Electronic Supplementary Information for

A computational study on the hydrogenation of CO_2 catalyzed by a tetraphos-ligated cobalt complex: monohydride *vs.* dihydride

Hui Gao,[a,b] Limin Chen,[b] Jinzhu Chen,*[a,c] Yuanyuan Guo[a] and Daiqi Ye[b]

[a] CAS Key Laboratory of Renewable Energy, Guangzhou Institute of Energy Conversion, Chinese Academy of Sciences, Guangzhou 510640, P. R. China; [b] Guangdong Provincial Key Laboratory of Atmospheric Environment and Pollution Control, College of Environment and Energy, South China University of Technology, Guangzhou 510006, P. R. China; [c] *State Key Laboratory of Elemento-organic Chemistry, Nankai University, Tianjin 300071, P. R. China.*

Fax/Tel.: +86 20 3722 3380

E-mail: chenjz@ms.giec.ac.cn

Contents of the Supporting Information

I. Complete list of authors for references with more than 10 authors……..…….... S2

II. **Fig. S1** The calculated structure of the tetraphos-ligated cobalt dihydride **2** optimized by the wB97XD and M06 functional, respectively……. ……...…..... ....…..... S3

III. **Fig. S2** Depicted is optimized structures of $\mathbf{TS_{associative}}$ in another alternative pathway via the carbon atom of CO_2 coordination to Co center……. ……...…..... ....…..... S3

IV. **Fig. S3** Relative free energy, zero-point corrected energy and enthalpy profiles for the hydrogenation of carbon dioxide catalyzed by tetraphos-ligated cobalt **monohydride** complex, respectively. ……..S4

V. **Fig. S4** Relative free energy, zero-point corrected energy and enthalpy profiles for the hydrogenation of carbon dioxide catalyzed by tetraphos-ligated cobalt **dihydride** complex, respectively. ……....S4

VI. **Table S1** Relative enthalpy and zero point energy profiles for the key transition state compared to the starting point structure **2** optimized by the wB97XD and M06 functional, respectively. ……....S4

VII. Cartesian coordinates for all of the relevant species (wB97XD/TZVP)…….…….....S5

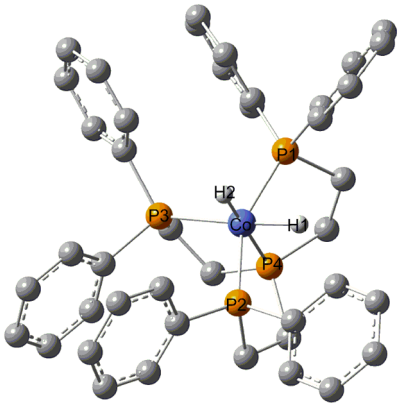
VIII. Electronic energies, zero-point corrected energies, enthalpies and free energies (wB97XD/TZVP) for all of the relevant species... ……..…....S22

IX. Electronic energies (wB97XD/6-311++G(d,p)(SDD for Co)//wB97XD/TZVP) for all of the relevant species……..…....S29

X. Electronic energies (wB97XD/6-31+G(d,p)//wB97XD/TZVP) for all of the relevant species……..…....S33

Complete list of authors for references with more than 10 authors:

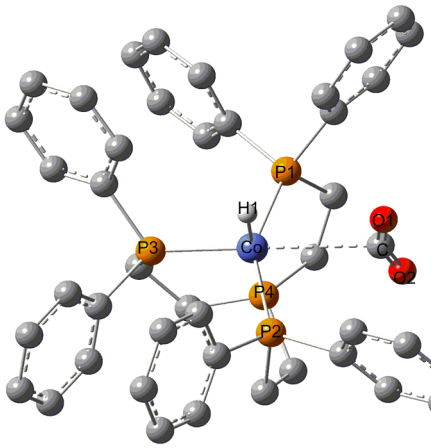
(45) M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian 09, Revision C.01, Gaussian, Inc., Wallingford CT, 2010.



	Calc. *w*B97XD	Calc. M06	Exp.
Co-P1	**2.19**	2.20	2.169(2)
Co-P2	**2.19**	2.21	2.165(2)
Co-P3	**2.24**	2.24	2.196(2)
Co-P4	**2.19**	2.19	2.138(2)
Co-H1	**1.47**	1.48	1.28(8)
Co-H2	**1.50**	1.52	1.51(6)
P1-Co-P2	**152.2**	151.5	152.54(8)
P1-Co-P3	**103.4**	103.2	103.08(8)
P2-Co-P3	**103.6**	104.5	104.00(8)
P4-Co-P1	**87.0**	87.2	88.24(8)
P4-Co-P2	**87.7**	87.4	87.99(7)
P4-Co-P3	**87.6**	87.3	88.65(8)
H1-Co-H2	**89.7**	89.3	88(4)
P4-Co-H1	**88.4**	88.6	
P4-Co-H2	**177.7**	**177.6**	

2

Fig. S1 The calculated structure of the tetraphos-ligated cobalt dihydride **2** optimized by the wB97XD and M06 functional, respectively, with some hydrogen atoms are omitted for clarity. The distances and angles are in Å and deg, respectively. The experimental values were cited from the X-ray data.[43]



Co-P1	2.19
Co-P2	2.22
Co-P3	2.24
Co-P4	2.17
Co-H1	1.52
Co-C	**2.82**
Co-O1	3.27
Co-O2	3.32
P1-Co-P2	149.7
P1-Co-P3	105.6
P2-Co-P3	103.4
P4-Co-P1	85.3
P4-Co-P2	87.3
P4-Co-P3	87.3
P4-Co-H1	177.5
P3-Co-C	**179.3**

$TS_{associative}$

Fig. S2 Depicted is optimized structures of **$TS_{associative}$** in another alternative pathway via the carbon atom of CO_2 coordination to Co. Some hydrogen atoms are omitted for clarity. The distances and angles are in Å and deg, respectively. The relevant Cartesian coordinates and energies are listed on page S20 and S28, respectively.

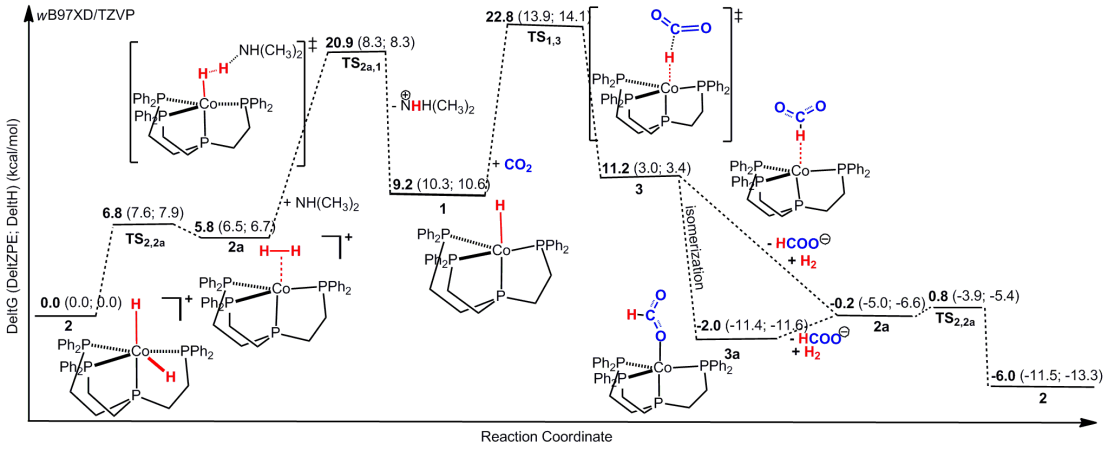


Fig. S3 Shown are relative free energy (G), zero-point corrected energy (ZPE) and enthalpy (H) profiles for the hydrogenation of carbon dioxide catalyzed by tetraphos-ligated cobalt **monohydride** complex, respectively.

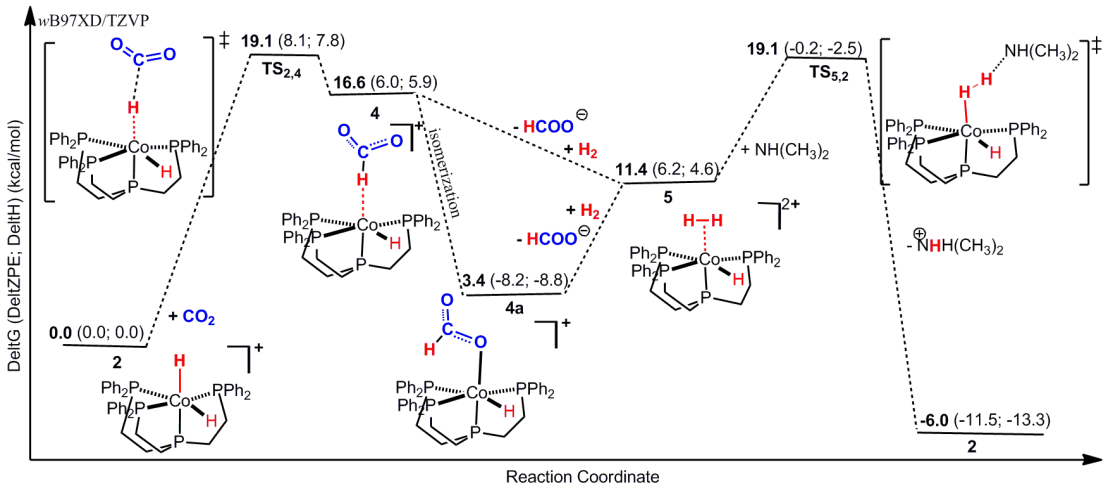


Fig. S4 Shown are relative free energy (G), zero-point corrected energy (ZPE) and enthalpy (H) profiles for the hydrogenation of carbon dioxide catalyzed by tetraphos-ligated cobalt **dihydride** complex, respectively.

Table S1 Relative enthalpy and zero point energy profiles for the key transition state compared to the starting point structure **2** optimized by the wB97XD and M06 functional, respectively.

DFT	Delt H (kcal mol^{-1})		Delt (ZPE) (kcal mol^{-1})	
	$TS_{1,3}$	**$TS_{2,4}$**	**$TS_{1,3}$**	**$TS_{2,4}$**
wB97XD	14.1	7.8	13.9	8.1
M06	13.3	9.9	13.5	10.5

Cartesian coordinates for all of the species (in Å) (wB97XD/TZVP).

1

P	0.680898	-1.891760	0.481445
P	1.513320	1.633261	0.385618
P	-0.061979	0.208810	2.455812
P	-2.170652	0.445743	0.388996
C	-0.553947	-3.250111	0.194407
C	-1.129713	-3.354065	-1.073830
C	-2.105173	-4.301667	-1.338478
C	-2.546658	-5.150484	-0.329968
C	-1.993543	-5.047682	0.937139
C	-1.000648	-4.108403	1.195998
C	2.094485	-2.526441	-0.534049
C	2.096736	-2.254962	-1.902574
C	3.105506	-2.737357	-2.722971
C	4.151012	-3.472990	-2.180633
C	4.173328	-3.728448	-0.816929
C	3.147508	-3.267578	-0.000459
C	3.229183	1.006820	0.084918
C	3.648047	0.791878	-1.228167
C	4.868677	0.191468	-1.495931
C	5.689961	-0.217734	-0.452656
C	5.284242	-0.008764	0.857631
C	4.063545	0.599544	1.123732
C	1.542241	3.156475	-0.666934
C	0.558129	3.343494	-1.630997
C	0.542578	4.492307	-2.413910
C	1.513478	5.466616	-2.235943
C	2.503209	5.288425	-1.275220
C	2.518293	4.139548	-0.499119
C	-2.905464	2.137167	0.118792
C	-2.161973	3.244140	0.525131
C	-2.665080	4.530885	0.392010
C	-3.920133	4.731443	-0.167000
C	-4.669856	3.637333	-0.578606
C	-4.168117	2.350416	-0.432202
C	-3.292747	-0.582951	-0.656218
C	-4.303234	-1.392096	-0.144425
C	-5.090176	-2.164394	-0.992034
C	-4.885060	-2.127488	-2.362733
C	-3.882264	-1.318452	-2.884511
C	-3.088787	-0.561997	-2.037253
C	1.256099	-2.175985	2.231772
C	0.314555	-1.450073	3.190863
C	1.600018	2.389057	2.098236
C	1.197331	1.371528	3.165194
C	-1.727209	0.681531	3.107528
C	-2.760091	0.114637	2.134733
H	-0.035336	0.131010	-1.218789
H	-0.822125	-2.677355	-1.862643
H	-2.535414	-4.367630	-2.330889
H	-3.318679	-5.883559	-0.532148
H	-2.330291	-5.703334	1.732047
H	-0.583085	-4.057449	2.193660
H	1.306316	-1.647538	-2.328216
H	3.084754	-2.521394	-3.784898
H	4.948161	-3.838655	-2.817334
H	4.989960	-4.293669	-0.382735
H	3.181664	-3.495906	1.057492
H	3.008941	1.087505	-2.053669
H	5.173762	0.030196	-2.523324
H	6.639096	-0.697637	-0.660132
H	5.918604	-0.320638	1.679518
H	3.772308	0.750133	2.155847
H	-0.204414	2.584435	-1.765933
H	-0.230438	4.623310	-3.162255
H	1.502552	6.364355	-2.843178
H	3.265631	6.045886	-1.134144
H	3.300097	4.007100	0.241142
H	-1.171706	3.096103	0.941046
H	-2.069511	5.377790	0.713282
H	-4.312106	5.735050	-0.284337
H	-5.649367	3.784615	-1.018952
H	-4.771181	1.510171	-0.755374
H	-4.494822	-1.430841	0.920328
H	-5.866894	-2.795067	-0.575175
H	-5.499594	-2.729040	-3.022146
H	-3.711142	-1.285101	-3.954264
H	-2.296245	0.050783	-2.453233
H	1.366229	-3.231385	2.484883
H	2.250208	-1.723133	2.280602
H	0.745030	-1.354273	4.189656
H	-0.636288	-1.980393	3.284723

H	2.579517	2.825617	2.302447
H	0.877284	3.207980	2.071650
H	0.812209	1.856622	4.064180
H	2.050220	0.758996	3.464877
H	-1.880609	0.314098	4.124281
H	-1.771313	1.773300	3.132260
H	-3.755063	0.526422	2.312877
H	-2.812877	-0.970930	2.251497
Co	-0.034355	0.142041	0.309683

1a

P	0.246470	-1.701787	0.397966
P	2.010372	1.237237	0.383538
P	0.017222	0.411042	2.530097
P	-2.124523	0.798412	0.341888
C	-1.218368	-2.807432	0.132969
C	-1.654436	-3.057957	-1.168215
C	-2.754178	-3.866803	-1.406913
C	-3.452248	-4.428042	-0.344627
C	-3.040505	-4.171096	0.953720
C	-1.930398	-3.368138	1.190345
C	1.462739	-2.546373	-0.712998
C	1.594330	-2.072862	-2.016838
C	2.444821	-2.697657	-2.917230
C	3.196983	-3.792949	-2.515585
C	3.087275	-4.261979	-1.213184
C	2.218617	-3.648760	-0.319417
C	3.499995	0.137844	0.350696
C	4.096352	-0.184888	-0.868198
C	5.142654	-1.092221	-0.930320
C	5.608042	-1.701838	0.228441
C	5.025190	-1.388067	1.447235
C	3.980293	-0.473743	1.506669
C	2.605744	2.607385	-0.716361
C	1.821991	2.993979	-1.796749
C	2.227428	4.025691	-2.636116
C	3.427678	4.679296	-2.399872
C	4.221729	4.298098	-1.323150
C	3.813611	3.268523	-0.488554
C	-2.799549	2.507478	0.019737
C	-1.995651	3.499411	-0.530676
C	-2.504728	4.765999	-0.795106
C	-3.830500	5.056533	-0.511698
C	-4.647124	4.071556	0.032101
C	-4.135646	2.808914	0.290771
C	-3.411468	-0.140465	-0.611134
C	-4.493472	-0.806349	-0.044091
C	-5.438664	-1.432438	-0.850178
C	-5.317468	-1.394506	-2.230675
C	-4.236459	-0.736826	-2.806495
C	-3.290443	-0.123656	-2.001303
C	0.828769	-2.190482	2.114287
C	0.176979	-1.316148	3.191383
C	2.171883	2.109045	2.056056
C	1.434911	1.404427	3.208044
C	-1.616642	1.050648	3.119186
C	-2.672468	0.537255	2.130300
H	-0.088254	1.944570	0.576822
H	-1.131083	-2.619565	-2.010113
H	-3.071825	-4.052679	-2.426144
H	-4.315752	-5.055730	-0.530734
H	-3.578135	-4.599683	1.791553
H	-1.629964	-3.195276	2.215110
H	1.034360	-1.194921	-2.321778
H	2.533526	-2.316377	-3.927896
H	3.873025	-4.275226	-3.211922
H	3.677416	-5.111908	-0.890491
H	2.136073	-4.041260	0.686832
H	3.736819	0.273505	-1.782715
H	5.591282	-1.330461	-1.887634
H	6.419594	-2.418360	0.179924
H	5.382947	-1.854394	2.357955
H	3.540329	-0.248278	2.469914
H	0.886807	2.474278	-1.979331
H	1.605457	4.314215	-3.475737
H	3.748342	5.481976	-3.053799
H	5.162639	4.803289	-1.137417
H	4.446741	2.974035	0.341410
H	-0.958442	3.281857	-0.754294
H	-1.859405	5.524151	-1.223925
H	-4.230179	6.043201	-0.714999
H	-5.686970	4.285746	0.250318
H	-4.794958	2.051026	0.699294
H	-4.620173	-0.841203	1.030560
H	-6.273670	-1.949680	-0.391670
H	-6.056436	-1.880694	-2.856833

H	-4.126934	-0.708062	-3.884471
H	-2.441070	0.375610	-2.457429
H	0.672738	-3.252900	2.310297
H	1.906631	-2.014394	2.102515
H	0.750557	-1.344549	4.120019
H	-0.833528	-1.661436	3.420386
H	3.222151	2.275602	2.303377
H	1.719244	3.086675	1.878548
H	1.085681	2.131806	3.943349
H	2.095479	0.711200	3.731408
H	-1.854092	0.741626	4.139438
H	-1.562887	2.142380	3.096685
H	-3.646266	0.987085	2.331539
H	-2.779141	-0.545159	2.251088
Co	0.006763	0.470829	0.407079

2

P	0.239839	-1.700786	0.401463
P	2.034655	1.273827	0.453596
P	-0.011129	0.495954	2.523729
P	-2.192539	0.792824	0.432063
C	-1.205846	-2.818784	0.150390
C	-1.619217	-3.110504	-1.149029
C	-2.690133	-3.960040	-1.374382
C	-3.374682	-4.520595	-0.303533
C	-2.982093	-4.222133	0.991772
C	-1.902861	-3.376574	1.218560
C	1.463808	-2.464855	-0.734407
C	1.576814	-1.971404	-2.031655
C	2.443142	-2.566463	-2.936937
C	3.217765	-3.650035	-2.547554
C	3.118271	-4.140006	-1.252040
C	2.239799	-3.556210	-0.349896
C	3.490821	0.146757	0.456376
C	4.084676	-0.208849	-0.753689
C	5.136697	-1.110408	-0.783692
C	5.605551	-1.674740	0.395709
C	5.024005	-1.322673	1.604688
C	3.973188	-0.415063	1.635624
C	2.565913	2.550707	-0.754823
C	1.769215	2.894603	-1.840147
C	2.186209	3.874616	-2.733218
C	3.400190	4.517328	-2.543969
C	4.201696	4.178094	-1.459626
C	3.788834	3.198485	-0.571130
C	-2.848486	2.482003	0.063246
C	-2.070031	3.451782	-0.557753
C	-2.607398	4.695254	-0.868999
C	-3.928931	4.979908	-0.562704
C	-4.717430	4.012872	0.049906
C	-4.183146	2.771141	0.354044
C	-3.343118	-0.196259	-0.600197
C	-4.434490	-0.881204	-0.077021
C	-5.323181	-1.528084	-0.927556
C	-5.130509	-1.490500	-2.300264
C	-4.036822	-0.813637	-2.826142
C	-3.145892	-0.173719	-1.980258
C	0.841169	-2.113305	2.110731
C	0.164343	-1.231011	3.160654
C	2.135324	2.197018	2.070958
C	1.384137	1.496403	3.207346
C	-1.642460	1.096301	3.125224
C	-2.702276	0.501864	2.194534
H	-0.059033	0.586891	-1.157853
H	-1.100787	-2.679290	-1.997095
H	-2.993196	-4.180686	-2.390785
H	-4.212300	-5.184726	-0.480491
H	-3.508968	-4.652695	1.835066
H	-1.613873	-3.174160	2.240884
H	0.993636	-1.108555	-2.331489
H	2.523022	-2.172469	-3.943134
H	3.903905	-4.108384	-3.249903
H	3.725199	-4.982110	-0.941147
H	2.163600	-3.961464	0.651717
H	3.726230	0.220143	-1.681808
H	5.587919	-1.376933	-1.731773
H	6.423028	-2.385518	0.371644
H	5.388831	-1.752020	2.530206
H	3.538332	-0.154312	2.591810
H	0.822542	2.391280	-1.990276
H	1.558982	4.131979	-3.578564
H	3.725804	5.279842	-3.241614
H	5.152312	4.675806	-1.309115
H	4.427907	2.933696	0.263847
H	-1.037404	3.242130	-0.804060
H	-1.987087	5.439653	-1.354146

H	-4.348318	5.949682	-0.803032
H	-5.754039	4.223460	0.284546
H	-4.820826	2.023200	0.811677
H	-4.608726	-0.914711	0.991069
H	-6.169537	-2.060959	-0.510713
H	-5.826723	-1.993898	-2.960483
H	-3.875120	-0.787720	-3.897219
H	-2.290495	0.347840	-2.395968
H	0.704274	-3.171731	2.334677
H	1.914496	-1.916577	2.092712
H	0.727544	-1.230388	4.095037
H	-0.842486	-1.585352	3.387781
H	3.175837	2.388848	2.335641
H	1.664092	3.156793	1.852659
H	1.000177	2.222339	3.925038
H	2.032941	0.812452	3.755013
H	-1.817264	0.811142	4.163449
H	-1.634657	2.186896	3.063117
H	-3.688560	0.913122	2.406845
H	-2.756349	-0.582108	2.328646
Co	-0.016476	0.522123	0.335796
H	-0.087799	1.986462	0.393503

2a

P	0.746009	-1.905128	0.490218
P	1.505881	1.677381	0.390838
P	-0.097220	0.205831	2.442153
P	-2.257361	0.406736	0.406240
C	-0.464064	-3.280765	0.236612
C	-1.115963	-3.353643	-0.995212
C	-2.045020	-4.349843	-1.247286
C	-2.359972	-5.274472	-0.258667
C	-1.729963	-5.200254	0.974283
C	-0.781252	-4.213801	1.219269
C	2.150512	-2.467000	-0.563034
C	2.069257	-2.261499	-1.940579
C	3.079720	-2.699560	-2.782099
C	4.201243	-3.326315	-2.254787
C	4.301034	-3.515611	-0.884441
C	3.279678	-3.093709	-0.041716
C	3.219483	1.052998	0.125892
C	3.629802	0.787710	-1.180941
C	4.866822	0.215808	-1.430104
C	5.708826	-0.113431	-0.374922
C	5.307859	0.142887	0.927513
C	4.069988	0.723536	1.177355
C	1.503535	3.180923	-0.675518
C	0.478989	3.394248	-1.590582
C	0.457108	4.545481	-2.369023
C	1.459811	5.493664	-2.233811
C	2.488183	5.288364	-1.320446
C	2.511300	4.137964	-0.548118
C	-2.987961	2.087903	0.150801
C	-2.235588	3.200876	0.518890
C	-2.752368	4.481997	0.384504
C	-4.026548	4.665324	-0.134488
C	-4.783911	3.562001	-0.506603
C	-4.269889	2.280902	-0.361474
C	-3.317484	-0.637410	-0.669378
C	-4.308596	-1.481243	-0.178013
C	-5.059988	-2.262929	-1.047650
C	-4.834431	-2.200938	-2.414401
C	-3.849483	-1.356231	-2.912926
C	-3.091514	-0.586576	-2.045456
C	1.341800	-2.105783	2.230684
C	0.332542	-1.439251	3.160874
C	1.515458	2.425476	2.094334
C	1.136595	1.388249	3.145506
C	-1.766003	0.635230	3.092975
C	-2.792336	0.024112	2.143384
H	-0.167567	-0.325099	-1.241758
H	-0.903356	-2.619612	-1.763884
H	-2.534694	-4.396200	-2.212404
H	-3.096634	-6.045919	-0.449024
H	-1.971346	-5.915230	1.752034
H	-0.297212	-4.186145	2.187018
H	1.211899	-1.752002	-2.365219
H	2.996985	-2.536975	-3.850179
H	4.996989	-3.659609	-2.910375
H	5.176836	-3.995165	-0.463414
H	3.376442	-3.265598	1.022784
H	2.976257	1.026831	-2.013251
H	5.170645	0.017748	-2.451067
H	6.671717	-0.570938	-0.568420
H	5.958458	-0.108957	1.756869
H	3.785269	0.916914	2.203657

H	-0.314598	2.663581	-1.694354
H	-0.346046	4.698501	-3.080178
H	1.443469	6.393015	-2.838230
H	3.274054	6.026715	-1.212840
H	3.321386	3.982937	0.156019
H	-1.231762	3.065467	0.903744
H	-2.152491	5.337136	0.673572
H	-4.428997	5.664619	-0.251877
H	-5.778273	3.698266	-0.915498
H	-4.874867	1.430959	-0.654362
H	-4.509256	-1.539892	0.884134
H	-5.823967	-2.921647	-0.651903
H	-5.422411	-2.810467	-3.090242
H	-3.666637	-1.303154	-3.979668
H	-2.318051	0.061892	-2.443031
H	1.522669	-3.146416	2.500260
H	2.300303	-1.582074	2.277819
H	0.725678	-1.321538	4.171998
H	-0.591480	-2.018894	3.221168
H	2.474686	2.897197	2.312940
H	0.763123	3.215845	2.053801
H	0.730687	1.852101	4.045933
H	2.001197	0.793615	3.444739
H	-1.886424	0.271156	4.114657
H	-1.842830	1.724840	3.108794
H	-3.799614	0.392449	2.340891
H	-2.793782	-1.063736	2.247740
Co	-0.064673	0.136663	0.271084
H	-0.063193	0.518940	-1.267602

$TS_{2,2a}$

P	0.238771	-1.798851	0.445030
P	1.954350	1.306261	0.368659
P	-0.081164	0.546107	2.405401
P	-2.194714	0.808809	0.367372
C	-1.231244	-2.895579	0.229778
C	-1.721801	-3.098278	-1.061065
C	-2.834119	-3.893994	-1.278407
C	-3.491426	-4.482723	-0.204703
C	-3.021446	-4.274610	1.082379
C	-1.894837	-3.488805	1.299734
C	1.477030	-2.677909	-0.593896
C	1.582758	-2.339030	-1.941128
C	2.453321	-3.025101	-2.774690
C	3.250247	-4.040447	-2.263618
C	3.168329	-4.368396	-0.917284
C	2.280964	-3.696664	-0.087215
C	3.421964	0.190835	0.393644
C	3.957527	-0.244803	-0.818030
C	5.000499	-1.156694	-0.840855
C	5.516517	-1.656285	0.348395
C	4.990277	-1.228588	1.558094
C	3.949321	-0.308757	1.580975
C	2.510904	2.579068	-0.844105
C	1.737465	2.950491	-1.937151
C	2.183244	3.931055	-2.816037
C	3.405103	4.550787	-2.606715
C	4.185418	4.186099	-1.515434
C	3.743035	3.205417	-0.642627
C	-2.678559	2.569495	0.080592
C	-1.717326	3.574611	0.124819
C	-2.082141	4.906363	-0.028556
C	-3.412391	5.243369	-0.231238
C	-4.378903	4.245658	-0.273134
C	-4.015482	2.916781	-0.114298
C	-3.387533	-0.092009	-0.690305
C	-4.490898	-0.769085	-0.181331
C	-5.372768	-1.411093	-1.042358
C	-5.160743	-1.377137	-2.412276
C	-4.056617	-0.706449	-2.924911
C	-3.171681	-0.072491	-2.067981
C	0.799996	-2.090397	2.188963
C	0.064300	-1.150153	3.140882
C	2.036665	2.264111	1.964532
C	1.307301	1.550403	3.100369
C	-1.700625	1.165502	3.027693
C	-2.766311	0.562474	2.113896
H	-0.046658	0.299555	-1.279026
H	-1.232966	-2.631449	-1.908342
H	-3.198346	-4.043874	-2.287672
H	-4.368151	-5.096639	-0.373345
H	-3.525303	-4.729597	1.927096
H	-1.542528	-3.359515	2.314867
H	0.986135	-1.526042	-2.339308
H	2.520692	-2.755671	-3.822110
H	3.938653	-4.570544	-2.911073

H	3.795605	-5.152234	-0.509329
H	2.222103	-3.977694	0.957070
H	3.558366	0.129838	-1.753824
H	5.405358	-1.486210	-1.790158
H	6.325387	-2.376985	0.330465
H	5.389197	-1.609832	2.490677
H	3.557144	0.011245	2.537499
H	0.780742	2.477688	-2.116648
H	1.570480	4.206454	-3.666242
H	3.752578	5.314072	-3.292842
H	5.142544	4.665171	-1.346613
H	4.367204	2.922556	0.197632
H	-0.675951	3.314506	0.274362
H	-1.322586	5.678461	0.005273
H	-3.696757	6.281163	-0.359419
H	-5.419652	4.501777	-0.432804
H	-4.780015	2.149071	-0.150797
H	-4.677854	-0.801492	0.884600
H	-6.228363	-1.937677	-0.636611
H	-5.850666	-1.877455	-3.081369
H	-3.881870	-0.682324	-3.993984
H	-2.306757	0.441250	-2.473953
H	0.685425	-3.131118	2.494368
H	1.868421	-1.863811	2.187399
H	0.566324	-1.088371	4.107723
H	-0.954328	-1.497759	3.322671
H	3.070965	2.495267	2.223853
H	1.533105	3.204920	1.732817
H	0.913340	2.262991	3.826234
H	1.965412	0.869290	3.639956
H	-1.855428	0.893449	4.072694
H	-1.691700	2.255197	2.951504
H	-3.743309	1.019631	2.273153
H	-2.856000	-0.513246	2.285550
Co	-0.045656	0.397156	0.214944
H	-0.197926	1.375626	-0.864805

$TS_{2a,1}$

P	-0.388896	-2.180168	0.378660
P	2.176986	0.661789	0.589965
P	0.167657	-0.185644	2.586897
P	-1.731544	1.222171	0.753664
C	-2.115272	-2.756870	0.038350
C	-2.464138	-3.411212	-1.140360
C	-3.784502	-3.766051	-1.389769
C	-4.774898	-3.472954	-0.464306
C	-4.438150	-2.816193	0.712836
C	-3.121654	-2.458883	0.957588
C	0.564701	-3.308252	-0.730821
C	1.141811	-2.790978	-1.887016
C	1.887939	-3.602517	-2.730555
C	2.072635	-4.942347	-2.420495
C	1.497895	-5.469374	-1.270609
C	0.742190	-4.659154	-0.434987
C	3.602443	-0.533985	0.497241
C	3.364620	-1.895537	0.618761
C	4.409293	-2.811882	0.626627
C	5.717241	-2.366795	0.516579
C	5.972194	-1.003629	0.408865
C	4.925248	-0.094943	0.403364
C	2.823954	1.996670	-0.499728
C	3.280218	1.652796	-1.773405
C	3.756007	2.623176	-2.640413
C	3.761008	3.958636	-2.254869
C	3.290814	4.311464	-0.998505
C	2.828310	3.336036	-0.122795
C	-1.635961	3.052751	0.470983
C	-0.564555	3.733991	1.048560
C	-0.393741	5.094691	0.849405
C	-1.283108	5.795741	0.044270
C	-2.346081	5.126890	-0.544784
C	-2.526740	3.765759	-0.327386
C	-3.306636	0.798305	-0.105752
C	-4.551620	1.150829	0.414469
C	-5.717467	0.810823	-0.256551
C	-5.653260	0.127410	-1.464112
C	-4.419260	-0.226752	-1.990174
C	-3.255560	0.096651	-1.306651
C	-0.057063	-2.900872	2.077723
C	-0.320367	-1.870011	3.173421
C	2.461669	1.254860	2.333654
C	1.843534	0.206170	3.256831
C	-0.984407	0.988298	3.423249
C	-2.227182	1.129313	2.553673
H	0.147640	-0.045589	-1.138013
H	-1.707221	-3.650206	-1.877462

H	-4.036034	-4.273313	-2.313998
H	-5.805120	-3.744824	-0.661203
H	-5.204037	-2.573757	1.440152
H	-2.885584	-1.928771	1.872090
H	1.024032	-1.739257	-2.119962
H	2.333663	-3.183352	-3.625022
H	2.665685	-5.575136	-3.070247
H	1.637566	-6.515602	-1.024865
H	0.293376	-5.088600	0.453095
H	2.349280	-2.248930	0.700833
H	4.195185	-3.870673	0.716467
H	6.536722	-3.075938	0.515913
H	6.992434	-0.646718	0.327968
H	5.143821	0.963202	0.318334
H	3.277803	0.615049	-2.088656
H	4.115675	2.338095	-3.622107
H	4.127871	4.719433	-2.933567
H	3.287526	5.350785	-0.691341
H	2.474695	3.634455	0.856089
H	0.159669	3.189075	1.641376
H	0.445374	5.604551	1.308019
H	-1.142929	6.856289	-0.127770
H	-3.040397	5.664412	-1.180064
H	-3.361896	3.263667	-0.799788
H	-4.620699	1.697690	1.347326
H	-6.678335	1.084626	0.163136
H	-6.564333	-0.134309	-1.989275
H	-4.360003	-0.772957	-2.924030
H	-2.300515	-0.229229	-1.699938
H	-0.643262	-3.806400	2.238064
H	0.996850	-3.186280	2.083606
H	0.206789	-2.120958	4.095865
H	-1.384762	-1.814923	3.411316
H	3.524490	1.400849	2.531565
H	1.955368	2.211884	2.465891
H	1.774807	0.555223	4.288458
H	2.429486	-0.716072	3.248038
H	-1.226558	0.642038	4.430062
H	-0.458496	1.941240	3.514171
H	-2.822385	1.996735	2.840539
H	-2.857774	0.242466	2.648880
Co	0.077032	-0.009519	0.424676
H	-0.125609	0.844688	-1.388771
N	-0.521441	1.751916	-2.460054
H	-1.517746	1.887122	-2.316545
C	0.119988	3.063764	-2.545333
H	0.046174	3.572278	-1.586739
H	1.170919	2.930613	-2.790483
H	-0.344541	3.684212	-3.318061
C	-0.324843	0.936879	-3.656929
H	0.742677	0.753717	-3.791405
H	-0.828612	-0.022639	-3.528454
H	-0.715022	1.425149	-4.554025

$TS_{1,3}$

P	0.201052	-2.017799	0.494412
P	1.910150	1.217721	0.554716
P	-0.020938	0.167410	2.540228
P	-2.096428	0.845653	0.513564
C	-1.321434	-3.055988	0.263739
C	-1.910260	-3.094674	-1.001818
C	-3.076025	-3.809098	-1.224571
C	-3.694323	-4.482027	-0.177578
C	-3.125579	-4.443699	1.085883
C	-1.944572	-3.742183	1.303630
C	1.379772	-2.958914	-0.573872
C	1.403255	-2.669359	-1.937964
C	2.254592	-3.351334	-2.793873
C	3.116186	-4.319041	-2.293612
C	3.113121	-4.603094	-0.935292
C	2.245582	-3.933216	-0.081530
C	3.401587	0.126176	0.428763
C	3.703249	-0.424083	-0.818353
C	4.759822	-1.306443	-0.970306
C	5.523293	-1.677271	0.130467
C	5.232676	-1.139630	1.374673
C	4.183974	-0.237537	1.521390
C	2.462692	2.674666	-0.448812
C	1.493477	3.551875	-0.928503
C	1.852615	4.699869	-1.621566
C	3.192237	4.982404	-1.849996
C	4.167637	4.115146	-1.374895
C	3.805927	2.971403	-0.676304
C	-2.523028	2.638211	0.268355
C	-1.641931	3.583592	0.793079
C	-1.899055	4.941442	0.675092

C	-3.041026	5.376503	0.015002
C	-3.925186	4.445171	-0.511818
C	-3.671472	3.085250	-0.381183
C	-3.424514	0.023758	-0.475965
C	-4.574985	-0.520182	0.091384
C	-5.539803	-1.125747	-0.705481
C	-5.376720	-1.183344	-2.081289
C	-4.235427	-0.640891	-2.657584
C	-3.266179	-0.053640	-1.859739
C	0.756578	-2.439313	2.220303
C	0.017995	-1.552526	3.219981
C	2.046896	1.961135	2.261114
C	1.432198	1.028352	3.298652
C	-1.549176	0.937218	3.228270
C	-2.683516	0.590053	2.271005
H	-0.058164	0.218854	-1.205154
H	-1.459945	-2.554086	-1.826047
H	-3.513909	-3.826705	-2.215449
H	-4.614876	-5.028026	-0.347145
H	-3.596825	-4.964351	1.911652
H	-1.519490	-3.745860	2.298939
H	0.759856	-1.892499	-2.333263
H	2.256439	-3.115227	-3.851685
H	3.791423	-4.844955	-2.958318
H	3.788341	-5.350657	-0.535143
H	2.256193	-4.180232	0.972610
H	3.102615	-0.160229	-1.680375
H	4.977619	-1.719900	-1.947904
H	6.339465	-2.381063	0.016716
H	5.825244	-1.415493	2.239457
H	3.995137	0.179427	2.501914
H	0.446316	3.335036	-0.762045
H	1.083183	5.369990	-1.987252
H	3.475905	5.874333	-2.396384
H	5.216038	4.328602	-1.548201
H	4.579899	2.307435	-0.310477
H	-0.734591	3.250077	1.285477
H	-1.199048	5.659955	1.085810
H	-3.238347	6.436631	-0.092926
H	-4.818345	4.776432	-1.029005
H	-4.377079	2.375029	-0.794964
H	-4.741567	-0.474388	1.159587
H	-6.424348	-1.549831	-0.244584
H	-6.131391	-1.652920	-2.701299
H	-4.092574	-0.685430	-3.731017
H	-2.377834	0.355902	-2.321160
H	0.644044	-3.498220	2.457359
H	1.825401	-2.207443	2.241401
H	0.490701	-1.570253	4.203661
H	-1.019068	-1.871043	3.343251
H	3.077753	2.228936	2.501709
H	1.475043	2.890472	2.201505
H	1.125336	1.562832	4.199657
H	2.137120	0.252871	3.602954
H	-1.747005	0.583125	4.241969
H	-1.384026	2.016017	3.273334
H	-3.586240	1.165001	2.482312
H	-2.922662	-0.472376	2.365673
Co	-0.012196	0.169649	0.374259
C	0.268830	1.111358	-2.642046
O	-0.624051	1.877437	-2.702847
O	1.245315	0.589668	-3.044271

3

P	0.291619	-2.035955	0.492520
P	1.910172	1.314089	0.513793
P	-0.033011	0.209362	2.500012
P	-2.186276	0.814879	0.511510
C	-1.198684	-3.107103	0.251350
C	-1.836772	-3.045782	-0.988495
C	-2.963328	-3.809210	-1.246224
C	-3.492173	-4.626955	-0.255061
C	-2.875698	-4.683819	0.985666
C	-1.731248	-3.934256	1.236500
C	1.522082	-2.958892	-0.525121
C	1.509267	-2.761258	-1.905547
C	2.398554	-3.438312	-2.725354
C	3.326091	-4.313128	-2.174450
C	3.354501	-4.506895	-0.800870
C	2.455228	-3.837706	0.020028
C	3.421663	0.255850	0.387234
C	3.713990	-0.304597	-0.857964
C	4.802960	-1.145389	-1.017736
C	5.606410	-1.462565	0.071034
C	5.323233	-0.914296	1.312361
C	4.241992	-0.053251	1.468697

C	2.410614	2.778327	-0.494311
C	1.426252	3.544259	-1.110933
C	1.762060	4.693631	-1.813945
C	3.089245	5.087113	-1.908678
C	4.079024	4.328255	-1.296002
C	3.742256	3.181077	-0.592112
C	-2.617841	2.597372	0.251112
C	-1.681615	3.554363	0.638302
C	-1.953433	4.908469	0.507037
C	-3.165516	5.323968	-0.027529
C	-4.104447	4.378468	-0.417799
C	-3.835635	3.023562	-0.274838
C	-3.521235	-0.047052	-0.426949
C	-4.604312	-0.667093	0.192139
C	-5.579902	-1.305436	-0.564685
C	-5.492294	-1.322659	-1.948330
C	-4.418152	-0.703128	-2.574092
C	-3.438430	-0.077138	-1.819715
C	0.825771	-2.368017	2.235511
C	-0.000429	-1.503186	3.181341
C	1.996496	2.040557	2.221417
C	1.427706	1.059431	3.238212
C	-1.545286	0.995394	3.186054
C	-2.699264	0.577732	2.284980
H	-0.231297	0.042898	-1.447730
H	-1.455828	-2.387606	-1.761301
H	-3.441264	-3.750452	-2.216581
H	-4.382890	-5.212600	-0.449841
H	-3.279964	-5.318552	1.765743
H	-1.264427	-4.010338	2.210492
H	0.808678	-2.062037	-2.345393
H	2.374401	-3.272117	-3.795954
H	4.027305	-4.837346	-2.812985
H	4.078202	-5.184161	-0.362398
H	2.494480	-4.012861	1.087626
H	3.079180	-0.081954	-1.707691
H	5.015156	-1.568544	-1.992321
H	6.448958	-2.133336	-0.049640
H	5.946999	-1.149526	2.167025
H	4.061620	0.376140	2.445502
H	0.390299	3.237679	-1.053201
H	0.983422	5.275666	-2.292956
H	3.354056	5.981213	-2.460981
H	5.117817	4.628636	-1.368373
H	4.524659	2.597113	-0.121395
H	-0.722699	3.235014	1.031363
H	-1.211638	5.637815	0.810758
H	-3.375486	6.380524	-0.145697
H	-5.051323	4.695795	-0.838987
H	-4.581470	2.301501	-0.584193
H	-4.711774	-0.658353	1.268606
H	-6.413592	-1.785853	-0.066095
H	-6.255180	-1.819141	-2.536486
H	-4.337516	-0.712637	-3.654874
H	-2.605111	0.404571	-2.316743
H	0.771126	-3.424158	2.500057
H	1.877563	-2.071395	2.280497
H	0.409448	-1.498992	4.192931
H	-1.032890	-1.855014	3.237523
H	3.010713	2.356110	2.472123
H	1.377018	2.939186	2.172099
H	1.136153	1.552581	4.167101
H	2.150792	0.282115	3.490089
H	-1.703419	0.691580	4.222458
H	-1.393863	2.076896	3.166149
H	-3.613084	1.129856	2.506781
H	-2.897435	-0.487747	2.422320
Co	-0.030302	0.188752	0.330118
C	0.077008	0.760909	-2.319020
O	-0.771340	1.604621	-2.631680
O	1.154401	0.481654	-2.857749

$TS_{2,4}$

P	0.212311	-1.850185	0.489671
P	2.087796	1.164158	0.582481
P	-0.008618	0.359701	2.612621
P	-2.201958	0.758478	0.542519
C	-1.275205	-2.919919	0.260567
C	-1.745762	-3.147918	-1.032065
C	-2.836044	-3.973275	-1.251347
C	-3.487112	-4.570374	-0.179708
C	-3.036042	-4.338110	1.109754
C	-1.934101	-3.520541	1.329774
C	1.402195	-2.695043	-0.620066
C	1.419079	-2.343146	-1.967091
C	2.244294	-3.013419	-2.857073

C	3.071701	-4.031973	-2.404801
C	3.068226	-4.378523	-1.060617
C	2.233334	-3.718010	-0.170105
C	3.484269	-0.017435	0.470402
C	3.912387	-0.440508	-0.788402
C	4.939709	-1.361384	-0.906156
C	5.533500	-1.892988	0.231784
C	5.102146	-1.489867	1.486160
C	4.085282	-0.550748	1.606498
C	2.614680	2.571480	-0.484279
C	1.670626	3.500643	-0.915498
C	2.061152	4.625485	-1.626743
C	3.402808	4.840399	-1.909035
C	4.351374	3.928802	-1.467767
C	3.962028	2.802424	-0.756702
C	-2.758448	2.488882	0.195447
C	-2.012127	3.570356	0.663391
C	-2.449952	4.871494	0.466705
C	-3.639339	5.113486	-0.206577
C	-4.391082	4.044819	-0.671438
C	-3.957563	2.741573	-0.468180
C	-3.388240	-0.233082	-0.439378
C	-4.490336	-0.860473	0.133633
C	-5.416401	-1.513703	-0.669982
C	-5.254564	-1.537591	-2.046894
C	-4.152288	-0.919618	-2.622468
C	-3.220407	-0.279299	-1.822590
C	0.796672	-2.241437	2.202357
C	0.066214	-1.375858	3.224437
C	2.205649	1.979291	2.248714
C	1.447738	1.227757	3.337033
C	-1.589293	1.055629	3.232500
C	-2.696453	0.530502	2.319042
H	-0.063109	0.516521	-1.153074
H	-1.258340	-2.684165	-1.880809
H	-3.184584	-4.142052	-2.262894
H	-4.343225	-5.211742	-0.351761
H	-3.534142	-4.799516	1.954162
H	-1.596151	-3.379397	2.347032
H	0.790141	-1.537827	-2.323437
H	2.247400	-2.731975	-3.903380
H	3.723311	-4.551873	-3.097041
H	3.719055	-5.166485	-0.700703
H	2.239557	-4.009347	0.872575
H	3.450735	-0.039940	-1.683067
H	5.269515	-1.674187	-1.889242
H	6.329126	-2.622617	0.139299
H	5.559776	-1.900097	2.378377
H	3.776542	-0.242777	2.597255
H	0.620216	3.353178	-0.699639
H	1.312115	5.333150	-1.961233
H	3.708432	5.717473	-2.467061
H	5.402318	4.093281	-1.673591
H	4.719150	2.108559	-0.415247
H	-1.077060	3.407345	1.184337
H	-1.854555	5.697502	0.837089
H	-3.977429	6.130119	-0.368330
H	-5.322646	4.220432	-1.196205
H	-4.566022	1.926304	-0.836882
H	-4.651224	-0.837849	1.203513
H	-6.269951	-2.000199	-0.213293
H	-5.982218	-2.042916	-2.670769
H	-4.012522	-0.941605	-3.696585
H	-2.367516	0.202028	-2.282312
H	0.686908	-3.302452	2.427856
H	1.864035	-2.009752	2.208645
H	0.564788	-1.400356	4.194202
H	-0.961590	-1.707586	3.374306
H	3.251703	2.141185	2.512743
H	1.750791	2.958056	2.087302
H	1.114151	1.903462	4.125559
H	2.070077	0.462609	3.801493
H	-1.758548	0.766069	4.270503
H	-1.512749	2.143586	3.188194
H	-3.646346	1.028379	2.514459
H	-2.832918	-0.542046	2.478641
Co	-0.000182	0.424354	0.415730
C	0.125098	1.280444	-2.489795
O	-0.788753	2.032340	-2.566422
O	1.102824	0.805180	-2.963642
H	-0.064006	1.874179	0.534804

4

P	0.232707	-1.868788	0.484326
P	2.102209	1.204262	0.590868
P	-0.029815	0.381867	2.591451

P	-2.251852	0.767178	0.546733	H	-1.286579	-2.620775	-1.874408
C	-1.241811	-2.950825	0.254930	H	-3.177954	-4.120704	-2.271659
C	-1.738373	-3.134827	-1.035128	H	-4.256176	-5.302204	-0.380457
C	-2.808726	-3.983220	-1.262879	H	-3.404810	-4.960923	1.921098
C	-3.415185	-4.642935	-0.201722	H	-1.492184	-3.506150	2.327525
C	-2.939328	-4.451934	1.085562	H	0.806899	-1.623634	-2.348791
C	-1.854681	-3.613998	1.314157	H	2.311698	-2.814784	-3.878558
C	1.449466	-2.702818	-0.602355	H	3.845471	-4.555417	-3.008544
C	1.459630	-2.394094	-1.960144	H	3.850303	-5.093405	-0.593666
C	2.312971	-3.063054	-2.823987	H	2.325004	-3.938258	0.935760
C	3.172812	-4.036951	-2.335713	H	3.398240	-0.030761	-1.682416
C	3.174499	-4.340474	-0.981300	H	5.257959	-1.616572	-1.915541
C	2.313438	-3.680980	-0.115592	H	6.413457	-2.485976	0.095756
C	3.507486	0.040486	0.467471	H	5.701910	-1.732880	2.343758
C	3.903535	-0.397172	-0.796865	H	3.882518	-0.118627	2.587747
C	4.953340	-1.289928	-0.928952	H	0.570265	3.332393	-0.730104
C	5.600538	-1.777261	0.199691	H	1.220605	5.325117	-1.995225
C	5.201316	-1.357729	1.459305	H	3.609112	5.769151	-2.484232
C	4.162407	-0.445241	1.594638	H	5.339990	4.193044	-1.673828
C	2.585793	2.613722	-0.486615	H	4.700260	2.198836	-0.405500
C	1.618469	3.511144	-0.932273	H	-1.094434	3.442432	1.057052
C	1.985115	4.640330	-1.648597	H	-1.900500	5.715780	0.679235
C	3.322912	4.888062	-1.922265	H	-4.081314	6.102631	-0.434281
C	4.292702	4.003946	-1.471067	H	-5.450512	4.164285	-1.147191
C	3.928728	2.873028	-0.754424	H	-4.662505	1.884652	-0.761323
C	-2.812610	2.487307	0.169766	H	-4.613622	-0.932022	1.252106
C	-2.051948	3.583966	0.572437	H	-6.214466	-2.150498	-0.138120
C	-2.507349	4.876716	0.360601	H	-5.983475	-2.158369	-2.601605
C	-3.728568	5.092835	-0.261721	H	-4.096015	-0.953833	-3.664177
C	-4.494780	4.007920	-0.661512	H	-2.472164	0.259034	-2.278913
C	-4.043402	2.713615	-0.444686	H	0.740422	-3.264604	2.452076
C	-3.421254	-0.256161	-0.416578	H	1.866656	-1.928581	2.223425
C	-4.479006	-0.936980	0.178475	H	0.481877	-1.365449	4.184817
C	-5.394398	-1.622598	-0.609753	H	-1.004735	-1.694491	3.301579
C	-5.264813	-1.625655	-1.990264	H	3.226170	2.185456	2.535928
C	-4.207594	-0.951089	-2.586584	H	1.713313	2.978074	2.103150
C	-3.286247	-0.274908	-1.804336	H	1.105915	1.863222	4.137278
C	0.809756	-2.205216	2.205763	H	2.056473	0.432746	3.749609
C	0.024556	-1.352185	3.194604	H	-1.740273	0.844532	4.254661
C	2.187074	2.007189	2.257002	H	-1.507776	2.191742	3.128707
C	1.435865	1.219800	3.320561	H	-3.662089	1.068252	2.525815
C	-1.593627	1.106395	3.205898	H	-2.853962	-0.505622	2.509471
C	-2.717324	0.562723	2.327047	Co	-0.009310	0.440799	0.408488
H	-0.086300	0.438640	-1.358806	C	0.117704	1.078784	-2.344047

O	-0.780671	1.870656	-2.617345
O	1.160863	0.768586	-2.911350
H	-0.086098	1.882832	0.589232

4a

P	0.286315	-1.796967	0.445367
P	2.109436	1.258404	0.568403
P	0.010419	0.431738	2.597261
P	-2.277070	0.851214	0.658402
C	-1.101177	-2.969853	0.114869
C	-1.470725	-3.225604	-1.206166
C	-2.472856	-4.137892	-1.494685
C	-3.118687	-4.813187	-0.467529
C	-2.760291	-4.563041	0.847613
C	-1.760654	-3.643694	1.138972
C	1.587202	-2.549478	-0.613099
C	1.730624	-2.125026	-1.931917
C	2.613305	-2.768510	-2.786475
C	3.380550	-3.827931	-2.325466
C	3.264097	-4.238508	-1.004355
C	2.367187	-3.608877	-0.152960
C	3.537422	0.108785	0.458824
C	4.104320	-0.153715	-0.786983
C	5.168761	-1.033805	-0.900721
C	5.672916	-1.669720	0.225973
C	5.111229	-1.416675	1.468345
C	4.049609	-0.529949	1.584922
C	2.647711	2.643530	-0.509982
C	1.813049	3.187964	-1.477908
C	2.229242	4.283989	-2.223873
C	3.478032	4.843265	-2.004103
C	4.319004	4.300309	-1.038880
C	3.908717	3.205306	-0.295941
C	-2.828029	2.543438	0.183426
C	-2.025999	3.374239	-0.588719
C	-2.480788	4.626996	-0.980272
C	-3.741394	5.058579	-0.598340
C	-4.552559	4.230106	0.168537
C	-4.103292	2.976401	0.550210
C	-3.555733	-0.164620	-0.186614
C	-4.132929	-1.281600	0.410583
C	-5.102813	-2.011156	-0.263570
C	-5.488769	-1.648447	-1.544996
C	-4.907820	-0.542712	-2.151638
C	-3.954021	0.198948	-1.474008
C	0.805306	-2.165534	2.183654
C	0.008497	-1.315138	3.168387
C	2.231168	2.040341	2.244898
C	1.500808	1.237081	3.314084
C	-1.489547	1.229975	3.275060
C	-2.677183	0.732192	2.462301
H	-1.472625	-0.614128	-2.022154
H	-0.959497	-2.735456	-2.025668
H	-2.742230	-4.326330	-2.526934
H	-3.898372	-5.530635	-0.693425
H	-3.258515	-5.082647	1.657412
H	-1.503156	-3.474303	2.175964
H	1.163755	-1.282202	-2.301279
H	2.709662	-2.428963	-3.810738
H	4.075089	-4.327494	-2.990308
H	3.869185	-5.057167	-0.633361
H	2.277142	-3.959091	0.867797
H	3.717746	0.331329	-1.675479
H	5.603085	-1.226117	-1.874156
H	6.500794	-2.362611	0.134407
H	5.501167	-1.904465	2.353596
H	3.635544	-0.344208	2.566466
H	0.851534	2.736529	-1.669544
H	1.571243	4.696218	-2.979613
H	3.801388	5.699132	-2.584723
H	5.297252	4.732114	-0.864640
H	4.576006	2.788375	0.449962
H	-1.045012	3.042167	-0.895209
H	-1.845692	5.261282	-1.587047
H	-4.097116	6.036380	-0.901000
H	-5.541583	4.558852	0.464738
H	-4.758973	2.334158	1.126468
H	-3.840180	-1.601662	1.401186
H	-5.549979	-2.873186	0.215802
H	-6.241720	-2.224296	-2.069811
H	-5.202027	-0.250620	-3.152566
H	-3.526201	1.071882	-1.952583
H	0.712398	-3.227354	2.411194
H	1.865821	-1.911534	2.237688
H	0.427782	-1.371877	4.173869
H	-1.032909	-1.636679	3.223331

H	3.276329	2.207386	2.506773
H	1.756360	3.015010	2.119192
H	1.192590	1.873396	4.144813
H	2.127422	0.446997	3.727123
H	-1.599488	0.998663	4.335378
H	-1.352621	2.307868	3.166262
H	-3.585750	1.287260	2.691022
H	-2.867184	-0.316559	2.691460
Co	-0.029998	0.520440	0.400680
C	-0.824899	0.187357	-2.408024
O	-0.084782	0.782330	-1.562387
O	-0.851269	0.446865	-3.614478
H	-0.098125	1.968528	0.622801

5

P	0.287621	-1.746669	0.445501
P	2.044031	1.355500	0.387922
P	-0.038690	0.582852	2.449236
P	-2.265768	0.771335	0.394019
C	-1.152698	-2.873947	0.245818
C	-1.580878	-3.196494	-1.041391
C	-2.634910	-4.074381	-1.231063
C	-3.286910	-4.629517	-0.137742
C	-2.877611	-4.300754	1.144783
C	-1.813498	-3.428588	1.337968
C	1.538504	-2.551335	-0.629118
C	1.587197	-2.247523	-1.987931
C	2.469771	-2.912454	-2.825083
C	3.324337	-3.876871	-2.310229
C	3.289693	-4.175710	-0.955752
C	2.397585	-3.521869	-0.117841
C	3.487034	0.230450	0.366882
C	4.001257	-0.184083	-0.860956
C	5.069325	-1.064418	-0.908276
C	5.622999	-1.552377	0.268551
C	5.110271	-1.149496	1.492441
C	4.046702	-0.258436	1.543649
C	2.478874	2.633141	-0.851320
C	1.543619	3.141023	-1.746914
C	1.897993	4.159879	-2.622058
C	3.182381	4.681592	-2.601833
C	4.118037	4.183275	-1.703408
C	3.770277	3.163352	-0.833122
C	-2.888974	2.467630	0.019225
C	-2.154156	3.596039	0.379106
C	-2.669466	4.867523	0.174638
C	-3.922366	5.028822	-0.399124
C	-4.661272	3.911163	-0.759343
C	-4.151186	2.638176	-0.549177
C	-3.340811	-0.292005	-0.622699
C	-4.416400	-0.989779	-0.083247
C	-5.261231	-1.709565	-0.917754
C	-5.041375	-1.728201	-2.286859
C	-3.964817	-1.036012	-2.826729
C	-3.113440	-0.324685	-1.997737
C	0.887116	-2.011060	2.172580
C	0.136026	-1.111924	3.145551
C	2.098321	2.300054	1.979309
C	1.353191	1.593688	3.107396
C	-1.666430	1.186510	3.037293
C	-2.733293	0.528768	2.163958
H	0.222208	0.286108	-1.335048
H	-1.087691	-2.772760	-1.907339
H	-2.951364	-4.319584	-2.237451
H	-4.111597	-5.316028	-0.287070
H	-3.377972	-4.729668	2.004622
H	-1.504327	-3.208814	2.350878
H	0.933235	-1.493503	-2.408964
H	2.493858	-2.670122	-3.880635
H	4.019250	-4.391805	-2.962630
H	3.959916	-4.921555	-0.545662
H	2.380463	-3.778929	0.933407
H	3.574550	0.186813	-1.785262
H	5.463881	-1.378638	-1.866612
H	6.452346	-2.248441	0.230213
H	5.538979	-1.525264	2.413519
H	3.666945	0.049106	2.509453
H	0.534063	2.753757	-1.770324
H	1.164114	4.543910	-3.320271
H	3.456863	5.475688	-3.285823
H	5.121567	4.590481	-1.679852
H	4.509759	2.780428	-0.139489
H	-1.174502	3.496036	0.828820
H	-2.085282	5.733529	0.461728
H	-4.322524	6.022036	-0.563852
H	-5.640232	4.026539	-1.208704

H	-4.747926	1.780674	-0.832575
H	-4.612843	-0.972829	0.981224
H	-6.096009	-2.253099	-0.492262
H	-5.704180	-2.289811	-2.934127
H	-3.784951	-1.054315	-3.894764
H	-2.276116	0.213971	-2.426776
H	0.807190	-3.059620	2.459080
H	1.946227	-1.747068	2.158040
H	0.653286	-1.044700	4.103536
H	-0.871553	-1.479968	3.342106
H	3.132258	2.515352	2.250222
H	1.609740	3.245404	1.738172
H	0.959774	2.310101	3.829266
H	2.003363	0.906594	3.648610
H	-1.796863	0.934060	4.090274
H	-1.682125	2.273125	2.938268
H	-3.720480	0.950062	2.352801
H	-2.772729	-0.548037	2.346130
H	-0.333407	0.883132	-1.295473
Co	-0.026411	0.524790	0.257795
H	-0.116700	1.975417	0.345305

$TS_{5,2}$

P	0.314281	-1.917842	0.442162
P	2.105913	1.141673	0.696455
P	0.066091	0.166258	2.704000
P	-2.189654	0.708360	0.730973
C	-1.081106	-3.099312	0.170115
C	-1.064481	-4.024235	-0.870803
C	-2.113603	-4.919598	-1.035234
C	-3.188034	-4.908797	-0.159604
C	-3.213088	-3.990465	0.881503
C	-2.171726	-3.090898	1.039112
C	1.564001	-2.562350	-0.726084
C	1.523113	-2.125976	-2.048214
C	2.371618	-2.677075	-2.995599
C	3.278016	-3.661019	-2.625293
C	3.332222	-4.089987	-1.306696
C	2.473703	-3.549695	-0.359143
C	3.546846	0.042924	0.435478
C	3.964535	-0.222217	-0.868379
C	5.055857	-1.041970	-1.099548
C	5.728108	-1.624920	-0.032391
C	5.309060	-1.376655	1.265369
C	4.225193	-0.539943	1.500683
C	2.517993	2.622666	-0.308386
C	1.506200	3.456816	-0.768287
C	1.813556	4.646238	-1.414339
C	3.137434	5.011357	-1.606005
C	4.154212	4.185621	-1.143364
C	3.848871	2.999710	-0.494036
C	-2.721865	2.414187	0.274367
C	-2.080395	3.506600	0.858524
C	-2.460023	4.800050	0.536656
C	-3.477664	5.019838	-0.383298
C	-4.119337	3.939329	-0.968240
C	-3.749192	2.642029	-0.637068
C	-3.395848	-0.349291	-0.140361
C	-4.696829	-0.499606	0.335462
C	-5.601332	-1.289570	-0.357909
C	-5.217571	-1.922395	-1.533283
C	-3.923882	-1.771539	-2.012520
C	-3.014580	-0.994302	-1.311375
C	0.910774	-2.383328	2.138172
C	0.139549	-1.603910	3.200005
C	2.256023	1.828728	2.410390
C	1.564335	0.946393	3.438432
C	-1.442343	0.917713	3.419153
C	-2.630766	0.562318	2.531687
H	-0.388047	0.937696	-1.319440
H	-0.237208	-4.060819	-1.566782
H	-2.084000	-5.631834	-1.851221
H	-4.003769	-5.610256	-0.287670
H	-4.049677	-3.965335	1.569388
H	-2.229634	-2.365664	1.838063
H	0.817614	-1.359994	-2.345640
H	2.326558	-2.333366	-4.022057
H	3.947925	-4.087534	-3.362347
H	4.043847	-4.851284	-1.010949
H	2.519195	-3.911625	0.660300
H	3.446714	0.224979	-1.708588
H	5.376240	-1.234112	-2.115977
H	6.577141	-2.272674	-0.215185
H	5.828493	-1.826640	2.102776
H	3.929616	-0.345273	2.523266
H	0.470418	3.183879	-0.620695

H	1.013571	5.284042	-1.770940
H	3.378013	5.937704	-2.113914
H	5.191149	4.465075	-1.285815
H	4.653716	2.372153	-0.132425
H	-1.273725	3.356439	1.566224
H	-1.954469	5.638285	1.000795
H	-3.765584	6.031567	-0.642760
H	-4.911049	4.100016	-1.690086
H	-4.260890	1.812809	-1.108428
H	-5.013782	-0.000103	1.243079
H	-6.609513	-1.408866	0.020148
H	-5.926517	-2.538456	-2.073429
H	-3.615516	-2.272580	-2.921908
H	-1.993952	-0.913482	-1.662231
H	0.816072	-3.457869	2.293631
H	1.971661	-2.125597	2.177283
H	0.623202	-1.680790	4.174835
H	-0.881286	-1.968179	3.313080
H	3.304979	2.002853	2.653085
H	1.761773	2.799909	2.350069
H	1.276383	1.512394	4.325381
H	2.210601	0.131267	3.765287
H	-1.590450	0.569249	4.442289
H	-1.271919	1.995452	3.446627
H	-3.490170	1.195622	2.750753
H	-2.928336	-0.474677	2.694327
H	0.271729	0.405893	-1.045548
Co	0.022089	0.366771	0.514898
H	-0.071511	1.801294	0.766993
N	-1.175127	1.547566	-2.595158
H	-2.152789	1.316864	-2.450766
C	-1.068544	2.982231	-2.852985
H	-1.374726	3.545346	-1.971950
H	-0.032178	3.227807	-3.082408
H	-1.691854	3.287758	-3.700865
C	-0.659446	0.749668	-3.704973
H	0.423000	0.880118	-3.769702
H	-0.872042	-0.306174	-3.535366
H	-1.102414	1.042019	-4.662728

CO_2

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.155676
O	0.000000	0.000000	-1.155676

H_2

H	0.000000	0.000000	0.372510
H	0.000000	0.000000	-0.372510

$HCOO^-$

C	0.000000	0.000000	0.338323
O	0.000000	1.120958	-0.217572
O	0.000000	-1.120958	-0.217572
H	0.000000	0.000000	1.451222

$NH(CH_3)_2$

N	0.000000	0.573283	-0.156524
H	0.000000	1.310383	0.537957
C	-1.204713	-0.224137	0.019967
H	-2.088296	0.412092	-0.054519
H	-1.266636	-0.975835	-0.771235
H	-1.241659	-0.753119	0.984811
C	1.204713	-0.224137	0.019966
H	1.266634	-0.975837	-0.771233
H	2.088297	0.412091	-0.054522
H	1.241661	-0.753116	0.984813

$NH_2(CH_3)_2^+$

N	0.000000	0.537729	-0.000002
H	0.000000	1.148927	-0.817085
C	1.241838	-0.273683	-0.000001
H	2.096032	0.398799	0.000005
H	1.247981	-0.893833	0.893076
H	1.247991	-0.893822	-0.893085
C	-1.241838	-0.273683	-0.000001
H	-1.247989	-0.893820	0.893085
H	-2.096032	0.398799	-0.000012
H	-1.247983	-0.893836	-0.893076

H	0.000000	1.148886	0.817116

$TS_{associative}$

P	-0.287985	1.790224	0.432201
P	-2.003684	-1.292108	0.417347
P	0.018369	-0.495979	2.418506
P	2.201411	-0.660610	0.325454
C	1.089993	3.026291	0.291610
C	1.400992	3.605700	-0.937517
C	2.439271	4.517727	-1.052425
C	3.194575	4.863666	0.060312
C	2.902212	4.286682	1.286795
C	1.860812	3.375168	1.399829
C	-1.528794	2.627038	-0.648426
C	-1.667150	2.190760	-1.963663
C	-2.541561	2.826719	-2.833588
C	-3.305237	3.897281	-2.390621
C	-3.184145	4.332162	-1.076993
C	-2.295323	3.706730	-0.213106
C	-3.443619	-0.114684	0.503612
C	-4.077900	0.311515	-0.662614
C	-5.108365	1.237912	-0.614589
C	-5.522849	1.760300	0.603560
C	-4.903562	1.340779	1.771637
C	-3.873855	0.409561	1.720710
C	-2.726584	-2.479984	-0.803444
C	-2.373345	-2.380161	-2.146511
C	-2.945297	-3.218331	-3.093499
C	-3.872249	-4.176167	-2.705634
C	-4.229071	-4.285674	-1.368137
C	-3.667178	-3.436573	-0.424372
C	3.180914	-2.193642	-0.100171
C	3.664029	-3.063033	0.875246
C	4.353082	-4.216994	0.521812
C	4.572991	-4.519367	-0.813574
C	4.096943	-3.659044	-1.795034
C	3.407063	-2.510791	-1.440381
C	3.228326	0.518990	-0.662067
C	4.402239	1.079542	-0.164438
C	5.202931	1.872829	-0.975412
C	4.852031	2.097478	-2.299417
C	3.681713	1.546322	-2.801924
C	2.868933	0.775310	-1.983578
C	-0.910732	2.133168	2.157870
C	-0.282158	1.178980	3.172430
C	-2.176882	-2.204806	2.043898
C	-1.263562	-1.632775	3.138150
C	1.688801	-0.961815	3.051805
C	2.710440	-0.344204	2.093301
H	-0.035228	-0.432346	-1.269167
H	0.826172	3.351432	-1.820194
H	2.660257	4.957612	-2.017888
H	4.004386	5.578079	-0.029332
H	3.483620	4.545249	2.164312
H	1.658827	2.944767	2.371270
H	-1.092396	1.337462	-2.304405
H	-2.635299	2.475843	-3.854707
H	-3.996701	4.389557	-3.064424
H	-3.781323	5.164449	-0.722989
H	-2.202828	4.072312	0.802627
H	-3.767518	-0.079217	-1.623968
H	-5.585625	1.556752	-1.533684
H	-6.323616	2.489419	0.640794
H	-5.219979	1.738189	2.729065
H	-3.405259	0.104932	2.648812
H	-1.633145	-1.649477	-2.451168
H	-2.661543	-3.125456	-4.135348
H	-4.312599	-4.837872	-3.442368
H	-4.952499	-5.030190	-1.056941
H	-3.972564	-3.527713	0.611022
H	3.502781	-2.861126	1.926400
H	4.718128	-4.880478	1.297236
H	5.110735	-5.419053	-1.088722
H	4.261248	-3.883029	-2.842615
H	3.034463	-1.861603	-2.223453
H	4.708043	0.899059	0.858862
H	6.108034	2.310413	-0.570331
H	5.482975	2.709498	-2.933230
H	3.392569	1.727581	-3.830564
H	1.944209	0.367665	-2.375321
H	-0.743354	3.173997	2.438303
H	-1.987754	1.974477	2.112675
H	-0.906062	1.082895	4.062812
H	0.690226	1.545708	3.505871
H	-3.217877	-2.209820	2.367004
H	-1.899255	-3.235249	1.829304

H	-0.755449	-2.434976	3.674416	O	0.459120	-3.584333	1.164441
H	-1.838699	-1.067150	3.871924	O	0.382777	-3.363860	-1.118507
H	1.838525	-0.608927	4.073945				
H	1.753366	-2.050597	3.055229				
H	3.720793	-0.698236	2.299649				
H	2.715984	0.742985	2.208941				
Co	-0.000257	-0.421582	0.249961				
C	0.378016	-3.204304	0.048778				

Electronic energies, zero-point energies, enthalpies and free energies (in Hartrees) for all of the relevant species (fully optimized (*w*B97XD/TZVP) using the PCM method with SMD atomic radii for methanol)

1

SCF Done: E(RwB97XD) = -4374.70015826 A.U. after 4 cycles
Convg = 0.5751D-08 -V/T = 2.0033
SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.11
(included in total energy above)

Zero-point correction= 0.738294 (Hartree/Particle)
Thermal correction to Energy= 0.781320
Thermal correction to Enthalpy= 0.782264
Thermal correction to Gibbs Free Energy= 0.662545
Sum of electronic and zero-point Energies= -4373.961865
Sum of electronic and thermal Energies= -4373.918839
Sum of electronic and thermal Enthalpies= -4373.917894
Sum of electronic and thermal Free Energies= -4374.037614

1a

SCF Done: E(RwB97XD) = -4374.66798493 A.U. after 3 cycles
Convg = 0.4353D-08 -V/T = 2.0033
SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.33
(included in total energy above)

Zero-point correction= 0.738806 (Hartree/Particle)
Thermal correction to Energy= 0.781758
Thermal correction to Enthalpy= 0.782702
Thermal correction to Gibbs Free Energy= 0.663628
Sum of electronic and zero-point Energies= -4373.929179
Sum of electronic and thermal Energies= -4373.886227
Sum of electronic and thermal Enthalpies= -4373.885283
Sum of electronic and thermal Free Energies= -4374.004357

2

SCF Done: E(RwB97XD) = -4375.18876976 A.U. after 3 cycles
Convg = 0.6165D-08 -V/T = 2.0033
SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.23
(included in total energy above)

Zero-point correction= 0.750061 (Hartree/Particle)
Thermal correction to Energy= 0.792841
Thermal correction to Enthalpy= 0.793786
Thermal correction to Gibbs Free Energy= 0.675726
Sum of electronic and zero-point Energies= -4374.438709
Sum of electronic and thermal Energies= -4374.395928
Sum of electronic and thermal Enthalpies= -4374.394984
Sum of electronic and thermal Free Energies= -4374.513044

2a

SCF Done: E(RwB97XD) = -4375.17950672 A.U. after 3 cycles
Convg = 0.6975D-08 -V/T = 2.0033
SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.05
(included in total energy above)

Zero-point correction= 0.751142 (Hartree/Particle)
Thermal correction to Energy= 0.794325
Thermal correction to Enthalpy= 0.795269
Thermal correction to Gibbs Free Energy= 0.675724
Sum of electronic and zero-point Energies= -4374.428365
Sum of electronic and thermal Energies= -4374.385182
Sum of electronic and thermal Enthalpies= -4374.384238
Sum of electronic and thermal Free Energies= -4374.503783

$TS_{2a,2}$

SCF Done: E(RwB97XD) = -4375.17354781 A.U. after 3 cycles
Convg = 0.5077D-08 -V/T = 2.0033
SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.20
(included in total energy above)

Zero-point correction= 0.747000 (Hartree/Particle)
Thermal correction to Energy= 0.790150
Thermal correction to Enthalpy= 0.791095
Thermal correction to Gibbs Free Energy= 0.671361
Sum of electronic and zero-point Energies= -4374.426548
Sum of electronic and thermal Energies= -4374.383397
Sum of electronic and thermal Enthalpies= -4374.382453
Sum of electronic and thermal Free Energies= -4374.502187

$TS_{2a,1}$

SCF Done: E(RwB97XD) = -4510.35271876 A.U. after 4 cycles
Convg = 0.6066D-08 -V/T = 2.0033
SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.82
(included in total energy above)

Zero-point correction= 0.844805 (Hartree/Particle)
Thermal correction to Energy= 0.892799
Thermal correction to Enthalpy= 0.893743
Thermal correction to Gibbs Free Energy= 0.764988
Sum of electronic and zero-point Energies= -4509.507914
Sum of electronic and thermal Energies= -4509.459920
Sum of electronic and thermal Enthalpies= -4509.458976
Sum of electronic and thermal Free Energies= -4509.587730

$TS_{1,3}$

SCF Done: E(RwB97XD) = -4563.28346303 A.U. after 16 cycles
Convg = 0.2880D-08 -V/T = 2.0033
SMD-CDS (non-electrostatic) energy (kcal/mol) = -0.82
(included in total energy above)

Zero-point correction= 0.750195 (Hartree/Particle)
Thermal correction to Energy= 0.796799
Thermal correction to Enthalpy= 0.797743
Thermal correction to Gibbs Free Energy= 0.669727
Sum of electronic and zero-point Energies= -4562.533268
Sum of electronic and thermal Energies= -4562.486664
Sum of electronic and thermal Enthalpies= -4562.485720
Sum of electronic and thermal Free Energies= -4562.613736

3

SCF Done: E(RwB97XD) = -4563.30479063 A.U. after 3 cycles
Convg = 0.6733D-08 -V/T = 2.0033
SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.25
(included in total energy above)

Zero-point correction= 0.754166 (Hartree/Particle)
Thermal correction to Energy= 0.801025
Thermal correction to Enthalpy= 0.801969

Thermal correction to Gibbs Free Energy= 0.672635
Sum of electronic and zero-point Energies= -4562.550625
Sum of electronic and thermal Energies= -4562.503766
Sum of electronic and thermal Enthalpies= -4562.502822
Sum of electronic and thermal Free Energies= -4562.632156

$TS_{2,4}$

SCF Done: E(RwB97XD) = -4563.76538006 A.U. after 4 cycles
Convg = 0.5528D-08 -V/T = 2.0033
SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.28
(included in total energy above)

Zero-point correction= 0.762592 (Hartree/Particle)
Thermal correction to Energy= 0.808467
Thermal correction to Enthalpy= 0.809412
Thermal correction to Gibbs Free Energy= 0.684980
Sum of electronic and zero-point Energies= -4563.002788
Sum of electronic and thermal Energies= -4562.956913
Sum of electronic and thermal Enthalpies= -4562.955968
Sum of electronic and thermal Free Energies= -4563.080400

4

SCF Done: E(RwB97XD) = -4563.77235025 A.U. after 4 cycles
Convg = 0.6572D-08 -V/T = 2.0033
SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.41
(included in total energy above)

Zero-point correction= 0.766198 (Hartree/Particle)
Thermal correction to Energy= 0.812378
Thermal correction to Enthalpy= 0.813322
Thermal correction to Gibbs Free Energy= 0.687976
Sum of electronic and zero-point Energies= -4563.006152
Sum of electronic and thermal Energies= -4562.959972
Sum of electronic and thermal Enthalpies= -4562.959028
Sum of electronic and thermal Free Energies= -4563.084374

5

SCF Done: E(RwB97XD) = -4375.63365904 A.U. after 4 cycles

Convg = 0.5170D-08 -V/T = 2.0033
SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.24
(included in total energy above)

Zero-point correction= 0.762855 (Hartree/Particle)
Thermal correction to Energy= 0.805903
Thermal correction to Enthalpy= 0.806848
Thermal correction to Gibbs Free Energy= 0.687839
Sum of electronic and zero-point Energies= -4374.870804
Sum of electronic and thermal Energies= -4374.827756
Sum of electronic and thermal Enthalpies= -4374.826812
Sum of electronic and thermal Free Energies= -4374.945820

$TS_{5,2}$

SCF Done: E(RwB97XD) = -4510.82084484 A.U. after 3 cycles
Convg = 0.9763D-08 -V/T = 2.0034
SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.04
(included in total energy above)

Zero-point correction= 0.857198 (Hartree/Particle)
Thermal correction to Energy= 0.904676
Thermal correction to Enthalpy= 0.905620
Thermal correction to Gibbs Free Energy= 0.779287
Sum of electronic and zero-point Energies= -4509.963646
Sum of electronic and thermal Energies= -4509.916169
Sum of electronic and thermal Enthalpies= -4509.915225
Sum of electronic and thermal Free Energies= -4510.041558

CO_2

SCF Done: E(RwB97XD) = -188.588767524 A.U. after 1 cycles
Convg = 0.1437D-09 -V/T = 2.0034
SMD-CDS (non-electrostatic) energy (kcal/mol) = 6.34
(included in total energy above)

Zero-point correction= 0.011725 (Hartree/Particle)
Thermal correction to Energy= 0.014345
Thermal correction to Enthalpy= 0.015289
Thermal correction to Gibbs Free Energy= -0.008960
Sum of electronic and zero-point Energies= -188.577042
Sum of electronic and thermal Energies= -188.574422

Sum of electronic and thermal Enthalpies= -188.573478
Sum of electronic and thermal Free Energies= -188.597727

H_2

SCF Done: E(RwB97XD) = -1.17590942502 A.U. after 1 cycles
Convg = 0.9522D-14 -V/T = 2.0364
SMD-CDS (non-electrostatic) energy (kcal/mol) = 0.44
(included in total energy above)

Zero-point correction= 0.010078 (Hartree/Particle)
Thermal correction to Energy= 0.012438
Thermal correction to Enthalpy= 0.013382
Thermal correction to Gibbs Free Energy= -0.001415
Sum of electronic and zero-point Energies= -1.165832
Sum of electronic and thermal Energies= -1.163471
Sum of electronic and thermal Enthalpies= -1.162527
Sum of electronic and thermal Free Energies= -1.177325

$HCOO^-$

SCF Done: E(RwB97XD) = -189.321728651 A.U. after 1 cycles
Convg = 0.1795D-09 -V/T = 2.0037
SMD-CDS (non-electrostatic) energy (kcal/mol) = 4.90
(included in total energy above)

Zero-point correction= 0.020900 (Hartree/Particle)
Thermal correction to Energy= 0.023863
Thermal correction to Enthalpy= 0.024807
Thermal correction to Gibbs Free Energy= -0.002249
Sum of electronic and zero-point Energies= -189.300829
Sum of electronic and thermal Energies= -189.297866
Sum of electronic and thermal Enthalpies= -189.296922
Sum of electronic and thermal Free Energies= -189.323978

$NH(CH_3)_2$

SCF Done: E(RwB97XD) = -135.175588764 A.U. after 1 cycles
Convg = 0.3567D-09 -V/T = 2.0055
SMD-CDS (non-electrostatic) energy (kcal/mol) = -0.44
(included in total energy above)

Zero-point correction= 0.093078 (Hartree/Particle)
Thermal correction to Energy= 0.097434
Thermal correction to Enthalpy= 0.098379
Thermal correction to Gibbs Free Energy= 0.067657
Sum of electronic and zero-point Energies= -135.082511
Sum of electronic and thermal Energies= -135.078154
Sum of electronic and thermal Enthalpies= -135.077210
Sum of electronic and thermal Free Energies= -135.107932

$NH_2(CH_3)_2^+$

SCF Done: E(RwB97XD) = -135.651726542 A.U. after 1 cycles
Convg = 0.2840D-09 -V/T = 2.0062
SMD-CDS (non-electrostatic) energy (kcal/mol) = 0.57
(included in total energy above)

Zero-point correction= 0.108861 (Hartree/Particle)
Thermal correction to Energy= 0.113348
Thermal correction to Enthalpy= 0.114292
Thermal correction to Gibbs Free Energy= 0.083098
Sum of electronic and zero-point Energies= -135.542865
Sum of electronic and thermal Energies= -135.538379
Sum of electronic and thermal Enthalpies= -135.537434
Sum of electronic and thermal Free Energies= -135.568629

$TS_{associative}$

SCF Done: E(RwB97XD) = -4563.27397377 A.U. after 3 cycles
Convg = 0.3858D-08 -V/T = 2.0033
SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.80
(included in total energy above)

Zero-point correction= 0.751998 (Hartree/Particle)
Thermal correction to Energy= 0.797810
Thermal correction to Enthalpy= 0.798755
Thermal correction to Gibbs Free Energy= 0.674266
Sum of electronic and zero-point Energies= -4562.521976
Sum of electronic and thermal Energies= -4562.476163
Sum of electronic and thermal Enthalpies= -4562.475219
Sum of electronic and thermal Free Energies= -4562.599708

Electronic energies (in Hartrees) for all of the relevant species (*w*B97XD/6-311++G(d,p) (SDD for Zn) single-point refinement calculations based on the optimized geometries from the *w*B97XD/TZVP calculations, methanol as the solvent**)**

1

SCF Done: E(RwB97XD) = -3137.61640944 A.U. after 28 cycles
Convg = 0.1315D-08 -V/T = 2.0218
SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.11
(included in total energy above)

1a

SCF Done: E(RwB97XD) = -3137.58489570 A.U. after 27 cycles
Convg = 0.4201D-08 -V/T = 2.0218
SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.33
(included in total energy above)

2

SCF Done: E(RwB97XD) = -3138.10285042 A.U. after 28 cycles
Convg = 0.4610D-08 -V/T = 2.0219
SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.23
(included in total energy above)

2a

SCF Done: E(RwB97XD) = -3138.09535443 A.U. after 26 cycles
Convg = 0.8476D-08 -V/T = 2.0218
SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.05
(included in total energy above)

$TS_{2,2a}$

SCF Done: E(RwB97XD) = -3138.08848518 A.U. after 27 cycles
Convg = 0.7833D-08 -V/T = 2.0219
SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.20
(included in total energy above)

$TS_{2a,1}$

SCF Done: E(RwB97XD) = -3273.26061863 A.U. after 42 cycles
Convg = 0.3481D-08 -V/T = 2.0210
SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.82
(included in total energy above)

$TS_{1,3}$

SCF Done: E(RwB97XD) = -3326.18827541 A.U. after 29 cycles
Convg = 0.7038D-08 -V/T = 2.0207
SMD-CDS (non-electrostatic) energy (kcal/mol) = -0.82
(included in total energy above)

3

SCF Done: E(RwB97XD) = -3326.21031201 A.U. after 29 cycles
Convg = 0.4014D-08 -V/T = 2.0206
SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.25
(included in total energy above)

$TS_{2,4}$

SCF Done: E(RwB97XD) = -3326.66831335 A.U. after 27 cycles
Convg = 0.9454D-08 -V/T = 2.0208
SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.28
(included in total energy above)

4

SCF Done: E(RwB97XD) = -3326.67557496 A.U. after 27 cycles
Convg = 0.8746D-08 -V/T = 2.0208
SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.41
(included in total energy above)

4a

SCF Done: E(RwB97XD) = -3326.69993409 A.U. after 25 cycles
Convg = 0.7191D-08 -V/T = 2.0208

SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.79
(included in total energy above)

5

SCF Done: E(RwB97XD) = -3138.54712588 A.U. after 44 cycles
Convg = 0.1150D-08 -V/T = 2.0219
SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.24
(included in total energy above)

$TS_{5,2}$

SCF Done: E(RwB97XD) = -3273.72700063 A.U. after 32 cycles
Convg = 0.8425D-08 -V/T = 2.0212
SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.04
(included in total energy above)

CO_2

SCF Done: E(RwB97XD) = -188.576221010 A.U. after 9 cycles
Convg = 0.5501D-08 -V/T = 2.0028
SMD-CDS (non-electrostatic) energy (kcal/mol) = 6.34
(included in total energy above)

H_2

SCF Done: E(RwB97XD) = -1.17584075569 A.U. after 6 cycles
Convg = 0.2652D-09 -V/T = 2.0365
SMD-CDS (non-electrostatic) energy (kcal/mol) = 0.44
(included in total energy above)

$HCOO^-$

SCF Done: E(RwB97XD) = -189.312749581 A.U. after 11 cycles
Convg = 0.3971D-08 -V/T = 2.0031
SMD-CDS (non-electrostatic) energy (kcal/mol) = 4.90
(included in total energy above)

$NH(CH_3)_2$

SCF Done: E(RwB97XD) = -135.168154114 A.U. after 11 cycles
Convg = 0.5860D-08 -V/T = 2.0048
SMD-CDS (non-electrostatic) energy (kcal/mol) = -0.44
(included in total energy above)

$NH_2(CH_3)_2^+$

SCF Done: E(RwB97XD) = -135.642236073 A.U. after 10 cycles
Convg = 0.3904D-08 -V/T = 2.0053
SMD-CDS (non-electrostatic) energy (kcal/mol) = 0.57
(included in total energy above)

Electronic energies (in Hartrees) for all of the relevant species (*w*B97XD/6-31+G(d,p) single-point refinement calculations based on the optimized geometries from the *w*B97XD/TZVP calculations, methanol as the solvent**)**

1

SCF Done: E(RwB97XD) = -4374.08187371 A.U. after 25 cycles
Convg = 0.5529D-08 -V/T = 2.0052
SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.11
(included in total energy above)

2

SCF Done: E(RwB97XD) = -4374.57100665 A.U. after 27 cycles
Convg = 0.2412D-08 -V/T = 2.0053
SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.23
(included in total energy above)

2a

SCF Done: E(RwB97XD) = -4374.56025777 A.U. after 25 cycles
Convg = 0.3081D-08 -V/T = 2.0053
SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.05
(included in total energy above)

$TS_{2,2a}$

SCF Done: E(RwB97XD) = -4374.55538332 A.U. after 26 cycles
Convg = 0.2115D-08 -V/T = 2.0053
SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.20
(included in total energy above)

$TS_{2a,1}$

SCF Done: E(RwB97XD) = -4509.69931465 A.U. after 25 cycles
Convg = 0.2521D-08 -V/T = 2.0054
SMD-CDS (non-electrostatic) energy (kcal/mol) = -3.82
(included in total energy above)

$TS_{1,3}$

SCF Done: E(RwB97XD) = -4562.60027106 A.U. after 25 cycles
Convg = 0.7883D-08 -V/T = 2.0054
SMD-CDS (non-electrostatic) energy (kcal/mol) = -0.82
(included in total energy above)

3

SCF Done: E(RwB97XD) = -4562.62390172 A.U. after 29 cycles
Convg = 0.6812D-08 -V/T = 2.0054
SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.25
(included in total energy above)

$TS_{2,4}$

SCF Done: E(RwB97XD) = -4563.08341773 A.U. after 24 cycles
Convg = 0.3097D-08 -V/T = 2.0054
SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.28
(included in total energy above)

4

SCF Done: E(RwB97XD) = -4563.09214656 A.U. after 27 cycles
Convg = 0.6364D-08 -V/T = 2.0054
SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.41
(included in total energy above)

4a

SCF Done: E(RwB97XD) = -4563.11829425 A.U. after 27 cycles
Convg = 0.5096D-08 -V/T = 2.0054
SMD-CDS (non-electrostatic) energy (kcal/mol) = -1.79
(included in total energy above)

5

SCF Done: E(RwB97XD) = -4375.01510356 A.U. after 25 cycles
Convg = 0.9012D-08 -V/T = 2.0053

SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.24
(included in total energy above)

$TS_{5,2}$

SCF Done: E(RwB97XD) = -4510.16836766 A.U. after 25 cycles
Convg = 0.3429D-08 -V/T = 2.0054
SMD-CDS (non-electrostatic) energy (kcal/mol) = -4.04
(included in total energy above)

CO_2

SCF Done: E(RwB97XD) = -188.521713607 A.U. after 9 cycles
Convg = 0.4031D-08 -V/T = 2.0082
SMD-CDS (non-electrostatic) energy (kcal/mol) = 6.34
(included in total energy above)

H_2

SCF Done: E(RwB97XD) = -1.17474443416 A.U. after 4 cycles
Convg = 0.5005D-10 -V/T = 2.0305
SMD-CDS (non-electrostatic) energy (kcal/mol) = 0.44
(included in total energy above)

$HCOO^-$

SCF Done: E(RwB97XD) = -189.263540994 A.U. after 11 cycles
Convg = 0.1836D-08 -V/T = 2.0087
SMD-CDS (non-electrostatic) energy (kcal/mol) = 4.90
(included in total energy above)

$NH(CH_3)_2$

SCF Done: E(RwB97XD) = -135.141922334 A.U. after 11 cycles
Convg = 0.6455D-08 -V/T = 2.0099
SMD-CDS (non-electrostatic) energy (kcal/mol) = -0.44
(included in total energy above)

$NH_2(CH_3)_2^+$

SCF Done: E(RwB97XD) = -135.616966186 A.U. after 10 cycles

Convg = 0.3464D-08 -V/T = 2.0104

SMD-CDS (non-electrostatic) energy (kcal/mol) = 0.57

(included in total energy above)