

Electronic Supplementary Information

Computational and Experimental Investigation of the Effect of Cation Structure on the Solubility of Anionic Flow Battery Active-Materials

Benjoe Rey B. Visayas,^a Shyam K. Pahari,^a Tugba Ceren Gokoglan,^b James A. Golen,^a Ertan Agar,^b
Patrick J. Cappillino^{*a} and Maricris L. Mayes^{*a}

^a *Department of Chemistry and Biochemistry, University of Massachusetts Dartmouth, MA 02747-2300, USA*

^b *Department of Mechanical Engineering, Energy Engineering Graduate Program, University of Massachusetts Lowell, Lowell, MA 01854, USA*

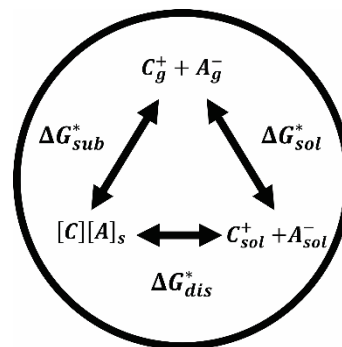
email: maricris.mayes@umassd.edu
pcappillino@umassd.edu

Computational Details

The intrinsic solubility (S_o) of a substance is directly related to the difference in its stabilities in both the solid and solvated states. This relationship is demonstrated from the well-known Born-Fajans-Haber thermochemical correlation¹ (Scheme 1), which translates to

$$\Delta G_{dis}^* = \Delta G_{sub}^* + \Delta G_{sol}^* = -RT \ln(S_o V_m) \quad (1)$$

where ΔG_{dis}^* is the free energy of dissolution and is the sum of the free energies of sublimation (ΔG_{sub}^*) and solvation (ΔG_{sol}^*) while R , T , and V_m are the gas constant, temperature, and the solid's molar volume, respectively. In this cycle, a substance first sublimates into the gas phase, then gets solvated into the solution phase and the free energies associated with each process determine its dissolution. The free energy of sublimation is roughly the negative of the lattice free energy (ΔG_{latt}^o).



Scheme 1. The Born-Fajans-Haber thermochemical correlation

Sublimation free energy ΔG_{sub}^*

The free energy of sublimation (ΔG_{sub}^*) was obtained from the negative of the lattice free energy (ΔG_{latt}^o) and the isothermal expansion of an ideal gas:²⁻⁴

$$\Delta G_{sub}^* = -\Delta G_{latt}^o - RT \ln \left(\frac{V_m p_o}{RT} \right) \quad (2)$$

where p_o is the standard condition pressure. The subsequent equations detail the calculation of the ΔG_{latt}^o .

$$\Delta G_{latt}^o = \Delta H_{latt}^o - T \Delta S_{latt}^o \quad (3)$$

$$\Delta H_{latt}^o = \Delta U_{latt} + p \Delta V = \Delta U_{latt} - (n + m)RT \quad (4)$$

where ΔH_{latt}^o , ΔS_{latt}^o , ΔU_{latt} , and ΔV are the lattice enthalpy, entropy, internal energy, and volume change, respectively. The $p \Delta V$ term in the enthalpy is generally negligible in solids at ordinary pressures, while $p \Delta V = RT$ for each gaseous species, hence the $(n + m)RT$ term in equation (4).²⁻⁶ The lattice internal energy can be expressed as the sum of the lattice potential energy, ΔU_o , and the internal energy change, ΔU_{therm} , as shown in equation (5).

$$U_{latt} = \Delta U_o + \Delta U_{therm} \quad (5)$$

ΔU_o can be expressed as

$$\Delta U_o = \frac{E_{total}^{[C]_n[A]_m} + E_{ZPE}^{[C]_n[A]_m}}{Z} - n \left(E_{total}^{C_{gas}^+} + E_{ZPE}^{C_{gas}^+} \right) - m \left(E_{total}^{A_{gas}^-} + E_{ZPE}^{A_{gas}^-} \right) \quad (6)$$

where E_{total}^X and E_{ZPE}^X ($X = C_{gas}^+$, A_{gas}^- , and $[C]_n[A]_m$) are the total energies and zero-point vibrational energies of the cations and anions in the gas phase and the solids, respectively. Z is the number of formula units included in the unit cell while n and m are the stoichiometric coefficients of the cation and anion, respectively, in one formula unit.⁵ In a similar manner, the ΔU_{therm} and ΔS_{latt}^o were estimated from the difference between the sum of the corresponding quantities of the gas-phase ions and the solid phase using the rigid-rotor harmonic oscillator approximation.^{5,7}

$$\Delta U_{therm} = \left(\frac{U_{vib}^{[C]_n[A]_m}}{Z} + (n + m)(3RT) \right) - n \left(U_{vib}^{C_{gas}^+} + U_{rot}^{C_{gas}^+} + U_{trans}^{C_{gas}^+} \right) - m \left(U_{vib}^{A_{gas}^-} + U_{rot}^{A_{gas}^-} + U_{trans}^{A_{gas}^-} \right) \quad (7)$$

$$\Delta S_{latt}^o = \frac{S_{vib}^{[C]_n[A]_m}}{Z} - n \left(S_{vib}^{C_{gas}^+} + S_{rot}^{C_{gas}^+} + S_{trans}^{C_{gas}^+} \right) - m \left(S_{vib}^{A_{gas}^-} + S_{rot}^{A_{gas}^-} + S_{trans}^{A_{gas}^-} \right) \quad (8)$$

Only the lattice vibrational contribution was considered for the internal energy and entropy whereas all three vibrational, rotational, and translational contributions were considered for the gas-phase ions. Additionally, three acoustic modes of the solids were approximated by $3RT$ per ion, hence the $(n + m)(3RT)$ term in equation (7).⁸

Solvation free energy ΔG_{sol}^* .

The standard free energy of solvation must be corrected for the free energy change ($\Delta G^{o \rightarrow *}$) associated with the solvation of 1 mole of each gaseous ion at 1 atmosphere (24.46 L/mol) into a 1 M solution. Thus,

$$\Delta G_{sol}^* = \Delta G_{sol}^o + (n + m)\Delta G^{o \rightarrow *} \quad (9)$$

where $\Delta G^{o \rightarrow *}$ is equal to 7.95 kJ/mol at 298 K.^{9,10} The standard free energy of solvation (G_{sol}^o) was obtained using

$$\Delta G_{sol}^o = n \left(E_{total,SMD}^{C_{sol}^+} - E_{total}^{C_{gas}^+} \right) + m \left(E_{total,SMD}^{A_{sol}^-} - E_{total}^{A_{gas}^-} \right) \quad (10)$$

where $E_{total,SMD}^{X_{sol}}$ and $E_{total}^{X_{gas}}$ are the final energies of species X in solution and in gas phase, respectively.

Under the solvation model based on density (SMD)¹¹ method, the solvation energy of each ion can be decomposed into bulk-electrostatic (ΔG_{ENP}) and non-electrostatic (ΔG_{CDS}) contributions as shown in (11).^{11,12}

$$\Delta G_{sol}^o = \Delta G_{ENP} + \Delta G_{CDS} \quad (11)$$

Table S1. Number of formula (Z), asymmetric (Z') units, and trapped solvent impurities in the crystallized $[N_{xxxx}]_y[VBH]$ active materials in the +4 (where $y=2$) and +5 (where $y=1$) states and the corresponding molar volume, $V_m(\text{exp})$, in $\text{L}\cdot\text{mol}^{-1}$. Also listed are the calculated molar volumes, $V_m(\text{calc})$, of the simplified crystals with the corresponding percent difference from $V_m(\text{exp})$.

xxxx	Vanadium (+4) species						Vanadium (+5) species					
	Z	Z'	Solvent	V_m (exp)	V_m (calc)	% Diff	Z	Z'	Solvent	V_m (exp)	V_m (calc)	% Diff
1111	2	1	4 H ₂ O, 2 MeOH	0.397	0.345	13.10	16	0.5	32 H ₂ O	0.302	0.259	14.24
2222	4	1	2 H ₂ O	0.435	0.427	1.84	2	1	---	0.322	0.315	2.17
3333	4	2	4 H ₂ O	0.605	0.573	5.29	2	1	---	0.378	0.380	0.53
4444	4	1	4 H ₂ O	0.723	0.726	0.41	4	1	4 MeCN	0.500	0.428	14.40

Table S2. SMD solvents used in ΔG_{sol}^* calculations.

Solvent	Dielectric Constant	Viscosity (25 °C), mPa·s
Dimethyl sulfoxide (DMSO)	46.826	2.00
N,N-dimethylacetamide	37.781	0.95
N,N-Dimethylformamide (DMF)	37.219	0.80
Nitromethane	36.562	0.63
Acetonitrile (MeCN)	35.688	0.34
Methanol	32.613	0.54
Propanonitrile	29.324	0.39 *
Nitroethane	28.29	0.66
Ethanol	24.852	1.08
1-Propanol	20.524	1.95
Acetone	20.493	0.30
2-Propanol	19.264	2.07
4-Methyl-2-pentanone	12.887	0.58 **
Dichloromethane	8.93	0.41
Tetrahydrofuran (THF)	7.4257	0.46
Ethyl acetate (Ethyl ethanoate)	5.9867	0.43
Toluene	2.3741	0.55
n-Hexane	1.8819	0.29

* at 30°C, ** at 20°C

Table S3. Calculated lattice thermodynamic properties, molar volumes, and free energies of sublimation of the $[N_{xxxx}]_y[VBH]$ active materials in the +4 (where $y=2$) and +5 (where $y=1$) states. Energy values are in units of $\text{kJ}\cdot\text{mol}^{-1}$ and molar volumes are in units of $\text{L}\cdot\text{mol}^{-1}$.

xxxx	Vanadium (+4) species					Vanadium (+5) species				
	ΔH_{latt}^o	$T\Delta S_{latt}^o$	ΔG_{latt}^o	V_m	ΔG_{sub}^*	ΔH_{latt}^o	$T\Delta S_{latt}^o$	ΔG_{latt}^o	V_m	ΔG_{sub}^*
Symmetric										
1111	-1253.0	-196.3	-1056.6	0.345	1067.2	-522.6	-141.6	-381.0	0.259	392.3
2222	-1176.8	-218.5	-958.3	0.427	968.4	-514.2	-147.9	-366.2	0.315	377.0
3333	-1164.8	-240.1	-924.7	0.573	934.0	-518.3	-161.1	-357.2	0.380	367.5
4444	-1105.1	-244.4	-860.7	0.726	869.4	-505.8	-168.9	-336.9	0.428	346.9
Monosubstituted										
1112	-1216.4	-197.6	-1018.9	0.397	1029.1	-515.7	-143.3	-372.4	0.284	383.5
1113	-1223.3	-205.3	-1018.1	0.405	1028.2	-524.4	-151.1	-373.3	0.285	384.3
1114	-1246.7	-216.3	-1030.4	0.415	1040.5	-516.0	-156.3	-359.7	0.298	370.6
Symmetric disubstituted										
1122	-1211.1	-207.7	-1003.4	0.406	1013.6	-515.0	-146.9	-368.1	0.294	379.1
1133	-1178.0	-216.2	-961.8	0.470	971.6	-506.5	-149.7	-356.8	0.337	367.4
1144	-1180.2	-219.8	-960.4	0.571	969.7	-504.6	-156.0	-348.7	0.353	359.2
Asymmetric disubstituted										
1123	-1191.0	-208.9	-982.1	0.431	992.1	-503.2	-144.1	-359.1	0.316	369.9
1124	-1166.4	-218.7	-947.8	0.517	957.3	-509.9	-149.9	-360.0	0.339	370.6
1134	-1184.5	-216.7	-967.9	0.518	977.4	-515.7	-155.3	-360.3	0.345	370.9
Monosubstituted										
444c	-1099.3	-235.7	-863.6	0.719	872.3	-498.8	-160.1	-338.7	0.417	348.8
4441	-1138.1	-237.3	-900.8	0.584	910.0	-493.9	-161.8	-332.1	0.406	342.3
444s	-1130.4	-235.1	-895.3	0.700	904.1	-492.0	-160.8	-331.3	0.435	341.2
444t	-1148.4	-240.6	-907.9	0.654	916.9	-463.0	-162.1	-300.9	0.449	310.8
Symmetric disubstituted										
44cc	-1152.2	-229.8	-922.3	0.560	931.7	-483.6	-147.6	-336.0	0.413	346.2
44ss	-1155.0	-243.4	-911.6	0.639	920.6	-480.6	-164.2	-316.3	0.434	326.3
44tt	-1130.9	-231.6	-899.3	0.676	908.2	-484.7	-154.8	-329.9	0.440	339.8
Asymmetric disubstituted										
441c	-1158.0	-223.3	-934.7	0.543	944.2	-512.0	-155.0	-357.1	0.368	367.5
44cs	-1135.1	-224.5	-910.6	0.647	919.6	-495.1	-152.5	-342.6	0.410	352.7
44ct	-1119.5	-226.2	-893.3	0.644	902.3	-483.4	-156.9	-326.6	0.425	336.6
441s	-1169.2	-230.9	-938.3	0.575	947.6	-504.2	-156.3	-347.9	0.382	358.2
441t	-1104.8	-229.2	-875.7	0.618	884.8	-494.8	-160.3	-334.5	0.385	344.8
44st	-1135.9	-230.1	-905.8	0.666	914.7	-486.1	-162.1	-324.0	0.422	334.0

Table S4. Heatmap of the free energies of solvation (ΔG_{sol}^*), in kJ/mol units, of the $[N_{xxxx}]_2[VBH]$ active materials. Red-yellow-green cell format indicates the favorability of solvation from least to most favorable ΔG_{sol}^* .

xxxx	Dimethyl sulfoxide	N,N-Dimethylacetate	N,N-Dimethylformamide	Nitromethane	Acetonitrile	Methanol	Propanonitrile	Nitroethane	Ethanol	1-Propanol	Acetone	2-Propanol	4-Methyl-2-pentanone	Dichloromethane	Tetrahydrofuran	Ethyl acetate	Toluene	n-Hexane
1111	-1099	-1106	-1103	-1098	-1107	-1156	-1099	-1091	-1143	-1131	-1089	-1127	-1055	-1022	-984	-951	-667	-541
2222	-1047	-1057	-1054	-1049	-1060	-1113	-1052	-1043	-1100	-1089	-1044	-1085	-1011	-983	-943	-912	-645	-525
3333	-1025	-1040	-1036	-1031	-1045	-1098	-1038	-1028	-1087	-1075	-1032	-1073	-1000	-975	-931	-902	-645	-528
4444	-1024	-1045	-1040	-1034	-1050	-1104	-1045	-1033	-1093	-1082	-1039	-1080	-1008	-985	-938	-910	-658	-541
1112	-1085	-1093	-1090	-1085	-1094	-1144	-1086	-1078	-1132	-1120	-1077	-1116	-1043	-1011	-973	-940	-661	-536
1113	-1079	-1088	-1084	-1079	-1089	-1140	-1081	-1073	-1127	-1116	-1073	-1112	-1039	-1008	-969	-937	-660	-536
1114	-1077	-1087	-1084	-1078	-1089	-1140	-1082	-1073	-1127	-1116	-1073	-1112	-1039	-1009	-969	-937	-662	-539
444c	-1024	-1041	-1036	-1030	-1045	-1101	-1039	-1028	-1089	-1078	-1033	-1075	-1001	-975	-931	-902	-644	-526
4441	-1040	-1056	-1052	-1046	-1061	-1113	-1055	-1044	-1102	-1091	-1048	-1088	-1016	-991	-946	-917	-658	-539
444s	-1016	-1036	-1031	-1026	-1041	-1095	-1036	-1024	-1084	-1073	-1030	-1071	-999	-976	-930	-902	-650	-534
444t	-1014	-1033	-1028	-1023	-1038	-1092	-1033	-1021	-1082	-1070	-1027	-1068	-996	-973	-927	-899	-647	-531
1122	-1072	-1081	-1077	-1072	-1083	-1134	-1074	-1066	-1121	-1109	-1066	-1106	-1032	-1002	-963	-931	-656	-533
1133	-1060	-1072	-1068	-1063	-1074	-1126	-1067	-1058	-1113	-1102	-1059	-1098	-1025	-997	-956	-925	-655	-533
1144	-1058	-1071	-1067	-1062	-1074	-1126	-1067	-1058	-1114	-1103	-1060	-1100	-1027	-999	-957	-926	-659	-538
44cc	-1011	-1025	-1021	-1015	-1029	-1087	-1022	-1011	-1074	-1062	-1016	-1060	-983	-956	-914	-885	-624	-507
44ss	-1008	-1027	-1022	-1017	-1032	-1086	-1027	-1015	-1075	-1064	-1021	-1062	-989	-967	-921	-893	-642	-527
44tt	-1003	-1020	-1016	-1011	-1026	-1079	-1020	-1008	-1068	-1057	-1013	-1054	-982	-959	-915	-887	-636	-521
1123	-1066	-1076	-1073	-1067	-1078	-1130	-1071	-1062	-1117	-1106	-1062	-1102	-1029	-999	-959	-928	-655	-533
1124	-1064	-1076	-1072	-1067	-1078	-1130	-1071	-1062	-1117	-1106	-1063	-1102	-1029	-1000	-960	-928	-657	-535
1134	-1059	-1071	-1068	-1062	-1074	-1126	-1067	-1058	-1114	-1102	-1059	-1099	-1026	-998	-957	-926	-657	-536
441c	-1046	-1060	-1056	-1050	-1063	-1118	-1056	-1046	-1106	-1094	-1049	-1091	-1016	-988	-946	-915	-647	-527
44cs	-1014	-1030	-1026	-1020	-1035	-1090	-1029	-1017	-1079	-1067	-1022	-1064	-990	-965	-922	-893	-636	-519
44ct	-1013	-1029	-1024	-1019	-1033	-1089	-1027	-1016	-1077	-1065	-1020	-1063	-988	-963	-920	-891	-634	-518
441s	-1032	-1048	-1044	-1038	-1053	-1105	-1046	-1036	-1094	-1083	-1039	-1080	-1008	-982	-938	-909	-650	-533
441t	-1030	-1046	-1042	-1036	-1050	-1103	-1044	-1033	-1092	-1080	-1037	-1078	-1005	-980	-936	-907	-648	-530
44st	-1007	-1024	-1020	-1015	-1030	-1084	-1024	-1013	-1073	-1062	-1018	-1059	-987	-964	-919	-891	-640	-525

Table S5. Heatmap of the free energies of solvation (ΔG_{sol}^*), in kJ/mol units, of the [N_{xxxx}][VBH] active materials. Red-yellow-green cell format indicates the favorability of solvation from least to most favorable ΔG_{sol}^* .

xxxx	Dimethyl sulfoxide	N,N-Dimethylacetate	N,N-Dimethylformamide	Nitromethane	Acetonitrile	Methanol	Propanonitrile	Nitroethane	Ethanol	1-Propanol	Acetone	2-Propanol	4-Methyl-2-pentanone	Dichloromethane	Tetrahydrofuran	Ethyl acetate	Toluene	n-Hexane
1111	-461	-467	-465	-452	-458	-461	-459	-454	-460	-455	-457	-458	-446	-421	-415	-402	-283	-229
2222	-435	-443	-440	-427	-434	-439	-436	-430	-439	-433	-434	-436	-425	-402	-394	-382	-272	-222
3333	-424	-435	-432	-418	-427	-432	-429	-422	-432	-427	-428	-430	-419	-398	-388	-377	-272	-223
4444	-424	-437	-433	-420	-429	-435	-432	-425	-435	-430	-431	-434	-423	-403	-392	-381	-279	-230
1112	-454	-461	-458	-445	-452	-455	-453	-447	-454	-449	-451	-452	-440	-416	-409	-396	-280	-227
1113	-451	-458	-456	-442	-449	-453	-451	-445	-452	-447	-448	-450	-438	-415	-407	-395	-280	-227
1114	-450	-458	-455	-442	-449	-453	-451	-445	-452	-447	-449	-450	-439	-415	-407	-395	-281	-228
444c	-423	-435	-432	-418	-427	-433	-430	-422	-433	-428	-428	-431	-419	-398	-388	-377	-271	-222
4441	-431	-442	-439	-426	-435	-440	-437	-430	-440	-434	-436	-438	-427	-406	-396	-385	-278	-228
444s	-420	-432	-429	-416	-425	-431	-428	-421	-431	-426	-427	-429	-418	-399	-387	-377	-275	-226
444t	-419	-431	-428	-414	-424	-429	-426	-419	-429	-424	-425	-428	-417	-397	-386	-376	-273	-225
1122	-447	-455	-452	-439	-446	-450	-447	-442	-449	-444	-445	-447	-435	-411	-404	-392	-278	-225
1133	-442	-450	-447	-434	-441	-446	-443	-437	-445	-440	-441	-443	-432	-409	-401	-389	-277	-226
1144	-440	-450	-447	-434	-442	-446	-444	-437	-446	-440	-442	-444	-432	-410	-401	-389	-279	-228
44cc	-417	-427	-424	-411	-419	-426	-421	-414	-426	-420	-420	-424	-410	-389	-380	-369	-261	-213
44ss	-415	-428	-425	-411	-421	-426	-423	-416	-426	-421	-422	-425	-414	-394	-383	-373	-271	-223
44tt	-413	-424	-421	-408	-417	-423	-420	-413	-423	-418	-419	-421	-410	-390	-380	-370	-268	-220
1123	-444	-452	-450	-437	-444	-448	-445	-439	-447	-442	-443	-445	-433	-410	-402	-390	-277	-225
1124	-444	-452	-449	-436	-443	-448	-445	-439	-447	-442	-443	-445	-434	-411	-403	-390	-278	-227
1134	-441	-450	-447	-434	-441	-446	-444	-437	-445	-440	-442	-443	-432	-410	-401	-389	-278	-227
441c	-434	-444	-441	-428	-436	-442	-438	-431	-441	-436	-436	-439	-427	-405	-395	-384	-273	-223
44cs	-418	-429	-426	-413	-422	-428	-424	-417	-428	-423	-423	-426	-414	-393	-383	-373	-268	-219
44ct	-418	-429	-426	-412	-421	-427	-423	-416	-427	-422	-422	-425	-413	-392	-383	-372	-267	-218
441s	-427	-438	-435	-422	-431	-436	-433	-426	-436	-430	-432	-434	-423	-402	-392	-381	-275	-225
441t	-426	-437	-434	-421	-429	-435	-432	-425	-434	-429	-430	-433	-421	-400	-391	-380	-274	-224
44st	-415	-427	-424	-411	-419	-425	-422	-415	-425	-420	-421	-423	-412	-393	-382	-372	-270	-221

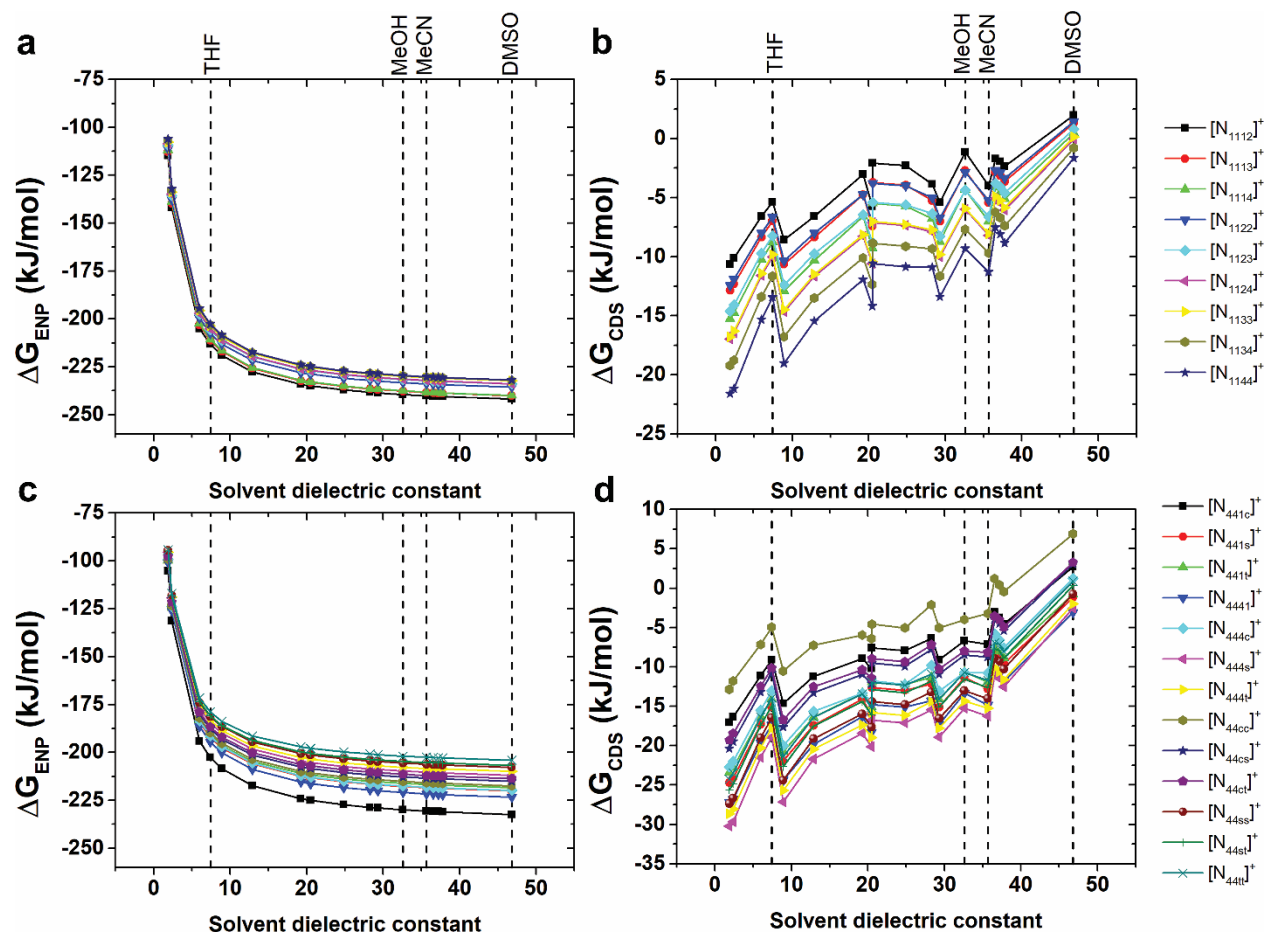


Fig. S1. The electrostatic (ΔG_{ENP}) and cavity-dispersion (ΔG_{CDS}) components of the SMD solvation energies of the asymmetric cations: **a** shows the ΔG_{ENP} while **b** shows the ΔG_{CDS} of the asymmetric $[N_{1111}]^+$ -based cations across the different solvents used; panels **c** and **d** show the ΔG_{ENP} and ΔG_{CDS} , respectively, of the $[N_{4444}]^+$ -based cations.

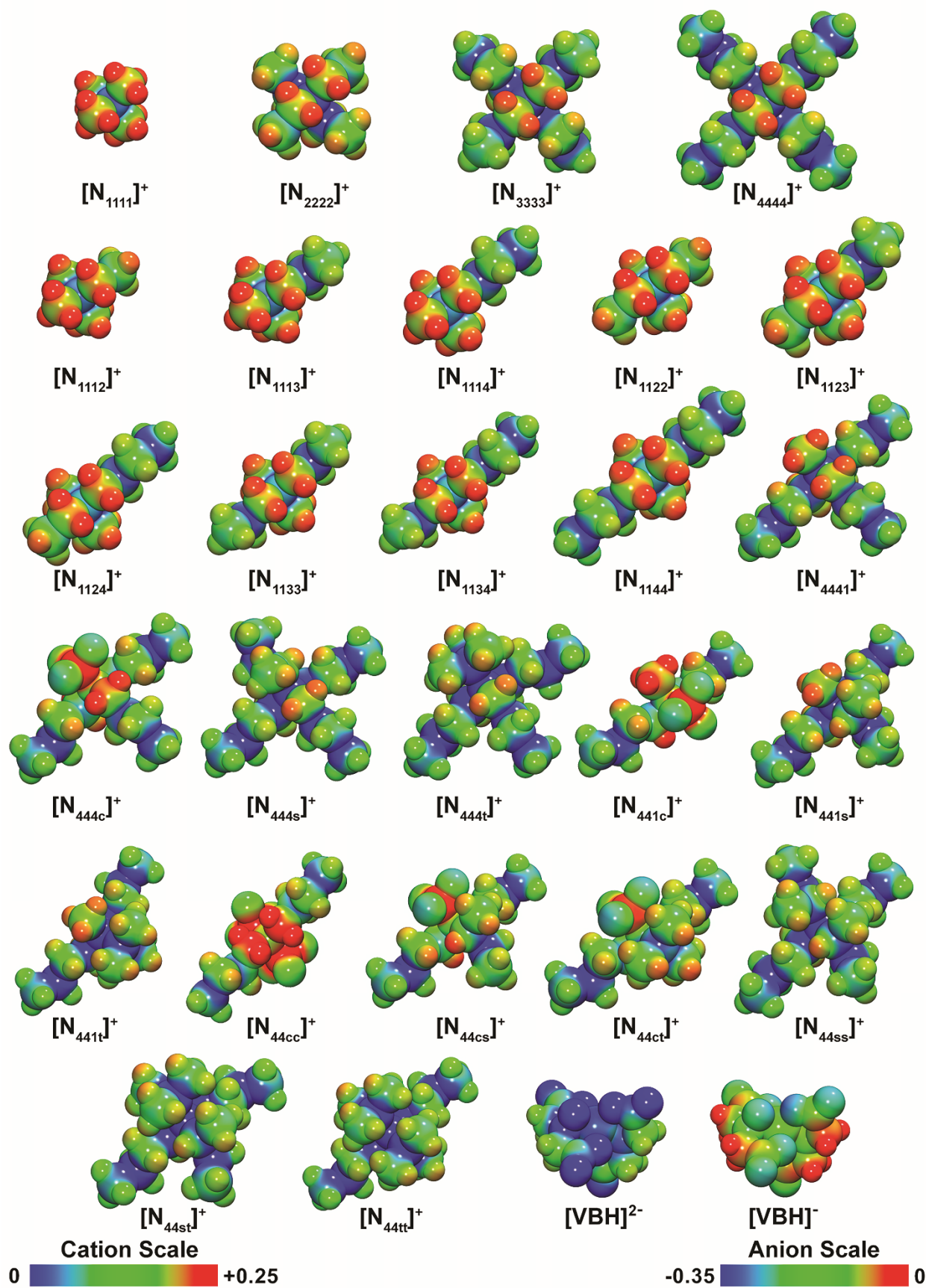


Fig. S2. Electrostatic potential maps from natural atomic charges of the free ions in the gas phase.

Table S6. Crystal data and structure refinement summary.

Compound	[N1111]VBH	[N2222]VBH	[N1114] ₂ VBH
Identification code	UMD702_a	UMD2266f_a	UMD1830B_a
Empirical formula	C ₁₂ H ₂₅ N ₃ O ₁₂ V	C ₁₆ H ₂₈ N ₃ O ₁₀ V	C ₂₂ H ₄₈ N ₄ O ₁₂ V
Formula weight	454.29	473.35	611.58
Temperature/K	200(2)	297(2)	200(2)
Crystal system	orthorhombic	monoclinic	monoclinic
Space group	Fddd	P2 ₁	P2 ₁ /c
a/Å	15.926(2)	11.8775(7)	13.3481(10)
b/Å	18.696(3)	8.1637(5)	12.7135(10)
c/Å	26.925(4)	12.1364(6)	18.0999(13)
α/°	90.00	90	90
β/°	90.00	114.799(2)	96.632(2)
γ/°	90.00	90	90
Volume/Å ³	8017(2)	1068.28(11)	3051.0(4)
Z	16	2	4
ρ _{calc} /g/cm ³	1.506	1.472	1.331
μ/mm ⁻¹	0.559	0.521	0.387
F(000)	3792.0	496.0	1308.0
Crystal size/mm ³	0.3 × 0.14 × 0.08	0.22 × 0.15 × 0.1	0.32 × 0.28 × 0.27
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2θ range for data collection/°	5.94 to 52.82	6.298 to 52.79	6.086 to 50.884
Index ranges	-19 ≤ h ≤ 19, -23 ≤ k ≤ 23, -33 ≤ l ≤ 33	-14 ≤ h ≤ 14, -10 ≤ k ≤ 10, -15 ≤ l ≤ 14	-16 ≤ h ≤ 16, -15 ≤ k ≤ 15, -21 ≤ l ≤ 21
Reflections collected	56007	34061	82551
Independent reflections	2073 [R _{int} = 0.0479, R _{sigma} = 0.0143]	4351 [R _{int} = 0.0329, R _{sigma} = 0.0207]	5619 [R _{int} = 0.0474, R _{sigma} = 0.0171]
Data/restraints/parameters	2073/2/138	4351/1/275	5619/370/390
Goodness-of-fit on F ²	1.096	1.016	1.085
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0297, wR ₂ = 0.0715	R ₁ = 0.0215, wR ₂ = 0.0564	R ₁ = 0.0358, wR ₂ = 0.0802
Final R indexes [all data]	R ₁ = 0.0392, wR ₂ = 0.0759	R ₁ = 0.0231, wR ₂ = 0.0575	R ₁ = 0.0443, wR ₂ = 0.0857
Largest diff. peak/hole / e Å ⁻³	0.24/-0.31	0.16/-0.14	0.75/-0.50

NMR spectra

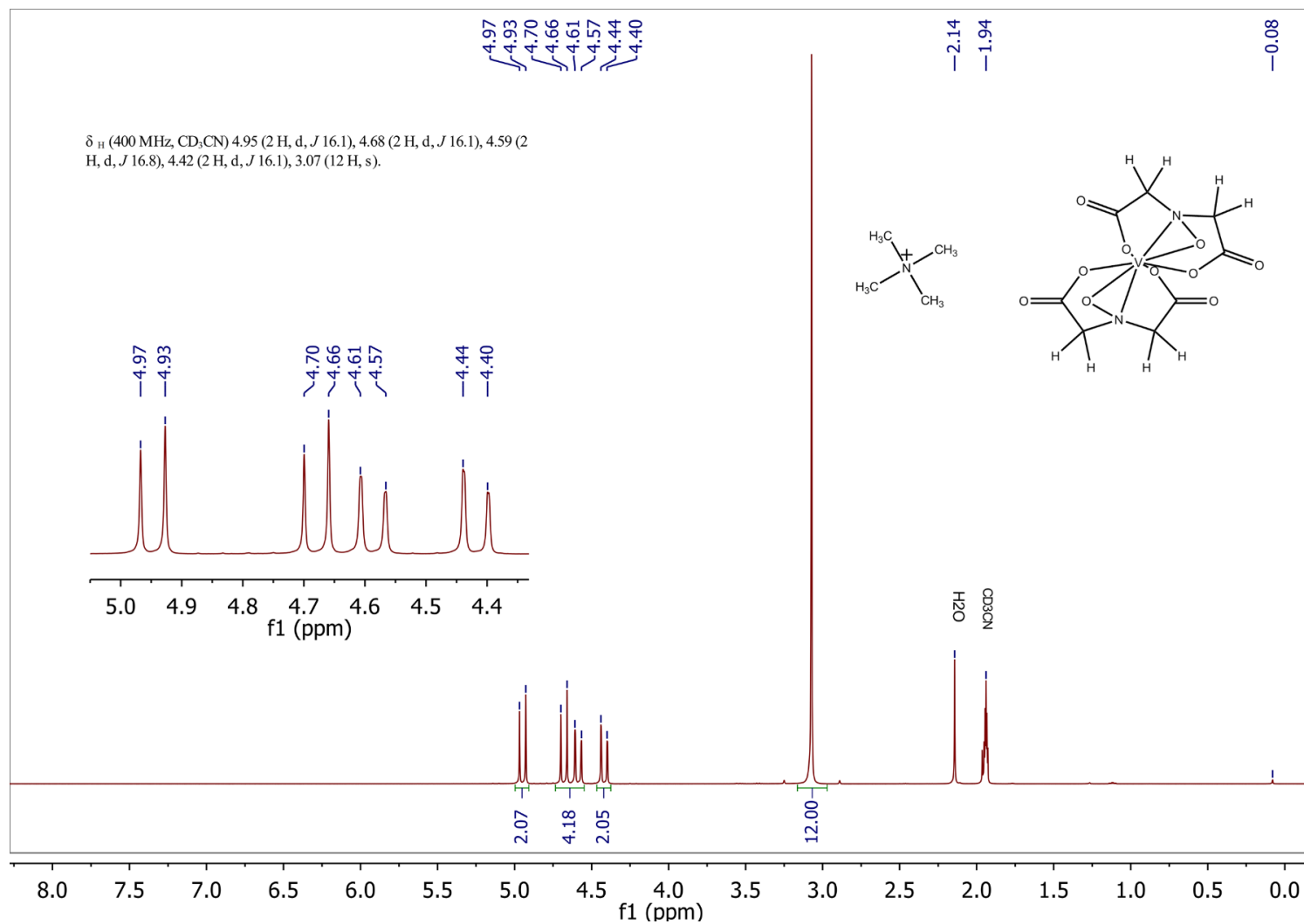


Fig. S3. ¹H-NMR of [N₁₁₁₁]VBH

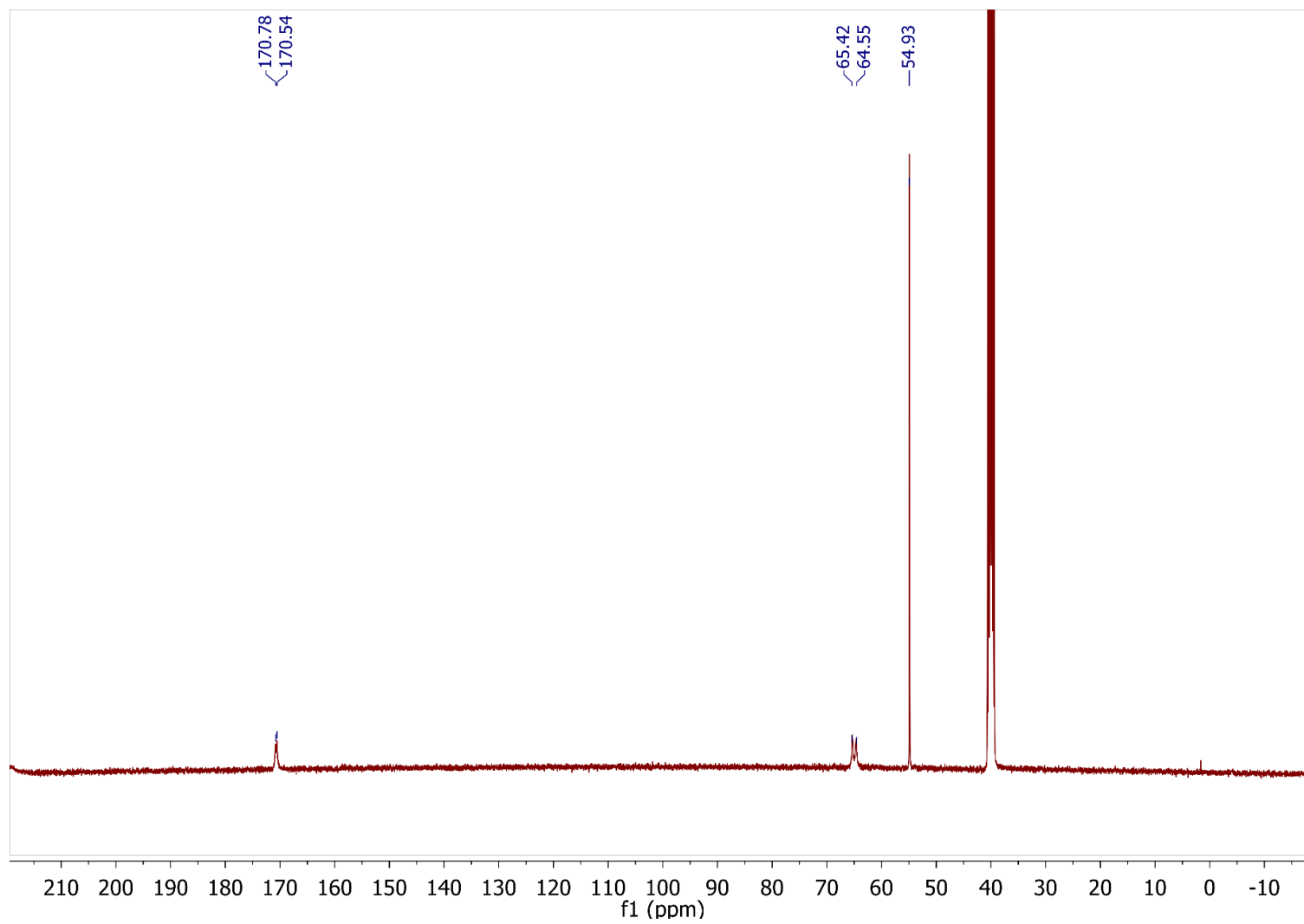


Fig. S4. ^{13}C -NMR of [N₁₁₁₁]VBH

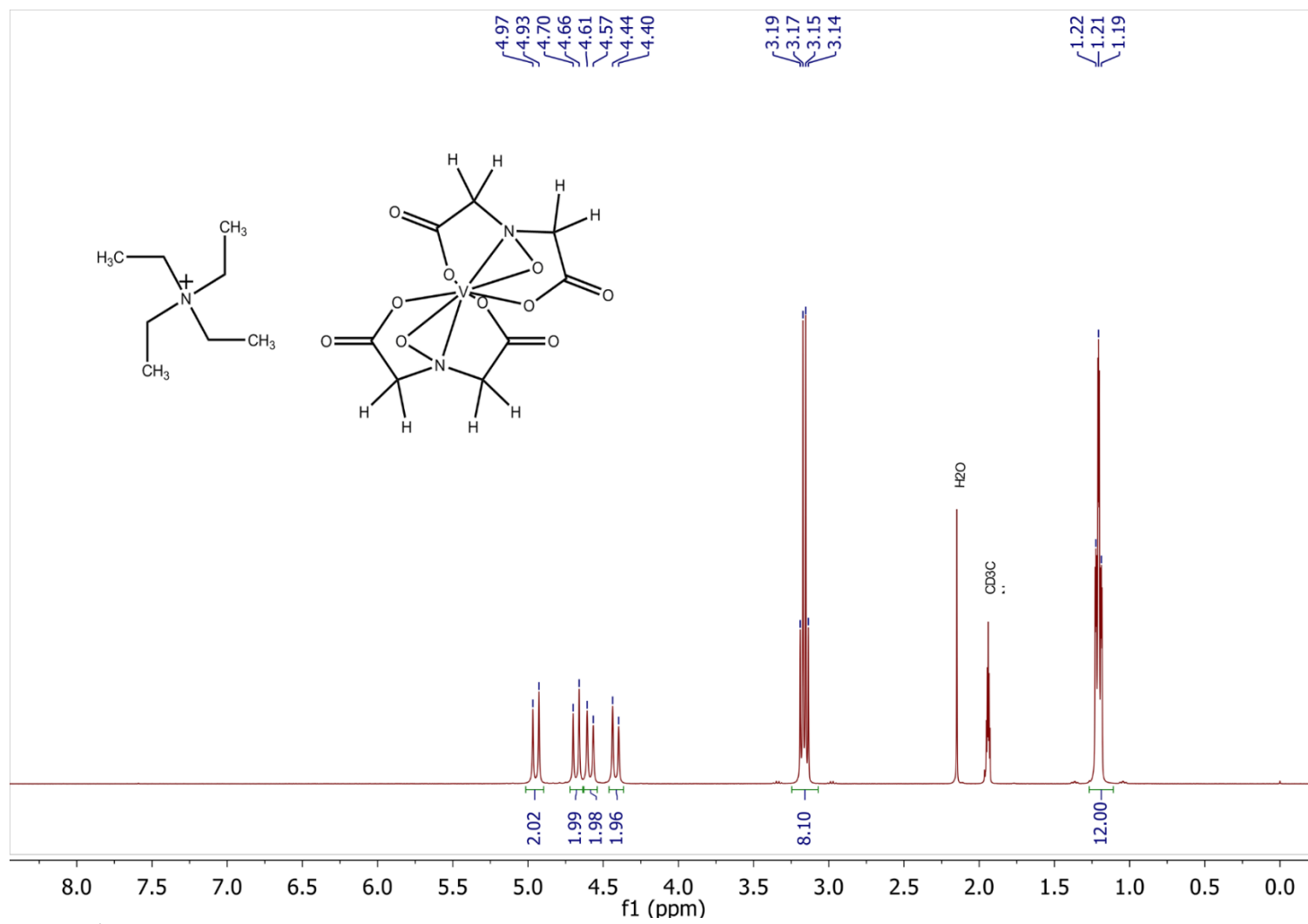


Fig. S5. $^1\text{H-NMR}$ of $[\text{N}_{2222}]\text{VBH}$

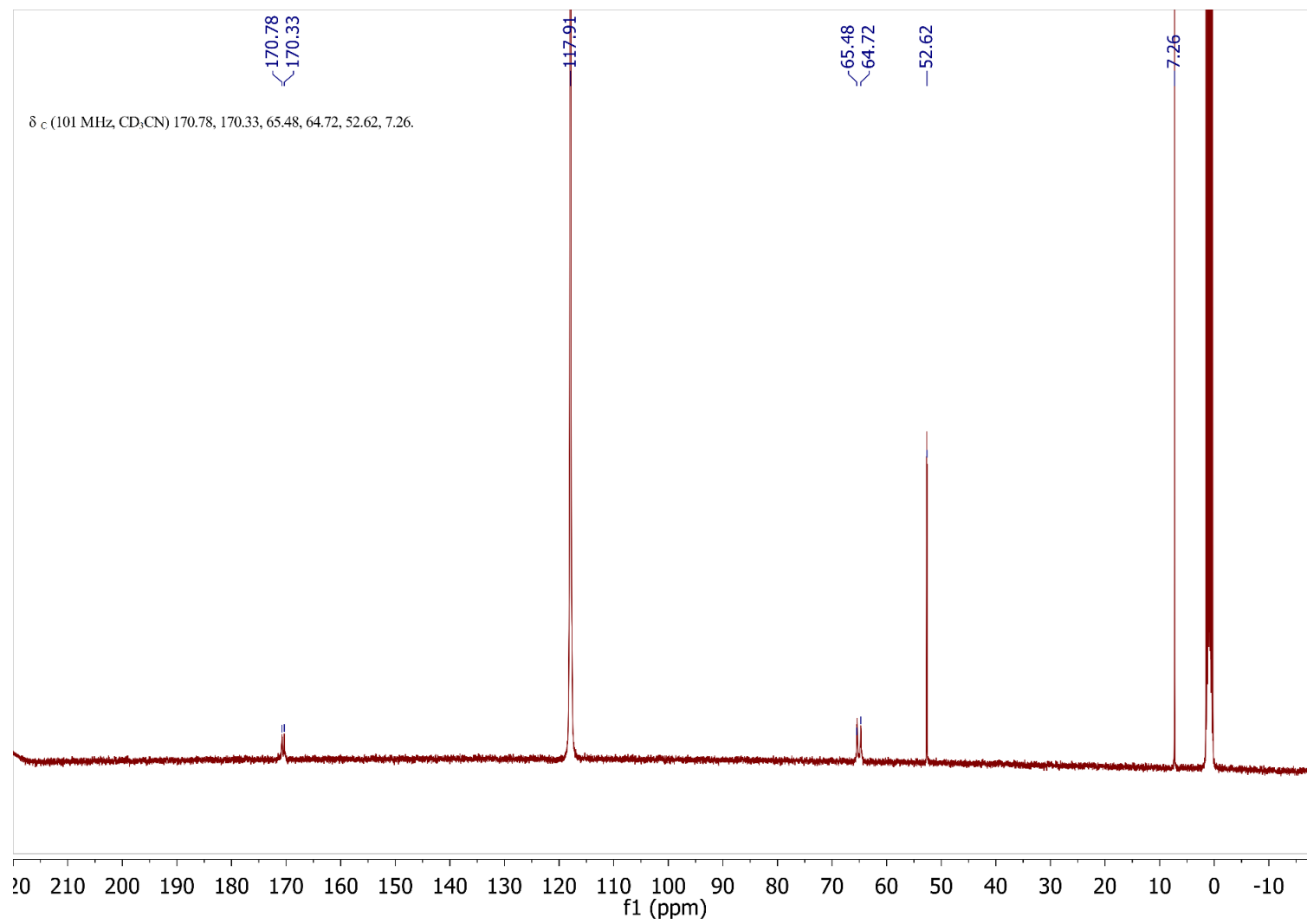


Fig. S6. ^{13}C -NMR of $[N_{2222}]VBH$

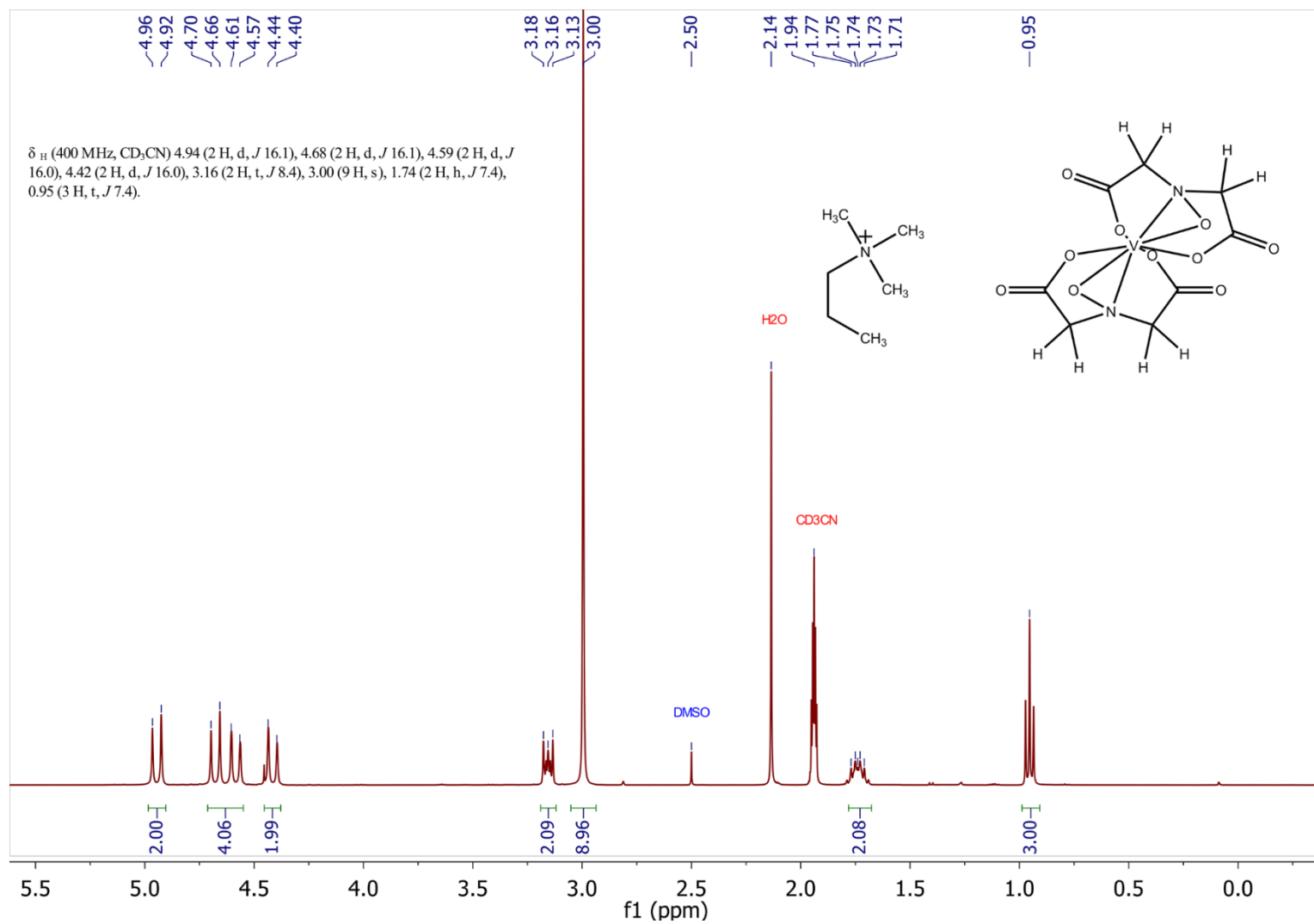


Fig. S7. ^1H -NMR of $[\text{N}_{1113}]\text{VBH}$

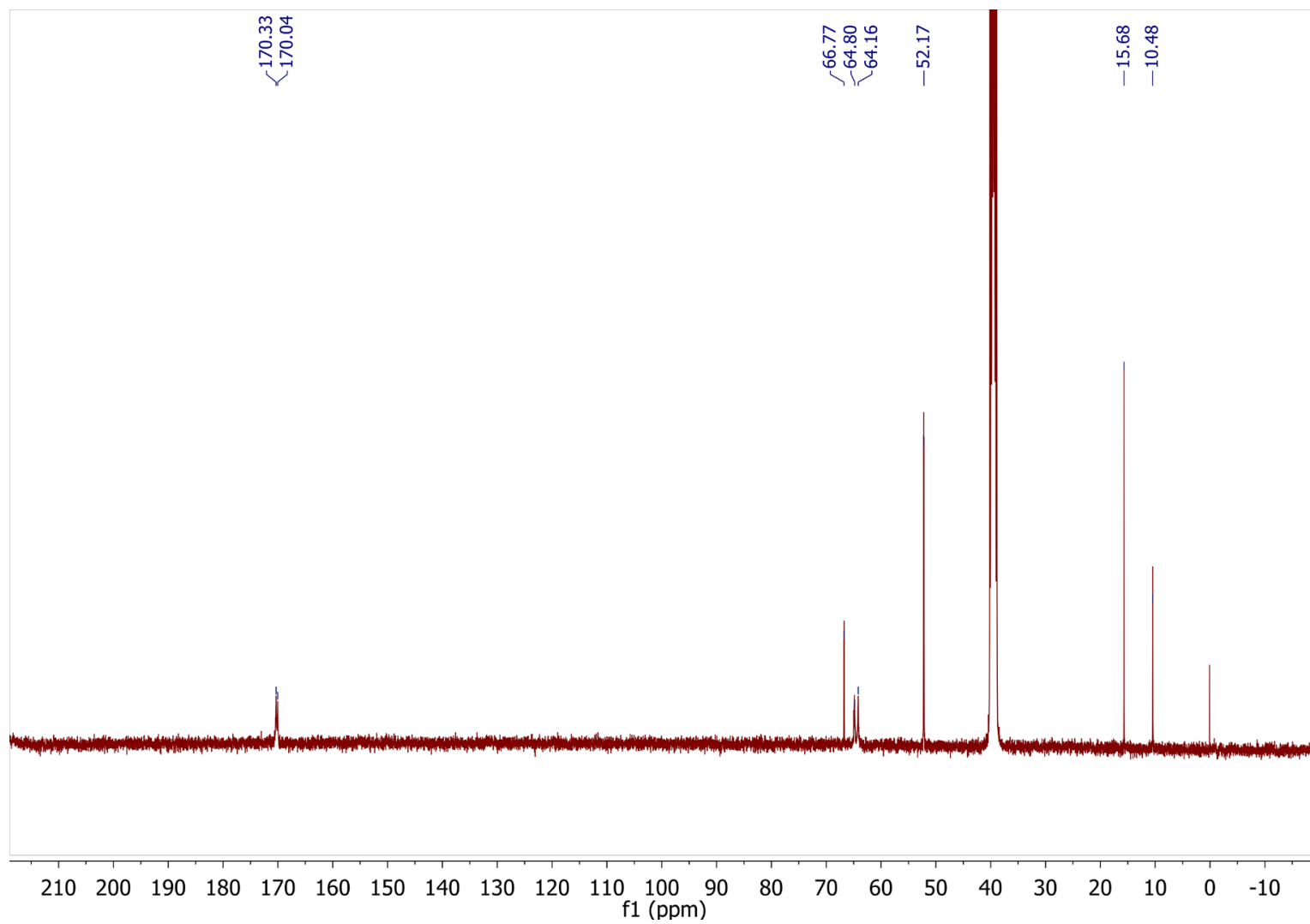


Fig. S8. ^{13}C -NMR of [N₁₁₁₃]VBH

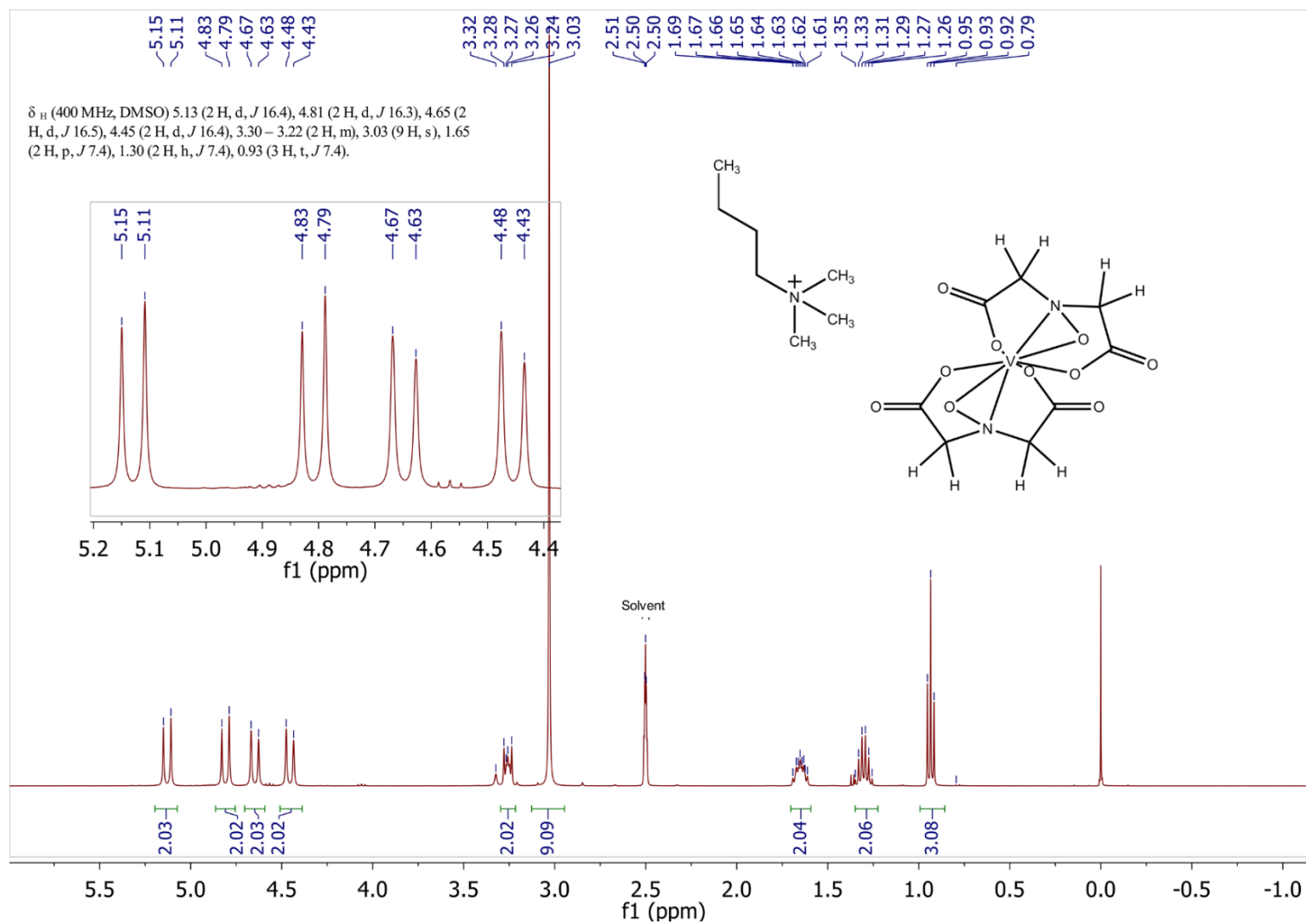


Fig. S9. $^1\text{H-NMR}$ of $[\text{N}_{1114}]\text{VBH}$

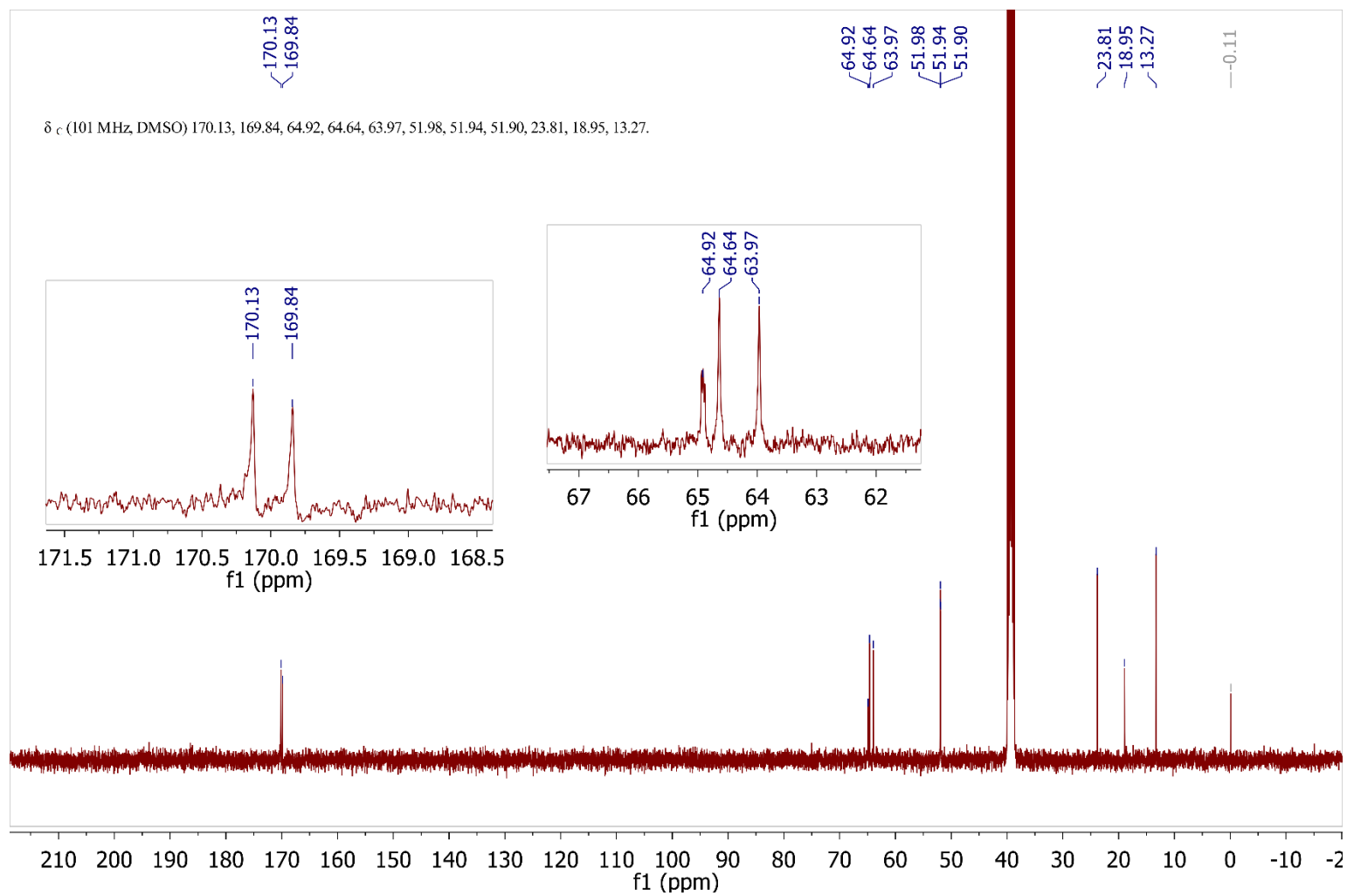
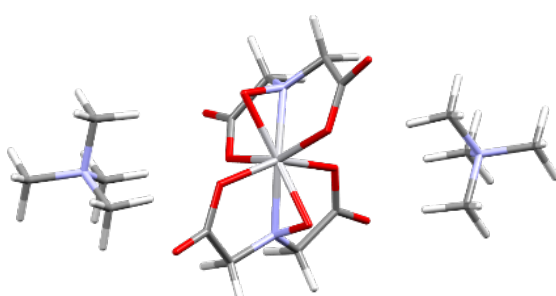
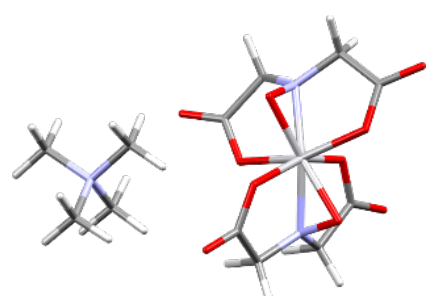


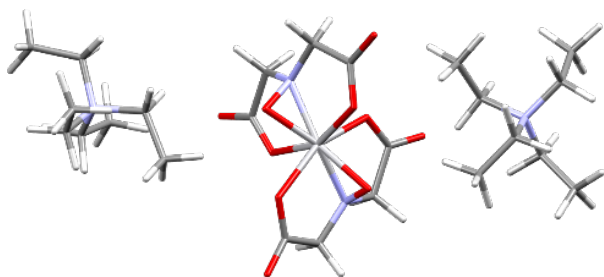
Fig. S10. ^{13}C -NMR of $[\text{N}_{1114}]\text{VBH}$

Table S7. Cartesian coordinates of the formula units in the DFT-optimized crystals.

Reduced (V^{+4}) State	Oxidized (V^{+5}) State
Symmetric	
$[N_{1111}]_2[VBH]$	$[N_{1111}][VBH]$
	
63	46
N -3.748725 -3.357626 2.163700 C -2.412568 -3.628849 2.793092 H -2.015621 -4.534117 2.321823 H -1.770597 -2.763102 2.596176 C -4.389490 -2.180383 2.832807 H -5.362844 -2.020155 2.356636 H -4.528982 -2.430695 3.888512 C -3.548468 -3.045905 0.708829 H -3.117303 -3.924972 0.220771 H -2.878830 -2.180301 0.656895 C -4.620280 -4.566178 2.340611 H -4.678703 -4.779597 3.412566 H -5.620122 -4.313560 1.976038 H -3.723152 -1.320187 2.704075 H -4.521206 -2.793852 0.273959 H -2.556736 -3.765551 3.871842 H -4.176360 -5.386851 1.766427 V 0.000000 0.000000 0.000000 O 1.941460 0.275732 -0.686253 O 4.107492 0.438703 -0.084252 O 0.926525 -1.278482 1.220936 O -1.960658 -0.156191 3.635925 O -1.505158 -0.281773 1.435983 O -0.185011 2.030842 0.498158 O -1.565272 3.805105 0.399149 O -0.422332 0.756447 -1.798111 O -1.889073 -2.734539 -2.454529 O -0.497044 -1.770525 -0.966725 N 1.060864 0.012147 1.718580 N -1.604238 0.550122 -1.096730 C 2.895705 0.391745 0.186365 C 2.432359 0.503962 1.640353 H 3.088858 -0.076807 2.301686 H 2.445212 1.550349 1.977492	O -1.528721 1.269096 0.103523 O -3.220906 2.013053 1.386607 O 2.336292 -2.213732 2.466184 O 1.281241 -1.425737 0.641797 O 0.757738 1.008673 1.476085 N -0.212294 0.181070 1.996565 C -2.135170 1.446602 1.257599 C -1.416311 0.862829 2.463962 H -2.041397 0.125616 2.983798 H -1.140857 1.672257 3.153073 C 0.288306 -0.977475 2.743762 H 0.567115 -0.692578 3.765087 H -0.536431 -1.702360 2.787340 C 1.412601 -1.591643 1.936868 V 0.000000 0.000000 0.000000 O 1.627991 0.826452 -0.833773 O 3.220868 0.613727 -2.397490 O -2.643423 -3.018049 -0.660417 O -1.426902 -1.393717 0.300288 O -0.620578 -0.016272 -1.858956 N 0.184973 -1.116701 -1.668437 C 2.187106 0.227402 -1.848464 C 1.496116 -1.053347 -2.308043 H 2.075089 -1.920652 -1.961409 H 1.412233 -1.086067 -3.402556 C -0.536750 -2.391688 -1.666782 H -0.933526 -2.582494 -2.672185 H 0.160588 -3.189836 -1.365393 C -1.641558 -2.294791 -0.617610 C 4.776390 -2.070314 0.095400 H 4.134260 -1.821233 -0.755912 H 4.160856 -2.412278 0.936558 C 4.531679 0.227449 0.948266 H 3.857163 0.464821 0.121559

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 H 0.690718 -0.241614 3.795364
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 C -1.280002 2.618903 0.139434
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 H -3.103753 1.466114 0.010457
 H -2.703231 2.324883 -1.492179
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 H -2.773368 -0.250536 -2.662917
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 C -1.548648 -1.785875 -1.727895
 N 2.121329 5.042326 -0.301367
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 C 2.833349 3.786134 0.109687
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 H 0.729209 5.658917 -1.780155
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 H 3.597457 6.406943 0.338996
 H 3.808037 5.769200 -1.343116
 H 2.028075 4.522259 -2.334486
 H 2.526677 7.007665 -0.949196
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[N₂₂₂₂]₂[VBH]

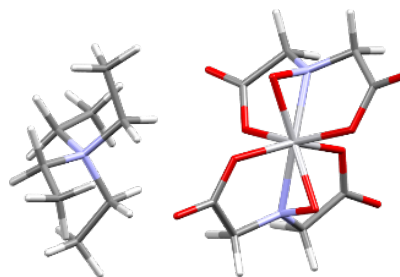


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 C 1.094621 4.813559 -0.556078
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 C 2.155321 4.197000 0.317555
 H 1.663961 3.798873 1.212036

H 3.969017 -0.181393 1.794911
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 H 6.792853 0.624249 -0.373188
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 H 5.516271 -2.823087 -0.196579
 H 5.109213 1.118382 1.220598
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[N₂₂₂₂][VBH]



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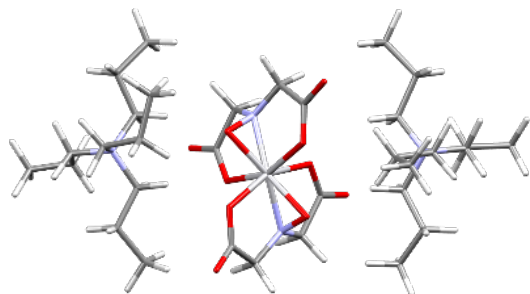
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 C -1.045768 2.169586 1.773672
 H -1.754864 1.776680 2.517637
 H -0.680152 3.149197 2.109210

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[N₃₃₃₃]₂[VBH]

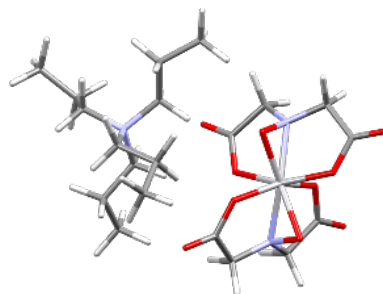


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 H -2.954691 -5.369520 3.499814
 H -1.914983 -4.969831 4.888406
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 H -1.453061 -2.781221 1.305936
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[N₃₃₃₃][VBH]



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 C -1.000073 1.541194 2.358959
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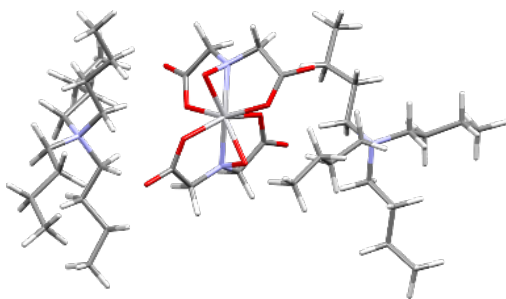
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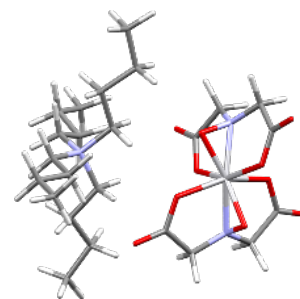
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[N₄₄₄₄][VBH]



82

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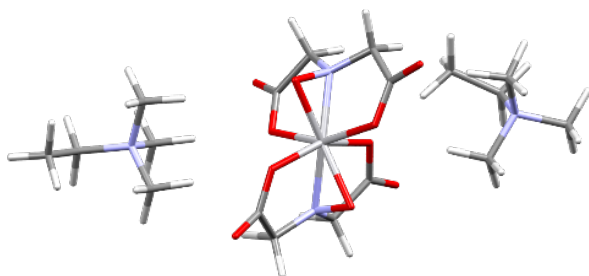
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Monosubstituted [N111x]

[N₁₁₁₂]₂[VBH]

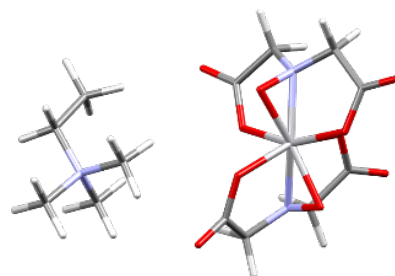


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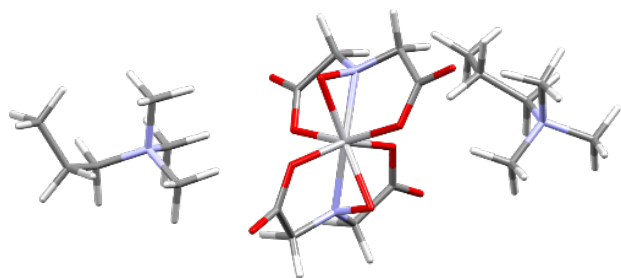
49

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[N₁₁₁₃]₂[VBH]

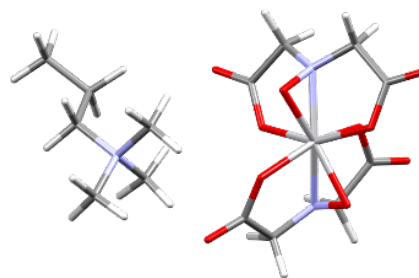


75

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[N₁₁₁₃][VBH]



52

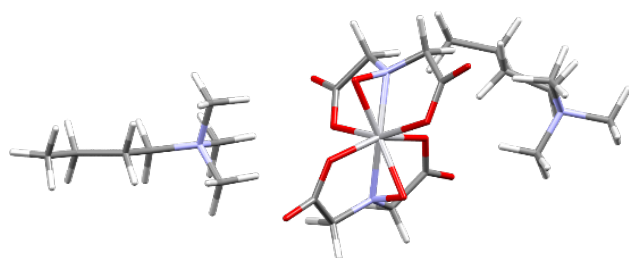
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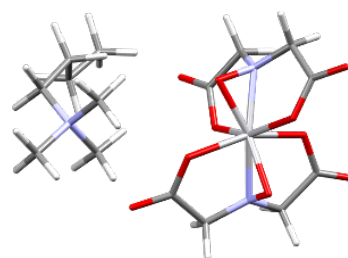
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[N₁₁₁₄][VBH]



55

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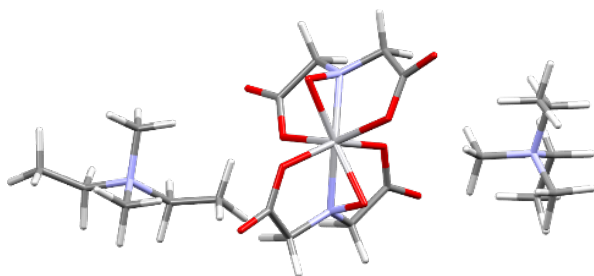
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Symmetric disubstituted [N11xx]

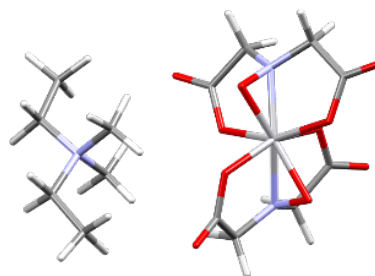
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[N₁₁₂₂][VBH]

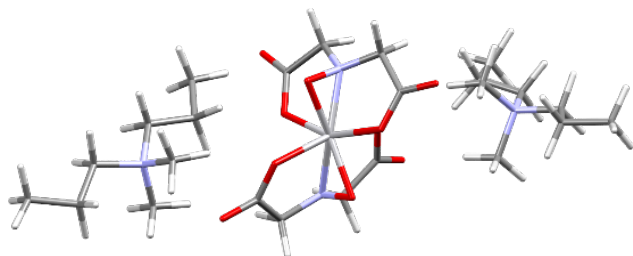


52

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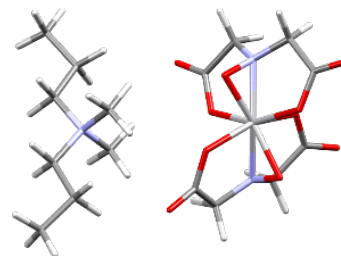
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H 2.593800 1.538126 1.750041
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H 0.405444 2.120883 2.689088
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C -0.391636 2.724238 -0.949083
C -1.595747 1.970766 -1.528099
H -2.484988 2.210891 -0.926260
H -1.769229 2.245920 -2.580125
C -2.454026 -0.397067 -1.576187
H -2.833517 -0.371107 -2.605672
H -3.260511 -0.107265 -0.883915
C -1.974323 -1.801380 -1.189975
N 3.240923 6.215281 -0.053449
C 2.376598 6.219296 1.200998
H 1.714728 7.086634 1.075584
C 4.249820 5.113371 0.029722
H 4.853707 5.274399 0.930221
H 4.860530 5.124684 -0.878862
C 2.385995 6.053120 -1.280176
H 1.788342 5.141508 -1.184659
H 1.721347 6.924247 -1.339494
C 3.939460 7.569903 -0.097557
H 4.464280 7.654719 0.860402
H 3.053215 5.982174 -2.145712
H 3.135814 8.310653 -0.102886
H 3.069855 6.430250 2.028577
H 3.722473 4.159767 0.094657
C 1.601392 4.937364 1.441753
H 0.864778 4.727802 0.656989
H 2.261728 4.067357 1.542386
H 1.092786 5.015071 2.412083
C 4.875118 7.774457 -1.269449
H 4.323530 7.864499 -2.213115
H 5.402577 8.717334 -1.084773
H 5.613112 6.975726 -1.391059

C 4.476390 0.149735 0.806077
H 3.755658 0.334384 0.006402
H 3.947645 -0.248096 1.674652
C 6.323519 -0.325510 -0.776929
H 6.853497 0.532815 -0.347315
H 7.051358 -1.116625 -0.996472
N 5.467806 -0.880555 0.356890
C 6.421377 -1.203048 1.501499
H 7.237137 -1.786524 1.055177
H 6.815778 -0.228970 1.813632
H 5.517616 -2.871536 -0.360779
H 5.023462 1.071035 1.032110
C 5.793079 -1.946127 2.662802
H 5.489381 -2.964969 2.393515
H 6.547244 -2.007907 3.453511
H 4.914532 -1.442386 3.082029
C 5.545416 0.086808 -2.007748
H 6.264333 0.483009 -2.738757
H 5.026493 -0.752788 -2.487005
H 4.831254 0.888006 -1.795172

[N₁₁₃₃]₂[VBH]

87

N -6.177971 -0.964721 0.087767
 C -4.768781 -1.429327 -0.128985
 H -4.647035 -1.767908 -1.162902
 H -4.078149 -0.607206 0.091163
 C -6.341007 -0.327195 1.469301
 H -6.091102 -1.111234 2.195755
 C -6.561043 0.026516 -0.964035
 H -6.424254 -0.423024 -1.951318
 H -5.904193 0.895173 -0.873085
 C -7.135813 -2.146760 0.059612
 H -6.768773 -2.845490 0.822172
 H -8.106912 -1.734017 0.362532
 H -7.414380 -0.113475 1.548376
 H -7.608678 0.309117 -0.801925
 H -4.581950 -2.262006 0.553893
 C -7.269767 -2.863587 -1.270545
 H -6.324297 -3.347197 -1.549334
 H -7.570658 -2.160054 -2.058240
 C -5.518748 0.922031 1.726841
 H -4.445919 0.697920 1.784240
 H -5.672179 1.674151 0.941289
 C -5.959930 1.521578 3.062863
 H -7.015026 1.837915 3.022646
 H -5.865893 0.778184 3.864977
 H -5.349065 2.395951 3.314105
 C -8.370901 -3.908838 -1.101850
 H -8.496305 -4.514974 -2.008604
 H -8.127871 -4.585321 -0.272572
 H -9.326894 -3.417760 -0.882786
 V 0.000000 0.000000 0.000000
 O 2.057210 -0.248526 -0.219490
 O 4.053686 -0.152500 0.833051
 O 0.261486 -1.400645 1.396073
 O -2.667577 0.565001 3.117718
 O -1.804447 0.272359 1.048462
 O 0.362309 2.026195 0.458939
 O -0.284691 4.142745 0.020021
 O 0.249005 0.660161 -1.838806
 O -2.543588 -2.153337 -2.462016
 O -0.942141 -1.589908 -0.963953

[N₁₁₃₃][VBH]

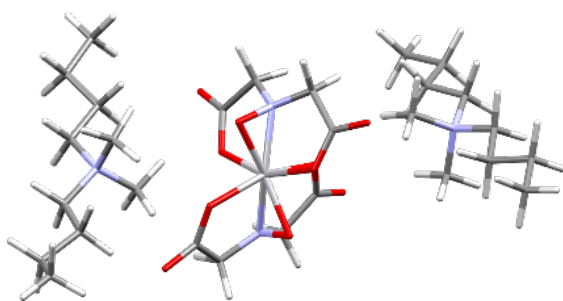
58

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 O -3.213097 1.969320 1.490697
 O 2.503750 -2.133130 2.410177
 O 1.414860 -1.309857 0.626136
 O 0.762441 1.132368 1.380483
 N -0.101386 0.265084 2.002166
 C -2.129147 1.413290 1.323378
 C -1.329593 0.882895 2.506223
 H -1.915765 0.111485 3.022421
 H -1.089120 1.695329 3.203982
 C 0.547880 -0.792277 2.784931
 H 0.965500 -0.383919 3.713425
 H -0.221693 -1.542664 3.017434
 C 1.589968 -1.472676 1.910948
 V 0.000000 0.000000 0.000000
 O 1.454487 0.924483 -0.980570
 O 2.682287 1.037017 -2.861099
 O -2.393936 -3.228404 -0.397787
 O -1.261326 -1.495077 0.472127
 O -0.786485 -0.197686 -1.790803
 N 0.175491 -1.171920 -1.635893
 C 1.897290 0.450729 -2.120595
 C 1.372602 -0.954150 -2.440881
 H 2.120223 -1.705053 -2.147788
 H 1.142942 -1.064858 -3.509476
 C -0.340573 -2.533450 -1.456992
 H -0.716212 -2.939874 -2.401972
 H 0.476333 -3.160123 -1.065943
 C -1.435950 -2.455274 -0.400564
 C 4.773868 -2.174808 -0.276416
 H 4.215529 -1.892686 -1.172672
 H 4.075882 -2.496126 0.502622
 C 4.562964 0.096831 0.633191
 H 3.921540 0.363488 -0.209880
 H 3.953804 -0.305113 1.446209
 C 6.453149 -0.458062 -0.887176
 H 7.052151 0.334664 -0.422003
 H 7.112228 -1.304631 -1.117244
 N 5.523588 -0.970845 0.205843
 C 6.416217 -1.350986 1.381742

N 0.625786 -0.168569 1.917337
N -1.050383 0.951125 -1.451748
C 2.801977 -0.167015 0.819146
C 2.059669 -0.047351 2.157606
H 2.401079 -0.825599 2.854990
H 2.260374 0.937776 2.599469
C -0.301095 0.350501 2.915880
H 0.007669 1.373605 3.170405
H -0.287561 -0.262263 3.826570
C -1.719896 0.399342 2.335864
C -0.333892 2.913957 -0.170255
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H -1.211851 2.941223 -2.165400
C -2.047937 0.162736 -2.166716
H -2.003522 0.363160 -3.248245
H -3.042161 0.444664 -1.790543
C -1.833427 -1.326060 -1.868151
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C 3.216205 5.550183 1.700710
H 3.236995 6.427744 1.041475
C 3.528508 3.080833 1.520566
H 4.005523 3.098678 2.505587
H 3.960897 2.290283 0.902582
C 3.047042 4.382739 -0.474284
H 1.975612 4.269653 -0.281977
H 3.254522 5.326102 -0.989507
C 5.233527 4.663214 0.661592
H 5.652580 4.804316 1.667398
H 3.421470 3.542288 -1.065298
H 5.288651 5.623042 0.132539
H 3.970607 5.731235 2.476875
H 2.448562 2.917642 1.595818
C 1.854572 5.329399 2.332110
H 1.104194 5.071001 1.570302
H 1.890693 4.477780 3.027972
C 6.003906 3.580035 -0.071172
H 5.551048 3.381202 -1.053768
H 5.992303 2.643203 0.504514
C 7.444680 4.063646 -0.229297
H 7.907285 4.276131 0.745774
H 8.068137 3.316370 -0.738729
H 7.470816 4.985381 -0.826201
C 1.457781 6.582214 3.116597
H 0.445395 6.489617 3.525023
H 2.120394 6.737616 3.979186
H 1.519353 7.490101 2.502886

H 7.246621 -1.928536 0.957154
H 6.803701 -0.395505 1.760524
H 5.491631 -2.964902 -0.513388
H 5.141323 0.972076 0.942961
C 5.728335 -2.146603 2.475753
H 5.412208 -3.124665 2.093043
H 4.819349 -1.645457 2.828660
C 6.688228 -2.353257 3.646139
H 6.204496 -2.980636 4.406948
H 7.611232 -2.858025 3.320409
H 6.956907 -1.398364 4.123403
C 5.777900 0.065330 -2.144419
H 5.091378 -0.680223 -2.569240
H 5.197520 0.968246 -1.918329
C 6.857608 0.374259 -3.186071
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H 6.412320 0.823247 -4.084154

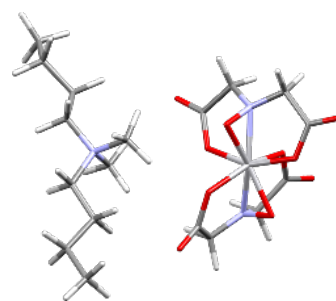
[N₁₁₄₄]₂[VBH]



99

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H -3.204531 -2.068214 0.832754
H -3.590664 -1.865435 2.549194
C -6.188020 -1.666082 2.424226
H -6.226627 -2.730108 2.697677
C -4.957253 -0.169430 0.875760
H -4.362520 -0.179682 -0.040733
H -4.361556 0.281549 1.676230
C -5.907858 -2.334436 0.100681
H -6.224058 -3.293890 0.532122
H -6.787291 -1.730405 -0.158730
H -7.159591 -1.352953 2.021768
H -5.920302 0.326565 0.721420
H -4.156425 -3.352870 1.663618
C -5.023123 -2.623717 -1.095087
H -4.119585 -3.154666 -0.773354
H -4.701387 -1.710056 -1.613295
C -5.819304 -0.814928 3.623180
H -4.771555 -0.958304 3.921440
H -5.931893 0.252270 3.381883
C -6.738872 -1.177574 4.788886
H -7.790456 -1.011290 4.505214
H -6.654907 -2.250008 5.018600
C -5.770439 -3.539652 -2.069404
H -6.334527 -4.283235 -1.485722
H -6.517614 -2.965715 -2.639023
C -6.412403 -0.375375 6.039425
H -7.074451 -0.671856 6.862430
H -5.374746 -0.570793 6.349400
H -6.514346 0.705991 5.856591
C -4.802674 -4.254162 -3.007562
H -4.111111 -4.887637 -2.434997
H -5.339446 -4.894096 -3.720352
H -4.182803 -3.534031 -3.556951
V 0.000000 0.000000 0.000000
O 2.031859 -0.038541 -0.404434
O 4.093339 0.049000 0.506027
O 0.446872 -1.587450 1.116352

[N₁₁₄₄][VBH]



64

O -1.587590 1.150523 0.332476
O -3.035332 1.985103 1.844103
O 2.505144 -2.437905 2.117280
O 1.402076 -1.399287 0.456783
O 0.872651 0.992220 1.410169
N 0.015067 0.110462 2.023139
C -2.011157 1.368069 1.559209
C -1.146635 0.742668 2.648459
H -1.719271 -0.030783 3.177539
H -0.820328 1.525457 3.347107
C 0.662863 -1.018100 2.697214
H 1.171919 -0.704234 3.617519
H -0.119260 -1.748326 2.950788
C 1.615187 -1.684520 1.716116
V 0.000000 0.000000 0.000000
O 1.391677 1.010781 -0.981978
O 2.331125 1.407009 -2.988279
O -2.363425 -3.263194 -0.500026
O -1.226914 -1.549095 0.399635
O -0.898691 -0.035562 -1.749892
N 0.070303 -1.016752 -1.752719
C 1.697011 0.690599 -2.221433
C 1.212085 -0.708921 -2.615040
H 2.002342 -1.444887 -2.404123
H 0.934712 -0.757692 -3.677806
C -0.449749 -2.387124 -1.687801
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C 4.800958 -2.243858 -0.295635
H 4.144574 -2.021140 -1.140202
H 4.211182 -2.692052 0.508356
C 4.320585 -0.037307 0.695029
H 3.503104 0.016609 -0.027178
H 3.950605 -0.455888 1.634751
C 6.160926 -0.287197 -0.946461
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N 5.394486 -0.951382 0.184237

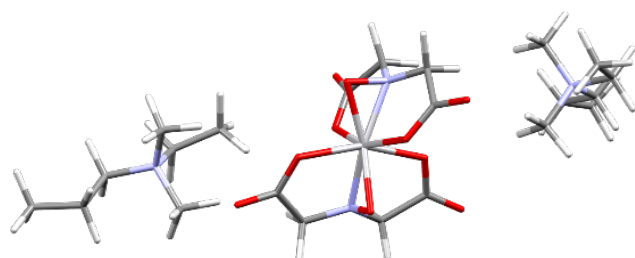
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O 0.067931 0.963116 -1.704533
O -2.312353 -1.924134 -2.851487
O -0.879407 -1.485793 -1.156339
N 0.782516 -0.443960 1.829633
N -1.221137 1.070525 -1.209508
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H 0.205844 0.775762 3.421984
H -0.011067 -0.973467 3.732905
C -1.547991 -0.051945 2.485943
C -0.541293 2.864168 0.324313
C -1.557797 2.412069 -0.736024
H -2.554520 2.376286 -0.275807
H -1.573352 3.120504 -1.574396
C -2.172644 0.328837 -2.027187
H -2.200766 0.735090 -3.050542
H -3.173950 0.430495 -1.587008
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C 3.392803 5.194401 2.956988
H 3.554533 6.247112 2.689943
C 3.241464 2.996404 1.822804
H 3.850186 2.591378 2.638848
H 3.448243 2.463318 0.892861
C 2.720662 5.036126 0.581732
H 1.674055 4.882728 0.862343
H 2.975736 6.094316 0.468506
C 5.064203 4.580309 1.269747
H 5.622745 4.156177 2.116218
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H 5.245992 5.662245 1.221033
H 4.185375 4.855122 3.640796
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C 2.034454 4.986030 3.612452
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H 7.161683 5.183259 -0.426156
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C 7.331012 3.391227 -1.636851

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H 6.405957 -0.258929 1.896379
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H 4.765777 0.953281 0.840450
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C 7.279349 -2.459259 3.234802
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H 7.078092 -1.703395 4.010877
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H 4.717843 -0.591407 -2.553705
H 4.647856 1.004649 -1.771798
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H 7.089159 1.313498 -2.663066
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H 4.804391 1.172501 -4.729787
H 5.060721 2.521589 -3.602913
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H 7.836364 -4.548329 3.139674
H 8.033510 -3.822268 4.752164
H 6.417169 -4.238948 4.161028

H 8.383858 3.563874 -1.894420
 H 7.178847 2.304608 -1.542094
 H 6.723405 3.731982 -2.486732
 C 0.392974 5.931679 5.306264
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Asymmetric disubstituted [N11xy]

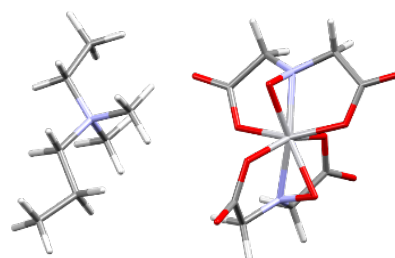
[N₁₁₂₃]₂[VBH]



81

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 C -6.917675 -0.853495 1.924477
 H -6.974033 -1.715713 2.600969
 C -6.103792 -0.239546 -0.343651
 H -5.643469 -0.643498 -1.249133
 H -5.454675 0.533866 0.074512
 C -7.165230 -2.425314 0.088408
 H -7.237352 -3.189623 0.869051
 H -8.132621 -1.924404 -0.040345
 H -7.929170 -0.568591 1.610356
 H -7.093930 0.169409 -0.564292
 H -5.065679 -2.815536 1.604149
 C -6.696893 -3.053197 -1.207983
 H -5.708180 -3.515009 -1.114955
 H -7.406297 -3.857276 -1.442422
 H -6.711123 -2.342889 -2.039688
 C -6.247291 0.320988 2.614222
 H -5.260263 0.036465 3.005311
 H -6.096944 1.153597 1.913077
 C -7.153567 0.795262 3.753471
 H -8.182660 0.932466 3.391478
 H -7.198766 0.054190 4.559555
 H -6.800309 1.757537 4.141016
 V 0.000000 0.000000 0.000000
 O 1.944670 0.197131 -0.662127
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 O 0.811380 -1.451561 1.103947

[N₁₁₂₃][VBH]

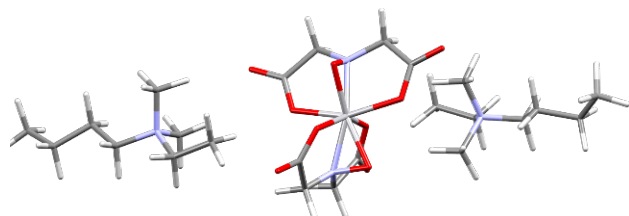


55

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 O 1.463310 -1.286933 0.532632
 O 0.724014 1.076881 1.441720
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 C -2.138652 1.276136 1.436594
 C -1.341833 0.636654 2.562673
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 H -1.147429 1.379912 3.344188
 C 0.641485 -0.918642 2.741033
 H 1.077293 -0.518574 3.667150
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 O 1.380847 1.064235 -0.943567
 O 2.344650 1.481390 -2.931033
 O -2.275979 -3.301876 -0.586027
 O -1.219996 -1.562404 0.364455
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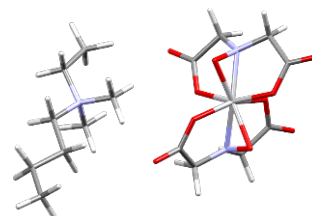
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[N₁₁₂₄]₂[VBH]

87

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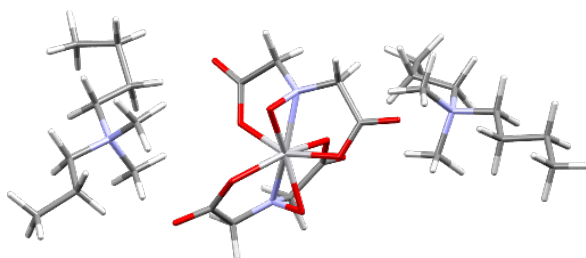
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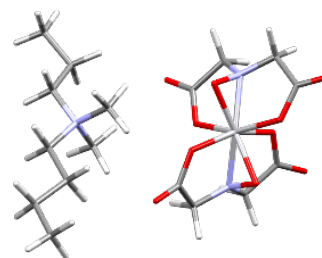
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[N₁₁₃₄]₂[VBH]

93

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[N₁₁₃₄][VBH]

61

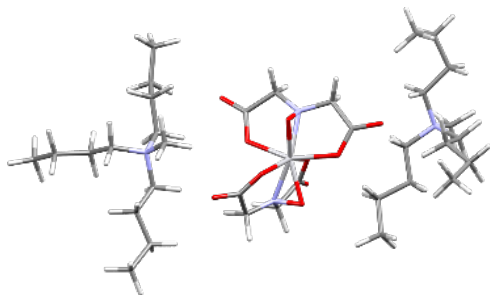
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Monosubstituted [N444x]

[N₄₄₄₁]₂[VBH]

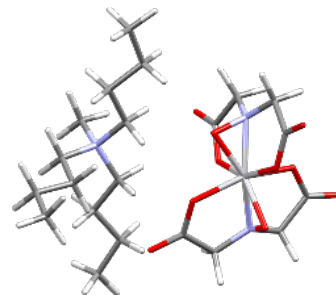


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[N₄₄₄₁][VBH]



73

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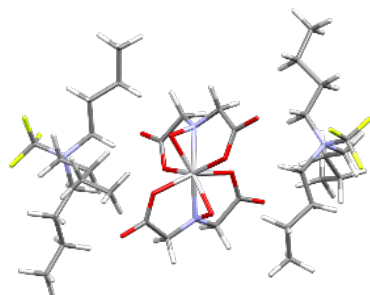
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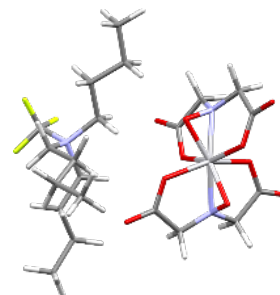
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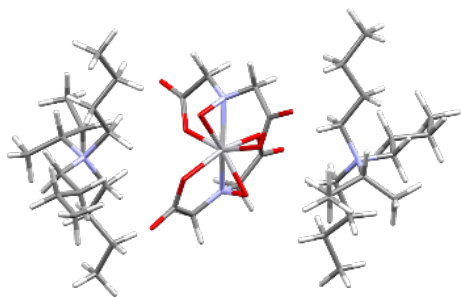
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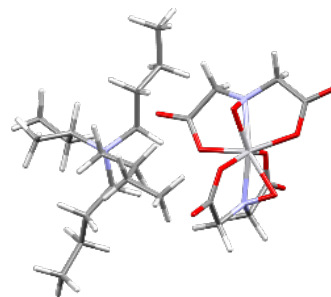
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135

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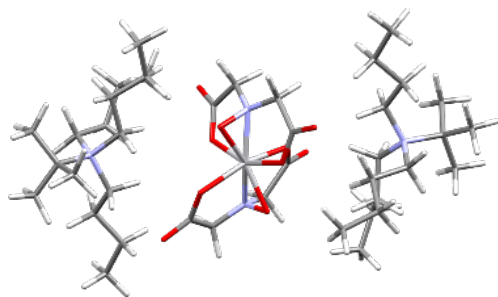
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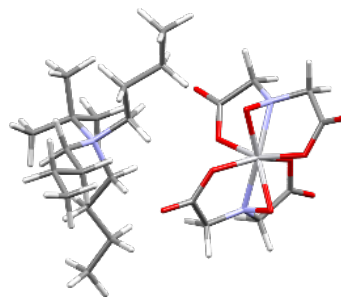
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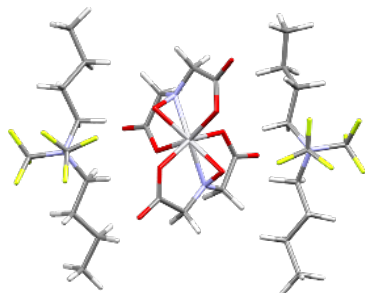
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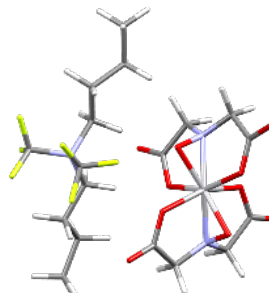


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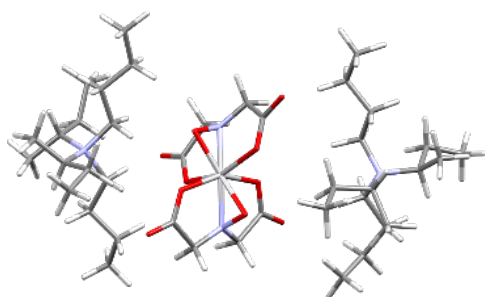
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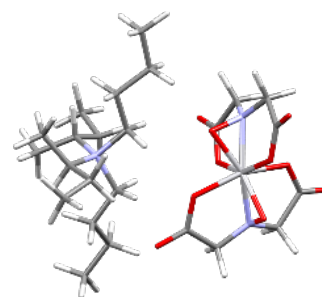
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[N_{44ss}][VBH]



82

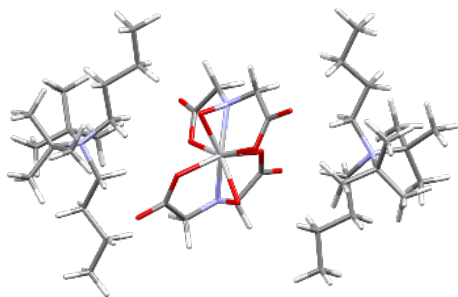
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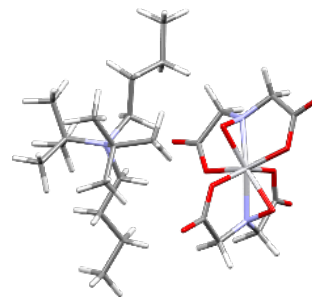
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82

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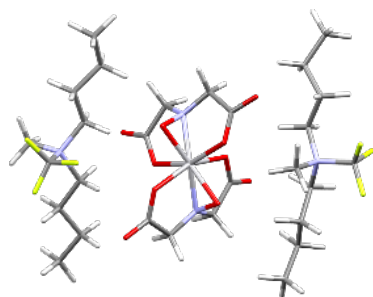
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Asymmetric disubstituted [N44xy]

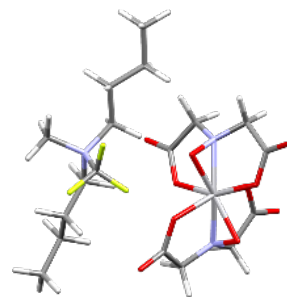
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[N441c][VBH]



64

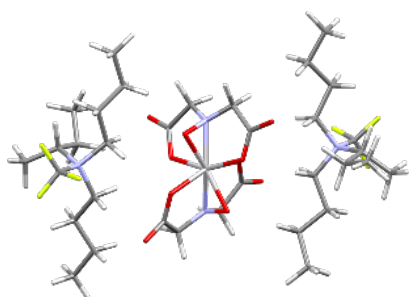
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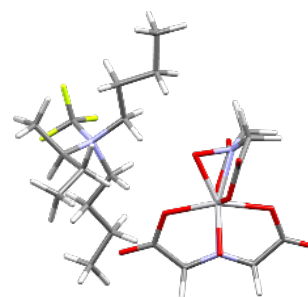
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117

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[N_{44cs}][VBH]



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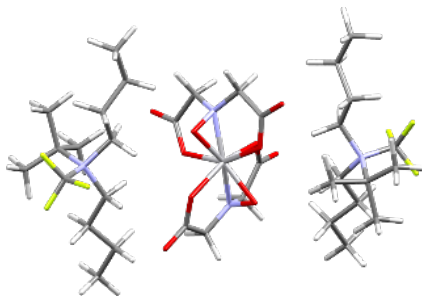
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C 5.336355 -3.918733 -2.219914
H 5.019178 -3.561719 -3.208317
H 6.435689 -3.974776 -2.224403
H 4.949908 -4.937366 -2.097064
C 4.347649 2.178182 -3.340274
H 5.105095 2.919983 -3.629145
H 4.560090 1.241711 -3.874749
C 6.872080 0.449358 0.681669
F 7.356988 1.571371 1.230862
F 6.757834 -0.481147 1.631882
F 7.732382 0.028680 -0.259200
H 3.373056 2.543180 -3.686644
C 6.677121 2.617312 -1.258190
H 6.426724 3.338537 -0.476058
H 7.711884 2.293433 -1.114858
H 6.636875 3.142529 -2.220224

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 H -0.702384 6.377583 -1.944262
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 O 4.086261 0.524976 0.069261
 O 0.845571 -0.855338 1.576822
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 N 0.929736 0.523234 1.723800
 N -1.465240 0.185911 -1.381801
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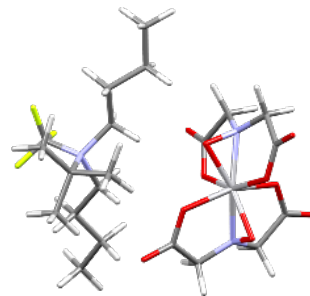
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117

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 H -1.139233 -2.289930 3.243337

[N_{44ct}][VBH]



73

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H -4.134756 -2.121705 2.188778
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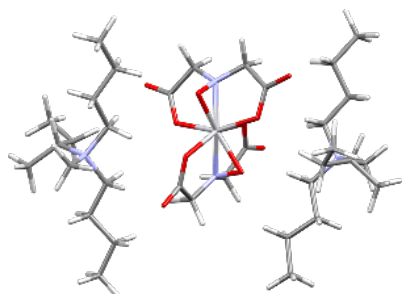
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H 3.787251 -3.126506 0.233248
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O -0.146847 0.433554 -1.918034
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H 0.332117 0.238962 3.832654
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H 4.406367 -5.179838 -1.075366
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H 7.706276 2.170198 -0.892005
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H 5.243469 -0.167229 -2.529465
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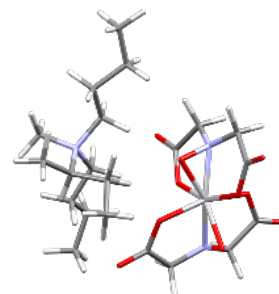
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117

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H -5.346907 -1.329569 -1.564430
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[N_{441s}][VBH]



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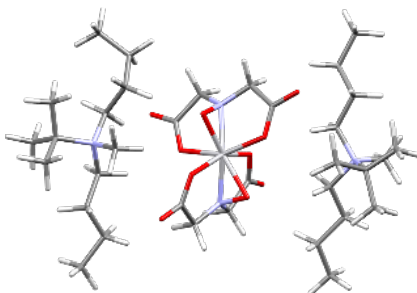
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 C -2.318168 -0.693214 -1.755131
 H -2.514902 -0.614886 -2.833615
 H -3.276545 -0.672754 -1.216656
 C -1.568190 -1.989783 -1.445774

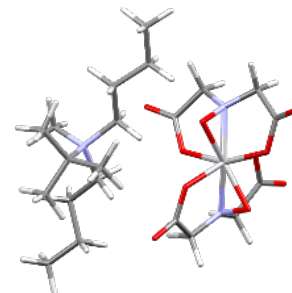
[N_{441t}]₂[VBH]



117

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 C -2.241660 -2.620353 3.445297
 H -1.252734 -2.570229 2.977733
 H -2.731997 -1.666742 3.222394

[N_{441t}][VBH]



73

O -1.177566 1.533195 -0.391143
 O -1.890325 3.553543 0.279404
 O 2.084142 -1.562636 3.151654
 O 1.062088 -1.281222 1.161932

C -4.143170 -4.196067 3.532873
H -4.800444 -4.836126 2.941579
H -3.744109 -4.755268 4.382268
C -3.619373 -2.954330 1.480220
H -2.778749 -2.453805 0.987630
H -4.227046 -2.169705 1.951864
C -2.045489 -4.893281 2.260511
C -2.131142 -2.764976 4.956940
H -3.060795 -2.442500 5.448359
H -1.943826 -3.795423 5.279534
C -0.982464 -1.881993 5.446233
H -1.201598 -0.845250 5.151379
H -0.059142 -2.168143 4.912262
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C -5.446490 -2.730304 -0.178478
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H -6.033808 -2.204981 0.590562
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H -0.410996 -3.002705 7.215213
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H -5.871080 -3.967168 -1.922169
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H -0.628449 -3.465277 1.349644
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H -0.514945 -4.503818 3.795999
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H -2.119933 -6.891543 1.521236
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C 3.116193 2.378938 -2.854562
H 4.128614 2.268241 -2.464136
H 3.086569 2.156070 -3.923542
C 1.137647 3.886011 -2.918904
H 0.636688 3.775323 -1.953267
H 0.955295 4.913282 -3.249565
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C 4.171061 4.148845 -0.516566
H 4.620239 5.128753 -0.719530

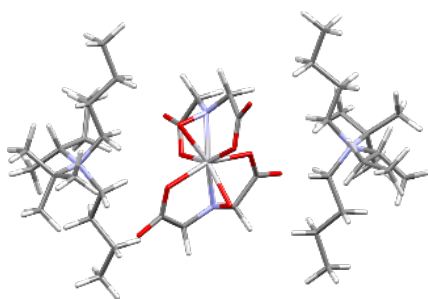
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H -1.843799 1.648270 2.464995
H -0.563403 2.909095 2.481347
C 0.444295 0.190335 2.934729
H 1.021256 0.799701 3.643540
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C 1.280684 -0.982975 2.412858
V 0.000000 0.000000 0.000000
O 1.636279 0.126493 -1.126945
O 2.815697 -0.694960 -2.851193
O -3.087324 -2.577467 0.620741
O -1.574171 -0.933392 0.863951
O -0.866905 -0.524354 -1.652390
N -0.192612 -1.632687 -1.186329
C 1.889878 -0.779835 -2.040115
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H 1.477727 -2.833195 -1.496163
H 0.649485 -2.292705 -2.998895
C -1.082566 -2.682985 -0.695870
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H -0.454415 -3.442259 -0.210010
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C 4.504600 -1.142685 -0.152745
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H 3.464563 1.070587 0.346643
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H 4.499030 1.181556 -1.787242
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H 4.846639 3.406621 -0.949564
C 4.137184 3.905767 1.005626
H 3.141131 4.155458 1.406387
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C -0.852882 3.262389 -4.299787
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H -1.397597 3.637847 -3.420048
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O 4.057462 0.772862 -0.029765
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O -2.165121 0.639157 3.479640
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O -0.143494 2.117814 0.042990
O -1.368319 3.871088 -0.697486
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O -2.066032 -3.159475 -1.718431
O -0.572742 -1.920835 -0.552780
N 0.977785 0.317829 1.762337
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H 0.276698 1.863952 2.971955
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H 6.879372 2.223448 1.088385
H 7.986494 0.856550 0.783439
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H 7.554211 -0.893087 -0.831598
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C -2.090933 1.671577 -1.280490
H -3.013657 1.578715 -0.689338
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C -2.323172 -0.780734 -1.704363
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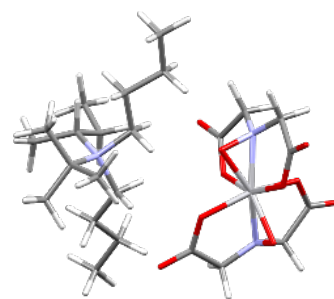
[N_{44st}]₂[VBH]



135

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H -2.380669 -1.850285 3.331618
C -4.713348 -2.756231 3.849072
C -3.760875 -3.183828 1.487560
H -2.893357 -3.605393 0.970866
H -3.642955 -2.098168 1.421840
C -3.645321 -5.067100 3.145891
C -1.404542 -3.368091 4.519580
H -2.027556 -3.495938 5.408271
H -0.904960 -4.331556 4.334899
C -0.356221 -2.286000 4.805327
H -0.875252 -1.319007 4.868492
H 0.323622 -2.207903 3.940214
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H -5.043650 -4.741493 0.697677
H -5.936017 -3.336369 1.306312
C -5.067219 -3.018373 -0.619082
H -4.127999 -3.226211 -1.152675
H -5.147059 -1.924890 -0.517779
C 0.415949 -2.517708 6.099002
H 1.178143 -1.736840 6.228193
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H -1.627427 -5.352541 2.403517

[N_{44st}][VBH]



82

O -1.394298 1.321079 -0.531714
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O 2.745636 -0.506678 3.007443
O 1.409226 -0.869522 1.232738
O 1.065111 1.596248 0.341278
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C -1.567331 2.421079 0.164223
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H -0.418532 3.419754 1.726954
C 0.897745 0.987601 2.647825
H 1.482658 1.799880 3.099875
H 0.113384 0.655911 3.344864
C 1.779705 -0.211733 2.294502
V 0.000000 0.000000 0.000000
O 1.423421 -0.129062 -1.365492
O 2.564932 -1.380458 -2.830368
O -2.338266 -2.520977 2.174825
O -1.212110 -0.735893 1.407871
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N -0.222920 -1.919639 -0.646715
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H -1.615271 -3.453189 -0.240140
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C -1.554862 -2.009190 1.384431
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H 4.006763 -0.249543 -1.342465

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H -6.749664 -2.947029 4.405048
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H	3.473001	7.013258	-1.015316
H	3.832051	6.928517	-2.748897
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H	1.582784	6.002077	-3.191861
C	-0.560324	6.442518	-1.915173
H	-0.476594	7.274534	-2.626680
H	-0.895895	5.537277	-2.434739
H	-1.338938	6.697154	-1.185427
C	4.950861	4.430043	-2.412957
H	5.185523	3.847973	-1.516818
H	5.714636	4.188901	-3.161635
H	5.054334	5.491097	-2.176239
C	3.489089	4.775612	-4.392213
H	3.553241	5.862592	-4.305373
H	4.351309	4.446614	-4.987117
H	2.587297	4.512814	-4.949512
C	3.614272	2.544790	-3.298747
H	2.788170	2.223002	-3.942521
H	4.549371	2.328628	-3.834372
H	3.622698	1.940201	-2.382198
V	0.000000	0.000000	0.000000
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O	4.019626	0.829384	-0.236639
O	1.014255	-1.048737	1.371371
O	-2.003214	0.357665	3.594725
O	-1.506849	-0.125770	1.454345
O	-0.189722	2.106816	0.253193
O	-1.532541	3.873477	-0.166914
O	-0.426708	0.489709	-1.856300
O	-1.917391	-2.995182	-2.066215
O	-0.514038	-1.900674	-0.672106
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C	2.819931	0.648365	0.051268
C	2.344694	0.950011	1.476413
H	3.093269	0.656539	2.221016
H	2.176430	2.033069	1.552580
C	0.260568	0.674914	2.858418
H	0.314597	1.766157	2.967336
H	0.647283	0.198545	3.771682
C	-1.205950	0.278297	2.636073
C	-1.262606	2.657405	-0.221546
C	-2.249059	1.706646	-0.894796
H	-3.115763	1.539321	-0.242499
H	-2.608176	2.129532	-1.842676
C	-2.436814	-0.731023	-1.481157
H	-2.880133	-0.615818	-2.477533
H	-3.256470	-0.790377	-0.752574
C	-1.565083	-1.987131	-1.420054

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