Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Three-centre electron sharing indices (3c-ESI) as a tool to differentiate among (an)agostic interactions and hydrogen bonds in transition metal complexes

Yago García-Rodeja[a] , Ferran Feixas,[a] Eduard Matito[b,c] and Miquel Solà*[a]

[a] *Institut de Química Computacional i Catàlisi and Departament de Química, Universitat de Girona, Campus Montilivi, 17071 Girona, Catalonia, Spain.* .[b] *Donostia International Physics Center (DIPC), Donostia, Euskadi, Spain.* [c] *Ikerbasque Foundation for Science, 48011 Bilbao, Euskadi, Spain.*

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COMPUTATIONAL DETAILS

All DFT calculations were performed with the Gaussian16 set of programs.[1] The initial geometry of the molecular systems, which was obtained previously from the Cambridge Crystallographic Data Centre (CCDC) from their corresponding CSD number, was optimized with the GGA functional of Becke's functional[2] with the gradient correction of Perdew along with his local correlation functional.[3] Pople's split-valence double-zeta basis set with diffuse functions for heavy atoms, one set of *d* polarization functions for heavy atoms and *p* polarization functions for hydrogen ones,[4] together with the Stuttgart-Dresden ECPs[5, 6] for Iodine and with a set of *f* polarization functions for transition metals[7] were used. The geometry optimizations were performed without symmetry constraints (except for the compound **GEGRIX** for which have been used the geometry obtained by X-Ray diffraction), and the characterization of the local stationary points was carried out by analytical frequency calculations. Corrections due to dispersion were included through the D3 Grimme's scheme method with the Becke-Johnson damping function (GD3BJ keyword in Gaussian).[8, 9] This method is denoted as BP86-D3BJ/6–31+G(d,p)~SDD+f(M)~SDD(I). The calculation of the 3c-ESI was performed with the ESI-3D program[10, 11] using the wavefunction generated by Gaussian16.

3C-ESI AS AN INDICATOR OF 3C-2E AND 3C-4E BONDING

Let us consider the example of the allyl cation and allyl anion. σ-Electrons in these systems are core electrons or they are localized in C–C and C–H bonds as 2c-2e bonds. As a consequence, the contribution to the 3c-ESI of the σ-system is close to zero. On the other hand, we have 2 π-electrons in the allyl cation that generate a 3c-2e π-bond and 4 π-electrons in the allyl cation that generate a 3c-4e π-bond (see Figure S1).

In the case of the allyl cation, taking into account that we have one α and one β electron, the contribution to the 3c-ESI from the π-system (which amounts as much as the total 3c-ESI) is given by:

$$\delta^{SD}(C_1,C_2,C_3) = 8S_{11}(C_1)S_{11}(C_2)S_{11}(C_3) \quad ,$$

where the subindex 1 refers to the occupied π-orbital in Figure S1. The latter is a positive quantity because $S_{11}(C_1)$, $S_{11}(C_2)$, and $S_{11}(C_3)$ are positive.

On the other hand, for the allyl anion, one has to consider not only the in phase bonding orbital **1** but also the non-bonding orbital **2**. So the expression one has to use to get the 3c-ESI is:

$$\begin{aligned}\delta^{SD}(C_1,C_2,C_3) &= 8\,[S_{11}(C_1)S_{11}(C_2)S_{11}(C_3) + S_{21}(C_1)S_{11}(C_2)S_{12}(C_3) + S_{12}(C_1)S_{21}(C_2)S_{11}(C_3) \\ &\quad + S_{11}(C_1)S_{12}(C_2)S_{21}(C_3) + S_{12}(C_1)S_{22}(C_2)S_{21}(C_3) + S_{21}(C_1)S_{12}(C_2)S_{22}(C_3) + S_{22}(C_1)S_{21}(C_2)S_{12}(C_3) + S_{22}(C_1)S_{22}(C_2)S_{22}(C_3)]\end{aligned}$$

,

where $S_{12}(C_2)$ = $S_{21}(C_2)$= $S_{22}(C_2)$ = 0 or close to zero because there is no contribution from atom C_2 to orbital **2** (see Figure S1).

Consequently, we get:

$$\delta^{SD}(C_1,C_2,C_3) \approx 8\,[S_{11}(C_1)S_{11}(C_2)S_{11}(C_3) + \underset{\text{(-)}}{S_{21}(C_1)}\underset{\text{(+)}}{S_{11}(C_2)}\underset{\text{(+)}}{S_{12}(C_3)}]$$

in which, according to the shape of the molecular orbitals of Figure S1, only $S_{21}(C_1) < 0$ and, consequently, the sign of the 3c-DI depends on whether $S_{11}(C_1) > |S_{21}(C_1)|$ or $S_{11}(C_1) < |S_{21}(C_1)|$. Since in most cases $S_{11}(C_1) < |S_{21}(C_1)|$, the final sign is negative or very close to zero.

Figure S1. Molecular orbitals of the allyl cation and anion with the value of the 3c-ESI computed at the BP86-D3BJ/6–31+G(d,p) level of theory.

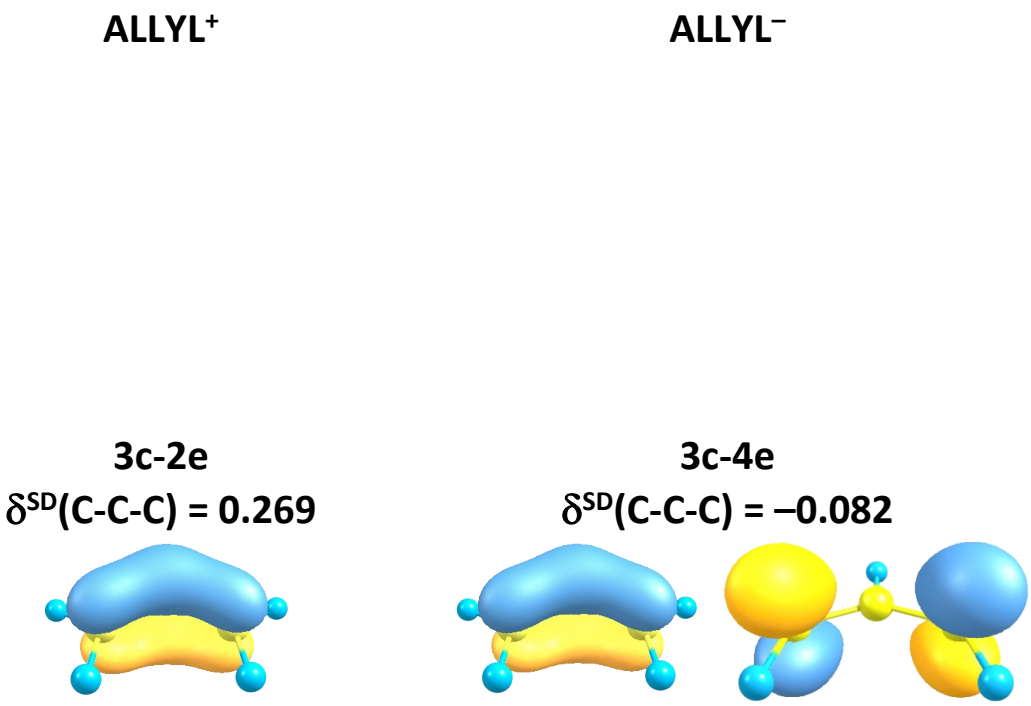

Table S1. QTAIM parameters for different transition metal complexes.

CCDC	d(M···H)	ρ	$\nabla^2\rho$	ε	3c-ESI
CIPKOB	2.006	0.0457	0.0188	0.0042	-0.0186
COCMOV	2.205	0.0362	0.0658	0.0449	-0.0002
WOCMUX	2.549	0.0165	0.0449	2.0935	0.0080
JODFAM	2.359	0.0190	0.0346	0.1335	0.0137
YACDIT	2.339	0.0272	0.0708	0.0542	0.0206
VIGIT[a]	2.287	0.0314	0.0734	0.0252	0.0248
No BCP found for systems with 3c-ESI values ranging from 0.025 to 0.050					
KEHLAK	2.123	0.0385	0.1619	1.8963	0.0575
WODFOK	1.889	0.0611	0.1974	0.3274	0.0648
IMOZIU	2.089	0.0429	0.1238	0.4225	0.0729
XAMPUY	1.966	0.0544	0.1702	0.5680	0.0838
$Cp^*Co(C_2H_2)_2$	1.659	0.0785	0.2943	0.6269	0.0909

As can be observed, the presence of a bond critical point (BCP) between the transition metal and the hydrogen is not enough to discriminate among (an)agostic interactions and hydrogen bonds. Although BCPs are found in the hydrogen bond region, there are no BCPs for complexes with 3c-ESI values lower than 0.050 and higher than 0.025. In our particular study, this problem affects 6 complexes that do not present a BCP, i.e., 15% of the systems.

Table S2. 3c-ESI computed at different levels of theory.

CCDC	Level	Metal	r(M)	d^n	d(M···H)	d(M···C)	d(C-H)	a(M···C-H)	d-r(M)	3c-ESI	SD
CIPKOB	**BP86-D3BJ/SDD+f(M), 6-31+G(d,p)**	Ni	1.24	10	2.006	3.114	1.108	179.73	0.766	-0.0186	**2.6E-03**
	BP86-D3BJ/def2-SVP				1.978	3.104	1.126	180.00	0.738	-0.0188	
	M062X/SDD+f(M), 6-31+G(d,p)				2.08	3.151	1.071	179.94	0.840	-0.0143	
	B3LYP-D3BJ/SDD+f(M), 6-31+G(d,p)				2.06	3.132	1.072	179.89	0.820	-0.0143	
KILKOF	**BP86-D3BJ/SDD+f(M), 6-31+G(d,p)**	Pt	1.36	8	1.919	2.394	1.195	97.80	0.559	0.1026	**7.4E-03**
	BP86-D3BJ/def2-SVP				1.919	2.395	1.198	97.70	0.559	0.0983	
	M062X/SDD+f(M), 6-31+G(d,p)				2.01	2.432	1.156	96.61	0.650	0.0863	
	B3LYP-D3BJ/SDD+f(M), 6-31+G(d,p)				1.919	2.398	1.18	98.58	0.559	0.1013	
WOCMUX	**BP86-D3BJ/SDD+f(M), 6-31+G(d,p)**	Ni	1.24	8	2.549	3.286	1.106	123.03	1.309	0.0076	**1.1E-03**
	BP86-D3BJ/def2-SVP				2.517	3.273	1.112	124.11	1.277	0.0053	
	M062X/SDD+f(M), 6-31+G(d,p)				2.654	3.365	1.095	121.97	1.414	0.0072	
	B3LYP-D3BJ/SDD+f(M), 6-31+G(d,p)				2.597	3.317	1.093	122.65	1.357	0.0077	
KEHLAK	**BP86-D3BJ/SDD+f(M), 6-31+G(d,p)**	Zr	1.75	0	2.123	2.537	1.139	97.49	0.373	0.0575	**5.8E-03**
	BP86-D3BJ/def2-SVP				2.130	2.537	1.147	96.84	0.380	0.0565	
	M062X/SDD+f(M), 6-31+G(d,p)				2.199	2.573	1.122	96.14	0.449	0.0450	
	B3LYP-D3BJ/SDD+f(M), 6-31+G(d,p)				2.163	2.564	1.121	97.51	0.413	0.0502	

CARTESIAN COORDINATES

Cartesian coordinates of all the compounds discussed in the text. Level of theory: BP86-D3BJ/6–31+G(d,p)~SDD+f(M)~SDD(I).

BIMHAH

Pt	0.053128	-0.011783	-0.198041
P	-2.273790	0.074646	-0.003949
P	2.368716	-0.074540	0.007855
C	0.051512	0.205956	-2.226093
H	0.364021	1.241862	-2.442442
H	-0.938163	0.020224	-2.664957
H	0.781442	-0.502082	-2.650745
C	-2.894047	1.838116	-0.061589
H	-3.978110	1.803610	0.154676
C	-2.180153	2.661742	1.027622
H	-1.088995	2.661983	0.853938
H	-2.365879	2.278324	2.044142
H	-2.531200	3.707082	0.997792
C	-2.681371	2.464389	-1.450773
H	-3.051034	3.503697	-1.445376
H	-3.221220	1.929038	-2.248326
H	-1.610190	2.490155	-1.711584
C	-3.199696	-0.853396	-1.339526
H	-2.983303	-0.230836	-2.229586
C	-4.726737	-0.900711	-1.158088
H	-5.194738	-1.278831	-2.083040
H	-5.162500	0.089171	-0.946035
H	-5.011020	-1.586920	-0.344071
C	-2.599657	-2.249363	-1.595540
H	-2.860139	-2.956211	-0.792895
H	-1.500464	-2.214686	-1.673457
H	-3.001372	-2.655948	-2.539102
C	-2.728213	-0.546511	1.712286
H	-1.996938	-0.005483	2.345167
C	-4.138323	-0.175880	2.206555
H	-4.923636	-0.682319	1.625617
H	-4.330799	0.907931	2.173281
H	-4.245452	-0.495599	3.257585
C	-2.451610	-2.055304	1.853639
H	-2.470574	-2.339641	2.919342
H	-1.471068	-2.343211	1.436836
H	-3.224899	-2.650074	1.341486
C	3.271984	1.541764	-0.222201
H	4.240998	1.441722	0.302082
C	2.459110	2.681387	0.421279
H	2.995671	3.637928	0.302087
H	2.291946	2.526320	1.499527
H	1.471528	2.774352	-0.062832
C	3.531902	1.816215	-1.714971
H	2.588976	1.858129	-2.285988
H	4.183819	1.059173	-2.178968

H	4.030058	2.794116	-1.826423
C	3.289477	-1.381852	-0.951105
H	3.235169	-1.022698	-1.996916
C	4.766091	-1.511458	-0.538166
H	4.858555	-1.893941	0.492566
H	5.310680	-0.555189	-0.602046
H	5.277285	-2.230315	-1.200818
C	2.537694	-2.723210	-0.864638
H	3.003784	-3.457306	-1.543052
H	1.476067	-2.614568	-1.143013
H	2.580064	-3.146833	0.153822
C	2.446956	-0.547510	1.825891
H	2.530306	-1.650450	1.805717
C	3.610364	0.023444	2.646539
H	3.565822	1.122937	2.712547
H	4.588378	-0.253684	2.222685
H	3.570799	-0.370980	3.676868
C	1.065658	-0.189916	2.420901
H	0.232070	-0.655900	1.813668
H	0.925336	-0.621620	3.428120
H	0.905411	0.897619	2.488606

BIXFUJ

Ti	-0.190694	0.921604	-0.014976
Cl	-2.495313	1.451444	-0.215405
Cl	0.080283	0.674786	-2.306118
Cl	-0.195566	0.770243	2.288810
P	1.814092	-0.654148	0.016896
P	-1.228116	-1.420317	0.032623
C	1.515424	2.212815	0.074958
C	0.480135	3.324739	0.136404
C	1.322534	-2.394552	-0.456786
C	0.032216	-2.773558	0.287921
H	2.141789	2.142176	0.974190
H	2.117286	2.228510	-0.841999
H	0.541335	4.017471	-0.717862
H	0.494891	3.875809	1.089117
H	-0.593456	2.961880	0.077874
H	1.156272	-2.387482	-1.549034
H	2.145992	-3.100465	-0.245915
H	0.216437	-2.845952	1.374879
H	-0.367787	-3.747282	-0.046077
C	3.231758	-0.323454	-1.116306
H	3.918741	-1.185665	-1.142127
H	2.837919	-0.124692	-2.124724
H	3.781121	0.565027	-0.769175
C	2.643497	-0.899428	1.649597
H	1.917347	-1.292760	2.376354
H	3.500510	-1.587485	1.556853
H	2.988307	0.076022	2.025797
C	-2.490866	-1.722560	1.335537
H	-3.314418	-1.008843	1.180591

H	-2.869318	-2.757391	1.290264
H	-2.040677	-1.520968	2.319363
C	-2.076885	-1.892161	-1.533629
H	-1.343727	-1.910593	-2.353906
H	-2.569421	-2.874182	-1.436982
H	-2.820266	-1.112523	-1.760849

BPPMBPmod

Pd	0.023057	0.054135	-0.306689
Br	0.053909	-2.208690	0.812687
P	2.320011	0.043351	-0.169034
P	-2.281090	0.018209	-0.131413
C	0.003155	1.711965	-1.408313
H	0.260999	1.526609	-2.464902
C	-0.281669	2.988593	-1.044827
H	-0.314719	3.756434	-1.833574
C	-0.574328	3.467491	0.305534
H	-1.126024	4.415817	0.365223
C	-0.201940	2.869097	1.464598
H	0.391035	1.946408	1.462034
H	-0.469321	3.295303	2.436667
C	2.907587	0.281842	1.557373
C	2.048981	0.007144	2.641859
C	4.209206	0.770042	1.801374
C	2.494660	0.218062	3.955295
C	4.649596	0.973627	3.118099
C	3.791694	0.700490	4.197395
H	1.044775	-0.384682	2.449874
H	4.872369	0.999701	0.961377
H	1.821585	0.003301	4.791601
H	5.660913	1.351952	3.299166
H	4.133339	0.866905	5.224312
C	3.259364	1.321950	-1.090949
C	4.153011	1.002102	-2.130330
C	3.030045	2.674563	-0.755353
C	4.813619	2.027004	-2.829805
C	3.698264	3.691158	-1.449656
C	4.588513	3.370692	-2.490948
H	4.336830	-0.044877	-2.389357
H	2.331208	2.928344	0.048024
H	5.508970	1.770804	-3.635837
H	3.515826	4.737138	-1.182965
H	5.104742	4.167903	-3.035717
C	3.008440	-1.549987	-0.749894
C	3.968423	-2.269731	-0.018849
C	2.510405	-2.069502	-1.963147
C	4.435464	-3.502046	-0.504706
C	2.987846	-3.293005	-2.450135
C	3.951798	-4.012099	-1.720256
H	4.330564	-1.881582	0.937762
H	1.733722	-1.520012	-2.506898
H	5.172448	-4.068132	0.074066

H	2.597409	-3.694002	-3.391013
H	4.314106	-4.975577	-2.093018
C	-2.771262	-0.509793	1.555453
C	-3.681046	-1.558237	1.775676
C	-2.167853	0.138239	2.653272
C	-3.990694	-1.950695	3.088337
C	-2.489436	-0.247646	3.960804
C	-3.400727	-1.296018	4.181275
H	-4.129069	-2.082367	0.926802
H	-1.443131	0.938424	2.471738
H	-4.689002	-2.777292	3.254752
H	-2.018582	0.261437	4.808165
H	-3.640927	-1.608518	5.202677
C	-3.068863	-1.177968	-1.283160
C	-2.292265	-2.207677	-1.852640
C	-4.436920	-1.067501	-1.611822
C	-2.884068	-3.115041	-2.744716
C	-5.022980	-1.981599	-2.500716
C	-4.246194	-3.005056	-3.071012
H	-1.235209	-2.297223	-1.582018
H	-5.038941	-0.263422	-1.176681
H	-2.275751	-3.911337	-3.185716
H	-6.084923	-1.890373	-2.751162
H	-4.702455	-3.713970	-3.769776
C	-3.237039	1.557351	-0.428500
C	-3.270643	2.079111	-1.739295
C	-3.877630	2.256156	0.611031
C	-3.945532	3.277644	-2.005687
C	-4.547798	3.461404	0.342604
C	-4.580944	3.975950	-0.963126
H	-2.766770	1.543606	-2.549540
H	-3.854753	1.860331	1.630080
H	-3.966737	3.672614	-3.026541
H	-5.044330	3.996613	1.158541
H	-5.102925	4.915802	-1.170602

BPPMBP

Pd	-0.193221	-0.859295	-0.060819
Br	-0.677114	-2.973867	1.129714
P	2.072868	-1.312975	0.250195
P	-2.444489	-0.274649	-0.144847
C	0.305627	0.616154	-1.309694
C	0.646226	1.919627	-1.068272
C	0.597373	2.552742	0.263393
C	0.146910	1.911402	1.376843
H	-0.222582	0.881065	1.275069
C	2.544139	-1.026787	2.000505
C	1.550360	-0.943042	2.994888
C	3.901493	-0.863827	2.353921
C	1.911586	-0.702068	4.328321
C	4.256760	-0.623953	3.689361
C	3.261601	-0.541372	4.678928

H	0.501050	-1.078823	2.721878
H	4.675370	-0.908142	1.581325
H	1.131195	-0.636991	5.092751
H	5.310730	-0.493941	3.954747
H	3.539789	-0.346217	5.719753
C	3.286834	-0.300552	-0.681448
C	3.892230	-0.779565	-1.858276
C	3.531880	1.023439	-0.259509
C	4.742578	0.056856	-2.598194
C	4.374244	1.857786	-1.005348
C	4.984364	1.374072	-2.175219
H	3.697245	-1.799175	-2.199858
H	3.059030	1.414839	0.645303
H	5.213581	-0.325784	-3.509668
H	4.522939	2.888696	-0.672942
H	5.643627	2.025545	-2.758703
C	2.470106	-3.055224	-0.143035
C	3.194514	-3.871888	0.742670
C	1.978766	-3.583073	-1.355735
C	3.443344	-5.212525	0.407389
C	2.238614	-4.919863	-1.686317
C	2.971229	-5.736760	-0.806863
H	3.541495	-3.471420	1.699532
H	1.388392	-2.945472	-2.022148
H	3.998500	-5.850075	1.103089
H	1.858060	-5.327712	-2.628434
H	3.162387	-6.784142	-1.062274
C	-3.436805	-0.908661	1.256154
C	-4.735475	-1.412780	1.065518
C	-2.881725	-0.855386	2.551656
C	-5.480759	-1.857140	2.170327
C	-3.635688	-1.285261	3.651051
C	-4.934094	-1.790965	3.462183
H	-5.160845	-1.465571	0.058638
H	-1.863115	-0.483490	2.693751
H	-6.488252	-2.257663	2.018944
H	-3.199127	-1.247854	4.654094
H	-5.515481	-2.141751	4.320970
C	-3.203868	-0.976361	-1.654470
C	-2.770329	-2.260208	-2.052559
C	-4.180017	-0.295118	-2.406627
C	-3.320008	-2.854135	-3.197655
C	-4.716164	-0.892383	-3.559441
C	-4.288539	-2.171051	-3.955094
H	-2.011576	-2.783428	-1.458782
H	-4.511174	0.700452	-2.095580
H	-2.985240	-3.850899	-3.502301
H	-5.471065	-0.358306	-4.145654
H	-4.707991	-2.634580	-4.853950
C	-2.775439	1.528300	-0.137599
C	-2.442194	2.309509	-1.265239
C	-3.190402	2.165088	1.050921

C	-2.507681	3.707797	-1.194850
C	-3.254408	3.564873	1.112663
C	-2.904364	4.338049	-0.004635
H	-2.099366	1.826841	-2.183409
H	-3.446639	1.571455	1.932005
H	-2.208036	4.303343	-2.061777
H	-3.563921	4.049514	2.044094
H	-2.926392	5.430316	0.054460
C	0.232851	0.005707	-2.665147
O	0.884715	-0.962221	-3.056414
O	-0.776531	0.563990	-3.407234
C	-1.068998	-0.117778	-4.652209
H	-0.196585	-0.081163	-5.323211
H	-1.338521	-1.165814	-4.449739
H	-1.922222	0.423654	-5.081223
C	1.043893	2.808762	-2.202964
O	0.790202	4.009637	-2.280628
O	1.730855	2.123683	-3.157352
C	2.103608	2.894425	-4.319749
H	1.204872	3.248884	-4.850525
H	2.713635	3.761056	-4.019994
H	2.684132	2.204003	-4.945515
C	1.200177	3.932397	0.399169
O	2.409649	4.127213	0.323179
O	0.273661	4.880584	0.636027
C	0.817150	6.203121	0.864293
H	1.447415	6.193970	1.767378
H	1.411986	6.523910	-0.005196
H	-0.057063	6.852745	1.003980
C	0.137720	2.455685	2.736830
O	0.698317	3.465356	3.159314
O	-0.609954	1.624394	3.548255
C	-0.669682	2.033724	4.930544
H	0.340329	2.040911	5.372193
H	-1.105024	3.042247	5.018123
H	-1.308653	1.290416	5.426833

CIPKOB

Ni	0.001407	0.000296	0.386762
P	-0.751097	-1.933099	-0.351237
P	2.051770	0.315219	-0.351276
P	-1.298690	1.616449	-0.351557
N	0.002576	0.001535	-2.726880
O	0.008592	0.004398	3.329513
C	0.004763	0.001920	2.155459
C	-0.475142	-1.375566	-3.105810
C	-1.485963	-1.897864	-2.078717
C	1.433524	0.276006	-3.106276
C	2.389919	-0.339046	-2.078564
C	-0.951345	1.102786	-3.107122
C	-0.902465	2.237848	-2.078632
C	-2.061958	-2.793824	0.617944

C	0.547120	-3.240663	-0.501436
C	3.453917	-0.386040	0.617866
C	2.531677	2.094396	-0.502787
C	-1.393004	3.181941	0.617382
C	-3.079140	1.141138	-0.501386
H	0.004499	0.003470	-1.619131
H	-0.898484	-1.322387	-4.123722
H	0.409907	-2.031153	-3.132843
H	-2.380931	-1.252177	-2.026013
H	-1.822487	-2.895004	-2.405832
H	1.598622	-0.117134	-4.124295
H	1.559502	1.370276	-3.132624
H	2.276853	-1.436713	-2.025533
H	3.422430	-0.132877	-2.404455
H	-0.691371	1.444083	-4.124045
H	-1.961017	0.662749	-3.137030
H	0.102179	2.694206	-2.025111
H	-1.600610	3.025580	-2.405463
C	-3.261807	-3.278629	0.062242
H	-3.478208	-3.162115	-1.002793
C	-4.217457	-3.903579	0.880838
H	-5.148987	-4.271059	0.438772
C	-3.980907	-4.054962	2.256036
H	-4.726925	-4.542083	2.891199
C	-2.781501	-3.577898	2.814412
H	-2.588295	-3.692115	3.885402
C	-1.830249	-2.946746	2.001647
H	-0.904758	-2.565558	2.444444
C	1.632673	-3.170903	0.395578
H	1.679918	-2.349669	1.117267
C	2.650616	-4.136057	0.359602
H	3.485241	-4.064285	1.062981
C	2.601683	-5.172976	-0.585979
H	3.399075	-5.921534	-0.623325
C	1.520520	-5.253323	-1.481890
H	1.471585	-6.067300	-2.212092
C	0.491789	-4.299503	-1.432917
H	-0.358179	-4.400912	-2.115706
C	3.473700	-0.101315	2.000010
H	2.682794	0.513390	2.441114
C	4.496645	-0.606940	2.813423
H	4.501484	-0.376898	3.883206
C	5.507016	-1.411849	2.257272
H	6.302618	-1.812095	2.892939
C	5.490325	-1.700742	0.883848
H	6.272205	-2.327712	0.443617
C	4.470055	-1.188937	0.064596
H	4.473683	-1.441441	-0.998902
C	1.924431	2.999954	0.390824
H	1.189876	2.629808	1.112160
C	2.247280	4.364996	0.352641
H	1.763593	5.052014	1.053026

C	3.171521	4.841332	-0.591035
H	3.418349	5.906753	-0.630141
C	3.787107	3.944631	-1.482689
H	4.518528	4.309368	-2.210796
C	3.478551	2.576117	-1.431879
H	3.995689	1.890466	-2.111068
C	-1.633151	3.056687	2.002337
H	-1.755941	2.063877	2.446133
C	-1.707384	4.195848	2.815136
H	-1.896331	4.084627	3.887199
C	-1.531836	5.474056	2.255423
H	-1.582941	6.363606	2.890517
C	-1.289919	5.604235	0.878959
H	-1.150698	6.595427	0.435815
C	-1.223494	4.464273	0.060421
H	-1.020482	4.594366	-1.005713
C	-3.561298	0.171166	0.400776
H	-2.874454	-0.274697	1.126577
C	-4.905553	-0.229815	0.365336
H	-5.260510	-0.985015	1.072493
C	-5.778629	0.323955	-0.584808
H	-6.824997	0.005654	-0.621909
C	-5.307766	1.295838	-1.485766
H	-5.987952	1.740398	-2.219156
C	-3.968004	1.711967	-1.437247
H	-3.631152	2.495575	-2.123823

COCMOVmod2

Pd	0.003444	-0.518603	-0.900748
P	1.051878	1.509583	-0.520736
P	-1.929360	-0.169151	0.248851
N	1.694511	-0.913385	-2.035234
N	-0.043634	-1.857008	2.002181
O	2.797803	-2.705327	-3.076467
O	0.859232	-2.248405	4.097703
C	1.804784	-2.219627	-2.494381
C	0.581506	-3.029521	-2.198991
C	-0.484204	-2.434973	-1.480011
C	-1.631087	-3.215832	-1.245571
C	-1.705176	-4.548053	-1.695217
C	-0.629135	-5.127555	-2.389585
C	0.517395	-4.362469	-2.642875
C	1.015502	-2.019347	2.888099
C	2.535914	1.308597	-1.554206
C	3.481401	2.340639	-1.689860
C	4.619806	2.157797	-2.482220
C	4.789705	0.923595	-3.139398
C	3.857849	-0.112976	-3.017629
C	2.692690	0.053836	-2.212925
C	0.922708	2.791186	2.005193
C	1.413948	3.097306	3.282061
C	2.666619	2.613143	3.692711

C	3.422843	1.812514	2.820854
C	2.937120	1.498345	1.543954
C	1.685893	1.998263	1.123753
C	-0.818518	2.674166	-2.197287
C	-1.574034	3.711365	-2.760558
C	-1.374083	5.036202	-2.332610
C	-0.402022	5.318119	-1.357553
C	0.361507	4.281030	-0.797648
C	0.145582	2.950554	-1.203819
C	-1.873323	1.196026	2.732987
C	-2.022780	2.318477	3.562162
C	-2.371276	3.563624	3.014098
C	-2.561128	3.685202	1.626158
C	-2.416576	2.565560	0.793424
C	-2.080703	1.309256	1.343283
C	-4.560528	0.623389	-0.500087
C	-5.602286	0.799327	-1.422767
C	-5.433068	0.405442	-2.761859
C	-4.218300	-0.164863	-3.176349
C	-3.173547	-0.343157	-2.256619
C	-3.339669	0.045256	-0.911569
C	2.594064	-2.110523	0.885485
C	3.877179	-1.958205	0.339347
C	4.950027	-1.596661	1.170707
C	4.739915	-1.407578	2.550023
C	3.456239	-1.547838	3.092738
C	2.369875	-1.880950	2.258940
C	-2.394582	-1.518373	1.416116
C	-3.744052	-1.890064	1.574303
C	-4.125437	-2.840712	2.528945
C	-3.143607	-3.426212	3.346551
C	-1.794548	-3.089891	3.196047
C	-1.398665	-2.149339	2.218018
H	0.187118	-1.495543	1.057142
H	-2.490021	-2.811386	-0.703907
H	-2.610037	-5.132968	-1.494569
H	-0.687492	-6.166252	-2.731090
H	1.380917	-4.766131	-3.182978
H	3.320659	3.286765	-1.161336
H	5.358562	2.957842	-2.588118
H	5.672705	0.760634	-3.767129
H	4.004704	-1.064390	-3.526758
H	-0.049260	3.178281	1.694957
H	0.809459	3.714232	3.954407
H	3.049859	2.853577	4.689598
H	4.394206	1.419911	3.133551
H	3.527679	0.864445	0.876015
H	-0.986762	1.635534	-2.505259
H	-2.327270	3.482418	-3.521024
H	-1.972248	5.847119	-2.760474
H	-0.237434	6.349452	-1.028745
H	1.109609	4.506133	-0.031741

H	-1.607861	0.232532	3.175608
H	-1.862254	2.213743	4.639549
H	-2.491946	4.436568	3.663567
H	-2.823160	4.651212	1.183783
H	-2.577255	2.671314	-0.281767
H	-4.688641	0.953513	0.535345
H	-6.544990	1.249562	-1.095705
H	-6.246098	0.548190	-3.480974
H	-4.078207	-0.470604	-4.217894
H	-2.222821	-0.786670	-2.571133
H	1.779145	-2.441010	0.236927
H	4.032597	-2.134330	-0.729131
H	5.951836	-1.475859	0.745877
H	5.580685	-1.144791	3.200793
H	3.266717	-1.397119	4.159383
H	-4.504177	-1.432070	0.935781
H	-5.178756	-3.116654	2.635360
H	-3.426792	-4.164479	4.103467
H	-1.028019	-3.541849	3.826581

COCMOVmod

Ni	0.033125	-0.461132	-0.942282
P	0.860785	1.533001	-0.479622
P	-1.804040	-0.339446	0.198397
N	1.677298	-0.650784	-2.108721
N	0.188890	-2.066585	1.799843
O	2.892015	-2.282131	-3.283392
O	1.144235	-2.380829	3.882089
C	1.882550	-1.912638	-2.645490
C	0.739062	-2.827748	-2.355701
C	-0.336981	-2.335898	-1.573976
C	-1.423965	-3.210143	-1.368554
C	-1.421589	-4.519263	-1.887523
C	-0.327918	-4.991415	-2.632367
C	0.755620	-4.135655	-2.870420
C	1.269280	-2.146649	2.669874
C	2.360277	1.575709	-1.506907
C	3.215751	2.687503	-1.566582
C	4.354518	2.650446	-2.380145
C	4.609900	1.485670	-3.130387
C	3.764411	0.370770	-3.080384
C	2.604713	0.390059	-2.252416
C	0.693088	2.756582	2.092152
C	1.192882	3.055027	3.368055
C	2.457867	2.588744	3.759069
C	3.220298	1.816058	2.867218
C	2.728251	1.514134	1.590216
C	1.460975	1.993120	1.190371
C	-1.115591	2.603870	-2.096796
C	-1.960081	3.593522	-2.617664
C	-1.868045	4.913512	-2.141690
C	-0.912540	5.239739	-1.163831

C	-0.062670	4.250024	-0.644485
C	-0.174595	2.920340	-1.093764
C	-1.831749	0.867315	2.762446
C	-2.093863	1.899714	3.675626
C	-2.608682	3.127450	3.228817
C	-2.848208	3.323176	1.857519
C	-2.590837	2.292364	0.940948
C	-2.092087	1.049506	1.388416
C	-4.498359	0.297614	-0.508746
C	-5.552929	0.453107	-1.420857
C	-5.361474	0.151247	-2.780217
C	-4.110890	-0.308411	-3.224625
C	-3.054778	-0.467346	-2.314911
C	-3.240495	-0.169606	-0.949000
C	2.811941	-2.030244	0.636023
C	4.064602	-1.737066	0.076889
C	5.121428	-1.331671	0.908596
C	4.928337	-1.242962	2.300534
C	3.673603	-1.523329	2.856496
C	2.599590	-1.897244	2.023907
C	-2.187433	-1.767901	1.315746
C	-3.520702	-2.173427	1.518567
C	-3.842206	-3.154414	2.464817
C	-2.817271	-3.737577	3.229419
C	-1.482861	-3.369101	3.030323
C	-1.150582	-2.396715	2.060990
H	0.379325	-1.734361	0.841993
H	-2.304230	-2.901114	-0.800429
H	-2.284141	-5.169379	-1.701817
H	-0.326311	-6.012551	-3.027550
H	1.629193	-4.445499	-3.454726
H	2.989681	3.575382	-0.966138
H	5.029405	3.510145	-2.431211
H	5.494676	1.440968	-3.775033
H	3.978099	-0.526002	-3.660005
H	-0.291352	3.126589	1.801710
H	0.583586	3.650450	4.055324
H	2.847237	2.822035	4.755283
H	4.203073	1.438919	3.162469
H	3.331186	0.912872	0.903012
H	-1.195718	1.570094	-2.450147
H	-2.695836	3.329489	-3.383795
H	-2.534663	5.687157	-2.536048
H	-0.828567	6.269282	-0.800724
H	0.673295	4.511432	0.121270
H	-1.435132	-0.082986	3.128800
H	-1.888856	1.739249	4.738451
H	-2.818777	3.929586	3.943585
H	-3.238620	4.278235	1.492578
H	-2.793757	2.456291	-0.119495
H	-4.648545	0.561264	0.542308
H	-6.523544	0.816331	-1.068133

H	-6.184470	0.278492	-3.490850
H	-3.951887	-0.543859	-4.281618
H	-2.078959	-0.829930	-2.654586
H	2.014625	-2.386632	-0.020935
H	4.207078	-1.834572	-1.003427
H	6.098147	-1.097008	0.473311
H	5.758551	-0.946625	2.950440
H	3.493427	-1.446897	3.932620
H	-4.317011	-1.718627	0.923900
H	-4.884558	-3.455451	2.606207
H	-3.054711	-4.498768	3.979247
H	-0.680280	-3.819784	3.615426

COCMOV

Pt	-0.002534	-0.501034	-0.829198
P	1.025337	1.548079	-0.501845
P	-1.929557	-0.139427	0.311242
N	1.703487	-0.917905	-1.944821
N	-0.007968	-1.765593	2.121239
O	2.811619	-2.711152	-2.980939
O	0.911523	-2.152342	4.213438
C	1.818364	-2.229901	-2.397828
C	0.602367	-3.044263	-2.092457
C	-0.460686	-2.438940	-1.374797
C	-1.601162	-3.226064	-1.119722
C	-1.671360	-4.563967	-1.549445
C	-0.598919	-5.148522	-2.245881
C	0.542557	-4.382268	-2.518760
C	1.055706	-1.929897	3.000792
C	2.528871	1.321615	-1.500064
C	3.477932	2.349779	-1.639033
C	4.630682	2.151405	-2.406040
C	4.811773	0.905040	-3.036035
C	3.877420	-0.128903	-2.910086
C	2.699980	0.053955	-2.128929
C	0.880654	2.932328	1.971243
C	1.358405	3.279102	3.243018
C	2.587600	2.775205	3.697822
C	3.333686	1.914104	2.876179
C	2.861538	1.559962	1.604615
C	1.633997	2.079082	1.140310
C	-0.842723	2.678887	-2.209215
C	-1.573838	3.710266	-2.814299
C	-1.335451	5.047103	-2.448452
C	-0.350175	5.346670	-1.492043
C	0.389223	4.315563	-0.890551
C	0.135191	2.974316	-1.235237
C	-1.874958	1.307106	2.748353
C	-2.040276	2.453320	3.541427
C	-2.406965	3.674959	2.953940
C	-2.597498	3.750163	1.562753
C	-2.437602	2.606277	0.766572

C	-2.084145	1.373381	1.356410
C	-4.581648	0.600520	-0.415926
C	-5.643857	0.732586	-1.322405
C	-5.496218	0.295883	-2.650706
C	-4.282148	-0.271841	-3.070497
C	-3.216805	-0.406342	-2.166897
C	-3.361683	0.024084	-0.832331
C	2.620404	-2.073175	0.991874
C	3.897222	-1.923373	0.430404
C	4.972105	-1.520128	1.239678
C	4.772036	-1.292229	2.614713
C	3.495126	-1.433271	3.173171
C	2.405313	-1.801379	2.358955
C	-2.364359	-1.460031	1.524057
C	-3.710216	-1.839933	1.697066
C	-4.083214	-2.767665	2.676857
C	-3.095037	-3.322590	3.507619
C	-1.749856	-2.977420	3.346163
C	-1.360825	-2.059774	2.342750
H	0.218418	-1.395172	1.173941
H	-2.455565	-2.817154	-0.574255
H	-2.570336	-5.151609	-1.331635
H	-0.655636	-6.191998	-2.572559
H	1.402903	-4.791042	-3.059467
H	3.308337	3.306124	-1.132311
H	5.371818	2.949000	-2.513481
H	5.705447	0.729407	-3.644803
H	4.032846	-1.089547	-3.398519
H	-0.074455	3.332921	1.626889
H	0.761719	3.942761	3.876717
H	2.960974	3.047647	4.690224
H	4.286770	1.506420	3.223617
H	3.446417	0.883081	0.974597
H	-1.038518	1.631319	-2.466842
H	-2.337397	3.468182	-3.560311
H	-1.913913	5.853823	-2.910061
H	-0.156130	6.386918	-1.210947
H	1.148567	4.555308	-0.140266
H	-1.596782	0.361330	3.220557
H	-1.878244	2.385745	4.621530
H	-2.541210	4.566065	3.575523
H	-2.873414	4.697855	1.090147
H	-2.601301	2.674479	-0.311194
H	-4.694053	0.962983	0.610490
H	-6.585623	1.181840	-0.991333
H	-6.325315	0.403730	-3.357453
H	-4.158479	-0.609956	-4.104100
H	-2.265942	-0.844524	-2.486831
H	1.801383	-2.430112	0.363220
H	4.046917	-2.131502	-0.633069
H	5.967991	-1.397733	0.801666
H	5.615191	-0.998753	3.249122

H	3.313070	-1.253859	4.236730
H	-4.475883	-1.407608	1.047692
H	-5.134031	-3.049797	2.791208
H	-3.369761	-4.043281	4.284386
H	-0.978776	-3.404668	3.988145

Cp*Co(C2H4)2

Co	0.057004	-0.495219	-0.447167
C	1.132854	0.809541	0.783097
C	0.378570	1.600537	-0.174500
C	-1.008878	1.309232	-0.007530
C	-1.122501	0.309391	1.047487
C	0.203306	0.011214	1.549515
C	1.558156	-1.788355	-0.443271
H	2.341762	-1.518461	0.270686
H	1.303632	-2.850249	-0.404676
C	1.619576	-1.137474	-1.776774
H	2.509640	-0.515271	-1.953509
H	0.754380	-0.315163	-1.941969
H	1.405779	-1.800836	-2.628855
C	-1.187277	-2.144084	-0.702561
H	-0.630077	-3.024402	-1.032551
H	-1.765420	-2.286447	0.214084
C	-1.527059	-1.144717	-1.628687
H	-1.211740	-1.229722	-2.674137
H	-2.384486	-0.487904	-1.464409
C	0.524051	-0.877242	2.712275
H	0.434335	-0.311928	3.657591
H	-0.163909	-1.734374	2.768914
H	1.549070	-1.272601	2.655786
C	2.610766	0.920259	1.000351
H	3.177682	0.897762	0.054676
H	2.839199	1.885761	1.486532
H	2.995822	0.125930	1.656187
C	0.968757	2.587135	-1.135515
H	1.976228	2.289392	-1.465861
H	0.334823	2.724137	-2.024642
H	1.067591	3.572340	-0.643791
C	-2.145865	2.002559	-0.694442
H	-2.348517	2.965791	-0.191865
H	-1.920541	2.221072	-1.749892
H	-3.077091	1.417351	-0.653731
C	-2.412370	-0.198432	1.608924
H	-2.846786	0.575008	2.268765
H	-3.160011	-0.407233	0.826392
H	-2.272994	-1.106425	2.213583

Cp*Ir(C2H4)2

Ir	0.511730	-0.047757	-0.159802
C	-1.140239	1.352760	0.409485
C	-1.634582	0.639126	-0.763116
C	-1.661716	-0.762254	-0.467531

C	-1.160678	-0.939827	0.899944
C	-0.892372	0.380438	1.465299
C	2.039471	1.305346	0.358749
H	1.642550	2.245632	0.759646
H	2.864587	0.906976	0.957058
C	2.186642	1.239595	-1.123271
H	1.969770	2.170201	-1.667342
H	1.324020	0.531406	-1.657573
H	3.094915	0.736384	-1.485761
C	1.963067	-1.580236	0.333563
H	2.995926	-1.214496	0.340966
H	1.668616	-2.102910	1.249427
C	1.345920	-1.907046	-0.912430
H	1.902023	-1.776341	-1.847378
H	0.569372	-2.677336	-0.962966
C	-0.537328	0.676855	2.891061
H	-1.459002	0.797864	3.488595
H	0.050713	-0.137388	3.339870
H	0.046562	1.604921	2.981109
C	-1.077482	2.844721	0.549814
H	-0.743588	3.331834	-0.379952
H	-2.079292	3.242995	0.790177
H	-0.401061	3.150752	1.361954
C	-2.070407	1.280365	-2.044552
H	-1.504827	2.200981	-2.254449
H	-1.959215	0.598687	-2.900995
H	-3.137624	1.559669	-1.975624
C	-2.182247	-1.850506	-1.355806
H	-3.272641	-1.958669	-1.211601
H	-2.004454	-1.633102	-2.419914
H	-1.726573	-2.824687	-1.122695
C	-1.142199	-2.236301	1.652187
H	-2.161068	-2.469899	2.008866
H	-0.814213	-3.077313	1.021169
H	-0.483826	-2.187099	2.531797

Cp*Rh(C2H4)2

Rh	0.553675	-0.246383	-0.227629
C	-0.521880	1.595948	0.374403
C	-1.277213	1.044458	-0.751883
C	-1.732366	-0.259271	-0.395427
C	-1.239407	-0.545406	0.957237
C	-0.547386	0.633069	1.456287
C	2.448868	0.486602	0.277984
H	2.367708	1.460366	0.774297
H	3.112756	-0.204981	0.804420
C	2.509297	0.503423	-1.209536
H	2.586114	1.502378	-1.663747
H	1.482257	0.127331	-1.727498
H	3.220004	-0.210543	-1.652287
C	1.404906	-2.221230	0.182108
H	2.498917	-2.197161	0.190755

H	0.948526	-2.609485	1.097524
C	0.713893	-2.268532	-1.047282
H	1.266773	-2.261809	-1.992736
H	-0.293923	-2.689752	-1.112012
C	-0.040397	0.835222	2.851877
H	-0.847526	1.239628	3.489549
H	0.300333	-0.109365	3.301597
H	0.797704	1.547299	2.884292
C	0.024459	2.990177	0.439885
H	0.458692	3.308367	-0.521253
H	-0.785736	3.700892	0.683762
H	0.794028	3.094518	1.219464
C	-1.554661	1.762279	-2.036743
H	-0.729364	2.434438	-2.318061
H	-1.731771	1.061638	-2.866465
H	-2.460588	2.386538	-1.927639
C	-2.630085	-1.145854	-1.202921
H	-3.686646	-0.893615	-0.998175
H	-2.462617	-1.027046	-2.284312
H	-2.498977	-2.208822	-0.948469
C	-1.585784	-1.764287	1.754600
H	-2.609235	-1.659201	2.158494
H	-1.571532	-2.679418	1.141398
H	-0.904755	-1.904531	2.606851

Cu(II)H33m

H	4.897927	0.000023	-1.373616
C	3.980174	0.000028	-0.777744
H	3.810502	-2.169894	-0.804348
H	3.810462	2.169945	-0.804451
C	3.376553	-1.233278	-0.440578
C	3.376529	1.233339	-0.440637
H	1.094285	-2.562859	1.648697
H	1.094302	2.563002	1.648601
C	2.218967	-1.240935	0.342312
C	2.218941	1.241011	0.342248
H	-1.249390	-2.890122	1.371167
C	1.309754	-2.419049	0.575505
C	1.690348	0.000045	0.793091
C	1.309709	2.419117	0.575407
H	1.703200	3.367170	0.172777
H	1.703289	-3.367121	0.172966
H	-1.249448	2.890040	1.371225
H	-3.063481	-1.193456	1.154188
C	-1.133851	-2.950000	0.275160
H	-0.866065	-3.993318	0.025778
N	0.003302	-2.055001	-0.104906
Cu	-0.315122	-0.000034	0.007812
N	0.003229	2.054996	-0.104901
H	-3.063573	1.193382	1.154190
C	-1.133926	2.949962	0.275219
H	-3.171677	-3.343433	-0.236203

C	-3.040285	-1.231931	0.051141
H	-0.866156	3.993294	0.025874
C	-2.429716	-2.549975	-0.430909
H	0.161604	-2.170227	-1.120158
H	0.161449	2.170180	-1.120170
H	-4.086488	-1.159079	-0.298672
N	-2.312210	-0.000004	-0.420263
C	-3.040341	1.231883	0.051145
C	-2.429797	2.549958	-0.430849
H	-2.293622	-2.544148	-1.530450
H	-3.171767	3.343395	-0.236093
H	-4.086529	1.159003	-0.298708
H	-2.359930	-0.000005	-1.452745
H	-2.293718	2.544185	-1.530393
H	1.024746	0.000061	1.681403

EtHfCl3

Hf	-0.096934	-0.000013	0.001155
Cl	0.456634	-2.012776	-1.089069
Cl	0.454924	2.013448	-1.088662
Cl	-2.347656	-0.001009	0.640407
C	1.056236	0.000291	1.843865
H	0.879253	0.892969	2.469163
H	0.879603	-0.892183	2.469538
C	2.461580	0.000438	1.182539
H	3.041101	0.898770	1.447051
H	2.445622	0.001515	0.061736
H	3.040460	-0.898778	1.445414

EtZrCl3

Zr	-0.104746	-0.000013	-0.000066
Cl	0.422218	-2.029812	-1.084080
Cl	0.420128	2.030584	-1.083635
Cl	-2.365669	-0.001251	0.624745
C	0.992431	0.000351	1.873340
H	0.808155	0.897636	2.488294
H	0.808692	-0.896634	2.488864
C	2.376194	0.000582	1.184411
H	2.962317	0.900821	1.425673
H	2.333630	0.001633	0.059655
H	2.961778	-0.900405	1.424139

FAZZAH10

Pt	2.325385	0.033366	-0.168932
Cl	3.155726	-1.307907	1.576404
Cl	2.070676	-1.897884	-1.526240
Cl	1.422160	1.379513	-1.907469
Cl	2.687198	1.965453	1.140207
Pt	-2.326523	-0.026384	0.018352
Cl	-4.192511	1.434756	-0.196530
Cl	-3.621347	-2.006153	0.012934
N	-0.633338	-1.166878	0.203455

N	-1.175287	1.678871	0.002600
C	-0.482570	-1.952102	1.458163
C	-0.757394	2.156581	1.348422
H	0.250476	-0.583904	0.103816
H	-0.565191	-1.808387	-0.601733
H	-1.781640	2.386433	-0.438786
H	-0.328568	1.578211	-0.608192
H	0.486057	-2.480798	1.437847
H	-1.332742	-2.643773	1.547644
H	-0.483271	-1.253815	2.308092
H	-0.176545	3.091057	1.260177
H	-0.094631	1.406592	1.801034
H	-1.657384	2.300733	1.965261

FEKMOX

Pt	-0.651618	-0.835005	-0.043045
As	1.587678	-1.460537	-0.227587
Cl	-0.556973	-0.359747	-2.348494
Cl	-0.812550	-1.491318	2.216180
N	-2.650198	-0.171878	0.052492
C	-2.921169	1.175916	0.028631
C	-4.264003	1.650708	0.005714
C	-5.292445	0.705256	0.038314
C	-5.000130	-0.671284	0.092707
C	-3.665349	-1.067897	0.093434
N	-1.867395	2.055551	-0.062012
C	-0.815870	1.835874	0.695204
C	0.496385	2.446154	0.503285
C	1.454774	2.292150	1.556098
C	2.745736	2.814295	1.388545
C	3.133763	3.471220	0.204694
C	2.186880	3.591706	-0.827200
C	0.874886	3.100337	-0.710763
C	1.853009	-2.920789	-1.534351
H	1.909567	-2.417014	-2.514071
H	2.827119	-3.396447	-1.325953
C	0.689467	-3.919216	-1.502219
H	-0.253251	-3.403528	-1.747218
H	0.564953	-4.376102	-0.506908
H	0.847903	-4.727933	-2.236930
C	2.729199	-0.016090	-0.910668
H	2.216966	0.329508	-1.823390
H	2.669666	0.796999	-0.172056
C	4.179117	-0.430469	-1.173179
H	4.250737	-1.247438	-1.911041
H	4.689600	-0.763975	-0.253378
H	4.751597	0.425073	-1.572027
C	2.451862	-2.059525	1.444442
H	3.535991	-1.870502	1.360272
H	2.036479	-1.402496	2.225877
C	2.151375	-3.526798	1.767611
H	2.559588	-4.210118	1.003849

H	1.064210	-3.692749	1.838910
H	2.596821	-3.807236	2.737862
C	-4.513903	3.135149	-0.031889
H	-5.585460	3.352365	-0.166872
H	-4.173948	3.620910	0.899776
H	-3.942764	3.601734	-0.852785
C	1.126972	1.556938	2.836129
H	0.804442	0.517985	2.637957
H	2.010538	1.524911	3.493325
H	0.308163	2.037804	3.399030
C	-0.061384	3.251259	-1.881186
H	0.468950	3.705665	-2.734346
H	-0.465779	2.269329	-2.184905
H	-0.933214	3.874070	-1.623315
C	4.523584	4.045010	0.057251
H	4.577923	5.058087	0.497300
H	5.273860	3.424449	0.575549
H	4.814268	4.130672	-1.002617
H	-0.930108	1.220090	1.600803
H	-3.361076	-2.117072	0.118312
H	-5.792153	-1.423264	0.119124
H	-6.333367	1.046913	0.026828
H	3.474266	2.692750	2.199167
H	2.478855	4.077663	-1.765919

FESXAC

Pt	0.359004	-0.457477	-0.003086
P	2.475734	0.303604	0.220947
Cl	-0.205777	0.459526	2.090481
Cl	0.779005	-1.694476	-1.958499
N	-1.675908	-0.999749	-0.162068
C	-2.051873	-2.256934	0.097769
C	-3.394131	-2.602701	0.376117
C	-4.349452	-1.598796	0.421834
C	-4.901408	0.830319	0.190515
C	-4.477712	2.122406	-0.083670
C	-3.142593	2.365253	-0.495896
C	-2.216016	1.329557	-0.607912
C	-2.614891	0.007369	-0.232773
C	-3.982106	-0.257583	0.123092
C	-0.904420	1.625299	-1.281727
O	-0.356163	2.733731	-1.216908
H	-0.566291	0.857245	-2.015074
C	3.198062	-0.113014	1.869869
H	4.217125	0.314899	1.911845
H	2.572454	0.405095	2.615379
C	3.199018	-1.626235	2.137409
H	3.805952	-2.176623	1.398872
H	2.169734	-2.019783	2.095456
H	3.609068	-1.839685	3.138705
C	3.701736	-0.358352	-1.002977
H	4.703946	-0.203774	-0.560125

H	3.520652	-1.443759	-1.070956
C	3.608081	0.283140	-2.396712
H	3.866297	1.354377	-2.373806
H	2.593823	0.170804	-2.809594
H	4.309022	-0.217190	-3.085877
C	2.620584	2.140746	0.037752
H	3.702209	2.351601	-0.070144
H	2.129447	2.386931	-0.919835
C	1.999756	2.978769	1.163018
H	2.459962	2.765041	2.141897
H	0.919972	2.789144	1.243720
H	2.147323	4.049191	0.942297
H	-1.249196	-2.998950	0.103805
H	-3.646532	-3.644829	0.586582
H	-5.387723	-1.821283	0.690509
H	-5.939313	0.626490	0.474015
H	-5.180740	2.957740	-0.011385
H	-2.815509	3.373525	-0.767977

IMOZIU

Pt	-0.033785	-0.786439	-0.041803
N	0.921228	1.022008	-0.024353
Cl	-1.036652	-2.885231	-0.088526
Cl	-0.062909	-0.666948	-2.393762
C	2.273334	1.170186	-0.040556
Cl	0.052622	-0.827538	2.313353
C	2.795330	2.476562	-0.075863
H	3.876302	2.618477	-0.085068
C	1.943239	3.586797	-0.091647
H	2.361046	4.597396	-0.121932
C	0.560804	3.397742	-0.065091
H	-0.125153	4.247021	-0.073469
C	0.052978	2.091063	-0.029779
C	-1.359889	1.726063	0.009209
C	-2.430954	2.645558	0.043899
H	-2.233737	3.721545	0.033984
C	-3.753621	2.196869	0.094325
H	-4.595468	2.892002	0.122581
F	-5.276926	0.379366	0.161432
C	-3.989065	0.815172	0.110540
C	-2.966592	-0.142232	0.075928
H	-3.189320	-1.209753	0.087082
C	-1.662425	0.341454	0.024137
C	3.216700	-0.039294	0.084537
C	4.493927	0.194051	-0.763136
H	5.104586	1.029709	-0.385251
H	4.245487	0.386667	-1.820192
H	5.125676	-0.708343	-0.716968
C	3.599679	-0.158703	1.586020
H	4.085377	0.764505	1.944252
H	4.307171	-0.995738	1.717295
H	2.707207	-0.351043	2.203106

C	2.617128	-1.378915	-0.395315
H	1.788656	-1.760586	0.262748
H	3.371267	-2.176107	-0.272384
H	2.304364	-1.360904	-1.448953

JODFAM

H	-5.933758	-1.272790	1.095567
H	-7.331763	-1.873638	0.156107
N	-3.889335	2.075448	1.144760
H	-3.384541	2.796702	1.661547
C	-5.259704	2.319969	0.946112
C	-5.836985	3.387518	1.671939
H	-5.220102	3.959467	2.374224
C	-7.187340	3.714059	1.502757
H	-7.616308	4.542963	2.073382
C	-7.991579	2.986076	0.613620
H	-9.046831	3.235868	0.479381
C	-7.409697	1.930358	-0.110910
C	-6.058449	1.589173	0.040644
H	-5.612702	0.776823	-0.528496
C	-8.277006	1.125856	-1.047338
F	-9.090218	0.249672	-0.363227
F	-9.110703	1.919580	-1.789622
F	-7.552333	0.371291	-1.930720
C	2.185178	1.100736	3.599439
H	2.277562	1.614557	2.629351
H	1.321551	1.537701	4.128877
H	3.096455	1.278904	4.194419
H	0.906872	-0.809945	5.240484
Ni	-0.013254	-0.376129	0.659310
S	-1.493871	-2.123546	1.045026
P	-2.907671	-1.411977	-0.223264
N	-3.677675	-0.018555	0.164037
C	-3.106865	0.991508	0.790178
S	-1.433532	1.231593	1.303584
O	-4.034359	-2.567372	-0.294146
C	-5.409915	-2.254015	-0.765690
H	-5.367675	-1.308880	-1.334322
C	-6.296728	-2.097368	0.462898
H	-6.295599	-3.028807	1.053501
C	-5.815922	-3.397010	-1.686821
H	-5.788227	-4.357265	-1.144940
H	-6.843229	-3.230045	-2.052088
H	-5.143076	-3.460989	-2.556387
O	-2.357414	-1.130346	-1.726360
C	-1.336164	-1.995943	-2.361118
H	-0.821720	-2.546957	-1.552741
C	-0.355593	-1.051627	-3.042103
H	0.095217	-0.372197	-2.300351
H	0.452800	-1.633369	-3.516700
H	-0.864729	-0.452915	-3.816598
C	-2.041919	-2.969684	-3.298313

H	-1.297357	-3.608711	-3.803237
H	-2.731423	-3.621119	-2.737918
H	-2.612002	-2.423297	-4.068999
S	1.495491	-2.039581	0.362296
P	3.183877	-1.180020	1.116897
O	3.135197	-0.969321	2.719121
C	1.954806	-0.391452	3.401247
H	1.071227	-0.549065	2.746073
C	1.783750	-1.186509	4.687510
H	2.675411	-1.085774	5.329496
H	1.625688	-2.253243	4.463669
O	4.422778	-2.206478	1.074138
C	5.214906	-2.397375	-0.164701
H	5.179118	-1.446350	-0.725644
C	4.595181	-3.524766	-0.984828
H	3.564938	-3.275793	-1.285804
H	5.194770	-3.692381	-1.895952
H	4.574983	-4.459885	-0.400398
C	6.635879	-2.680353	0.304398
H	7.296316	-2.812024	-0.568494
H	6.664691	-3.601021	0.911262
N	3.689288	0.163974	0.324848
C	2.918423	1.087456	-0.210841
S	1.175130	1.346874	-0.067399
H	7.022692	-1.845236	0.907937
N	3.499689	2.073646	-0.985712
H	2.825617	2.722893	-1.393980
C	4.843703	2.309659	-1.323828
C	5.093626	3.335611	-2.266943
H	4.252131	3.892734	-2.694406
C	6.401087	3.641004	-2.655931
H	6.573692	4.437746	-3.385399
C	7.489351	2.934161	-2.119515
H	8.513034	3.166929	-2.420462
C	7.235473	1.923836	-1.177519
C	5.930836	1.601282	-0.770697
H	5.743636	0.824122	-0.031401
C	8.378967	1.111188	-0.621001
F	8.556504	-0.059970	-1.325095
F	8.177702	0.748335	0.683625
F	9.571491	1.778524	-0.673326

KEHCEF

Pt	1.889204	-0.246800	-0.235031
Cl	2.412636	-1.623612	1.538195
N	1.364238	0.989010	-1.862852
N	3.933466	0.185209	-0.268506
N	-0.013423	-0.847973	-0.139949
N	-3.664595	1.049593	-0.203473
C	-0.212675	2.004519	0.735153
C	-0.349811	3.383571	0.868124
C	-1.591978	3.998738	0.577068

C	-2.689128	3.226780	0.209111
C	-4.868452	-1.052587	-0.277868
C	-4.860838	-2.441832	-0.196475
C	-3.650317	-3.139877	0.025094
C	-2.454784	-2.436116	0.133020
C	-1.178287	-0.247025	0.069588
C	-3.657657	-0.332960	-0.147334
C	-2.422279	-1.020592	0.033307
C	-1.294246	1.191743	0.299883
C	-2.561315	1.820153	0.097768
H	0.733590	1.511193	0.993846
H	0.488423	3.985726	1.229625
H	-1.703940	5.082375	0.675175
H	-3.662273	3.694650	0.026892
H	-5.806835	-0.508111	-0.426621
H	-5.801103	-2.992842	-0.287098
H	-3.654577	-4.228445	0.122170
H	-1.534228	-2.992302	0.338340
H	-0.085858	-1.865474	-0.232652
H	-4.558560	1.520250	-0.342458
H	4.176326	1.172474	-0.116132
H	4.314250	-0.357429	0.527441
H	4.418060	-0.138963	-1.115857
H	0.578176	0.553055	-2.364013
H	1.032668	1.905458	-1.526106
H	2.105984	1.152245	-2.554626

KEHLAKmod2

Zr	1.033907	-0.575927	-0.012785
I	2.125100	2.215956	0.124975
Si	-2.459908	-2.194131	-0.072153
C	-1.179011	-0.837902	-0.096249
C	-1.248920	0.506149	-0.161794
C	-1.679450	-3.831247	-0.641524
C	-3.109367	-2.451403	1.696973
C	-3.873959	-1.837228	-1.288874
C	0.727519	-2.313880	1.822061
C	0.432213	-1.063522	2.449592
C	1.615835	-0.282828	2.458323
C	2.657738	-1.045096	1.832447
C	2.110026	-2.311449	1.469646
C	1.464912	-2.398614	-1.664607
C	0.554410	-1.514608	-2.316751
C	1.219329	-0.272675	-2.526263
C	2.566055	-0.406351	-2.056586
C	2.719254	-1.712077	-1.525534
C	-2.323748	1.508943	-0.083855
C	-3.598061	1.211706	0.450865
C	-4.596897	2.192068	0.498954
C	-4.339216	3.490756	0.022682
C	-3.067568	3.805486	-0.486631
C	-2.065795	2.826364	-0.531924

H	-0.276186	1.092797	-0.291743
H	-1.353942	-3.778690	-1.694406
H	-0.805838	-4.121085	-0.034929
H	-2.423566	-4.643922	-0.567406
H	-2.293108	-2.748952	2.377503
H	-3.572930	-1.542157	2.115092
H	-3.866952	-3.254999	1.710847
H	-4.410827	-0.901836	-1.066578
H	-3.474091	-1.753029	-2.314705
H	-4.603122	-2.667078	-1.280414
H	0.028041	-3.133058	1.666748
H	-0.546851	-0.746035	2.806854
H	1.713216	0.734547	2.832058
H	3.682451	-0.709163	1.674034
H	2.646847	-3.133029	0.996891
H	1.250321	-3.421437	-1.356300
H	-0.477857	-1.737222	-2.578504
H	0.785095	0.627866	-2.960370
H	3.322216	0.376070	-2.065677
H	3.628416	-2.114551	-1.079681
H	-3.792011	0.214062	0.851347
H	-5.577857	1.946780	0.919176
H	-5.121182	4.255656	0.063133
H	-2.852937	4.818438	-0.841845
H	-1.066990	3.073707	-0.908977

KEHLAKmod

Zr	-1.391909	-0.418274	0.056654
Cl	-1.271799	-2.893576	0.570196
Si	1.207492	2.397013	-0.255217
C	0.565667	0.643910	-0.140141
C	1.212100	-0.547167	-0.151919
C	-0.111243	3.487917	-1.088228
C	1.558162	3.136831	1.463453
C	2.745668	2.522752	-1.363040
C	-1.819286	1.570100	1.611823
C	-1.080691	0.629560	2.397082
C	-1.879257	-0.531054	2.561171
C	-3.114799	-0.324091	1.866497
C	-3.083167	0.989588	1.306024
C	-2.492384	0.831307	-1.821428
C	-1.283639	0.316986	-2.375184
C	-1.379106	-1.105541	-2.393773
C	-2.668225	-1.470964	-1.894677
C	-3.355130	-0.281404	-1.537447
C	2.631965	-0.923224	-0.012353
C	3.562150	-0.105501	0.667844
C	4.906720	-0.484425	0.771804
C	5.346766	-1.695108	0.206804
C	4.425574	-2.532645	-0.446104
C	3.079216	-2.155341	-0.543735
H	0.604712	-1.487543	-0.276970

H	-0.278610	3.183125	-2.135471
H	-1.085052	3.456277	-0.572945
H	0.228499	4.538707	-1.102018
H	0.647805	3.171623	2.085401
H	2.319336	2.566548	2.022245
H	1.928387	4.171908	1.354485
H	3.621983	1.999915	-0.949789
H	2.534787	2.082733	-2.353560
H	3.013580	3.583670	-1.515878
H	-1.481922	2.560856	1.314468
H	-0.064217	0.766213	2.764728
H	-1.583792	-1.448462	3.066817
H	-3.931178	-1.042473	1.792097
H	-3.881441	1.465161	0.737390
H	-2.723133	1.884461	-1.663109
H	-0.428009	0.903633	-2.702083
H	-0.603399	-1.798850	-2.718664
H	-3.028820	-2.488028	-1.750817
H	-4.357496	-0.227397	-1.113138
H	3.214562	0.817786	1.138157
H	5.612647	0.159783	1.306416
H	6.397195	-1.991319	0.290575
H	4.755919	-3.485390	-0.872454
H	2.357353	-2.814313	-1.039163

KEHLAK

Zr	-1.255817	-0.007643	0.006959
Br	-1.409149	-2.711728	-0.034543
Si	1.544437	2.628414	-0.015257
C	0.775074	0.931665	-0.000216
C	1.261693	-0.324997	0.007199
C	0.181813	3.949180	-0.078054
C	2.541197	2.924411	1.577929
C	2.626849	2.875113	-1.559591
C	-1.078367	1.261244	2.202118
C	-1.098695	-0.121920	2.555749
C	-2.385749	-0.641996	2.228486
C	-3.147402	0.398649	1.630988
C	-2.334961	1.583326	1.611655
C	-2.223901	1.681506	-1.580866
C	-1.046987	1.195962	-2.223198
C	-1.247178	-0.182057	-2.528202
C	-2.572620	-0.535435	-2.122926
C	-3.175105	0.607393	-1.535373
C	2.581171	-0.975434	0.004707
C	3.803895	-0.266607	0.042207
C	5.024090	-0.953872	0.034622
C	5.048773	-2.360354	-0.009677
C	3.839717	-3.076267	-0.043844
C	2.617701	-2.391515	-0.034787
H	0.512449	-1.183385	0.014946
H	-0.378777	3.908737	-1.026938

H	-0.539372	3.834539	0.748482
H	0.625862	4.957036	0.002002
H	1.873982	2.937684	2.457637
H	3.302490	2.147551	1.755898
H	3.051331	3.903219	1.533998
H	3.416877	2.113073	-1.656144
H	2.010688	2.827616	-2.474695
H	3.107675	3.869358	-1.534716
H	-0.245293	1.944766	2.351428
H	-0.270190	-0.687697	2.982063
H	-2.705714	-1.673933	2.357188
H	-4.173899	0.314127	1.276950
H	-2.638432	2.563096	1.244517
H	-2.384830	2.697790	-1.224016
H	-0.144501	1.768573	-2.426965
H	-0.516274	-0.857380	-2.973034
H	-3.017499	-1.525432	-2.203078
H	-4.183857	0.661110	-1.128229
H	3.796132	0.824341	0.080439
H	5.962780	-0.390721	0.064683
H	6.005286	-2.892589	-0.015946
H	3.849191	-4.170517	-0.076325
H	1.668606	-2.940552	-0.059461

KEKZAB

Pt	0.637155	-0.045181	-0.670272
S	-3.741309	1.536679	-0.485294
S	-3.813444	-1.484923	-0.980810
N	-0.997059	1.303342	-0.849782
N	-1.046266	-1.329328	-0.892236
C	-0.782512	2.754045	-0.812848
C	-1.993144	3.587169	-1.230247
C	-3.209929	3.297500	-0.353210
C	-3.330646	-3.247257	-0.756265
C	-0.860781	-2.777633	-1.026771
C	-2.063065	-3.562621	-1.550362
C	-2.181399	0.751862	-0.764739
C	-2.211262	-0.737006	-0.878687
C	2.657841	1.707463	0.712656
C	3.584137	2.761467	0.796462
C	3.974843	3.460444	-0.358956
C	3.432127	3.089748	-1.600959
C	2.496249	2.042204	-1.680238
C	2.078338	1.337284	-0.523883
C	1.926189	-2.329815	0.753896
C	2.858632	-3.360450	0.965136
C	3.935994	-3.531053	0.079436
C	4.077386	-2.649351	-1.006369
C	3.153366	-1.608889	-1.203342
C	2.041417	-1.438453	-0.342443
H	0.085699	2.955742	-1.461037
H	-0.453811	3.006311	0.212634

H	-1.729898	4.655798	-1.137155
H	-2.238765	3.400039	-2.290826
H	-2.997068	3.504181	0.708251
H	-4.092462	3.882019	-0.657571
H	-4.199849	-3.824120	-1.108809
H	-3.193921	-3.436886	0.321269
H	0.018722	-2.915575	-1.676157
H	-0.547424	-3.142895	-0.030422
H	-1.835044	-4.640264	-1.465056
H	-2.231878	-3.346292	-2.619829
H	2.388653	1.161341	1.622850
H	4.009954	3.030750	1.769947
H	4.701913	4.276863	-0.293554
H	3.738450	3.614597	-2.513518
H	2.087722	1.764976	-2.660266
H	1.099039	-2.218477	1.464838
H	2.743828	-4.027061	1.827819
H	4.663489	-4.333830	0.240185
H	4.921173	-2.762077	-1.696962
H	3.298973	-0.913267	-2.036315
Cl	-1.761951	-1.203186	2.456336
Cl	0.723948	-0.196985	3.717005
Cl	-1.269788	1.711426	2.647450
C	-0.503927	0.091033	2.451107
H	-0.002942	0.068554	1.443049

KILKOF

Pt	-0.021393	-0.497798	-0.758060
P	1.811247	0.300446	0.487255
P	-1.738868	0.297787	0.478545
C	-1.028923	-1.636728	-2.205212
C	0.377708	-1.842811	-2.698160
C	1.393737	1.176500	2.071747
C	-1.192246	1.117384	2.059555
C	2.834446	-1.196079	1.095895
C	3.831722	-0.842791	2.220565
C	1.802489	-2.208242	1.644783
C	3.588188	-1.850334	-0.079280
C	2.883721	1.527769	-0.504565
C	4.286528	1.743717	0.093953
C	2.992041	1.019692	-1.958967
C	2.138298	2.880024	-0.527572
C	-2.857821	-1.112033	1.128684
C	-3.805632	-1.618996	0.023423
C	-3.691259	-0.685552	2.360024
C	-1.909650	-2.257411	1.548419
C	-2.745035	1.628652	-0.454324
C	-4.048541	1.992610	0.286221
C	-1.867222	2.893433	-0.570340
C	-3.064975	1.147242	-1.883785
H	4.336990	-1.770463	2.543606
H	4.611673	-0.139968	1.897208

H	3.333703	-0.422936	3.109058
H	2.333469	-3.099504	2.023670
H	1.215015	-1.794949	2.482178
H	1.094872	-2.528509	0.861492
H	4.049392	-2.790723	0.270434
H	2.914250	-2.108188	-0.913665
H	4.397682	-1.213132	-0.467474
H	4.791810	2.551083	-0.465577
H	4.249036	2.055308	1.151365
H	4.919533	0.846898	0.014846
H	3.600668	1.730106	-2.545882
H	3.472412	0.032078	-2.033447
H	1.995156	0.962085	-2.429403
H	2.674211	3.569103	-1.203885
H	1.111192	2.770586	-0.911687
H	2.100970	3.358588	0.464347
H	-4.307610	-2.534159	0.383670
H	-4.593457	-0.889392	-0.218930
H	-3.268398	-1.875422	-0.900838
H	-4.319651	-1.543191	2.658403
H	-3.065503	-0.429660	3.229029
H	-4.365530	0.157534	2.154461
H	-2.510694	-3.086985	1.960817
H	-1.330064	-2.637206	0.691965
H	-1.197122	-1.945314	2.330274
H	-4.513537	2.849243	-0.233055
H	-4.780865	1.171605	0.280366
H	-3.874646	2.304197	1.329553
H	-2.378575	3.615590	-1.230825
H	-1.711555	3.391428	0.399390
H	-0.889115	2.662018	-1.022825
H	-3.673775	1.919983	-2.385263
H	-2.139564	1.011646	-2.464761
H	-3.633283	0.206569	-1.906221
C	0.083256	1.981357	2.046874
H	-1.691301	-1.092294	-2.887246
H	-1.507221	-2.539108	-1.802430
H	0.601551	-1.376571	-3.668706
H	0.739993	-2.880450	-2.644789
H	1.191143	-1.307042	-2.005565
H	-1.067344	0.305997	2.798187
H	-2.048721	1.720819	2.407551
H	0.077645	2.677201	1.197318
H	0.059838	2.609492	2.955713
H	1.331446	0.406380	2.860300
H	2.241873	1.829991	2.341363

MIJDOBmod

C	-3.127231	0.960088	0.449181
C	-4.441205	0.778030	0.030241
C	-4.729092	-0.177171	-0.962697
C	-3.662523	-0.906283	-1.483729

C	-2.350868	-0.683042	-1.020740
C	-1.195893	-1.410924	-1.509026
C	-1.223699	-2.451798	-2.446584
C	-0.029241	-3.076845	-2.834241
C	1.172708	-2.622568	-2.283050
C	1.175266	-1.572976	-1.347867
C	2.355294	-0.987706	-0.754620
C	3.673156	-1.361931	-1.089443
C	4.766275	-0.699065	-0.539776
C	4.504174	0.371531	0.344945
C	3.194545	0.701554	0.655129
C	-1.959137	-2.145928	2.131756
C	1.105313	3.879810	-0.544860
C	-0.800744	1.953547	1.929974
C	0.613875	1.991626	2.406456
Mo	0.044148	0.475100	0.551396
N	-2.058392	0.258694	-0.045658
N	-0.013724	-0.976051	-0.931832
N	2.092096	0.035837	0.156513
P	-0.293267	-1.339328	2.185998
P	0.267391	2.311579	-1.069420
H	-2.902638	1.701250	1.210860
H	-5.227830	1.388728	0.480895
H	-5.749889	-0.341852	-1.316510
H	-3.833796	-1.656693	-2.258693
H	-2.176641	-2.775204	-2.870240
H	2.119404	-3.077004	-2.582386
H	3.827226	-2.176508	-1.800855
H	5.788275	-0.986533	-0.796796
H	5.315043	0.951196	0.793829
H	2.988459	1.533017	1.330758
H	-2.737271	-1.402941	2.368218
H	-2.022650	-2.982571	2.846843
H	-2.147263	-2.526217	1.115030
H	2.130220	3.653916	-0.208129
H	0.553153	4.343669	0.288824
H	1.156291	4.601074	-1.377255
H	-1.159417	2.897698	1.494253
H	-1.507497	1.573674	2.682852
H	1.213705	1.088427	1.980877
H	1.182783	2.891948	2.136461
H	0.735162	1.764195	3.477607
H	-0.037037	-3.894492	-3.558528
C	-1.308102	2.942928	-1.807262
H	-1.116658	3.739275	-2.545199
H	-1.836875	2.110735	-2.298564
H	-1.960129	3.337337	-1.011604
C	1.244055	1.837727	-2.567425
H	1.286725	2.661503	-3.298766
H	2.268277	1.566760	-2.265509
H	0.781239	0.956220	-3.038999
C	0.840737	-2.780979	1.936506

H	0.708921	-3.176708	0.916714
H	1.885629	-2.448604	2.042442
H	0.636426	-3.583764	2.664176
C	-0.089479	-0.995541	3.996056
H	-0.309934	-1.895129	4.594128
H	0.946119	-0.679608	4.201320
H	-0.772544	-0.188627	4.307936

MULSAO

C	-4.174252	-0.334378	1.014691
H	-5.029110	-1.013397	1.173337
H	-4.439092	0.337853	0.182473
H	-4.079144	0.277148	1.923947
C	-2.913126	-1.172869	0.732728
H	-2.546381	-1.580428	1.692134
C	-1.715825	-0.431784	-0.031196
C	-1.644840	-1.184762	-1.404465
H	-1.193851	-0.573982	-2.202399
C	-3.215754	-2.335734	-0.254699
H	-4.174199	-2.830586	-0.032341
C	-3.117081	-1.609192	-1.616045
H	-3.820739	-0.767156	-1.718890
H	-3.238482	-2.276179	-2.485911
C	-0.971631	-2.556077	-1.202153
H	-0.829835	-3.062200	-2.172299
H	0.022373	-2.452218	-0.735889
C	-2.009613	-3.314141	-0.307618
H	-2.298990	-4.278185	-0.756353
H	-1.624542	-3.531767	0.705302
C	-0.349251	1.562712	-0.723206
C	-0.067988	2.811588	0.117723
C	-1.770347	1.100890	-0.256112
C	-0.621124	2.367518	1.495969
C	-1.100802	3.908181	-0.307382
H	0.969785	3.173484	0.101123
C	-2.032776	2.048843	0.959791
H	-2.535576	1.286744	-1.034347
H	-0.618601	3.169999	2.252687
H	-0.090277	1.487557	1.912020
H	-0.785514	4.892305	0.078836
H	-1.175361	3.995159	-1.404638
C	-2.431368	3.420464	0.355763
H	-2.744085	1.664613	1.698903
H	-2.753936	4.111707	1.151908
H	-3.262560	3.332461	-0.363605
H	-0.217244	1.673289	-1.813414
H	-0.817614	-0.714992	0.640572
Pd	0.819860	0.043265	0.016506
N	2.138701	-1.415033	1.219732
N	2.663480	0.531431	-0.970465
C	1.870597	-1.187438	2.662668
H	2.587336	-1.741921	3.301281

H	1.943597	-0.111639	2.884504
H	0.850784	-1.529025	2.897243
C	1.988172	-2.860348	0.919791
H	2.691349	-3.464739	1.527481
H	0.959081	-3.174380	1.147641
H	2.180032	-3.052149	-0.146120
C	3.268948	1.824516	-0.542253
H	4.264914	1.948406	-1.009552
H	2.618523	2.647527	-0.863970
H	3.367375	1.858802	0.551290
C	2.471837	0.562350	-2.451125
H	1.819240	1.406004	-2.714260
H	3.447645	0.687435	-2.959381
H	2.000303	-0.375397	-2.777624
C	3.581551	-0.609950	-0.621299
H	4.617282	-0.350548	-0.916368
H	3.269145	-1.476396	-1.226722
C	3.509778	-0.948045	0.862270
H	4.269790	-1.715105	1.113688
H	3.737106	-0.057171	1.470492

PCAuIII

P	1.549969	-1.404549	0.334847
C	-5.105107	-0.746733	1.059730
H	-5.893281	-1.512641	1.152980
H	-5.461797	0.005673	0.337652
H	-5.017464	-0.258600	2.040699
Au	-0.113760	0.279424	-0.204570
C	-3.799333	-1.432374	0.613641
H	-3.373280	-1.964610	1.483018
C	-2.679720	-0.484090	-0.038563
H	-1.732116	-0.720976	0.572071
C	1.944689	-2.638295	-1.018950
H	1.174675	-3.425993	-0.903936
C	1.500834	1.446664	-0.653034
C	2.772109	0.999841	-0.162866
C	1.372513	2.637599	-1.347048
C	2.978634	-0.284004	0.447246
C	3.904422	1.887073	-0.313592
C	2.510347	3.473197	-1.537829
H	0.407660	2.961446	-1.741555
C	4.227312	-0.631372	0.959209
C	5.159923	1.494230	0.237636
C	3.740244	3.120135	-1.009205
H	2.390592	4.410348	-2.089473
C	5.316254	0.274644	0.879524
H	4.383201	-1.612796	1.414021
H	6.008369	2.179643	0.140609
H	4.605808	3.780051	-1.125119
H	6.285250	-0.006948	1.301068
C	1.194463	-2.241179	1.965974
H	0.178900	-2.654064	1.798424

C	3.346872	-3.264776	-0.919538
H	3.533351	-3.764990	0.042261
H	3.459643	-4.019536	-1.716479
H	4.126917	-2.500915	-1.070379
C	1.757974	-1.931559	-2.376747
H	2.467044	-1.092775	-2.482460
H	1.955301	-2.644238	-3.195064
H	0.738681	-1.533713	-2.505336
C	1.109144	-1.151557	3.052393
H	2.098271	-0.702975	3.241391
H	0.418774	-0.337684	2.770643
H	0.746348	-1.592977	3.995444
C	2.122787	-3.397775	2.370892
H	3.158920	-3.056618	2.528245
H	1.770716	-3.823228	3.326414
H	2.126896	-4.211093	1.629106
C	-2.537780	-1.067589	-1.484913
H	-2.098843	-0.356700	-2.204496
C	-4.070116	-2.439626	-0.542206
H	-5.017951	-2.983064	-0.403825
C	-3.983377	-1.526106	-1.785535
H	-4.719473	-0.705607	-1.785816
H	-4.062979	-2.070957	-2.741038
C	-1.797372	-2.426915	-1.407722
H	-1.521240	-2.777820	-2.415923
H	-0.862637	-2.353733	-0.823263
C	-2.847336	-3.367833	-0.730396
H	-3.096684	-4.221194	-1.382364
H	-2.494826	-3.782181	0.230287
C	-2.894406	1.052034	-0.035701
H	-3.724471	1.264056	-0.735902
C	-1.580977	1.782428	-0.495049
H	-1.572286	2.091736	-1.553597
C	-1.786029	2.198906	1.833207
H	-1.840962	2.870356	2.706343
H	-1.111493	1.358092	2.083604
C	-3.180539	1.765979	1.330100
H	-3.775145	1.180845	2.039717
C	-1.400506	2.919768	0.520829
H	-0.412010	3.401091	0.496478
C	-2.590420	3.911966	0.338608
H	-2.384530	4.857626	0.867839
H	-2.755396	4.161347	-0.723525
C	-3.798233	3.143630	0.976064
H	-4.659763	3.052066	0.293370
H	-4.152781	3.650117	1.889218

RUCLTP

Cl	0.033297	1.017160	2.227079
Cl	-0.033220	0.841850	-2.496720
C	-2.249381	2.740183	-0.143986
C	-4.455961	0.111406	4.100305

C	-3.468792	-0.770004	3.627926
C	-2.806370	-0.501449	2.421931
C	-3.629324	0.400117	-1.154157
C	-4.966242	0.220206	-0.739279
C	-5.957807	-0.121471	-1.671364
C	-5.629442	-0.290041	-3.026259
C	-4.297921	-0.126673	-3.439655
C	-3.301074	0.210476	-2.512955
C	2.602590	2.549591	0.468372
C	-1.898330	3.547438	0.960672
C	3.826963	3.014889	0.988312
C	4.019309	4.384781	1.218268
C	2.998005	5.301421	0.909345
C	1.784396	4.843354	0.372085
C	1.586055	3.471208	0.155152
C	3.603546	0.642922	-1.298734
C	3.274708	1.197413	-2.554556
C	4.198616	1.161277	-3.609040
C	5.469388	0.590802	-3.420957
C	5.814805	0.073256	-2.162196
C	-1.758567	4.933760	0.802063
C	4.890730	0.102539	-1.105823
C	3.105049	-0.174122	1.437873
C	3.126858	0.341239	2.751212
C	3.558740	-0.463807	3.817768
C	3.970054	-1.787455	3.589045
C	3.956581	-2.303331	2.282679
C	3.527514	-1.502910	1.215156
C	-1.502274	-2.370711	-1.217264
C	-1.321132	-2.686386	-2.578596
C	-2.396719	-3.159640	-3.344661
C	-1.939642	5.524135	-0.460497
C	-3.663093	-3.326986	-2.760731
C	-3.854331	-3.000697	-1.409139
C	-2.785217	-2.511540	-0.646722
C	-0.222423	-2.676829	1.358293
C	-0.908038	-3.911250	1.421339
C	-0.938715	-4.644530	2.617874
C	-0.276512	-4.161296	3.759757
C	0.423319	-2.945595	3.694721
C	0.453581	-2.208034	2.502294
C	1.354308	-2.539581	-1.024262
C	-2.263452	4.719766	-1.566619
C	1.855287	-3.774238	-0.558718
C	2.988024	-4.344716	-1.158913
C	3.631746	-3.691268	-2.225525
C	3.120881	-2.475702	-2.706996
C	1.985280	-1.904667	-2.112518
C	-2.420006	3.334448	-1.411365
C	-3.133769	0.640431	1.666497
C	-4.119693	1.526085	2.147074
C	-4.775519	1.262870	3.360788

P	-2.304461	0.900448	0.042239
P	2.341568	0.769998	0.057427
P	-0.095049	-1.710333	-0.218662
Ru	-0.015818	0.482466	-0.116737
H	4.629161	2.303721	1.211022
H	4.969622	4.738235	1.631833
H	3.151496	6.371478	1.083876
H	0.983854	5.545401	0.122969
H	0.634243	3.127427	-0.266149
H	-2.669023	2.714604	-2.276502
H	-1.709555	3.082802	1.932189
H	-1.491377	5.549150	1.667228
H	-2.395256	5.170227	-2.555646
H	-1.823237	6.606072	-0.583924
H	-4.371562	2.424307	1.574531
H	-5.236718	0.331343	0.313261
H	-6.404436	-0.558690	-3.751830
H	-6.990215	-0.259316	-1.332650
H	-4.022860	-0.277961	-4.488443
H	-2.259933	0.309056	-2.832860
H	-2.001381	-1.160539	2.090996
H	-3.193280	-1.658009	4.205466
H	-4.966892	-0.091142	5.047348
H	-5.537200	1.959230	3.726788
H	2.283357	1.630805	-2.709462
H	5.180023	-0.301313	-0.132896
H	3.921429	1.582936	-4.580861
H	6.188919	0.560702	-4.245896
H	6.808302	-0.356672	-1.996320
H	3.511777	-1.920842	0.207527
H	2.785045	1.360775	2.939834
H	3.562395	-0.053383	4.832808
H	4.297221	-2.414399	4.424996
H	4.267243	-3.334830	2.088814
H	1.383731	-4.273904	0.291075
H	3.378292	-5.295364	-0.780333
H	4.530157	-4.127231	-2.674539
H	3.617992	-1.947307	-3.526436
H	1.591664	-0.952313	-2.479200
H	-1.414093	-4.303526	0.535282
H	0.971529	-1.249321	2.471058
H	-1.479421	-5.596118	2.654090
H	0.948729	-2.558024	4.572820
H	-0.305565	-4.732177	4.693918
H	-2.955571	-2.245143	0.400489
H	-4.842554	-3.099726	-0.950696
H	-4.501713	-3.695533	-3.359715
H	-2.242033	-3.398376	-4.401948
H	-0.338039	-2.567003	-3.040531

TBPPPD

Pd	-0.000012	-0.760506	-0.000173

P	2.267256	-0.493449	-0.073041
C	2.686512	1.289651	0.212388
C	3.927416	1.895759	-0.080702
C	4.135279	3.261878	0.169803
C	3.110082	4.042876	0.730763
C	1.874441	3.449575	1.038998
C	1.665802	2.086801	0.776578
C	3.234526	-1.372804	1.322958
C	2.470016	-0.993679	2.612446
C	3.116618	-2.893489	1.099581
C	4.708004	-0.956280	1.478039
C	2.945781	-0.939382	-1.808443
C	2.470774	0.199248	-2.739009
C	2.215923	-2.237455	-2.228088
C	4.463917	-1.147592	-1.951425
H	4.741214	1.306836	-0.511235
H	5.101971	3.716065	-0.072628
H	3.275007	5.108081	0.924036
H	1.066348	4.046969	1.473973
H	0.698788	1.608753	0.987110
H	2.923064	-1.517790	3.475082
H	1.405523	-1.277858	2.538385
H	2.519038	0.091260	2.807216
H	2.065922	-3.186534	0.926526
H	3.481196	-3.427499	1.996946
H	5.149579	-1.499274	2.335110
H	4.801554	0.122152	1.685157
H	5.312490	-1.193520	0.589381
H	2.998768	1.146116	-2.542324
H	1.387423	0.376241	-2.612875
H	2.654237	-0.088958	-3.790836
H	2.448728	-2.463295	-3.285961
H	1.122181	-2.118402	-2.117434
H	2.522145	-3.103951	-1.620566
H	5.047376	-0.254169	-1.678061
H	4.698265	-1.379597	-3.007771
H	4.821732	-1.994589	-1.343765
P	-2.267269	-0.493479	0.072894
C	-2.686577	1.289597	-0.212655
C	-3.234912	-1.373083	-1.322651
C	-2.945323	-0.939047	1.808611
C	-3.927497	1.895698	0.080405
C	-1.665854	2.086748	-0.776810
C	-2.470644	-0.994285	-2.612388
C	-3.117064	-2.893723	-1.098957
C	-4.708396	-0.956506	-1.477524
C	-2.469814	0.199677	2.738807
C	-2.215602	-2.237178	2.228274
C	-4.463455	-1.146905	1.952109
C	-4.135342	3.261822	-0.170074
H	-4.741307	1.306773	0.510907
C	-1.874473	3.449536	-1.039187

H	-0.698853	1.608675	-0.987362
H	-2.924020	-1.518399	-3.474850
H	-1.406192	-1.278677	-2.538542
H	-2.519483	0.090646	-2.807266
H	-2.066370	-3.186812	-0.925977
H	-3.481798	-3.427897	-1.996159
H	-5.150229	-1.499759	-2.334299
H	-4.801919	0.121860	-1.684984
H	-5.312689	-1.193392	-0.588632
H	-2.997657	1.146618	2.542055
H	-1.386457	0.376405	2.612326
H	-2.653054	-0.088251	3.790752
H	-2.447942	-2.462655	3.286328
H	-1.121874	-2.118453	2.117068
H	-2.522376	-3.103764	1.621159
H	-5.046769	-0.253371	1.678794
H	-4.697515	-1.378665	3.008576
H	-4.821678	-1.993930	1.344730
C	-3.110116	4.042835	-0.730967
H	-5.102042	3.716007	0.072332
H	-1.066364	4.046937	-1.474123
H	-3.275026	5.108047	-0.924208
H	-3.721040	-3.234772	-0.241453
H	3.720686	-3.234777	0.242235

TBPPPT

Pt	-0.000010	-0.531924	0.000116
P	2.268064	-0.404246	-0.084071
C	2.822212	1.342676	0.181847
C	4.121221	1.830700	-0.075991
C	4.441363	3.176579	0.165665
C	3.470871	4.053212	0.680110
C	2.176872	3.576860	0.949728
C	1.855445	2.234174	0.697830
C	3.136194	-1.349957	1.329602
C	2.415047	-0.870329	2.610704
C	2.863676	-2.854143	1.129482
C	4.644395	-1.082301	1.478521
C	2.901692	-0.922636	-1.814108
C	2.501400	0.237679	-2.753523
C	2.090639	-2.175749	-2.220428
C	4.403073	-1.230069	-1.952687
H	4.893230	1.165861	-0.471145
H	5.452502	3.539474	-0.047144
H	3.723686	5.101949	0.868332
H	1.412548	4.250843	1.350767
H	0.845639	1.841005	0.883307
H	2.806282	-1.429991	3.481089
H	1.325940	-1.034875	2.533077
H	2.583804	0.205143	2.790278
H	1.789219	-3.037805	0.952090
H	3.167028	-3.407034	2.038034

H	5.026163	-1.653082	2.345977
H	4.847661	-0.016005	1.668978
H	5.222858	-1.395836	0.596191
H	3.090490	1.149235	-2.562742
H	1.431941	0.484498	-2.628033
H	2.667416	-0.070327	-3.802563
H	2.298787	-2.415294	-3.280323
H	1.008000	-1.991415	-2.094162
H	2.353888	-3.057482	-1.614915
H	5.044519	-0.375888	-1.684051
H	4.620630	-1.481974	-3.007913
H	4.702640	-2.096853	-1.341464
P	-2.268067	-0.404238	0.084050
C	-2.822129	1.342734	-0.181776
C	-3.136106	-1.349776	-1.329794
C	-2.901918	-0.922771	1.813968
C	-4.121071	1.830857	0.076206
C	-1.855364	2.234162	-0.697892
C	-2.414689	-0.870194	-2.610763
C	-2.863784	-2.853992	-1.129692
C	-4.644239	-1.081903	-1.478916
C	-2.501842	0.237515	2.753521
C	-2.090868	-2.175873	2.220308
C	-4.403310	-1.230292	1.952326
C	-4.441146	3.176756	-0.165421
H	-4.893082	1.166076	0.471451
C	-2.176727	3.576867	-0.949770
H	-0.845602	1.840928	-0.883474
H	-2.805822	-1.429786	-3.481242
H	-1.325613	-1.034861	-2.532948
H	-2.583293	0.205300	-2.790351
H	-1.789366	-3.037773	-0.952182
H	-3.167083	-3.406825	-2.038299
H	-5.025957	-1.652575	-2.346466
H	-4.847331	-0.015566	-1.669323
H	-5.222864	-1.395413	-0.596686
H	-3.090961	1.149041	2.562680
H	-1.432381	0.484420	2.628215
H	-2.668019	-0.070547	3.802518
H	-2.299115	-2.415471	3.280167
H	-1.008219	-1.991508	2.094154
H	-2.354055	-3.057572	1.614720
H	-5.044757	-0.376127	1.683642
H	-4.621005	-1.482253	3.007508
H	-4.702758	-2.097066	1.341028
C	-3.470657	4.053317	-0.679994
H	-5.452233	3.539723	0.047511
H	-1.412399	4.250788	-1.350904
H	-3.723423	5.102070	-0.868194
H	-3.435658	-3.268120	-0.282332
H	3.435411	-3.268303	0.282044

VIGVITmod2

Pt	-1.206174	-0.185752	-0.139376
P	0.886826	0.785586	-0.227447
P	-3.254678	-1.179507	-0.092334
Si	-0.270068	-1.989506	-1.468877
Si	-1.892613	1.790373	1.138884
Si	1.606018	-2.642624	1.110015
C	2.341233	0.056101	-1.117046
C	3.376318	0.929418	-1.522699
H	3.270395	2.004526	-1.354885
C	4.539336	0.450903	-2.135586
H	5.323811	1.150072	-2.441266
C	4.680934	-0.930768	-2.349653
H	5.576741	-1.327274	-2.839064
C	3.678116	-1.804463	-1.918169
H	3.798627	-2.884076	-2.063465
C	2.502313	-1.349189	-1.272079
C	1.506026	-2.357947	-0.776663
H	1.803735	-3.345549	-1.188773
C	0.660464	2.455519	-0.954278
C	0.947817	2.665151	-2.320483
H	1.431156	1.873629	-2.900152
C	0.609651	3.869787	-2.950711
H	0.840623	4.013839	-4.010738
C	-0.029320	4.879411	-2.211795
H	-0.294785	5.828784	-2.688775
C	-0.344606	4.664375	-0.863672
H	-0.868616	5.441106	-0.295451
C	-0.031374	3.454085	-0.204847
C	-0.537007	3.193370	1.178212
H	-0.999672	4.105329	1.596253
H	0.256545	2.876296	1.871757
C	1.718010	0.976122	1.409884
C	2.552852	2.090813	1.627432
H	2.618526	2.867677	0.857877
C	3.270975	2.230215	2.820834
H	3.906830	3.106767	2.979049
C	3.156529	1.238208	3.810061
H	3.706224	1.332178	4.752313
C	2.334163	0.125851	3.591676
H	2.249968	-0.646532	4.364662
C	1.600787	-0.039627	2.393667
C	0.787248	-1.286447	2.191773
H	-0.202023	-1.045656	1.726396
H	0.584396	-1.761543	3.169518
C	-0.018224	-1.438879	-3.285228
H	-0.995748	-1.317217	-3.785014
H	0.573183	-2.177971	-3.857026
H	0.501430	-0.467930	-3.340022
C	-0.979149	-3.772055	-1.642798
H	-0.941504	-4.344254	-0.701289
H	-0.344391	-4.310271	-2.372125

H	-2.013658	-3.815369	-2.022832
C	-3.366777	2.796159	0.429592
H	-3.214511	2.982121	-0.648008
H	-3.422163	3.778640	0.934945
H	-4.343973	2.306458	0.557235
C	-2.215235	1.454968	2.997075
H	-3.009189	0.705118	3.160086
H	-2.503316	2.376252	3.536645
H	-1.292503	1.060949	3.459551
C	3.430329	-2.761123	1.599733
H	3.948297	-1.813398	1.373538
H	3.943210	-3.565847	1.044799
H	3.544223	-2.960038	2.679737
C	0.693541	-4.248761	1.546296
H	0.938294	-4.557102	2.578025
H	0.968672	-5.075729	0.869584
H	-0.399457	-4.109326	1.488900
C	-4.740483	-0.383680	0.678462
H	-4.506752	-0.040579	1.697207
H	-5.047748	0.484606	0.078285
H	-5.572578	-1.107423	0.717738
C	-3.241373	-2.779299	0.832944
H	-2.954524	-2.570186	1.875959
H	-4.237531	-3.253095	0.816174
H	-2.499613	-3.458492	0.393829
C	-3.957203	-1.581170	-1.754889
H	-4.912017	-2.126129	-1.659919
H	-4.129276	-0.634020	-2.290566
H	-3.242105	-2.179591	-2.335222

VIGVITmod

Pt	0.189366	-0.029494	0.074148
P	-1.951941	0.701795	-0.251645
P	2.450431	-0.207339	0.020654
Si	0.359587	1.732412	1.824589
Si	-0.299160	-1.913236	-1.353033
Si	-2.646565	-2.823852	0.743513
C	-1.646084	2.412059	-0.849525
C	-1.148291	3.402017	0.053278
C	-0.695558	4.620526	-0.501513
H	-0.314832	5.387956	0.181672
C	-0.694378	4.854961	-1.883538
H	-0.330522	5.811808	-2.273416
C	-1.145628	3.856817	-2.762863
H	-1.126875	4.014581	-3.845660
C	-1.615787	2.643476	-2.242615
H	-1.944440	1.856872	-2.927608
C	-0.974456	3.131993	1.512775
H	-1.906333	2.791321	1.990050
H	-0.647078	4.047351	2.036287
C	-3.114426	-0.063776	-1.463526
C	-4.100238	0.757056	-2.057127

H	-4.127956	1.823995	-1.816770
C	-5.041292	0.234126	-2.950560
H	-5.794254	0.889112	-3.399738
C	-5.002076	-1.137042	-3.258786
H	-5.720863	-1.565943	-3.964955
C	-4.050567	-1.960406	-2.648383
H	-4.035609	-3.032786	-2.874114
C	-3.100806	-1.463337	-1.721795
C	-3.078705	0.740045	1.199948
C	-4.021268	1.780209	1.324226
H	-4.020754	2.592998	0.589310
C	-4.934283	1.797590	2.385337
H	-5.655219	2.615893	2.476623
C	-4.905133	0.758133	3.331518
H	-5.606755	0.758531	4.172064
C	-3.974100	-0.280466	3.203623
H	-3.956140	-1.087380	3.945008
C	-3.043371	-0.322990	2.140012
C	-2.108225	-1.493792	2.017919
C	-2.155161	-2.420753	-1.054404
H	-2.268286	-3.401746	-1.564041
C	-0.040820	1.094183	3.582273
H	0.716059	0.366813	3.920727
H	-1.029463	0.607621	3.617068
H	-0.046018	1.935239	4.300371
C	1.943837	2.790809	2.033997
H	2.132437	3.419079	1.147866
H	2.847446	2.189048	2.218889
H	1.800795	3.458940	2.903964
C	-0.250196	-1.600354	-3.238932
H	0.776361	-1.390886	-3.580906
H	-0.881542	-0.735907	-3.505389
H	-0.623103	-2.480491	-3.795642
C	0.669464	-3.536230	-1.045623
H	0.986103	-3.649050	0.004440
H	1.576882	-3.574114	-1.668493
H	0.043422	-4.408471	-1.308772
C	-1.812769	-4.441163	1.275448
H	-2.230204	-4.785991	2.237917
H	-0.725215	-4.310634	1.400172
H	-1.970233	-5.240282	0.530751
C	-4.529863	-2.990427	0.834236
H	-5.012639	-2.040549	0.547447
H	-4.862207	-3.244249	1.856060
H	-4.894507	-3.774361	0.147894
C	3.209468	-0.434999	1.681279
C	2.480212	-1.235109	2.585167
H	1.500017	-1.620520	2.280190
C	2.990318	-1.505609	3.863575
H	2.415507	-2.127278	4.557517
C	4.223922	-0.959247	4.256697
H	4.616483	-1.155414	5.259558

C	4.946472	-0.149432	3.364064
H	5.900588	0.290752	3.671534
C	4.447662	0.104826	2.076395
H	5.012155	0.744692	1.392920
C	3.153341	1.284511	-0.798181
C	4.531893	1.390558	-1.078926
H	5.210806	0.574096	-0.812132
C	5.030646	2.522127	-1.741909
H	6.103068	2.602033	-1.947445
C	4.152974	3.539335	-2.157523
H	4.543869	4.417923	-2.681313
C	2.774542	3.417264	-1.916847
H	2.075919	4.189316	-2.252784
C	2.276392	2.295511	-1.238503
H	1.201956	2.186915	-1.046714
C	3.301390	-1.527571	-0.952396
C	3.270580	-1.440879	-2.359974
H	2.808125	-0.570705	-2.836974
C	3.824531	-2.460901	-3.144029
H	3.789388	-2.386543	-4.235708
C	4.419132	-3.578272	-2.529350
H	4.847073	-4.378287	-3.141808
C	4.464709	-3.661516	-1.128527
H	4.929796	-4.526155	-0.643954
C	3.908729	-2.639985	-0.340734
H	3.941908	-2.713900	0.750157
H	-1.082544	-1.159033	1.730479
H	-2.024968	-2.006274	2.993683

WOCMUX

Br	-0.243942	0.035189	-2.302318
N	2.747103	1.116806	-0.022541
C	1.868803	0.083960	-0.190549
C	6.452742	0.466832	0.151228
H	7.434570	0.933948	0.272380
C	5.304466	1.274526	0.164709
H	5.382735	2.355934	0.293375
C	4.062685	0.638659	0.021019
C	2.268178	2.503472	0.155082
C	2.768920	3.407316	-0.978473
H	3.862015	3.548119	-0.944542
H	2.501797	2.977469	-1.957436
H	2.319230	-2.408383	-2.606862
H	1.824276	-3.976453	-1.911852
H	-0.901329	-2.108729	0.615120
C	-2.086394	-3.205025	-0.816822
H	-1.640161	-2.653230	-1.660792
H	-1.548238	-4.160141	-0.693469
H	-3.137591	-3.434602	-1.059907
H	-1.821300	-3.973636	1.915256
N	2.612800	-1.057841	-0.301868
C	3.974929	-0.770704	-0.153463

C	5.125807	-1.571963	-0.180739
H	5.066878	-2.654123	-0.311747
C	6.364844	-0.932554	-0.016682
H	7.279603	-1.532580	-0.022646
C	1.964054	-2.376242	-0.465858
H	0.902457	-2.109608	-0.617337
C	2.084360	-3.202790	0.819720
H	3.135141	-3.430810	1.066081
H	1.547457	-4.158671	0.696918
H	1.635375	-2.649645	1.661359
C	2.441658	-3.079044	-1.741192
H	3.495110	-3.398112	-1.682769
N	-2.747161	1.116814	0.021775
C	-4.062758	0.638502	-0.020606
C	-5.304723	1.274160	-0.163457
H	-5.383199	2.355501	-0.292662
C	-6.452920	0.466371	-0.148383
H	-7.434907	0.933306	-0.268838
C	-2.268299	2.503265	-0.157649
H	-1.171337	2.394199	-0.061948
C	-2.580364	3.010622	-1.570487
H	-3.665329	3.107728	-1.743250
H	-2.121312	4.002557	-1.717584
H	-2.160490	2.313836	-2.313860
C	-2.767997	3.408352	0.975347
H	-3.861093	3.549416	0.942070
H	1.171313	2.394400	0.058578
C	2.579138	3.012365	1.567611
H	2.158543	2.316420	2.311364
H	2.120064	4.004493	1.713208
H	3.663956	3.109567	1.741205
H	2.298008	4.400715	-0.892869
H	-2.500267	2.979354	1.954526
H	-2.296861	4.401532	0.888453
N	-2.612418	-1.057730	0.301629
C	-1.868677	0.084111	0.189416
C	-6.364741	-0.932919	0.020354
H	-7.279453	-1.532983	0.027698
C	-5.125475	-1.572119	0.183518
H	-5.066270	-2.654196	0.315242
C	-3.974708	-0.770795	0.154461
C	-1.963303	-2.375777	0.466718
C	-2.437991	-3.075734	1.744689
H	-3.492084	-3.393402	1.689851
H	-2.312188	-2.403506	2.608681
Ni	0.000021	0.130933	-0.000691
Br	0.243332	0.039690	2.301127

WOCNIM

N	-2.285904	-0.397154	-1.776071
C	-4.602981	-0.398899	-2.902399
H	-4.367258	-1.036265	-3.756586

C	-1.461167	-1.293159	-2.619633
H	-0.455262	-1.208649	-2.171566
C	-1.937794	-2.742804	-2.469021
H	-1.914862	-3.034848	-1.406392
H	-1.265862	-3.415488	-3.026860
H	-2.963133	-2.880710	-2.851971
C	-1.375498	-0.786212	-4.062902
H	-2.336314	-0.866474	-4.597019
H	-0.631867	-1.387599	-4.611633
Br	-0.747241	-1.415430	1.720368
N	-2.823748	0.841121	-0.044501
C	-1.788524	0.158894	-0.627583
C	-3.640536	-0.072842	-1.934970
C	-5.892901	0.131247	-2.734415
H	-6.662940	-0.102025	-3.475740
C	-6.217319	0.960261	-1.636946
H	-7.230777	1.362280	-1.547913
C	-5.260499	1.283532	-0.661541
C	-3.979195	0.743137	-0.823943
H	-1.044753	0.264438	-4.072142
H	-0.743096	2.843638	-0.089444
H	-0.339357	5.291725	-0.172957
H	-5.500381	1.934766	0.182825
C	-2.735349	1.514684	1.256110
H	-1.906407	1.017694	1.788425
H	-3.660460	1.289744	1.813596
C	-2.514084	3.010576	1.163487
C	-1.413500	3.523023	0.448733
C	-1.193840	4.906513	0.392930
C	-2.061758	5.791964	1.056970
H	-1.888319	6.872014	1.009652
C	-3.155426	5.285330	1.777614
H	-3.838085	5.966927	2.295494
C	-3.377533	3.898389	1.829443
H	-4.232681	3.502787	2.391009
H	5.500381	-1.934766	-0.182825
C	2.735349	-1.514684	-1.256110
H	1.906407	-1.017694	-1.788425
H	3.660460	-1.289744	-1.813596
C	2.514084	-3.010576	-1.163487
C	1.413500	-3.523023	-0.448733
C	1.193840	-4.906513	-0.392930
C	2.061758	-5.791964	-1.056970
H	1.888319	-6.872014	-1.009652
C	3.155426	-5.285330	-1.777614
H	3.838085	-5.966927	-2.295494
C	3.377533	-3.898389	-1.829443
H	4.232681	-3.502787	-2.391009
N	2.823748	-0.841121	0.044501
C	1.788524	-0.158894	0.627583
C	3.640536	0.072842	1.934970
C	5.892901	-0.131247	2.734415

H	6.662940	0.102025	3.475740
C	6.217319	-0.960261	1.636946
H	7.230777	-1.362280	1.547913
C	5.260499	-1.283532	0.661541
C	3.979195	-0.743137	0.823943
H	1.044753	-0.264438	4.072142
H	0.743096	-2.843638	0.089444
H	0.339357	-5.291725	0.172957
Br	0.747241	1.415430	-1.720368
Ni	0.000000	0.000000	0.000000
N	2.285904	0.397154	1.776071
C	4.602981	0.398899	2.902399
H	4.367258	1.036265	3.756586
C	1.461167	1.293159	2.619633
H	0.455262	1.208649	2.171566
C	1.937794	2.742804	2.469021
H	1.914862	3.034848	1.406392
H	1.265862	3.415488	3.026860
H	2.963133	2.880710	2.851971
C	1.375498	0.786212	4.062902
H	2.336314	0.866474	4.597019
H	0.631867	1.387599	4.611633

WODFOK

Ru	-0.165601	-0.464119	-0.229021
P	2.140197	-1.027239	-0.004319
P	-2.534782	-0.502602	-0.343276
N	-0.177871	0.895699	1.362545
C	-0.627428	0.558247	2.603162
H	-0.955145	-0.475006	2.713858
C	-0.668650	1.455638	3.668986
H	-1.032343	1.116120	4.641928
C	-0.250862	2.780679	3.458273
H	-0.287467	3.517643	4.265079
C	0.208763	3.138040	2.188850
H	0.525770	4.162606	1.980947
C	0.259131	2.183150	1.154435
C	0.795645	2.487403	-0.180430
C	1.751949	3.504980	-0.384616
H	2.118468	4.089426	0.464576
C	2.272578	3.746113	-1.664170
H	3.019743	4.532544	-1.804431
C	1.839196	2.981060	-2.762628
H	2.235448	3.181655	-3.762361
C	0.899212	1.958274	-2.571320
H	0.549772	1.365297	-3.420733
C	0.403021	1.689476	-1.285306
C	2.455809	-2.831013	-0.497411
H	2.324078	-2.793451	-1.595688
C	2.945413	-0.843325	1.683455
H	3.981438	-1.196482	1.528099
C	3.287044	-0.029680	-1.137320

H	2.864011	0.985311	-1.047470
C	-3.384655	0.919471	0.564201
H	-2.812454	0.958495	1.509941
C	-3.188917	-0.587576	-2.113882
H	-2.879319	-1.608799	-2.408475
C	-3.310119	-2.034685	0.431104
H	-4.401393	-1.903050	0.312571
C	1.424336	-3.837687	0.046469
H	0.393223	-3.568243	-0.221792
H	1.467175	-3.927692	1.143271
H	1.636788	-4.834799	-0.376756
C	3.883107	-3.328206	-0.200110
H	4.659794	-2.696344	-0.653450
H	4.007970	-4.347170	-0.605554
H	4.077657	-3.385149	0.884227
C	2.286357	-1.729757	2.753499
H	2.439614	-2.802306	2.561811
H	1.200502	-1.546869	2.810378
H	2.720722	-1.504255	3.743227
C	3.001431	0.625022	2.153455
H	3.226109	1.336912	1.343129
H	3.783761	0.735341	2.923899
H	2.048512	0.925289	2.611574
C	4.779914	0.068179	-0.772075
H	4.951288	0.421589	0.255885
H	5.260665	0.795192	-1.450455
H	5.311033	-0.887971	-0.896831
C	3.112138	-0.481855	-2.597933
H	2.051328	-0.615273	-2.868757
H	3.638913	-1.432060	-2.790025
H	3.538026	0.275638	-3.277839
C	-4.867949	0.731920	0.933585
H	-5.052272	-0.183008	1.517484
H	-5.518354	0.707588	0.046712
H	-5.191582	1.585050	1.555738
C	-3.161684	2.260987	-0.159063
H	-2.107937	2.429541	-0.431204
H	-3.470653	3.092060	0.497862
H	-3.767189	2.327038	-1.077927
C	-4.717687	-0.491135	-2.259773
H	-5.257760	-1.162689	-1.573499
H	-5.007597	-0.767755	-3.288329
H	-5.072952	0.537906	-2.087016
C	-2.475129	0.382952	-3.072269
H	-1.392210	0.186783	-3.106636
H	-2.626382	1.438569	-2.795795
H	-2.869607	0.248130	-4.094272
C	-2.894430	-3.329959	-0.285317
H	-3.197946	-3.353030	-1.343914
H	-3.369341	-4.194531	0.209619
H	-1.802329	-3.476203	-0.231507
C	-2.986254	-2.129685	1.931613

H	-3.251030	-1.215367	2.488019
H	-1.910109	-2.330690	2.076023
H	-3.544521	-2.967210	2.383643
H	-0.302540	-1.667106	0.781576
H	-0.564424	1.083821	-1.235408
H	-0.023776	-1.151631	-1.724540
H	-0.340557	-1.844611	-1.092202

XAMPUY

Pt	0.016652	-0.886038	-0.062057
Cl	-0.938296	-2.989446	-0.133019
N	0.888875	0.918350	-0.046919
C	2.242571	1.096208	-0.051033
C	2.764359	2.396319	-0.130343
H	3.844903	2.545439	-0.141151
C	1.899601	3.500676	-0.187778
H	2.307275	4.513737	-0.253408
C	0.517952	3.297881	-0.152787
H	-0.174291	4.142320	-0.185811
C	0.014164	1.989710	-0.080296
C	-1.387736	1.590969	-0.025639
C	-2.474393	2.490383	-0.000334
H	-2.301302	3.570778	-0.038375
C	-3.787383	2.015025	0.078786
H	-4.646168	2.689559	0.101736
F	-5.266800	0.164208	0.210200
C	-3.983399	0.627183	0.131439
C	-2.940982	-0.304003	0.105358
H	-3.150547	-1.374791	0.140881
C	-1.624975	0.178960	0.024173
C	3.131873	-0.139507	0.146795
C	3.299512	-0.336286	1.678943
H	3.794506	0.536889	2.135472
H	3.914618	-1.230781	1.879834
H	2.316753	-0.474087	2.160819
C	4.517848	0.059195	-0.507784
H	4.428963	0.266622	-1.587643
H	5.117613	-0.857456	-0.381246
H	5.084200	0.880624	-0.039598
C	2.507216	-1.422860	-0.452985
H	2.177357	-1.308173	-1.497900
H	1.698872	-1.866328	0.213502
H	3.241134	-2.248250	-0.427817

YABXOS

Au	0.111021	-1.580923	-0.497507
Cl	1.017362	-3.627244	-1.078860
C	-2.588056	0.120060	0.577852
H	-3.059910	1.097045	0.798349
P	-0.835312	0.410747	0.022778
C	-2.592238	-0.746925	1.856611
H	-2.051553	-1.689274	1.639679

H	-2.035890	-0.241480	2.665287
C	-4.029368	-1.067202	2.305275
H	-4.001819	-1.711635	3.202188
H	-4.538050	-0.128548	2.604955
C	-4.825951	-0.879790	-0.095707
H	-5.367915	-1.389875	-0.912183
H	-5.368311	0.066824	0.102302
C	-4.828943	-1.743576	1.177758
H	-5.865760	-1.940568	1.504758
H	-4.373354	-2.727288	0.950029
C	-3.391856	-0.555750	-0.555619
H	-3.420898	0.092031	-1.450069
H	-2.873472	-1.488820	-0.852176
C	0.495796	1.827149	-1.995240
H	1.029450	0.879887	-2.191056
H	1.063839	2.364250	-1.211305
C	-0.924229	1.531748	-1.467913
H	-1.453010	0.921637	-2.227267
C	-0.044949	1.436551	1.340600
C	-1.711568	2.833118	-1.222207
H	-2.739638	2.609348	-0.883681
H	-1.221224	3.403336	-0.410150
C	-1.756272	3.697189	-2.498472
H	-2.333421	3.162016	-3.278722
H	-2.299259	4.637255	-2.291991
C	-0.341465	3.994129	-3.026862
H	-0.396662	4.588311	-3.956667
H	0.200254	4.614015	-2.284638
C	0.444260	2.692652	-3.266737
H	1.471770	2.916039	-3.605726
H	-0.039035	2.114984	-4.079430
C	-0.885520	2.266883	2.119675
H	-1.963505	2.277056	1.938393
C	-0.371208	3.086028	3.131504
H	-1.045458	3.716558	3.719335
C	1.009736	3.083604	3.380700
H	1.431252	3.712384	4.171598
C	1.850087	2.272097	2.609847
H	2.925896	2.275812	2.811499
C	1.358835	1.442821	1.576918
C	2.347531	0.581810	0.812654
H	1.828199	0.142351	-0.060741
C	3.553427	1.365984	0.248615
H	3.196244	2.211175	-0.368292
H	4.143013	1.805961	1.076895
C	4.461684	0.433446	-0.572296
H	3.893046	0.048381	-1.442020
H	5.319286	1.001066	-0.977439
C	4.950362	-0.753151	0.278900
H	5.579404	-1.426897	-0.330376
H	5.595168	-0.367730	1.095326
C	3.768263	-1.533351	0.880893

H	3.193341	-2.022482	0.071527
H	4.133766	-2.345906	1.534309
C	2.823830	-0.614632	1.674678
H	3.333814	-0.224891	2.578759
H	1.941123	-1.182798	2.022155

YACDIT

Au	-2.404650	-0.174978	-1.038001
Cl	-3.646491	0.545683	-2.875425
S	1.491470	-0.511653	2.164824
P	0.932563	1.301968	-0.282656
P	-1.132093	-0.852763	0.727031
O	0.746297	-1.598979	2.876457
O	2.010587	0.639782	2.968875
C	0.452283	0.004774	0.831482
C	2.976501	-1.301913	1.484915
C	4.203659	-0.627168	1.501631
H	4.281902	0.337315	2.010954
C	5.319887	-1.215401	0.885110
H	6.279590	-0.686692	0.893574
C	5.229564	-2.475382	0.261668
C	3.992622	-3.157925	0.309978
H	3.907572	-4.154548	-0.137880
C	2.873367	-2.582411	0.919600
H	1.923783	-3.120234	0.961355
C	6.421200	-3.094063	-0.432868
H	6.258050	-3.150128	-1.524452
H	6.601153	-4.124114	-0.079526
H	7.337957	-2.508096	-0.260250
C	-0.472846	2.415816	-0.766247
C	-1.387360	2.892811	0.374848
H	-1.677065	2.031727	0.995365
H	-0.854515	3.600837	1.032620
C	-2.642140	3.561339	-0.216478
H	-3.290083	3.920911	0.603174
H	-3.218983	2.800944	-0.777579
C	-2.270867	4.718678	-1.160449
H	-3.182465	5.153351	-1.607669
H	-1.782615	5.527643	-0.579174
C	-1.315113	4.244544	-2.269853
H	-1.024077	5.089200	-2.920334
H	-1.836567	3.504655	-2.907251
C	-0.050781	3.585769	-1.680662
H	0.520387	4.332939	-1.096822
H	0.605743	3.241565	-2.498614
C	2.309211	2.291611	0.485243
H	2.910860	1.535691	1.015972
C	3.253175	3.012120	-0.503244
H	3.656176	2.312141	-1.253662
H	2.706746	3.800212	-1.052966
C	4.425890	3.643506	0.275873
H	5.092400	4.174653	-0.427585

H	5.026887	2.829753	0.729104
C	3.940308	4.593062	1.385273
H	3.435740	5.463897	0.920237
H	4.803058	4.992101	1.948670
C	2.956030	3.885428	2.332413
H	3.471328	3.075626	2.883502
H	2.573121	4.591608	3.090810
C	1.779384	3.273130	1.554526
H	1.214027	4.082487	1.055728
H	1.099472	2.749122	2.243169
C	1.605472	0.708232	-1.924292
H	2.037215	1.614482	-2.393772
C	0.521767	0.158290	-2.874180
H	-0.031527	-0.655403	-2.374119
H	-0.227526	0.932081	-3.109348
C	1.137767	-0.369414	-4.182531
H	0.335362	-0.792875	-4.811864
H	1.572238	0.478453	-4.750018
C	2.235630	-1.413372	-3.917635
H	2.669244	-1.767740	-4.870144
H	1.787130	-2.297205	-3.421774
C	3.330198	-0.828408	-3.010019
H	3.841715	0.001306	-3.538666
H	4.102211	-1.586198	-2.784022
C	2.735465	-0.311449	-1.690572
H	2.326899	-1.163126	-1.123160
H	3.530962	0.117297	-1.057856
C	-2.076176	-0.739195	2.353196
H	-1.776734	-1.654709	2.898848
C	-3.600588	-0.756609	2.098857
H	-3.878084	0.171296	1.560882
H	-3.890170	-1.588162	1.434715
C	-4.371767	-0.841540	3.429756
H	-5.459168	-0.834210	3.232168
H	-4.143775	-1.810756	3.917502
C	-3.986680	0.308575	4.377320
H	-4.332131	1.266375	3.938674
H	-4.505528	0.198945	5.347162
C	-2.462790	0.373321	4.584795
H	-2.120788	-0.532573	5.123292
H	-2.195147	1.237852	5.219316
C	-1.713217	0.465168	3.242178
H	-0.629316	0.521568	3.417646
H	-2.008457	1.401272	2.733628
C	-0.824210	-2.686662	0.494048
H	-0.152918	-2.975651	1.323432
C	-2.118874	-3.518392	0.597908
H	-2.592384	-3.379652	1.584554
H	-2.841344	-3.163291	-0.164132
C	-1.824556	-5.016082	0.378926
H	-1.182945	-5.380579	1.205983
H	-2.767188	-5.590268	0.432586

C	-1.115709	-5.271019	-0.962918
H	-0.886308	-6.345759	-1.079082
H	-1.797449	-4.997769	-1.792517
C	0.167773	-4.429414	-1.073009
H	0.648259	-4.576535	-2.057842
H	0.895619	-4.773321	-0.309965
C	-0.136125	-2.937361	-0.859643
H	-0.808793	-2.585083	-1.666984
H	0.785630	-2.336965	-0.933003
H	-1.096489	1.732956	-1.383460

ZIYJID

C	0.240832	-0.286567	1.990295
C	-0.232832	0.556383	3.025568
H	-0.812828	1.441826	2.761962
C	0.008355	0.291142	4.378846
H	-0.381583	0.971169	5.141389
C	0.748839	-0.840825	4.748771
H	0.949744	-1.058620	5.801120
C	1.228603	-1.701029	3.753642
H	1.800220	-2.590297	4.035823
C	0.974792	-1.427893	2.401906
C	3.001111	-2.471857	1.354591
H	3.390185	-2.924872	2.276629
H	3.271845	-3.079489	0.478706
H	3.384539	-1.449630	1.238314
C	0.864626	-3.768560	1.522356
H	-0.225171	-3.635417	1.544292
H	1.154339	-4.340212	0.628104
H	1.209864	-4.267480	2.437988
C	-2.002452	0.486487	0.108102
C	-2.678911	-0.682637	0.876152
H	-2.295495	-1.649110	0.492523
H	-2.432864	-0.630597	1.951736
C	-4.213299	-0.607867	0.691597
H	-4.673243	-1.440625	1.253853
C	-2.371578	0.362962	-1.401954
H	-1.997883	-0.601197	-1.798260
H	-1.885875	1.163784	-1.985517
C	-4.071103	1.902368	0.458875
H	-4.427440	2.870295	0.855288
C	-4.423303	1.785901	-1.039053
H	-5.517542	1.855207	-1.176662
H	-3.972676	2.623588	-1.604270
C	-3.905710	0.435929	-1.579261
H	-4.132462	0.348375	-2.656847
C	-2.532045	1.844467	0.633158
H	-2.065682	2.675140	0.074435
H	-2.289867	1.984526	1.701023
C	-4.563700	-0.727277	-0.807088
H	-5.660114	-0.699644	-0.941642
H	-4.212141	-1.697133	-1.206317

C	-4.722493	0.742372	1.244015
H	-4.484441	0.828478	2.321646
H	-5.822196	0.796849	1.151876
C	0.958485	1.735023	-0.054415
C	3.070361	2.889267	-1.789814
H	3.773581	3.695049	-2.067326
H	3.198297	2.077745	-2.530439
C	1.778748	4.032200	0.615963
H	1.647491	4.840006	1.358347
C	0.642248	2.273116	-1.476423
H	-0.395393	2.650615	-1.516615
H	0.728283	1.455932	-2.218341
C	3.396177	2.373121	-0.370719
H	4.429957	1.983424	-0.341293
C	0.812572	2.875908	0.982255
H	1.064298	2.505403	1.991865
H	-0.223649	3.253084	1.008858
C	1.620332	3.419082	-1.824990
H	1.379733	3.785936	-2.838806
C	3.232941	3.515665	0.654888
H	3.484096	3.157165	1.671502
H	3.933368	4.337297	0.419688
C	2.426915	1.221535	-0.015528
H	2.553644	0.387483	-0.733132
H	2.655810	0.838016	0.998569
C	1.449515	4.559508	-0.797686
H	2.119509	5.400993	-1.050704
H	0.414636	4.950065	-0.829625
Au	0.467146	-1.412875	-1.253890
Cl	1.193957	-3.199673	-2.510339
N	1.499562	-2.406165	1.417109
P	-0.130335	0.224113	0.237566
H	1.193241	-2.047676	0.445761

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