

Supplementary Information

- Comparison of selected energy levels and orbital plots for metal-metal bonded structures of

page S1: Ta, W, Re species

page S2: Nb, Mo, Tc species

page S3: V, Cr, Mn species

- Comparison of the relative stability of $[(NR_2)_2M-(\mu_2, \eta^2, \eta^2-N_2)-M(NR_2)_2]$ systems with planar and perpendicular orientation of central and terminal moieties

page S4: Zr and Re species

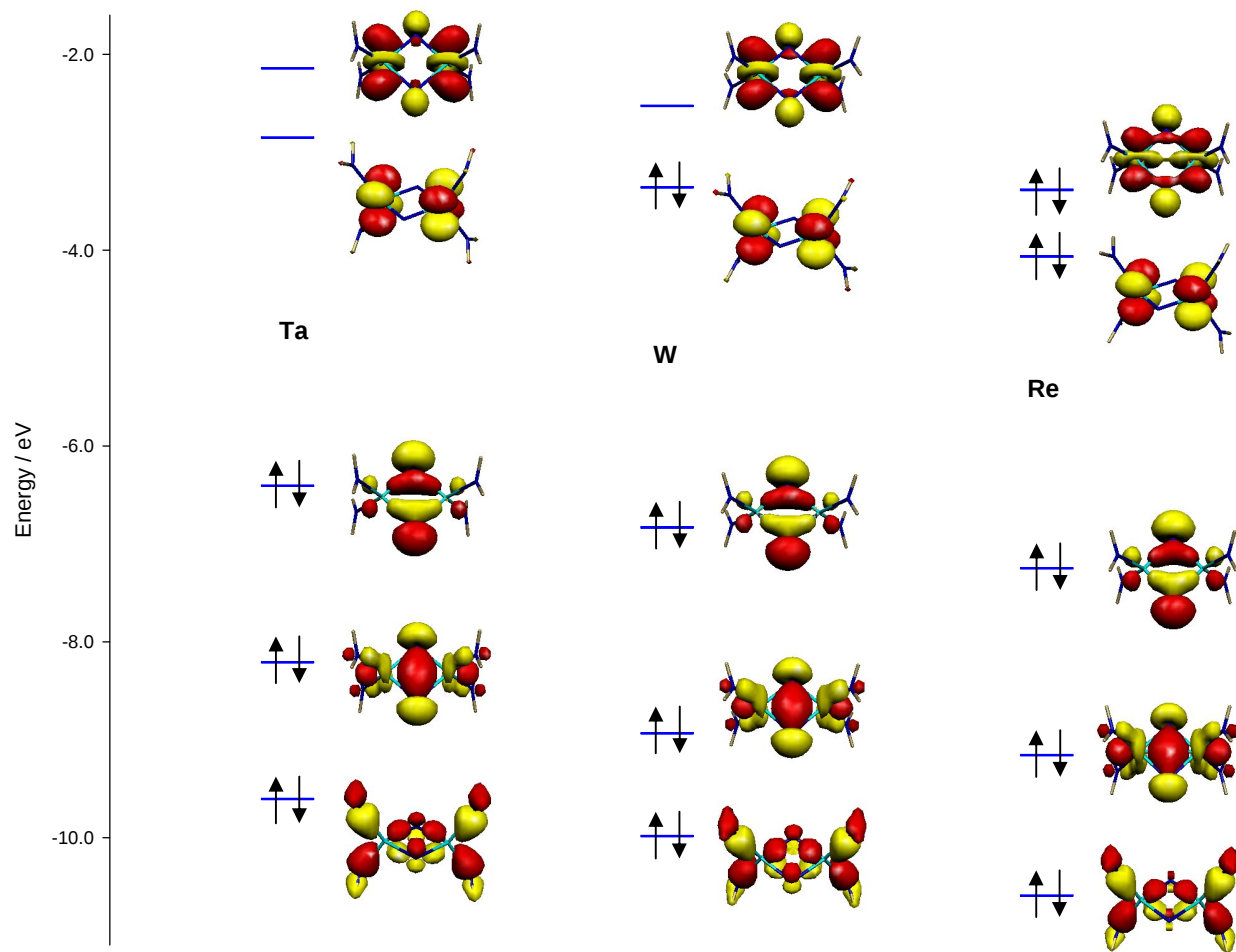
- Cartesian coordinates corresponding to selected optimized structures

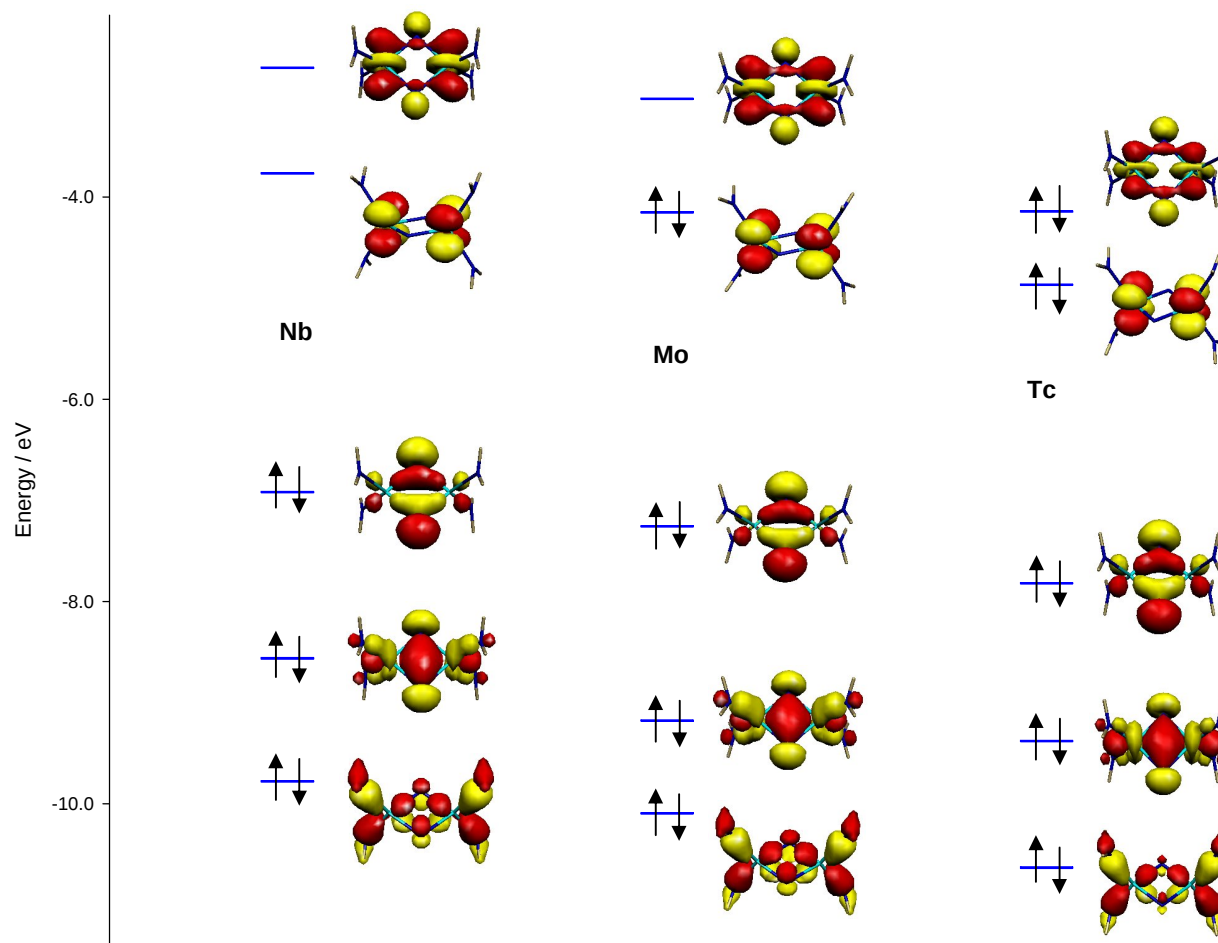
page S5: (NH₂) amide complexes containing elements in groups 4, 5, 6, and 7

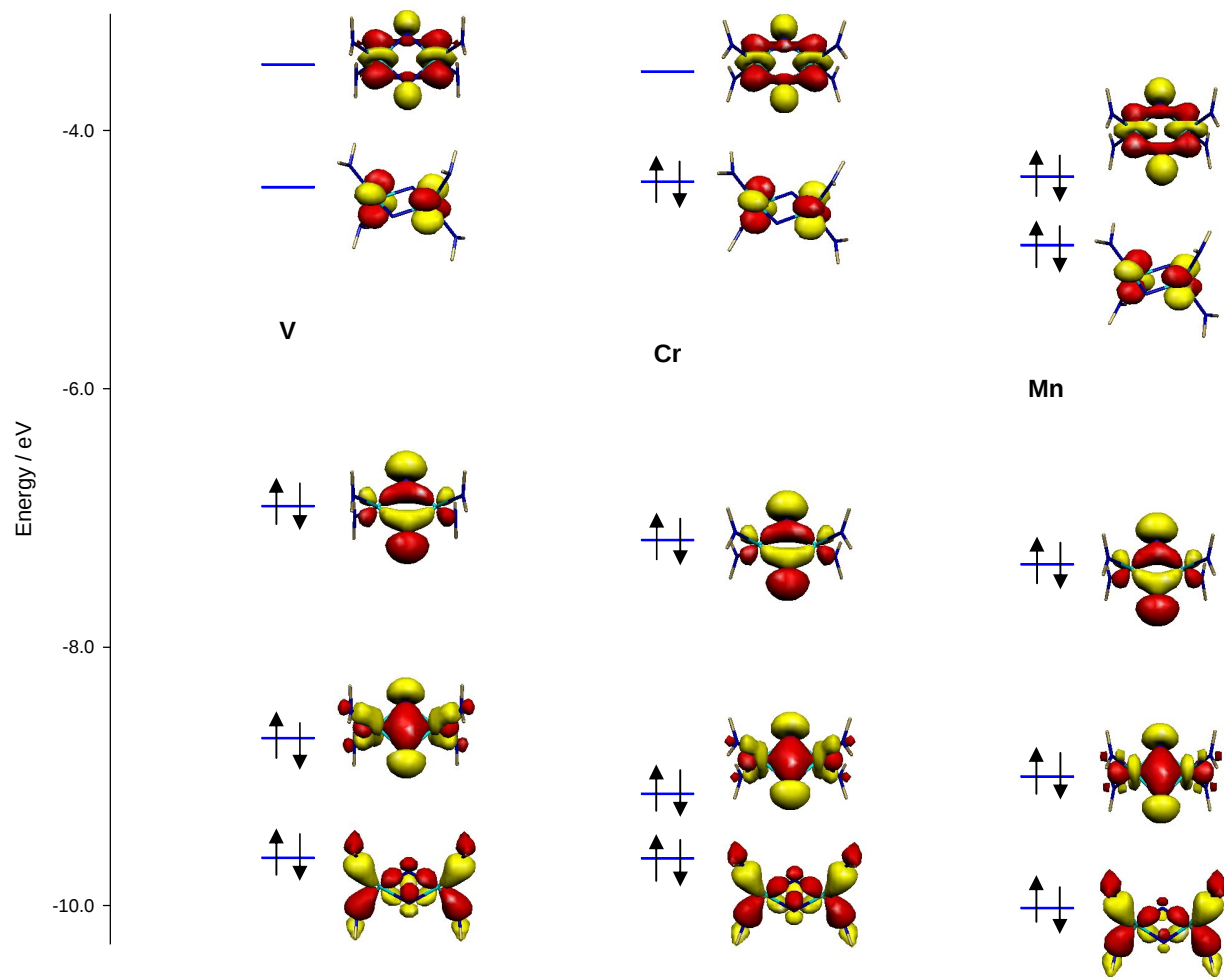
page S11: cyclopentadienyl complexes of Ti, Zr, and Hf

page S17: (methyl and isopropyl) amide complexes of Zr and Re

S 1







Comparison of the relative stability ($E_{[90]} - E_{[0]}$ in $\text{kJ}\cdot\text{mol}^{-1}$) of $[(\text{NR}_2)_2\text{M}-(\mu_2, \eta^2, \eta^2\text{-N}_2)\text{-M}(\text{NR}_2)_2]$ systems with planar (twist angle = 0 degrees) and perpendicular (twist angle = 90 degrees) orientation of central and terminal moieties.

Metal	Organic Group (R)	$E_{[90]} - E_{[0]}$
Zr	Methyl	-178
	Isopropyl	-141
Re	Methyl	-530
	Isopropyl	-336

Cartesian Coordinates for (NH₂) amide complexes containing elements in groups 4, 5, 6, and 7.

- Ti

N	0.763253	-0.026607	0.001595
Ti	-0.005687	1.743267	0.000919
N	-0.763256	0.026962	0.000470
Ti	0.005922	-1.743190	0.001147
N	-0.008370	2.825294	-1.597683
N	-0.010719	2.825495	1.599379
N	0.010441	-2.825784	-1.596988
N	0.008093	-2.825583	1.599422
H	0.770430	3.434621	-1.864749
H	-0.625950	2.722565	-2.405530
H	-0.057859	2.470587	2.556504
H	-0.056228	3.845990	1.620346
H	-0.769036	-3.433677	-1.865369
H	0.630178	-2.724522	-2.403414
H	0.056184	-2.469824	2.556182
H	0.048845	-3.846316	1.621653

- V

N	1.224485	-0.146277	-0.000776
V	0.001703	1.284276	-0.000140
N	-1.231112	0.150557	0.000812
V	-0.006661	-1.280601	0.000176
N	0.010788	2.246489	-1.600846
N	0.012906	2.246877	1.600318
N	-0.003974	-2.253069	-1.593459
N	-0.001865	-2.252682	1.594041
H	0.679729	2.989818	-1.813671
H	-0.614183	2.094384	-2.391924
H	-0.620417	2.106539	2.387024
H	0.699514	2.971201	1.822586
H	-0.670711	-2.997271	-1.810971
H	0.640305	-2.116868	-2.371831
H	0.643701	-2.117601	2.371122
H	-0.663316	-3.003334	1.804602

- Cr

N	1.189679	-0.002460	-0.000074
Cr	0.002797	1.243219	-0.000074
N	-1.189679	0.002460	-0.000074
Cr	-0.002797	-1.243219	-0.000074
N	0.005024	2.236851	-1.538362
N	0.005024	2.236851	1.538215
N	-0.005024	-2.236851	-1.538362
N	-0.005024	-2.236851	1.538215
H	0.826994	2.344123	-2.132770
H	-0.822068	2.649670	-1.970870
H	-0.815149	2.342409	2.135394
H	0.835924	2.637294	1.975104
H	-0.826994	-2.344123	-2.132770
H	0.822068	-2.649670	-1.970870
H	0.815149	-2.342409	2.135394
H	-0.835924	-2.637294	1.975104

- Mn

N	1.312394	-0.001620	-0.000027
Mn	0.001523	1.135449	-0.000027
N	-1.312394	0.001620	-0.000027
Mn	-0.001523	-1.135449	-0.000027
N	0.002837	2.114152	-1.512429
N	0.002837	2.114152	1.512376
N	-0.002837	-2.114152	-1.512429
N	-0.002837	-2.114152	1.512376
H	0.728798	1.994309	-2.218744
H	-0.850764	2.509200	-1.910546
H	0.858911	2.503011	1.911455
H	-0.720999	1.990531	2.220393
H	-0.728798	-1.994309	-2.218744
H	0.850764	-2.509200	-1.910546
H	-0.858911	-2.503011	1.911455
H	0.720999	-1.990531	2.220393

- Zr

N	0.837292	0.000295	-0.000149
Zr	0.002416	1.854347	-0.000033
N	-0.833583	0.000268	0.000141
Zr	0.000430	-1.853573	0.000025
N	-0.003321	2.942661	-1.780059
N	-0.002703	2.942716	1.779961
N	-0.006492	-2.944728	-1.778206
N	-0.005875	-2.944673	1.778292
H	-0.007540	3.961773	-1.870784
H	0.000719	2.547493	-2.722566
H	-0.005000	2.546233	2.721914
H	-0.006644	3.961690	1.872050
H	-0.006503	-3.964401	-1.863255
H	-0.010284	-2.554825	-2.722832
H	-0.006061	-2.554546	2.722833
H	-0.008574	-3.964403	1.863587

- Nb

N	1.299938	-0.119185	0.000531
Nb	0.002048	1.407404	-0.000026
N	-1.298328	0.117985	-0.000503
Nb	-0.001249	-1.408570	0.000054
N	0.001982	2.446911	-1.732858
N	0.000612	2.447011	1.732746
N	-0.003815	-2.443067	-1.736260
N	-0.005188	-2.442967	1.736425
H	0.639136	3.216121	-1.949180
H	-0.554559	2.230019	-2.560024
H	-0.570540	2.235636	2.551164
H	0.662665	3.189261	1.967707
H	-0.671998	-3.179547	-1.972254
H	0.567069	-2.233965	-2.555535
H	0.558116	-2.226957	2.559256
H	-0.636830	-3.215936	1.955155

- Mo

N 1.258507 -0.001285 -0.000335
Mo 0.000748 1.371394 0.000563
N -1.259829 0.000501 0.000360
Mo -0.001675 -1.371641 -0.000538
N 0.003208 2.459533 -1.648655
N 0.004118 2.458208 1.650653
N -0.001063 -2.457512 -1.651734
N -0.000153 -2.458838 1.649785
H 0.842152 2.743555 -2.156315
H -0.833275 2.745039 -2.159502
H -0.832106 2.749600 2.158556
H 0.843404 2.743157 2.157167
H -0.837921 -2.741338 -2.162904
H 0.837258 -2.741219 -2.160710
H 0.839473 -2.738522 2.158464
H -0.835454 -2.744657 2.161803

- Tc

N 1.182973 -0.001261 -0.000011
Tc 0.001561 1.409819 -0.000011
N -1.182973 0.001261 -0.000011
Tc -0.001561 -1.409819 -0.000011
N 0.002946 2.659822 -1.510689
N 0.002946 2.659822 1.510666
N -0.002946 -2.659822 -1.510689
N -0.002946 -2.659822 1.510666
H 0.718818 3.393882 -1.558168
H -0.161963 2.293960 -2.452941
H 0.169228 2.293825 2.452592
H -0.712365 3.394372 1.560108
H -0.718818 -3.393882 -1.558168
H 0.161963 -2.293960 -2.452941
H -0.169228 -2.293825 2.452592
H 0.712365 -3.394372 1.560108

- Hf

N	0.898196	0.004143	-0.000337
Hf	0.000587	1.791983	-0.000015
N	-0.909111	0.005266	0.000347
Hf	-0.000330	-1.792700	0.000021
N	0.001488	2.872774	-1.750669
N	0.002812	2.872809	1.750616
N	-0.000006	-2.872938	-1.751226
N	0.001319	-2.872903	1.751288
H	0.025485	3.891061	-1.831315
H	-0.004314	2.487160	-2.695883
H	-0.000536	2.486450	2.695485
H	-0.002451	3.891125	1.832176
H	-0.017758	-3.891044	-1.834578
H	0.005549	-2.485104	-2.695565
H	0.002398	-2.487415	2.696447
H	0.019450	-3.891366	1.831981

- Ta

N	1.298908	-0.083972	0.000335
Ta	0.002717	1.394836	0.000050
N	-1.298192	0.082937	-0.000308
Ta	-0.003178	-1.395715	-0.000024
N	0.006393	2.448239	-1.709976
N	0.005541	2.448150	1.710134
N	-0.004045	-2.443237	-1.713283
N	-0.004898	-2.443326	1.713181
H	0.676318	3.183719	-1.938652
H	-0.535899	2.222969	-2.543140
H	-0.541933	2.225657	2.540598
H	0.674915	3.183476	1.939877
H	-0.675709	-3.173227	-1.953705
H	0.542929	-2.208784	-2.540872
H	0.558068	-2.218442	2.532635
H	-0.667423	-3.179766	1.957326

- W

N	0.769610	0.002673	-0.000113
W	-0.005104	1.778282	-0.000117
N	-0.761273	-0.002852	0.000043
W	0.008295	-1.777218	0.000048
N	-0.021322	2.846594	-1.641123
N	-0.020988	2.846748	1.640791
N	0.000004	-2.855214	-1.634864
N	0.000337	-2.855060	1.635064
H	0.822154	3.085050	-2.167288
H	-0.825124	3.352246	-2.020107
H	-0.870040	3.047867	2.172880
H	0.766667	3.374124	2.024183
H	-0.836434	-3.018713	-2.198550
H	0.785789	-3.392903	-2.007512
H	0.835895	-3.029692	2.196736
H	-0.793991	-3.374512	2.015049

- Re

N	1.396695	-0.002308	-0.000597
Re	-0.000114	1.286070	0.000314
N	-1.396883	-0.002106	0.000570
Re	-0.000391	-1.286953	-0.000339
N	0.001181	2.326739	-1.631518
N	0.002545	2.325911	1.632672
N	0.000637	-2.321273	-1.636845
N	0.002004	-2.322103	1.635641
H	0.843773	2.569017	-2.152033
H	-0.842856	2.585060	-2.141993
H	0.846698	2.595724	2.137039
H	-0.840288	2.590679	2.142030
H	-0.844563	-2.573224	-2.147996
H	0.843273	-2.568352	-2.154844
H	-0.841933	-2.551575	2.160203
H	0.843557	-2.551119	2.163369

Cartesian Coordinates for cyclopentadienyl complexes of Ti, Zr, and Hf.

• Ti

C	2.2007430	-5.1086440	2.3133580
C	1.3401070	-4.1356660	2.9280300
C	2.0567420	-3.5448460	4.0173700
C	3.3781900	-4.0588290	3.9812780
C	3.4757230	-5.0311130	2.9397180
Ti	3.1503410	-2.7184980	1.9827670
C	4.6595860	-2.5188480	-0.0248080
C	3.7466100	-1.4118040	-0.0824110
C	2.4264970	-1.9233020	-0.2102340
C	2.5377360	-3.3495560	-0.2752940
C	3.9121350	-3.7150060	-0.2121030
C	4.1698190	0.0187800	-0.1910010
C	1.1630890	-1.1468960	-0.4680190
C	4.5081750	-5.0582520	-0.5249280
C	6.1567230	-2.4035920	0.0201950
C	-0.1288140	-3.9820130	2.6418800
C	1.4642670	-2.7025950	5.1047530
C	4.6486540	-5.9588440	2.7712110
C	1.7254750	-6.1705930	1.3635690
N	2.8441420	-1.0685190	3.1117220
N	4.0805300	-1.0498120	2.7023870
Ti	3.7321970	0.5957150	3.8607010
C	1.4390700	1.4707670	3.6885830
C	2.1047390	1.5964770	2.4323130
C	3.1165340	2.5937920	2.5325170
C	3.0515890	3.1165360	3.8637390
C	2.0303870	2.4162060	4.5752630
C	3.9050800	3.2102280	1.4071520
C	3.7383200	4.3679050	4.3298910
C	1.5499680	2.7484380	5.9593960
C	0.2330400	0.6200190	3.9538730
C	5.9695870	1.3013560	4.5335270
C	6.1180260	-0.1211210	4.5256390
C	5.2890220	-0.6650430	5.5455650
C	4.5943890	0.4089370	6.1832780
C	5.0531470	1.6169250	5.5832810
C	6.8178580	2.2708570	3.7544930
C	7.0580690	-0.9020280	3.6571900
C	5.3456270	-2.0741730	6.0540850
C	3.7736260	0.2842720	7.4386760
XX	3.3980900	-0.9420580	2.8571520
XX	3.5411470	-1.8374890	0.1341410
XX	2.2188310	1.6070500	3.0949920
XX	2.9534130	-3.8127680	3.1413410
XX	5.0437640	0.3210940	5.0071810
H	1.8720850	1.0086220	1.5515540
H	4.7897010	2.6154640	5.9133550

H	1.7080630	-4.0268790	-0.4548060
H	4.1684760	-3.8191900	4.6808060
H	1.1174170	-3.3468860	5.9298480
H	2.1949740	-1.9878750	5.5022210
H	0.6033610	-2.1237090	4.7523130
H	7.9228070	-1.2665810	4.2359330
H	6.5550560	-1.7714700	3.2107470
H	7.4525500	-0.2859500	2.8387530
H	7.8299050	2.3423160	4.1862130
H	6.9362510	1.9749220	2.7026870
H	6.3910580	3.2807810	3.7697500
H	4.4254610	0.1011470	8.3096770
H	3.2065420	1.1993740	7.6450140
H	3.0598700	-0.5501190	7.3922540
H	3.1176570	5.2503380	4.0964630
H	3.9106050	4.3850190	5.4144760
H	4.7058170	4.5223060	3.8357370
H	0.7770680	3.5348380	5.9257960
H	1.1037110	1.8796720	6.4611490
H	2.3599970	3.1261470	6.5982390
H	3.5433490	4.2312130	1.2015900
H	4.9787270	3.2884640	1.6297090
H	3.8003450	2.6368800	0.4810340
H	-0.6937240	1.1645890	3.7074600
H	0.2643480	-0.2901620	3.3408230
H	0.1640120	0.3182580	5.0075190
H	-0.7195690	-4.7582250	3.1586310
H	-0.5083000	-3.0088610	2.9787210
H	-0.3501670	-4.0713360	1.5693250
H	0.9973570	-6.8248560	1.8708060
H	1.2195500	-5.7694920	0.4738670
H	2.5449160	-6.8135740	1.0214540
H	4.6804190	-6.6822840	3.6017800
H	4.6016810	-6.5354800	1.8413550
H	5.6045540	-5.4158960	2.7815670
H	0.9915540	-1.0284590	-1.5508170
H	0.2832300	-1.6559500	-0.0525170
H	1.1940040	-0.1402470	-0.0345320
H	6.5715580	-2.2038390	-0.9830650
H	6.4758990	-1.5836490	0.6761840
H	6.6257380	-3.3268720	0.3859830
H	4.8396720	-5.0780130	-1.5763220
H	5.3890100	-5.2854620	0.0891380
H	3.7843600	-5.8709210	-0.4020220
H	6.0015700	-2.1273470	6.9404590
H	4.3653180	-2.4586010	6.3632310
H	5.7637180	-2.7556450	5.3052670
H	4.6342860	0.2057550	-1.1742550
H	3.3135310	0.6961200	-0.1044480
H	4.8932420	0.2934070	0.5872750

• Zr

C	6.1861310	1.5312160	4.7140980
C	6.2961260	0.1044210	4.6799450
C	5.4472130	-0.4345530	5.6902930
C	4.7952770	0.6523830	6.3585110
C	5.2823090	1.8568670	5.7690210
Zr	3.8195800	0.7669770	3.9699060
C	1.8367800	1.7485930	2.7122040
C	2.8651540	2.7127680	2.5183230
C	3.0855450	3.3538840	3.7851570
C	2.1930730	2.7789910	4.7373060
C	1.4323040	1.7612820	4.0829310
C	3.3957070	3.2116600	1.1990330
C	3.9057560	4.5984680	3.9801920
C	1.9592590	3.2801360	6.1340000
C	0.2752580	0.9920980	4.6572730
C	7.2194110	-0.6897220	3.8041290
C	3.9630770	0.5387640	7.6083230
C	7.0331970	2.5012110	3.9325030
N	2.8936990	-0.9955930	3.2064580
N	4.1873840	-0.9656420	2.7705920
Zr	3.2265560	-2.7092930	1.9916890
C	4.0163330	-1.4082990	-0.1469440
C	2.6535820	-1.7815900	-0.3321060
C	2.6254040	-3.2112160	-0.4595610
C	3.9537320	-3.7115280	-0.3787330
C	4.8147360	-2.6029290	-0.1225530
C	1.4867890	-0.8612630	-0.5773840
C	4.4240860	-5.0981240	-0.7182450
C	6.3175740	-2.6541870	-0.0605700
C	1.2947080	-4.2114900	2.9274720
C	1.9589740	-3.6495130	4.0658270
C	3.2739540	-4.1819040	4.0948930
C	3.4244350	-5.1205790	3.0243620
C	2.1840300	-5.1652710	2.3242400
C	-0.1583770	-4.0400610	2.5730230
C	1.3257460	-2.7908920	5.1185840
C	4.5970020	-6.0529050	2.8699730
C	1.7635460	-6.1819090	1.3001690
XX	3.3774230	-0.8574610	2.9190110
XX	3.5411470	-1.8374890	0.1341410
XX	2.3499600	1.8618760	3.2086790
XX	2.9534130	-3.8127680	3.1413410
XX	5.1703970	0.5109360	5.0823090
C	4.5690730	-0.0170410	-0.1709800
C	5.3989570	-1.8747280	6.1092990
H	1.4226430	1.0956080	1.9500360
H	5.0239640	2.8626170	6.0877370
H	1.7389860	-3.7997800	-0.6848790
H	4.0283170	-3.9600650	4.8433880

H	0.8862500	-3.4198120	5.9100450
H	2.0582570	-2.1151700	5.5764570
H	0.5216340	-2.1671840	4.7089720
H	8.0736020	-1.0798940	4.3808990
H	6.6946410	-1.5429530	3.3494790
H	7.6282120	-0.0757660	2.9912650
H	8.0552330	2.5496560	4.3423420
H	7.1237860	2.2229850	2.8735210
H	6.6191600	3.5156450	3.9766940
H	4.6034160	0.3533880	8.4867510
H	3.4041640	1.4615930	7.8042870
H	3.2404590	-0.2872550	7.5570870
H	3.2939780	5.4978380	3.7957460
H	4.3041010	4.6892140	4.9995320
H	4.7544440	4.6439310	3.2852700
H	1.2349230	4.1117780	6.1314710
H	1.5455530	2.4996540	6.7858180
H	2.8769150	3.6582730	6.6035790
H	3.0417070	4.2379970	1.0082050
H	4.4933860	3.2345110	1.1499270
H	3.0400400	2.5921980	0.3678240
H	-0.6637520	1.5631340	4.5648110
H	0.1407770	0.0416960	4.1254680
H	0.4120370	0.7626660	5.7225540
H	-0.7831860	-4.8037560	3.0670260
H	-0.5399220	-3.0590560	2.8842750
H	-0.3311030	-4.1343670	1.4922800
H	1.0468040	-6.8919070	1.7446120
H	1.2667150	-5.7349020	0.4270620
H	2.6120250	-6.7726590	0.9361030
H	4.4928590	-6.9183060	3.5447230
H	4.6895730	-6.4488300	1.8515040
H	5.5440290	-5.5567110	3.1238470
H	1.3745960	-0.6449480	-1.6532790
H	0.5408510	-1.3031030	-0.2360020
H	1.6089390	0.1011010	-0.0655460
H	6.7658670	-2.5055060	-1.0578340
H	6.7236370	-1.8755610	0.5982490
H	6.6765450	-3.6232980	0.3117590
H	4.8948450	-5.0980850	-1.7147660
H	5.1784010	-5.4784960	-0.0156390
H	3.5959030	-5.8143060	-0.7510340
H	6.1069090	-2.0633790	6.9338600
H	4.4039660	-2.1740570	6.4660670
H	5.6727390	-2.5390070	5.2805350
H	4.8055060	0.2843890	-1.2059800
H	3.8555360	0.7076580	0.2332210
H	5.4860600	0.0659090	0.4236010

• Hf

C	1.0118480	-4.3431800	2.9940840
C	1.6551540	-3.8315340	4.1592150
C	3.0063810	-4.3104270	4.1754720
C	3.1665790	-5.1514140	3.0378900
C	1.9552610	-5.1515600	2.2797430
Hf	2.9588570	-2.7972500	2.1120970
C	5.0807780	-3.8433200	0.8601260
C	5.6276930	-2.9732180	1.8548830
C	5.1953020	-1.6414410	1.5694050
C	4.3896870	-1.6997500	0.3960410
C	4.2826830	-3.0552600	-0.0359650
XX	4.4875470	-1.3091480	0.9114000
XX	2.6318020	-3.8633620	2.7342000
N	2.3252380	-0.8187910	2.3406340
N	1.2800190	-1.5963480	1.7933400
Hf	0.6414370	0.3782890	2.0279480
C	-0.7310460	1.8694200	0.5014230
C	-1.2814620	0.5609590	0.3391600
C	-0.3060470	-0.2218110	-0.3597990
C	0.8395620	0.5950660	-0.5907130
C	0.5895710	1.8908280	-0.0306000
C	1.4807510	1.5046970	4.1879980
C	0.6818860	0.3727510	4.5176380
C	-0.6778810	0.6412730	4.1792160
C	-0.7260750	1.9856690	3.6781460
C	0.6049610	2.5079180	3.6696690
XX	1.9178100	-1.1035410	1.9553720
XX	0.1379720	0.1895860	0.1325720
XX	0.1379730	0.1895870	3.7781720
C	3.6728430	-3.5367610	-1.3272540
H	3.9068860	-0.8460080	-0.0629950
C	5.6051940	-0.3773860	2.2696360
C	6.6377220	-3.3597160	2.9001370
C	5.4752090	-5.2770630	0.6366870
C	-0.4346760	-4.1536490	2.6396120
C	1.6468990	-6.0276730	1.0929120
H	4.0624430	-5.7130070	2.7945200
C	3.9760880	-4.1560820	5.3175660
C	0.9766340	-3.1259980	5.2970560
C	-0.4929740	-1.6255950	-0.8579400
C	-2.7027700	0.1485540	0.6237600
H	-1.2404020	2.7167780	0.9479860
C	1.4642720	3.1046920	-0.2034970
C	2.0008600	0.2451820	-1.4747850
H	1.0643290	-0.5549140	4.9247240
C	2.9482150	1.6396190	4.4778070
C	0.9920150	3.9283330	3.3625790
C	-1.8694900	-0.2136670	4.5260760
C	-1.9820460	2.7796220	3.4482500

H	3.1151880	2.0007050	5.5059300
H	3.4486210	0.6675690	4.3732290
H	3.4427820	2.3484220	3.8002660
H	0.6031130	-3.8570320	6.0343860
H	1.6561840	-2.4521750	5.8355430
H	0.1150240	-2.5397780	4.9583600
H	-1.0876700	-4.7132490	3.3290730
H	-0.7159700	-3.0913710	2.6815250
H	-0.6493550	-4.5116870	1.6245390
H	1.1459550	-6.9574710	1.4090420
H	0.9856800	-5.5339310	0.3678850
H	2.5609640	-6.3213670	0.5616420
H	3.6985100	-4.8149110	6.1569010
H	4.9962150	-4.4249850	5.0177570
H	4.0024650	-3.1291490	5.7083670
H	6.3093320	-5.3406720	-0.0822900
H	5.8174780	-5.7657460	1.5587120
H	4.6554460	-5.8816450	0.2257190
H	7.6626540	-3.2773930	2.5017070
H	6.5840680	-2.7098110	3.7839480
H	6.5090480	-4.3960220	3.2404210
H	4.4278370	-3.5700920	-2.1308150
H	3.2503510	-4.5465340	-1.2389250
H	2.8679590	-2.8722920	-1.6647350
H	6.5043590	0.0577830	1.8035560
H	4.7988220	0.3663700	2.2133410
H	5.8373230	-0.5429350	3.3302310
H	0.9378360	4.5517160	4.2704740
H	2.0207640	4.0006970	2.9848910
H	0.3298780	4.3897100	2.6179170
H	-2.3750240	3.1667690	4.4034720
H	-1.8131450	3.6506140	2.8013100
H	-2.7831730	2.1803710	2.9950180
H	-2.2903540	0.0759900	5.5034770
H	-2.6770910	-0.1257820	3.7876410
H	-1.5980080	-1.2746750	4.5910660
H	1.3745600	3.5100690	-1.2249010
H	1.1808840	3.9055800	0.4897830
H	2.5272830	2.8804600	-0.0375820
H	1.7883640	0.5305330	-2.5191250
H	2.9203720	0.7699340	-1.1831840
H	2.2080430	-0.8307860	-1.4689710
H	-0.5958610	-1.6454470	-1.9549260
H	0.3602530	-2.2610090	-0.5781030
H	-1.3972200	-2.0833010	-0.4369500
H	-3.3265180	0.2346090	-0.2804960
H	-2.7753780	-0.8910090	0.9704580
H	-3.1601960	0.7863090	1.3905510

Cartesian Coordinates for (methyl and isopropyl) amide complexes of Zr and Re.

• Zr (Me)

Zr	0.0000000	1.8633710	0.0000000
N	0.8307700	0.0000000	0.0000000
Zr	0.0000000	-1.8633710	0.0000000
N	-0.8307700	0.0000000	0.0000000
N	0.0000000	-2.9359540	1.7998640
N	0.0000000	-2.9359540	-1.7998640
N	0.0000000	2.9359540	-1.7998640
N	0.0000000	2.9359540	1.7998640
C	0.0000000	-4.4038110	1.8443260
C	0.0000000	-2.2563100	3.1032780
C	0.0000000	-4.4038110	-1.8443260
C	0.0000000	-2.2563100	-3.1032780
C	0.0000000	4.4038110	1.8443260
C	0.0000000	2.2563100	3.1032780
C	0.0000000	4.4038110	-1.8443260
C	0.0000000	2.2563100	-3.1032780
H	0.0000000	2.9848240	3.9306240
H	-0.8880890	1.6151950	3.2367500
H	0.8880890	1.6151950	3.2367500
H	0.0000000	4.7684610	2.8850200
H	0.8896200	4.8467700	1.3586340
H	-0.8896200	4.8467700	1.3586340
H	0.0000000	-2.9848240	3.9306240
H	0.8880890	-1.6151950	3.2367500
H	-0.8880890	-1.6151950	3.2367500
H	0.0000000	-4.7684610	2.8850200
H	-0.8896200	-4.8467700	1.3586340
H	0.8896200	-4.8467700	1.3586340
H	0.0000000	-4.7684610	-2.8850200
H	0.8896200	-4.8467700	-1.3586340
H	-0.8896200	-4.8467700	-1.3586340
H	0.0000000	-2.9848240	-3.9306240
H	-0.8880890	-1.6151950	-3.2367500
H	0.8880890	-1.6151950	-3.2367500
H	0.0000000	2.9848240	-3.9306240
H	0.8880890	1.6151950	-3.2367500
H	-0.8880890	1.6151950	-3.2367500
H	0.0000000	4.7684610	-2.8850200
H	-0.8896200	4.8467700	-1.3586340
H	0.8896200	4.8467700	-1.3586340

• Zr (Pr)

Zr	0.0000000	1.8714770	0.0000000
N	0.8242330	0.0000000	0.0000000
Zr	0.0000000	-1.8714770	0.0000000
N	-0.8242330	0.0000000	0.0000000
N	-0.0250690	-2.9097630	1.8211330
N	0.0250690	-2.9097630	-1.8211330
N	-0.0250690	2.9097630	-1.8211330
N	0.0250690	2.9097630	1.8211330
C	-0.3147330	-4.3551000	1.9199940
C	0.1942570	-2.0623750	3.0187550
C	0.3147330	-4.3551000	-1.9199940
C	-0.1942570	-2.0623750	-3.0187550
C	0.3147330	4.3551000	1.9199940
C	-0.1942570	2.0623750	3.0187550
C	-0.3147330	4.3551000	-1.9199940
C	0.1942570	2.0623750	-3.0187550
C	0.8841780	2.1565650	4.1139260
C	-1.6088380	2.1796830	3.6288710
H	-0.1328550	1.0290920	2.6293160
C	-0.6685090	5.1856520	2.7693550
C	1.7777870	4.6958350	2.2888940
H	0.1909170	4.7298770	0.8860780
C	-0.8841780	-2.1565650	4.1139260
C	1.6088380	-2.1796830	3.6288710
H	0.1328550	-1.0290920	2.6293160
C	0.6685090	-5.1856520	2.7693550
C	-1.7777870	-4.6958350	2.2888940
H	-0.1909170	-4.7298770	0.8860780
C	-0.6685090	-5.1856520	-2.7693550
C	1.7777870	-4.6958350	-2.2888940
H	0.1909170	-4.7298770	-0.8860780
C	0.8841780	-2.1565650	-4.1139260
C	-1.6088380	-2.1796830	-3.6288710
H	-0.1328550	-1.0290920	-2.6293160
C	-0.8841780	2.1565650	-4.1139260
C	1.6088380	2.1796830	-3.6288710
H	0.1328550	1.0290920	-2.6293160
C	0.6685090	5.1856520	-2.7693550
C	-1.7777870	4.6958350	-2.2888940
H	-0.1909170	4.7298770	-0.8860780
H	1.7802270	-1.3594800	4.3439290
H	1.7564130	-3.1270930	4.1651680
H	2.3726390	-2.1056760	2.8415220

H	-1.7802270	1.3594800	4.3439290
H	-1.7564130	3.1270930	4.1651680
H	-2.3726390	2.1056760	2.8415220
H	-0.7221950	-1.3652250	4.8622280
H	-1.8902900	-2.0268150	3.6922730
H	-0.8490690	-3.1190950	4.6454660
H	0.7221950	1.3652250	4.8622280
H	1.8902900	2.0268150	3.6922730
H	0.8490690	3.1190950	4.6454660
H	0.7221950	-1.3652250	-4.8622280
H	1.8902900	-2.0268150	-3.6922730
H	0.8490690	-3.1190950	-4.6454660
H	-0.7221950	1.3652250	-4.8622280
H	-1.8902900	2.0268150	-3.6922730
H	-0.8490690	3.1190950	-4.6454660
H	-1.7802270	-1.3594800	-4.3439290
H	-1.7564130	-3.1270930	-4.1651680
H	-2.3726390	-2.1056760	-2.8415220
H	1.7802270	1.3594800	-4.3439290
H	1.7564130	3.1270930	-4.1651680
H	2.3726390	2.1056760	-2.8415220
H	1.9775150	-5.7616840	-2.0931950
H	1.9967530	-4.5040830	-3.3478170
H	2.4767570	-4.1008830	-1.6840550
H	-1.9775150	-5.7616840	2.0931950
H	-1.9967530	-4.5040830	3.3478170
H	-2.4767570	-4.1008830	1.6840550
H	-0.4769110	-6.2596630	-2.6180740
H	-1.7104770	-4.9795260	-2.4872190
H	-0.5536690	-4.9803300	-3.8437830
H	0.4769110	-6.2596630	2.6180740
H	1.7104770	-4.9795260	2.4872190
H	0.5536690	-4.9803300	3.8437830
H	-0.4769110	6.2596630	2.6180740
H	-1.7104770	4.9795260	2.4872190
H	-0.5536690	4.9803300	3.8437830
H	0.4769110	6.2596630	-2.6180740
H	1.7104770	4.9795260	-2.4872190
H	0.5536690	4.9803300	-3.8437830
H	-1.9775150	5.7616840	-2.0931950
H	-1.9967530	4.5040830	-3.3478170
H	-2.4767570	4.1008830	-1.6840550
H	1.9775150	5.7616840	2.0931950
H	1.9967530	4.5040830	3.3478170
H	2.4767570	4.1008830	1.6840550

- Re (Me)

Re	0.0000000	1.3015940	0.0000000
N	1.3920260	0.0000000	0.0000000
Re	0.0000000	-1.3015940	0.0000000
N	-1.3920260	0.0000000	0.0000000
N	0.0000000	-2.3814540	1.6104740
N	0.0000000	-2.3814540	-1.6104740
N	0.0000000	2.3814540	-1.6104740
N	0.0000000	2.3814540	1.6104740
C	-1.2228350	-2.9077690	2.2150920
C	1.2228350	-2.9077690	2.2150920
C	1.2228350	-2.9077690	-2.2150920
C	-1.2228350	-2.9077690	-2.2150920
C	1.2228350	2.9077690	2.2150920
C	-1.2228350	2.9077690	2.2150920
C	-1.2228350	2.9077690	-2.2150920
C	1.2228350	2.9077690	-2.2150920
H	1.1858460	-2.8051220	3.3155150
H	1.3645700	-3.9803320	1.9825580
H	2.0940170	-2.3521560	1.8467200
H	-1.1858460	-2.8051220	3.3155150
H	-2.0940170	-2.3521560	1.8467200
H	-1.3645700	-3.9803320	1.9825580
H	1.1858460	-2.8051220	-3.3155150
H	2.0940170	-2.3521560	-1.8467200
H	1.3645700	-3.9803320	-1.9825580
H	-1.1858460	-2.8051220	-3.3155150
H	-1.3645700	-3.9803320	-1.9825580
H	-2.0940170	-2.3521560	-1.8467200
H	1.1858460	2.8051220	3.3155150
H	2.0940170	2.3521560	1.8467200
H	1.3645700	3.9803320	1.9825580
H	-1.1858460	2.8051220	3.3155150
H	-1.3645700	3.9803320	1.9825580
H	-2.0940170	2.3521560	1.8467200
H	-1.1858460	2.8051220	-3.3155150
H	-2.0940170	2.3521560	-1.8467200
H	-1.3645700	3.9803320	-1.9825580
H	1.1858460	2.8051220	-3.3155150
H	1.3645700	3.9803320	-1.9825580
H	2.0940170	2.3521560	-1.8467200

- Re (Pr)

Re	0.0000000	1.2781240	0.0000000
N	1.4098740	0.0000000	0.0000000
Re	0.0000000	-1.2781240	0.0000000
N	-1.4098740	0.0000000	0.0000000
N	0.0000000	-2.2507560	1.6955410
N	0.0000000	-2.2507560	-1.6955410
N	0.0000000	2.2507560	-1.6955410
N	0.0000000	2.2507560	1.6955410
C	-1.3194620	-2.6096690	2.2950380
C	1.3194620	-2.6096690	2.2950380
C	1.3194620	-2.6096690	-2.2950380
C	-1.3194620	-2.6096690	-2.2950380
C	1.3194620	2.6096690	2.2950380
C	-1.3194620	2.6096690	2.2950380
C	-1.3194620	2.6096690	-2.2950380
C	1.3194620	2.6096690	-2.2950380
C	1.5434690	-2.1610020	3.7527470
C	1.7145980	-4.0868470	2.1252860
H	2.0316910	-2.0213540	1.6933590
C	-1.5434690	-2.1610020	3.7527470
H	-2.0316910	-2.0213540	1.6933590
C	-1.7145980	-4.0868470	2.1252860
C	1.5434690	-2.1610020	-3.7527470
H	2.0316910	-2.0213540	-1.6933590
C	1.7145980	-4.0868470	-2.1252860
C	-1.5434690	-2.1610020	-3.7527470
C	-1.7145980	-4.0868470	-2.1252860
H	-2.0316910	-2.0213540	-1.6933590
C	1.5434690	2.1610020	3.7527470
H	2.0316910	2.0213540	1.6933590
C	1.7145980	4.0868470	2.1252860
C	-1.5434690	2.1610020	3.7527470
C	-1.7145980	4.0868470	2.1252860
H	-2.0316910	2.0213540	1.6933590
C	-1.5434690	2.1610020	-3.7527470
H	-2.0316910	2.0213540	-1.6933590
C	-1.7145980	4.0868470	-2.1252860
C	1.5434690	2.1610020	-3.7527470
C	1.7145980	4.0868470	-2.1252860
H	2.0316910	2.0213540	-1.6933590
H	-2.6221680	-2.1873100	3.9691770
H	-1.0478920	-2.8222740	4.4767490
H	-1.1931640	-1.1344980	3.9171230

H	2.6221680	-2.1873100	3.9691770
H	1.1931640	-1.1344980	3.9171230
H	1.0478920	-2.8222740	4.4767490
H	2.6221680	2.1873100	3.9691770
H	1.0478920	2.8222740	4.4767490
H	1.1931640	1.1344980	3.9171230
H	-2.6221680	2.1873100	3.9691770
H	-1.1931640	1.1344980	3.9171230
H	-1.0478920	2.8222740	4.4767490
H	2.6221680	2.1873100	-3.9691770
H	1.1931640	1.1344980	-3.9171230
H	1.0478920	2.8222740	-4.4767490
H	-2.6221680	2.1873100	-3.9691770
H	-1.0478920	2.8222740	-4.4767490
H	-1.1931640	1.1344980	-3.9171230
H	-2.6221680	-2.1873100	-3.9691770
H	-1.1931640	-1.1344980	-3.9171230
H	-1.0478920	-2.8222740	-4.4767490
H	2.6221680	-2.1873100	-3.9691770
H	1.0478920	-2.8222740	-4.4767490
H	1.1931640	-1.1344980	-3.9171230
H	-2.7618190	-4.2261680	2.4368540
H	-1.6275200	-4.3961890	1.0751600
H	-1.0930150	-4.7562180	2.7358800
H	2.7618190	-4.2261680	2.4368540
H	1.0930150	-4.7562180	2.7358800
H	1.6275200	-4.3961890	1.0751600
H	-2.7618190	4.2261680	2.4368540
H	-1.0930150	4.7562180	2.7358800
H	-1.6275200	4.3961890	1.0751600
H	2.7618190	4.2261680	2.4368540
H	1.6275200	4.3961890	1.0751600
H	1.0930150	4.7562180	2.7358800
H	2.7618190	-4.2261680	-2.4368540
H	1.6275200	-4.3961890	-1.0751600
H	1.0930150	-4.7562180	-2.7358800
H	-2.7618190	-4.2261680	-2.4368540
H	-1.0930150	-4.7562180	-2.7358800
H	-1.6275200	-4.3961890	-1.0751600
H	-2.7618190	4.2261680	-2.4368540
H	-1.6275200	4.3961890	-1.0751600
H	-1.0930150	4.7562180	-2.7358800
H	2.7618190	4.2261680	-2.4368540
H	1.0930150	4.7562180	-2.7358800
H	1.6275200	4.3961890	-1.0751600