.282049	15.380070	1.956611
C	1.375834	15.280274	3.933065
H	1.471788	14.202754	4.013498
C	0.812095	16.030464	4.947231
H	0.448271	15.557892	5.855486
C	0.707468	17.432689	4.803019
C	1.191378	18.001066	3.598830
C	0.139118	18.286660	5.807976
H	-0.225953	17.831868	6.724565
C	0.057535	19.634750	5.619366
H	-0.372741	20.276048	6.383545
C	0.535749	20.242394	4.409329
C	0.474895	21.633370	4.163670
H	0.051505	22.291302	4.917701
C	0.954774	22.136039	2.969802
H	0.923210	23.198230	2.751055
C	1.492957	21.246097	2.020721
H	1.873511	21.594398	1.066302
C	1.100399	19.428501	3.395967
N	1.738304	17.248443	2.611147
N	1.564172	19.937423	2.227259
F	0.192194	19.765433	-0.454246
F	0.761212	18.348360	-2.038707
F	-0.587613	17.831078	1.125411
F	-1.232677	17.346313	-0.885217
F	0.455075	16.287944	-0.018255
C	0.795151	18.573066	-0.684478
C	-0.152353	17.491550	-0.097036
Cu	2.482797	18.377415	1.005973
Cl	4.715813	18.193568	1.413566
C	2.720655	19.155540	-0.801497
C	3.510031	18.233978	-1.664603
C	3.273569	16.857939	-1.674253
C	4.549316	18.774786	-2.435582
C	4.080332	16.026111	-2.445122
H	2.472519	16.435797	-1.081735
C	5.349322	17.934629	-3.206643
H	4.728420	19.844465	-2.412378
C	5.120249	16.557081	-3.214069
H	6.158666	18.350606	-3.798705
H	5.747291	15.899581	-3.806682
O	2.749317	20.360418	-0.835610
C	3.781850	14.553686	-2.468714
F	2.775306	14.256675	-3.328086
F	3.390288	14.102882	-1.251730
F	4.850057	13.818957	-2.847144

47
V_mCF3_B3LYP
Cu 2.725354 16.229148 0.727647
C 0.521862 16.176192 3.200446
H -0.158712 15.728066 2.481307
C 0.100446 16.465712 4.513881
H -0.916849 16.238011 4.815319
C 0.999915 17.036368 5.393203
H 0.712434 17.272616 6.414280
C 2.314866 17.320145 4.957556
C 2.637934 16.994201 3.616029
C 3.310797 17.919027 5.800048
H 3.044960 18.158612 6.826022
C 4.560786 18.185853 5.325437
H 5.310936 18.642561 5.965064
C 4.917968 17.883956 3.967743
C 6.187177 18.182849 3.424490
H 6.943476 18.643357 4.054276
C 6.443833 17.894359 2.098482
H 7.404041 18.117278 1.645717
C 5.432633 17.305130 1.320143
H 5.596447 17.070536 0.273916
C 3.959943 17.287654 3.110545
N 1.748377 16.429648 2.765888
N 4.227391 17.007819 1.805260
Cl 1.656934 15.387200 -0.988076
O 0.470753 19.411108 1.595728
C 0.908716 20.477503 1.208607
C 0.211104 21.768575 1.431795
C 2.287037 20.427770 0.471550
C 0.703134 23.014225 1.008764
C -1.016419 21.709109 2.119376
C 3.482524 20.766830 1.397168
F 2.330534 21.272616 -0.596899
F 2.486675 19.172016 0.010636
C -0.027928 24.169417 1.278325
H 1.641677 23.102063 0.482387
C -1.737773 22.868087 2.380920
H -1.388095 20.743518 2.444846
F 3.342358 20.127254 2.570890
F 3.535149 22.086488 1.638338
F 4.637159 20.388496 0.835677
C -1.246486 24.105102 1.959473
H -2.681858 22.812867 2.913530
H -1.802536 25.014608 2.162861
C 0.464667 25.496968 0.769277
F -0.074522 25.798621 -0.437106
F 0.136997 26.509630 1.603885
F 1.807290 25.518692 0.613925

17
C6H5COCl_mCF3_B3LYP
C -1.417277 -0.630226 0.305487
C -0.027657 -0.628124 0.219877
C 0.641413 0.573201 -0.046522
C -0.091314 1.760922 -0.225056
C -1.479585 1.744120 -0.137840
C -2.147963 0.548636 0.126405
H 0.522462 -1.548882 0.364604
H 0.436031 2.686383 -0.428605
H -2.042075 2.662329 -0.273279
H -3.230710 0.529969 0.199430
C 2.112509 0.690610 -0.156462
O 2.730477 1.685167 -0.390648
Cl 3.056534 -0.873028 0.095988
C -2.152358 -1.922326 0.538942
F -3.246583 -1.741761 1.313603
F -2.585717 -2.466672 -0.624377
F -1.378194 -2.850827 1.141801

23
C6H5COC2F5_mCF3_B3LYP
C -1.459204 -0.583052 0.390480
C -0.078837 -0.628164 0.206825
C 0.619413 0.552610 -0.092674
C -0.090867 1.763078 -0.205440
C -1.468376 1.795098 -0.024492
C -2.159793 0.620462 0.276720
H 0.428950 -1.576720 0.299088
H 0.455385 2.671184 -0.436337
H -2.007474 2.732489 -0.118032
H -3.235586 0.637168 0.417960
C 2.088616 0.623457 -0.294791
C 2.976338 -0.660724 -0.209449
C 3.347486 -1.065573 1.236370
F 4.140673 -0.421479 -0.856363
F 2.377293 -1.731958 -0.805529
F 2.251781 -1.424654 1.926810
F 3.924441 -0.027145 1.858959
F 4.201366 -2.096771 1.227340
O 2.680593 1.661556 -0.520343
C -2.195505 -1.837688 0.774023
F -2.281398 -1.974884 2.120378
F -1.584161 -2.950017 0.308031
F -3.462475 -1.843921 0.301460

48
III_pOMe_B3LYP
Cu 2.842414 17.085866 0.851855
C 0.344350 14.850083 1.308116
H 0.462215 14.627054 0.251958
C -0.612215 14.173128 2.092075
H -1.246395 13.419609 1.636446
C -0.718601 14.486384 3.433657
H -1.443504 13.985089 4.069483
C 0.124494 15.477548 3.986364
C 1.045725 16.105094 3.110504
C 0.068513 15.881951 5.362497
H -0.640237 15.385942 6.020049
C 0.879148 16.871920 5.834912
H 0.826779 17.182961 6.874198
C 1.817074 17.535215 4.973915
C 2.655402 18.582225 5.416578
H 2.603611 18.908282 6.451574
C 3.525821 19.178764 4.525292
H 4.182919 19.986183 4.829984
C 3.557431 18.724842 3.195484
H 4.230664 19.166082 2.468493
C 1.907898 17.150411 3.613452
N 1.143373 15.786606 1.799783
N 2.774731 17.743556 2.747318
F 2.556064 17.020815 -1.965295
F 4.648633 17.389709 -1.323235
F 2.702852 14.470157 -1.005267
F 4.264560 14.987330 -2.429972
F 4.743943 14.816618 -0.313325
C 3.465923 16.718364 -0.940173
C 3.799894 15.247114 -1.185183
O 0.767848 19.556530 -0.847253
C 0.030042 18.884158 -0.188698
C -0.277087 19.034743 1.237097
Cl -0.871102 17.503155 -1.048176
C -1.243549 18.289920 1.929206
C 0.458052 20.018187 1.937942
C -1.486221 18.516092 3.279170
C 0.230645 20.241963 3.281166
C -0.745747 19.492076 3.967065
H -1.812398 17.523484 1.417077
H -2.236925 17.924633 3.787460
H 0.797526 20.985840 3.830581
H 1.211386 20.593045 1.410539
O -0.889521 19.779121 5.276933
C -1.917939 19.114111 6.019026
H -1.753468 18.031794 6.042964
H -1.854371 19.513191 7.032871
H -2.908174 19.332171 5.601870

48
OATS_pOMe_B3LYP
C 1.103176 15.961791 2.979939
H 1.401276 15.371398 2.118838
C 0.567900 15.352125 4.129577
H 0.464504 14.272718 4.166918
C 0.179811 16.148718 5.189966
H -0.240431 15.712499 6.092157
C 0.328029 17.551364 5.098987
C 0.880393 18.071632 3.901021
C -0.051850 18.451485 6.151520
H -0.473751 18.033219 7.061180
C 0.112229 19.798506 6.016701
H -0.176123 20.474338 6.817120
C 0.667793 20.359583 4.817226
C 0.860131 21.747382 4.629316
H 0.578964 22.438040 5.419695
C 1.404827 22.204945 3.444876
H 1.568482 23.263243 3.270094
C 1.753506 21.272206 2.449490
H 2.194469 21.588766 1.509003
C 1.050457 19.500282 3.756543
N 1.259475 17.275938 2.869199
N 1.580267 19.964449 2.597461
F -0.148369 19.107588 -0.452017
F 1.491436 18.365791 -1.736580
F -0.619542 16.630314 0.460933

F	-0.515623	16.676175	-1.711916	C	3.913600	18.117915	-1.425258	H	4.785654	19.780487	-2.334480
F	1.126407	15.818179	-0.566672	C	3.934373	16.726976	-1.268123	H	6.188377	18.267939	-3.733047
C	0.916949	18.183535	-0.479077	C	4.549381	18.696281	-2.543744	H	3.759932	14.919040	-2.513466
C	0.217013	16.826587	-0.584242	C	4.572915	15.913070	-2.195224	H	2.380841	16.416700	-1.148423
Cu	1.978730	18.380357	1.159483	C	5.186271	17.895718	-3.474089	O	5.898420	15.771811	-3.995392
Cl	4.402586	18.402166	1.935911	C	5.202991	16.496084	-3.309732	C	5.705153	14.356606	-4.067235
C	3.954934	19.086924	0.042318	O	3.181972	20.204818	-0.498096	H	4.720018	14.107668	-4.480006
C	4.257453	18.065744	-0.962112	H	4.531611	19.774311	-2.668394	H	6.481905	13.985614	-4.738394
C	4.239456	16.687096	-0.714635	H	5.678770	18.324391	-4.341277	H	5.822193	13.889054	-3.082050
C	4.492702	18.529115	-2.273621	H	4.577614	14.839988	-2.048511				
C	4.458148	15.777725	-1.741057	H	3.451694	16.278815	-0.405075	48			
C	4.720732	17.630851	-3.299365	O	5.845825	15.802980	-4.273217	V_pOMe_B3LYP			
C	4.700051	16.245679	-3.045499	C	5.897935	14.376178	-4.176909	Cu	2.665399	16.309854	0.743540
O	3.891362	20.274770	-0.053303	H	6.456144	14.041512	-5.053032	C	0.605720	15.782771	3.306163
H	4.489978	19.595167	-2.473497	H	6.421200	14.056975	-3.267572	H	-0.076229	15.357037	2.574592
H	4.908034	17.972928	-4.312207	H	4.892213	13.939580	-4.198507	C	0.245636	15.870353	4.666206
H	4.431652	14.716981	-1.523610					H	-0.724656	15.508844	4.990963
H	4.031864	16.323540	0.284737	48				C	1.144155	16.418628	5.560436
O	4.921816	15.451369	-4.113780	RETS_pOMe_B3LYP				H	0.903463	16.501915	6.616983
C	4.860636	14.032453	-3.940462	C	1.756561	15.919381	2.822311	C	2.396178	16.881419	5.093829
H	3.871895	13.717130	-3.585917	H	2.187684	15.350332	2.004551	C	2.660537	16.750621	3.706808
H	5.043041	13.606211	-4.928550	C	1.326017	15.285370	4.001884	C	3.385429	17.469083	5.951620
H	5.632767	13.681141	-3.245419	H	1.423415	14.209295	4.099197	H	3.164180	17.557776	7.011729
				C	0.785468	16.053687	5.015037	C	4.574258	17.909349	5.450058
48				H	0.440825	15.597860	5.939226	H	5.319764	18.355943	6.102030
IV_pOMe_B3LYP				C	0.680427	17.453225	4.848672	C	4.872222	17.802536	4.049457
C	1.430394	15.899318	2.828343	C	1.145822	18.001446	3.627312	C	6.081234	18.268581	3.485914
H	1.800838	15.323019	1.987118	C	0.129699	18.323539	5.849372	H	6.831305	18.721575	4.128484
C	0.973340	15.265663	3.996178	H	-0.221960	17.883467	6.778354	C	6.288494	18.146693	2.126375
H	0.990776	14.182998	4.060561	C	0.046259	19.668460	5.641112	H	7.200942	18.500028	1.658252
C	0.507024	16.043114	5.038413	H	-0.373636	20.321887	6.400876	C	5.288404	17.557460	1.333739
H	0.141067	15.587852	5.954600	C	0.513351	20.257323	4.417592	H	5.415022	17.450090	0.262001
C	0.507306	17.450333	4.913389	C	0.453740	21.644987	4.154282	C	3.919072	17.223489	3.174902
C	0.993412	18.001429	3.700803	H	0.034171	22.313435	4.901222	N	1.772960	16.205881	2.841365
C	0.042591	18.326802	5.951817	C	0.930648	22.130842	2.952437	N	4.138710	17.108118	1.835715
H	-0.328344	17.883235	6.871541	H	0.899452	23.190070	2.719362	Cl	1.597881	15.481563	-0.978334
C	0.064773	19.680458	5.791083	C	1.467284	21.227507	2.015121	O	0.624911	19.531033	1.794429
H	-0.288673	20.337923	6.580680	H	1.850216	21.562144	1.057081	C	1.017500	20.598620	1.349026
C	0.558398	20.271165	4.579328	C	1.067144	19.428072	3.410151	C	0.341432	21.881722	1.585930
C	0.611441	21.667487	4.363360	N	1.666082	17.231024	2.638998	C	2.333614	20.534186	0.508276
H	0.264029	22.342264	5.141147	N	1.533002	19.920888	2.236056	C	0.799917	23.132357	1.129001
C	1.105563	22.152571	3.168168	F	0.234482	19.845238	-0.448727	C	-0.854435	21.842551	2.341884
H	1.160345	23.218338	2.971290	F	0.736693	18.404269	-2.033659	C	3.599825	20.868269	1.330388
C	1.548434	21.237540	2.191677	F	-0.634364	17.942243	1.127958	F	2.308707	21.370943	-0.569050
H	1.950778	21.575374	1.241468	F	-1.296943	17.502675	-0.885381	F	2.495103	19.273144	0.039793
C	1.024203	19.435985	3.532243	F	0.335751	16.359500	-0.023911	C	0.101155	24.300687	1.412925
N	1.434086	17.219412	2.682321	C	0.790814	18.627954	-0.677330	C	-1.557307	22.995135	2.625476
N	1.510551	19.924816	2.368160	C	-0.210020	17.592274	-0.095419	F	3.609626	20.152195	2.466714
F	0.390670	19.489004	-0.534865	Cu	2.445802	18.332026	1.017092	F	3.628389	22.172105	1.652198
F	1.023964	17.612533	-1.511460	Cl	4.669965	18.101450	1.509767	F	4.706198	20.580191	0.630289
F	-0.959108	18.034991	1.349434	C	2.728236	19.129459	-0.794121	C	-1.085480	24.241361	2.162848
F	-1.479325	17.569509	-0.706184	C	3.487775	18.199129	-1.645513	H	-1.214777	20.883786	2.699398
F	-0.256886	16.177156	0.432452	C	3.215072	16.826553	-1.706073	H	-2.475875	22.968148	3.203017
C	0.781665	18.192467	-0.278980	C	4.568548	18.718661	-2.385210	H	0.482289	25.245878	1.046109
C	-0.493384	17.487314	0.211958	C	3.995300	15.975958	-2.481074	H	1.709206	23.215172	0.550562
Cu	2.288223	18.174103	1.034627	C	5.351191	17.882516	-3.159591	O	-1.838262	25.309206	2.491791
Cl	4.374436	18.062777	1.968662	C	5.074865	16.501781	-3.212312	C	-1.419283	26.609450	2.061941
C	3.228771	19.007268	-0.479054	O	2.804318	20.334794	-0.782520	H	-1.390043	26.675594	0.967907

H	-2.168232	27.303180	2.447624	C	0.266386	14.830261	4.850420	H	1.616928	23.241695	3.286747
H	-0.437095	26.867095	2.475607	H	-0.255695	14.509010	5.746978	C	1.780841	21.258706	2.443266
				C	1.172412	15.912807	4.923728	H	2.216993	21.581927	1.503041
18				C	1.822834	16.296991	3.724147	C	1.075895	19.477642	3.737727
pOMe-C6H4COCl_B3LYP				C	1.434003	16.633787	6.136234	N	1.266235	17.261617	2.825742
C	-1.422183	-0.557627	0.261527	H	0.918217	16.327165	7.041670	N	1.599712	19.950609	2.579312
C	-0.046500	-0.613441	0.138276	C	2.303196	17.684175	6.151407	F	-0.155291	19.114074	-0.476006
C	0.696046	0.562349	-0.090522	H	2.497386	18.230197	7.070337	F	1.483048	18.400874	-1.776364
C	0.012283	1.790302	-0.187945	C	2.980155	18.101757	4.955868	F	-0.613070	16.621036	0.399197
C	-1.367630	1.855758	-0.062744	C	3.869022	19.199709	4.923250	F	-0.515442	16.700026	-1.773358
C	-2.097959	0.674575	0.163444	H	4.071218	19.751254	5.837477	F	1.133856	15.833013	-0.645240
C	2.150948	0.616761	-0.238633	C	4.465143	19.558005	3.730301	C	0.911192	18.195241	-0.523159
O	2.831719	1.575469	-0.456438	H	5.151538	20.395582	3.668380	C	0.218702	16.835475	-0.645962
Cl	3.027868	-1.022272	-0.059694	C	4.166360	18.821236	2.571269	Cu	1.959470	18.380250	1.124741
H	0.577984	2.699213	-0.363456	H	4.606368	19.079484	1.615084	Cl	4.420055	18.426048	1.880801
H	-1.864586	2.814920	-0.141564	C	2.740787	17.413132	3.740801	C	3.926077	19.101064	0.048193
H	-2.003808	-1.456845	0.436715	N	1.607883	15.673498	2.541665	C	4.220962	18.087122	-0.987501
H	0.454100	-1.570874	0.217740	N	3.329515	17.783857	2.569965	C	4.219947	16.707183	-0.750454
O	-3.436766	0.617206	0.299075	F	2.995047	17.210993	-1.925633	C	4.444831	18.575264	-2.283928
C	-4.195047	1.831580	0.229819	F	3.905832	15.312862	-1.225066	C	4.444005	15.816913	-1.795883
H	-5.235945	1.535578	0.370098	F	0.483956	16.165198	-1.214094	C	4.676650	17.691861	-3.334786
H	-3.902721	2.526944	1.025448	F	1.635105	15.070520	-2.700846	C	4.670231	16.319736	-3.079589
H	-4.081629	2.315408	-0.747391	F	1.475815	14.297683	-0.672745	O	3.858816	20.289741	-0.064127
				C	2.850487	16.212535	-0.949078	H	4.430336	19.643942	-2.467651
24				C	1.611381	15.437212	-1.399201	H	4.851306	18.073357	-4.334491
pOMe-C6H5COC2F5_B3LYP				O	2.234070	20.584844	0.863296	H	4.433770	14.749309	-1.607888
C	-1.441266	-0.504716	0.349014	C	1.285245	19.881685	0.668020	H	4.023124	16.326347	0.244715
C	-0.067328	-0.577286	0.207227	C	0.420532	19.268209	1.698475	I	5.010659	14.948183	-4.700685
C	0.684973	0.578657	-0.102946	Cl	0.766227	19.577041	-1.061248				
C	-0.003629	1.797326	-0.265108	C	-0.457297	18.204175	1.447516	44			
C	-1.380976	1.880103	-0.131374	C	0.524608	19.797754	2.995989	IV_pI_B3LYP			
C	-2.114269	0.720007	0.180157	C	-1.243768	17.689192	2.476509	C	1.466490	15.892727	2.770620
C	2.146175	0.618527	-0.260756	C	-0.266719	19.298350	4.024782	H	1.837537	15.327673	1.922212
C	2.996862	-0.689195	-0.156620	C	-1.151338	18.251898	3.750578	C	1.022791	15.244845	3.935555
C	3.347474	-1.092431	1.293295	H	-0.511739	17.757075	0.462241	H	1.051287	14.161936	3.990175
F	4.175652	-0.491792	-0.796101	H	-1.912859	16.859627	2.279862	C	0.555393	16.008513	4.987513
F	2.379166	-1.754905	-0.746550	H	-0.190474	19.717980	5.021007	H	0.199732	15.541378	5.901730
F	2.237943	-1.405589	1.984646	H	1.221448	20.605218	3.191875	C	0.541140	17.416756	4.875486
F	3.961151	-0.072121	1.911249	I	-2.404426	17.507048	5.326884	C	1.014581	17.983558	3.665397
F	4.163596	-2.156041	1.299849					C	0.074910	18.279580	5.924592
O	2.783990	1.638930	-0.469562	44				H	-0.286152	17.824398	6.842521
H	0.566675	2.689600	-0.501214	OATS_pI_B3LYP				C	0.083814	19.634817	5.776007
H	-1.874969	2.834594	-0.266722	C	1.102899	15.946999	2.923328	H	-0.270569	20.281902	6.573666
H	-2.023741	-1.387957	0.590974	H	1.392044	15.363691	2.054512	C	0.564783	20.240983	4.566828
H	0.413094	-1.535562	0.346649	C	0.570574	15.329032	4.069794	C	0.604558	21.639581	4.362913
O	-3.452143	0.679100	0.337709	H	0.460299	14.250056	4.096187	H	0.255948	22.304355	5.148702
C	-4.204100	1.890275	0.192680	C	0.193500	16.116819	5.140687	C	1.087767	22.139493	3.169331
H	-5.243021	1.615558	0.382664	H	-0.224523	15.673633	6.040470	H	1.132220	23.207340	2.981584
H	-3.886679	2.644218	0.922367	C	0.349971	17.519458	5.063842	C	1.533221	21.237269	2.182280
H	-4.112957	2.294303	-0.822525	C	0.898175	18.048922	3.868328	H	1.927211	21.587577	1.233116
				C	-0.017607	18.410854	6.128067	C	1.031670	19.419416	3.509788
44				H	-0.436903	17.985618	7.035646	N	1.456259	17.214387	2.637161
III_pI_B3LYP				C	0.154965	19.758127	6.006819	N	1.507637	19.922702	2.347438
Cu	2.855958	16.803955	0.889517	H	-0.123621	20.427191	6.816280	F	0.382983	19.509614	-0.537941
C	0.748077	14.664808	2.501858	C	0.706684	20.328243	4.809869	F	1.038800	17.659453	-1.547522
H	0.599432	14.201072	1.531431	C	0.907800	21.716566	4.635076	F	-0.951688	18.008804	1.319004
C	0.050787	14.205814	3.637701	H	0.637900	22.400821	5.434855	F	-1.465228	17.566133	-0.743581
H	-0.642579	13.376156	3.545740	C	1.446691	22.182865	3.451429	F	-0.223475	16.174443	0.375366

C 0.784934 18.214012 -0.306907
C -0.479951 17.483404 0.174044
Cu 2.290310 18.190216 1.006510
Cl 4.386395 18.096116 1.914609
C 3.220504 19.033108 -0.492734
C 3.924146 18.146391 -1.450677
C 3.938204 16.755295 -1.300908
C 4.571521 18.741902 -2.543950
C 4.593796 15.955309 -2.231957
C 5.231840 17.951395 -3.481367
C 5.234046 16.564874 -3.314113
O 3.175986 20.229087 -0.526339
H 4.554835 19.821287 -2.655614
H 5.732770 18.412922 -4.325023
H 3.442195 16.297603 -0.450620
H 4.604074 14.877918 -2.112422
I 6.247326 15.336015 -4.761043

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RETS_pI_B3LYP
C 1.797107 15.927731 2.810053
H 2.245870 15.365113 1.997580
C 1.345088 15.285569 3.977009
H 1.442699 14.209091 4.068944
C 0.783619 16.046101 4.984674
H 0.422815 15.583263 5.899119
C 0.678238 17.446563 4.825560
C 1.160678 18.002792 3.614874
C 0.111555 18.310461 5.822846
H -0.252565 17.864688 6.744241
C 0.030283 19.656622 5.621276
H -0.399369 20.305430 6.379456
C 0.510143 20.252510 4.406084
C 0.452006 21.641393 4.148584
H 0.027215 22.306291 4.895680
C 0.936809 22.133113 2.952248
H 0.907399 23.193436 2.724291
C 1.478333 21.234465 2.013311
H 1.864991 21.574169 1.058436
C 1.075105 19.428914 3.400604
N 1.703697 17.240079 2.632857
N 1.545889 19.927232 2.230244
F 0.220232 19.769441 -0.472263
F 0.790115 18.339661 -2.044185
F -0.600759 17.852391 1.106492
F -1.225611 17.364599 -0.909387
F 0.439633 16.292746 -0.016320
C 0.814085 18.569631 -0.690545
C -0.153119 17.502480 -0.108689
Cu 2.470618 18.354185 1.022783
Cl 4.694850 18.147101 1.474388
C 2.742476 19.131171 -0.782456
C 3.535682 18.214574 -1.642891
C 3.292996 16.836946 -1.696469
C 4.585709 18.768791 -2.388197
C 4.089159 16.012650 -2.486753
C 5.391215 17.953721 -3.179549
C 5.133475 16.581774 -3.218822
O 2.781912 20.336898 -0.802279
H 4.774036 19.836106 -2.337945
H 6.205006 18.385441 -3.751527
H 3.894637 14.946873 -2.527418
H 2.478448 16.403513 -1.128215
I 6.374167 15.314209 -4.437014

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V_pI_B3LYP
Cu 2.789081 16.132078 0.720776
C 0.595228 16.349006 3.199876
H -0.120489 15.924437 2.501060
C 0.204080 16.720494 4.501822
H -0.825415 16.580754 4.815181
C 1.147793 17.259374 5.354417
H 0.883726 17.557759 6.365485
C 2.476743 17.430171 4.903216
C 2.767063 17.026997 3.575615
C 3.516779 17.995447 5.715076
H 3.274667 18.296048 6.730769
C 4.778341 18.157673 5.224376
H 5.561822 18.590174 5.840382
C 5.105411 17.772738 3.880303
C 6.390693 17.952507 3.322582
H 7.181608 18.385810 3.928608
C 6.621014 17.580578 2.012579
H 7.593716 17.708660 1.549796
C 5.566220 17.031083 1.263765
H 5.709067 16.733482 0.230501
C 4.103120 17.207307 3.053423
N 1.834621 16.493827 2.752157
N 4.344161 16.846619 1.762946
Cl 1.662261 15.292815 -0.955796
O 0.280603 19.451398 1.692889
C 0.832244 20.503710 1.428727
C 0.173066 21.823309 1.564330
C 2.316693 20.397364 0.948800
C 0.797173 23.056089 1.302750
C -1.166546 21.814150 1.998222
C 3.345793 20.659473 2.078683
F 2.588631 21.254083 -0.075596
F 2.536530 19.139070 0.501848
C 0.100334 24.250560 1.476665
C -1.870522 22.999176 2.171069
F 2.942932 20.055835 3.209987
F 3.465151 21.974130 2.320411
F 4.550101 20.179050 1.741446
C -1.225584 24.211638 1.908371
H -2.901838 22.976899 2.504662
H -1.650024 20.863986 2.198914
H 0.593131 25.194660 1.273742
H 1.822633 23.107401 0.965884
I -2.298938 26.053719 2.175520

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III'_pI_B3LYP
Cu 2.869238 17.006866 0.991649
C 0.438180 14.961894 2.289103
H 0.292533 14.608210 1.272424
C -0.295579 14.413089 3.360546
H -1.021521 13.628961 3.171515
C -0.068919 14.889068 4.637613
H -0.613763 14.491214 5.489495
C 0.882711 15.915032 4.839354
C 1.557871 16.407821 3.693277
C 1.161980 16.481896 6.127427
H 0.635937 16.088170 6.992212
C 2.048537 17.508778 6.261911
H 2.244044 17.948031 7.235332
C 2.731756 18.050504 5.121343
C 3.613957 19.150140 5.211807
H 3.798721 19.608822 6.179232
C 4.220212 19.632162 4.068049
H 4.898118 20.478374 4.099431
C 3.959234 18.999150 2.841004
H 4.432229 19.336584 1.925162
C 2.505126 17.491023 3.838838
N 1.332061 15.928123 2.448494
N 3.131800 17.959890 2.724115
F 2.852952 17.213063 -1.845436
F 4.442229 15.875103 -1.060466
F 0.951766 15.383216 -1.027737
F 2.468742 14.615183 -2.387599
F 2.529816 14.077090 -0.278323
C 3.128035 16.315366 -0.796070
C 2.273723 15.093371 -1.136777
O -1.661883 18.361454 6.583530
C -0.940514 19.106488 5.990423
C -0.695437 19.136787 4.537046
Cl -0.037131 20.390035 6.973696
C 0.192421 20.018372 3.903498
C -1.405155 18.193478 3.769967
C 0.364468 19.967060 2.522504
C -1.239811 18.138094 2.391254
C -0.355934 19.030610 1.777210
H 0.757136 20.741853 4.478317
H 1.057589 20.646582 2.040206
H -1.784772 17.404479 1.808530
H -2.082167 17.503565 4.260965
I -0.094687 18.955372 -0.344057

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OATS'_pI_B3LYP
N 1.548055 1.067499 -1.085442
N 1.553581 -0.825244 0.873282
C 1.539780 2.033877 -1.996513
C 2.710663 2.532633 -2.597748
C 3.930264 1.999500 -2.228530
C 5.202129 0.389336 -0.794115
C 5.201096 -0.573597 0.170984
C 3.921242 -1.997294 1.785727
C 2.699676 -2.360320 2.320725
C 1.533907 -1.741783 1.834610
C 2.741578 0.549072 -0.699698
C 3.975730 0.981291 -1.249754
C 3.973284 -1.020662 0.765913

C	2.743326	-0.462373	0.333317
H	0.566808	2.437568	-2.259134
H	2.639818	3.322592	-3.338202
H	4.855229	2.356001	-2.673547
H	6.134399	0.731703	-1.234453
H	6.132005	-1.015608	0.514806
H	4.843337	-2.449525	2.140514
H	2.625698	-3.105430	3.105909
H	0.556365	-1.993524	2.235414
C	-0.861026	1.546161	1.419920
F	-1.475680	2.646003	0.813241
F	-1.826750	1.034967	2.294756
C	-2.026103	0.030406	-0.944813
C	-2.058782	1.057334	-1.909675
C	-3.117174	-0.165728	-0.072352
C	-3.104512	1.966473	-1.905731
H	-1.257821	1.147654	-2.632857
C	-4.156472	0.744841	-0.081847
H	-3.113203	-0.989777	0.631082
C	-4.163609	1.831356	-0.988264
H	-3.100924	2.776537	-2.625541
H	-4.978160	0.631886	0.617655
Cu	-0.149967	0.238253	0.103782
I	-0.869732	-1.864547	-1.561988
C	-5.309230	2.734655	-0.901695
O	-6.246355	2.665865	-0.160287
Cl	-5.283085	4.167646	-2.103514
C	0.190114	2.162780	2.341812
F	0.778346	1.209987	3.101583
F	1.162570	2.767456	1.620189
F	-0.311119	3.092199	3.189573

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IV'_pI_B3LYP

N	1.362204	0.766910	-0.300042
N	0.331979	-0.997418	1.537800
C	1.839443	1.631973	-1.191403
C	3.170193	2.075852	-1.174064
C	4.017532	1.599768	-0.192726
C	4.358160	0.155337	1.814869
C	3.855595	-0.724358	2.725591
C	1.921455	-2.049878	3.592384
C	0.592102	-2.401851	3.474533
C	-0.167535	-1.844891	2.426585
C	2.173226	0.286926	0.677822
C	3.532110	0.685138	0.767591
C	2.484578	-1.143503	2.665696
C	1.635077	-0.642897	1.644400
H	1.139024	1.984846	-1.939669
H	3.508812	2.780982	-1.925069
H	5.054295	1.920819	-0.146235
H	5.395364	0.474359	1.862209
H	4.484246	-1.123849	3.516390
H	2.541355	-2.456196	4.386878
H	0.125909	-3.092667	4.169250
H	-1.217506	-2.100616	2.318560
C	-0.195488	-1.406293	-1.512345
F	-0.935402	-2.509110	-1.209123
C	-2.425550	-0.125020	-0.797223
C	-3.129294	-1.062237	-0.041247
C	-3.066127	0.623990	-1.787075
C	-4.492404	-1.234350	-0.257606
H	-2.623083	-1.661111	0.705960
C	-4.428537	0.447954	-2.013013
H	-2.514330	1.349318	-2.375399
C	-5.154297	-0.479976	-1.246532
H	-5.051506	-1.954637	0.330549
H	-4.920898	1.035175	-2.779125
Cu	-0.581181	0.203364	-0.402328
I	-1.310957	2.374087	0.956969
C	-0.286857	-1.185408	-3.034408
F	0.212606	0.026153	-3.361067
F	-1.556807	-1.245861	-3.458991
F	0.418613	-2.113914	-3.706548
F	1.106675	-1.753253	-1.260088
C	-6.595276	-0.736508	-1.397562
O	-7.269767	-1.490818	-0.761770
Cl	-7.438518	0.232681	-2.741953

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RETS'_pI_B3LYP

N	-0.463733	1.292438	0.482712
N	-1.312472	-0.734123	-1.107195
C	-0.014938	2.259202	1.273618
C	-0.821021	3.343192	1.664601
C	-2.125494	3.408572	1.210610
C	-3.965298	2.371558	-0.147737
C	-4.393291	1.356557	-0.952191
C	-3.915324	-0.803200	-2.133331
C	-3.011221	-1.807302	-2.421263
C	-1.713094	-1.735802	-1.884087
C	-1.741299	1.335969	0.031789
C	-2.626011	2.388640	0.369439
C	-3.520089	0.272880	-1.307021
C	-2.192247	0.260391	-0.815572
H	1.015252	2.166168	1.604430
H	-0.410537	4.108882	2.313983
H	-2.773374	4.233587	1.493371
H	-4.631750	3.186999	0.118249
H	-5.408011	1.347461	-1.339780
H	-4.925935	-0.829158	-2.531046
H	-3.282490	-2.648352	-3.050223
H	-0.979738	-2.507146	-2.086812
C	2.046084	-1.512773	-1.225249
F	3.211214	-2.000977	-0.748283
F	1.158831	-2.574164	-1.126330
C	2.318999	0.358144	-0.411065
C	2.300227	1.451295	-1.284164
C	3.179055	0.317954	0.690523
C	3.116436	2.547502	-1.018459
H	1.648123	1.462598	-2.148831
C	3.990486	1.415381	0.951800
H	3.189470	-0.546104	1.343593
C	3.965396	2.537408	0.098938
H	3.085975	3.401962	-1.683528
H	4.647279	1.410155	1.815029
Cu	0.562365	-0.390382	-0.165928
I	0.385926	-1.877411	2.324593
C	2.203612	-1.286837	-2.751344
F	1.129477	-0.637221	-3.244315
F	2.302033	-2.466296	-3.382333
F	3.302367	-0.573800	-3.028344
C	4.867746	3.649366	0.462287
O	5.610701	3.692231	1.396545
Cl	4.817196	5.113416	-0.665394

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V'_pI_B3LYP

Cu	-0.091081	18.968413	1.807454
C	-0.207070	16.880988	4.232317
H	-1.277763	16.862705	4.049718
C	0.369285	16.100254	5.253527
H	-0.263903	15.470681	5.869656
C	1.733688	16.162859	5.455141
H	2.211622	15.581084	6.238448
C	2.520737	17.003893	4.635396
C	1.849426	17.745455	3.631762
C	3.941390	17.142539	4.785950
H	4.436468	16.568157	5.563726
C	4.653156	17.982239	3.981620
H	5.727196	18.089875	4.104253
C	4.005737	18.747188	2.953281
C	4.700911	19.632555	2.098375
H	5.774020	19.756456	2.215213
C	4.005830	20.323585	1.125469
H	4.506205	21.009692	0.450348
C	2.617904	20.127700	1.008515
H	2.044031	20.645420	0.251347
C	2.605782	18.625143	2.769987
N	0.506768	17.676661	3.445580
N	1.933684	19.312239	1.807115
O	0.339091	19.201293	6.456907
C	1.123471	19.977377	5.998921
C	0.884110	20.916087	4.879136
C	1.857609	21.781080	4.357302
C	-0.408847	20.901208	4.328511
C	1.532451	22.640317	3.312879
C	-0.731732	21.759103	3.281470
C	0.236273	22.636238	2.784975
H	-1.727107	21.739525	2.855528
H	-1.153903	20.219045	4.719719
H	2.283118	23.314721	2.916260
H	2.862055	21.790079	4.761549
I	-2.382679	19.093640	0.712924
Cl	2.799475	20.060386	6.757773
C	-0.104285	23.576851	1.657819
C	0.432697	23.134262	0.276412
F	-0.015396	21.903670	-0.030723
F	0.038589	23.982834	-0.680060
F	1.779252	23.104375	0.292220
F	0.428973	24.816036	1.885731
F	-1.451865	23.717947	1.517794

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V'_pI_B3LYP
Cu -0.902358 -0.021652 0.072758
N 0.715924 1.370545 0.018899
N 0.701309 -1.344586 0.022678
C 0.699010 2.699149 0.021214
C 1.873210 3.476074 -0.001132
C 3.098312 2.838164 -0.026943
C 4.375848 0.680263 -0.055310
C 4.368949 -0.683451 -0.056543
C 3.074808 -2.829949 -0.030563
C 1.845197 -3.458819 -0.003648
C 0.676636 -2.674945 0.023070
C 1.913112 0.731547 -0.006020
C 3.148422 1.425162 -0.030078
C 3.134663 -1.417647 -0.031522
C 1.905558 -0.713340 -0.005413
H -0.281693 3.165339 0.042027
H 1.800283 4.558515 0.002385
H 4.024423 3.406145 -0.044342
H 5.312856 1.229757 -0.073752
H 5.300462 -1.242133 -0.076153
H 3.996903 -3.404308 -0.050570
H 1.764003 -4.540573 -0.002189
H -0.305998 -3.135304 0.045789
I -3.417301 0.270918 0.235837

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VII'_pI_B3LYP
Cu 11.148110 3.687465 1.312911
C 11.316602 0.584930 1.816825
H 12.385076 0.768774 1.882623
C 10.780915 -0.686776 2.092210
H 11.442762 -1.498803 2.374629
C 9.415046 -0.872673 1.995568
H 8.965644 -1.840583 2.200491
C 8.590137 0.213156 1.625008
C 9.222824 1.456722 1.371434
C 7.162914 0.109116 1.505084
H 6.697301 -0.853424 1.698405
C 6.406814 1.189615 1.158579
H 5.327259 1.104986 1.069366
C 7.012835 2.467400 0.908939
C 8.420260 2.605503 1.016964
C 6.269753 3.620098 0.567864
H 5.189202 3.552207 0.475035
C 6.928952 4.816451 0.359371
H 6.389125 5.720329 0.096700
C 8.328792 4.857284 0.498755
H 8.878130 5.782118 0.352594
C 10.665341 6.057731 3.703633
C 10.446067 6.967976 2.656275
H 10.835763 6.746228 1.665179
C 9.729973 8.144479 2.882050
H 9.567639 8.843206 2.065646
C 9.215515 8.416603 4.153325
H 8.651560 9.328992 4.328491
C 9.421884 7.511041 5.197705
H 9.021322 7.718476 6.186616
C 10.145149 6.336495 4.976556
H 10.298732 5.636428 5.792751
C 13.369050 4.977760 3.680753
C 14.368694 4.343608 2.927037
H 14.085732 3.655865 2.134056
C 15.716350 4.609617 3.178766
H 16.483297 4.115704 2.588282
C 16.073827 5.518837 4.177629
H 17.122129 5.732678 4.368752
C 15.082129 6.161084 4.926070
H 15.358261 6.872161 5.700263
C 13.734498 5.892174 4.681263
H 12.969508 6.396016 5.265353
C 11.145930 3.351142 4.631085
C 9.848445 2.811399 4.561976
H 9.168253 3.146364 3.783260
C 9.434163 1.842889 5.474071
H 8.430108 1.432380 5.405352
C 10.314459 1.391906 6.464226
H 9.995948 0.629593 7.170205
C 11.603876 1.921549 6.538847
H 12.291883 1.575982 7.306104
C 12.019954 2.898982 5.628617
H 13.025791 3.301885 5.697559
N 10.566363 1.624609 1.468315
N 9.054601 3.790870 0.819014
P 11.625991 4.541061 3.310059
I 12.660282 4.130583 -0.895316

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III_2_pI_B3LYP
Cu 2.949356 16.982740 0.762854
C 0.534255 14.961566 2.192096
H 0.350947 14.591491 1.187778
C -0.192404 14.462619 3.292075
H -0.948591 13.699560 3.138451
C 0.077988 14.962203 4.551068
H -0.462110 14.606654 5.423815
C 1.069079 15.958093 4.706486
C 1.738744 16.397056 3.535529
C 1.395265 16.542678 5.975113
H 0.868997 16.190547 6.857496
C 2.334492 17.526014 6.069745
H 2.574137 17.973970 7.030083
C 3.023539 18.006284 4.905084
C 3.968220 19.055543 4.958130
H 4.205174 19.513558 5.914594
C 4.569992 19.490108 3.793646
H 5.294831 20.297104 3.796243
C 4.231194 18.868360 2.580246
H 4.680787 19.183621 1.645780
C 2.736012 17.440528 3.637345
N 1.465452 15.897726 2.308009
N 3.346008 17.874817 2.498621
F 2.847893 17.140382 -2.091513
F 4.314919 15.674879 -1.300153
F 0.796400 15.508949 -1.126680
F 2.167145 14.605760 -2.556288
F 2.296608 14.080524 -0.446864
C 3.055398 16.255267 -1.024393
C 2.080687 15.109413 -1.303378
O 2.152948 20.596790 0.971101
C 1.200981 19.861991 0.773803
C 0.335092 19.347028 1.860763
C -0.700800 18.413169 1.682620
C 0.595360 19.839158 3.153298
C -1.457128 17.982053 2.770999
C -0.156478 19.421099 4.243850
C -1.178889 18.490139 4.039392
H -0.927799 18.005903 0.707865
H -2.245992 17.253804 2.623264
H 0.057372 19.806490 5.233854
H 1.402116 20.550393 3.292564
I -2.342909 17.825191 5.715288
C 0.879317 19.556711 -0.722218
C -0.249854 20.452354 -1.282254
F 0.507989 18.261348 -0.926941
F 1.981013 19.803252 -1.464745
F -0.413847 20.232983 -2.592194
F 0.058303 21.744316 -1.092389
F -1.409945 20.190995 -0.655437

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OATS_2_pI_B3LYP
N 1.132902 1.339612 -0.607274
N 1.490915 -0.953484 0.822709
C 0.953523 2.481216 -1.261206
C 2.011933 3.217357 -1.826694
C 3.301095 2.737834 -1.700212
C 4.837459 0.974982 -0.806973
C 5.012659 -0.181075 -0.106158
C 4.024832 -2.065828 1.213028
C 2.898635 -2.668370 1.740853
C 1.643827 -2.072329 1.522641
C 2.396896 0.869172 -0.457348
C 3.528338 1.533396 -0.997036
C 3.893076 -0.872425 0.468303
C 2.585432 -0.351308 0.294430
H -0.070175 2.834562 -1.339211
H 1.802068 4.143374 -2.351896
H 4.143323 3.274939 -2.127915
H 5.688209 1.498871 -1.233820
H 6.005386 -0.598929 0.036205
H 5.011618 -2.495241 1.363522
H 2.965541 -3.584692 2.317733
H 0.736374 -2.510792 1.927084
C -1.028727 0.915741 2.157042
F -1.758004 2.082234 1.909584
F -1.878391 0.120378 2.932632
C -2.328438 -0.045721 -0.408808
C -2.572646 1.187257 -1.042924
C -3.293272 -0.609669 0.452016
C -3.703524 1.917167 -0.709693
H -1.868557 1.571877 -1.770582
C -4.421041 0.123224 0.763970

H	-3.125849	-1.583962	0.895871
C	-4.647382	1.404154	0.206659
H	-3.850395	2.876129	-1.187458
H	-5.152976	-0.281789	1.455148
Cu	-0.362061	0.059279	0.490782
I	-1.091402	-1.568187	-1.639938
C	-5.881896	2.087503	0.610336
O	-6.754643	1.575690	1.297920
C	0.065947	1.354936	3.128694
F	0.774392	0.288719	3.566579
F	0.931755	2.199140	2.520807
F	-0.407607	1.993634	4.224677
C	-6.163172	3.556792	0.167117
C	-6.869573	3.655606	-1.201947
F	-5.029123	4.313302	0.101022
F	-6.992137	4.134412	1.070985
F	-8.027034	2.980284	-1.166862
F	-6.097939	3.131688	-2.171624
F	-7.124351	4.935261	-1.509230

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IV_2_pI_B3LYP

N	0.448408	1.391197	0.202853
N	1.369251	-0.698103	-1.233399
C	-0.036651	2.378976	0.949586
C	0.787253	3.375144	1.498932
C	2.146894	3.338797	1.256498
C	4.084787	2.171821	0.169886
C	4.549459	1.135065	-0.584423
C	4.086055	-0.969845	-1.865871
C	3.156843	-1.892829	-2.302037
C	1.803400	-1.724762	-1.960533
C	1.786007	1.329131	-0.033461
C	2.686901	2.295894	0.471056
C	3.657379	0.131291	-1.091789
C	2.274265	0.227121	-0.809659
H	-1.106150	2.376859	1.121161
H	0.340848	4.156675	2.103652
H	2.807941	4.097916	1.664653
H	4.764178	2.923801	0.559958
H	5.607716	1.043948	-0.810899
H	5.139862	-1.078376	-2.105878
H	3.448253	-2.751145	-2.897367
H	1.062068	-2.443608	-2.279069
C	-1.640898	-1.600130	-1.384540
F	-2.820776	-1.901942	-0.790907
C	-2.209005	0.800419	-0.653411
C	-3.112355	0.702969	0.400269
C	-2.327740	1.762354	-1.651801
C	-4.156996	1.621012	0.462271
H	-2.994349	-0.061392	1.160951
C	-3.381126	2.674845	-1.587638
H	-1.619974	1.809190	-2.472932
C	-4.304014	2.615399	-0.526000
H	-4.870045	1.578160	1.278999
H	-3.463295	3.421204	-2.365153
Cu	-0.564185	-0.166456	-0.592983
I	-0.238823	-1.543895	2.305703
C	-1.902880	-1.444515	-2.903023
F	-0.862432	-0.833251	-3.509931
F	-3.003355	-0.713064	-3.122516
F	-2.070290	-2.643394	-3.485750
F	-0.850271	-2.709546	-1.232992
C	-5.443967	3.547336	-0.357202
O	-6.234401	3.481384	0.566251
C	-5.680269	4.718776	-1.364930
C	-4.789188	5.950616	-1.087337
F	-5.476124	4.336883	-2.658577
F	-6.962382	5.135965	-1.253110
F	-3.490669	5.649395	-1.263335
F	-4.965118	6.356291	0.178794
F	-5.107613	6.954241	-1.914219

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RETS_2_pI_B3LYP

N	-0.251280	1.389156	0.454506
N	-1.171141	-0.656409	-1.068046
C	0.232510	2.365253	1.212743
C	-0.542529	3.476865	1.588779
C	-1.852424	3.561068	1.153740
C	-3.735309	2.535505	-0.153583
C	-4.197545	1.512717	-0.928708
C	-3.786689	-0.685424	-2.063657
C	-2.910359	-1.717526	-2.338243
C	-1.604737	-1.665481	-1.817289
C	-1.534649	1.451166	0.022743
C	-2.389144	2.532875	0.345603
C	-3.355661	0.399596	-1.267443
C	-2.022535	0.366371	-0.791553
H	1.265908	2.257174	1.528382
H	-0.104293	4.249009	2.211852
H	-2.476655	4.407775	1.425363
H	-4.378510	3.372966	0.101039
H	-5.216927	1.519416	-1.303812
H	-4.802304	-0.696039	-2.449172
H	-3.208778	-2.565711	-2.944984
H	-0.892778	-2.459007	-2.010338
C	2.160485	-1.522428	-1.199791
F	3.318759	-2.035758	-0.731356
F	1.245477	-2.558171	-1.067287
C	2.503646	0.350508	-0.411523
C	2.528623	1.435420	-1.293369
C	3.354562	0.291477	0.696632
C	3.363887	2.516397	-1.019201
H	1.889490	1.457917	-2.167756
C	4.189083	1.369537	0.958640
H	3.336085	-0.569309	1.353613
C	4.199708	2.497349	0.112855
H	3.353925	3.357085	-1.698458
H	4.838943	1.352568	1.827013
Cu	0.724493	-0.334709	-0.160784
I	0.511896	-1.750849	2.387621
C	2.301660	-1.331684	-2.731799
F	1.233393	-0.672412	-3.224660
F	2.369485	-2.525990	-3.338770
F	3.409801	-0.645873	-3.038878
C	5.124670	3.592494	0.489802
O	5.938305	3.502421	1.390772
C	5.096965	4.960356	-0.262360
C	5.988626	4.984356	-1.523042
F	3.834120	5.314323	-0.636503
F	5.569787	5.918825	0.568132
F	7.249587	4.676467	-1.191370
F	5.550620	4.088716	-2.425600
F	5.969498	6.199363	-2.085039

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V_2_pI_B3LYP

Cu	-0.063742	18.952421	1.892350
C	-0.174103	16.854184	4.284671
H	-1.247185	16.854827	4.116625
C	0.404361	16.052057	5.288232
H	-0.230480	15.427802	5.908029
C	1.772849	16.084879	5.465827
H	2.252646	15.484334	6.233608
C	2.562590	16.919934	4.642167
C	1.887670	17.695281	3.667266
C	3.988114	17.028324	4.768910
H	4.486306	16.425997	5.523242
C	4.699899	17.875765	3.973184
H	5.777633	17.962271	4.078996
C	4.046871	18.685152	2.983415
C	4.739508	19.593589	2.151142
H	5.816091	19.698758	2.253826
C	4.037275	20.333006	1.219549
H	4.535471	21.039970	0.564582
C	2.645136	20.158742	1.117640
H	2.065810	20.711763	0.390190
C	2.642649	18.590043	2.820165
N	0.541223	17.649234	3.499118
N	1.964053	19.319667	1.893942
O	0.120162	19.286622	6.389682
C	0.993994	20.015113	5.957713
C	0.780653	20.981224	4.851210
C	1.742603	21.907902	4.408821
C	-0.477379	20.942966	4.222705
C	1.442233	22.782183	3.368673
C	-0.775149	21.811550	3.178695
C	0.185121	22.736144	2.758478
H	-1.740604	21.759930	2.690814
H	-1.215452	20.222384	4.553941
H	2.184288	23.500210	3.037561
H	2.718766	21.967383	4.867468
I	-2.338833	19.044695	0.758154
C	-0.116322	23.662831	1.610476
C	0.439876	23.175358	0.251546
F	-0.009450	21.936960	-0.022523
F	0.066174	23.994195	-0.738475
F	1.785692	23.139400	0.290685
F	0.434175	24.896965	1.819983
F	-1.459023	23.823017	1.440473
C	2.384632	19.892456	6.656886
C	2.589754	20.914094	7.797502
F	3.417040	20.039779	5.778482

F 2.483905 18.662887 7.215412
F 1.600718 20.797558 8.693801
F 2.586773 22.167670 7.312534
F 3.760489 20.697124 8.410134

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III'_2_pI_B3LYP
Cu 2.850632 16.810136 0.907043
C 0.675451 14.754167 2.576565
H 0.489570 14.291834 1.611695
C -0.022828 14.336285 3.726592
H -0.759984 13.543507 3.651971
C 0.241296 14.958836 4.930826
H -0.287719 14.674442 5.835792
C 1.199924 15.995605 4.982348
C 1.843481 16.345208 3.767717
C 1.512821 16.713030 6.185166
H 0.998773 16.435806 7.100742
C 2.423154 17.727307 6.176998
H 2.655822 18.271547 7.088014
C 3.091258 18.112421 4.965479
C 4.017683 19.177918 4.909560
H 4.257453 19.725466 5.817068
C 4.601171 19.510701 3.703136
H 5.315000 20.323432 3.623149
C 4.251134 18.781615 2.553987
H 4.677862 19.022240 1.587171
C 2.803118 17.426647 3.759535
N 1.577856 15.726222 2.594010
N 3.378852 17.773713 2.574982
F 2.941236 17.219549 -1.906198
F 3.817943 15.296720 -1.227781
F 0.422652 16.244308 -1.179935
F 1.528367 15.092006 -2.657204
F 1.358114 14.354306 -0.616728
C 2.790201 16.220573 -0.930740
C 1.524870 15.477787 -1.361074
O 2.290341 20.604931 0.943841
C 1.330725 19.931840 0.704317
C 0.437516 19.295299 1.702355
Cl 0.837738 19.699021 -1.039784
C -0.465040 18.270345 1.389240
C 0.549790 19.757153 3.025492
C -1.261743 17.721012 2.389965
C -0.253561 19.215940 4.020750
C -1.155116 18.194221 3.699567
H -0.528832 17.882648 0.380752
H -1.952975 16.920619 2.153229
H -0.173342 19.572241 5.041333
H 1.264540 20.537121 3.262069
C -2.051141 17.634720 4.772170
C -3.339175 18.462693 4.984040
F -2.456722 16.365697 4.475341
F -1.414466 17.597921 5.981749
F -3.025185 19.719313 5.339683
F -4.051056 18.500241 3.846790
F -4.097273 17.921571 5.947823

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OATS'_2_pI_B3LYP
C 1.128756 15.953954 2.904508
H 1.416440 15.378008 2.030275
C 0.605766 15.325124 4.049306
H 0.502438 14.245322 4.068925
C 0.228517 16.103352 5.127138
H -0.182615 15.651440 6.025733
C 0.375315 17.507507 5.058750
C 0.914805 18.048245 3.864431
C 0.006327 18.389794 6.130044
H -0.406353 17.955986 7.036600
C 0.169529 19.738945 6.016699
H -0.109883 20.400876 6.831704
C 0.711805 20.320349 4.820795
C 0.902338 21.711072 4.653096
H 0.632174 22.388706 5.458413
C 1.431044 22.188271 3.469141
H 1.592888 23.249247 3.310016
C 1.764719 21.272791 2.452979
H 2.191480 21.604863 1.511398
C 1.081003 19.478937 3.741557
N 1.283604 17.270312 2.815077
N 1.593336 19.962663 2.582458
F -0.169104 19.162176 -0.482716
F 1.455418 18.426918 -1.787467
F -0.643906 16.672287 0.407028
F -0.567935 16.749882 -1.766491
F 1.085057 15.868063 -0.655090
C 0.885665 18.231314 -0.532235
C 0.178714 16.878295 -0.646880
Cu 1.937448 18.407355 1.112792
Cl 4.425333 18.492070 1.839612
C 3.899483 19.129317 0.021385
C 4.189144 18.098556 -1.006978
C 4.177480 16.722760 -0.747488
C 4.431365 18.571013 -2.305730
C 4.407316 15.821988 -1.779700
C 4.670957 17.669122 -3.336991
C 4.647235 16.296604 -3.073970
O 3.821334 20.315052 -0.116826
H 4.426580 19.637456 -2.500108
H 4.865368 18.029469 -4.341217
H 4.390524 14.755732 -1.583905
H 3.969628 16.360338 0.251861
C 4.941204 15.320930 -4.180792
C 6.444416 14.988264 -4.315128
F 4.301872 14.130708 -3.978592
F 4.546526 15.810122 -5.392964
F 7.143279 16.109602 -4.557222
F 6.897010 14.435219 -3.177295
F 6.656231 14.127692 -5.321133

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IV'_2_pI_B3LYP
C 1.406033 15.891614 2.782170
H 1.774419 15.320652 1.936599
C 0.939064 15.251040 3.941951
H 0.946936 14.167735 3.995485
C 0.475946 16.022151 4.990378
H 0.103016 15.560581 5.900517
C 0.488759 17.430554 4.879964
C 0.983557 17.989820 3.675026
C 0.028768 18.300832 5.925681
H -0.348698 17.851420 6.839832
C 0.063446 19.655811 5.778503
H -0.286377 20.308464 6.573618
C 0.565544 20.254176 4.574035
C 0.630948 21.651974 4.371011
H 0.287164 22.322462 5.154050
C 1.131998 22.143920 3.181484
H 1.195954 23.210909 2.994500
C 1.569986 21.234562 2.197651
H 1.977464 21.578548 1.251838
C 1.027188 19.425199 3.520573
N 1.421257 17.213501 2.650298
N 1.520895 19.920615 2.362238
F 0.429541 19.524956 -0.544997
F 1.059538 17.654869 -1.534015
F -0.958750 18.062533 1.305743
F -1.458920 17.622480 -0.760761
F -0.260916 16.208604 0.377735
C 0.799619 18.222665 -0.301126
C -0.486398 17.521843 0.168312
Cu 2.286617 18.173523 1.032267
Cl 4.373352 18.057328 1.957771
C 3.251137 18.996842 -0.452140
C 3.942751 18.092703 -1.411485
C 3.937482 16.702803 -1.250314
C 4.585060 18.676449 -2.513852
C 4.569883 15.893675 -2.186864
C 5.218831 17.868286 -3.452087
C 5.200539 16.479337 -3.290165
O 3.235688 20.192755 -0.491884
H 4.580272 19.755107 -2.628672
H 5.718103 18.311942 -4.306591
H 3.443393 16.259980 -0.391820
H 4.569696 14.815982 -2.067395
C 5.910883 15.605309 -4.288655
C 7.391106 15.344754 -3.930208
F 5.909248 16.170168 -5.532023
F 5.317868 14.378462 -4.383789
F 7.976231 14.572656 -4.857495
F 7.473697 14.723466 -2.742290
F 8.059259 16.507302 -3.857337

50
RETS'_2_pI_B3LYP
C 1.789903 15.917554 2.806324
H 2.231562 15.354317 1.990304
C 1.355417 15.277675 3.981037
H 1.460012 14.202138 4.076047
C 0.802078 16.039320 4.992399
H 0.454280 15.578109 5.912685
C 0.688374 17.438706 4.829797
C 1.157879 17.993722 3.613485

C 0.125556 18.302763 5.829146
H -0.229326 17.857880 6.754552
C 0.035047 19.647744 5.623898
H -0.393806 20.296399 6.382662
C 0.506102 20.242922 4.404950
C 0.439827 21.630868 4.144433
H 0.011632 22.295002 4.890258
C 0.921241 22.122617 2.946775
H 0.885167 23.182161 2.716133
C 1.468732 21.225121 2.010235
H 1.854888 21.565539 1.055499
C 1.071273 19.419838 3.399149
N 1.690340 17.229312 2.626772
N 1.540943 19.918339 2.228547
F 0.257898 19.842148 -0.467771
F 0.792676 18.402428 -2.042998
F -0.619682 17.934259 1.103125
F -1.262151 17.499262 -0.918728
F 0.364222 16.356608 -0.043653
C 0.817638 18.627471 -0.687722
C -0.185246 17.586945 -0.117054
Cu 2.458550 18.331885 1.015710
Cl 4.679085 18.104196 1.462613
C 2.750832 19.128039 -0.772587
C 3.525838 18.196700 -1.642770
C 3.251100 16.825239 -1.703270
C 4.587928 18.736706 -2.381418
C 4.037689 15.993437 -2.491944
C 5.376319 17.906473 -3.170363
C 5.096784 16.537025 -3.226056
O 2.825998 20.331993 -0.787662
H 4.794075 19.799804 -2.323630
H 6.203214 18.317798 -3.739196
H 3.829300 14.930422 -2.540677
H 2.423496 16.409390 -1.141505
C 5.985025 15.632375 -4.035131
C 7.210795 15.119915 -3.245704
F 6.477559 16.273995 -5.136284
F 5.311703 14.523146 -4.462349
F 7.960506 16.155478 -2.835128
F 6.805946 14.425257 -2.169830
F 7.969789 14.320103 -4.009738

50
V'_2_pI_B3LYP
Cu -0.032004 19.029908 1.699817
C -0.190101 16.877088 4.282439
H -1.264483 16.869315 4.117711
C 0.391143 16.096553 5.302904
H -0.239891 15.482502 5.936893
C 1.759430 16.139914 5.477902
H 2.243788 15.558857 6.257787
C 2.544006 16.961443 4.635706
C 1.862317 17.713156 3.644983
C 3.968465 17.078460 4.761049
H 4.469794 16.494797 5.527982
C 4.674889 17.913671 3.948696
H 5.752035 18.009760 4.052352
C 4.017756 18.698659 2.941958
C 4.713140 19.590362 2.095074
H 5.788718 19.700524 2.202707
C 4.015230 20.306648 1.142884
H 4.514270 21.000961 0.475338
C 2.626554 20.123806 1.034853
H 2.051420 20.657629 0.290619
C 2.613511 18.592304 2.776824
N 0.518773 17.658201 3.480606
N 1.939652 19.298932 1.825746
O 0.101577 19.283351 6.422489
C 0.981821 20.002591 5.988635
C 0.780233 20.959813 4.871656
C 1.746082 21.885179 4.434042
C -0.470279 20.916286 4.230679
C 1.453951 22.756038 3.389142
C -0.757978 21.777603 3.177230
C 0.203083 22.705685 2.765915
H -1.716635 21.717839 2.676800
H -1.208846 20.193428 4.555591
H 2.196892 23.476497 3.065513
H 2.717167 21.948703 4.902848
Cl -2.114293 18.959904 1.013608
C -0.090297 23.641815 1.623111
C 0.487159 23.182239 0.263728
F 0.018624 21.962742 -0.058373
F 0.151300 24.037521 -0.709307
F 1.830480 23.117143 0.329692
F 0.447445 24.877719 1.856863
F -1.431695 23.793801 1.436576
C 2.367357 19.880496 6.697515
C 2.565934 20.906561 7.835325
F 3.405603 20.022848 5.825651
F 2.461344 18.653148 7.262168
F 1.571842 20.793953 8.726465
F 2.566086 22.158301 7.345416
F 3.733108 20.691947 8.455696

14
pI-C6H4COCl_B3LYP
C -1.426847 -0.641701 0.295837
C -0.041774 -0.636987 0.147143
C 0.638320 0.566991 -0.087488
C -0.085498 1.771374 -0.167865
C -1.467824 1.774589 -0.018859
C -2.126584 0.563611 0.210672
C 2.100227 0.676226 -0.264182
O 2.721871 1.671787 -0.487497
Cl 3.038956 -0.909224 -0.119809
H 0.441250 2.702306 -0.347727
H -2.018084 2.706532 -0.082024
H -1.946826 -1.575944 0.474439
H 0.498242 -1.573883 0.213033
I -4.263144 0.556540 0.432992

20
pI-C6H4COC2F5_B3LYP
C -1.467233 -0.592675 0.412211
C -0.083600 -0.622753 0.248305
C 0.620252 0.550008 -0.079516
C -0.094575 1.752212 -0.241737
C -1.474778 1.790883 -0.087342
C -2.150259 0.611611 0.240536
C 2.089321 0.626513 -0.255426
C 2.975537 -0.658028 -0.181731
C 3.371840 -1.049247 1.259771
F 4.129141 -0.424868 -0.850378
F 2.368009 -1.735189 -0.756388
F 2.285274 -1.383191 1.977228
F 3.977705 -0.013222 1.857240
F 4.209263 -2.094083 1.245806
O 2.687498 1.667811 -0.456314
H 0.446701 2.658621 -0.491166
H -2.011790 2.723558 -0.218779
H -1.998469 -1.502334 0.668539
H 0.426801 -1.565399 0.386556
I -4.284049 0.655292 0.486864

20
p-C2F5-C6H6COCl_B3LYP
C -1.412363 -0.647716 0.263891
C -0.028588 -0.646205 0.118589
C 0.648449 0.562172 -0.097473
C -0.071043 1.769276 -0.162881
C -1.451877 1.766118 -0.014772
C -2.120072 0.554899 0.191421
C 2.116155 0.672052 -0.268458
O 2.732074 1.671798 -0.484747
Cl 3.054641 -0.906852 -0.126321
H 0.458562 2.700668 -0.328491
H -2.007111 2.696281 -0.062076
H -1.938830 -1.580794 0.430119
H 0.513156 -1.582405 0.171782
C -3.613663 0.553057 0.389521
C -4.034465 0.713820 1.868819
F -5.369510 0.717546 1.987256
F -3.557059 1.869638 2.359481
F -3.541207 -0.299955 2.599072
F -4.168433 -0.616354 -0.045887
F -4.203286 1.577482 -0.294101

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p-C2F5-C6H4COC2F5_B3LYP
C -1.549669 -0.649097 0.196691
C -0.159068 -0.666748 0.139721
C 0.556017 0.537425 0.016148
C -0.148875 1.753985 -0.048871
C -1.535436 1.771317 0.003049
C -2.234925 0.564915 0.118164
C 2.038836 0.629812 -0.038002
O 2.640558 1.686014 -0.068492
H 0.405355 2.681313 -0.141761
H -2.073033 2.711601 -0.049547

H	-2.098114	-1.579183	0.296459
H	0.348183	-1.618849	0.199402
C	-3.737886	0.581573	0.214102
C	-4.259793	0.712675	1.663773
F	-5.599773	0.745933	1.686399
F	-3.793383	1.842729	2.220596
F	-3.844587	-0.332723	2.397985
F	-4.278253	-0.567848	-0.288160
F	-4.264583	1.632398	-0.481803
C	2.925145	-0.657423	-0.046557
C	3.206278	-1.220187	1.365461
F	3.805682	-0.282151	2.112427
F	2.059860	-1.580078	1.968745
F	4.003327	-2.293276	1.289907
F	4.126238	-0.350615	-0.589987
F	2.369617	-1.654137	-0.793430

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III_oBr_B3LYP

Cu	2.547978	16.997279	0.974312
C	0.622615	14.797659	2.799403
H	0.286179	14.406921	1.843518
C	0.068217	14.330625	4.008630
H	-0.701800	13.565957	3.989748
C	0.526095	14.860190	5.199627
H	0.126710	14.523213	6.152481
C	1.532111	15.853875	5.179402
C	2.016143	16.261209	3.909029
C	2.068249	16.451311	6.369358
H	1.684234	16.124730	7.331818
C	3.043100	17.401601	6.295970
H	3.453130	17.847109	7.197995
C	3.552011	17.844875	5.028216
C	4.558609	18.829705	4.912015
H	4.981997	19.269118	5.811052
C	4.985898	19.221655	3.659455
H	5.754564	19.976388	3.533064
C	4.394096	18.639842	2.525825
H	4.684573	18.941403	1.526008
C	3.030286	17.290778	3.832599
N	1.562976	15.730207	2.750273
N	3.447084	17.704592	2.603135
F	1.249027	17.764356	-1.426412
F	3.000970	16.435767	-1.750903
F	-0.132820	15.674903	-0.334522
F	0.668410	15.272887	-2.317998
F	1.592645	14.362459	-0.568873
C	1.957746	16.692062	-0.839937
C	1.019216	15.499720	-1.031714
O	2.147953	20.537338	0.349216
C	1.001481	20.217120	0.348755
C	0.262491	19.444801	1.380071
Cl	-0.067140	20.754770	-1.052515
C	-0.618840	18.425809	0.977910
C	0.464014	19.645147	2.756854
C	-1.266055	17.629962	1.916114
C	-0.200468	18.868438	3.701527
C	-1.062659	17.855572	3.277146
H	-0.745005	18.232920	-0.078957
H	-1.917180	16.829609	1.581173
H	-0.045423	19.046403	4.759587
H	-1.562720	17.240047	4.018488
Br	1.617109	21.066527	3.453108

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OATS_oBr_B3LYP

C	1.131319	15.953632	2.965266
H	1.416560	15.371998	2.093892
C	0.621968	15.330544	4.119372
H	0.528186	14.250086	4.149488
C	0.245825	16.115203	5.192909
H	-0.154826	15.667968	6.098552
C	0.378918	17.519945	5.110315
C	0.906249	18.054309	3.907604
C	0.006153	18.408856	6.174786
H	-0.396133	17.979916	7.088306
C	0.151729	19.758583	6.045694
H	-0.131811	20.426013	6.854783
C	0.679626	20.333704	4.840373
C	0.847329	21.725173	4.655661
H	0.570500	22.407874	5.454415
C	1.361329	22.196400	3.463003
H	1.504393	23.257855	3.289625
C	1.704294	21.274336	2.455972
H	2.119729	21.602577	1.508341
C	1.055136	19.485526	3.768624
N	1.275573	17.270223	2.863058
N	1.554676	19.963084	2.601238
F	-0.142966	19.172444	-0.524000
F	1.494447	18.358367	-1.766513
F	-0.688502	16.710991	0.434643
F	-0.595361	16.747669	-1.739520
F	1.026091	15.843501	-0.600347
C	0.888012	18.213273	-0.519476
C	0.146884	16.877654	-0.616708
Cu	1.903663	18.400854	1.145106
Cl	4.424586	18.501135	1.864873
C	3.878096	19.161954	0.026406
C	4.220852	18.146260	-1.000821
C	4.089887	16.774983	-0.716378
C	4.621684	18.509998	-2.301075
C	4.334671	15.805948	-1.677968
C	4.878933	17.541743	-3.270235
C	4.728897	16.190450	-2.961002
O	3.739859	20.341014	-0.060549
H	5.193306	17.839335	-4.264247
H	4.211957	14.756825	-1.428678
H	3.762183	16.482305	0.273493
H	4.922957	15.444891	-3.726340
Br	4.896432	20.363584	-2.875722

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IV_oBr_B3LYP

C	1.456282	15.905680	2.808353
H	1.843374	15.341676	1.966388
C	0.983018	15.256223	3.960635
H	1.005045	14.173007	4.012441
C	0.494854	16.018863	5.003938
H	0.115654	15.550576	5.908055
C	0.489205	17.427408	4.895949
C	0.993605	17.995793	3.699114
C	0.000189	18.288968	5.935623
H	-0.384341	17.832642	6.843409
C	0.015312	19.644397	5.789735
H	-0.357449	20.290802	6.579527
C	0.526688	20.251971	4.593778
C	0.571606	21.650874	4.393376
H	0.203640	22.314474	5.171305
C	1.083793	22.152352	3.212757
H	1.132654	23.220408	3.027338
C	1.554163	21.251679	2.235879
H	1.972087	21.604521	1.298242
C	1.019085	19.432005	3.547045
N	1.455335	17.227809	2.679237
N	1.524707	19.936656	2.397732
F	0.474471	19.539710	-0.535800
F	1.107916	17.658301	-1.501698
F	-0.921683	18.091789	1.325662
F	-1.414805	17.640807	-0.740013
F	-0.223886	16.231295	0.410918
C	0.843840	18.239208	-0.275244
C	-0.445440	17.543965	0.193119
Cu	2.327106	18.199232	1.064542
Cl	4.410652	18.069285	2.005188
C	3.290663	19.053879	-0.417150
C	3.941809	18.178845	-1.430374
C	4.018911	16.795052	-1.191712
C	4.468868	18.661846	-2.644342
C	4.609657	15.929216	-2.101771
C	5.058138	17.801142	-3.567894
C	5.132166	16.434946	-3.293240
O	3.278832	20.246569	-0.366602
H	5.456741	18.190787	-4.498029
H	4.659726	14.867103	-1.884029
H	3.612893	16.406347	-0.264585
H	5.595179	15.771944	-4.018169
Br	4.401365	20.548254	-3.174090

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RETS_oBr_B3LYP

C	1.815963	15.952605	2.807417
H	2.288778	15.402855	1.999746
C	1.324591	15.291078	3.947328
H	1.414794	14.212642	4.022469
C	0.734040	16.035694	4.950206
H	0.342508	15.557851	5.844087
C	0.637736	17.439147	4.812942
C	1.156475	18.014644	3.626545
C	0.042626	18.287013	5.807313
H	-0.349070	17.826598	6.710034
C	-0.030637	19.636429	5.625419
H	-0.480754	20.273683	6.381511
C	0.481696	20.250982	4.432947
C	0.429755	21.643786	4.196030

H	-0.011851	22.297059	4.943642	C	1.271982	20.073110	0.722977	C	-0.830180	17.720229	4.202808
C	0.941333	22.153485	3.018625	C	1.305490	20.907176	1.953530	C	-0.175839	18.459064	1.996636
H	0.917938	23.217208	2.806495	C	1.616421	20.730027	-0.652918	C	-0.823240	17.537705	2.820933
C	1.501072	21.269031	2.076780	C	2.324802	21.865475	2.117891	H	-0.183881	18.946884	5.830343
H	1.904445	21.624030	1.134586	C	0.390806	20.738728	3.011746	H	-1.322533	17.003293	4.851243
C	1.072277	19.443332	3.429325	C	3.004436	20.342467	-1.210240	H	-0.156163	18.304973	0.926111
N	1.730371	17.268035	2.650137	F	1.560537	22.088079	-0.602820	H	-1.301025	16.674793	2.369931
N	1.565496	19.958621	2.275134	F	0.696900	20.300441	-1.553181	Br	1.344428	20.734475	1.259922
F	0.209494	19.796517	-0.443557	C	2.443291	22.601708	3.292113				
F	0.761728	18.376058	-2.029635	C	0.487447	21.487756	4.179212	44			
F	-0.589262	17.886266	1.138724	F	3.079646	19.023469	-1.411329	OATS'_oBr_B3LYP			
F	-1.242622	17.394840	-0.868279	F	3.971033	20.697072	-0.336910	Cu	2.706743	17.488679	1.015446
F	0.429840	16.320540	0.007748	F	3.230372	20.974336	-2.367991	C	2.576951	15.691791	3.552956
C	0.800652	18.598315	-0.675924	C	1.523029	22.414412	4.322305	H	1.686677	15.315606	3.059282
C	-0.159351	17.532392	-0.081747	H	-0.235832	21.353016	4.975432	C	2.991492	15.194565	4.802504
Cu	2.504126	18.407931	1.057256	H	3.249472	23.320768	3.396621	H	2.417010	14.411580	5.286213
Cl	4.735446	18.197097	1.445161	H	3.047316	22.016149	1.327202	C	4.128428	15.718422	5.388170
C	2.737691	19.194094	-0.767313	H	1.598266	22.988607	5.240985	H	4.478140	15.357347	6.351588
C	3.531630	18.283872	-1.644108	Br	-1.143236	19.523925	2.895948	C	4.847482	16.739496	4.725859
C	3.239922	16.907847	-1.637628					C	4.351057	17.175735	3.471896
C	4.592776	18.717649	-2.459391	44				C	6.036944	17.339524	5.261763
C	3.962204	16.000973	-2.400243	III'_oBr_B3LYP				H	6.400960	16.992928	6.225016
C	5.329112	17.816081	-3.225884	Cu	2.303107	16.350466	1.319125	C	6.697574	18.318355	4.579890
C	5.014094	16.457297	-3.196231	C	0.785841	14.166637	3.477015	H	7.598710	18.766770	4.989058
O	2.734856	20.396191	-0.752590	H	0.470111	13.624401	2.588986	C	6.223664	18.781304	3.305633
H	6.146172	18.169889	-3.844834	C	0.375091	13.758094	4.762595	C	6.878261	19.785085	2.556287
H	3.706793	14.946376	-2.372889	H	-0.266357	12.890020	4.874601	H	7.782404	20.242374	2.948860
H	2.425856	16.555658	-1.017476	C	0.805823	14.479650	5.859349	C	6.361008	20.167307	1.333487
H	5.593398	15.763374	-3.798149	H	0.512060	14.195915	6.866421	H	6.842238	20.929841	0.730068
Br	5.152193	20.590732	-2.601055	C	1.638545	15.607140	5.670223	C	5.182892	19.551611	0.870084
				C	1.988666	15.937392	4.335921	H	4.749989	19.826579	-0.087404
44				C	2.111644	16.424125	6.750793	C	5.046004	18.218340	2.751120
V_oBr_B3LYP				H	1.831574	16.155789	7.765707	N	3.235624	16.648910	2.910237
Cu	3.344807	16.763442	0.873107	C	2.891616	17.516299	6.511177	N	4.538690	18.615142	1.556576
C	0.832120	15.674685	2.745249	H	3.244573	18.136108	7.329806	F	1.623787	15.609649	-0.892202
H	0.625613	14.982668	1.932927	C	3.259268	17.885271	5.173431	F	3.168705	16.964239	-1.712816
C	0.045930	15.672640	3.915945	C	4.041470	19.026383	4.885865	F	3.517640	14.361788	0.631676
H	-0.777751	14.972396	4.009654	H	4.396005	19.650509	5.700613	F	3.979445	14.408505	-1.495433
C	0.349025	16.565122	4.924878	C	4.337631	19.334860	3.572970	F	5.056141	15.714013	-0.125741
H	-0.231075	16.591323	5.843360	H	4.931252	20.205208	3.315428	C	2.793660	16.284292	-0.550270
C	1.430151	17.460925	4.759614	C	3.847354	18.503947	2.551279	C	3.840055	15.181431	-0.393601
C	2.153539	17.386750	3.542947	H	4.053060	18.718217	1.508952	O	-0.120473	16.441318	1.612806
C	1.814029	18.420520	5.754832	C	2.806822	17.103006	4.082385	C	-0.546740	16.851204	0.571975
H	1.245864	18.461657	6.680162	N	1.564815	15.218778	3.271400	C	0.013276	17.894701	-0.286601
C	2.864855	19.263682	5.546073	N	3.100416	17.425963	2.790538	Cl	-2.132888	16.089260	-0.036949
H	3.151755	19.991046	6.299964	F	2.582027	15.658191	-1.429059	C	-0.373368	18.054307	-1.632553
C	3.619832	19.217125	4.326068	F	1.490805	14.164566	-0.194640	C	1.114539	18.669285	0.183687
C	4.714698	20.072278	4.070035	F	0.446814	17.383988	-1.175513	C	0.266957	18.953261	-2.471761
H	5.009366	20.801917	4.818982	F	-0.032224	15.430426	-2.006969	C	1.709134	19.635734	-0.650478
C	5.392860	19.968531	2.871443	F	-0.612057	15.907027	0.036323	C	1.314692	19.744109	-1.975461
H	6.238264	20.607962	2.640864	C	1.707178	15.555644	-0.331892	H	-1.174167	17.437897	-2.022677
C	4.973035	19.012316	1.930878	C	0.375397	16.061166	-0.883389	H	-0.050883	19.048142	-3.504953
H	5.480029	18.904780	0.978985	O	1.482220	21.960597	4.026593	H	2.487583	20.274469	-0.251308
C	3.264987	18.283509	3.320650	C	1.119527	20.959168	4.557936	H	1.813411	20.461644	-2.621246
N	1.852482	16.500365	2.565002	C	0.473179	19.772787	3.952851	Br	1.148108	19.292944	2.215045
N	3.941642	18.194176	2.141013	Cl	1.382937	20.856110	6.401575				
Cl	3.349630	15.397008	-0.838293	C	-0.182534	18.817305	4.756381				
O	0.959346	18.902561	0.689958	C	0.456951	19.565955	2.553584				

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IV'_oBr_B3LYP

Cu	2.322105	17.415092	1.213812
C	2.599840	15.615106	3.504657
H	1.700924	15.215961	3.052480
C	3.071567	15.140237	4.738095
H	2.530333	14.350364	5.247277
C	4.216141	15.696005	5.275145
H	4.608653	15.354813	6.229095
C	4.886821	16.724404	4.576921
C	4.343807	17.144408	3.336497
C	6.080202	17.348098	5.074940
H	6.475585	17.011516	6.029036
C	6.703005	18.334224	4.370298
H	7.607324	18.801119	4.750510
C	6.181876	18.778654	3.109116
C	6.798436	19.788003	2.335035
H	7.705007	20.263149	2.699810
C	6.240902	20.150549	1.125140
H	6.691153	20.916303	0.502011
C	5.061877	19.506075	0.699920
H	4.606655	19.766208	-0.251396
C	4.998634	18.192659	2.589243
N	3.218112	16.579471	2.827308
N	4.453882	18.565341	1.407720
F	2.101452	15.576938	-0.985271
F	3.733670	17.050262	-1.142649
F	3.422434	14.292880	1.008560
F	4.488672	14.499216	-0.875242
F	5.091408	15.692469	0.832948
C	3.035521	16.269066	-0.260011
C	4.027954	15.176788	0.195717
O	0.228274	15.765030	1.286746
C	-0.429438	16.254844	0.410075
C	-0.080550	17.421385	-0.412075
Cl	-2.050480	15.463910	0.052075
C	-0.924464	17.943192	-1.412350
C	1.167224	18.036678	-0.177736
C	-0.528437	19.044028	-2.161956
C	1.561996	19.132636	-0.932974
C	0.715194	19.638438	-1.923495
H	-1.888283	17.484185	-1.598587
H	-1.185699	19.437947	-2.930968
H	2.519055	19.604623	-0.745287
H	1.029721	20.498703	-2.508555
Br	1.177991	18.992092	2.677870

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RETS'_oBr_B3LYP

Cu	2.343395	17.529550	1.063710
C	2.652617	15.471927	3.246312
H	1.746273	15.090476	2.791728
C	3.184455	14.898210	4.413931
H	2.681657	14.053092	4.871780
C	4.339946	15.428631	4.953391
H	4.779818	15.011814	5.855361
C	4.958199	16.533264	4.325981
C	4.351708	17.044900	3.151195
C	6.154231	17.145951	4.830488
H	6.602628	16.735956	5.731064
C	6.712835	18.216602	4.198881
H	7.616517	18.679859	4.585251
C	6.121077	18.763050	3.010671
C	6.660514	19.876823	2.328582
H	7.562852	20.349764	2.706431
C	6.029691	20.348350	1.194749
H	6.413941	21.202403	0.646882
C	4.861376	19.701132	0.748381
H	4.343904	20.056656	-0.137274
C	4.940919	18.180982	2.479882
N	3.220559	16.504767	2.632834
N	4.331204	18.652703	1.363798
F	2.064677	15.887657	-1.808439
F	3.696517	17.364811	-1.590510
F	3.077111	14.558867	0.414892
F	4.265938	14.753680	-1.389384
F	4.788159	15.916524	0.357043
C	2.832348	16.568493	-0.902298
C	3.752761	15.429633	-0.342264
O	0.491052	15.478127	0.784317
C	-0.230515	16.049518	0.014518
C	0.038480	17.333782	-0.643879
C	-0.953366	18.075237	-1.301614
C	1.353146	17.867231	-0.555037
C	-0.657434	19.310778	-1.871864
C	1.652527	19.074609	-1.184717
C	0.646247	19.808327	-1.814412
H	-1.965528	17.691541	-1.349878
H	-1.439520	19.875204	-2.369528
H	2.667423	19.447935	-1.174640
H	0.888776	20.764441	-2.269473
Br	0.881022	18.881340	2.553397
Cl	-1.817151	15.238439	-0.415500

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V'_oBr_B3LYP

Cu	2.946363	17.343376	0.836508
C	0.464279	16.616925	2.441846
H	-0.016971	16.605730	1.469821
C	-0.257542	16.324231	3.613060
H	-1.313999	16.087138	3.544665
C	0.399819	16.338052	4.827813
H	-0.125024	16.108688	5.751238
C	1.775914	16.655679	4.870065
C	2.414698	16.957034	3.642101
C	2.535937	16.685599	6.088085
H	2.027876	16.441037	7.016809
C	3.858483	17.016432	6.083865
H	4.426715	17.040481	7.009636
C	4.528811	17.359322	4.861583
C	5.885399	17.752112	4.805071
H	6.470071	17.789440	5.720283
C	6.446503	18.088121	3.588031
H	7.483409	18.398432	3.511187
C	5.649705	18.023609	2.428209
H	6.057859	18.276498	1.453536
C	3.810592	17.329973	3.640165
N	1.758981	16.924885	2.450565
N	4.374934	17.654886	2.450962
O	2.108384	19.890262	1.084478
C	1.006675	20.342987	1.069051
C	0.557440	21.612946	1.709163
C	0.127178	22.645723	0.867491
C	0.639431	21.828227	3.097327
C	-0.178645	23.899173	1.394860
C	0.313697	23.084902	3.615612
C	-0.081241	24.119973	2.769124
H	0.359130	23.247224	4.686525
H	-0.496848	24.697283	0.731306
H	0.050186	22.466704	-0.200209
H	-0.326625	25.091264	3.187265
Cl	-0.315382	19.503431	0.135349
C	0.999534	20.738805	4.078490
C	2.473652	20.744104	4.547810
F	0.745735	19.498216	3.565739
F	0.254715	20.866206	5.217603
F	2.767403	21.931859	5.104123
F	2.670033	19.784546	5.464693
F	3.306607	20.531699	3.521489
Br	3.450514	17.062679	-1.448476

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V'_oBr_B3LYP

Cu	-0.906998	-0.088899	0.082828
N	0.713533	1.367924	0.017375
N	0.701782	-1.348327	0.030036
C	0.695039	2.695550	0.019632
C	1.868368	3.474692	-0.001938
C	3.094266	2.838391	-0.027767
C	4.374257	0.681729	-0.057180
C	4.368216	-0.681926	-0.058938
C	3.077275	-2.829285	-0.031183
C	1.849063	-3.460643	-0.001100
C	0.679522	-2.679801	0.030170
C	1.911035	0.731254	-0.006211
C	3.146221	1.425401	-0.031042
C	3.134543	-1.417045	-0.031882
C	1.905108	-0.713549	-0.003073
H	-0.285993	3.161727	0.039797
H	1.794353	4.557101	0.002007
H	4.019726	3.407488	-0.044962
H	5.310966	1.231718	-0.076360
H	5.299823	-1.240340	-0.080026
H	4.000329	-3.401933	-0.053944
H	1.769359	-4.542438	-0.000186
H	-0.301970	-3.141695	0.056330
Br	-3.213514	0.302613	0.213858

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VII'_oBr_B3LYP

Cu	11.307058	3.620085	1.197434
C	11.195970	0.574712	2.087804
H	12.277384	0.667170	2.131781
C	10.550286	-0.589333	2.545025

H	11.138598	-1.407347	2.947518	C	0.778753	14.414817	2.575277	H	4.447733	15.437269	6.412663
C	9.172470	-0.662856	2.470063	H	0.539533	14.023793	1.590700	C	4.823466	16.773495	4.750351
H	8.639173	-1.545962	2.811472	C	0.227843	13.838125	3.737698	C	4.307587	17.208550	3.503477
C	8.446192	0.428806	1.943384	H	-0.444879	12.990888	3.652495	C	6.054246	17.329204	5.238681
C	9.187153	1.562617	1.521417	C	0.562259	14.369052	4.968289	H	6.432936	16.982746	6.196331
C	7.014620	0.437959	1.832379	H	0.159614	13.950684	5.886829	C	6.736432	18.264664	4.518486
H	6.465924	-0.441862	2.157421	C	1.441021	15.474890	5.034334	H	7.670071	18.677717	4.890390
C	6.356349	1.521241	1.329835	C	1.933304	15.986925	3.806343	C	6.243286	18.726519	3.251302
H	5.273086	1.521365	1.245196	C	1.834924	16.090539	6.269836	C	6.919444	19.685441	2.463492
C	7.073099	2.691708	0.906927	H	1.447916	15.681264	7.198892	H	7.856289	20.105733	2.819143
C	8.487873	2.720166	1.009538	C	2.675794	17.163537	6.278990	C	6.381535	20.070611	1.250673
C	6.433958	3.841861	0.391508	H	2.974690	17.626615	7.215222	H	6.877816	20.799365	0.618237
H	5.351609	3.854940	0.295337	C	3.181126	17.719127	5.054789	C	5.162161	19.501832	0.835868
C	7.195853	4.931761	0.016643	C	4.032106	18.846580	5.021200	H	4.712362	19.780591	-0.112703
H	6.738252	5.829089	-0.386906	H	4.343403	19.309568	5.953600	C	5.024299	18.208460	2.743409
C	8.593474	4.871528	0.171108	C	4.445324	19.350607	3.804453	N	3.156555	16.715532	2.983240
H	9.221029	5.713945	-0.102951	H	5.088538	20.221263	3.740808	N	4.498382	18.607237	1.558083
C	10.595515	5.909410	3.651744	C	4.000379	18.732815	2.623410	F	1.609058	15.712074	-0.990279
C	10.299568	6.810655	2.616269	H	4.267514	19.126951	1.650412	F	3.281946	17.012512	-1.624801
H	10.691707	6.625100	1.619372	C	2.803149	17.142383	3.816506	F	3.297283	14.350086	0.681273
C	9.505951	7.933231	2.858374	N	1.602622	15.453520	2.606954	F	3.924758	14.395390	-1.403265
H	9.284887	8.623357	2.048404	N	3.208579	17.660375	2.623630	F	4.961190	15.623622	0.065050
C	8.989939	8.160950	4.137141	F	1.119161	17.809681	-1.400049	C	2.770790	16.321944	-0.520314
H	8.366256	9.030662	4.326205	F	2.849160	16.480350	-1.827151	C	3.742183	15.162895	-0.303552
C	9.273635	7.265175	5.172082	F	-0.256342	15.698571	-0.362004	O	0.031328	16.491671	1.577743
H	8.873023	7.437717	6.167649	F	0.463859	15.393436	-2.394334	C	-0.506269	16.868380	0.543784
C	10.073266	6.145296	4.933285	F	1.429051	14.363421	-0.736696	C	0.000688	17.961760	-0.286934
H	10.282107	5.452170	5.742826	C	1.833514	16.698493	-0.882448	C	-0.360588	18.116629	-1.644308
C	13.363826	5.028377	3.664928	C	0.864443	15.538346	-1.111902	C	1.077078	18.762642	0.195508
C	14.406888	4.674661	2.796401	O	2.421071	20.407433	0.153063	C	0.293366	19.014474	-2.474717
H	14.180185	4.126994	1.884316	C	1.231199	20.200674	0.244436	C	1.694327	19.719262	-0.630524
C	15.722288	5.044907	3.091039	C	0.565321	19.677273	1.474188	C	1.330720	19.810801	-1.966138
H	16.525027	4.768698	2.412334	C	-0.222472	18.514298	1.392600	H	-1.140727	17.496675	-2.062842
C	16.000974	5.774565	4.248596	C	0.789209	20.232556	2.742753	H	-0.003309	19.100336	-3.515147
H	17.023101	6.066337	4.475540	C	-0.746363	17.924332	2.540591	H	2.461403	20.364108	-0.219429
C	14.962883	6.136840	5.114516	C	0.257547	19.662056	3.894211	H	1.842910	20.520907	-2.609637
H	15.177475	6.708643	6.013662	C	-0.505462	18.495583	3.789038	Br	1.084891	19.374322	2.207652
C	13.649812	5.765190	4.826102	H	-0.375858	18.050327	0.429109	C	-1.770380	16.058076	0.137826
H	12.848145	6.051107	5.501496	H	-1.325811	17.010952	2.454771	C	-1.449109	14.788621	-0.685047
C	11.251062	3.217377	4.512292	H	0.431978	20.116509	4.862944	F	-2.385875	15.634466	1.271108
C	9.915720	2.783424	4.601410	H	-0.905845	18.040673	4.690037	F	-2.673063	16.795057	-0.570564
H	9.151438	3.260665	3.993855	Br	1.785103	21.912015	2.963599	F	-0.563067	14.026638	-0.030690
C	9.565329	1.737496	5.452894	C	0.341978	20.605856	-0.966632	F	-0.939003	15.114868	-1.883779
H	8.529774	1.412188	5.506980	C	-0.119422	22.076112	-0.830598	F	-2.567584	14.073578	-0.883472
C	10.545010	1.101195	6.223413	F	-0.781721	19.848142	-1.072874				
H	10.273224	0.280682	6.882091	F	1.048544	20.507097	-2.113516	50			
C	11.872766	1.522870	6.138326	F	0.940630	22.896024	-0.820953	IV_2_oBr_B3LYP			
H	12.639857	1.034636	6.733884	F	-0.794995	22.232571	0.322845	Cu	2.258082	17.428797	1.280145
C	12.226423	2.575756	5.288115	F	-0.920743	22.413368	-1.847973	C	2.539393	15.713864	3.625236
H	13.263720	2.891665	5.230960					H	1.620672	15.326316	3.203861
N	10.540626	1.617933	1.592417	50				C	3.015465	15.275255	4.870367
N	9.223396	3.806987	0.656724	OATS_2_oBr_B3LYP				H	2.458218	14.524147	5.419484
P	11.666919	4.473186	3.231813	Cu	2.619393	17.488608	1.066047	C	4.183358	15.818214	5.368195
Br	12.828572	3.755067	-0.740773	C	2.480670	15.795895	3.662780	H	4.579048	15.506268	6.330818
				H	1.564845	15.444311	3.199326	C	4.874384	16.794987	4.617641
50				C	2.910997	15.306555	4.910013	C	4.327657	17.179170	3.366766
III_2_oBr_B3LYP				H	2.320734	14.555390	5.424362	C	6.091877	17.402078	5.076128
Cu	2.431323	16.907611	0.942849	C	4.084147	15.795038	5.453129	H	6.488081	17.094011	6.039511

C	6.735498	18.338278	4.324053	C	6.020024	20.342333	1.189869	N	1.784888	16.881045	2.498620
H	7.657552	18.793440	4.674707	H	6.404142	21.196211	0.641535	N	4.371133	17.712993	2.488820
C	6.214119	18.742956	3.049903	C	4.855582	19.689982	0.740263	O	1.965465	19.809202	1.140948
C	6.854550	19.697350	2.226991	H	4.342744	20.042835	-0.149042	C	0.866989	20.314364	1.081623
H	7.778063	20.160095	2.564301	C	4.929967	18.174797	2.474789	C	0.527788	21.619231	1.730689
C	6.299237	20.021328	1.005301	N	3.211636	16.493182	2.631434	C	0.109921	22.677859	0.910575
H	6.767717	20.743525	0.344639	N	4.324598	18.641816	1.354702	C	0.684917	21.839105	3.114445
C	5.098780	19.392684	0.617332	F	2.060003	15.892277	-1.819197	C	-0.103795	23.947033	1.445764
H	4.645924	19.619657	-0.343788	F	3.698461	17.364317	-1.598596	C	0.447668	23.111344	3.642237
C	5.008167	18.171381	2.566234	F	3.071515	14.547629	0.388282	C	0.068295	24.165394	2.812013
N	3.175569	16.629942	2.899074	F	4.268982	14.761053	-1.407849	H	0.549633	23.274187	4.709082
N	4.467351	18.505715	1.371840	F	4.780134	15.908573	0.352389	H	-0.409101	24.759319	0.793349
F	1.955359	15.557517	-0.891981	C	2.830313	16.570331	-0.911322	H	-0.028728	22.511684	-0.151046
F	3.643718	16.958722	-1.084796	C	3.748938	15.427520	-0.357257	H	-0.105268	25.148739	3.237982
F	3.221792	14.272842	1.138341	O	0.556398	15.583881	0.844705	C	1.033120	20.745698	4.098588
F	4.282065	14.375182	-0.757704	C	-0.214345	16.077167	0.031105	C	2.515220	20.716217	4.543297
F	4.954337	15.584904	0.911992	C	0.045562	17.348951	-0.645627	F	0.733880	19.503846	3.617438
C	2.918024	16.228951	-0.180702	C	-0.948564	18.096155	-1.302334	F	0.314827	20.910269	5.251881
C	3.862175	15.104248	0.296494	C	1.360777	17.883152	-0.565476	F	2.845482	21.893088	5.103637
O	0.210837	15.935668	1.453892	C	-0.648007	19.329712	-1.872987	F	2.701343	19.746823	5.452940
C	-0.457154	16.298368	0.494133	C	1.666507	19.086421	-1.197325	F	3.329370	20.492038	3.505720
C	-0.121273	17.465480	-0.332801	C	0.658881	19.821259	-1.824189	Br	3.540316	17.138106	-1.390535
C	-0.959628	17.983043	-1.346048	H	-1.965422	17.730901	-1.345683	C	-0.232217	19.603288	0.230070
C	1.129540	18.079635	-0.114464	H	-1.429931	19.899519	-2.364968	C	-1.598256	19.417918	0.930583
C	-0.550919	19.069940	-2.108851	H	2.682248	19.456346	-1.193422	F	-0.451192	20.332147	-0.904172
C	1.541271	19.158731	-0.882519	H	0.902066	20.775481	-2.283088	F	0.200206	18.376181	-0.131710
C	0.698661	19.656759	-1.880806	Br	0.867492	18.873085	2.545866	F	-2.400741	18.660206	0.172844
H	-1.927229	17.539865	-1.536949	C	-1.500085	15.249376	-0.244084	F	-1.428083	18.811942	2.118393
H	-1.204424	19.459903	-2.883266	C	-2.630911	15.557127	0.763958	F	-2.191234	20.602681	1.132980
H	2.504298	19.621159	-0.700992	F	-1.992711	15.445808	-1.497384				
H	1.021394	20.503122	-2.481622	F	-1.201577	13.933768	-0.114341	50			
Br	1.238273	19.127145	2.703771	F	-2.217576	15.288555	2.009156	III'_2_oBr_B3LYP			
C	-1.657769	15.370987	0.143614	F	-3.710584	14.812907	0.493240	Cu	2.582917	17.029024	0.971208
C	-1.354789	14.431688	-1.047447	F	-2.975936	16.855228	0.694974	C	0.686245	14.748248	2.763828
F	-1.926703	14.575865	1.204858					H	0.372466	14.351581	1.802728
F	-2.791173	16.070939	-0.147671	50				C	0.115106	14.276118	3.963266
F	-2.373629	13.583259	-1.239334	V_2_oBr_B3LYP				H	-0.644234	13.501259	3.931608
F	-0.243024	13.725516	-0.790768	Cu	2.938719	17.414567	0.881398	C	0.541582	14.815870	5.161229
F	-1.167454	15.135204	-2.174970	C	0.503000	16.525549	2.498590	H	0.126977	14.477585	6.107124
				H	0.010568	16.515476	1.533321	C	1.534207	15.823042	5.157758
50				C	-0.197254	16.192039	3.671952	C	2.040569	16.230892	3.896009
RETS_2_oBr_B3LYP				H	-1.246244	15.922526	3.609274	C	2.034266	16.434215	6.356155
Cu	2.307174	17.487149	1.063303	C	0.470650	16.212450	4.880500	H	1.630348	16.109862	7.311182
C	2.648030	15.458810	3.246925	H	-0.036926	15.953578	5.805783	C	2.999888	17.394927	6.299535
H	1.742375	15.074615	2.793694	C	1.835667	16.576493	4.913688	H	3.382616	17.851753	7.207794
C	3.181978	14.888782	4.415234	C	2.451148	16.918618	3.684495	C	3.537850	17.831568	5.041920
H	2.682258	14.042496	4.874340	C	2.606820	16.612810	6.124486	C	4.542597	18.820469	4.945844
C	4.334748	15.425029	4.954146	H	2.116562	16.337711	7.054254	H	4.936662	19.271037	5.852546
H	4.776147	15.012250	5.857265	C	3.918774	16.983497	6.112351	C	5.007944	19.198744	3.703270
C	4.948579	16.530822	4.324677	H	4.495586	17.009560	7.032795	H	5.778393	19.953887	3.591646
C	4.341519	17.038558	3.147931	C	4.564807	17.367992	4.889398	C	4.446147	18.609042	2.558557
C	6.141613	17.147583	4.831000	C	5.906700	17.807291	4.826156	H	4.762662	18.905387	1.564902
H	6.589158	16.739993	5.733107	H	6.500512	17.845312	5.735466	C	3.047977	17.268296	3.837425
C	6.698087	18.219011	4.199319	C	6.441261	18.189094	3.610598	N	1.615627	15.692401	2.730237
H	7.599421	18.685920	4.586884	H	7.466100	18.536213	3.529103	N	3.492348	17.679319	2.615996
C	6.107392	18.760964	3.008768	C	5.632151	18.125163	2.459418	F	1.178384	17.828968	-1.368971
C	6.647202	19.874759	2.327049	H	6.017741	18.415811	1.486050	F	2.961671	16.569435	-1.781655
H	7.546955	20.350286	2.707892	C	3.833499	17.339356	3.675655	F	-0.106453	15.676044	-0.300870

F	0.655422	15.344503	-2.312596	C	4.269175	18.366847	0.480872	C	4.964918	17.615484	-3.481549
F	1.648804	14.419562	-0.609950	C	4.393449	17.806482	-0.888504	C	5.387344	16.346074	-3.085983
C	1.939915	16.766108	-0.832817	C	4.702224	16.455129	-1.090204	O	3.853299	20.170997	-0.032455
C	1.032058	15.550678	-1.030193	C	4.235651	18.653906	-2.014398	H	5.077765	17.919848	-4.515612
O	1.998231	20.501355	0.220337	C	4.891968	15.946991	-2.372124	H	5.509460	14.943300	-1.450528
C	0.852614	20.235273	0.383785	C	4.429411	18.125484	-3.292674	H	4.467838	16.487899	0.177826
C	0.208608	19.417203	1.454600	C	4.760648	16.783646	-3.477598	H	5.841407	15.680182	-3.813478
Cl	-0.384852	20.896272	-0.822593	O	4.660212	19.399016	0.923156	C	3.905570	19.822317	-3.127045
C	-0.662140	18.398652	1.043926	H	4.305806	18.768351	-4.155958	C	5.003157	20.915302	-3.169726
C	0.472504	19.589554	2.834134	H	5.141011	14.897970	-2.498935	F	2.835751	20.326262	-2.457594
C	-1.271528	17.561395	1.974378	H	4.801435	15.801915	-0.234562	F	3.511399	19.665054	-4.430818
C	-0.180006	18.765269	3.756056	H	4.903283	16.399223	-4.482784	F	5.965995	20.541129	-4.032627
C	-1.041507	17.753789	3.333671	C	3.840284	20.117886	-1.966484	F	4.487194	22.081254	-3.586396
H	-0.824728	18.238225	-0.013089	C	5.046404	21.091662	-2.013349	F	5.562871	21.099197	-1.968147
H	-1.918744	16.761475	1.630160	F	3.094308	20.453681	-0.877987				
H	-0.007275	18.912174	4.814830	F	3.084794	20.432381	-3.062825	50			
H	-1.517326	17.113985	4.069673	F	5.671360	20.975094	-3.198545	RETS'_2_oBr_B3LYP			
C	1.334936	20.697229	3.401370	F	4.628391	22.358783	-1.874373	C	1.690738	15.877330	2.841379
C	0.639243	22.079333	3.395902	F	5.929035	20.823375	-1.042559	H	2.178973	15.332814	2.039227
F	2.514453	20.853450	2.741233					C	1.150063	15.204674	3.951884
F	1.647031	20.443606	4.708850	50				H	1.217288	14.123498	4.009682
F	1.438659	23.013980	3.925735	IV'_2_oBr_B3LYP				C	0.541824	15.942640	4.949017
F	-0.493777	22.024105	4.112449	C	1.254293	15.901044	2.666455	H	0.112057	15.456729	5.820695
F	0.334275	22.441458	2.136226	H	1.664373	15.354151	1.823961	C	0.477953	17.349919	4.835516
				C	0.621381	15.233809	3.728276	C	1.050344	17.937543	3.679790
50				H	0.539219	14.152470	3.709016	C	-0.137591	18.189866	5.824047
OATS'_2_oBr_B3LYP				C	0.113872	15.977634	4.775957	H	-0.571562	17.719950	6.702219
C	0.611391	15.962248	3.115144	H	-0.385042	15.495922	5.612333	C	-0.179169	19.543521	5.665857
H	0.851808	15.247092	2.336665	C	0.246108	17.384054	4.762837	H	-0.647105	20.174902	6.416057
C	-0.105412	15.572297	4.261214	C	0.903734	17.971531	3.652887	C	0.393842	20.170994	4.508291
H	-0.414135	14.538377	4.374590	C	-0.252381	18.225203	5.814814	C	0.379607	21.569169	4.300063
C	-0.407241	16.522866	5.216770	H	-0.754353	17.754557	6.655481	H	-0.084391	22.215188	5.040429
H	-0.968035	16.260940	6.109891	C	-0.100878	19.579106	5.762910	C	0.956498	22.092691	3.159646
C	0.022431	17.856123	5.032122	H	-0.480423	20.210106	6.561876	H	0.963158	23.160791	2.969289
C	0.754269	18.148765	3.852913	C	0.565751	20.204964	4.656191	C	1.545734	21.216890	2.227624
C	-0.247808	18.903089	5.976443	C	0.756586	21.602327	4.555359	H	2.005067	21.584726	1.316832
H	-0.815076	18.658100	6.870171	H	0.384515	22.250912	5.343939	C	1.011133	19.372321	3.513215
C	0.191371	20.174606	5.756326	C	1.415637	22.121777	3.458036	N	1.638392	17.197099	2.707599
H	-0.019901	20.966102	6.469936	H	1.580399	23.189087	3.352077	N	1.572349	19.901041	2.397152
C	0.948946	20.502059	4.581463	C	1.884763	21.239654	2.463647	F	0.394190	19.908686	-0.401723
C	1.428844	21.803756	4.314675	H	2.415963	21.605308	1.589976	F	0.961388	18.493560	-1.988876
H	1.219528	22.606141	5.016860	C	1.070980	19.405395	3.599778	F	-0.590553	18.005424	1.084305
C	2.156115	22.035532	3.163888	N	1.385448	17.222558	2.627774	F	-1.158262	17.608438	-0.968742
H	2.535777	23.023163	2.923898	N	1.718604	19.927001	2.532733	F	0.401644	16.417433	-0.039576
C	2.415134	20.962175	2.291691	F	0.943490	19.823370	-0.468615	C	0.934815	18.685928	-0.630200
H	2.996249	21.107616	1.389155	F	1.444410	17.935207	-1.500849	C	-0.113825	17.660859	-0.121364
C	1.243697	19.489894	3.632449	F	-0.757618	18.443460	1.181193	Cu	2.525589	18.337861	1.164250
N	1.021831	17.208966	2.911782	F	-1.118877	18.187368	-0.944150	Cl	4.718079	18.005929	1.658046
N	1.981431	19.726650	2.517091	F	-0.205314	16.573079	0.190950	C	2.896339	19.182809	-0.614540
F	-0.165453	18.454181	-0.146529	C	1.142771	18.477335	-0.266871	C	3.659101	18.284317	-1.542189
F	1.479227	18.407813	-1.623115	C	-0.252448	17.913073	0.052942	C	3.415474	16.907137	-1.448469
F	-0.007277	15.788478	0.162419	Cu	2.501844	18.191284	1.176842	C	4.631763	18.738781	-2.467753
F	-0.115165	16.359765	-1.933071	Cl	4.432741	17.876842	2.374954	C	4.135195	15.980885	-2.194143
F	1.769719	15.663541	-1.096791	C	3.665879	19.000766	-0.166902	C	5.362584	17.796216	-3.199379
C	1.064732	17.827981	-0.426564	C	4.230255	18.095735	-1.220155	C	5.127390	16.428393	-3.063242
C	0.670958	16.406236	-0.833109	C	4.613478	16.801357	-0.848724	O	2.965412	20.376618	-0.498913
Cu	2.151172	17.972615	1.224666	C	4.379402	18.496729	-2.568456	H	6.120557	18.136529	-3.893900
Cl	4.220120	16.872916	1.985906	C	5.202074	15.935174	-1.767895	H	3.923846	14.921018	-2.090892

H 2.647170 16.560986 -0.767126
H 5.711270 15.722931 -3.646548
C 4.959893 20.193916 -2.749752
C 5.981868 20.823135 -1.766089
F 5.559133 20.309805 -3.979775
F 3.856008 20.983388 -2.801591
F 6.096559 22.140953 -1.997201
F 7.182766 20.248194 -1.964674
F 5.639548 20.641518 -0.487240

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V'_2_oBr_B3LYP
Cu 3.011200 17.125409 0.835127
C 0.576608 16.636405 2.435030
H 0.116092 16.617925 1.454648
C -0.185778 16.417320 3.594903
H -1.249712 16.226669 3.504960
C 0.440279 16.451668 4.824527
H -0.115666 16.279914 5.742198
C 1.826377 16.716507 4.891245
C 2.513262 16.944294 3.672592
C 2.548052 16.762087 6.131536
H 1.999968 16.577055 7.051224
C 3.884287 17.029003 6.158359
H 4.425014 17.061620 7.100228
C 4.606217 17.289984 4.946290
C 5.983782 17.605679 4.921334
H 6.539683 17.644298 5.854304
C 6.601045 17.864600 3.712978
H 7.656096 18.112933 3.659705
C 5.835054 17.804116 2.531377
H 6.287126 18.001494 1.562577
C 3.925665 17.253652 3.702233
N 1.884105 16.890961 2.464873
N 4.542669 17.508530 2.524928
O 1.937731 20.004966 1.001396
C 0.806068 20.429201 1.013093
C 0.396745 21.668822 1.744205
C -0.173842 22.714382 1.003525
C 0.641926 21.852325 3.120809
C -0.450584 23.941185 1.604923
C 0.342232 23.080401 3.716487
C -0.187267 24.126559 2.961274
H 0.512111 23.213898 4.778823
H -0.874411 24.745673 1.011787
H -0.381282 22.574074 -0.050780
H -0.406887 25.076092 3.439564
C 1.141521 20.754040 4.032601
C 2.653671 20.801534 4.362275
F 0.878596 19.513055 3.530881
F 0.509427 20.836072 5.244495
F 2.965603 21.999321 4.888366
F 2.953234 19.852231 5.263957

F 3.399884 20.603627 3.271590
Cl 3.770690 16.964795 -1.213285
C -0.268251 19.677382 0.163763
C -1.608631 19.407840 0.887198
F -0.543004 20.409171 -0.955869
F 0.229213 18.481720 -0.223160
F -2.335662 18.517143 0.201827
F -1.372800 18.915610 2.116830
F -2.315767 20.539812 1.008041

14
o-Br-C6H4COCl_B3LYP
C -1.414066 -0.563334 0.184872
C -0.029758 -0.591740 0.059164
C 0.710627 0.592156 -0.116048
C 0.008165 1.813920 -0.142033
C -1.374455 1.850575 0.010337
C -2.085979 0.658798 0.164034
C 2.175136 0.522496 -0.342570
O 2.845918 1.214599 -1.040431
Cl 3.014632 -0.823703 0.612443
H -1.897870 2.800016 0.011722
H -1.962402 -1.492218 0.304226
H 0.491322 -1.541799 0.075188
H -3.165748 0.696144 0.273232
Br 0.901477 3.552678 -0.299727

20
o-Br-C6H4COC2F5_B3LYP
C -1.465509 -0.429879 0.517432
C -0.075122 -0.412789 0.556289
C 0.654101 0.703495 0.102365
C -0.069421 1.790703 -0.418726
C -1.458300 1.772480 -0.488714
C -2.156628 0.661798 -0.007849
C 2.133544 0.716941 0.263579
C 2.942302 -0.567376 -0.110303
C 3.547125 -1.300709 1.106659
F 3.979267 -0.180914 -0.897483
F 2.194346 -1.467000 -0.801232
F 2.564694 -1.698365 1.939338
F 4.374546 -0.493671 1.777890
F 4.225530 -2.382270 0.702786
O 2.783005 1.665923 0.645270
H -1.996150 2.611845 -0.915081
H -2.003824 -1.295904 0.889333
H 0.456442 -1.262812 0.965845
H -3.241556 0.655672 -0.055611
Br 0.819421 3.369021 -1.179980

20
o-C2F5-C6H6COCl_B3LYP
C -1.466210 -0.462531 0.340231
C -0.080025 -0.599597 0.326297
C 0.740391 0.483594 -0.015476
C 0.155008 1.733409 -0.307214
C -1.235808 1.862199 -0.267993
C -2.045030 0.769893 0.042076
C 2.205174 0.238433 -0.141785
O 2.915546 0.492286 -1.060216
H -1.685930 2.827312 -0.470755
H -2.087270 -1.317055 0.590246
H 0.371170 -1.556791 0.563510
H -3.123695 0.890159 0.062194
Cl 2.921122 -0.604230 1.335736
C 0.949045 2.982215 -0.622214
C 1.079229 3.291278 -2.135103
F 0.330341 4.077113 -0.080866
F 2.207312 2.938741 -0.102164
F 1.849016 4.372446 -2.326247
F 1.614937 2.258679 -2.796669
F -0.140460 3.538527 -2.647048

26
o-C2F5-C6H4COC2F5_B3LYP
C -1.513770 -0.554966 0.015923
C -0.134014 -0.751132 -0.007078
C 0.740714 0.326586 -0.211592
C 0.206582 1.625957 -0.347386
C -1.177467 1.812119 -0.303131
C -2.037116 0.727421 -0.134739
C 2.205245 0.040876 -0.345621
O 2.877450 0.371318 -1.294359
H -1.583310 2.813387 -0.390160
H -2.173644 -1.405473 0.156914
H 0.263809 -1.750965 0.113697
H -3.109911 0.891594 -0.108196
C 1.052960 2.871674 -0.492353
C 1.191206 3.386184 -1.947627
F 0.483119 3.905936 0.202816
F 2.310843 2.708007 0.006715
F 2.011409 4.446909 -1.992274
F 1.672045 2.436976 -2.757255
F -0.018325 3.762934 -2.403645
C 2.912264 -0.754057 0.801319
C 2.776492 -0.105934 2.197009
F 2.404555 -2.020438 0.880473
F 4.230589 -0.844549 0.525102
F 3.163661 1.178361 2.136089
F 1.502875 -0.153734 2.617260
F 3.543693 -0.749011 3.086921