Electronic Supplementary Material (ESI) for Dalton Transactions
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Electronic Supporting Information

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)

$$\Delta S_1 = R \ln V^s_{m,liq}/V_{m,gas} \quad (1)$$

$$\Delta S_2 = R \ln V^\circ_m/V^s_{m,liq} \quad (2)$$

$$\alpha = \frac{S^{o,s}_{liq} - (S^{o,s}_{gas} + R \ln V^s_{m,liq}/V_{m,gas})}{(S^{o,s}_{gas} + R \ln V^s_{m,liq}/V_{m,gas})} \quad (3)$$

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

$$S_g + [(-12.21 \text{ cal/mol·K}) - 0.23(S_g - 12.21 \text{ cal/mol·K}) + 5.87 \text{ cal/mol·K}] \quad (4)$$

where S_g – gas-phase entropy of solute, ΔS_{sol} – solvation entropy, $S^{o,s}_{liq}$, $S^{o,s}_{gas}$, and $V^s_{m,liq}$ – standard entropies and molar volume of the solvent in liquid or gas phases (149.62 and 245.48 J/mol•K and 52.16 mL/mol, respectively, for CH_3CN), $V_{m,gas}$ – 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).

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Additional information on single crystal X-ray diffraction studies of complexes 1

Table S1 Hydrogen bonds data and symmetry operations.

D-H	H...A	D...A	<(DHA)	
0.79(3)	1.98(3)	2.7589(19)	171(3)	O1W-H1O...N1
0.82(3)	2.01(3)	2.8205(18)	171(3)	N3-H3N...O1_$1
0.81(3)	1.94(3)	2.731(2)	165(2)	O5-H5...O1W_$2

$1 [x, -y+1/2, z-1/2]

$2 [x, -y-1/2, z-1/2]

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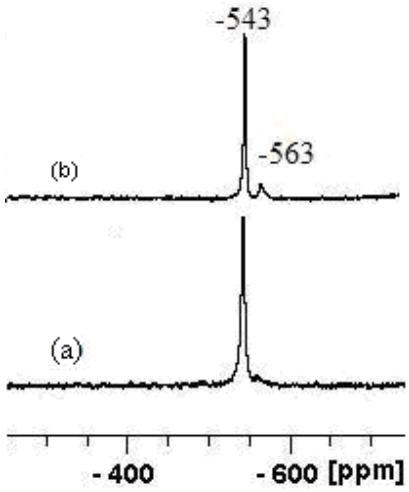

Figure S1 ^{51}V NMR spectra of ca. 4 mM solutions of (a) [$V^{V}O_2$(pydx-aebmz)] **3** and (b) [$V^{V}O(O)_2$(pydx-aebmz)] **4** prepared in DMSO.

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Studying the best catalytic conditions for higher conversion of styrene using $[V^{V}O_2(pydx\text{-}aebmz)]$-Y. Comparison with $[V^{V}O_2(pydx\text{-}ambmz)]$-Y

For three different amounts of catalyst $[V^{V}O_2(pydx\text{-}aebmz)]$-Y (viz. 0.005, 0.015, and 0.020 g) and with a H_2O_2 to styrene molar ratio of 3:1, 0.005 g gave only 30 % oxidative conversion while 0.015 g and 0.020 g have shown nearly identical results with ca. 68 % conversion in 6 h of contact time; Fig. S3. Thus, 0.015 g catalyst may be considered adequate to run the reaction under the above conditions.

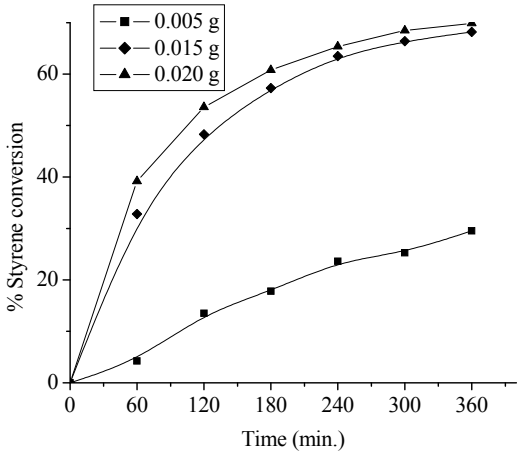

Figure S2 Effect of amount of catalyst on the convertion of styrene. Reaction conditions: styrene (0.50 g, 0.005 mol), aqueous 30 % H_2O_2 (1.70g, 0.015 mol), acetonitrile (10 mL) and catalyst precursor (0.005g, 0.0010g or 0.015 g) at ca. 75 ºC with continuous stirring. The reaction took place during 6 h counted after addition of the catalyst.

Considering these selected "optimized" reaction conditions, the catalyst precursor $[V^{V}O_2(pydx\text{-}ambmz)]$-Y was also tested under the same conditions. Thus, for 5 mmol of styrene, 15 mmol of 30 % H_2O_2 and 0.015 g of $[V^{V}O_2(pydx\text{-}ambmz)]$-Y were taken in 10 mL of CH_3CN and the reaction was carried out at 75 °C. A maximum of ca. 65 % conversion was achieved after 6 h of reaction time which is marginally less than that observed for $[V^{V}O_2(pydx\text{-}ambmz)]$-Y; Fig. S4. The turn over rate calculated for these The turn over rate calculated for these catalysts is ca. 55 h^{-1}).

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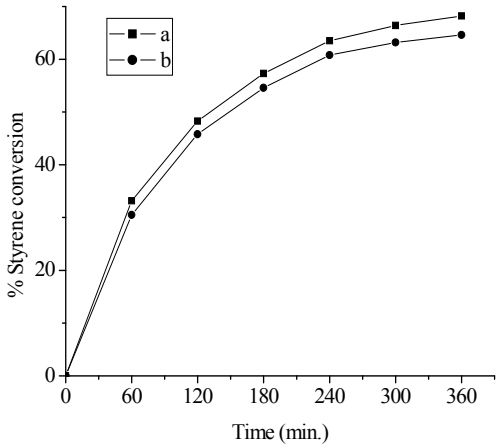

Figure S3 Effect of [$V^{V}O_2$(pydx-aebmz)]-Y (a) and [$V^{V}O_2$(pydx-ambmz)]-Y (b) on the oxidation of styrene. For reaction conditions see text.

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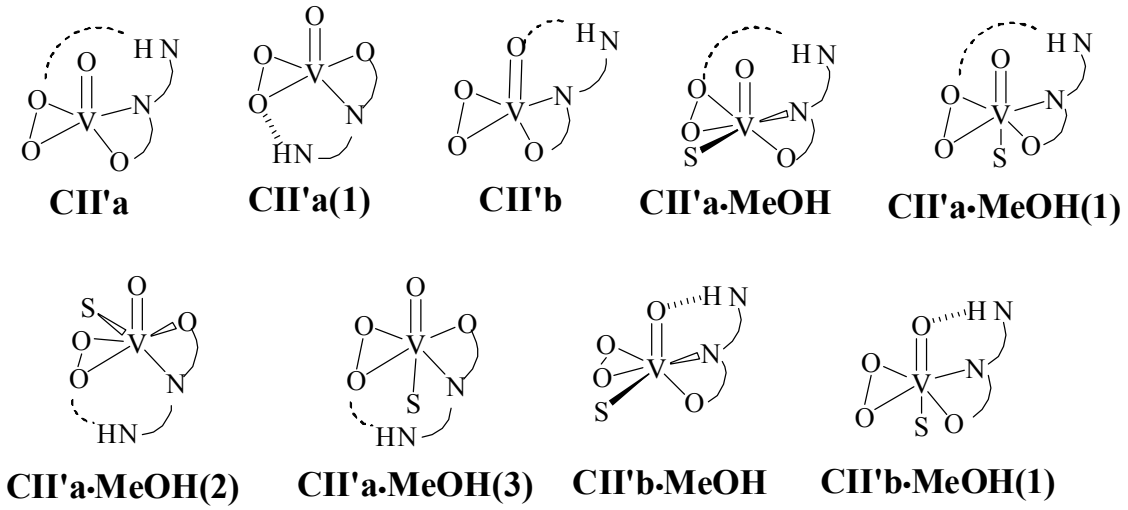

Figure S4. (1TS). Schematic structures of the calculated isomers of complexes **CII'a**, **CII'b**, **CII'·MeOH**, and **CII'b·MeOH**.

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Table S2. Total energies, enthalpies, Gibbs free energies (Hartree) and entropies (cal/mol•K) in gas-phase and CH_3CN solution.

	E_g	E_s	H_g	H_s	S_g	S_s	G_g	G_s
H_2O_2	–151.851341	–151.924440	–151.820524	–151.893623	55.72	39.37	–151.846996	–151.912329
H_2O	–76.587853	–76.639176	–76.562685	–76.614008	46.50	32.27	–76.584777	–76.629341
C_2H_4	–78.873560	–78.896307	–78.818209	–78.840956	52.32	36.75	–78.843069	–78.858417
$HOO^{\bullet}$	–151.196237	–151.258505	–151.178189	–151.240457	54.66	38.56	–151.204158	–151.258778
$HO^{\bullet}$	–75.879308	–75.919088	–75.867578	–75.907358	42.60	29.27	–75.887818	–75.921265
CH_2CH_2O	–154.218112	–154.268941	–154.156061	–154.206890	57.87	41.03	–154.183555	–154.226384
3'	–944.924368	–945.167486	–944.682899	–944.926017	130.66	97.08	–944.744979	–944.972143
3'•MeOH	–1060.981826		–1060.682005		150.42		–1060.753472	
TI	–1096.797110	–1097.099362	–1096.522553	–1096.824805	145.97	108.87	–1096.591906	–1096.876533
TIIa	–1096.786260	–1097.084967	–1096.513072	–1096.811779	141.06	105.08	–1096.580096	–1096.861708
TIIb	–1096.796521	–1097.083189	–1096.523464	–1096.810132	147.16	109.78	–1096.593383	–1096.862292
TIIc	–1096.785664	–1097.084568	–1096.512997	–1096.811901	142.37	106.09	–1096.580640	–1096.862308
TIIIb	–1096.811756	–1097.108101	–1096.537915	–1096.834260	140.82	104.90	–1096.604820	–1096.884101
TIIIa	–1096.813391	–1097.101256	–1096.539416	–1096.827281	145.26	108.32	–1096.608434	–1096.878747
4'	–1020.202888	–1020.462737	–1019.957381	–1020.217230	132.29	98.33	–1020.020234	–1020.263950
CI'a	–1061.358893		–1061.045910		150.74		–1061.117531	
CI'a•MeOH	–1177.429103		–1177.057783		167.39		–1177.137314	
CIb'	–945.315718		–945.062142		128.64		–945.123263	
CIb'•MeOH	–1061.376432		–1061.064318		148.21		–1061.134736	
CII'a	–1020.592482		–1020.333294		134.62		–1020.397258	
CII'a(1)	–1020.585832		–1020.327184		134.73		–1020.391200	
CII'a•MeOH	–1136.664111		–1136.346120		151.81		–1136.418247	
CII'a•MeOH(1)	–1136.650254		–1136.332624		152.36		–1136.405015	
CII'a•MeOH(2)	–1136.656279		–1136.338768		153.50		–1136.411700	
CII'a•MeOH(3)	–1136.640010		–1136.322608		155.33		–1136.396411	
CII'b	–1020.592676		–1020.333631		133.49		–1020.397055	
CII'b•MeOH	–1136.664502		–1136.346790		150.78		–1136.418431	
CII'b•MeOH(1)	–1136.648482		–1136.330938		151.76		–1136.403045	
TIV	–945.565002	–945.814734	–945.312663	–945.562395	132.27	98.32	–945.375507	–945.609110
TV	–1097.439569	–1097.749953	–1097.154201	–1097.464585	150.74	112.54	–1097.225821	–1097.518056
TVI	–1020.826044	–1021.099698	–1020.568797	–1020.842451	142.40	106.12	–1020.636456	–1020.892872
TS1	–1173.399306	–1173.735219	–1173.103965	–1173.439878	147.28	109.87	–1173.173941	–1173.492081
TS2	–1173.404498	–1173.727761	–1173.108845	–1173.432108	151.18	112.88	–1173.180676	–1173.485741
TS3	–1173.403287	–1173.736160	–1173.105940	–1173.438813	143.99	107.34	–1173.174352	–1173.489814
TS4	–1099.039682	–1099.317468	–1098.738477	–1099.016263	150.03	111.99	–1098.809760	–1099.069473
TS5	–1174.040241	–1174.384349	–1173.733615	–1174.077723	155.45	116.16	–1173.807476	–1174.132914
TS6	–1020.800259	–1021.076198	–1020.546014	–1020.821953	143.95	107.31	–1020.614410	–1020.872939

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Table S3. Cartesian atomic coordinates (Å) of the calculated equilibrium structures.

	1'		
V	1.250314	-0.545497	0.253892
O	2.372716	-1.595930	0.615506
O	1.185113	-0.548838	-1.683250
O	2.251820	1.146080	0.146638
O	-0.523199	0.767742	0.075720
N	0.854592	-0.093618	2.308151
N	-0.310066	-1.961757	0.289430
N	-0.105452	-0.005889	4.265975
H	-0.767073	-0.179432	5.007415
C	1.932026	2.291554	-0.327191
C	1.602115	0.722886	3.119970
C	1.015068	0.791934	4.349528
C	-0.172026	-0.524998	3.015955
C	-1.238636	-1.442040	2.528694
H	-2.017275	-0.866317	2.012808
H	-1.708795	-1.939935	3.385041
C	-0.700805	-2.516045	1.574290
H	0.178294	-2.996380	2.018742
H	-1.475672	-3.282598	1.436755
C	-0.916630	-2.401901	-0.760622
H	-1.703426	-3.154315	-0.621470
C	-0.667602	-2.025479	-2.121682
C	-1.472085	-2.585080	-3.135135
H	-2.269470	-3.275718	-2.867707
C	-1.248538	-2.257354	-4.453329
H	-1.860344	-2.674115	-5.249226
N	-0.266556	-1.413093	-4.832972
C	0.499985	-0.886380	-3.900584
H	1.292560	-0.209723	-4.216386
C	0.371005	-1.132224	-2.501224
C	-0.520933	1.949878	-0.368621
H	1.285613	1.313039	5.254034
H	2.500744	1.192098	2.751267
C	-1.872510	2.563973	-0.648455
C	0.636084	2.720187	-0.607351
C	3.093404	3.220143	-0.562864
H	2.777474	4.208017	-0.905417
H	3.759336	2.776204	-1.310764
H	3.675413	3.325891	0.358876
H	-2.387280	1.965213	-1.407649
H	-1.806362	3.597383	-0.996548
H	-2.484968	2.529540	0.258978
H	0.509344	3.723833	-0.996144

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		3'	
V	0.194955	1.410264	0.212283
N	-1.872500	0.976311	0.539425
N	0.331754	-0.875107	0.500845
N	-3.892871	0.177100	0.327900
H	-4.641832	-0.473541	0.142888
O	0.160141	1.486855	-1.374097
O	-0.115266	2.844401	0.839291
O	2.013834	1.288467	0.702458
C	-2.769703	1.973585	0.854571
C	-4.036592	1.489840	0.727155
C	-2.575337	-0.098251	0.219165
C	-1.993544	-1.414802	-0.141210
H	-1.658147	-1.412656	-1.186083
H	-2.752431	-2.198642	-0.039790
C	-0.809268	-1.737346	0.770972
H	-1.112236	-1.598201	1.816085
H	-0.533525	-2.793257	0.643846
C	1.436561	-1.488633	0.232295
H	1.426438	-2.585913	0.188905
C	2.721088	-0.887403	0.013024
C	3.811562	-1.681763	-0.386400
H	3.665765	-2.738723	-0.598364
C	5.059234	-1.107024	-0.506688
H	5.917444	-1.692131	-0.826956
N	5.293239	0.190732	-0.231597
C	4.282056	0.943939	0.158768
H	4.481617	1.989450	0.385212
C	2.948729	0.478025	0.290476
H	-5.002922	1.943469	0.878581
H	-2.411213	2.952425	1.131880
		4'	
V	0.004028	1.219684	0.369574
N	1.605024	0.233104	-0.594951
N	-0.920371	-0.985962	0.063789
N	3.189211	-1.196389	-1.039095
H	3.725519	-2.051304	-1.032657
O	0.688809	0.531018	1.906652
O	0.713814	2.580673	0.021763
O	-1.678994	1.624897	-0.319345
C	2.543041	0.859113	-1.385388
C	3.538492	-0.023877	-1.676330
C	2.021533	-1.007760	-0.387278
C	1.298066	-2.033169	0.406211

H	1.272705	-1.726897	1.457204
H	1.818294	-2.994574	0.335935
C	-0.132790	-2.197859	-0.103606
H	-0.101960	-2.439894	-1.175079
H	-0.605554	-3.047227	0.409584
C	-2.170527	-1.163048	0.299907
H	-2.553541	-2.184871	0.435603
C	-3.172561	-0.125027	0.355284
C	-4.499934	-0.453343	0.668785
H	-4.758195	-1.474821	0.938795
C	-5.472231	0.529070	0.627465
H	-6.505766	0.301038	0.876346
N	-5.211773	1.799082	0.277523
C	-3.963581	2.118966	-0.026176
H	-3.757713	3.149098	-0.309910
C	-2.883838	1.209689	0.004161
H	4.442819	0.070718	-2.255739
H	2.428293	1.896963	-1.655428
O	-0.539328	1.235668	2.078180

3'·MeOH

V	1.130216	0.815633	1.463694
N	-0.944346	0.769305	2.031250
N	0.268518	0.174277	-0.483007
N	-3.117740	0.930464	2.151996
H	-4.086418	0.927361	1.869782
O	1.177104	2.396044	1.374474
O	1.464090	0.330834	2.967514
O	2.743994	0.319566	0.608351
C	-1.290222	1.020252	3.340361
C	-2.645434	1.124804	3.432159
C	-2.063467	0.721452	1.330912
C	-2.160409	0.454674	-0.127288
H	-2.125348	1.395190	-0.693407
H	-3.122338	-0.021005	-0.352014
C	-1.033768	-0.464790	-0.593573
H	-1.002819	-1.361932	0.033765
H	-1.224761	-0.767624	-1.631970
C	0.913675	0.371766	-1.582223
H	0.418078	0.131120	-2.531557
C	2.276278	0.819338	-1.683604
C	2.814778	1.211225	-2.921439
H	2.174053	1.278134	-3.797813
C	4.158017	1.514130	-3.008070
H	4.598956	1.840476	-3.946497
N	4.996635	1.415670	-1.959427

C	4.508111	1.024318	-0.796604
H	5.195977	0.940392	0.042493
C	3.141672	0.723828	-0.570189
H	-3.301869	1.308169	4.267640
H	-0.527210	1.098869	4.098577
O	0.629443	-1.967767	1.786331
C	1.696910	-2.808157	1.381965
H	0.951163	-1.403800	2.523172
H	1.377491	-3.329053	0.474936
H	1.931376	-3.562604	2.145298
H	2.601410	-2.230338	1.156237

CI'a

V	1.162881	1.421871	-0.302772
N	-2.094881	-2.924241	-0.436100
N	0.764203	-0.392969	1.068837
N	-0.829482	-1.551942	-1.494038
H	-0.309307	-0.650491	-1.681183
O	0.222070	0.856842	-1.495749
O	1.440667	2.955248	-0.567460
O	2.857489	0.762622	-0.334809
C	-1.720433	-3.557495	-1.602525
C	-0.917547	-2.682296	-2.267764
C	-1.548533	-1.697082	-0.382314
C	-1.695279	-0.677859	0.690949
H	-2.620707	-0.864901	1.245684
H	-1.796465	0.300283	0.214430
C	-0.530416	-0.628762	1.701419
H	-0.751795	0.186300	2.394164
H	-0.506693	-1.561161	2.281184
C	1.615491	-1.363457	1.179724
H	1.324171	-2.246179	1.762223
C	2.925719	-1.440016	0.596432
C	3.696350	-2.605211	0.768906
H	3.312476	-3.433575	1.359025
C	4.943377	-2.681052	0.179237
H	5.561809	-3.567058	0.291109
N	5.463432	-1.683175	-0.555270
C	4.758602	-0.577111	-0.717247
H	5.195635	0.226664	-1.305452
C	3.474803	-0.389892	-0.163761
H	-0.414823	-2.769667	-3.217933
H	-2.056833	-4.550589	-1.854330
O	-0.314446	2.165363	1.077955
H	-0.707850	2.855141	0.513592
C	0.261470	2.841636	2.227065

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H	0.759346	2.074663	2.821452
H	-0.542085	3.297885	2.808528
H	0.983319	3.592048	1.897195
H	-2.717106	-3.308772	0.262856

CI'a·MeOH

V	-0.596159	-0.518774	2.566595
N	-1.110786	2.599022	-1.926587
N	-0.302586	-0.759372	0.234814
N	-0.510655	2.380027	0.123312
H	-0.483952	1.957580	1.101002
O	-0.763643	1.084303	2.381364
O	-0.999549	-0.875814	4.059885
O	1.190954	-0.930251	2.602435
C	-0.219089	3.619136	-1.669237
C	0.157641	3.472841	-0.369202
C	-1.284876	1.851588	-0.822370
C	-2.154240	0.657607	-0.652836
H	-2.932916	0.657845	-1.422559
H	-2.652865	0.738675	0.315641
C	-1.406954	-0.692576	-0.711948
H	-2.139720	-1.466334	-0.470295
H	-1.049968	-0.872425	-1.735516
C	0.876470	-0.782366	-0.292802
H	0.962246	-0.796143	-1.387610
C	2.137194	-0.766563	0.402762
C	3.330055	-0.699157	-0.340749
H	3.294859	-0.679492	-1.427372
C	4.541289	-0.655620	0.322454
H	5.477870	-0.600475	-0.225232
N	4.636399	-0.679292	1.662331
C	3.526346	-0.755296	2.375432
H	3.617298	-0.780243	3.459269
C	2.234225	-0.804536	1.807992
H	0.833903	4.053994	0.237492
H	0.056648	4.347080	-2.415386
O	-2.558361	-1.052823	1.941654
C	-3.644007	-0.598818	2.783465
H	-3.463247	-0.886666	3.820881
H	-4.579280	-1.019442	2.407246
H	-3.660634	0.488144	2.711720
H	-1.590879	2.449888	-2.804303
O	-0.921181	-2.988722	2.447012
H	-2.448642	-2.024327	2.043767
C	-0.040652	-3.956676	1.862616
H	-0.807894	-2.980161	3.414318

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H	-0.171598	-3.889464	0.782500
H	-0.305609	-4.963485	2.196845
H	0.998372	-3.733904	2.119276

CI'b

V	0.033831	1.207860	0.664487
N	-0.892537	1.259157	-1.204781
N	-0.116460	-0.946103	0.329194
N	-1.856561	0.841359	-3.116024
H	-2.307812	0.330780	-3.863898
O	0.188464	2.952999	0.513569
O	-0.939249	1.010084	1.857804
O	1.724851	0.821858	1.044929
C	-0.987162	2.444113	-1.924717
C	-1.584908	2.190049	-3.116776
C	-1.430842	0.297644	-1.963709
C	-1.537734	-1.153713	-1.657251
H	-0.767447	-1.703037	-2.215354
H	-2.508125	-1.530726	-1.999936
C	-1.392618	-1.442060	-0.171256
H	-2.189160	-0.945882	0.394183
H	-1.481519	-2.520884	-0.000722
C	0.726653	-1.816049	0.772502
H	0.459883	-2.876183	0.713400
C	1.999570	-1.519274	1.377257
C	2.827318	-2.544561	1.856592
H	2.524023	-3.584327	1.772010
C	4.036524	-2.205681	2.443817
H	4.700916	-2.972937	2.830734
N	4.456791	-0.939886	2.572077
C	3.687704	0.040710	2.121364
H	4.046179	1.061585	2.228628
C	2.445431	-0.196255	1.516600
H	-1.839755	2.833546	-3.943858
H	-0.605313	3.368108	-1.525021
H	-0.294684	3.514158	1.143176

CI'b·MeOH

V	0.984250	0.669682	1.560277
N	1.797909	0.272116	-0.345525
N	-0.878034	0.652109	0.461846
N	2.198238	0.012609	-2.473804
H	2.042737	-0.042009	-3.471412
O	2.520277	0.129647	2.265087
O	1.156256	2.212009	1.488001
O	-0.110578	0.452568	2.990487

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C	3.147831	0.015368	-0.514540
C	3.406561	-0.149999	-1.839669
C	1.244863	0.265295	-1.555503
C	-0.186280	0.483464	-1.892808
H	-0.695155	-0.483207	-2.005263
H	-0.260555	0.997431	-2.857727
C	-0.904345	1.315659	-0.838302
H	-0.419890	2.290504	-0.725192
H	-1.938774	1.486418	-1.156586
C	-1.994358	0.183633	0.906634
H	-2.881154	0.256570	0.268952
C	-2.200467	-0.383029	2.215108
C	-3.401555	-1.026398	2.553115
H	-4.173345	-1.180640	1.804059
C	-3.582744	-1.463548	3.854262
H	-4.492095	-1.980024	4.147506
N	-2.671538	-1.272834	4.820818
C	-1.545865	-0.642300	4.527291
H	-0.828299	-0.478730	5.328035
C	-1.243646	-0.183188	3.230398
H	4.320294	-0.357646	-2.373626
H	3.815514	-0.038348	0.328529
H	3.094375	0.842758	2.591467
O	0.654916	-1.681417	1.362781
H	0.016445	-1.956064	2.038980
C	1.740694	-2.621987	1.385694
H	2.307885	-2.542952	2.316288
H	2.388572	-2.373876	0.546030
H	1.354672	-3.636594	1.253989

CII'a

V	0.629649	0.879069	2.343651
N	-2.871600	1.035298	1.046602
N	0.919308	0.711003	0.308893
N	-3.593417	2.357818	-0.476604
H	-3.612729	2.983271	-1.271946
O	0.271984	2.407586	2.302496
O	-0.514232	0.037837	3.420836
O	2.366246	0.552393	2.593500
C	-4.224999	1.166977	1.249245
C	-4.688019	2.007748	0.286164
C	-2.487946	1.762339	-0.003071
C	-1.098329	1.939100	-0.511401
H	-0.591281	2.664153	0.139190
H	-1.151049	2.390907	-1.506295
C	-0.249896	0.640546	-0.568609

H	-0.835434	-0.233872	-0.270278
H	0.080662	0.464572	-1.597352
C	2.095538	0.725226	-0.236180
H	2.147572	0.689394	-1.327861
C	3.360177	0.774896	0.444546
C	4.554573	0.875911	-0.291189
H	4.530251	0.936421	-1.375606
C	5.758595	0.901902	0.389233
H	6.699463	0.987268	-0.146433
N	5.843307	0.821148	1.726064
C	4.731885	0.713673	2.436234
H	4.820986	0.641141	3.517453
C	3.457682	0.691067	1.847850
H	-5.679488	2.376323	0.076789
H	-4.737676	0.657177	2.049431
O	-0.764955	-0.305817	2.064963
H	-2.191436	0.467786	1.602484

CII'a(1)

V	1.021082	1.255834	2.056166
N	-1.373588	-1.630340	1.944311
N	-0.346247	1.205342	0.517323
N	-2.499240	-2.612304	0.406710
H	-3.081154	-2.762020	-0.407854
O	1.224693	2.798970	2.126095
O	0.952775	0.532603	3.682027
O	2.214802	0.511946	0.927913
C	-1.307211	-2.979498	2.204061
C	-2.021585	-3.606985	1.232490
C	-2.099753	-1.407541	0.850421
C	-2.478498	-0.105466	0.219354
H	-3.560046	0.034019	0.351100
H	-2.313093	-0.189996	-0.862196
C	-1.794779	1.162129	0.749350
H	-2.265376	2.017361	0.252162
H	-1.970207	1.281805	1.820270
C	0.068198	1.430888	-0.693493
H	-0.682262	1.630359	-1.465148
C	1.431782	1.401944	-1.140113
C	1.758876	1.766670	-2.460292
H	0.996792	2.158453	-3.128175
C	3.065686	1.626942	-2.887068
H	3.357585	1.914043	-3.892921
N	4.040377	1.129251	-2.107401
C	3.752505	0.766326	-0.869340
H	4.553810	0.362107	-0.255303

C	2.466115	0.899444	-0.318465
H	-2.226894	-4.651157	1.057753
H	-0.762153	-3.372367	3.047825
O	-0.342489	0.524725	3.092438
H	-0.903285	-0.865657	2.501790

CII'a·MeOH

V	0.447895	-1.796741	0.368006
N	-2.913032	-0.743623	-0.501625
N	0.757140	-0.807696	-1.506497
N	-3.565026	1.274768	-0.804375
H	-3.560617	2.254676	-1.055820
O	-0.047554	-0.444579	1.008239
O	-0.777836	-3.092239	0.656215
O	2.269072	-2.133410	0.304419
C	-4.219083	-0.683901	-0.076621
C	-4.638015	0.595698	-0.264929
C	-2.515020	0.448981	-0.940541
C	-1.161106	0.818027	-1.439061
H	-0.552009	1.113162	-0.575757
H	-1.263312	1.700243	-2.078824
C	-0.422601	-0.301369	-2.213317
H	-1.082888	-1.149262	-2.415654
H	-0.115070	0.090629	-3.188375
C	1.892476	-0.631672	-2.099643
H	1.895124	-0.105124	-3.059084
C	3.176237	-1.067347	-1.632882
C	4.336677	-0.776642	-2.371508
H	4.270875	-0.210308	-3.296658
C	5.558123	-1.221461	-1.902115
H	6.475890	-1.011736	-2.443653
N	5.685876	-1.931012	-0.769049
C	4.602226	-2.214754	-0.067610
H	4.727508	-2.800153	0.841167
C	3.308449	-1.806087	-0.445514
H	-5.586368	1.072137	-0.074804
H	-4.734974	-1.546352	0.314225
O	-0.920088	-2.537290	-0.632058
H	-2.263647	-1.567477	-0.485616
O	0.951364	-2.522934	2.326919
H	1.911679	-2.397446	2.398083
C	0.273656	-2.075559	3.510091
H	0.700395	-2.583100	4.378154
H	-0.768741	-2.368042	3.394693
H	0.348694	-0.989915	3.614440

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CII'a·MeOH(1)			
V	0.250592	0.771414	2.263352
N	-2.996047	1.161118	0.851389
N	0.697542	0.690921	0.258450
N	-3.601200	2.720600	-0.487775
H	-3.570195	3.425983	-1.212442
O	-0.416638	2.190765	2.205614
O	-0.926438	-0.196277	3.232030
O	1.981242	1.108316	2.647129
C	-4.312829	1.435778	1.134164
C	-4.702471	2.425738	0.287880
C	-2.561868	1.948148	-0.131325
C	-1.188735	2.025334	-0.709528
H	-0.624247	2.776702	-0.143357
H	-1.278148	2.399517	-1.734498
C	-0.388467	0.700677	-0.720716
H	-1.038140	-0.155952	-0.515838
H	0.031349	0.547331	-1.720259
C	1.913335	0.573894	-0.171380
H	2.059336	0.468276	-1.250313
C	3.115619	0.588362	0.616445
C	4.358219	0.378129	-0.005906
H	4.410666	0.167380	-1.070532
C	5.511884	0.437642	0.755516
H	6.486240	0.269244	0.306286
N	5.502428	0.708324	2.069443
C	4.343436	0.925357	2.670636
H	4.356949	1.156264	3.733518
C	3.108782	0.867962	2.000164
H	-5.646723	2.931839	0.166457
H	-4.854337	0.910032	1.904281
O	-1.100364	-0.467022	1.848356
H	-2.372704	0.475517	1.347014
O	1.281254	-1.488184	2.171912
C	1.908565	-2.093552	3.306034
H	0.424411	-1.920172	2.024499
H	2.870980	-1.598784	3.440488
H	2.083326	-3.158402	3.124630
H	1.302994	-1.964877	4.209272
CII'a·MeOH(2)			
V	0.241685	-2.277671	1.376401
N	-1.825192	-0.309348	-1.213242
N	0.482322	-0.173722	1.051299
N	-1.828589	1.621496	-2.144792

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H	-1.728157	2.619261	-2.280707
O	0.420306	-2.053884	2.914216
O	-1.236657	-3.243542	0.978688
O	1.661380	-2.385350	0.186129
C	-2.274002	-0.489732	-2.500596
C	-2.279378	0.732202	-3.096177
C	-1.556452	0.976376	-0.996275
C	-1.080478	1.641698	0.255212
H	-1.894017	2.269951	0.642313
H	-0.272449	2.331477	-0.019558
C	-0.626722	0.725092	1.400052
H	-0.325469	1.367725	2.234652
H	-1.457586	0.113986	1.754056
C	1.621583	0.380779	0.792295
H	1.704529	1.470252	0.876354
C	2.806713	-0.301715	0.359723
C	4.011447	0.395198	0.161132
H	4.082979	1.451565	0.406799
C	5.101155	-0.286329	-0.347248
H	6.052840	0.214411	-0.499653
N	5.053364	-1.585584	-0.686043
C	3.925395	-2.251997	-0.510223
H	3.908160	-3.301714	-0.795873
C	2.761991	-1.671031	0.031475
H	-2.556234	1.041470	-4.091404
H	-2.547267	-1.461842	-2.879080
O	-1.499972	-1.861048	0.891015
H	-1.698632	-1.065737	-0.484727
O	0.984174	-4.257577	1.701670
H	1.147893	-4.700605	0.854397
C	0.340120	-5.153839	2.628148
H	-0.645627	-5.451555	2.263786
H	0.242741	-4.598055	3.559072
H	0.981776	-6.024660	2.779423

CII'a·MeOH(3)

V	1.168176	1.010506	1.307060
N	-1.078561	-1.982885	1.161561
N	0.225065	0.696337	-0.508657
N	-1.767856	-3.323547	-0.363375
H	-2.110346	-3.669686	-1.250350
O	1.245264	2.555308	1.131661
O	0.556077	0.781965	2.983800
O	2.763051	0.509928	0.483588
C	-1.119551	-3.236195	1.723021
C	-1.559569	-4.090950	0.762076

C	-1.471125	-2.036460	-0.107320
C	-1.624739	-0.922210	-1.090409
H	-2.684352	-0.875212	-1.375104
H	-1.074751	-1.182779	-2.003971
C	-1.221399	0.484531	-0.629708
H	-1.621918	1.187650	-1.367769
H	-1.683277	0.735598	0.327640
C	0.863285	1.002690	-1.598575
H	0.282528	1.079664	-2.523499
C	2.269123	1.245217	-1.732289
C	2.791693	1.687650	-2.963760
H	2.126763	1.911431	-3.793426
C	4.156981	1.843209	-3.095922
H	4.592294	2.196711	-4.025885
N	5.021507	1.567120	-2.103770
C	4.552817	1.136746	-0.946323
H	5.269378	0.918143	-0.157485
C	3.178356	0.970172	-0.685531
H	-1.740072	-5.153921	0.778000
H	-0.836148	-3.412035	2.747976
O	-0.448536	0.455977	2.046817
H	-0.739455	-1.102845	1.634468
O	1.781157	-1.360807	1.871075
C	2.126174	-1.745755	3.205811
H	2.581529	-1.377207	1.323561
H	1.261300	-1.530292	3.832777
H	2.976176	-1.167475	3.581943
H	2.362777	-2.814263	3.247021

CII'b

V	-1.379650	1.118622	0.844794
N	-1.302633	-3.695659	-1.506337
N	-0.632632	-0.717735	1.433372
N	-0.852515	-1.613517	-1.737017
H	-0.862756	-0.589393	-1.535280
O	-1.139720	0.846852	-0.712764
O	-2.963292	1.843254	1.119680
O	0.018688	1.915302	1.625516
C	-0.513024	-3.590309	-2.631419
C	-0.228929	-2.267177	-2.772304
C	-1.509416	-2.482749	-0.967302
C	-2.319152	-2.160156	0.238280
H	-2.990537	-2.999129	0.448653
H	-2.958064	-1.298146	0.022087
C	-1.516205	-1.879080	1.522092
H	-2.244736	-1.680821	2.314982

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H	-0.933666	-2.761176	1.813267
C	0.613932	-0.873053	1.757102
H	0.951861	-1.882645	2.008013
C	1.610707	0.157561	1.855791
C	2.956043	-0.180571	2.092815
H	3.258094	-1.221990	2.160751
C	3.885531	0.832748	2.235836
H	4.933808	0.607596	2.408908
N	3.560919	2.134507	2.180290
C	2.298925	2.474354	1.978199
H	2.052282	3.532990	1.949204
C	1.277144	1.526507	1.798741
H	0.350558	-1.744903	-3.517040
H	-0.234503	-4.446626	-3.224782
O	-2.904443	0.524607	1.617408
H	-1.701490	-4.555926	-1.152308

CII'b·MeOH

V	0.150099	-2.261817	1.828325
N	0.602358	1.424215	-2.146278
N	-0.183019	-0.135826	1.705496
N	-0.285489	-0.429409	-1.538025
H	-0.412487	-1.294279	-0.958989
O	-0.099674	-2.366510	0.241120
O	1.690524	-3.029388	2.317489
O	-1.238552	-2.226193	3.014054
C	-0.382433	1.141534	-3.069693
C	-0.942547	-0.035141	-2.678193
C	0.657081	0.455756	-1.216730
C	1.566421	0.368340	-0.044685
H	2.416902	1.040162	-0.199329
H	1.968590	-0.646665	0.022943
C	0.916421	0.737559	1.300178
H	1.698822	0.658584	2.061683
H	0.573719	1.779784	1.280779
C	-1.288757	0.443727	2.043033
H	-1.367309	1.527994	1.911719
C	-2.431516	-0.196372	2.631410
C	-3.631278	0.510063	2.825737
H	-3.728809	1.534414	2.475897
C	-4.681037	-0.118496	3.468371
H	-5.627294	0.391624	3.623793
N	-4.598882	-1.373041	3.942093
C	-3.470731	-2.043078	3.784081
H	-3.419199	-3.052622	4.185596
C	-2.345944	-1.512441	3.122459

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H	-1.738986	-0.616113	-3.115307
H	-0.589194	1.785321	-3.909657
O	1.791130	-1.634118	2.244867
H	1.217272	2.227276	-2.174550
O	-0.423374	-4.349782	1.840497
H	-0.010807	-4.749182	1.058413
C	-0.207405	-5.189405	2.990043
H	-0.672310	-6.161691	2.811607
H	-0.703418	-4.693297	3.822710
H	0.858819	-5.300625	3.201284

CII'b·MeOH(1)

V	-1.044225	-1.761032	2.950225
N	-2.941413	2.483877	0.238034
N	-1.241540	-1.282141	0.945321
N	-1.615181	1.766571	1.761623
H	-1.179915	1.110730	2.452213
O	-0.721069	-0.238160	3.314726
O	-2.244629	-2.263161	4.162577
O	0.676880	-2.365148	2.634870
C	-2.095635	3.529486	0.541371
C	-1.255198	3.067946	1.506415
C	-2.645175	1.411026	0.990616
C	-3.335306	0.094579	0.994156
H	-4.291343	0.189628	0.469398
H	-3.561731	-0.181633	2.029086
C	-2.551048	-1.065218	0.342125
H	-3.146321	-1.972196	0.479043
H	-2.436291	-0.891849	-0.734606
C	-0.192063	-1.075087	0.212004
H	-0.353448	-0.750170	-0.820551
C	1.182323	-1.224715	0.600437
C	2.200934	-0.783142	-0.267524
H	1.948322	-0.310816	-1.213115
C	3.520506	-0.953324	0.099736
H	4.328399	-0.614973	-0.542405
N	3.885158	-1.544600	1.251064
C	2.947024	-1.986986	2.068066
H	3.261635	-2.471714	2.989736
C	1.567103	-1.854625	1.806361
H	-0.447060	3.553400	2.030224
H	-2.169190	4.491333	0.059493
O	-2.846984	-2.060139	2.910936
H	-3.701482	2.522097	-0.428931
O	-1.152150	-4.054561	2.395774
H	-0.252206	-4.401890	2.484002

C	-2.095206	-4.998905	2.913866
H	-2.038638	-5.933777	2.348670
H	-3.078683	-4.549911	2.785797
H	-1.923811	-5.187711	3.977729

H_2O

O	-0.045055	0.109067	0.000000
H	0.885122	-0.151706	0.000000
H	-0.520021	-0.732145	0.000000

H_2O_2

O	0.046716	-0.040072	-0.284198
O	1.367259	0.128344	0.264492
H	-0.416616	0.684698	0.166547
H	1.862641	0.327030	-0.546840

$HOO^{\bullet}$

O	0.208833	0.134805	0.000000
O	1.506331	-0.108877	0.000000
H	1.934835	0.774072	0.000000

$HO^{\bullet}$

O	0.010217	0.000000	0.000000
H	0.989783	0.000000	0.000000

C_2H_4

C	0.045569	0.000000	0.000000
C	1.374431	0.000000	0.000000
H	-0.527411	0.923720	0.000000
H	-0.527411	-0.923720	0.000000
H	1.947411	0.923720	0.000000
H	1.947411	-0.923720	0.000000

CH_2CH_2O

O	0.000000	-0.027702	0.000000
C	-0.731948	-1.246731	0.000000
C	0.731948	-1.246731	0.000000
H	-1.270380	-1.469709	0.920875
H	-1.270380	-1.469709	-0.920875
H	1.270380	-1.469709	0.920875
H	1.270380	-1.469709	-0.920875

TI

V	1.568607	0.745932	0.103234
N	1.421263	0.495666	2.246940

N	-0.642813	0.188187	0.221825
N	0.801442	0.729876	4.327271
H	0.204158	0.841906	5.133237
O	1.322628	2.309706	0.171133
O	3.157807	0.459618	0.237681
O	1.327959	0.331518	-1.706108
C	2.549645	0.513970	3.038800
C	2.177919	0.657367	4.341985
C	0.376550	0.636792	3.047110
C	-1.043043	0.678149	2.610997
H	-1.315272	1.699602	2.315126
H	-1.694389	0.394963	3.445852
C	-1.296740	-0.267363	1.435848
H	-0.916054	-1.266638	1.680934
H	-2.380744	-0.359580	1.281222
C	-1.410559	0.384270	-0.794685
H	-2.492488	0.242506	-0.669863
C	-0.992673	0.741914	-2.123545
C	-1.953716	1.071817	-3.095620
H	-3.005601	1.124960	-2.823684
C	-1.550064	1.328473	-4.389680
H	-2.269931	1.600660	-5.157305
N	-0.264315	1.250318	-4.780321
C	0.646719	0.923824	-3.881897
H	1.682563	0.854133	-4.207743
C	0.361214	0.668154	-2.517609
H	2.748801	0.714907	5.254953
H	3.527718	0.444885	2.588143
O	1.571154	-1.789780	0.424067
O	2.886905	-2.167540	-0.020300
H	3.277012	-1.254115	-0.093645
H	1.666686	-1.874808	1.387919

TIIa

V	1.072714	0.405686	0.290557
N	0.483220	0.603038	2.358607
N	-1.084614	0.072784	-0.061884
N	-0.616331	0.790036	4.233063
H	-1.388641	0.806990	4.882117
O	0.775789	1.949306	0.059683
O	2.763713	0.370988	0.835492
O	1.190345	-0.100684	-1.507122
C	1.381284	0.870120	3.365619
C	0.709066	0.989150	4.545423
C	-0.720388	0.563115	2.901581
C	-2.017423	0.355198	2.200381
H	-2.438730	1.326903	1.908286

H	-2.731032	-0.105160	2.894165
C	-1.903912	-0.536925	0.965656
H	-1.422652	-1.485710	1.220329
H	-2.912342	-0.742885	0.581888
C	-1.614347	0.338463	-1.197427
H	-2.691863	0.184559	-1.336721
C	-0.869897	0.764249	-2.366370
C	-1.522322	1.325556	-3.472182
H	-2.588059	1.536307	-3.428364
C	-0.794940	1.615058	-4.613344
H	-1.272739	2.070377	-5.477282
N	0.514505	1.348713	-4.731658
C	1.137002	0.793247	-3.702422
H	2.196661	0.571342	-3.810595
C	0.509111	0.487967	-2.479496
H	1.043313	1.183767	5.551898
H	2.434085	0.958189	3.149426
O	0.967010	-1.508328	0.736575
O	0.367033	-2.394146	-0.213764
H	0.690774	-2.002031	-1.048367
H	2.955781	-0.579796	0.953138

TIIb

V	2.643498	-0.290442	-0.262233
N	-2.609103	1.531442	0.885267
N	0.556426	-0.464190	-0.745183
N	-0.516643	1.369081	1.594693
H	0.430153	1.012649	1.698952
O	2.289838	0.401197	1.108112
O	4.445589	-0.467400	-0.226096
O	2.691653	0.784459	-1.744069
C	-2.204887	2.736138	1.401875
C	-0.908426	2.662726	1.838636
C	-1.572571	0.727999	1.015072
C	-1.572661	-0.714746	0.619404
H	-2.319485	-0.835206	-0.171869
H	-1.929161	-1.340140	1.449574
C	-0.204538	-1.272093	0.225863
H	0.426162	-1.365785	1.110610
H	-0.302932	-2.285934	-0.176338
C	-0.090033	0.131646	-1.685042
H	-1.173089	0.006013	-1.749918
C	0.500463	1.002132	-2.669217
C	-0.287922	1.602505	-3.662264
H	-1.354353	1.398563	-3.708489
C	0.309047	2.457778	-4.570449

H	-0.274744	2.936992	-5.351705
N	1.618948	2.751337	-4.544293
C	2.371274	2.198402	-3.606341
H	3.430282	2.447488	-3.591029
C	1.870823	1.306967	-2.637642
H	-0.241168	3.386182	2.281762
H	-2.869355	3.588968	1.426416
O	2.396147	-2.087857	-0.190126
O	3.214375	-2.573307	0.868013
H	4.076722	-2.144576	0.652246
H	4.857401	-0.605290	-1.094643

TIIc

V	1.497429	-0.241408	-0.017509
N	1.388279	0.069452	2.179373
N	-0.665707	-0.391700	0.170767
N	0.742574	0.459018	4.229600
H	0.137749	0.568163	5.029724
O	1.491702	1.376256	-0.051918
O	3.296912	-0.299971	0.108480
O	1.158151	-0.551704	-1.809384
C	2.496038	0.379255	2.933829
C	2.108926	0.624721	4.218829
C	0.339657	0.128084	2.976517
C	-1.083164	-0.082711	2.589391
H	-1.563074	0.886184	2.393362
H	-1.625537	-0.540760	3.425763
C	-1.246399	-0.980732	1.363540
H	-0.728174	-1.931934	1.520862
H	-2.315698	-1.179867	1.212269
C	-1.451410	-0.028997	-0.779708
H	-2.536047	-0.097919	-0.629068
C	-1.014525	0.404879	-2.084885
C	-1.906364	1.021366	-2.976517
H	-2.915373	1.268400	-2.655017
C	-1.486103	1.316197	-4.259050
H	-2.148415	1.813629	-4.963036
N	-0.260723	1.004326	-4.715556
C	0.580622	0.397885	-3.895687
H	1.565528	0.137435	-4.277636
C	0.279947	0.081187	-2.551284
H	2.665561	0.887488	5.104396
H	3.477324	0.421599	2.485644
O	1.535542	-2.037407	0.491413
H	2.129641	-2.340528	1.190424
O	4.041487	0.895469	0.110785

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H	3.324453	1.552854	-0.063815

TIIIa

V	2.398737	-0.534173	-0.048540
N	-1.553199	3.503493	0.543189
N	0.343792	-0.128092	0.120926
N	0.588358	2.950979	0.690975
H	1.418919	2.369892	0.802961
O	2.681512	0.881285	0.608113
O	4.377751	-0.462842	-0.994188
O	2.077371	-0.713725	-1.886964
C	-0.782826	4.504013	0.008017
C	0.546877	4.180151	0.080507
C	-0.699710	2.583339	0.945866
C	-1.091967	1.317916	1.641193
H	-2.094177	1.046275	1.294018
H	-1.200270	1.493914	2.720501
C	-0.089885	0.173223	1.498338
H	0.816111	0.404188	2.059519
H	-0.496574	-0.746746	1.932637
C	-0.526021	-0.072394	-0.823763
H	-1.554006	0.202317	-0.577715
C	-0.266151	-0.332797	-2.217618
C	-1.310453	-0.269804	-3.152590
H	-2.317865	-0.025838	-2.825873
C	-1.042037	-0.517279	-4.486413
H	-1.831643	-0.476404	-5.231825
N	0.186573	-0.814610	-4.937322
C	1.179925	-0.868388	-4.064773
H	2.171294	-1.108422	-4.445573
C	1.024611	-0.637672	-2.683714
H	1.443887	4.687724	-0.240156
H	-1.229626	5.399244	-0.402579
O	1.912601	-1.791786	1.153972
O	3.274462	-1.855454	0.815863
H	4.148985	-0.759351	-1.892424
H	4.931464	-1.153715	-0.596536

TIIIb

V	1.438536	-0.405408	0.373586
N	1.220770	-0.058346	2.550303
N	-0.719896	-0.459023	0.578612
N	0.572019	0.574062	4.541171
H	-0.035654	0.772120	5.321857

O	3.003283	-1.079756	1.096620
O	0.905640	-0.826709	-1.472044
C	2.328894	0.331074	3.273273
C	1.940493	0.726337	4.517250
C	0.170801	0.104263	3.336695
C	-1.246146	-0.156879	2.975013
H	-1.765368	0.791864	2.779649
H	-1.764731	-0.637834	3.813955
C	-1.350465	-1.055709	1.749916
H	-0.851189	-2.010670	1.933044
H	-2.409542	-1.257920	1.547125
C	-1.510359	0.042359	-0.312193
H	-2.584364	0.081189	-0.092833
C	-1.110977	0.451341	-1.623825
C	-1.963074	1.187329	-2.466855
H	-2.890398	1.603295	-2.079343
C	-1.603528	1.377423	-3.783583
H	-2.224098	1.964827	-4.455432
N	-0.486394	0.844478	-4.319936
C	0.305369	0.127406	-3.547001
H	1.198850	-0.305503	-3.993119
C	0.079651	-0.095473	-2.160704
H	2.496659	1.090336	5.366335
H	3.311173	0.296424	2.830368
O	1.597373	1.141337	0.186954
O	1.016070	-2.793555	0.813632
O	2.943818	-1.194473	-0.302173
H	1.922285	-2.700626	1.174714
H	1.159269	-3.009156	-0.122233

TIV

V	0.844014	1.150615	0.512149
N	0.406582	0.569134	2.489825
N	-1.073970	0.352773	-0.016912
N	-0.700811	0.433918	4.363221
H	-1.473080	0.423362	5.012500
O	0.558690	2.701333	0.622571
O	2.542668	0.598235	0.971672
O	1.373227	0.826801	-1.339236
C	1.310727	0.362816	3.504385
C	0.633675	0.276819	4.684749
C	-0.799158	0.613274	3.027578
C	-2.048339	0.792882	2.242394
H	-2.160343	1.844029	1.947863
H	-2.917895	0.525792	2.853130
C	-2.036523	-0.089207	0.989837

H	-1.783493	-1.116203	1.283158
H	-3.046230	-0.109100	0.558908
C	-1.508257	0.373758	-1.239011
H	-2.561109	0.117106	-1.411446
C	-0.761160	0.666073	-2.422608
C	-1.430409	0.695130	-3.664707
H	-2.508756	0.554605	-3.699847
C	-0.715469	0.899428	-4.822094
H	-1.208750	0.935265	-5.789762
N	0.625660	1.059085	-4.829608
C	1.267863	1.026799	-3.681271
H	2.349100	1.154131	-3.698653
C	0.647140	0.847238	-2.410281
H	0.963835	0.120712	5.699370
H	2.363433	0.302397	3.274999
H	3.109309	0.572922	0.185587

TV

V	1.528785	0.592156	0.519041
N	1.082627	0.045879	2.521001
N	-0.441518	-0.023832	-0.028843
N	-0.049807	0.072019	4.384505
H	-0.826814	0.148094	5.024047
O	1.204347	2.124274	0.710985
O	3.336362	0.216750	0.969203
O	2.054819	0.437948	-1.337665
C	1.962536	-0.153836	3.558857
C	1.268319	-0.143618	4.732847
C	-0.125310	0.189662	3.039836
C	-1.353164	0.464240	2.245327
H	-1.373393	1.523945	1.960542
H	-2.241936	0.267547	2.855426
C	-1.426126	-0.397643	0.980317
H	-1.265679	-1.449030	1.256188
H	-2.439120	-0.326238	0.562630
C	-0.858628	0.009123	-1.253126
H	-1.920239	-0.197921	-1.438839
C	-0.083824	0.271497	-2.428679
C	-0.742504	0.303998	-3.676124
H	-1.821026	0.166789	-3.718456
C	-0.020761	0.506527	-4.829924
H	-0.508406	0.541125	-5.800520
N	1.319441	0.666837	-4.828291
C	1.952199	0.633892	-3.674453
H	3.033595	0.760437	-3.683348
C	1.325157	0.449301	-2.407955

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H	1.578534	-0.266188	5.758340
H	3.017930	-0.262482	3.361738
O	1.618441	-1.973659	0.491405
O	2.997101	-2.334553	0.713604
H	3.357628	-1.396550	0.815330
H	1.231074	-2.202962	1.352090
H	3.905613	0.527433	0.248178

TVI

V	1.687156	0.790685	0.422016
N	1.668621	-0.048664	2.362637
N	-0.384652	0.150710	0.292799
N	0.989696	-0.355740	4.412873
H	0.384635	-0.378763	5.220127
O	1.507458	2.333424	0.717658
O	3.471037	0.310883	0.575757
O	1.733946	0.515612	-1.480275
C	2.733528	-0.511322	3.102047
C	2.324577	-0.709470	4.386637
C	0.628308	0.042546	3.174298
C	-0.724373	0.478263	2.743144
H	-0.726708	1.559493	2.557180
H	-1.455165	0.273492	3.533102
C	-1.148031	-0.258321	1.469879
H	-1.005783	-1.336583	1.620909
H	-2.219588	-0.089364	1.300564
C	-1.075736	0.273937	-0.797916
H	-2.160620	0.118957	-0.738976
C	-0.578653	0.561813	-2.106131
C	-1.483564	0.699125	-3.179678
H	-2.554436	0.643822	-2.995208
C	-1.002579	0.899569	-4.453086
H	-1.677200	1.017385	-5.297001
N	0.317645	0.954143	-4.733430
C	1.176454	0.820485	-3.744428
H	2.238648	0.860097	-3.978851
C	0.810581	0.634779	-2.379515
H	2.842902	-1.059955	5.264827
H	3.696290	-0.641328	2.632576
O	4.340115	0.564662	-0.537853
H	4.533592	1.507387	-0.402055

TS1

V	1.067019	0.542096	0.306500
N	0.479073	0.622865	2.358379
N	-1.105624	0.122063	-0.054807

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N	-0.602930	0.727314	4.248200
H	-1.370134	0.722238	4.903584
O	0.777163	2.074212	0.060563
O	2.680181	0.443988	0.801698
O	1.196805	-0.041381	-1.482925
C	1.391194	0.811421	3.372614
C	0.729226	0.878226	4.561292
C	-0.722897	0.578559	2.909045
C	-2.026029	0.428715	2.206522
H	-2.403863	1.417082	1.911526
H	-2.759919	-0.000522	2.898694
C	-1.937962	-0.468684	0.973921
H	-1.472823	-1.424362	1.235761
H	-2.951598	-0.654725	0.593253
C	-1.627667	0.342053	-1.204334
H	-2.701110	0.164838	-1.349154
C	-0.883597	0.746373	-2.380099
C	-1.540918	1.260895	-3.505867
H	-2.611404	1.448850	-3.474539
C	-0.812662	1.533238	-4.650418
H	-1.294288	1.952627	-5.530274
N	0.503314	1.293089	-4.752186
C	1.130032	0.782779	-3.702381
H	2.195493	0.582738	-3.796272
C	0.500980	0.498289	-2.474804
H	1.074856	1.005764	5.574504
H	2.444790	0.883739	3.155336
O	0.830670	-1.574756	0.795468
H	2.032845	-1.911908	1.165339
O	0.557773	-2.429834	-0.338647
H	0.812888	-1.830755	-1.070714
O	3.136014	-1.839511	1.420691
H	3.055142	-0.613586	1.087449
H	3.611025	-2.317587	0.725173

TS2

V	-0.832878	0.736839	0.495271
N	-5.117232	-1.840654	3.354689
N	-2.531249	-0.590273	0.400634
N	-3.214152	-0.713089	3.482538
H	-2.306521	-0.341720	3.210685
O	-0.920690	0.548247	2.054483
O	0.239903	2.340011	0.221665
O	-2.073799	1.985555	-0.230929
C	-5.211904	-0.889928	4.338773
C	-4.047964	-0.172712	4.430471

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C	-3.903579	-1.710538	2.857743
C	-3.336302	-2.577469	1.778580
H	-4.172069	-2.932792	1.167180
H	-2.893192	-3.484540	2.212805
C	-2.230891	-1.929178	0.945170
H	-1.331607	-1.819742	1.552354
H	-1.953548	-2.582722	0.111547
C	-3.742931	-0.337732	0.054093
H	-4.497172	-1.121096	0.154019
C	-4.216279	0.926048	-0.441685
C	-5.560273	1.090221	-0.810792
H	-6.251514	0.255077	-0.732411
C	-5.989030	2.322646	-1.266196
H	-7.023083	2.481553	-1.560090
N	-5.171998	3.384126	-1.368211
C	-3.905765	3.239375	-1.015714
H	-3.255641	4.108668	-1.100688
C	-3.353846	2.029492	-0.540809
H	-3.741695	0.651985	5.055821
H	-6.114480	-0.773194	4.922972
O	-0.198047	-0.717399	-0.390146
O	0.934290	-0.072596	0.157988
H	1.151843	2.146307	-0.709315
H	-0.383006	3.062405	0.044704
O	1.867047	1.542135	-1.328793
H	1.542478	1.500944	-2.241419
H	1.501185	0.600782	-0.736716

TS3

V	1.711978	-0.215857	-0.650338
N	1.585092	1.155118	1.107802
N	-0.481781	-0.068117	-0.473037
N	0.939720	2.577704	2.640163
H	0.331243	3.091479	3.259554
O	3.606390	-0.179644	-0.026713
O	1.150204	-1.469779	-2.007033
C	2.689506	1.825726	1.588274
C	2.304608	2.712097	2.547881
C	0.536122	1.636143	1.752881
C	-0.897581	1.306313	1.533515
H	-1.367054	2.101514	0.937042
H	-1.419357	1.282959	2.498504
C	-1.099491	-0.033818	0.842010
H	-0.618693	-0.830120	1.418200
H	-2.175887	-0.235615	0.765922
C	-1.255936	-0.085694	-1.499302

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H	-2.335800	0.040154	-1.351695
C	-0.817745	-0.385883	-2.836425
C	-1.624362	-0.139952	-3.958290
H	-2.547367	0.426041	-3.855458
C	-1.227231	-0.620472	-5.190404
H	-1.814941	-0.423011	-6.083474
N	-0.117255	-1.361820	-5.361905
C	0.634420	-1.623052	-4.307107
H	1.524131	-2.232278	-4.454395
C	0.363838	-1.143543	-3.001457
H	2.863422	3.401464	3.160338
H	3.675833	1.636238	1.197821
O	1.692101	1.094991	-1.524596
O	1.316403	-1.630663	0.809548
O	3.303600	-1.026611	-1.118019
H	1.122608	-2.418488	0.277659
H	2.525451	-1.864159	1.526876
O	3.544459	-1.782309	1.832348
H	3.698805	-0.870128	0.816262
H	3.976660	-2.603766	1.556136

TS4

V	0.936114	1.102100	-0.803139
N	2.393231	-0.431236	-0.965419
N	1.096798	0.031914	1.403825
N	4.080169	-1.729834	-0.498685
H	4.881103	-2.109368	-0.016590
O	2.004161	2.213140	-0.074410
O	0.970809	1.334651	-2.364223
O	-0.677535	0.111264	-0.721166
C	2.538578	-1.331476	-1.992954
C	3.589460	-2.154966	-1.715729
C	3.339989	-0.681398	-0.072227
C	3.573157	0.119848	1.155736
H	3.788121	1.143195	0.832145
H	4.448278	-0.258531	1.694794
C	2.356645	0.164034	2.108166
H	2.451627	-0.612797	2.881546
H	2.365648	1.139916	2.605239
C	0.164357	-0.615292	1.992669
H	0.339123	-1.053111	2.987783
C	-1.158246	-0.829779	1.444236
C	-2.134483	-1.462408	2.227085
H	-1.893985	-1.772902	3.241728
C	-3.397915	-1.682691	1.708698
H	-4.170027	-2.165022	2.303260

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N	-3.742546	-1.323360	0.462174
C	-2.825899	-0.734707	-0.290427
H	-3.108855	-0.454696	-1.303879
C	-1.503467	-0.447925	0.126911
H	4.024037	-2.980734	-2.256015
H	1.880581	-1.307342	-2.847618
O	0.297150	2.671938	0.018979
C	-1.731809	2.988132	0.561687
C	-1.440567	3.381673	-0.705845
H	-1.627217	2.732855	-1.555034
H	-1.102038	4.388062	-0.923259
H	-1.587343	3.656155	1.403651
H	-2.145835	2.008671	0.771018

TS5

V	1.156052	0.351794	0.298984
N	0.699044	0.058946	2.335072
N	-0.832933	-0.092095	-0.242333
N	-0.462360	-0.009367	4.178401
H	-1.254745	-0.000257	4.802421
O	0.939289	1.915751	0.360968
O	3.110018	0.199483	0.801055
O	1.695801	0.073437	-1.543070
C	1.569279	-0.106787	3.383293
C	0.859089	-0.150162	4.546721
C	-0.521665	0.117130	2.832765
C	-1.765500	0.290364	2.032398
H	-1.888299	1.344945	1.753779
H	-2.632624	0.010771	2.641598
C	-1.760736	-0.575670	0.767444
H	-1.442428	-1.590537	1.036539
H	-2.778125	-0.620679	0.355072
C	-1.254122	-0.002834	-1.455330
H	-2.315895	-0.198987	-1.651681
C	-0.455153	0.286904	-2.617788
C	-1.104757	0.493138	-3.849560
H	-2.192018	0.496066	-3.889839
C	-0.365572	0.690322	-4.996407
H	-0.849398	0.862606	-5.954397
N	0.980973	0.672955	-5.000845
C	1.604769	0.467788	-3.857012
H	2.693795	0.452087	-3.871879
C	0.964909	0.273729	-2.602290
H	1.160339	-0.271244	5.574921
H	2.631090	-0.176761	3.207197
O	1.182419	-1.892004	0.250165

H	2.412248	-2.118769	0.136712
O	0.740300	-2.622830	1.419044
H	0.560449	-3.486301	1.014343
O	3.571890	-2.030219	0.038065
H	3.488595	-0.843888	0.418988
H	3.730391	-1.994121	-0.917523
H	3.583933	0.896484	0.324011

TS6

V	0.851291	0.070732	-0.036815
N	1.143366	-1.146617	1.678500
N	-1.299075	-0.594862	0.231489
N	0.953762	-1.925438	3.707761
H	0.546614	-2.159650	4.601049
O	0.712616	1.507009	0.616559
O	2.466988	-0.246941	-0.307614
O	0.335278	0.171317	-1.845815
C	2.356466	-1.683677	2.050613
C	2.253578	-2.175959	3.316322
C	0.313231	-1.298809	2.698229
C	-1.113333	-0.891413	2.686806
H	-1.197598	0.198363	2.781348
H	-1.638370	-1.340771	3.536756
C	-1.779878	-1.342948	1.385951
H	-1.564524	-2.407272	1.225980
H	-2.868934	-1.238356	1.483480
C	-2.220162	-0.146020	-0.557604
H	-3.269082	-0.314712	-0.280826
C	-2.027003	0.533615	-1.805141
C	-3.135768	1.037399	-2.511563
H	-4.131792	0.971417	-2.079111
C	-2.944974	1.611413	-3.750069
H	-3.780129	2.020156	-4.312993
N	-1.734429	1.694529	-4.337181
C	-0.687595	1.215059	-3.692960
H	0.285825	1.278896	-4.174927
C	-0.749954	0.628613	-2.401637
H	2.964453	-2.666991	3.961360
H	3.193471	-1.647675	1.370575
O	3.356903	0.489158	-1.719892
H	3.395228	1.339903	-1.247328