

Supplementary Information

Vanadyl cationic complexes as catalysts in olefin oxidation

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Crystal Structure of the imid of naphthalene-1,8-dicarboxylic acid

The C=O distances of 1.215(1) Å are within the expected value for a carbonyl group, and the bond distances N(1)-C(2) (1.401(1) Å), N(1)-C(11) (1.455(2) Å), and C(2)-C(3) (1.480(2) Å) are intermediate between single and double C-C or N-C bonds. The terminal phenyl ring is almost perpendicular to the diquinone fragment making with it a dihedral angle of 83.25(9) °. The structure contains a C2 crystallographic axis of symmetry running along the main axis of the molecule. The methyl group is disordered with hydrogen atoms occupying two alternative positions. The crystal packing diagram shown in Figure S1 shows the existence of π - π stacking interactions between two molecules, at an interplanar distance of 3.46 Å, in the unit cell.

¹ Present address: ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxfordshire X11 0QX, United Kingdom

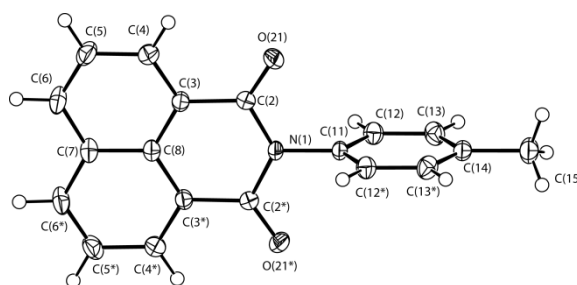


Figure S1. Ortep view of **4** with ellipsoids at 50 % level and the labelling scheme adopted (* denotes the symmetry operation: $-x, y, 3/2-z$). One unique set of positions of the disordered methyl group is shown.

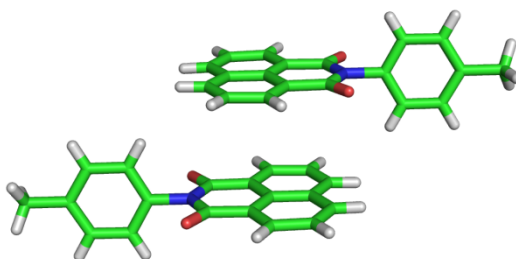


Figure S2. Crystal packing diagram showing the parallel disposition consistent with the existence of π - π stacking interactions between diquinone fragments.

Crystallography

Crystal data: $C_{19}H_{13}NO_2$, $M_r = 299.31$, Monoclinic, space group $C2/c$, $Z = 4$, $a = 12.112(2)$ Å, $b = 14.402(3)$ Å, $c = 9.294(2)$ Å, $\beta = 121.416(7)^\circ$, $U = 1383.6(4)$ Å³, $T = 180(2)$ K, $\rho(\text{calc}) = 1.379$ Mg m⁻³, (Mo-K α) 0.090 mm⁻¹. 18509 intensities collected, 1603 independent reflections (R_{int} of 0.0453), which were used in solution and structure refinement. The final R and R_w indices were $R_1 = 0.0416$ and $wR_2 = 0.1054$ for 1172 reflections with $I > 2\sigma(I)$ and $R_1 = 0.0622$ and $wR_2 = 0.1168$ for all hkl data.

The X-ray data were collected at room temperature on a Bruker APEX II diffractometer equipped with a CCD area detector using graphite monochromatized Mo-K α radiation ($\lambda = 0.71073$ Å) with the crystal positioned at 35 mm from the CCD and the spots were measured using a counting time of 5 s. The data reduction was carried out using the SAINT-NT software package.ⁱ Subsequently a multi-scan absorption correction was applied using the SADABS program.ⁱⁱ The structure was solved by direct methods and by subsequent difference Fourier syntheses and refined by full matrix least squares on F^2 using the SHELX-97 software suite.ⁱⁱⁱ ³Anisotropic thermal parameters were used for all non-hydrogen atoms. Hydrogen atoms bonded to the carbon atoms were included in the refinement in calculated positions with isotropic parameters equivalent 1.2 times those of the atom

to which they are attached.^{iv} . Molecular diagrams presented are drawn with the PLATON^v and PYMOL^{vi} graphical packages.

EPR studies

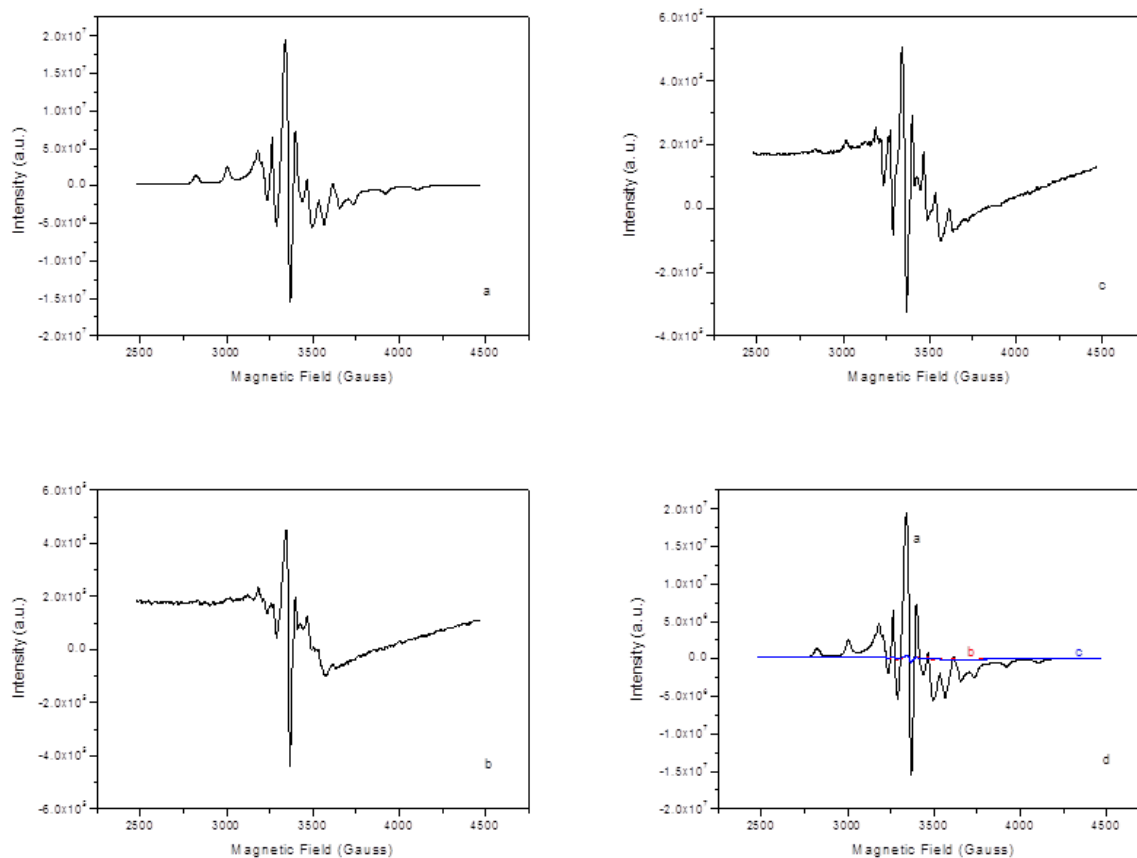


Figure S3. EPR spectra obtained at 100 K in frozen dichloromethane matrix of: complex $[\text{VO}(\text{acac})(\text{H-BIAN})]\text{Cl}$ (**1**, top left, a), **1** + tbhp (bottom left, b), **1** + cy8 + tbhp (top right, c), and all (bottom right, d).

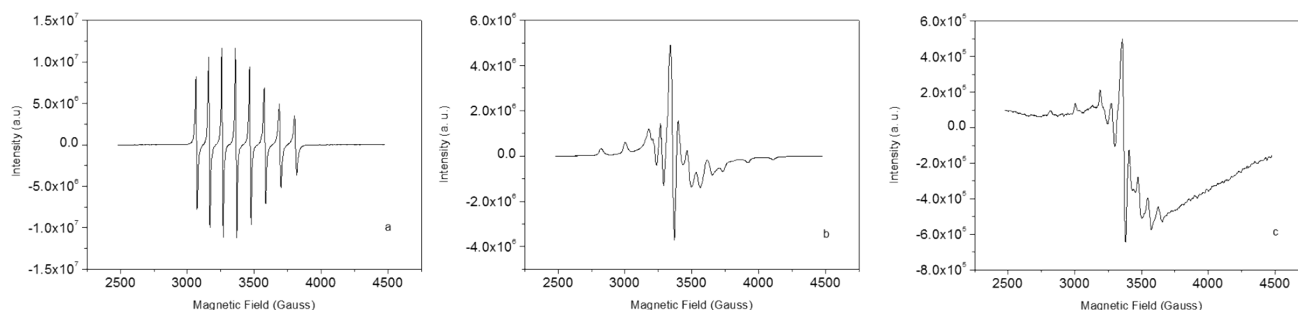


Figure S4. EPR signal of complex $[\text{VO}(\text{acac})(\text{H-BIAN})]\text{Cl}$ (**1**) at 296 K (a) and 100 K in frozen dichloromethane (b), and **1** + cy8 + tbhp at 100 K in frozen dichloromethane 24 hours later (c).

Atomic Coordinates for all the optimized molecules (PBE1PBE/b1)

MeOOH

C	-0.996537	-0.259389	-0.236558
O	0.032841	0.572458	0.239965
O	1.096412	-0.296173	0.644389
H	1.760617	-0.084629	-0.026498
H	-1.814560	0.422134	-0.488319
H	-1.331116	-0.964249	0.533198
H	-0.692071	-0.815249	-1.133203

MeOH

C	-0.476279	-0.051405	0.070908
O	0.555682	0.779749	0.545500
H	1.299299	0.217987	0.780535
H	-1.314871	0.597757	-0.193321
H	-0.831645	-0.767510	0.827108
H	-0.191986	-0.615678	-0.830031

CH₂=CH₂

C	0.662916	-0.028420	0.018139
C	-0.663369	0.028471	-0.018195
H	1.276431	0.862788	-0.082884
H	1.191466	-0.968632	0.150425
H	-1.276883	-0.862737	0.082828
H	-1.191918	0.968683	-0.150481

Hacac

H	-0.349696	-1.264150	1.302349
O	-1.682879	-0.735187	0.742563
C	-1.269073	0.022923	-0.159672
O	0.666835	-1.309192	1.311012
C	1.044896	-0.497749	0.348198
C	0.134276	0.189733	-0.415420
H	0.475522	0.850838	-1.202281
C	2.521607	-0.400904	0.172303
H	2.787887	0.280854	-0.636214
H	2.980889	-0.055773	1.104052
H	2.932510	-1.393118	-0.039474
C	-2.260503	0.784855	-0.996941
H	-2.124058	1.862399	-0.855697
H	-2.105906	0.576246	-2.060502
H	-3.274804	0.506327	-0.709877

1⁺

V	3.837571	-0.335597	-0.226971
C	3.916360	-0.908854	4.073599
C	4.887041	-1.339897	4.959094
C	4.519079	-1.577599	6.301430
C	3.225336	-1.399148	6.753751
C	2.204025	-0.972650	5.868014
C	2.586014	-0.730922	4.538137
C	0.833608	-0.785110	6.178230
C	-0.062736	-0.401454	5.198647
C	0.333873	-0.170628	3.863378
C	1.666914	-0.330513	3.531929
C	3.866385	-0.633780	2.643505
C	2.444763	-0.266618	2.300992
N	4.701297	-0.709775	1.662305
N	2.182606	-0.056174	1.054790
C	6.073167	-1.026760	1.839056
C	0.896364	0.315515	0.586068
C	0.299628	-0.465500	-0.405097
C	-0.953212	-0.107408	-0.889436
C	-1.588889	1.040042	-0.418820
C	-0.968954	1.835174	0.543354
C	0.274696	1.476092	1.052248
C	6.893667	-0.221654	2.632151
C	8.243763	-0.533797	2.752954
C	8.769102	-1.642555	2.092007
C	7.945080	-2.431010	1.291085
C	6.598634	-2.117491	1.144732
H	5.912844	-1.494978	4.645372
H	5.281731	-1.913403	6.996624
H	2.984010	-1.594370	7.794934
H	0.486453	-0.952967	7.193950
H	-1.108583	-0.273400	5.458486

H	-0.402803	0.126535	3.125983
H	0.815593	-1.346479	-0.775319
H	-1.430452	-0.724013	-1.644729
H	-2.561499	1.321370	-0.810202
H	-1.451024	2.741983	0.895575
H	0.774034	2.099491	1.788480
H	6.479277	0.650970	3.129062
H	8.887050	0.095245	3.360676
H	9.822417	-1.884914	2.192319
H	8.353275	-3.290972	0.769306
H	5.948607	-2.712122	0.509648
O	3.051330	1.003316	-1.359561
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O	5.557325	0.340419	-0.756422
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C	4.936278	1.611573	-2.650644
H	5.289319	2.159769	-3.514611
C	7.339147	1.128358	-2.068856
H	7.558710	1.717116	-2.959720
H	7.821778	1.585504	-1.199224
H	7.765202	0.125880	-2.178075
C	2.603198	2.379068	-3.210171
H	2.079416	3.110736	-2.586833
H	3.088688	2.889817	-4.041987
H	1.845263	1.689507	-3.595381
O	3.618428	-1.743096	-0.871972

A

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C	-4.162702	-0.512977	1.757968
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C	-3.386786	-0.401383	0.526190
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H	-5.070273	1.954970	0.115773
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O	-2.733069	0.883266	-3.281542
C	-2.233204	1.177220	-4.435744
O	-0.224583	0.083973	-2.691230
C	0.057273	0.501404	-3.865929
C	-0.897757	0.980222	-4.776168
H	-0.564755	1.287679	-5.759224
C	1.509578	0.479637	-4.220469
H	1.699503	0.826348	-5.236503
H	2.056641	1.108641	-3.510856
H	1.890415	-0.539340	-4.101182
C	-3.192950	1.797419	-5.400289
H	-3.637810	2.691943	-4.952711
H	-2.722229	2.060465	-6.347817
H	-4.012719	1.095048	-5.582977
O	-2.265653	-1.784260	-2.549834

TS_{AB}

V	-2.101366	0.121447	-1.712776
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C	-0.811246	-1.933583	3.072267
O	-1.830408	3.020177	-1.557713
C	-1.102586	-2.430081	4.361347
O	-2.781793	2.096209	-2.098536
C	-2.357291	-2.313182	4.929861
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C	-3.414711	-1.684893	4.224894
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H	-3.366681	4.069131	-0.624051
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C	-4.952248	0.744645	-0.603993
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C	-6.760347	2.285021	-0.211275
C	-5.531993	1.755695	0.168051
C	1.108158	-0.435234	0.833530
C	2.434999	-0.854104	0.811317
C	2.825760	-1.904046	-0.017518
C	1.888993	-2.526734	-0.841295
C	0.563438	-2.105418	-0.842267
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H	-0.312533	-2.922722	4.918871
H	-2.540113	-2.713057	5.923403
H	-5.044538	-1.896533	5.642267
H	-6.715469	-0.830317	4.196276
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H	-7.314055	0.445687	-3.014920
H	-8.368097	2.224013	-1.641057
H	-7.208764	3.077599	0.380035
H	-5.009151	2.136925	1.040711
H	0.796600	0.393328	1.462950
H	3.165375	-0.353737	1.439733
H	3.860972	-2.230453	-0.028456
H	2.191123	-3.341537	-1.492011
H	-0.174561	-2.568149	-1.490562
O	-2.527689	1.009684	-4.230378
C	-1.574332	0.819593	-5.035832
O	-0.392588	0.681385	-2.291346
C	0.301207	0.790185	-3.381975
C	-0.201916	0.798216	-4.670355
H	0.523410	0.781238	-5.475092
C	1.777049	0.887412	-3.141449

H	1.978645	1.774546	-2.531920
H	2.110365	0.019524	-2.563207
H	2.346944	0.953858	-4.068766
C	-1.941646	0.602725	-6.476109
H	-2.670100	1.356262	-6.787066
H	-1.079817	0.617489	-7.144730
H	-2.434434	-0.372461	-6.560364
O	-2.498425	-1.204074	-2.432343

B

V	-2.252868	0.257045	-1.705455
C	-1.762896	-1.186559	2.358731
C	-2.858510	3.667710	-1.061369
C	-0.694133	-1.760184	3.022338
O	-2.088101	2.597465	-1.579487
C	-0.909377	-2.279301	4.317514
O	-2.933080	1.864783	-2.489335
C	-2.149520	-2.244651	4.927738
H	-2.345561	1.754619	-3.907924
C	-3.266985	-1.675747	4.266173
H	-2.194886	4.173866	-0.355235
C	-3.034202	-1.142284	2.987801
H	-3.757491	3.307460	-0.554754
H	-3.135253	4.351946	-1.868466
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C	-5.596422	-1.053955	3.971567
C	-5.345314	-0.518409	2.688628
C	-4.054532	-0.552395	2.194471
C	-1.965353	-0.613711	1.036958
C	-3.406077	-0.185118	0.935814
N	-1.224949	-0.475180	-0.008182
N	-3.777968	0.313890	-0.193972
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C	-5.087331	0.791446	-0.438794
C	-5.739838	0.379739	-1.603506
C	-7.018222	0.853745	-1.872254
C	-7.629069	1.764604	-1.012546
C	-6.958335	2.202184	0.128144
C	-5.689740	1.715177	0.422451
C	1.111345	-0.105683	0.606587
C	2.433786	-0.541245	0.614162
C	2.776180	-1.759560	0.030740
C	1.793454	-2.540761	-0.574972
C	0.469039	-2.111570	-0.598794
H	0.290237	-1.816614	2.571985
H	-0.072410	-2.726090	4.844362
H	-2.274195	-2.664462	5.922116
H	-4.832870	-2.003290	5.733401
H	-6.611212	-1.023650	4.355119
H	-6.161782	-0.092690	2.117130
H	-5.245672	-0.316450	-2.273774
H	-7.534213	0.518781	-2.766517
H	-8.620739	2.144110	-1.237787
H	-7.420139	2.930344	0.787920
H	-5.154145	2.066149	1.300224
H	0.833512	0.843631	1.054715
H	3.197594	0.075034	1.078622
H	3.807753	-2.097174	0.043369
H	2.055945	-3.489759	-1.032571
H	-0.305499	-2.705566	-1.074891
O	-2.324438	1.632817	-4.913838
C	-1.263068	1.154052	-5.483774
O	-0.521099	0.621073	-2.539156
C	0.269394	0.598395	-3.530915
C	-0.077537	0.738499	-4.890128
H	0.720253	0.518630	-5.589290
C	1.715876	0.391619	-3.187000
H	2.027357	1.188262	-2.504012
H	1.827809	-0.551765	-2.643241
H	2.366147	0.394241	-4.061946
C	-1.396240	1.123618	-6.971486
H	-1.589299	2.135504	-7.341580
H	-0.512744	0.716744	-7.461977
H	-2.268889	0.517747	-7.235642
O	-2.789981	-0.986158	-2.488629

TS_{BC}

V	-2.259743	0.247696	-1.719506
C	-1.753585	-1.128631	2.359278
C	-2.791582	3.575622	-0.878807
C	-0.659498	-1.618034	3.048527
O	-2.043385	2.536807	-1.487332
C	-0.856748	-2.101538	4.360286
O	-2.902559	1.894746	-2.452223
C	-2.102699	-2.116212	4.960090
H	-2.226060	1.934156	-3.842027
C	-3.243770	-1.628077	4.274477
H	-2.116338	4.009986	-0.136834
C	-3.028951	-1.124123	2.981212
H	-3.695881	3.191862	-0.400014
H	-3.056752	4.327529	-1.626981
C	-4.579705	-1.608846	4.748245
C	-5.597209	-1.121905	3.950527
C	-5.362085	-0.605861	2.656393
C	-4.068373	-0.595929	2.169602
C	-1.972473	-0.595892	1.024306
C	-3.425977	-0.217975	0.910375
N	-1.224424	-0.435327	-0.012278
N	-3.802080	0.273322	-0.220874
C	0.145884	-0.831010	0.030868
C	-5.119221	0.721937	-0.477379
C	-5.746539	0.308561	-1.655531
C	-7.031682	0.756424	-1.936672
C	-7.675062	1.643182	-1.075601
C	-7.030300	2.082542	0.079288
C	-5.755203	1.621308	0.385904
C	1.125574	0.104449	0.358302
C	2.457720	-0.297155	0.411055
C	2.807343	-1.616487	0.128986
C	1.820487	-2.539070	-0.212529
C	0.484003	-2.151135	-0.265600
H	0.329463	-1.638760	2.604874
H	-0.001174	-2.482816	4.908284
H	-2.212561	-2.510767	5.966494
H	-4.802897	-1.986662	5.742064
H	-6.614780	-1.127778	4.327832
H	-6.192518	-0.227932	2.071468
H	-5.227622	-0.369487	-2.325521
H	-7.527753	0.419728	-2.841498
H	-8.671961	2.002679	-1.310378
H	-7.517622	2.792387	0.740648
H	-5.241047	1.973989	1.275703
H	0.841899	1.130981	0.568587
H	3.224176	0.425618	0.674000
H	3.847493	-1.923973	0.171519
H	2.088148	-3.567053	-0.437444
H	-0.294834	-2.858345	-0.535326
O	-2.150094	2.021048	-4.848342
C	-1.190346	1.435467	-5.491642
O	-0.550263	0.559735	-2.636175
C	0.181216	0.350929	-3.653078
C	-0.131538	0.691459	-4.983049
H	0.587614	0.366742	-5.724811
C	1.504405	-0.300991	-3.379910
H	2.036582	0.282279	-2.622461
H	1.330252	-1.290425	-2.944491
H	2.125723	-0.397905	-4.270423
C	-1.286228	1.670027	-6.964294
H	-1.255433	2.746363	-7.161698
H	-0.489828	1.175522	-7.519192
H	-2.256665	1.310501	-7.320706
O	-2.814230	-0.993880	-2.495767

C

V	-2.697860	-0.017203	-1.860010
C	-1.666495	-0.815732	2.277325
C	-3.261525	3.300205	-1.199594
C	-0.463493	-1.072853	2.908596
O	-2.561964	2.269004	-1.874629
C	-0.479567	-1.360487	4.290526
O	-3.533925	1.485944	-2.599054
C	-1.654261	-1.412129	5.018649

H	-0.858029	2.114618	-3.291999
C	-2.903038	-1.156033	4.398501
H	-2.496653	3.861069	-0.655719
C	-2.869319	-0.840678	3.029918
H	-4.002099	2.889093	-0.508359
H	-3.754994	3.947691	-1.928953
C	-4.181925	-1.193901	5.009059
C	-5.318044	-0.933662	4.267613
C	-5.264924	-0.597419	2.895992
C	-4.032609	-0.539030	2.273342
C	-2.067533	-0.497793	0.915134
C	-3.558630	-0.283272	0.912392
N	-1.442957	-0.387707	-0.207614
N	-4.093627	0.004265	-0.224280
C	-0.054330	-0.688594	-0.308586
C	-5.467980	0.284658	-0.399930
C	-6.142648	-0.344030	-1.449933
C	-7.487516	-0.065006	-1.659781
C	-8.148978	0.864715	-0.859850
C	-7.461484	1.517795	0.161564
C	-6.122953	1.227671	0.399445
C	0.861575	0.337473	-0.538165
C	2.213733	0.029054	-0.654245
C	2.645805	-1.292632	-0.564705
C	1.720718	-2.314017	-0.358215
C	0.366845	-2.017824	-0.228413
H	0.476054	-1.064171	2.367803
H	0.462508	-1.559033	4.791364
H	-1.622937	-1.654586	6.077325
H	-4.266093	-1.434466	6.065124
H	-6.288331	-0.978992	4.751723
H	-6.183251	-0.388561	2.359535
H	-5.609934	-1.051770	-2.077226
H	-8.017659	-0.567238	-2.462831
H	-9.194888	1.091584	-1.040940
H	-7.965773	2.261723	0.770679
H	-5.577700	1.746776	1.182791
H	0.511237	1.361488	-0.620897
H	2.931730	0.826666	-0.818554
H	3.701147	-1.527119	-0.662087
H	2.050879	-3.346654	-0.298828
H	-0.365711	-2.805232	-0.076134
O	-0.293977	2.736475	-3.814300
C	0.419885	2.058503	-4.676563
O	-1.119656	0.419379	-3.038330
C	-0.419385	-0.129082	-3.952527
C	0.395873	0.677496	-4.775719
H	1.008173	0.205360	-5.532694
C	-0.464204	-1.608632	-4.125062
H	-0.070190	-2.081429	-3.218137
H	-1.504287	-1.934370	-4.221791
H	0.116974	-1.939426	-4.986000
C	1.258143	2.913757	-5.557746
H	1.896992	3.557913	-4.945535
H	1.875453	2.321661	-6.232808
H	0.609698	3.573263	-6.143980
O	-3.129382	-1.408935	-2.450876

TS_{CD}

V	-2.703887	0.100344	-1.456623
C	-1.854889	-0.823769	2.663049
C	-1.268051	2.812126	-1.728596
C	-0.703051	-1.165580	3.349447
O	-1.897002	1.718674	-2.403768
C	-0.819443	-1.614028	4.682408
O	-3.306249	1.713902	-2.107715
C	-2.041796	-1.724933	5.319202
H	0.504208	0.739499	-3.533626
C	-3.241959	-1.397847	4.639899
H	-0.223215	2.764787	-2.040788
C	-3.110789	-0.946288	3.316297
H	-1.366917	2.715063	-0.642708
H	-1.731987	3.738094	-2.071780
C	-4.561622	-1.500275	5.147807
C	-5.646517	-1.184311	4.352272
C	-5.499768	-0.740752	3.019586

C	-4.224630	-0.615409	2.500389
C	-2.165035	-0.417171	1.299944
C	-3.663255	-0.288547	1.195914
N	-1.477923	-0.209163	0.222056
N	-4.140484	0.006898	0.033383
C	-0.058822	-0.184459	0.202726
C	-5.506960	0.266683	-0.229139
C	-6.112547	-0.376244	-1.312119
C	-7.444852	-0.106523	-1.601852
C	-8.156327	0.823528	-0.846794
C	-7.533458	1.489534	0.207818
C	-6.208938	1.213446	0.524112
C	0.646137	0.675487	1.052720
C	2.033054	0.722456	0.978557
C	2.713530	-0.083517	0.066329
C	2.002149	-0.922811	-0.787811
C	0.612760	-0.968412	-0.736759
H	0.275389	-1.094790	2.888479
H	0.084219	-1.880695	5.220881
H	-2.086382	-2.074200	6.347045
H	-4.718296	-1.838548	6.168238
H	-6.647890	-1.279973	4.759453
H	-6.378761	-0.506455	2.429986
H	-5.539556	-1.085323	-1.901754
H	-7.924904	-0.617790	-2.430199
H	-9.191429	1.042206	-1.089483
H	-8.076624	2.235994	0.779010
H	-5.707875	1.748629	1.325495
H	0.107688	1.312286	1.749310
H	2.582555	1.396732	1.628216
H	3.796838	-0.043746	0.011242
H	2.527473	-1.539374	-1.510109
H	0.051381	-1.587597	-1.428707
O	0.895073	1.602469	-3.933288
C	0.519561	1.564378	-5.193613
O	-0.307308	-0.504271	-3.571824
C	-0.652344	-0.517809	-4.786701
C	-0.245697	0.523761	-5.673159
H	-0.539049	0.504197	-6.714492
C	-1.495016	-1.654572	-5.278655
H	-0.929173	-2.586875	-5.180162
H	-2.376100	-1.746180	-4.636557
H	-1.800328	-1.531373	-6.318816
C	0.987890	2.707573	-6.022802
H	2.081921	2.746668	-6.010222
H	0.641690	2.627236	-7.053474
H	0.628479	3.648277	-5.593335
O	-3.024186	-1.225717	-2.231034

D

V	-2.588604	0.204062	-1.377995
C	-1.881744	-0.876990	2.723544
C	-0.994877	2.810760	-1.711556
C	-0.759038	-1.273805	3.428583
O	-1.693646	1.737160	-2.351069
C	-0.925289	-1.785899	4.732972
O	-3.103893	1.832899	-2.064734
C	-2.169017	-1.906059	5.325000
H	0.616272	0.721826	-3.763110
C	-3.340933	-1.526096	4.624295
H	0.040484	2.697325	-2.036135
C	-3.159942	-1.012443	3.329523
H	-1.085567	2.748574	-0.622732
H	-1.410104	3.750841	-2.077181
C	-4.677976	-1.633454	5.083420
C	-5.732015	-1.264609	4.269203
C	-5.535484	-0.761230	2.964734
C	-4.242096	-0.628720	2.494324
C	-2.141671	-0.401989	1.371887
C	-3.634754	-0.252502	1.224782
N	-1.420239	-0.148363	0.325558
N	-4.072669	0.098609	0.061250
C	-0.004038	-0.109979	0.328453
C	-5.426507	0.385616	-0.235078
C	-5.999062	-0.200996	-1.367077
C	-7.317021	0.096946	-1.692356

C	-8.046062	1.000281	-0.921790
C	-7.455362	1.610864	0.183708
C	-6.145955	1.305804	0.534557
C	0.689543	0.642816	1.284261
C	2.075306	0.717286	1.219469
C	2.767210	0.048159	0.209646
C	2.067664	-0.679133	-0.750432
C	0.679204	-0.751610	-0.707374
H	0.235146	-1.199655	3.003085
H	-0.043656	-2.094958	5.285114
H	-2.252646	-2.304321	6.332364
H	-4.872662	-2.017977	6.080666
H	-6.747421	-1.365492	4.638585
H	-6.391329	-0.488565	2.357879
H	-5.413510	-0.891425	-1.966726
H	-7.771722	-0.371079	-2.559627
H	-9.069437	1.241634	-1.191215
H	-8.011655	2.337013	0.768270
H	-5.668960	1.799064	1.376491
H	0.142551	1.183363	2.051562
H	2.615535	1.309745	1.951456
H	3.849875	0.110679	0.162375
H	2.598854	-1.184718	-1.550440
H	0.135926	-1.287007	-1.480992
O	0.807272	1.630052	-4.207315
C	0.224458	1.533083	-5.382418
O	0.004276	-0.626250	-3.686977
C	-0.545710	-0.694503	-4.820762
C	-0.456209	0.390814	-5.743287
H	-0.922666	0.324072	-6.717309
C	-1.307875	-1.935834	-5.171834
H	-0.668538	-2.809594	-5.015589
H	-2.154903	-2.027979	-4.483719
H	-1.672164	-1.929054	-6.200287
C	0.370840	2.728392	-6.256580
H	1.432995	2.930525	-6.428164
H	-0.129799	2.590805	-7.215261
H	-0.046363	3.607375	-5.754664
O	-2.861918	-1.108556	-2.192435

E

V	-1.901291	-0.429356	-3.115204
C	-1.148781	-2.132051	0.742947
C	-4.350407	-1.072760	-6.857589
C	-0.234379	2.134202	-3.092789
C	-0.014107	-2.642095	1.349880
C	-4.496658	0.227023	-6.611750
O	-0.936331	1.161633	-3.873004
C	-0.157443	-3.348514	2.562239
H	-5.014016	-1.603994	-7.535023
O	-2.356999	1.284213	-3.644617
C	-1.390815	-3.552221	-3.154336
H	-3.550521	-1.650341	-6.400501
C	-2.573944	-3.058614	2.549716
H	-3.825893	0.762011	-5.943259
H	0.823320	1.922050	-3.260810
C	-2.415480	-2.345248	1.350456
H	-5.285675	0.810890	-7.079369
H	-0.488159	2.043839	-2.032475
H	-0.496036	3.125228	-3.465582
C	-3.901986	-3.233637	3.014450
C	-4.968798	-2.735310	2.291215
C	-4.794239	-2.026340	1.082564
C	-3.509991	-1.821685	0.611825
C	-1.431335	-1.452286	-0.509807
C	-2.924402	-1.253738	-0.595903
N	-0.728405	-1.058876	-1.524798
N	-3.375371	-0.715627	-1.683479
C	0.687026	-1.090082	-1.589224
C	-4.715613	-0.334347	-1.911933
C	-5.270794	-0.598897	-3.167817
C	-6.571983	-0.193453	-3.436741
C	-7.304408	0.501221	-2.476775
C	-6.730103	0.800398	-1.240770
C	-5.436827	0.386050	-0.951447
C	1.466636	-0.474076	-0.604697

C	2.850265	-0.458425	-0.741713	H	3.253410	-2.279895	-3.573902
C	3.453734	-1.051901	-1.849731	H	0.770798	-2.309922	-3.489860
C	2.669585	-1.651558	-2.833275	O	-1.934243	-2.005558	-4.245239
C	1.283815	-1.660199	-2.717476	F			
H	0.970553	-2.512751	0.915422				
H	0.731717	-3.746794	3.040041		V	-1.940963	-0.166873
H	-1.457349	-4.104915	4.087358		C	-1.265888	-2.170568
H	-4.079382	-3.773107	3.940543		C	-4.148723	0.244170
H	-5.977764	-2.892010	2.658700		C	0.194993	1.915318
H	-5.661409	-1.657735	0.546657		C	-0.153387	-2.666675
H	-4.694402	-1.123603	-3.923944		C	-3.117929	1.227421
H	-6.999419	-0.407755	-4.410790		O	-1.013241	1.350102
H	-8.315119	0.830178	-2.696994		C	-0.333668	-3.345438
H	-7.286125	1.374151	-0.505847		H	-5.193869	0.538101
H	-4.970032	0.652975	-0.007979		O	-3.366316	0.866509
H	0.988966	0.006010	0.244824		C	-1.579141	-3.519466
H	3.458087	0.027413	0.015358		H	-3.928947	-0.810010
H	4.534258	-1.037127	-1.950988		C	-2.741712	-3.029847
H	3.136259	-2.110470	-3.699090		H	-2.166006	0.875811
H	0.662511	-2.124080	-3.479319		H	0.135123	2.217642
O	-2.088043	-1.621006	-4.115721		C	-2.547216	-2.373411
TS_{EF}					H	-3.395680	2.251898
	V	-1.842291	-0.668189		H	1.030512	1.213480
	C	-1.214830	-1.991115		H	0.403851	2.808041
	C	-4.233609	1.719430		C	-4.080711	-3.136245
	C	-0.019170	1.678642		C	-5.124597	-2.621334
	C	-0.095022	-2.375337		C	-4.916998	-1.985762
	C	-3.992564	0.806150		C	-3.620850	-1.865900
	O	-0.535385	0.570678		C	-1.513287	-1.473312
	C	-0.272723	-2.973340		C	-3.004453	-1.296620
	H	-3.913495	2.749742		N	-0.801697	-1.052270
	O	-2.227731	0.887153		N	-3.448957	-0.709261
	C	-1.524837	-3.191138		C	0.612015	-1.078995
	H	-4.795532	1.462942		C	-4.847710	-0.589035
	C	-2.693372	-2.826108		C	-5.580534	-1.719371
	H	-4.356248	-0.213263		C	-6.937618	-1.590521
	H	1.029100	1.461065		C	-7.556821	-0.345122
	C	-2.501338	-2.224459		C	-6.813905	0.778298
	H	-3.493591	1.077367		C	-5.453656	0.665367
	H	-0.564812	1.877788		C	1.355956	-0.477052
	H	-0.069599	2.563216		C	2.743889	-0.467454
	C	-4.035891	-3.027625		C	3.386462	-1.059318
	C	-5.083936	-2.661223		C	2.636770	-1.645076
	C	-4.876061	-2.069940		C	1.247487	-1.641515
	C	-3.577517	-1.843561		H	0.844520	-2.542282
	C	-1.460618	-1.440054		H	0.541898	-3.734716
	C	-2.955025	-1.344138		H	-1.671755	-4.036861
	N	-0.734974	-1.123316		H	-4.287185	-3.630173
	N	-3.387584	-0.940616		H	-6.139268	-2.715729
	C	0.681484	-1.124722		H	-5.762372	-1.611812
	C	-4.778674	-0.829823		H	-5.084413	-2.682895
	C	-5.326336	-1.613680		H	-7.510116	-2.466560
	C	-6.683496	-1.501199		H	-8.616163	-0.249158
	C	-7.480209	-0.597302		H	-7.293308	1.750099
	C	-6.920335	0.196714		H	-4.862381	1.535666
	C	-5.568365	0.083047		H	0.846065	0.005885
	C	1.397934	-0.407494		H	3.324087	0.012793
	C	2.786482	-0.374957		H	4.470322	-1.051839
	C	3.456291	-1.055678		H	3.134953	-2.099283
	C	2.734304	-1.756925		H	0.646322	-2.075057
	C	1.345103	-1.780047		O	-1.692281	-1.286283
	H	0.905979	-2.228394		G		
	H	0.607309	-3.271429			V	0.536307
	H	-1.617919	-3.654644			C	0.846449
	H	-4.239477	-3.483527			C	-2.425661
	H	-6.102894	-2.835449			C	2.760696
	H	-5.727387	-1.805461			C	1.896060
	H	-4.690136	-2.310093			O	-1.158197
	H	-7.117662	-2.120936			O	-0.721922
	H	-8.535205	-0.505899			O	1.500787
	H	-7.535173	0.912172			C	1.606657
	H	-5.119649	0.706102			H	-0.147483
	H	0.867366	0.142474			H	-2.719981
	H	3.345542	0.192155			C	0.314022
	H	4.540316	-1.027879			C	-0.785595
							-0.737555
							-1.682908
							1.325934
							1.177503
							-2.000344
							1.214119
							-0.141322
							0.737289
							-2.386299
							-0.083563
							2.358715
							-2.459193
							-2.153520
							3.620158

H	-3.457759	0.262110	-0.131356
H	2.716337	1.375620	-0.873230
H	5.190234	1.483488	-0.641100
H	6.496120	-0.596520	-0.288505
H	5.329541	-2.784427	-0.158549
H	2.854283	-2.886423	-0.362160
O	0.250679	-2.080818	-3.262591

I

V	-1.223667	-0.212002	-3.082798
C	-0.238136	-1.231713	1.006329
C	-0.988854	2.956636	-2.238618
C	-0.066869	0.101397	-5.429186
C	0.929449	-1.658496	1.613157
O	-0.678114	1.951557	-3.193677
C	0.879812	-2.023538	2.975682
C	0.884725	-0.267133	-4.554205
O	-1.919104	1.406010	-3.680871
C	-0.292743	-1.980498	3.708293
H	-0.638626	-0.636458	-5.984642
C	-1.506934	-1.556925	3.110989
H	-0.022550	3.357948	-1.922557
C	-1.439784	-1.176493	1.760967
H	-0.284258	1.146906	-5.622068
H	-1.529992	2.542888	-1.382070
H	1.497646	0.471806	-4.044920
H	-1.583275	3.739640	-2.714705
C	-2.783298	-1.491381	3.725026
C	-3.887659	-1.081247	3.002806
H	1.138742	-1.312960	-4.404714
C	-3.802457	-0.694761	1.646440
C	-2.569779	-0.733834	1.022593
C	-0.607371	-0.820089	-0.337074
C	-2.075191	-0.486344	-0.328963
N	0.025055	-0.728218	-1.458246
N	-2.580933	-0.132988	-1.460276
C	1.410731	-1.075034	-1.511852
C	-3.925265	0.272230	-1.633888
C	-4.662420	-0.297376	-2.675343
C	-5.976530	0.106970	-2.877767
C	-6.540963	1.097704	-2.076936
C	-5.787927	1.687947	-1.063251
C	-4.480316	1.276452	-0.834346
C	2.378355	-0.110862	-1.231749
C	3.724848	-0.460445	-1.295351
C	4.098638	-1.758065	-1.637948
C	3.122864	-2.711087	-1.923355
C	1.773224	-2.374586	-1.865829
H	1.865152	-1.718226	1.068760
H	1.793006	-2.355922	3.458610
H	-0.287064	-2.280130	4.752700
H	-2.892172	-1.772843	4.768649
H	-4.856779	-1.049196	3.490161
H	-4.695077	-0.374868	1.121137
H	-4.205526	-1.058712	-3.299773
H	-6.558295	-0.347545	-3.673381
H	-7.562410	1.420752	-2.251310
H	-6.216154	2.478641	-0.454965
H	-3.880693	1.748324	-0.061093
H	2.075878	0.897896	-0.966212
H	4.482458	0.285900	-1.077069
H	5.149480	-2.024815	-1.688104
H	3.410337	-3.722264	-2.194388
H	1.001933	-3.105053	-2.092723
O	-1.754549	-1.552599	-3.705377

TS_{II}

V	-1.028914	-0.435804	-3.004724
C	-0.138702	-1.338124	1.137630
C	-2.208538	3.049625	-3.170295
C	-0.116477	0.744866	-5.108229
C	0.992497	-1.833624	1.760676
O	-1.325628	1.939182	-3.119902
C	0.905494	-2.194004	3.122551
C	0.699930	-0.027100	-4.271354
O	-1.760402	1.005840	-4.123143

C	-0.270199	-2.078821	3.841327
H	-0.628921	0.281968	-5.948512
C	-1.449810	-1.588255	3.226921
H	-1.845591	3.728411	-2.394489
C	-1.344903	-1.215333	1.876778
H	0.009319	1.821171	-5.172124
H	-3.236372	2.744126	-2.960638
H	1.468326	0.479146	-3.690829
H	-2.144488	3.532462	-4.149693
C	-2.728443	-1.455439	3.824521
C	-3.801432	-0.995388	3.085814
H	0.930591	-1.044030	-4.580746
C	-3.679496	-0.623781	1.728277
C	-2.442135	-0.724649	1.120188
C	-0.472445	-0.930660	-0.217714
C	-1.922866	-0.523519	-0.231475
N	0.165642	-0.908759	-1.339740
N	-2.406032	-0.171626	-1.373742
C	1.539749	-1.283119	-1.410886
C	-3.724021	0.299301	-1.560971
C	-4.470813	-0.222692	-2.621460
C	-5.757866	0.251356	-2.848039
C	-6.285585	1.266571	-2.052650
C	-5.522652	1.810862	-1.019975
C	-4.242990	1.329744	-0.767931
C	2.523348	-0.434465	-0.900621
C	3.861910	-0.801593	-1.008518
C	4.213237	-2.004729	-1.616906
C	3.223270	-2.840171	-2.130092
C	1.882362	-2.479365	-2.041109
H	1.930489	-1.946742	1.229456
H	1.791932	-2.579304	3.615920
H	-0.295238	-2.374278	4.886625
H	-2.864493	-1.727014	4.867570
H	-4.774425	-0.913415	3.559501
H	-4.550834	-0.269274	1.189809
H	-4.043725	-1.005013	-3.241383
H	-6.346546	-0.168077	-3.657736
H	-7.285614	1.642706	-2.244218
H	-5.921714	2.618440	-0.413829
H	-3.632415	1.767767	0.016372
H	2.239399	0.504517	-0.433895
H	4.630962	-0.141945	-0.618468
H	5.258098	-2.286956	-1.698251
H	3.493861	-3.776703	-2.607756
H	1.101187	-3.116681	-2.445460
O	-1.550285	-1.784700	-3.591737

J

V	-0.925838	-0.506432	-2.917263
C	-0.103095	-1.429527	1.232372
C	-2.726426	2.927329	-3.734795
C	-0.336068	1.007170	-4.931097
C	0.984226	-1.991825	1.875666
O	-1.674885	2.071966	-3.314026
C	0.855935	-2.345188	3.236594
C	0.614780	0.384969	-3.955385
O	-1.661091	0.964432	-4.242178
C	-0.318509	-2.154619	3.939719
H	-0.518520	0.391177	-5.815904
C	-1.456399	-1.596108	3.304988
H	-2.707080	3.744891	-3.009920
C	-1.311072	-1.238101	1.954394
H	-0.179953	2.049524	-5.222921
H	-3.690287	2.413106	-3.696479
H	1.153383	1.113073	-3.340003
H	-2.530560	3.316042	-4.738809
C	-2.732589	-1.383187	3.883931
C	-3.768822	-0.866054	3.129571
H	1.310710	-0.331105	-4.392793
C	-3.610085	-0.518274	1.770550
C	-2.372365	-0.698173	1.180055
C	-0.399447	-1.019839	-0.134072
C	-1.831922	-0.543912	-0.165915
N	0.232924	-1.050784	-1.259197
N	-2.296645	-0.182377	-1.314197

C	1.595035	-1.433078	-1.371296
C	-3.605889	0.319141	-1.509978
C	-4.393333	-0.268045	-2.506842
C	-5.671033	0.233603	-2.744996
C	-6.148413	1.324847	-2.021281
C	-5.343730	1.923433	-1.052425
C	-4.071949	1.424602	-0.791597
C	2.587233	-0.740849	-0.672010
C	3.919302	-1.105365	-0.837742
C	4.258324	-2.155551	-1.688531
C	3.262890	-2.831561	-2.391943
C	1.929573	-2.463222	-2.252888
H	1.922518	-2.162555	1.360784
H	1.710787	-2.783206	3.741618
H	-0.376239	-2.442165	4.985831
H	-2.897102	-1.638687	4.927005
H	-4.740200	-0.722434	3.591672
H	-4.452506	-0.120999	1.216184
H	-4.008408	-1.108840	-3.070068
H	-6.292312	-0.231907	-3.503688
H	-7.142071	1.714829	-2.218222
H	-5.704715	2.786420	-0.501127
H	-3.430667	1.898705	-0.054186
H	2.315882	0.089113	-0.025672
H	4.693984	-0.560745	-0.306784
H	5.298882	-2.437953	-1.813422
H	3.525251	-3.644553	-3.061645
H	1.144666	-2.967705	-2.808697
O	-1.245462	-1.855550	-3.640238

TS_{JK}

V	-0.974930	-0.324806	-2.907868
C	-0.119274	-1.373266	1.214610
C	-2.672063	2.608262	-3.699251
C	-0.012719	1.022365	-5.116553
C	0.981137	-1.942871	1.828469
O	-1.580915	1.702024	-3.578965
C	0.871436	-2.338036	3.179613
C	0.671638	0.363479	-3.947598
O	-1.451792	1.025909	-4.857642
C	-0.297226	-2.182066	3.900636
H	0.035044	0.432839	-6.036803
C	-1.447918	-1.616606	3.295709
H	-2.747368	3.090585	-2.723171
C	-1.321002	-1.215812	1.955388
H	0.286806	2.054662	-5.324846
H	-3.597446	2.076222	-3.930491
H	1.248092	1.063198	-3.332216
H	-2.436490	3.343316	-4.471958
C	-2.719749	-1.434437	3.894450
C	-3.769137	-0.904305	3.167826
H	1.314554	-0.468722	-4.238991
C	-3.628630	-0.512469	1.818767
C	-2.395817	-0.661861	1.210075
C	-0.434549	-0.920786	-0.133803
C	-1.868292	-0.452086	-0.133561
N	0.181958	-0.923442	-1.267475
N	-2.343105	-0.056052	-1.264715
C	1.536948	-1.336972	-1.388710
C	-3.671946	0.402215	-1.436673
C	-4.449079	-0.196649	-2.432424
C	-5.741851	0.265377	-2.659159
C	-6.245282	1.338000	-1.925047
C	-5.454438	1.949015	-0.953100
C	-4.167447	1.483819	-0.701963
C	2.550847	-0.635666	-0.732741
C	3.872953	-1.037534	-0.896167
C	4.178239	-2.132755	-1.701452
C	3.159617	-2.818620	-2.360879
C	1.836106	-2.415268	-2.223140
H	1.915445	-2.087121	1.298607
H	1.736457	-2.781413	3.662138
H	-0.340338	-2.502153	4.937972
H	-2.870453	-1.723762	4.930756
H	-4.736646	-0.784889	3.644687
H	-4.480990	-0.106985	1.286059

H	-4.041332	-1.026236	-3.004134
H	-6.354393	-0.211937	-3.417689
H	-7.249831	1.702586	-2.114955
H	-5.838052	2.794894	-0.390739
H	-3.538877	1.966155	0.041562
H	2.303680	0.225277	-0.117948
H	4.665674	-0.487781	-0.398156
H	5.210700	-2.444045	-1.824850
H	3.395920	-3.667477	-2.994879
H	1.032648	-2.925204	-2.746287
O	-1.345919	-1.687205	-3.579623

K

V	-0.901729	-0.134586	-2.880877
C	-0.163896	-1.558935	1.165697
C	-3.046932	1.003371	-4.739989
C	0.206722	2.217414	-4.183638
C	0.855353	-2.273775	1.766381
O	-1.879779	1.326283	-3.974091
C	0.696945	-2.680615	3.110194
C	0.716671	0.969108	-3.500659
O	-0.969259	1.941886	-4.934200
C	-0.434508	-2.381115	3.844699
H	0.872984	2.609925	-4.962483
C	-1.503183	-1.659208	3.255342
H	-3.750730	0.561221	-4.033274
C	-1.337013	-1.275372	1.914933
H	-0.000657	3.027732	-3.470551
H	-2.781082	0.291584	-5.523930
H	1.361616	1.217476	-2.648819
H	-3.450893	1.927243	-5.156601
C	-2.726489	-1.290753	3.870293
C	-3.695519	-0.600888	3.163749
H	1.287122	0.330647	-4.184272
C	-3.526283	-0.243802	1.809053
C	-2.340491	-0.586080	1.184268
C	-0.413161	-1.014301	-0.166367
C	-1.800056	-0.420074	-0.153169
N	0.215104	-0.977577	-1.291650
N	-2.245722	0.086528	-1.253057
C	1.544401	-1.439893	-1.459735
C	-3.578004	0.590583	-1.336029
C	-4.640781	-0.303915	-1.481532
C	-5.934763	0.192381	-1.614129
C	-6.165294	1.566712	-1.600975
C	-5.096879	2.449997	-1.461665
C	-3.796777	1.968058	-1.337000
C	2.575594	-0.963983	-0.643866
C	3.878226	-1.394963	-0.868505
C	4.150476	-2.299702	-1.893276
C	3.119157	-2.756947	-2.711384
C	1.816029	-2.314927	-2.514773
H	1.766044	-2.522358	1.233604
H	1.498881	-3.242020	3.578669
H	-0.510294	-2.703457	4.879372
H	-2.904207	-1.557877	4.908384
H	-4.621925	-0.332386	3.660995
H	-4.316301	0.280045	1.282669
H	-4.447554	-1.372589	-1.502033
H	-6.763218	-0.499504	-1.730850
H	-7.175846	1.948769	-1.705046
H	-5.272527	3.521255	-1.453641
H	-2.957372	2.649357	-1.238446
H	2.359307	-0.240604	0.137172
H	4.683418	-1.014542	-0.247584
H	5.168534	-2.635471	-2.063490
H	3.330674	-3.452744	-3.517175
H	1.005763	-2.642988	-3.158651
O	-1.115297	-1.394720	-3.786363

TS_{KL}

V	-0.975470	-0.090534	-2.923401
C	-0.159007	-1.502998	1.157015
C	-2.980206	1.093414	-4.707775
C	0.358928	2.230329	-4.050057
C	0.874292	-2.198865	1.755832

O	-1.886405	1.253594	-3.813768
C	0.728794	-2.600491	3.102672
C	0.735859	0.822001	-3.627182
O	-0.761668	2.287751	-4.829034
C	-0.404063	-2.315482	3.841005
H	1.131607	2.626244	-4.741120
C	-1.486936	-1.613052	3.253913
H	-3.816885	0.692906	-4.126146
C	-1.332349	-1.231729	1.911590
H	0.310486	2.924309	-3.194012
H	-2.713752	0.402386	-5.510732
H	1.551669	0.828608	-2.898008
H	-3.243874	2.074433	-5.105575
C	-2.714132	-1.262501	3.872084
C	-3.697669	-0.592128	3.166793
H	1.027521	0.200533	-4.481410
C	-3.539583	-0.236309	1.810235
C	-2.349876	-0.559856	1.183735
C	-0.422567	-0.962631	-0.173974
C	-1.816766	-0.393552	-0.155521
N	0.191590	-0.915981	-1.305227
N	-2.273924	0.080145	-1.262674
C	1.514104	-1.402655	-1.475899
C	-3.619303	0.551019	-1.349979
C	-4.651270	-0.371007	-1.532069
C	-5.960174	0.088803	-1.651373
C	-6.233533	1.453625	-1.590763
C	-5.193455	2.364881	-1.418151
C	-3.879448	1.920172	-1.304500
C	2.563636	-0.903761	-0.698905
C	3.856882	-1.365283	-0.921298
C	4.100485	-2.321647	-1.905257
C	3.050020	-2.802327	-2.684652
C	1.756251	-2.332028	-2.489976
H	1.785508	-2.436798	1.219211
H	1.541479	-3.146939	3.570292
H	-0.469927	-2.634773	4.877321
H	-2.883424	-1.528505	4.911865
H	-4.626634	-0.337969	3.666781
H	-4.339267	0.273088	1.283990
H	-4.424171	-1.431634	-1.588416
H	-6.766081	-0.624237	-1.795194
H	-7.255238	1.807523	-1.685176
H	-5.402459	3.429328	-1.375994
H	-3.061197	2.623029	-1.183713
H	2.368251	-0.143816	0.052482
H	4.676437	-0.969425	-0.329466
H	5.110723	-2.680966	-2.073804
H	3.238844	-3.540009	-3.458242
H	0.931292	-2.680584	-3.103675
O	-1.219343	-1.402745	-3.733000

L

V	-1.101530	0.082062	-2.905137
C	-0.134716	-1.427184	1.181273
C	-2.952220	1.446603	-4.694451
C	0.619580	1.639518	-4.781280
C	0.944201	-2.080263	1.746191
O	-2.049761	1.327741	-3.613163
C	0.836170	-2.531631	3.080737
C	0.696857	0.801428	-3.509676
O	-0.078631	1.115883	-5.820781
C	-0.307692	-2.344633	3.833285
H	1.636749	1.912060	-5.130301
C	-1.436279	-1.689236	3.278450
H	-3.941133	1.686901	-4.291862
C	-1.312602	-1.241427	1.953545
H	0.146507	2.621486	-4.572082
H	-2.985029	0.517064	-5.269461
H	1.057626	1.406192	-2.663755
H	-2.614261	2.264592	-5.337156
C	-2.682468	-1.451782	3.911697
C	-3.711982	-0.823509	3.234396
H	1.372460	-0.047137	-3.640932
C	-3.578713	-0.388588	1.898405
C	-2.370604	-0.595842	1.257780

C	-0.444175	-0.867730	-0.130280
C	-1.856954	-0.361160	-0.080267
N	0.145100	-0.785191	-1.269996
N	-2.342681	0.074846	-1.189670
C	1.468340	-1.284334	-1.433050
C	-3.685763	0.545708	-1.277654
C	-4.610104	-0.193536	-2.015828
C	-5.919996	0.265768	-2.116918
C	-6.295181	1.462213	-1.508903
C	-5.357155	2.204632	-0.794166
C	-4.047119	1.750305	-0.673544
C	2.539209	-0.672725	-0.778759
C	3.827677	-1.160429	-0.977580
C	4.043140	-2.250151	-1.818300
C	2.968194	-2.846003	-2.475637
C	1.677658	-2.357942	-2.300238
H	1.860286	-2.247925	1.191705
H	1.684136	-3.042804	3.524961
H	-0.347847	-2.707266	4.856600
H	-2.830171	-1.773532	4.938917
H	-4.656895	-0.660128	3.742372
H	-4.410106	0.096700	1.399856
H	-4.302154	-1.119223	-2.493563
H	-6.647710	-0.313534	-2.676674
H	-7.315923	1.820093	-1.598716
H	-5.642440	3.144449	-0.331620
H	-3.305411	2.327683	-0.129307
H	2.362340	0.183226	-0.133467
H	4.664507	-0.681648	-0.478408
H	5.049336	-2.627573	-1.970435
H	3.133994	-3.689991	-3.137825
H	0.833935	-2.796508	-2.824352
O	-1.318995	-1.231684	-3.707280

TS_{LM}

V	-1.047194	0.131361	-2.943780
C	-0.128232	-1.412145	1.149015
C	-2.940818	1.645454	-4.522220
C	0.615717	1.416967	-4.817340
C	0.937341	-2.083898	1.717410
O	-2.031825	1.468645	-3.457810
C	0.810968	-2.549883	3.045259
C	0.810178	0.990010	-3.374965
O	-0.223655	0.359966	-5.145042
C	-0.337747	-2.358490	3.789328
H	1.515068	1.461377	-5.442240
C	-1.453649	-1.684705	3.231249
H	-3.880543	1.130013	-4.296848
C	-1.312396	-1.224508	1.912369
H	0.068407	2.371991	-4.852298
H	-2.511793	1.239580	-5.445288
H	0.795893	1.812538	-2.648849
H	-3.136802	2.715564	-4.633604
C	-2.703383	-1.440066	3.855185
C	-3.719560	-0.794329	3.174725
H	1.649737	0.313592	-3.246513
C	-3.569987	-0.350287	1.842902
C	-2.358117	-0.564192	1.213360
C	-0.418785	-0.827353	-0.156705
C	-1.827492	-0.320392	-0.117070
N	0.178605	-0.728491	-1.290538
N	-2.300116	0.116213	-1.228904
C	1.488854	-1.259353	-1.458734
C	-3.654057	0.554097	-1.320442
C	-4.582787	-0.263869	-1.963929
C	-5.906449	0.157921	-2.058171
C	-6.291414	1.390320	-1.534444
C	-5.349509	2.207724	-0.912592
C	-4.024965	1.794604	-0.802357
C	2.571359	-0.703452	-0.773301
C	3.846327	-1.223591	-0.977164
C	4.036953	-2.289086	-1.854422
C	2.951351	-2.827088	-2.543385
C	1.674209	-2.306677	-2.362843
H	1.857146	-2.256116	1.170655
H	1.648825	-3.075906	3.491356

H	-0.391481	-2.732210	4.808035
H	-2.864144	-1.770649	4.877619
H	-4.667274	-0.625420	3.675661
H	-4.391791	0.146182	1.339158
H	-4.266679	-1.218021	-2.375358
H	-6.637018	-0.480323	-2.545522
H	-7.323283	1.716763	-1.616770
H	-5.643635	3.173758	-0.513908
H	-3.279923	2.427887	-0.330190
H	2.413946	0.135372	-0.101143
H	4.692136	-0.788896	-0.453389
H	5.032736	-2.691738	-2.010482
H	3.098463	-3.651390	-3.234171
H	0.822269	-2.697936	-2.910296
O	-1.366384	-1.272534	-3.542562

M

V	-1.192365	-0.152641	-3.094644
C	-0.150589	-1.447398	1.031232
C	-3.130072	1.477540	-4.524082
C	1.294232	0.970522	-3.903763
C	0.938184	-2.095275	1.584894
O	-2.056249	1.256641	-3.635370
C	0.871740	-2.490899	2.938923
C	0.985877	2.017714	-2.895451
O	0.299742	-0.041152	-4.003927
C	-0.240914	-2.253621	3.724399
H	2.246217	0.473128	-3.686523
C	-1.379189	-1.603167	3.184664
H	-3.557407	0.528446	-4.863814
C	-1.297870	-1.213451	1.838145
H	1.375631	1.412174	-4.910812
H	-2.756598	2.040145	-5.386282
H	0.060069	2.580755	-2.968603
H	-3.898724	2.065737	-4.013331
C	-2.597802	-1.319720	3.852520
C	-3.641779	-0.704979	3.186442
H	1.755269	2.373787	-2.219363
C	-3.551624	-0.330851	1.827423
C	-2.371844	-0.584686	1.154903
C	-0.504011	-0.945747	-0.291409
C	-1.904892	-0.417325	-0.212666
N	0.040197	-0.918306	-1.458697
N	-2.416016	-0.014029	-1.318028
C	1.368940	-1.376552	-1.666798
C	-3.745993	0.487493	-1.382038
C	-4.724826	-0.271255	-2.023954
C	-6.022995	0.224033	-2.102200
C	-6.334249	1.473036	-1.568523
C	-5.343051	2.232368	-0.949290
C	-4.043518	1.743554	-0.851459
C	2.434649	-0.773151	-0.993537
C	3.733052	-1.209882	-1.237897
C	3.964909	-2.242369	-2.144705
C	2.896351	-2.830365	-2.819903
C	1.596271	-2.390610	-2.598367
H	1.831502	-2.300254	1.006344
H	1.727220	-2.998286	3.372999
H	-0.248236	-2.573621	4.762638
H	-2.711826	-1.595849	4.897109
H	-4.565245	-0.505295	3.720296
H	-4.394056	0.143600	1.336653
H	-4.463657	-1.235269	-2.449784
H	-6.792198	-0.368406	-2.587908
H	-7.346661	1.857675	-1.640885
H	-5.579031	3.211024	-0.542706

H	-3.260355	2.331370	-0.381831
H	2.243499	0.042302	-0.301642
H	4.564175	-0.736946	-0.723710
H	4.978721	-2.581199	-2.333320
H	3.075580	-3.629088	-3.532674
H	0.758946	-2.825162	-3.134868
O	-1.903529	-1.409330	-3.671122

TS_{MF}

V	-1.286123	-0.250397	-2.923922
C	-0.198307	-1.260858	1.190227
C	-2.643699	1.712454	-4.582038
C	0.757983	1.095125	-4.634185
C	0.944099	-1.820259	1.736751
O	-2.081791	1.279868	-3.371618
C	0.928335	-2.190259	3.097744
C	2.003130	0.356094	-4.360499
O	-0.005726	-0.017640	-4.229146
C	-0.188337	-2.018108	3.896057
H	0.578033	1.319046	-5.689365
C	-1.379179	-1.463342	3.365164
H	-2.796892	2.796152	-4.534755
C	-1.346831	-1.090450	2.011173
H	0.590264	1.983198	-4.017025
H	-3.613265	1.228307	-4.752047
H	2.450459	0.369812	-3.374013
H	-1.988059	1.481478	-5.433169
C	-2.605317	-1.265722	4.049836
C	-3.700615	-0.747692	3.387301
H	2.356741	-0.367763	-5.085379
C	-3.654933	-0.385622	2.021422
C	-2.470065	-0.551948	1.332590
C	-0.601722	-0.817048	-0.135029
C	-2.037981	-0.383414	-0.053917
N	-0.034559	-0.778927	-1.297668
N	-2.588707	-0.061778	-1.167787
C	1.324333	-1.169352	-1.459567
C	-3.917097	0.404996	-1.276303
C	-4.772561	-0.222990	-2.185430
C	-6.078728	0.233545	-2.316454
C	-6.518755	1.333258	-1.581413
C	-5.647709	1.979432	-0.706505
C	-4.346086	1.517055	-0.546362
C	2.345859	-0.414049	-0.877300
C	3.672036	-0.785267	-1.082791
C	3.975351	-1.902472	-1.860551
C	2.949492	-2.644775	-2.442394
C	1.620362	-2.275329	-2.257251
H	1.839442	-1.977776	1.146808
H	1.823870	-2.626992	3.527811
H	-0.157177	-2.319153	4.939633
H	-2.682127	-1.532465	5.100111
H	-4.632026	-0.613268	3.927865
H	-4.539564	0.014096	1.538952
H	-4.407880	-1.066449	-2.763524
H	-6.753209	-0.266677	-3.004493
H	-7.535300	1.694823	-1.700446
H	-5.978667	2.852424	-0.152317
H	-3.652709	2.030296	0.113622
H	2.098725	0.457789	-0.277925
H	4.468645	-0.198837	-0.635065
H	5.010327	-2.190442	-2.015784
H	3.182435	-3.514151	-3.049438
H	0.812677	-2.836174	-2.718410
O	-1.977296	-1.554499	-3.438087

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