Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information

Effect of coordination sites on vanadium complexes having $[VO]^{2+}$, $[VO]^{3+}$ and $[VO_2]^{+}$ cores with hydrazones of 2,6-diformyl-4-methylphenol: Synthesis, characterization, reactivity, and catalytic potential

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Molecular structures of $[V^{V}O(OMe)(MeOH)\{Hdfmp(bhz)_2\}]$ (6) and $[V^{V}O_2\{H_2dfmp(inh)_2\}]$ (7)

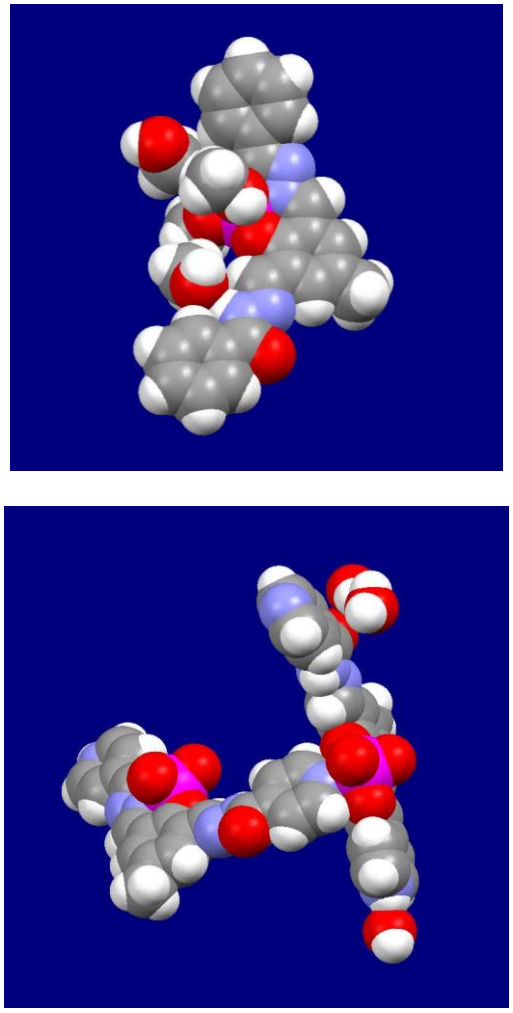

Fig. S1 Above: Space-filling representation of compound **6** colored by atom type where we can observe the hydrogen bond interaction between the methanol molecule and protonated hydrazone group occupying the position of the VO group (up) in the lower part of the ligand showed in the figure. Below: Space-filling representation of compound **7**, also colored by atom type, where we can observe the sixth coordinate position occupied by the $N_{pyridine}$ atom of a neighboring complex.

Table S1 Distances [Å] and angles [º] of hydrogen bonds for $[V^{V}O(OMe)(MeOH)\{Hdfmp(bhz)_2\}]\cdot 2MeOH$ (**6**) and for $[V^{V}O_2\{H_2dfmp(inh)_2\}]_n\cdot 5H_2O$ (**7**).

Compound	D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)	
6	N(2)-H(2N)...O(3M)	0.84(3)	2.08(4)	2.904(3)	167(3)	
6	O(2M)-H(2O)...O(4)#1	0.66(3)	2.09(3)	2.743(3)	173(4)	
6	O(3M)-H(3O)...O(4M)#2	0.90(3)	1.80(3)	2.677(3)	165.5	
6	O(4M)-H(4O)...O(4)#3	0.82	1.99	2.718(3)	148.6	
6	O(4M)-H(4O)...N(1)#3	0.82	2.49	3.157(3)	139.8	
7	O(3W)-H(3WB)...O(5W)	1.00	2.01	2.965(5)	158.5	
7	O(4W)-H(4WA)...O(1W)#4	0.80(4)	2.02(4)	2.805(5)	169(4)	
7	N(5)-H(5N)...O(3W)#5	0.80(5)	2.15(5)	2.930(5)	165(4)	
7	O(5W)-H(5WB)...O(1W)#6	1.00	2.44	3.208(5)	132.3	
7	O(5W)-H(5WA)...O(1W)#7	1.02	1.86	2.841(6)	160.2	

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+2,-z+1 #2 -x,-y+1,-z+1 #3 x,y-1,z

#4 -x+1/2,-y,z+1/2 #5 -x-1/2,y-1/2,z

#6 -x-1/2,y+1/2,z #7 x-1/2,-y+1/2,-z

^{51}V NMR studies

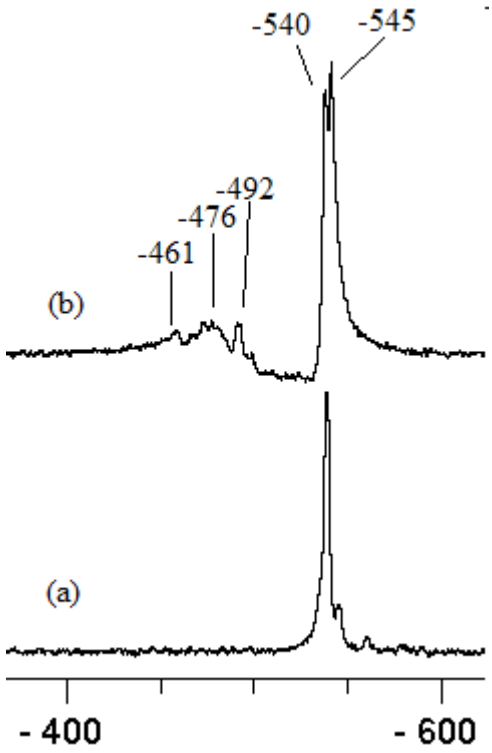

Fig. S2 ^{51}V NMR spectra for solutions (ca. 4 mM) in MeOD (a) of (**7**); (b) solution of (a) upon adding 1.0 equiv. of HCl [aqueous solution (11.6 M)].

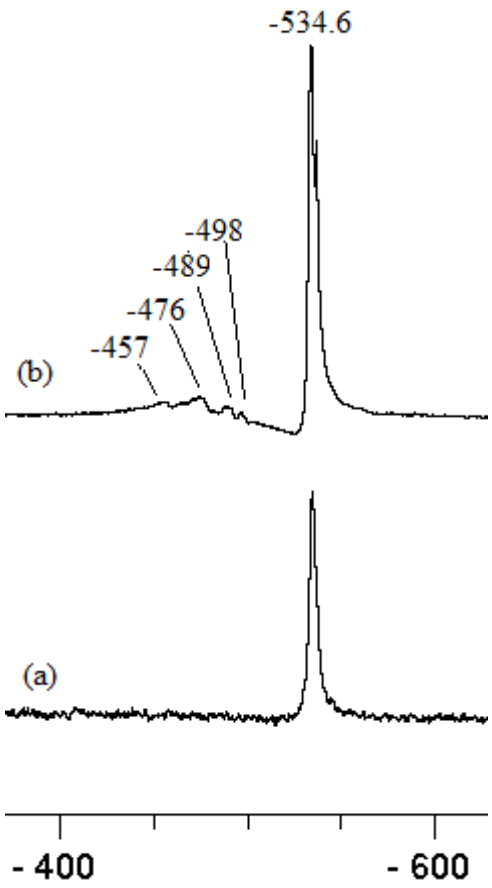

Fig. S3 ^{51}V NMR spectra for solutions (ca. 4 mM) in MeOD (a) of (**9**); (b) solution of (a) upon adding 1.0 equiv. of HCl [aqueous solution (11.6 M)].

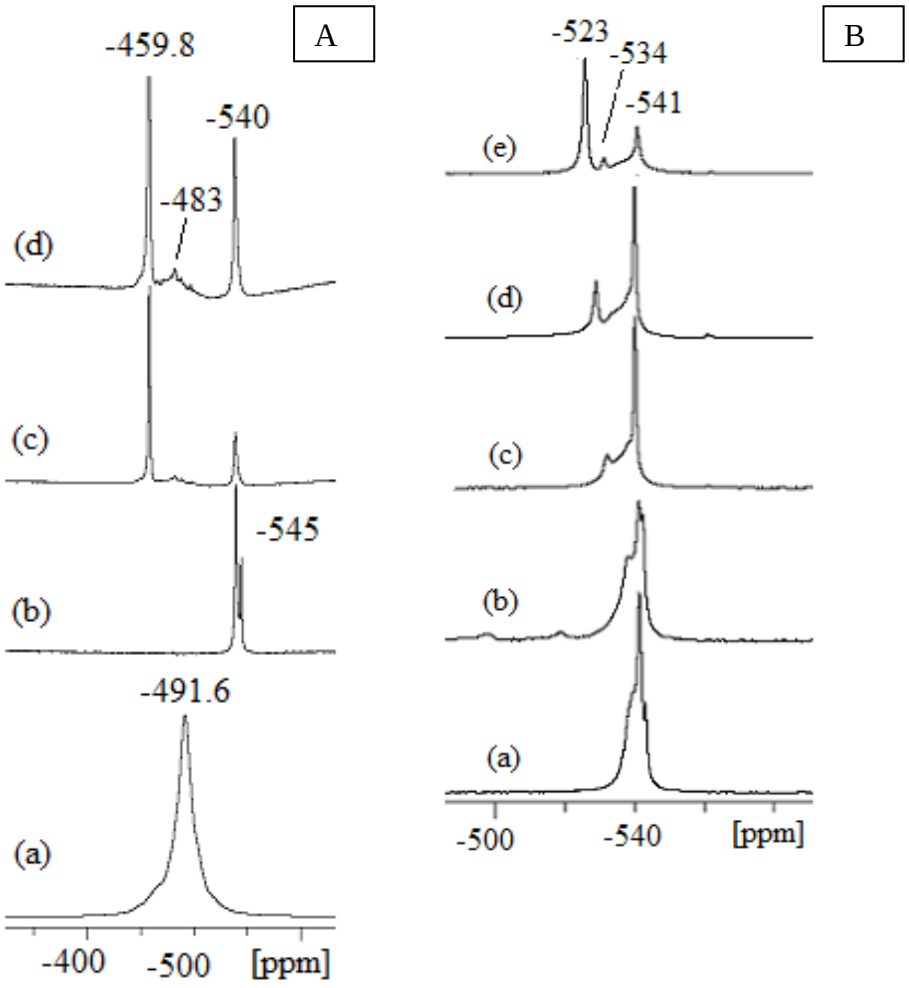

Fig. S4 (A) ^{51}V NMR spectra of solutions in MeOD (a) of the '$[V^{V}O]^{3+}$ solution' (ca. 8 mM); (b) of $[V^{V}O_2\{H_2dfmp(inh)_2\}]$ **7** (ca. 4 mM) in MeOD; (c) solution of (b) after addition of 1.0 equiv. of '$[V^{V}O]^{3+}$ solution'; (d) solution of (c) after additions of 2.0 equiv. of '$[V^{V}O]^{3+}$ solution'; the final pH of solution of (d) was ~5.0. (B) ^{51}V NMR spectra for solutions in MeOD (a) of $[V^{V}O_2\{H_2dfmp(inh)_2\}]$ **7**;(ca. 4 mM) (pH~ 6.8 to 7.0) (b) solution of (a) after addition of 0.5 equiv. of an 'aqueous $NaVO_3$ solution'; (c-e) solution of (b) after addition of 1.0 equiv. of an 'aqueous $NaVO_3$ solution'; the final pH of solution of (e) was ~7.4.

Oxidative bromination of styrene

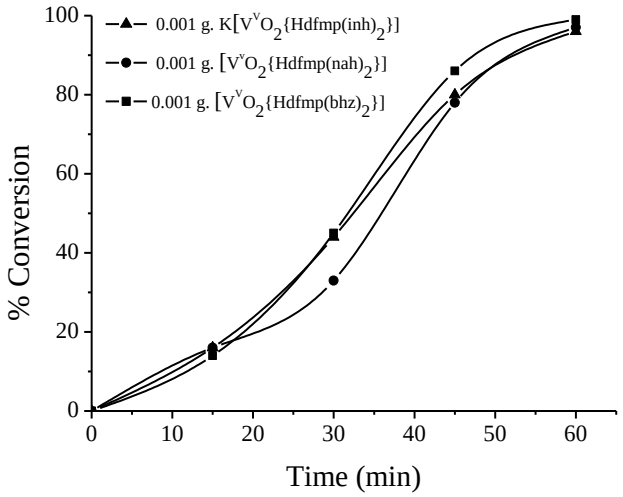

Fig. S5 Effect of different catalyst precursors on the conversion of oxidative bromination of styrene.

Calculations of entropies in solution

The entropies in solutions (S_s) were calculated according to the procedure described by Wertz and Cooper and Ziegler using equations (1) – (4)

$$\Delta S_1 = R\ln(V_m/V_{m,hi,liq}) \quad (1)$$

$$\Delta S_2 = R\ln(V_{m,hi}/V_{m,hi}) \quad (2)$$

$$\alpha = \frac{S_{g,abs,liq} - S_{g,abs,hi,liq}}{S_{g,abs,liq} - S_{g,abs,hi,gas}} \quad (3)$$

$$S_s = S_g + \Delta S_{sol} = S_g + [\Delta S_1 + \alpha(S_g + \Delta S_1) + \Delta S_2] =$$

$$S_g + [(-11.80\ \text{cal/mol·K}) - 0.21(S_g - 11.80\ \text{cal/mol·K}) + 5.45\ \text{cal/mol·K}] \quad (4)$$

where S_g = gas-phase entropy of solute, ΔS_{sol} = solvation entropy, $S^{\circ,s}_{liq}$, $S^{\circ,s}_{gas}$, and $V^{s}_{m,liq}$ = standard entropies and molar volume of the solvent in liquid or gas phases (127.2 and 239.9 J/mol•K and 40.46 mL/mol, respectively, for MeOH), $V_{m,gas}$ = molar volume of the ideal gas at

25 °C (24450 mL/mol), $V°_m$ = molar volume of the solution corresponding to the standard conditions (1000 mL/mol).

Table 1TS. Calculated total energies (E), enthalpies (H), Gibbs free energies (G) (in Hartree), and entropies (S) (in cal/mol•K) in gas-phase and MeOH solution.

	E_g	E_s	H_g	H_s	S_g	S_s	G_g	G_s
H_2O	-76.587853	-76.598524	-76.562685	-76.573356	46.50	29.34	-76.584777	-76.587297
H_2O_2	-151.851341	-151.869775	-151.820524	-151.838958	55.72	35.61	151.846996	-151.855877
HBr	-2573.126798	-2573.129022	-2573.117492	-2573.119716	47.44	29.98	-2573.140034	-2573.133960
HCl	-461.137649	-461.140404	-461.127579	-461.130334	44.60	28.05	-461.148770	-461.143661
$[V(=O)(acac)_2]$	-839.857103	-839.873605	-839.605278	-839.621780	143.95	95.61	-839.673673	-839.667206
$VOCl_3$	-1529.101289	-1529.096879	-1529.085743	-1529.081333	83.96	54.81	-1529.125636	-1529.107375
II	-1368.963767	-1369.015633	-1368.566506	-1368.618372	190.55	127.29	-1368.657041	-1368.678854
Hacac	-346.770595	-346.779122	-346.637969	-346.646496	87.76	57.40	-346.679666	-346.673767
MeOH	-116.037606	-116.046873	-115.981628	-115.990895	56.68	36.26	-116.008560	-116.008125
1a	1591.882843	-1591.930849	-1591.473724	-1591.521730	205.52	137.47	-1591.571373	-1591.587046
1	-1591.898667	-1591.940963	-1591.489761	-1591.532057	198.69	132.83	-1591.584165	-1591.595169
1•MeOH	-1707.949119	-1707.989769	-1707.481738	-1707.522388	218.47	146.30	-1707.585541	-1707.591900
2	-1591.885051	-1591.931780	-1591.475819	-1591.522548	205.64	137.56	-1591.573527	-1591.587905
5	-1746.765333	-1746.795685	-1746.279601	-1746.309953	227.52	152.43	-1746.387700	-1746.382379
8	-1590.749345		-1590.364456		197.97		-1590.458517	
8Ha	-1591.259162	-1591.298399	-1590.862270	-1590.901507	197.40	131.95	-1590.956060	-1590.964202
8Hb	-1591.189957	-1591.285287	-1590.791409	-1590.886739	200.55	134.09	-1590.886695	-1590.950452
8Ha•MeOH	-1707.313900	-1707.351827	-1706.858400	-1706.896327	217.55	145.65	-1706.961764	-1706.965530
11	-3105.942951	-3105.972160	-3105.173164	-3105.202373	340.98	229.59	-3105.335176	-3105.311457
14	-1666.025633		-1665.636349		201.74		-1665.732203	
14Ha	-1666.519189	-1666.550969	-1666.118473	-1666.150253	199.04	133.07	-1666.213044	-1666.213478
14Hb	-1666.476948	-1666.540235	-1666.074147	-1666.137434	193.54	129.33	-1666.166106	-1666.198883
14Hc	-1666.511903	-1666.540198	-1666.109545	-1666.137840	192.04	128.31	-1666.200790	-1666.198803
CVIIHa	-2314.088091	-2314.160729	-2313.644142	-2313.716780	232.29	155.68	-2313.754512	-2313.790747
CVIIHb	-1813.465672	-1813.545699	-1813.066802	-1813.146829	205.60	137.53	-1813.164491	-1813.212173
CVIII	-1666.893919		-1666.478359		190.97		-1666.569093	
CX	-1777.651507	-1777.675947	-1777.228150	-1777.252590	213.11	142.64	-1777.329405	-1777.320363
CXI^-	-4314.481949		-4314.072992		219.61		-4314.177338	
CXI-Ha	-4314.961519	-4315.012611	-4314.538610	-4314.589702	217.41	145.56	-4314.641909	-4314.658862
CXI-Hb	-4314.929357	-4315.002049	-4314.506540	-4314.579232	221.62	148.42	-4314.611837	-4314.649752
CXI-OH	-4314.968935	-4314.996053	-4314.547888	-4314.575006	220.58	147.71	-4314.652691	-4314.645188
CXI-OOH	-4314.959316	-4314.985328	-4314.537296	-4314.563308	219.70	147.12	-4314.641680	-4314.633208
CXII	-4163.110261	-4163.139070	-4162.721596	-4162.750405	209.96	140.49	-4162.821352	-4162.817158

Table 2TS. Cartesian atomic coordinates (Å) of the calculated equilibrium structures.

II

N	-3.606709	0.612266	0.023046
C	-7.102854	-0.551050	-0.005142
N	-4.720767	-0.147176	-0.028536
H	-4.629983	-1.160762	-0.046132
C	-7.043772	-1.767596	-0.691705
H	-6.139536	-2.066567	-1.221796
O	-0.082639	-1.339628	-0.112440
N	-8.064700	-2.619019	-0.791075
N	3.598447	0.579510	-0.131573
O	6.112690	1.498673	-0.736989
O	-6.153498	1.605083	0.314836
C	-9.209313	-2.270398	-0.200135
H	-10.025691	-2.985100	-0.286140
N	4.717826	-0.156667	0.007050
C	-9.391351	-1.069470	0.484605
H	-10.352089	-0.832218	0.930643
C	-8.320602	-0.193708	0.577451
H	-8.395180	0.763338	1.084353
C	-5.971051	0.420786	0.106917
C	-2.483581	-0.006451	-0.022097
H	-2.425091	-1.098165	-0.093491
C	-1.224207	0.726454	0.017617
C	-1.194193	2.122296	0.089415
H	-2.146770	2.643537	0.127026
C	0.004788	2.835422	0.102887
C	1.195089	2.115973	0.073102
H	2.151233	2.630066	0.108528
C	1.213341	0.714314	0.021802
C	-0.008830	0.023337	-0.031588
C	0.005236	4.339000	0.146135
H	0.987687	4.728787	0.427357
H	-0.250483	4.763068	-0.832398
H	-0.729093	4.717822	0.864454
C	2.476926	-0.011226	0.067259
H	2.451894	-1.080566	0.330322
C	5.957311	0.378221	-0.293318
C	7.102433	-0.550017	-0.045138
C	7.087146	-1.603068	0.874525
H	6.212070	-1.788313	1.497561
N	8.119608	-2.416614	1.094628
C	9.232040	-2.193843	0.391954
H	10.058491	-2.876183	0.581399
C	9.370225	-1.155894	-0.528918
H	10.306823	-1.013369	-1.058620
C	8.287959	-0.316932	-0.745706

H	8.330315	0.517920	-1.438293
H	0.735629	-1.685977	-0.492577
H	4.642063	-1.146125	0.234418

1a

V	1.901472	-0.730294	0.686151
N	-3.585621	1.012957	-0.245138
C	-6.665251	-1.008495	-0.167752
O	1.123277	-2.437257	-0.229888
O	1.790221	-0.792738	2.249209
N	-4.467092	-0.008003	-0.203131
H	-4.132292	-0.945535	0.010044
C	-6.257950	-2.259285	-0.635544
H	-5.289171	-2.407816	-1.104561
O	0.366938	0.088165	-0.091424
C	-7.145360	-3.328476	-0.540650
N	2.921622	0.928896	0.182727
O	3.591486	-1.432799	0.037723
O	-6.314303	1.344662	-0.268208
N	-8.369958	-3.233816	-0.021650
N	4.277288	0.762038	0.020028
C	-8.753928	-2.029029	0.411239
H	-9.758815	-1.969885	0.824577
C	-7.953203	-0.894238	0.354189
H	-8.305545	0.071440	0.700416
C	-5.825692	0.233242	-0.222806
C	-2.344760	0.715118	-0.112258
H	-2.005315	-0.317806	0.025418
C	-1.320240	1.750281	-0.111031
C	-1.664802	3.101183	-0.136306
H	-2.723536	3.345605	-0.172060
C	-0.709722	4.123997	-0.113112
C	0.623681	3.752706	-0.052696
H	1.395374	4.519557	-0.029987
C	1.025294	2.403097	-0.006676
C	0.044551	1.371480	-0.056098
C	-1.130190	5.567115	-0.144953
H	-0.264196	6.235180	-0.136086
H	-1.717650	5.791138	-1.042433
H	-1.754858	5.818380	0.719687
C	2.426472	2.116335	0.001380
H	3.134433	2.924301	-0.188795
C	4.534519	-0.518500	-0.034864
C	5.929051	-0.963543	-0.205078
C	6.972558	-0.047377	-0.363454
H	6.768658	1.017369	-0.362038
C	8.263566	-0.535498	-0.520114
N	8.576156	-1.835510	-0.528752

C	7.571129	-2.699429	-0.372987
H	7.843237	-3.753417	-0.377731
C	6.241515	-2.323346	-0.209639
H	5.460702	-3.064215	-0.080211
H	1.836737	-2.872217	-0.726325
H	0.443271	-2.148307	-0.861235
H	-6.855667	-4.311861	-0.906701
H	9.095661	0.154626	-0.646059

1

V	-1.142464	-0.365350	0.565449
N	2.615886	0.836956	-0.240759
C	5.309184	-1.646650	-0.127718
O	-1.005728	-0.360793	2.131076
O	0.216713	-1.724520	-0.153258
N	3.840740	0.266259	-0.232960
H	4.683844	0.833822	-0.157743
C	6.396239	-1.028407	-0.749107
H	6.286224	-0.107210	-1.314440
O	0.023638	0.870347	-0.249924
C	7.641357	-1.648122	-0.680717
N	-2.590306	1.004029	0.127055
O	-2.637547	-1.465846	0.001440
O	2.941125	-1.825801	-0.049103
N	7.862731	-2.802343	-0.050638
N	-3.855183	0.491566	-0.008465
C	6.812830	-3.390539	0.529402
H	7.012909	-4.334235	1.032530
C	5.525455	-2.865695	0.514225
H	4.696827	-3.380554	0.987826
C	3.924202	-1.091933	-0.137078
C	2.549960	2.120003	-0.222643
H	3.463613	2.734796	-0.211768
C	1.293862	2.847202	-0.183278
C	1.310331	4.241123	-0.131201
H	2.273630	4.749758	-0.154413
C	0.142828	5.009560	-0.043466
C	-1.069820	4.334963	0.006919
H	-1.994288	4.904621	0.081635
C	-1.149514	2.931810	-0.021430
C	0.043093	2.164847	-0.144428
C	0.212808	6.511457	0.003895
H	-0.785078	6.952064	0.083129
H	0.796961	6.859667	0.863772
H	0.685610	6.921511	-0.896240
C	-2.432679	2.286883	-0.009095
H	-3.332196	2.887788	-0.152041
C	-3.772115	-0.816852	-0.052598

C	-5.014899	-1.599025	-0.196658
C	-6.267054	-0.981295	-0.253987
H	-6.344963	0.098162	-0.191120
C	-7.394335	-1.781268	-0.391606
N	-7.360283	-3.115416	-0.474792
C	-6.157792	-3.692230	-0.418558
H	-6.146915	-4.778696	-0.487038
C	-4.964305	-2.990633	-0.281377
H	-4.009987	-3.503321	-0.240276
H	1.181613	-1.478795	-0.129157
H	0.149154	-2.641417	0.147510
H	-8.382535	-1.327118	-0.438084
H	8.503740	-1.193447	-1.164298

1•MeOH

V	1.093093	-0.340711	-0.446251
N	-2.758292	0.861079	0.177253
C	-5.501807	-1.564122	-0.064500
O	0.882309	-0.286677	-2.006167
O	-0.385063	-1.850475	-0.158771
N	-3.994749	0.311940	0.120409
H	-4.819682	0.899420	0.006454
C	-6.595314	-0.926081	0.524795
H	-6.484128	-0.010092	1.098294
O	-0.141847	0.912660	0.312260
C	-7.850706	-1.517865	0.411762
N	2.515637	1.087599	-0.143588
O	2.728611	-1.404064	-0.210620
O	-3.136213	-1.794863	-0.082721
N	-8.076501	-2.663706	-0.232009
N	3.808376	0.635848	-0.106895
C	-7.020887	-3.271420	-0.780876
H	-7.224569	-4.208047	-1.295714
C	-5.723802	-2.774591	-0.720537
H	-4.890836	-3.304974	-1.168731
C	-4.104633	-1.041436	-0.007300
C	-2.681628	2.143809	0.130315
H	-3.593213	2.758445	0.060333
C	-1.429182	2.873989	0.117289
C	-1.461594	4.267821	0.017964
H	-2.431758	4.763540	0.000619
C	-0.303811	5.044176	-0.071587
C	0.915934	4.376000	-0.087756
H	1.835641	4.951288	-0.178379
C	1.012202	2.978005	-0.007002
C	-0.173213	2.201193	0.138029
C	-0.380560	6.544733	-0.147016
H	0.575152	6.975893	-0.459060

H	-1.142541	6.872888	-0.862447
H	-0.637202	6.984840	0.824632
C	2.314645	2.363859	-0.032286
H	3.197224	3.001007	0.044421
C	3.805842	-0.677421	-0.160661
C	5.110484	-1.372944	-0.147900
C	6.316688	-0.673983	-0.055143
H	6.313688	0.408289	0.006439
C	7.502831	-1.397138	-0.043985
N	7.568209	-2.730775	-0.117645
C	6.408455	-3.385849	-0.208187
H	6.478019	-4.470697	-0.269792
C	5.163676	-2.764928	-0.226574
H	4.246829	-3.338610	-0.303671
H	-1.314083	-1.511001	-0.077950
H	-0.398750	-2.403503	-0.954019
H	8.456986	-0.877941	0.028235
H	-8.718508	-1.046746	0.869305
O	1.128432	-0.686147	1.902413
H	0.300234	-0.240452	2.138844
C	1.220580	-1.953308	2.543260
H	1.285552	-1.833309	3.630737
H	2.138515	-2.411112	2.174859
H	0.372480	-2.595135	2.283887

2

V	1.903194	-0.726599	0.698275
N	-3.587884	1.014249	-0.221013
C	-6.665825	-1.007975	-0.162284
O	1.107163	-2.437696	-0.196730
O	1.804535	-0.773567	2.262837
N	-4.467968	-0.007613	-0.177150
H	-4.129577	-0.945401	0.028453
C	-6.248608	-2.262987	-0.615368
H	-5.261444	-2.395250	-1.058148
O	0.364291	0.086376	-0.075891
N	-7.008187	-3.358021	-0.586485
N	2.922314	0.924592	0.169596
O	3.586448	-1.440467	0.045169
O	-6.316354	1.342951	-0.238069
C	-8.243312	-3.229857	-0.097564
H	-8.841833	-4.138598	-0.073695
N	4.275745	0.753816	-0.001741
C	-8.774872	-2.022340	0.353782
H	-9.793824	-1.976211	0.724982
C	-7.973358	-0.891704	0.313745
H	-8.327106	0.082526	0.636522
C	-5.827756	0.230056	-0.201354

C	-2.346451	0.716653	-0.092491
H	-2.006994	-0.316473	0.043533
C	-1.321080	1.750878	-0.096710
C	-1.664253	3.102199	-0.124577
H	-2.722856	3.347779	-0.155797
C	-0.707625	4.123363	-0.109920
C	0.625903	3.750420	-0.057538
H	1.398784	4.516297	-0.043351
C	1.025971	2.400738	-0.009481
C	0.043438	1.370799	-0.046892
C	-1.125799	5.567203	-0.143101
H	-0.258496	6.233683	-0.143092
H	-1.719844	5.789639	-1.036668
H	-1.743195	5.822527	0.725619
C	2.427349	2.111647	-0.013046
H	3.134736	2.917370	-0.214396
C	4.531831	-0.528145	-0.045143
C	5.919174	-0.980361	-0.218440
C	6.961787	-0.067745	-0.433658
H	6.739931	0.995339	-0.476577
N	8.233663	-0.423202	-0.593361
C	8.517675	-1.728872	-0.540232
H	9.565502	-1.993060	-0.671227
C	7.562459	-2.720008	-0.331385
H	7.854060	-3.764997	-0.294503
C	6.237451	-2.338565	-0.168514
H	5.451901	-3.066802	0.003953
H	1.807385	-2.871648	-0.712102
H	0.412356	-2.144866	-0.810249

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V	-1.646213	-0.625660	-0.486427
N	3.754707	1.190171	0.102112
C	6.783781	-0.906415	0.048627
O	-1.032897	-2.274331	-0.369592
O	-1.548373	-0.320532	-2.014908
C	-0.730966	-3.196474	-1.386227
H	0.211739	-3.700184	-1.141533
H	-1.524074	-3.951979	-1.441187
H	-0.640539	-2.695511	-2.357667
N	4.609179	0.146132	0.090589
H	4.239124	-0.796635	-0.010886
C	6.360653	-2.121657	0.595376
H	5.388414	-2.207104	1.080733
O	-0.216036	0.344450	0.189934
O	-1.795864	-0.885753	1.908766
H	-0.888775	-0.636622	2.141214
C	-2.126751	-2.132949	2.509950

H	-3.145018	-2.361971	2.195405
H	-1.461141	-2.930966	2.165447
H	-2.095597	-2.056239	3.602605
N	7.098885	-3.231644	0.608866
N	-2.724405	1.151382	-0.011364
O	-3.474175	-1.155634	-0.298992
O	6.485914	1.450807	-0.036518
C	8.317630	-3.159902	0.069949
H	8.898179	-4.080469	0.083233
N	-4.080933	1.019282	0.081082
C	8.854194	-1.994481	-0.475904
H	9.859664	-1.992399	-0.884840
C	8.074842	-0.847823	-0.480186
H	8.433621	0.096645	-0.877309
C	5.972933	0.350445	0.034306
C	2.502362	0.913533	0.062207
H	2.133315	-0.118036	0.023160
C	1.500879	1.970620	0.055190
C	1.862066	3.319787	0.019684
H	2.923517	3.552846	-0.001986
C	0.915973	4.347861	0.011878
C	-0.426897	3.991673	0.039188
H	-1.190447	4.766915	0.034220
C	-0.839394	2.649419	0.062581
C	0.132715	1.623137	0.082098
C	1.347063	5.787760	-0.038372
H	0.497360	6.463405	0.096150
H	2.081874	6.011467	0.742459
H	1.814592	6.029455	-1.000080
C	-2.241255	2.345954	0.111331
H	-2.952421	3.160620	0.252881
C	-4.386068	-0.236066	-0.102214
C	-5.791946	-0.660745	-0.078614
C	-6.823745	0.256378	0.165626
H	-6.579052	1.301344	0.337336
N	-8.111610	-0.074879	0.204092
C	-8.421933	-1.358622	-0.005892
H	-9.482092	-1.603098	0.029987
C	-7.478827	-2.351161	-0.258929
H	-7.792128	-3.377321	-0.424065
C	-6.137111	-1.995903	-0.295684
H	-5.357693	-2.725361	-0.490425

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V	1.816097	1.330483	-0.195407
C	8.586831	2.054822	0.604582
H	9.609859	2.419935	0.694228
C	8.329709	0.685405	0.574394

H	9.146414	-0.028245	0.639288
O	3.704010	1.788558	0.200701
N	4.285462	-0.437162	0.236687
C	7.013665	0.260975	0.459220
H	6.745107	-0.790064	0.429617
O	-6.317970	-0.961523	0.123776
O	1.219555	2.602405	0.569601
N	2.928114	-0.563512	0.110759
C	6.002095	1.220487	0.378494
N	7.637210	2.990049	0.528733
O	1.725554	1.526371	-1.776291
N	-3.554778	-0.798982	-0.056125
O	0.348402	0.136929	0.210568
N	-4.389175	0.272974	0.025860
H	-3.981869	1.198220	0.147342
C	6.374389	2.568724	0.418098
H	5.601223	3.329865	0.356165
C	-7.997698	3.690635	0.282325
C	4.577726	0.843512	0.257586
C	2.481482	-1.776085	0.025805
H	3.216485	-2.585266	0.042632
C	1.094590	-2.116878	-0.093278
C	0.730333	-3.461353	-0.259480
H	1.525250	-4.204724	-0.315410
C	-0.595077	-3.871111	-0.356832
C	-1.583446	-2.887570	-0.272423
H	-2.634448	-3.159295	-0.340515
C	-1.274249	-1.538692	-0.100045
C	-2.299858	-0.518301	-0.010250
H	-1.933527	0.509507	0.098286
C	-5.744721	0.116842	0.097067
C	-6.515011	1.403455	0.162898
C	-6.073866	2.635149	-0.331412
H	-5.106895	2.724313	-0.825363
N	-6.788909	3.760965	-0.277288
C	-8.549605	2.513180	0.783597
H	-9.546585	2.513320	1.214261
C	-7.796521	1.350841	0.713649
H	-8.166993	0.393309	1.066497
C	-0.957911	-5.317178	-0.562891
H	-1.336851	-5.500415	-1.576740
H	-0.090509	-5.969161	-0.415136
H	-1.740289	-5.639929	0.133900
C	0.085464	-1.115454	-0.002805
H	-8.557627	4.623838	0.323909

8Ha

V	2.245496	0.735047	-1.045588

C	8.656559	-0.949065	-2.444558
H	9.709537	-0.964173	-2.720070
C	7.960910	-2.143897	-2.258982
H	8.463107	-3.097248	-2.389354
O	4.130825	0.521593	-1.214820
N	3.875482	-1.742799	-1.194353
C	6.622209	-2.082738	-1.906430
H	6.030493	-2.978443	-1.748159
O	-5.081498	1.997541	2.858137
O	2.511408	2.433104	-0.626084
N	2.616173	-1.321049	-0.874689
C	6.029004	-0.825409	-1.753066
N	8.107423	0.259573	-2.305074
O	1.589178	0.688492	-2.458000
N	-2.782156	1.204132	1.597328
O	0.922017	0.351692	0.150444
N	-3.060247	2.485530	1.903571
H	-2.341772	3.195235	1.776738
C	6.819663	0.309545	-1.967192
H	6.379669	1.297687	-1.861320
C	-4.824167	6.938228	3.235261
C	4.619153	-0.687827	-1.378860
C	1.742355	-2.237740	-0.581701
H	2.068301	-3.274033	-0.670223
C	0.415202	-1.959106	-0.133756
C	-0.508497	-3.008215	0.026182
H	-0.204078	-4.015648	-0.249063
C	-1.787411	-2.780775	0.512741
C	-2.133105	-1.469224	0.862488
H	-3.125020	-1.252496	1.250612
C	-1.246689	-0.399088	0.737806
C	-1.620193	0.958719	1.112422
H	-0.870951	1.742526	0.955551
C	-4.251274	2.818919	2.520096
C	-4.432209	4.282845	2.762332
C	-3.810341	5.296274	2.026297
H	-3.155692	5.058795	1.187804
N	-3.990697	6.597870	2.250387
C	-5.520648	6.013984	4.013022
H	-6.199541	6.351148	4.789939
C	-5.324346	4.663901	3.766983
H	-5.842558	3.890761	4.325662
C	-2.784302	-3.896499	0.660000
H	-3.631808	-3.762833	-0.022077
H	-2.331629	-4.867998	0.442228
H	-3.191260	-3.934240	1.676226
C	0.046348	-0.644361	0.229666

H	-4.947465	8.006136	3.405576
H	3.213009	2.638580	0.012018

8Hb

V	1.367032	1.086753	0.147863
C	8.014189	2.613455	0.370054
H	8.984622	3.107794	0.388001
C	7.934751	1.224928	0.275987
H	8.838862	0.626038	0.219586
O	3.195897	1.725461	0.394084
N	4.046663	-0.408547	0.238994
C	6.680307	0.633305	0.255050
H	6.551406	-0.441575	0.182010
O	-6.480588	-0.692350	-0.151294
O	0.650320	2.229080	1.012139
N	2.715566	-0.701020	0.219406
C	5.551525	1.453199	0.329701
N	6.949179	3.415465	0.442205
O	1.052028	1.292675	-1.400941
N	-3.657345	-1.202257	0.089049
O	0.130657	-0.314918	0.658449
N	-4.304702	-0.008646	0.216763
H	-3.734650	0.782332	0.514870
C	5.747688	2.835648	0.421572
H	4.882377	3.490400	0.480364
C	-7.015451	4.224672	0.179259
C	4.185379	0.898096	0.313830
C	2.407297	-1.952406	0.090042
H	3.222765	-2.672864	-0.006447
C	1.050678	-2.427665	0.031512
C	0.775265	-3.761680	-0.267593
H	1.615642	-4.433086	-0.440060
C	-0.529617	-4.269825	-0.372147
C	-1.588941	-3.392811	-0.180396
H	-2.614075	-3.739794	-0.282953
C	-1.368054	-2.045934	0.140516
C	-2.383678	-1.052100	0.279819
H	-1.974435	-0.065453	0.535561
C	-5.634466	0.164506	0.049406
C	-6.052858	1.610503	0.127424
C	-5.212041	2.694417	-0.069537
H	-4.152262	2.622045	-0.287026
N	-5.709339	3.946412	-0.033812
C	-7.897107	3.175602	0.355412
H	-8.948374	3.386629	0.513907
C	-7.421159	1.869475	0.314945
H	-8.078109	1.010580	0.413456
C	-0.758067	-5.720778	-0.695551

H	-1.822748	-5.933210	-0.828575
H	-0.241475	-6.013877	-1.616968
H	-0.387031	-6.374287	0.103544
C	-0.036165	-1.540026	0.285239
H	-7.296717	5.269808	0.186113
H	-5.065911	4.717410	-0.187373

8Ha•MeOH

V	-1.710604	-0.756355	-0.533567
C	-8.414332	-1.734518	0.011229
H	-9.426775	-2.134071	0.031811
C	-8.193158	-0.368920	0.190033
H	-9.028325	0.305776	0.349943
O	-3.531220	-1.306115	-0.265534
N	-4.148432	0.872413	0.052467
C	-6.889606	0.100835	0.158987
H	-6.655191	1.151753	0.293022
O	6.402113	1.379935	0.195949
O	-1.097793	-2.427856	-0.347254
N	-2.792323	1.008094	-0.052242
C	-5.854095	-0.815018	-0.051495
N	-7.439934	-2.624062	-0.191567
O	-1.692601	-0.498058	-2.072031
N	3.682995	1.103582	-0.054215
O	-0.284318	0.232129	0.047167
N	4.547001	0.068643	-0.080943
H	4.184131	-0.882159	-0.064657
C	-6.189895	-2.162797	-0.221409
H	-5.402985	-2.893078	-0.391808
C	8.298158	-3.190495	-0.171394
C	-4.450306	-0.387712	-0.093411
C	-2.316346	2.207729	0.059630
H	-3.035575	3.014251	0.205479
C	-0.921085	2.529215	-0.002448
C	-0.520111	3.875451	-0.003332
H	-1.289211	4.644830	0.018183
C	0.819666	4.240958	-0.038893
C	1.773675	3.219430	-0.061214
H	2.833063	3.461508	-0.084775
C	1.424498	1.867077	-0.050792
C	2.432581	0.816139	-0.063203
H	2.070184	-0.218176	-0.082104
C	5.906302	0.281726	0.031435
C	6.733287	-0.962090	-0.044150
C	6.341590	-2.143377	-0.681533
H	5.384444	-2.208867	-1.198880
N	7.095405	-3.240932	-0.747159
C	8.803888	-2.057520	0.464773

H	9.797994	-2.070385	0.900438
C	8.008731	-0.923326	0.523224
H	8.343478	-0.003042	0.991686
C	1.241363	5.684235	-0.061570
H	1.712059	5.945960	-1.016384
H	0.386729	6.351918	0.081022
H	1.970917	5.898621	0.726825
C	0.058759	1.511509	-0.020668
H	8.891344	-4.101231	-0.229290
O	-1.927918	-1.153573	1.854532
C	-0.775919	-1.499401	2.617620
H	-2.487130	-1.939654	1.758156
H	-0.215712	-2.310478	2.140719
H	-1.059338	-1.786507	3.636582
H	-0.151707	-0.606833	2.659074
H	-0.943445	-2.884618	-1.188537

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V	-1.663353	-1.267648	-1.123642
C	-7.093797	-5.261992	-1.264630
H	-8.007433	-5.807957	-1.036514
C	-6.342689	-5.589068	-2.393840
H	-6.662794	-6.389805	-3.052867
O	-3.336097	-2.109342	-1.093947
N	-2.843433	-3.250589	-3.001760
C	-5.185488	-4.871302	-2.650114
H	-4.561106	-5.080833	-3.512520
O	3.275507	5.093080	-0.204882
O	-2.165887	-0.000001	-0.000112
N	-1.792948	-2.381149	-2.919732
C	-4.824276	-3.851151	-1.764015
N	-6.764787	-4.292280	-0.408271
O	-0.646759	-2.221651	-0.406707
N	2.339053	2.503516	-2.346492
O	-0.671688	-0.185506	-2.187874
N	2.302801	3.484195	-1.420637
H	1.592270	3.463068	-0.686316
C	-5.651408	-3.606288	-0.661225
H	-5.391143	-2.818552	0.040938
C	6.420347	4.965868	-4.000787
C	-3.615600	-3.052401	-1.970901
C	-0.941066	-2.385783	-3.901882
H	-1.101645	-3.119231	-4.692100
C	0.161913	-1.481889	-3.998689
C	1.126493	-1.635881	-5.011400
H	1.038642	-2.480240	-5.691355
C	2.183384	-0.746681	-5.145217
C	2.259668	0.328705	-4.249403

H	3.078374	1.039399	-4.328743
C	1.318775	0.534696	-3.240432
C	1.381826	1.647558	-2.304079
H	0.586873	1.715417	-1.557406
C	3.307189	4.404992	-1.215989
C	4.397733	4.549192	-2.222714
C	4.273656	4.308442	-3.596187
H	3.336905	3.946061	-4.005991
N	5.257101	4.512615	-4.473721
C	6.647371	5.260322	-2.658351
H	7.609699	5.643177	-2.333217
C	5.611858	5.059585	-1.757931
H	5.713502	5.291051	-0.702351
C	3.227386	-0.922220	-6.212908
H	4.217445	-1.091741	-5.774705
H	2.998245	-1.774460	-6.858782
H	3.302879	-0.030842	-6.845274
C	0.257845	-0.386860	-3.114983
H	7.209830	5.108567	-4.736917
V	-1.663516	1.267615	1.123532
C	-7.094300	5.261496	1.264409
H	-8.007964	5.807401	1.036265
C	-6.343289	5.588570	2.393684
H	-6.663499	6.389246	3.052734
O	-3.336342	2.109149	1.093797
N	-2.843877	3.250347	3.001688
C	-5.186046	4.870883	2.649991
H	-4.561735	5.080417	3.512447
O	3.276013	-5.092657	0.204869
N	-1.793317	2.380993	2.919679
C	-4.824697	3.850809	1.763859
N	-6.765159	4.291856	0.408018
O	-0.647003	2.221772	0.406686
N	2.339125	-2.503335	2.346564
O	-0.671765	0.185521	2.187732
N	2.303032	-3.483983	1.420670
H	1.592591	-3.462852	0.686262
C	-5.651740	3.605940	0.661004
H	-5.391369	2.818262	-0.041186
C	6.420536	-4.965526	4.001026
C	-3.615970	3.052144	1.970777
C	-0.941503	2.385645	3.901888
H	-1.102201	3.119037	4.692134
C	0.161543	1.481839	3.998729
C	1.126015	1.635845	5.011542
H	1.038028	2.480154	5.691543
C	2.182966	0.746723	5.145405

C	2.259416	-0.328602	4.249533
H	3.078168	-1.039239	4.328909
C	1.318636	-0.534606	3.240460
C	1.381863	-1.647419	2.304062
H	0.587007	-1.715289	1.557286
C	3.307493	-4.404714	1.216081
C	4.397983	-4.548888	2.222871
C	4.273790	-4.308312	3.596366
H	3.336969	-3.946101	4.006155
N	5.257205	-4.512468	4.473937
C	6.647679	-5.259803	2.658572
H	7.610073	-5.642505	2.333455
C	5.612199	-5.059085	1.758110
H	5.713937	-5.290419	0.702510
C	3.226851	0.922279	6.213205
H	4.216943	1.091879	5.775106
H	2.997597	1.774477	6.859095
H	3.302336	0.030878	6.845540
C	0.257650	0.386878	3.114957
H	7.209989	-5.108216	4.737190

14

V	-2.210142	-0.488678	-0.535734
C	-8.902704	0.615046	0.580845
H	-9.983559	0.542500	0.700843
C	-8.274474	1.858761	0.610130
H	-8.856735	2.765016	0.752142
O	-4.153063	-0.455250	-0.045079
N	-4.085944	1.827886	0.127991
C	-6.896646	1.908513	0.453435
H	-6.347071	2.844252	0.466146
O	6.278868	-0.379956	-0.117192
O	-1.202163	-1.970648	-0.171134
N	-2.750579	1.575924	-0.057306
C	-6.196640	0.713608	0.272924
N	-8.254966	-0.539697	0.409974
O	-2.247672	-0.284528	-2.092264
N	3.568689	0.185772	-0.286898
O	-0.445999	0.273162	-0.037836
N	4.097236	-1.068248	-0.258985
H	3.463212	-1.860933	-0.178779
C	-6.928960	-0.478675	0.259959
H	-6.401404	-1.418410	0.120144
C	6.701079	-5.309638	-0.178974
C	-4.728946	0.687282	0.100247
C	-2.007967	2.640961	-0.090330
H	-2.526034	3.597595	0.005571
C	-0.589132	2.646462	-0.235429

C	0.100119	3.864394	-0.347234
H	-0.480847	4.786285	-0.361593
C	1.484987	3.926538	-0.440235
C	2.192792	2.719841	-0.404174
H	3.278570	2.721402	-0.471172
C	1.554570	1.487437	-0.284509
C	2.283394	0.235161	-0.246748
H	1.662330	-0.666446	-0.183295
C	5.446409	-1.271229	-0.189142
C	5.858150	-2.714759	-0.186137
C	5.115774	-3.768196	-0.729563
H	4.159549	-3.583808	-1.217991
N	5.516615	-5.041419	-0.730637
C	7.536228	-4.337493	0.368457
H	8.498202	-4.613462	0.790261
C	7.108255	-3.018507	0.355489
H	7.711794	-2.205177	0.746450
C	2.206103	5.239340	-0.586998
H	2.654699	5.347220	-1.582993
H	1.525176	6.084507	-0.441156
H	3.019477	5.336982	0.141785
C	0.128975	1.419843	-0.197007
H	7.001530	-6.356475	-0.182964
O	-2.584702	-2.238231	-0.181061

14Ha

V	-0.667415	-0.263425	0.338569
C	-7.180867	-1.713181	-0.657285
H	-8.150491	-2.193333	-0.776920
C	-7.098996	-0.335853	-0.452146
H	-8.000346	0.267320	-0.409388
O	-2.350861	-0.873635	-0.301878
N	-3.174396	1.229483	-0.040485
C	-5.845962	0.237532	-0.305089
H	-5.719787	1.303153	-0.143527
O	5.738462	-2.089389	-1.425146
O	-0.023016	0.173293	1.933938
N	-1.835931	1.438194	0.080543
C	-4.721651	-0.591379	-0.367662
N	-6.119177	-2.520001	-0.720581
O	0.115939	-1.654504	-0.367018
N	3.394792	0.342749	-0.541927
O	0.626472	0.838601	-0.419986
N	4.545918	-0.284512	-0.863573
H	5.295520	0.231445	-1.326621
C	-4.918096	-1.961614	-0.577212
H	-4.058860	-2.625346	-0.628823
C	2.278229	-4.423265	1.112275

C	-3.366783	-0.055365	-0.217354
C	-1.421889	2.673741	0.118047
H	-2.188373	3.448743	0.135661
C	-0.048824	3.051835	0.088985
C	0.299705	4.409275	0.236201
H	-0.487641	5.128016	0.452097
C	1.607958	4.837014	0.107675
C	2.582523	3.870552	-0.189665
H	3.616399	4.193742	-0.300775
C	2.301266	2.513566	-0.336741
C	3.414502	1.625260	-0.636157
H	4.340501	2.134995	-0.937826
C	4.750669	-1.652963	-0.853814
C	3.802618	-2.534144	-0.123900
C	3.722339	-3.865300	-0.555712
H	4.302171	-4.174161	-1.422046
N	2.972915	-4.794013	0.031955
C	2.301799	-3.136635	1.643620
H	1.718304	-2.893057	2.525189
C	3.075765	-2.169491	1.013237
H	3.115292	-1.157133	1.398745
C	1.992224	6.279907	0.278008
H	2.530277	6.656303	-0.599223
H	1.111945	6.911237	0.426702
H	2.649491	6.416848	1.144607
C	0.951741	2.086883	-0.201665
H	1.673784	-5.198744	1.578541
H	1.057171	-1.517075	-0.585560
O	-1.208653	-0.598832	1.994926

14Hb

V	-0.533208	-0.096495	0.426042
C	-6.816484	-2.605231	-0.418621
H	-7.693183	-3.242665	-0.524154
C	-6.904986	-1.239044	-0.682497
H	-7.847962	-0.800467	-0.994623
O	-2.271044	-0.968142	0.427581
N	-3.337296	0.972132	-0.179316
C	-5.766165	-0.460985	-0.538182
H	-5.771428	0.607098	-0.729685
O	5.271094	-0.488151	-0.885984
O	0.826853	-0.813831	1.492069
N	-2.073683	1.443633	0.013272
C	-4.579687	-1.078795	-0.133394
N	-5.693981	-3.215307	-0.030812
O	0.028234	0.008508	-1.032084
N	3.291262	1.290023	0.115537
O	0.137059	1.465576	1.292815

N	3.441810	-0.048527	0.445821
H	2.595277	-0.463091	0.875237
C	-4.605031	-2.457073	0.106587
H	-3.693656	-2.956134	0.424725
C	3.510603	-5.042676	-0.451092
C	-3.331205	-0.317957	0.038656
C	-1.900670	2.721756	-0.146734
H	-2.761128	3.312912	-0.464385
C	-0.615099	3.339486	0.021236
C	-0.283379	4.595590	-0.517147
H	-1.062573	5.184452	-0.997945
C	1.022113	5.073964	-0.502961
C	2.037950	4.250878	0.022612
H	3.076482	4.563040	-0.057393
C	1.732794	3.038905	0.615493
C	2.593707	1.908278	0.999642
H	2.348566	1.424354	1.948255
C	4.277538	-0.834244	-0.260875
C	3.911984	-2.302007	-0.236674
C	4.938026	-3.156026	-0.605736
H	5.922602	-2.773591	-0.850541
N	4.716397	-4.478394	-0.692317
C	2.455059	-4.230327	-0.105683
H	1.475075	-4.656699	0.075620
C	2.643773	-2.848276	0.000741
H	1.770236	-2.241831	0.255138
C	1.363901	6.421691	-1.077445
H	2.248007	6.369811	-1.722717
H	0.538111	6.822136	-1.673252
H	1.583540	7.151444	-0.287884
C	0.385459	2.602091	0.678372
H	3.447196	-6.118575	-0.555958
H	5.488560	-5.078912	-0.961659
O	-0.021288	-1.817562	0.943001

14Hc

V	-0.756883	-0.280715	0.292634
C	-7.401848	-1.438652	-0.241557
H	-8.396241	-1.879242	-0.288580
C	-7.214395	-0.091724	-0.551989
H	-8.057524	0.526903	-0.842954
O	-2.574636	-0.776944	0.365887
N	-3.220705	1.317740	-0.251078
C	-5.933323	0.432136	-0.480343
H	-5.725879	1.472193	-0.710173
O	5.790376	-0.936414	-0.916437
O	0.112529	-1.323860	1.535876
N	-1.871278	1.484260	-0.100304

C	-4.886875	-0.413597	-0.099330
N	-6.416000	-2.261398	0.123086
O	-0.136263	-0.407483	-1.137701
N	4.051444	0.920024	0.496384
O	0.365935	1.006224	1.085982
N	4.518023	-0.312607	0.912140
H	3.914508	-0.763110	1.602490
C	-5.187319	-1.749735	0.190270
H	-4.389878	-2.425080	0.489066
C	2.282949	-4.444747	-0.661957
C	-3.508294	0.073128	0.000297
C	-1.419394	2.693932	-0.262376
H	-2.142010	3.452349	-0.563856
C	-0.048904	3.046821	-0.081201
C	0.463399	4.275641	-0.542592
H	-0.216817	4.978883	-1.018688
C	1.810116	4.584992	-0.438455
C	2.667791	3.630301	0.139708
H	3.736716	3.823667	0.184280
C	2.192883	2.431855	0.650171
C	3.015972	1.323512	1.132347
H	2.583106	0.726773	1.944580
C	4.909434	-1.180408	-0.125175
C	4.054405	-2.407710	-0.229856
C	2.688236	-2.304246	0.040257
H	2.253771	-1.382285	0.411981
N	1.813992	-3.291326	-0.176003
C	3.627026	-4.643127	-0.973487
H	3.952337	-5.595579	-1.378480
C	4.525039	-3.602081	-0.775397
H	5.574214	-3.693853	-1.040102
C	2.360359	5.888520	-0.947063
H	3.161205	5.724934	-1.676955
H	1.583587	6.487090	-1.431372
H	2.783654	6.488104	-0.132616
C	0.809415	2.136789	0.567656
H	1.551789	-5.233633	-0.816264
H	0.236353	-2.747193	0.263073
O	-0.553310	-2.305388	0.739497

CVIIHa

V	2.854547	1.319172	-0.210104
V	-4.041706	-1.415953	0.452453
O	4.785855	1.470705	0.324954
O	1.241898	0.267143	-0.119391
O	2.918396	1.822921	-1.719011
O	-4.130306	-2.367297	-0.784552
O	-5.037966	0.160906	0.252010

C	5.508310	0.414203	0.221279
N	5.079786	-0.796553	-0.028826
N	3.724017	-0.727026	-0.200674
C	3.143318	-1.850770	-0.507135
C	1.744610	-1.990046	-0.729595
C	0.852886	-0.894003	-0.528998
C	-0.545780	-1.124808	-0.743387
C	-0.983607	-2.378016	-1.169829
H	-2.040265	-2.514863	-1.379851
C	-0.107520	-3.455028	-1.372175
C	1.239553	-3.240924	-1.133153
H	1.945545	-4.057983	-1.274973
C	-1.399383	0.034280	-0.627653
C	-0.625486	-4.779138	-1.862924
H	0.153505	-5.546899	-1.832236
H	-0.981604	-4.708790	-2.897605
H	-1.469589	-5.131526	-1.259719
N	-2.673530	0.066203	-0.375761
C	-4.475774	1.279930	-0.155188
N	-3.225196	1.321714	-0.495202
H	3.777736	-2.734757	-0.606326
H	-0.920325	1.000072	-0.783898
C	9.657450	1.104850	0.784439
H	10.688108	1.396428	0.939920
C	9.240899	-0.192888	0.547322
H	9.977174	-0.987225	0.509865
C	7.887344	-0.454745	0.359406
H	7.523495	-1.459181	0.168294
C	6.953339	0.587278	0.411150
N	8.732461	2.086208	0.827588
C	7.416729	1.877091	0.653013
H	6.738218	2.721099	0.702298
C	-6.949838	4.650478	-0.289611
C	-5.307431	2.485608	-0.215526
C	-6.656541	2.435459	0.153168
H	-7.086179	1.495120	0.488970
N	-7.469968	3.491241	0.119302
C	-5.619556	4.812046	-0.676451
H	-5.254895	5.782564	-0.998118
C	-4.780740	3.709430	-0.639944
H	-3.736433	3.772075	-0.928366
H	-7.633389	5.497821	-0.308780
Cl	-5.619014	-2.234305	1.794905
O	2.410060	2.502227	0.759459
O	-2.710962	-1.883147	1.473487
C	-2.264486	-3.158804	1.861883
H	-2.995351	-3.585959	2.560715

H	-1.293847	-3.052289	2.355328
H	-2.165782	-3.822898	0.995637
H	9.043208	3.037253	1.000243

CVIIHb

V	-1.083858	-0.319076	-0.802543
V	1.256380	-0.051882	1.400909
O	-2.629101	-1.424663	-0.561592
O	-0.070001	0.972274	0.333439
O	-1.120508	0.315316	-2.255346
O	1.752984	0.989878	2.493587
O	2.826361	-1.159399	0.955708
C	-3.744040	-0.897224	-0.144536
N	-3.858084	0.349454	0.258224
N	-2.646374	0.954415	0.130409
C	-2.573604	2.223398	0.358946
C	-1.338599	2.960073	0.177043
C	-0.101720	2.288414	0.105182
C	1.067425	2.989441	-0.256579
C	0.985014	4.376751	-0.456009
H	1.887319	4.913929	-0.741381
C	-0.206058	5.077897	-0.296011
C	-1.358495	4.348052	0.008469
H	-2.311879	4.866688	0.089015
C	2.311747	2.299162	-0.510917
C	-0.261274	6.572225	-0.456459
H	-0.304686	7.075155	0.517374
H	-1.146091	6.882237	-1.022065
H	0.621442	6.949269	-0.981324
N	2.488017	1.067943	-0.168958
C	3.700463	-0.683744	0.137210
N	3.666691	0.465353	-0.491016
H	-3.483916	2.763414	0.626494
H	3.119754	2.842401	-1.008097
C	-7.055378	-3.466369	-0.088270
H	-7.884090	-4.172925	-0.092856
C	-7.250417	-2.157869	0.351711
H	-8.228636	-1.833690	0.693458
C	-6.170628	-1.288078	0.341109
H	-6.258303	-0.258137	0.670753
C	-4.934819	-1.761360	-0.108489
N	-5.884125	-3.938324	-0.521647
C	-4.851364	-3.094474	-0.526529
H	-3.899326	-3.483251	-0.877526
C	6.877402	-3.385305	-0.651671
C	4.840447	-1.566555	-0.155217
C	4.834363	-2.831991	0.421295
H	4.030446	-3.152807	1.073907

N	5.838194	-3.684732	0.154921
C	6.923868	-2.137569	-1.244726
H	7.753934	-1.890381	-1.896095
C	5.901264	-1.224719	-1.000537
H	5.895180	-0.239961	-1.456689
H	7.625514	-4.155031	-0.791522
O	0.350358	-1.122438	2.148283
O	0.140786	-1.359566	-0.702882
H	5.804490	-4.605793	0.580920

CVIII

V	-0.700602	-0.284444	0.300575
C	-7.451929	-1.254196	-0.261072
H	-8.437641	-1.701332	-0.291987
C	-7.188180	0.068154	-0.569728
H	-8.003595	0.718159	-0.864722
O	-2.566331	-0.776549	0.366410
N	-3.145783	1.347565	-0.265844
C	-5.881732	0.538882	-0.495967
H	-5.642205	1.571031	-0.730841
O	5.754829	-1.020735	-0.994344
O	0.114755	-1.324376	1.571332
N	-1.795899	1.490117	-0.106577
C	-4.842186	-0.320523	-0.112485
N	-6.430313	-2.053961	0.104331
O	-0.064252	-0.418006	-1.119079
N	4.059380	0.846441	0.460011
O	0.431672	0.992255	1.082913
N	4.562277	-0.361864	0.876307
H	4.022460	-0.803119	1.623285
C	-5.153443	-1.640490	0.188811
H	-4.400416	-2.357008	0.494692
C	2.160188	-4.430025	-0.627449
C	-3.446066	0.112776	-0.006581
C	-1.328977	2.702872	-0.273761
H	-2.041954	3.464660	-0.589154
C	0.031205	3.042334	-0.081109
C	0.551456	4.277399	-0.533612
H	-0.122898	4.987248	-1.007072
C	1.896486	4.572240	-0.424013
C	2.744483	3.603704	0.158835
H	3.813793	3.792960	0.208921
C	2.266154	2.407685	0.666742
C	3.092046	1.302125	1.163036
H	2.721069	0.765383	2.044738
C	4.901419	-1.247093	-0.172832
C	4.011861	-2.451937	-0.247914
C	2.660684	-2.300957	0.062766

H	2.272102	-1.364765	0.447149
N	1.747653	-3.258170	-0.130639
C	3.487406	-4.673223	-0.973274
H	3.769437	-5.636888	-1.383410
C	4.426117	-3.662562	-0.804077
H	5.463181	-3.792761	-1.098456
C	2.468126	5.867605	-0.925523
H	3.248343	5.691600	-1.674220
H	1.698252	6.494235	-1.383344
H	2.925633	6.439914	-0.110705
C	0.883865	2.119483	0.569014
H	1.398398	-5.192789	-0.760131
H	0.290766	-2.747272	0.285566
O	-0.538497	-2.282565	0.740673
H	-6.633404	-3.023642	0.331258

CX

V	1.340478	-0.295246	0.803347
V	-1.327889	-0.308841	-0.764454
O	2.851515	-1.382875	0.286399
O	-0.000134	0.950552	0.019301
O	-0.009650	-1.488569	0.053995
O	1.257618	-0.220627	2.366638
O	-1.202633	-0.260428	-2.325983
O	-2.854572	-1.389509	-0.274270
C	3.950857	-0.708280	0.086207
N	3.980763	0.604632	-0.005076
N	2.710293	1.084933	0.163911
C	2.511295	2.349764	-0.031021
C	1.220659	2.997651	0.010437
C	-0.000723	2.285248	0.005755
C	-1.223044	2.995722	-0.018616
C	-1.191872	4.398744	-0.014323
H	-2.139851	4.932470	-0.017452
C	-0.002646	5.122698	-0.018891
C	1.187437	4.400415	-0.019602
H	2.134623	4.935337	-0.036664
C	-2.513672	2.347118	0.013959
C	-0.003394	6.626110	-0.000603
H	0.880258	7.031507	-0.502276
H	-0.001139	7.008764	1.027224
H	-0.888850	7.031214	-0.499119
N	-2.709828	1.079985	-0.169107
C	-3.955069	-0.711026	-0.095355
N	-3.983426	0.602588	-0.014910
C	0.005216	-2.910284	0.026088
H	3.385103	2.959675	-0.264191
H	-1.022858	-3.273864	-0.056643

H	0.447654	-3.288663	0.952043
H	0.592753	-3.259440	-0.828177
H	-3.391154	2.959404	0.226189
C	7.456909	-2.962141	-0.328809
H	8.337998	-3.593586	-0.429347
C	7.568806	-1.576349	-0.439364
H	8.534431	-1.116987	-0.625788
C	6.423491	-0.807017	-0.306409
H	6.448210	0.274864	-0.383372
C	5.207406	-1.454600	-0.066902
N	6.306105	-3.599136	-0.100215
C	5.210596	-2.851256	0.026526
H	4.277797	-3.375889	0.213993
C	-7.473331	-2.952288	0.285325
C	-5.215799	-1.452966	0.044696
C	-5.221953	-2.850191	-0.038618
H	-4.288298	-3.379069	-0.209130
N	-6.321213	-3.594105	0.077805
C	-7.582688	-1.565422	0.384191
H	-8.549501	-1.101957	0.553503
C	-6.433347	-0.800321	0.262065
H	-6.455984	0.282146	0.330893
H	-8.357561	-3.580538	0.377872

CXI

V	-0.079678	-0.198007	1.439322
C	-7.217606	-1.994786	-0.618242
H	-8.072631	-2.668178	-0.663626
C	-5.924784	-2.505405	-0.556093
H	-5.754505	-3.577625	-0.561581
O	-4.291632	1.938061	-0.937268
N	-2.931576	0.430102	0.142171
C	-4.858329	-1.615672	-0.496334
H	-3.835024	-1.983519	-0.482376
O	6.908355	-0.577186	-0.378598
O	-0.097052	1.101621	2.682318
N	-1.720971	1.044280	0.192609
C	-5.132398	-0.246565	-0.497633
N	-7.501352	-0.688500	-0.636782
O	1.062455	-1.225042	1.804718
N	3.779568	0.990998	-0.188156
O	0.957504	0.874796	0.237958
N	5.099832	0.697599	-0.129502
H	5.785390	1.454444	-0.086892
C	-6.469762	0.153548	-0.583240
H	-6.695653	1.216848	-0.611387
C	3.643975	-4.188384	-0.699494
C	-4.083227	0.822126	-0.461852

C	-1.556410	2.257225	-0.215422
H	-2.407220	2.833405	-0.572261
C	-0.254427	2.881881	-0.241359
C	-0.212615	4.249260	-0.542186
H	-1.158195	4.770312	-0.685986
C	0.980278	4.952520	-0.650303
C	2.157711	4.222781	-0.497241
H	3.112261	4.739013	-0.598868
C	2.181180	2.848219	-0.234113
C	3.500118	2.244245	-0.155376
H	4.326462	2.973173	-0.106437
C	5.681617	-0.535764	-0.308626
C	4.847335	-1.762551	-0.417305
C	5.482423	-2.881920	-0.974378
H	6.513104	-2.784098	-1.306771
N	4.907723	-4.072454	-1.129184
C	2.924252	-3.152925	-0.116403
H	1.903036	-3.291931	0.222470
C	3.529778	-1.908110	0.024666
H	2.977669	-1.090548	0.472104
C	1.004071	6.434360	-0.906901
H	1.095921	7.005879	0.026259
H	1.848256	6.719435	-1.544704
H	0.085141	6.766939	-1.400884
C	0.951025	2.144617	-0.054719
H	3.189497	-5.170593	-0.827313
O	-1.104142	0.111576	2.909047
H	-2.817820	-0.496540	0.570746
O	-1.473561	-1.521237	1.081349
Br	-0.926752	-2.337411	-0.476739

CXIHa

V	-0.337774	-0.737953	-0.050451
C	7.272492	-1.378387	-0.363612
H	8.189608	-1.965059	-0.371389
C	6.153803	-1.832711	0.329186
H	6.188149	-2.769001	0.877299
O	4.009787	2.294051	-0.605452
N	2.644013	0.457744	-0.398126
C	5.001141	-1.056728	0.312648
H	4.121472	-1.362370	0.874243
O	-6.107975	-1.874432	0.844471
O	-0.969505	-0.227271	-1.676058
N	1.401354	0.983887	-0.245576
C	5.016700	0.144617	-0.398676
N	7.311336	-0.225276	-1.038288
O	-1.348718	-1.788281	0.562474
N	-3.850752	0.728945	0.332926

O	-1.087818	0.793471	0.714148
N	-5.021640	0.102719	0.618708
H	-5.709189	0.521463	1.246938
C	6.203593	0.513649	-1.040582
H	6.240163	1.458475	-1.577722
C	-2.304534	-3.280049	-2.011587
C	3.856254	1.083336	-0.473336
C	1.207853	2.261817	-0.244573
H	2.041490	2.939348	-0.412666
C	-0.106594	2.831243	-0.043716
C	-0.259460	4.213168	-0.223076
H	0.616269	4.792744	-0.509832
C	-1.476397	4.861463	-0.041970
C	-2.576826	4.072681	0.300283
H	-3.551340	4.545277	0.418604
C	-2.482514	2.689414	0.466551
C	-3.704894	1.939411	0.726583
H	-4.521331	2.470012	1.238564
C	-5.183576	-1.229948	0.371189
C	-4.166924	-1.879185	-0.519364
C	-3.764621	-3.147143	-0.150948
H	-4.137673	-3.638625	0.738172
N	-2.850882	-3.797255	-0.887204
C	-2.735403	-2.052837	-2.459725
H	-2.298378	-1.630392	-3.353491
C	-3.635723	-1.323745	-1.688725
H	-3.920182	-0.324775	-1.993148
C	-1.615933	6.346269	-0.237421
H	-2.164334	6.810642	0.589808
H	-0.637375	6.830966	-0.301586
H	-2.160649	6.582921	-1.159904
C	-1.216008	2.048756	0.360972
H	-1.542516	-3.869210	-2.502452
O	-0.036592	-1.298715	-1.776328
H	2.569901	-0.559619	-0.335752
O	1.292277	-1.699160	0.312529
Br	1.445443	-1.471127	2.134966
H	-2.485989	-4.673615	-0.533058

CXIHb

V	0.383101	-0.565041	0.311258
C	6.231908	-2.587610	-1.437643
H	6.857220	-3.410927	-1.759575
C	5.204772	-2.704678	-0.527900
H	4.978485	-3.673361	-0.098090
O	4.008580	1.780931	-1.492734
N	3.091840	0.913404	0.435960
C	4.446148	-1.580119	-0.190841

H	3.606947	-1.689275	0.496709
O	-6.807727	-0.899674	0.109975
O	0.499821	-0.525182	-1.487930
N	1.789961	1.361546	0.356731
C	4.747887	-0.341182	-0.771547
N	6.486135	-1.380098	-1.988347
O	-0.606021	-1.723231	0.698455
N	-3.723117	0.757335	0.037456
O	-0.816123	0.894024	0.432972
N	-4.992647	0.370387	0.292453
H	-5.678115	1.068797	0.587421
C	5.778079	-0.275468	-1.692269
H	6.009418	0.646147	-2.213811
C	-3.668561	-4.204711	-1.631886
C	3.916997	0.909856	-0.636622
C	1.524326	2.540512	-0.081449
H	2.324963	3.232948	-0.340518
C	0.164658	2.987952	-0.225764
C	-0.025818	4.328199	-0.598139
H	0.854275	4.935014	-0.804716
C	-1.285468	4.895333	-0.687819
C	-2.370642	4.065067	-0.393951
H	-3.374833	4.484089	-0.446152
C	-2.246706	2.714272	-0.060663
C	-3.502724	2.013468	0.183382
H	-4.339931	2.675329	0.455936
C	-5.593709	-0.828163	-0.045912
C	-4.800952	-1.962479	-0.583002
C	-5.531418	-2.960230	-1.245056
H	-6.607686	-2.842661	-1.343451
N	-4.992025	-4.056816	-1.770982
C	-2.850755	-3.289078	-0.980357
H	-1.783267	-3.453825	-0.879228
C	-3.423068	-2.139333	-0.447469
H	-2.801336	-1.413611	0.060391
C	-1.489544	6.329397	-1.089832
H	-2.165646	6.847984	-0.400750
H	-0.542146	6.876510	-1.102382
H	-1.928430	6.406951	-2.092127
C	-0.946239	2.135203	0.044517
H	-3.246255	-5.111027	-2.064362
O	1.602241	-1.223182	-0.908901
H	3.015847	0.058289	1.006034
O	1.827299	-1.083999	1.526339
Br	1.194781	-0.718022	3.213888
H	7.231205	-1.305707	-2.673301

CXIOH

V	0.062764	-0.576842	0.501097
C	-7.361272	-1.861015	0.012034
H	-8.242763	-2.498174	-0.026603
C	-6.142737	-2.317046	-0.484627
H	-6.062226	-3.305741	-0.924569
O	-4.328924	2.005569	0.240149
N	-2.870216	0.241742	0.435419
C	-5.040840	-1.474506	-0.414493
H	-4.084794	-1.782942	-0.831174
O	6.466112	-0.883058	-1.479033
O	0.486793	0.077301	2.083974
N	-1.647072	0.836529	0.359806
C	-5.205346	-0.208522	0.152013
N	-7.540407	-0.648332	0.544446
O	1.348599	-1.633501	-0.010216
N	3.674105	1.003003	-0.559978
O	0.879850	0.824102	-0.354561
N	4.919711	0.647013	-0.951605
H	5.455830	1.265521	-1.560882
C	-6.480399	0.153702	0.600993
H	-6.631377	1.143634	1.024888
C	4.010814	-3.553984	1.798348
C	-4.114000	0.799568	0.268183
C	-1.539545	2.130854	0.319330
H	-2.445724	2.725560	0.394834
C	-0.285232	2.817620	0.154594
C	-0.270532	4.218229	0.250238
H	-1.196640	4.731489	0.499348
C	0.886014	4.952856	0.026058
C	2.047200	4.248420	-0.310911
H	2.963641	4.806591	-0.495433
C	2.092624	2.855103	-0.406438
C	3.366184	2.238579	-0.747970
H	4.113715	2.925676	-1.168165
C	5.470302	-0.615618	-0.824547
C	4.866138	-1.575876	0.134753
C	5.021036	-2.939928	-0.146046
H	5.516058	-3.236552	-1.067645
N	4.597010	-3.915247	0.652575
C	3.828740	-2.230901	2.192137
H	3.350399	-1.998151	3.137618
C	4.260647	-1.219278	1.343262
H	4.136499	-0.177186	1.616670
C	0.903772	6.450969	0.148517
H	1.399711	6.916916	-0.709689
H	-0.109685	6.856611	0.211626
H	1.443744	6.769821	1.048142

C	0.899257	2.128381	-0.181159
H	3.673659	-4.367735	2.437266
H	2.174458	-1.141142	-0.198464
O	-0.416577	-1.014446	2.167261
H	-2.753767	-0.769134	0.478107
O	-1.275992	-1.807023	0.025994
Br	-1.275202	-1.808224	-1.812855

CXIOOH

V	-0.331247	-0.689347	0.056664
C	7.281562	-1.749992	-0.376100
H	8.166153	-2.384095	-0.367726
C	6.155375	-2.105714	0.361817
H	6.152715	-3.010489	0.961100
O	4.198822	2.067784	-0.765490
N	2.750575	0.312415	-0.462729
C	5.045476	-1.271340	0.321800
H	4.164053	-1.497975	0.917461
O	-6.205394	-1.386457	1.122091
O	-0.877297	-0.289592	-1.645251
N	1.538456	0.908203	-0.320000
C	5.108907	-0.113807	-0.457031
N	7.366121	-0.639332	-1.114638
O	-1.415213	-1.659706	0.626022
N	-3.700364	0.928675	0.422163
O	-0.931547	0.877820	0.694675
N	-4.881710	0.384427	0.768198
H	-5.499003	0.862982	1.426167
C	6.299933	0.156608	-1.139845
H	6.375184	1.065599	-1.731979
C	-3.273396	-3.513199	-2.146385
C	3.997489	0.874992	-0.571116
C	1.414455	2.194888	-0.358127
H	2.278572	2.822463	-0.560754
C	0.135213	2.840112	-0.149564
C	0.043924	4.220408	-0.384595
H	0.934706	4.745938	-0.721950
C	-1.138835	4.925620	-0.197774
C	-2.267206	4.205952	0.209350
H	-3.213980	4.729594	0.330691
C	-2.235178	2.829965	0.438101
C	-3.477715	2.140254	0.780155
H	-4.240357	2.723596	1.314895
C	-5.234677	-0.931935	0.536238
C	-4.458998	-1.744336	-0.442660
C	-4.459300	-3.132750	-0.242684
H	-4.967375	-3.537825	0.628654
N	-3.870573	-4.005603	-1.055025

C	-3.230415	-2.155707	-2.456757
H	-2.770500	-1.811009	-3.378942
C	-3.825147	-1.248954	-1.579492
H	-3.797160	-0.186054	-1.784149
C	-1.218712	6.406685	-0.442920
H	-1.552855	6.941627	0.453410
H	-0.246364	6.815003	-0.731658
H	-1.929740	6.641626	-1.243469
C	-1.002467	2.146307	0.311823
H	-2.823549	-4.247182	-2.814060
O	-0.193889	-1.545208	-1.794953
H	2.645379	-0.691688	-0.338177
O	1.221362	-1.683223	0.457030
Br	1.432451	-1.373103	2.253263
H	-0.947023	-2.185713	-1.831181

CXII

V	2.635586	1.590001	-0.752253
N	-1.826243	-1.819833	0.262189
C	-5.256398	-0.785798	1.110045
O	2.402013	1.706538	-2.287741
N	-2.911981	-1.103495	0.609016
H	-2.835344	-0.091841	0.691275
C	-5.077701	0.373685	1.870916
H	-4.088845	0.663068	2.226399
O	1.711138	0.151349	-0.154687
O	1.671772	2.811344	0.131629
Br	1.250590	4.422348	-0.591829
N	-6.071797	1.176038	2.251175
N	4.211492	0.186597	-0.803276
O	4.218890	2.569182	-0.437781
O	-4.350604	-2.872990	0.418672
C	-7.307518	0.834539	1.881121
H	-8.101197	1.510226	2.194355
N	5.472742	0.711921	-0.848660
C	-7.605930	-0.313287	1.147762
H	-8.633764	-0.548322	0.889951
C	-6.561815	-1.139456	0.761693
H	-6.722748	-2.054446	0.200189
C	-4.155374	-1.703347	0.686027
C	-0.724750	-1.178562	0.118101
H	-0.652115	-0.095258	0.265360
C	0.495048	-1.880166	-0.260725
C	0.515742	-3.257249	-0.489034
H	-0.421411	-3.795626	-0.373738
C	1.680528	-3.944261	-0.851568
C	2.852933	-3.213299	-0.984532
H	3.776984	-3.715740	-1.262009

C	2.880239	-1.822925	-0.776110
C	1.693894	-1.154089	-0.406791
C	1.646929	-5.428106	-1.091364
H	2.646616	-5.822597	-1.293708
H	1.243540	-5.961436	-0.223765
H	1.009567	-5.676472	-1.947612
C	4.112723	-1.106741	-0.881314
H	5.039463	-1.663214	-1.021750
C	5.382038	1.999676	-0.667253
C	6.573194	2.851156	-0.685301
C	7.848550	2.307103	-0.892818
H	7.956498	1.235399	-1.039463
N	8.962028	3.033173	-0.922906
C	8.839094	4.352996	-0.744703
H	9.765150	4.924093	-0.775207
C	7.622516	4.996136	-0.530738
H	7.586693	6.072059	-0.392619
C	6.464870	4.231058	-0.499394
H	5.489022	4.677093	-0.337467

Hacac

C	1.238133	0.001914	0.002873
C	2.543181	-0.750908	-0.005026
C	0.008242	-0.742651	0.003166
O	1.249421	1.251211	0.002188
H	3.373709	-0.049303	0.086160
H	2.647697	-1.314749	-0.939546
H	2.578915	-1.476288	0.815176
C	-1.194487	-0.082690	0.000338
H	0.026380	-1.825906	0.004805
C	-2.519961	-0.765381	-0.000649
O	-1.269567	1.235047	-0.001364
H	-2.413264	-1.851608	0.001849
H	-3.093358	-0.461067	-0.882992
H	-3.096390	-0.457228	0.878353
H	-0.305497	1.556167	-0.000500

$[V(=O)(acac)_2]$

C	-1.592534	-1.561392	0.286352
C	-2.344896	-2.860651	0.270854
C	4.189708	2.178943	-0.819856
C	3.481184	0.900556	-0.476251
C	4.154279	-0.323084	-0.543566
C	3.506866	-1.544806	-0.335605
C	4.242446	-2.839005	-0.531584
C	-2.397046	2.157571	-0.011465
C	-1.617898	0.884161	0.148999
C	-2.279133	-0.344181	0.243705
O	-0.347527	1.023045	0.164874

O	-0.319489	-1.671411	0.315770
O	2.251126	1.030944	-0.154555
O	2.279554	-1.663254	0.000665
O	1.225088	-0.196590	2.208608
V	1.035947	-0.286723	0.656258
H	3.659538	2.677330	-1.638122
H	5.230536	2.016856	-1.106997
H	4.151475	2.852739	0.042529
H	5.279990	-2.689059	-0.836640
H	3.723813	-3.438632	-1.286905
H	4.217228	-3.410451	0.402207
H	-3.475339	1.988311	-0.037709
H	-2.084622	2.658617	-0.933636
H	-2.155193	2.832422	0.816308
H	-2.020495	-3.455861	-0.589112
H	-3.426422	-2.717922	0.226393
H	-2.090517	-3.432743	1.169269
H	5.196822	-0.328984	-0.837014
H	-3.361621	-0.357295	0.210614

$VOCl_3$

V	0.617188	-0.904333	0.274477
O	0.551969	0.638270	0.259915
Cl	1.652093	-1.547356	-1.463031
Cl	-1.366353	-1.658510	0.281577
Cl	1.650993	-1.514370	2.024382