Metal effects on ligand non-innocence in Group 5 complexes of the redox-active [ONO] pincer ligand

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Supporting Information

Figure S1. ^{1}H NMR spectrum of [ONO]VCl_2(THF) (**1-V**) in C_6D_6.

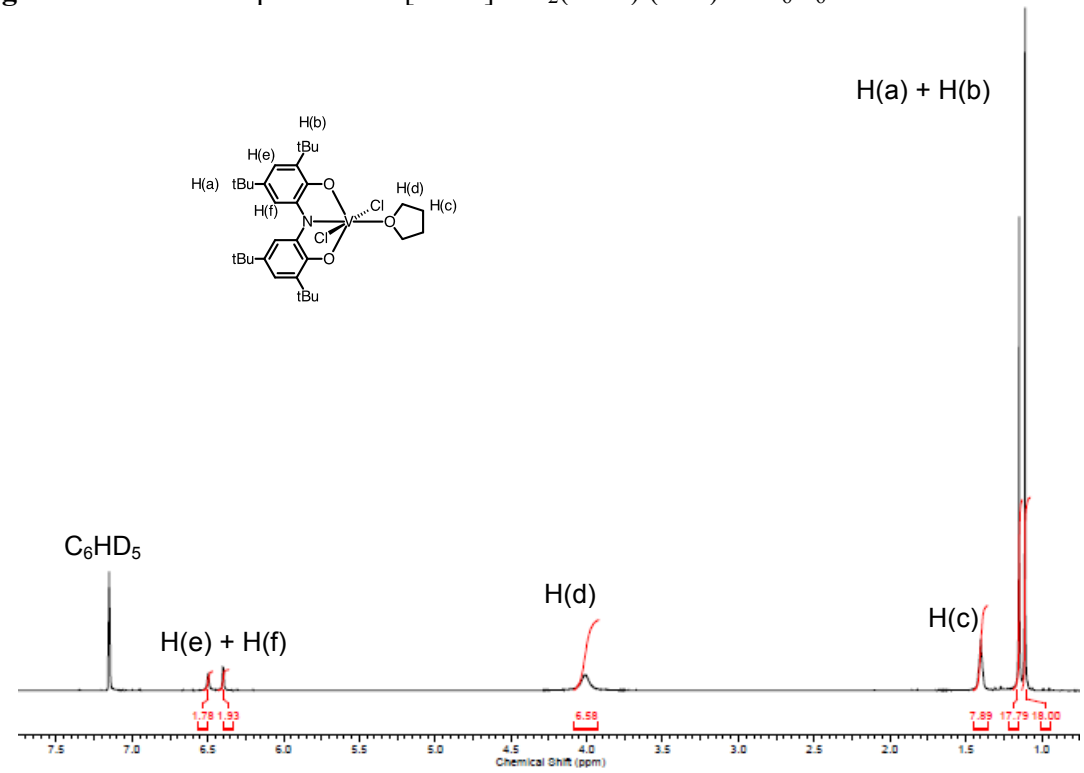


Figure S2. ^{1}H NMR spectrum of [ONO]$NbCl_2(OEt_2)$ (**1-Nb**) in C_6D_6.

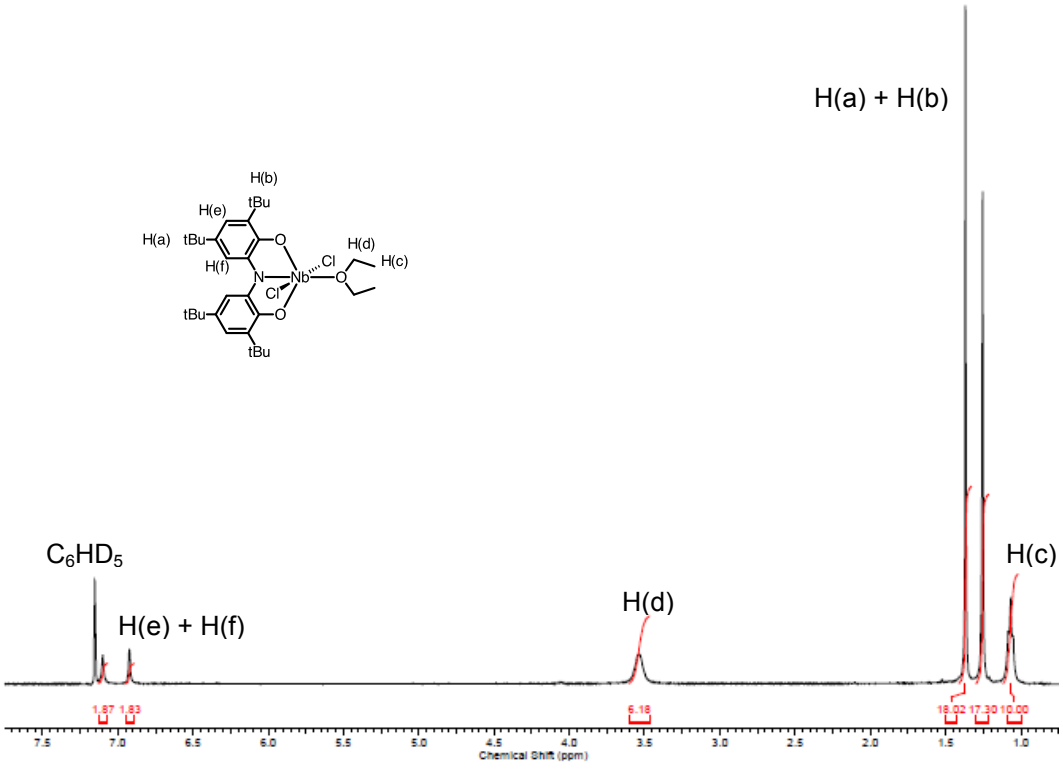


Figure S3. ^{1}H NMR spectrum of [BnNEt$_3$][[ONO]VCl$_3$] ([BnNEt$_3$][**2-V**]) in C_6D_6.

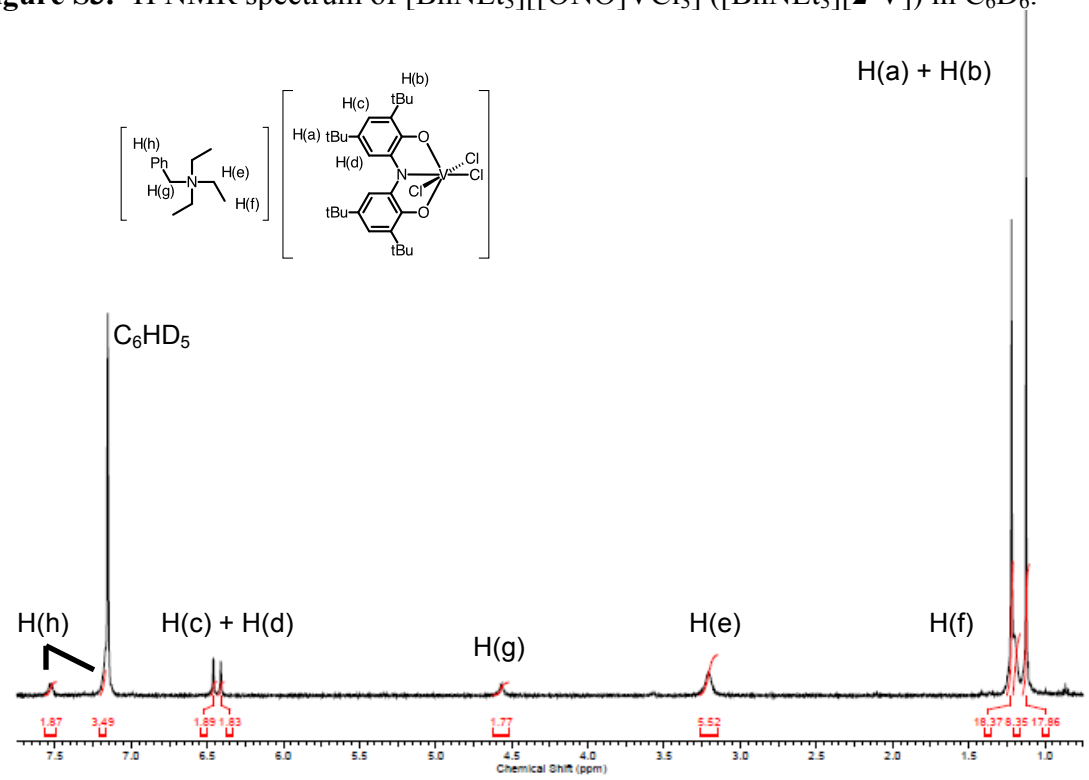


Figure S4. ^{1}H NMR spectrum of [BnNEt$_3$][[ONO]NbCl$_3$] ([BnNEt$_3$][**2-Nb**]) in C_6D_6.

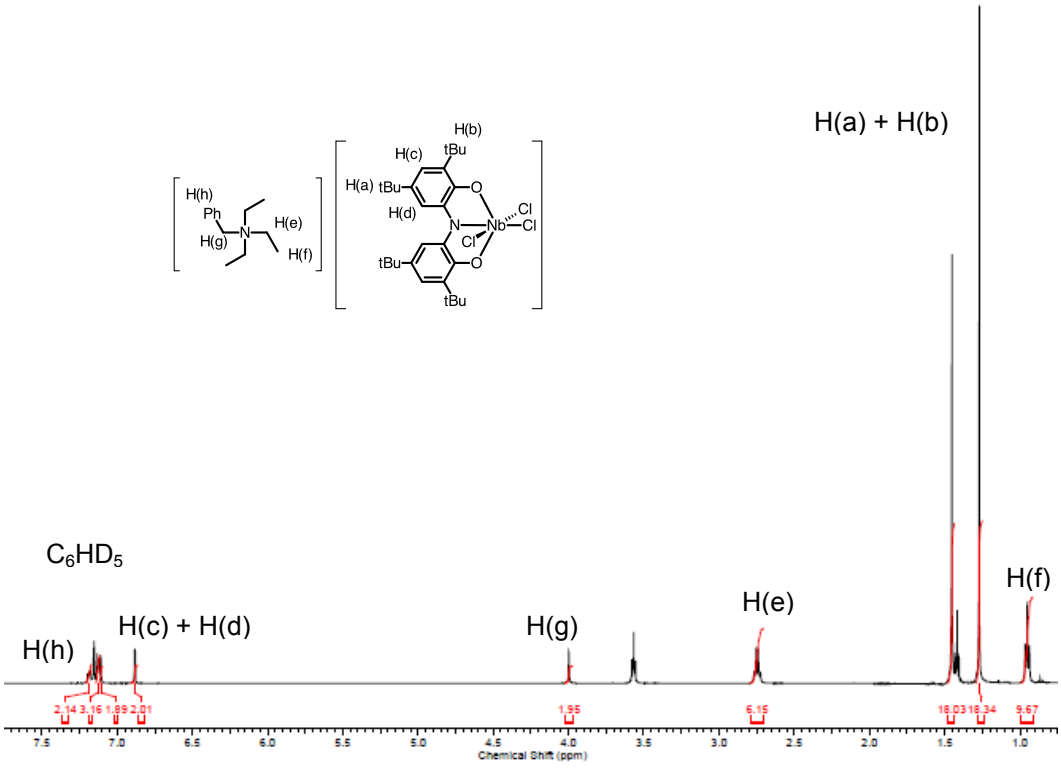
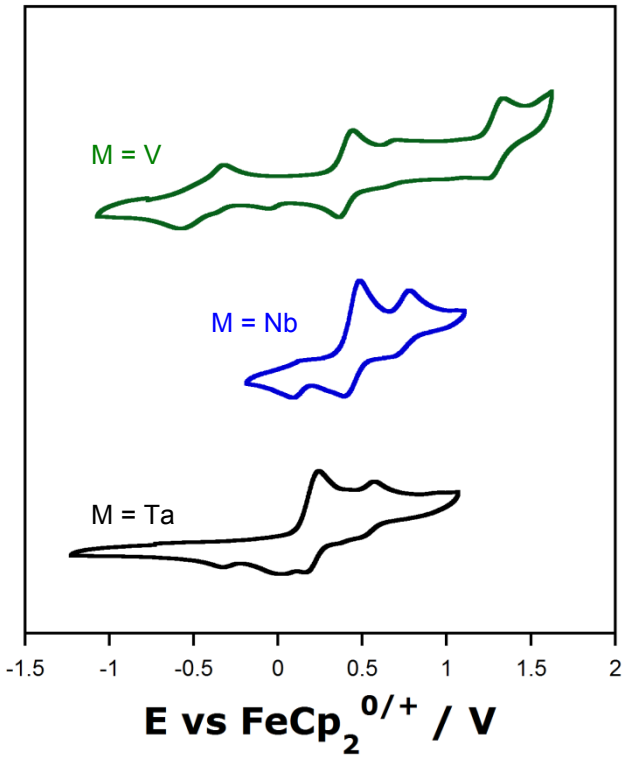


Figure S5. Cyclic voltammograms of $[BnNEt_3][[ONO]MCl_3]$ ($[BnNEt_3][$**2-M**$]$; M = V, Nb, Ta) in MeCN containing 0.1 M $[Bu_4N][PF_6]$ (3 mm diameter glassy carbon working electrode, Pt^0 wire counter electrode, and Ag^0 wire pseudo-reference. Potentials were referenced to the $FeCp_2^{+/0}$ using $[CoCp_2][PF_6]$ as an internal standard



1-V [ONO]VCl_2-Et_2O

Energy = -3392.801826445

V	-6.7849795	11.8073329	-1.4699098
Cl	-7.4840680	11.8361304	0.7147306
Cl	-5.5377409	11.8344339	-3.3947442
O	-7.1763658	13.5550174	-1.6517868
O	-7.0655553	10.0396238	-1.6076401
O	-4.8055818	11.8314270	-0.5286402
N	-8.5373470	11.7448138	-2.3038522
C	-9.1865713	12.9483251	-2.4800146
C	-8.3310491	13.9983429	-2.1086766
C	-8.6984498	15.3462733	-2.2122031
C	-9.9883952	15.5722870	-2.6613680
H	-10.3212634	16.5973890	-2.7529940
C	-10.9002620	14.5539449	-2.9827251
C	-10.4912454	13.2362635	-2.8894909
H	-11.1922513	12.4459451	-3.0909050
C	-7.7342900	16.4668911	-1.8455865
C	-6.4835729	16.3718375	-2.7299663
H	-6.7407901	16.5292846	-3.7806309
H	-5.9979742	15.3993493	-2.6474023
H	-5.7641176	17.1421360	-2.4388695
C	-7.3451844	16.3496275	-0.3660375
H	-8.2243365	16.4539556	0.2747083
H	-6.6395984	17.1435115	-0.1055335
H	-6.8800564	15.3896382	-0.1434011
C	-8.3556012	17.8448634	-2.0589752
H	-9.2352675	17.9995414	-1.4288556
H	-8.6412596	18.0081216	-3.1014556
H	-7.6231905	18.6114184	-1.7951301
C	-12.3134333	14.9371451	-3.4149239
C	-12.2433449	15.8141959	-4.6705171
H	-11.7707282	15.2781040	-5.4971498
H	-11.6736330	16.7292147	-4.4969490
H	-13.2504145	16.1043392	-4.9832082
C	-13.1736079	13.7181337	-3.7355542
H	-12.7549706	13.1298109	-4.5568070
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H	-12.4497936	16.6320612	-2.0379590
C	-9.0081648	10.4980374	-2.6673398
C	-8.1186133	9.5106276	-2.2066596
C	-8.3439200	8.1458852	-2.3932404
C	-9.4909456	7.8244335	-3.1118266
H	-9.7015947	6.7794342	-3.2829160
C	-10.3699134	8.7736289	-3.6424828
C	-10.1190002	10.1200981	-3.4151298
H	-10.7677530	10.8590376	-3.8552699
C	-7.3825282	7.0959506	-1.8505028
C	-6.0020831	7.2801888	-2.4943080
H	-5.3035714	6.5413132	-2.0908942
H	-5.5967856	8.2742435	-2.3065789
H	-6.0572328	7.1380776	-3.5764891
C	-7.2767926	7.2397318	-0.3264543
H	-6.5519952	6.5202764	0.0649539
H	-8.2409131	7.0400142	0.1482961
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C	-7.8554893	5.6767880	-2.1552652
H	-7.1415755	4.9651979	-1.7337587
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C	-11.5946675	8.3776332	-4.4671008
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H	-10.8670458	6.4327636	-5.1440162
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H	-11.8408367	6.3614868	-3.6640269
C	-11.4895170	8.9966022	-5.8659357
H	-11.4411251	10.0867133	-5.8262065
H	-12.3622838	8.7237575	-6.4659612
H	-10.5947674	8.6423412	-6.3838298
C	-12.8625884	8.8956544	-3.7781217
H	-12.8531684	9.9829320	-3.6764648
H	-12.9667035	8.4676678	-2.7779718
H	-13.7473546	8.6230079	-4.3601956
C	-3.6958306	13.9923079	-0.3259352
H	-3.4137665	14.7557823	0.4032332
H	-4.3573646	14.4491909	-1.0632028
H	-2.7887856	13.6644220	-0.8377621
C	-4.3904985	12.8555028	0.3851137
H	-3.7443305	12.3980964	1.1404064
H	-5.2968697	13.1881647	0.8893492
C	-3.7886682	10.8645392	-0.8233266
H	-2.8298734	11.3859488	-0.9008709
H	-4.0260944	10.4748707	-1.8121973
C	-3.7445934	9.7685444	0.2144195
H	-2.9769963	9.0410498	-0.0610651
H	-4.7036556	9.2522344	0.2708471
H	-3.5017934	10.1506911	1.2081413

1-Nb [ONO]$NbCl_2$-Et_2O

Energy = -2506.071299419

Nb	-6.6804944	11.8706056	-1.3894906
Cl	-7.2864878	12.0024925	0.9062990
Cl	-5.3041211	11.8849789	-3.3297763
O	-7.1859042	13.6805761	-1.6690115
O	-7.0716773	10.0182486	-1.5392415
O	-4.5846361	11.7315041	-0.3999709
N	-8.5307034	11.7847157	-2.2697827
C	-9.2032828	12.9935859	-2.4630263
C	-8.3807190	14.0767969	-2.1358795
C	-8.7816463	15.4048330	-2.2584228
C	-10.0883603	15.5957692	-2.6941384
H	-10.4460685	16.6102038	-2.8056544
C	-10.9697030	14.5495510	-2.9698863
C	-10.5184177	13.2414514	-2.8469200
H	-11.2031425	12.4276643	-3.0074759
C	-7.8450619	16.5605897	-1.9214696
C	-6.5914243	16.4840194	-2.8029831
H	-6.8553039	16.5862051	-3.8587807
H	-6.0630387	15.5386590	-2.6792985
H	-5.9067529	17.2972083	-2.5457117
C	-7.4503424	16.4928463	-0.4402963
H	-8.3320487	16.5845916	0.1988908
H	-6.7705374	17.3154535	-0.1998017
H	-6.9537355	15.5544489	-0.1948060
C	-8.5027122	17.9166330	-2.1664589
H	-9.3845877	18.0632690	-1.5378711
H	-8.7961052	18.0456895	-3.2114640
H	-7.7899873	18.7086327	-1.9239215
C	-12.4020388	14.8738122	-3.3920314
C	-12.3796763	15.7074417	-4.6785922
H	-11.9020394	15.1567748	-5.4927485
H	-11.8355421	16.6446012	-4.5458642
H	-13.3999067	15.9548292	-4.9860253
C	-13.2294055	13.6191192	-3.6568387
H	-12.8066091	13.0164666	-4.4655567
H	-14.2405858	13.9053795	-3.9566696
H	-13.3165800	12.9920911	-2.7657326
C	-13.0935493	15.6744736	-2.2825341
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H	-12.5691738	16.6085564	-2.0714941
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C	-6.0508582	7.2503533	-2.4484546
H	-5.3740505	6.4909873	-2.0452990
H	-5.6269235	8.2327757	-2.2414077
H	-6.0931494	7.1240817	-3.5331504
C	-7.3574425	7.2124646	-0.3012256
H	-6.6638067	6.4641778	0.0934440
H	-8.3351248	7.0401553	0.1561522
H	-7.0120648	8.1983347	0.0096133
C	-7.9362718	5.6804090	-2.1514814
H	-7.2413212	4.9536928	-1.7236513
H	-7.9812506	5.4987614	-3.2280766
H	-8.9233680	5.4837621	-1.7252488
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C	-11.7088325	6.9502638	-4.7387620
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C	-11.4311666	9.1115609	-5.9133561
H	-11.3731125	10.1996034	-5.8440690
H	-12.2948763	8.8635391	-6.5368711
H	-10.5300141	8.7621110	-6.4235713
C	-12.8460040	8.9650147	-3.8570137
H	-12.8270338	10.0481390	-3.7191667
H	-12.9758289	8.5056373	-2.8737758
H	-13.7209288	8.7210376	-4.4663604
C	-3.3918035	13.8584507	-0.3267979
H	-3.0043078	14.6113971	0.3636258
H	-4.1002439	14.3467234	-0.9990730
H	-2.5577440	13.4857642	-0.9244084
C	-4.0594239	12.7568372	0.4599509
H	-3.3668306	12.2851875	1.1624455
H	-4.9081943	13.1274464	1.0343962
C	-3.6455501	10.6897246	-0.7148049
H	-2.6595742	11.1461576	-0.8407892
H	-3.9461019	10.2975166	-1.6857885
C	-3.6371538	9.6134244	0.3423723
H	-2.9262940	8.8340381	0.0575683
H	-4.6236887	9.1577721	0.4390997
H	-3.3378216	9.9988143	1.3191169

1-Ta [ONO]$TaCl_2$-Et_2O

Energy = -2506.133000289

Ta	0.4779047	4.1874930	0.9902185
Cl	2.0368091	4.6080476	2.7327042
Cl	-0.2158269	3.9749249	-1.2639803
O	0.1736786	2.3446132	1.4314220
O	-0.0889164	6.0149711	1.0432456
N	-1.2962078	4.1686957	2.0173719
C	-1.8445799	2.9207738	2.3290819
C	-0.9587903	1.8866836	2.0113801
C	-1.2476574	0.5443890	2.2394267
C	-2.5067430	0.2819113	2.7731386
H	-2.7735350	-0.7473983	2.9690536
C	-3.4494825	1.2719425	3.0420739
C	-3.1094954	2.5999305	2.8105906
H	-3.8438470	3.3716112	2.9626253
C	-0.2556131	-0.5653236	1.9047346
C	1.0542173	-0.3391616	2.6701525
H	0.8836410	-0.3997918	3.7480448
H	1.4902315	0.6368853	2.4585198
H	1.7829766	-1.1092772	2.4005713
C	0.0043018	-0.5821868	0.3928589
H	-0.9155868	-0.8094307	-0.1517092
H	0.7411014	-1.3531103	0.1477048
H	0.3742449	0.3770790	0.0313386
C	-0.7827476	-1.9442567	2.2967566
H	-1.6958081	-2.2036064	1.7552736
H	-0.9832684	-2.0144236	3.3687569
H	-0.0300479	-2.6978170	2.0514408
C	-4.8235793	0.8699389	3.5767327
C	-4.6567531	0.1367646	4.9127190
H	-5.6328631	-0.1662127	5.3028516
H	-4.1780765	0.7810500	5.6544358
H	-4.0460568	-0.7620718	4.8074105
C	-5.5134521	-0.0604372	2.5722730
H	-5.6524328	0.4387239	1.6101114
H	-6.4965835	-0.3598090	2.9468993
H	-4.9324850	-0.9679226	2.3969535
C	-5.7328493	2.0735378	3.8087020
H	-5.9191787	2.6286517	2.8856877
H	-5.3147448	2.7616035	4.5484731
H	-6.6992889	1.7326442	4.1879256
C	-1.8506714	5.4095784	2.3610801
C	-1.1482358	6.4582688	1.7511206
C	-1.4948780	7.7928896	1.9026172
C	-2.5786929	8.0448278	2.7488051
H	-2.8809384	9.0707619	2.8934689
C	-3.2630445	7.0453547	3.4285790
C	-2.8860432	5.7164342	3.2295037
H	-3.3812483	4.9401821	3.7900626
C	-0.7182783	8.9094350	1.2107925
C	-0.7178083	8.6846575	-0.3067936
H	-0.2828986	7.7230377	-0.5776380
H	-0.1404898	9.4730239	-0.7986107
H	-1.7367747	8.7176351	-0.7012296
C	-1.3336705	10.2823464	1.4733439
H	-2.3643093	10.3423974	1.1146339
H	-0.7535632	11.0411168	0.9420415
H	-1.3206622	10.5424955	2.5346600
C	0.7217649	8.9351896	1.7397118
H	1.2261749	7.9808771	1.5892839
H	0.7354198	9.1557379	2.8101247
H	1.2947634	9.7130932	1.2262686
C	-4.4133294	7.3504850	4.3878145
C	-5.6966660	6.6872055	3.8748477
H	-6.5273313	6.8870096	4.5581343
H	-5.5858716	5.6038959	3.7919331
H	-5.9662939	7.0715718	2.8879643
C	-4.0815964	6.7999826	5.7797517
H	-3.1714627	7.2591891	6.1733564
H	-3.9292887	5.7187935	5.7655219
H	-4.8995283	7.0112025	6.4747064
C	-4.6774176	8.8477634	4.5238716
H	-4.9629213	9.2990491	3.5703105
H	-3.8051573	9.3811334	4.9101186
H	-5.5008726	9.0090774	5.2240635
O	2.5040458	3.6435718	-0.0532019
C	3.5570386	4.6054297	-0.2195775
C	2.9758266	2.2837689	-0.0825171
C	3.0736716	1.7592296	-1.4939104
H	3.9364940	2.2493017	0.4409927
H	2.2622640	1.7013360	0.4978010
H	3.7926630	2.3197216	-2.0950305
H	2.1005006	1.8043455	-1.9846339
H	3.4020521	0.7175067	-1.4681044
C	2.9945919	5.9270658	-0.6679733
H	4.0850696	4.6961112	0.7350139
H	4.2462122	4.2102860	-0.9702061
H	2.3426392	6.3717230	0.0885970
H	2.4356660	5.8234045	-1.5989535
H	3.8159229	6.6284081	-0.8286713

3-V [ONO]VCl_3

Energy = -3619.254478358

V	0.1799476	13.9417102	14.6558182
Cl	0.3213966	13.9413289	16.8455289
Cl	2.4200618	13.5379648	14.3314777
O	-0.1643242	12.1162610	14.3177760
N	0.0189951	13.8006574	12.4925641
C	-0.2880821	12.5864448	12.0513281
C	-0.3640322	11.6487516	13.1538637
C	-0.6469265	10.2659102	12.9234826
C	-0.8668690	9.9200859	11.6212079
C	-0.8444611	10.8235704	10.5103404
C	-0.5546581	12.1351896	10.7336318
C	-0.7008291	9.2742853	14.0771899
C	-1.0089242	7.8629516	13.5832578
C	-1.8056888	9.6832011	15.0622917
C	-1.1577856	10.2709562	9.1278566
C	-1.0941483	11.3468761	8.0484591
C	-2.5708790	9.6730266	9.1321514
C	-0.1407927	9.1763603	8.7789182
H	0.8758345	9.5761194	8.7594331
H	-2.7822560	9.6917234	14.5711181
H	-1.3231302	10.9019549	7.0778234
H	-2.6728769	8.8637382	9.8579035
H	-0.0982281	11.7923868	7.9772964
H	-2.8029410	9.2629109	8.1459193
H	-1.8459634	8.9582923	15.8793958
H	-3.3180901	10.4338841	9.3697005
H	-0.5616774	12.8323536	9.9146551
H	-0.3641981	8.7649243	7.7912275
H	-0.2448530	7.4912025	12.8946559
H	-1.0897269	8.8836678	11.4051125
H	-1.8227834	12.1429529	8.2231014
H	-1.9840494	7.8013760	13.0918899
H	-1.6295738	10.6678035	15.4927630
H	-0.1634180	8.3500236	9.4920662
H	-1.0327258	7.1863818	14.4398747
C	0.2470313	14.9645850	11.8658492
C	0.3127182	15.2556879	10.4878280
C	0.4750406	16.0156707	12.8223851
O	0.4491438	15.6775816	14.0614712
C	0.7140592	17.3492288	12.4004719
C	0.7409446	17.5489957	11.0407738
C	0.5599875	16.5337118	10.0639001
H	0.9262476	18.5525752	10.6870455
H	0.1997450	14.4693643	9.7598413
C	0.6562378	9.2390892	14.7949864
H	1.4496596	8.9203473	14.1138446
H	0.6100757	8.5207142	15.6173792
H	0.9283333	10.2089202	15.2089920
C	0.9352482	18.4671084	13.4112550
C	-0.3005993	18.6037776	14.3121313
H	-1.1850633	18.8614704	13.7235720
H	-0.1333365	19.4051187	15.0365379
H	-0.5113235	17.6886277	14.8636022
C	2.1750420	18.1582812	14.2629944
H	2.0705232	17.2288412	14.8206047
H	2.3317916	18.9684445	14.9800000
H	3.0684685	18.0843076	13.6375054
C	1.1632879	19.8096064	12.7207257
H	0.3055565	20.1122936	12.1135942
H	2.0549626	19.8020133	12.0876646
H	1.3111093	20.5774773	13.4828857
C	0.6415100	16.8342799	8.5670476
C	-0.6952425	16.4765440	7.9060697
H	-0.9403993	15.4199893	8.0339402
H	-0.6499279	16.6807475	6.8330322
H	-1.5133536	17.0634797	8.3304148
C	1.7594304	15.9916292	7.9409342
H	1.5797506	14.9214354	8.0627213
H	2.7263523	16.2216682	8.3946609
H	1.8280661	16.1974826	6.8693933
C	0.9361695	18.3044083	8.2774202
H	0.1560925	18.9640917	8.6658661
H	0.9826032	18.4549866	7.1966355
H	1.8962685	18.6203444	8.6932231
Cl	-2.0841231	14.3396264	14.6207055

3-Nb [ONO]$NbCl_3$

Energy = -2730.836167433

Nb	-0.2206679	3.2385023	0.2507466
Cl	-0.3788638	5.5507908	0.4181769
Cl	-0.7766333	2.9172721	2.5273802
O	-1.9561875	2.5843464	-0.2486190
N	-0.0737651	1.0052962	0.0947861
C	-1.2055767	0.3925560	-0.3544190
C	-2.2729357	1.3280991	-0.5243750
C	-3.5539429	0.9386284	-0.9603047
C	-3.7058572	-0.4164032	-1.2421684
H	-4.6811347	-0.7601155	-1.5854595
C	-2.6702269	-1.3760566	-1.1322546
C	-1.4253962	-0.9612752	-0.6894313
H	-0.6097963	-1.6726235	-0.6333839
C	-4.6857072	1.9573913	-1.1220674
C	-5.9823997	1.2878674	-1.5846791
H	-6.3403966	0.5352990	-0.8646490
H	-5.8737887	0.8058431	-2.5689031
H	-6.7694970	2.0508508	-1.6803278
C	-4.9596703	2.6432554	0.2271845
H	-4.0770497	3.1751747	0.6054786
H	-5.2685118	1.9076408	0.9859330
H	-5.7747358	3.3755707	0.1139987
C	-4.2861308	3.0033638	-2.1774824
H	-3.3780847	3.5505074	-1.8919310
H	-5.0987439	3.7363435	-2.3034113
H	-4.1061063	2.5263846	-3.1533509
C	-2.9636743	-2.8303108	-1.5137721
C	-1.7393370	-3.7310673	-1.3371215
H	-1.3919420	-3.7524428	-0.2923843
H	-0.9006367	-3.4153047	-1.9770307
H	-1.9949027	-4.7637505	-1.6186998
C	-3.3995334	-2.8905438	-2.9869167
H	-3.6173714	-3.9302927	-3.2785142
H	-2.6075286	-2.5086219	-3.6493359
H	-4.3074040	-2.2976961	-3.1732068
C	-4.0920793	-3.3690888	-0.6189823
H	-3.8043086	-3.3362036	0.4430833
H	-4.3183925	-4.4151870	-0.8797183
H	-5.0216465	-2.7915436	-0.7321433
H	4.9231759	2.6487592	-0.7337700
H	4.1484280	-2.7492995	-0.8456569
C	4.4702923	-2.8786623	0.1991604
C	4.5528982	3.2444989	0.1151409
H	5.3244251	-2.2070503	0.3723203
H	3.5984798	3.7012876	-0.1782468
H	4.8322819	-3.9120529	0.3197119
H	5.2747961	4.0555840	0.2997726
H	6.2196140	1.2132518	0.9102408
H	1.8311007	-3.5597159	-0.1343624
C	4.4133145	2.3742491	1.3759544
C	3.7388145	-0.1003808	1.2061144
C	3.3119690	-2.6039341	1.1718554
C	3.4097971	1.2490085	1.1092898
C	5.7974673	1.8214208	1.7255527
C	2.8287094	-1.1625842	0.9847752
C	2.2037031	-3.6232578	0.8998979
C	2.0763218	1.5245416	0.7505988
C	1.5310859	-0.8568430	0.6105085
C	1.1340481	0.4897551	0.4599327
O	1.5927744	2.7541712	0.6590819
H	4.7600678	-0.3569964	1.4863408
H	2.5933064	-4.6420091	1.0455615
H	6.4885781	2.6595442	1.9004529
H	0.8106530	-1.6537708	0.4674613
H	5.7825630	1.2134875	2.6436315
C	3.7969470	-2.7928068	2.6185194
H	1.3511179	-3.4974694	1.5854594
C	3.9281916	3.2287781	2.5595191
H	4.1512435	-3.8247749	2.7705910
H	2.9527852	3.6918187	2.3603515
H	4.6290368	-2.1172238	2.8665137
H	4.6525076	4.0342040	2.7587077
H	2.9845191	-2.6010082	3.3361501
H	3.8388375	2.6202906	3.4728829
Cl	0.3567119	3.3227334	-2.0417399

3-Ta [ONO]$TaCl_3$

Energy = -2732.744610861

Ta	0.2394078	13.9300100	14.8043397
Cl	0.4076360	14.0787076	17.1188748
Cl	2.4972141	13.2593198	14.5923834
O	-0.3042810	12.1197428	14.3858617
N	0.0678788	13.7961067	12.5871080
C	-0.1969753	12.5522948	12.1089824
C	-0.4330826	11.6248301	13.1628626
C	-0.7721706	10.2877240	12.9162769
C	-0.8195318	9.9176697	11.5831605
C	-0.5344195	10.7823175	10.5071641
C	-0.2230942	12.0935561	10.7801539
C	-1.0584972	9.3108769	14.0529023
C	-1.4263035	7.9253251	13.5264426
C	-2.2393254	9.8205763	14.8899442
C	-0.5715110	10.2297027	9.0863244
C	-0.2504091	11.2956626	8.0426672
C	-1.9721972	9.6786895	8.7928160
C	0.4575751	9.1007211	8.9532408
H	1.4683870	9.4674948	9.1475909
H	-3.1444733	9.8926059	14.2811866
H	-0.2953504	10.8532450	7.0451113
H	-2.2484559	8.8775667	9.4809702
H	0.7542166	11.7061307	8.1740092
H	-2.0093409	9.2719252	7.7786411
H	-2.4377390	9.1211657	15.7062464
H	-2.7276059	10.4643878	8.8725748
H	0.0429962	12.7569904	9.9763031
H	0.4331245	8.6877632	7.9412508
H	-0.6131606	7.4728748	12.9525405
H	-1.0727886	8.8924778	11.3508060
H	-0.9694413	12.1193441	8.0681832
H	-2.3243213	7.9472661	12.9031873
H	-2.0419033	10.7997114	15.3245810
H	0.2577794	8.2843616	9.6501281
H	-1.6325679	7.2679248	14.3739107
C	0.2327345	14.9804023	11.9301506
C	0.0395196	15.2844523	10.5774406
C	0.6094391	16.0242402	12.8213366
O	0.6902526	15.6665972	14.1001161
C	0.8582162	17.3248705	12.3796740
C	0.6817263	17.5465094	11.0179739
C	0.2624358	16.5646377	10.1087603
H	0.8620039	18.5426427	10.6435336
H	-0.3252410	14.5313204	9.8986990
C	0.1871586	9.1600915	14.9361874
H	1.0276658	8.7669695	14.3582529
H	-0.0226600	8.4569796	15.7465938
H	0.4920775	10.1065584	15.3801995
C	1.2809661	18.4323682	13.3414903
C	0.1778685	18.6648285	14.3830869
H	-0.7525303	18.9745403	13.9002520
H	0.4830859	19.4600682	15.0682422
H	-0.0250620	17.7709347	14.9711716
C	2.5903890	18.0431080	14.0407359
H	2.4933474	17.1182687	14.6076479
H	2.8846043	18.8359898	14.7334062
H	3.3960914	17.9155422	13.3130087
C	1.5193046	19.7536778	12.6136406
H	0.6143540	20.1260413	12.1264191
H	2.3111238	19.6732459	11.8638726
H	1.8316462	20.5063631	13.3407629
C	0.0412581	16.8690636	8.6269520
C	-1.4112895	16.5521025	8.2515319
H	-1.6561636	15.5014881	8.4200752
H	-1.5813079	16.7669635	7.1928986
H	-2.1080612	17.1558099	8.8379213
C	0.9834796	16.0000741	7.7853093
H	0.8047310	14.9347628	7.9472696
H	2.0287711	16.2049862	8.0295608
H	0.8356200	16.2049419	6.7213088
C	0.3116219	18.3320686	8.2841897
H	-0.3504495	19.0087435	8.8302130
H	0.1369040	18.4912248	7.2174997
H	1.3458575	18.6165676	8.4931364
Cl	-2.0393565	14.5647067	14.8417290