

SUPPORTING INFORMATION FOR

Carbene-Enabled Ether Activation Through the Formation of

Oxonium: A Theoretical View

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Part 1: Computational details

All the calculations were performed with the Gaussian 09 suite of programs by using density functional theory.¹ Geometry optimizations were carried out with the B3LYP functional and the 6-31G (d, p) basis sets. The stationary points were optimized in THF solvent using the integral equation formalism polarizable continuum model (IEF-PCM).² All the optimized stationary points had been identified as minima (zero imaginary frequencies) and transition states (one imaginary frequency), via the vibrational analysis. The solution translational entropy correction has been calculated with Fang's THERMO program,³ which is based on the free volume that a solute molecule could move along three axes within the cavity. Moreover, we further refined the energy by employing the single-point energy calculations at the B3LYP/6-311++G(2df,2pd)/IEF-PCM_{THF} level based on the B3LYP/6-31G(d,p)/IEF-PCM_{THF} optimized structures.

Energy decomposition analysis (EDA) calculations were performed using Q-Chem 5.2.⁴ The second-generation ALMO-EDA calculations were performed in THF using B3LYP and 6-311++G(2df,2pd) basis set in Q-Chem 5.2.

For analyzing the local nucleophilicity and electrophilicity, we have also performed the Parr function analysis, pioneered by Domingo and coworkers, the nucleophilic (P_k^-) and electrophilic (P_k^+) Parr functions which allow for the characterization of the nucleophilic and electrophilic sites of a molecule, can be obtained through the analysis of Mulliken atomic spin density (ASD) of the corresponding radical cations (RC) or anions (RA) of the studies molecules, separately. According to Domingo's definition, the Parr functions can be expressed by the following equations:

$$P^-(r) = \rho_S^{rc}(r) \text{ for the electrophilic attacks} \quad (1)$$

$$P^+(r) = \rho_S^{ra}(r) \text{ for the nucleophilic attacks} \quad (2)$$

where $\rho_S^{rc}(r)$ is the ASD of the radical cation and $\rho_S^{ra}(r)$ is the ASD of the radical anion. Each ASD condensed at the different atoms of the radical cation and radical anion provides the local nucleophilic P_k^- and electrophilic P_k^+ Parr functions of the neutral system, respectively.

For the global reactivity index (GRI) analysis, the relevant parameters of GRI, i.e., global electrophilicity index ω , electronic chemical potential μ , chemical hardness η , one-electron energies of the frontier molecular orbital HOMO (E_L) and LUMO (E_H), The HOMO energies obtained within the Kohn–Sham scheme, global nucleophilicity index N was generally utilized to judge the

nucleophilicity character. In addition, according to Domingo's definition, the local electrophilicity (ω_k) and local nucleophilicity (N_k) index can be expressed by the following equations:

$$N_k = N \times P_k^+ \quad (3)$$

$$\omega_k = \omega \times P_k^- \quad (4)$$

Part 2: The formation of ammonium carbamate salt **R2'**

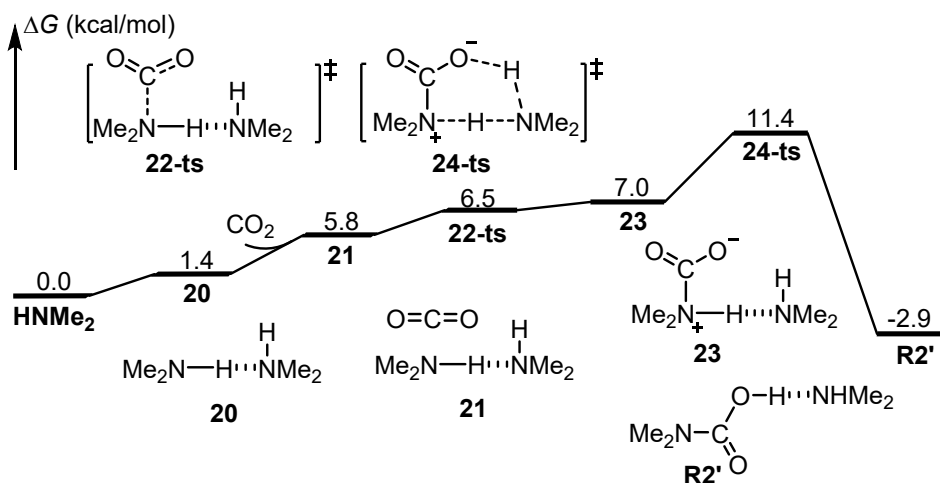


Figure S1. The energy profile for the formation of **R2'** in THF solvent.

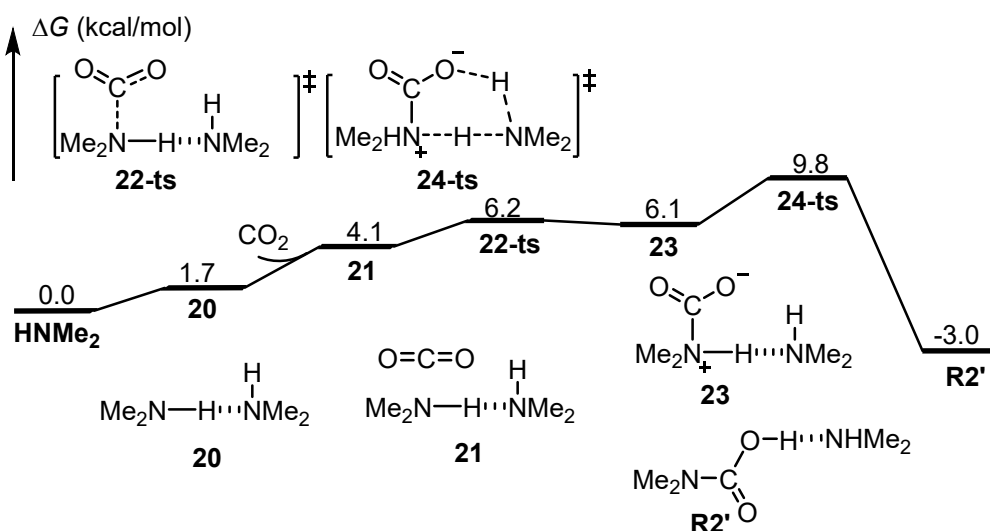


Figure S2. The energy profile for the formation of **R2'** in a mixed 1,4-dioxane/MeCN solvent.

As shown in Figure S1, two molecules of **HNMe₂** form intermediate **20** through hydrogen bonding. The reaction is initiated with nucleophilic addition of the hydrogen-bonded intermediate **20** to **CO₂** through transition state **22-ts** ($\Delta G^\ddagger = 6.5$ kcal/mol) forming the zwitterionic intermediate **23**. It should be noted that the Gibbs free energy difference between **22-ts** and **23** is negative (-0.5 kcal/mol) with zero-point and thermal corrections, while the relative electron energy is positive ($+2.1$ kcal/mol). Then the zwitterionic intermediate **23** undergoes intramolecular hydrogen atom transfer through the transition state **24-ts** ($\Delta G^\ddagger = 11.4$ kcal/mol) to obtain the final ammonium carbamate **R2'**.

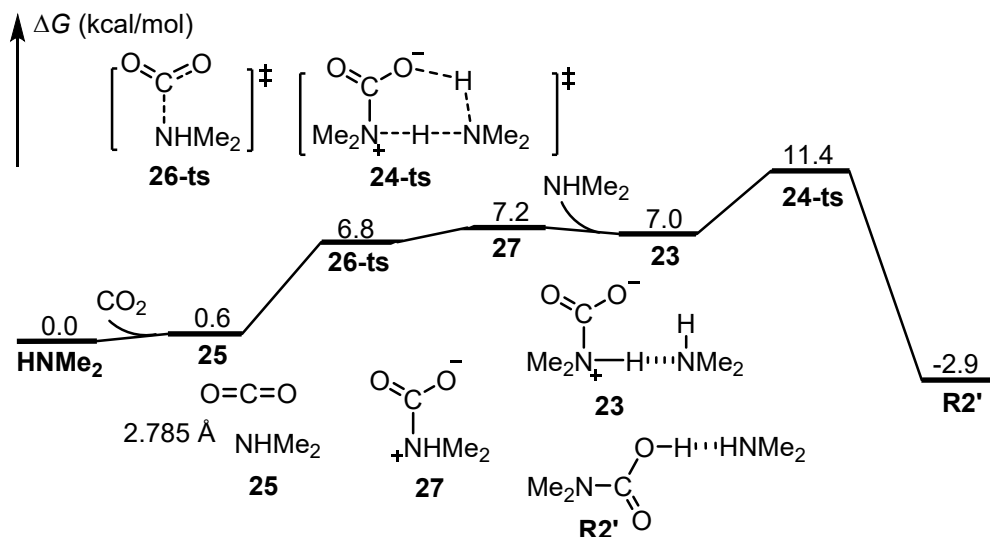


Figure S1a. The energy profile for Carbon dioxide first react with an amine to generate **R2'** in THF solvent.

At the same time, we also considered the possibility of carbon dioxide reacting with only one amine in Scheme 1a. In our DFT calculation, we found that the energy barrier of the nucleophilic addition of carbon dioxide with an amine to the zwitterionic intermediate **27** is higher than **23** for only 0.3 kcal/mol. Hence, both of two pathways for the formation of ammonium carbamate **R2'** are feasible.

Part 3: The relative Gibbs free energy profiles using THP as nucleophile in THF solvent

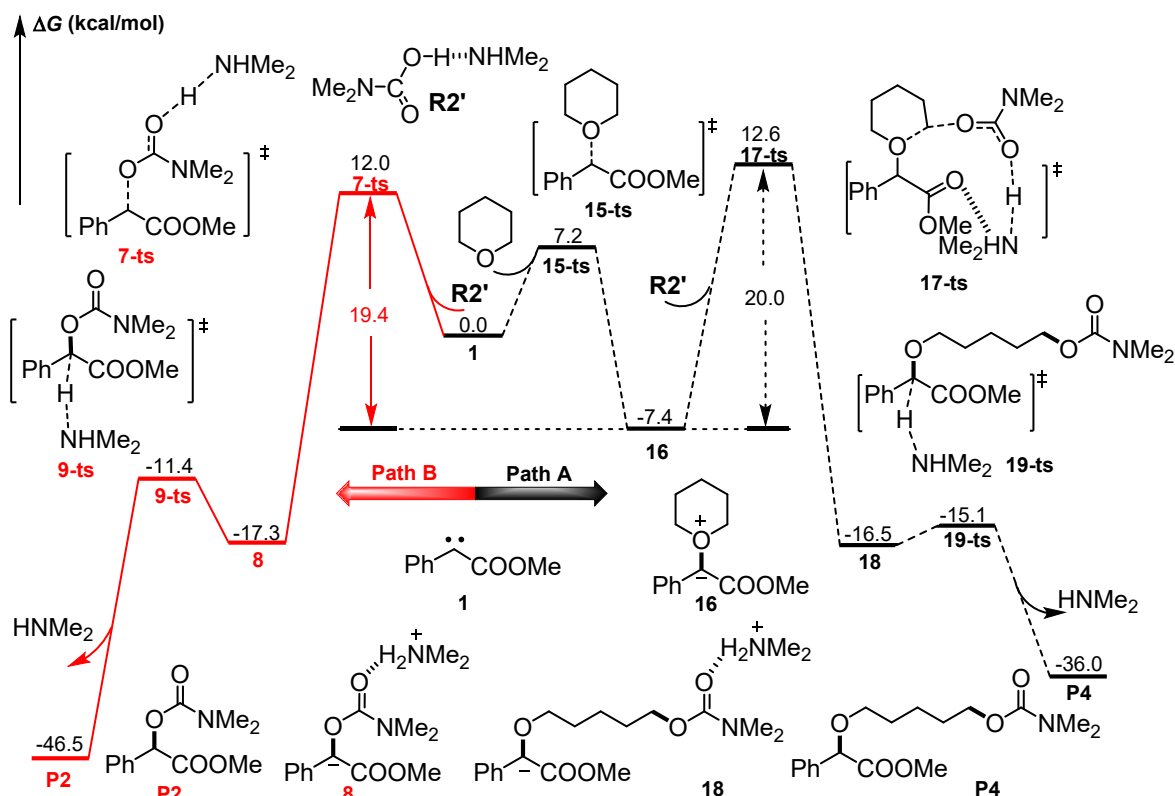


Figure S3. The energy profiles for the two possible reactions in THF computed at the B3LYP/6-311++G(2df,2pd)/IEF-PCM_{THF}//B3LYP/6-31G(d, p)/IEF-PCM_{THF} level (unit: kcal/mol)

In order to understand the influence of different cyclic ethers on the reaction, we also explored two possible reaction paths of 1,4-dihydropyran as a nucleophile in THF solution. As shown in Figure S3, THP also plays as an alternative nucleophile, which could attack electron-deficient carbene species **1**, forming the zwitterionic intermediate **16** via transition state **15-ts** with an energy barrier of 7.2 kcal/mol. It can be clearly found that the formation of intermediate **16** is exothermic, and the free energy is 7.4 kcal/mol. Then a sequential reaction with ammonium carbamate salt **R2'** takes place via transition state **17-ts** ($\Delta G^\ddagger = 20.0$ kcal/mol) to achieve nucleophilic substitution products methoxyenolate intermediate **18**, the generated methoxyenolate intermediate **18** could be protonated by ammonium through a rapid process via transition state **19-ts** to generate the ester-inserted alkyloxyargioacetate product **P4**. In an alternative pathway has been described in the text. The relative free energy of transition state **7-ts** is 0.6 kcal/mol lower than that of **17-ts**. Therefore, pathway B is favorable.

Part 4: The change of Gibbs free energy of intermediate **3** and transition state **4-ts** with eps

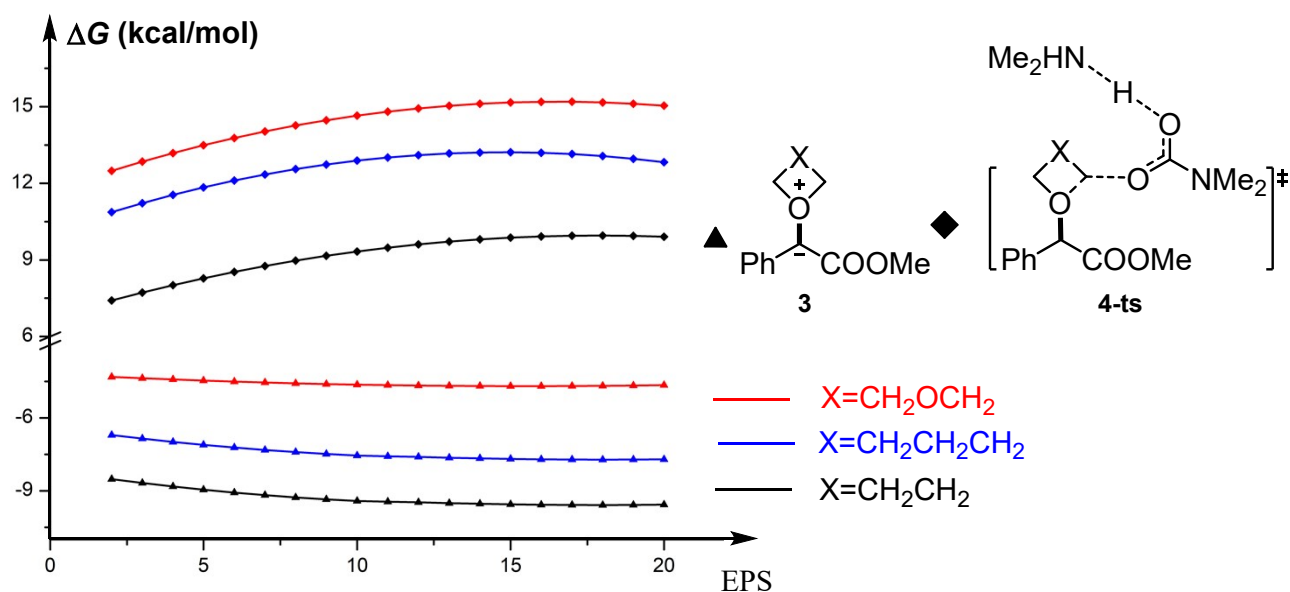


Figure S4. The change of Gibbs free energy of intermediate **3** and transition state **4-ts** with eps

In order to explore the reasons for the three/four-components coupling reaction, the solvation effect can easily be considered as the main influencing factor. Therefore, we have calculated the relative free energy of transition states **7-ts** and **4-ts** with different dielectric constants. As shown in the Figure S4, DFT calculations result that the relative free energy of every transition state is slightly increased with a higher dielectric constant. However, the trend of energy difference is remained unchanged. Therefore, dielectric constant is not a key factor affecting the results.

Part 5: Electrostatic potential map of different oxonium ion intermediates

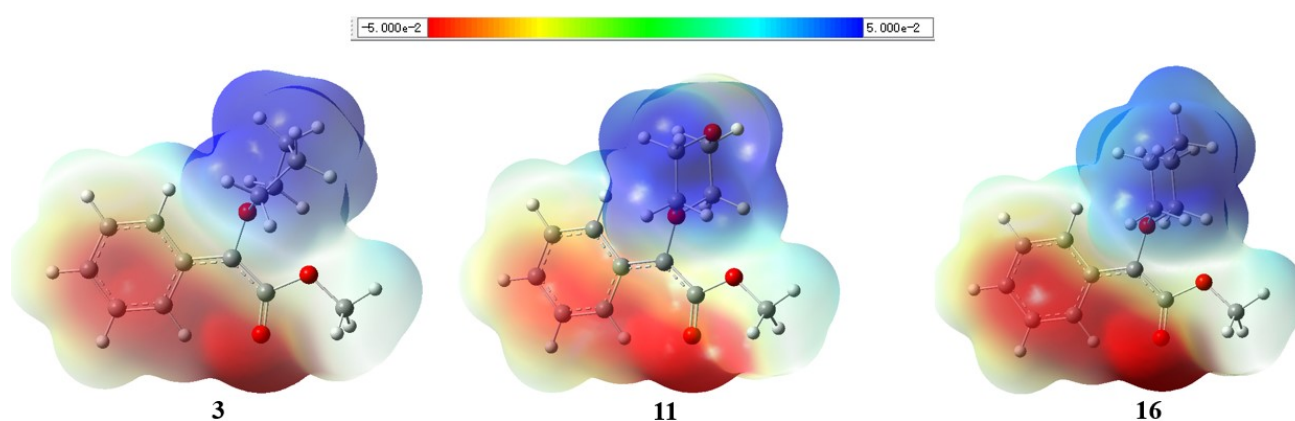


Figure S5. Electrostatic potential map of different oxonium ion intermediates **3,11,16**.

The electrostatic potential map of intermediates **3,11,16** were analyzed to investigate the stability of these oxonium ion. In Figure S5, blue represents the positively charged area, whereas red represents the negatively charged area. We found that the oxonium ion intermediate **3** is a highly separated structure of positive and negative charges. Relative to intermediate 3, the positive and negative charges of intermediate **11** are not completely separated.

Part 6: Detailed information of reactivity index calculation

Table S1. Nucleophilicity (N , eV) and Electrophilicity (ω , eV) values of the complexes THF, 1,4-Dioxane, and THP, involved in the reaction pathway.

species	E_H (a.u.)	E_L (a.u.)	μ (a.u.)	η (a.u.)	ω (eV)	N (eV)	P_k^+	P_k^-	N_k (eV)	ω_k (eV)
THF	-0.24139	0.09113	-0.07513	0.33252	0.231	3.799	0.702	-0.007	2.667	-0.002
1,4-Dioxane	-0.23796	0.09534	-0.07131	0.3333	0.208	3.892	0.353	0.009	1.374	0.002
THP	-0.24587	0.09236	-0.076755	0.33823	0.237	3.677	0.615	0.003	2.261	0.001
TCNE	-0.38099	-0.09281								

Part 7: Absolute single-point energies and Gibbs free energy (GFE) of the structures optimized

Table S3. The single-point energies (E), Gibbs free energy corrections (GFEC)¹, and GFE ($=E+GFEC$) energies of the stationary points involved in the reaction of mechanistic view of carbene enabled ether activations (unit: a.u.)

SP	GFEC (B3LYP/6-31G(d,p)/ IEFPCM _{THF})	E (B3LYP/6- 31++G(2df,2pd)/ IEFPCM _{THF})	GFE
1	-0.163587	-498.01019	-498.173777
THF	-0.074312	-232.3631	-232.437412
2-ts	-0.231453	-730.36562	-730.597073
3	-0.229169	-730.39681	-730.625979
R2'	-0.1544	-458.79344	-458.94784
4-ts	-0.377238	-1189.1673	-1189.544518
5	-0.379318	-1189.2122	-1189.591478
6-ts	-0.375399	-1189.2129	-1189.588289
HNMe₂	-0.045159	-135.09833	-135.143489
P1	-0.338249	-1054.143	-1054.481229
7-ts	-0.310749	-956.79313	-957.103879
8	-0.310549	-956.83724	-957.147789
9-ts	-0.308941	-956.83066	-957.139601
P2	-0.267492	-821.78558	-822.053072
1,4-Dioxane	-0.103957	-307.56811	-307.672067
10-ts	-0.263486	-805.57225	-805.835736
11	-0.258575	-805.59645	-805.855025
12-ts	-0.407083	-1264.3656	-1264.772683
13	-0.406446	-1264.4179	-1264.824306
14-ts	-0.40486	-1264.4157	-1264.82053

P3	-0.045216	-135.09875	-135.143966
THP	-0.083565	-271.65762	-271.741185
15-ts	-0.243331	-769.66013	-769.903461
16	-0.238574	-769.68818	-769.926754
17-ts	-0.386744	-1228.456	-1228.842694
18	-0.38676	-1228.5023	-1228.88902
19-ts	-0.385253	-1228.5016	-1228.886893
P4	-0.346401	-1093.4303	-1093.776721
CO₂	-0.076064	-188.58022	-188.656284
20	-0.08711	-270.19748	-270.28459
21	-0.155443	-458.77855	-458.933993
22-ts	-0.157128	-458.77575	-458.932878
23	-0.157227	-458.77489	-458.932117
24-ts	-0.158312	-458.76682	-458.925132
25	-0.118129	-323.68063	-323.798759
26-ts	-0.116945	-323.67194	-323.788885
27	-0.117498	-323.67088	-323.788378

¹ The solution translational entropy correction has been calculated with Fang's THERMO program

Part 8: List of the Cartesian coordinates of all the SPs involved in the reaction

1				C	1.812688	-1.406332	1.291461
Cartesian coordinates				C	3.292475	-1.573288	0.900218
C	-3.299520	0.652939	-0.097178	C	3.284796	-1.227175	-0.597406
C	-2.192504	1.490340	0.110075	H	1.981475	-2.862444	-1.208126
C	-0.921198	0.943345	0.163292	H	1.502241	-1.289067	-1.905728
C	-0.724653	-0.462592	0.018726	H	1.616046	-0.421710	1.727564
C	-1.871408	-1.282127	-0.180969	H	1.477991	-2.176512	1.997533
C	-3.143038	-0.730574	-0.244970	H	3.952269	-0.931148	1.489962
H	-2.337060	2.559741	0.223420	H	3.615133	-2.609754	1.047393
H	-0.057844	1.581008	0.325763	H	3.306152	-0.142575	-0.739823
H	-1.714638	-2.350419	-0.285839	H	4.118141	-1.671302	-1.148855
H	-4.011268	-1.361549	-0.402922	C	-4.028543	-0.934527	0.579620
C	0.543489	-1.098161	0.036818	C	-3.462988	0.196988	1.183927
C	1.748560	-0.360127	0.281771	C	-2.270941	0.712391	0.696970
O	2.151652	-0.197949	1.435004	C	-1.623654	0.119311	-0.422812
O	2.445591	-0.011546	-0.822982	C	-2.230373	-1.016532	-1.020548
H	-4.294311	1.086463	-0.142338	C	-3.412587	-1.544621	-0.519368
C	3.757839	0.537046	-0.585114	H	-3.955264	0.660602	2.032873
H	4.173047	0.735318	-1.572466	H	-1.828992	1.590684	1.157110
H	3.694289	1.463035	-0.009188	H	-1.736199	-1.461532	-1.877426
H	4.384434	-0.178168	-0.047314	H	-3.863594	-2.418002	-0.979084
THF				C	-0.404166	0.598357	-0.985764
Cartesian coordinates				C	0.217184	1.797833	-0.509575
C	-0.732893	-0.995559	0.228643	O	-0.218714	2.881635	-0.910472
C	0.732962	-0.995502	-0.228669	O	1.341895	1.672837	0.230160
C	1.168363	0.428020	0.132050	C	2.032066	2.906633	0.512738
C	-1.168400	0.427960	-0.131993	H	1.396019	3.588083	1.082167
H	-1.343635	-1.759338	-0.259922	H	2.343373	3.396740	-0.412470
H	-0.793652	-1.151442	1.311473	H	-4.958338	-1.340280	0.967648
H	0.793739	-1.151317	-1.311509	H	2.903087	2.623102	1.102181
H	1.343749	-1.759269	0.259859	3			
H	1.535708	0.478099	1.168085	Cartesian coordinates			
H	1.953775	0.819569	-0.524260	C	-1.572303	-1.230385	1.246938
H	-1.953756	0.819440	0.524428	O	-0.801247	-0.820305	0.021244
H	-1.535877	0.478056	-1.167979	C	-1.483150	-1.285808	-1.226142
O	-0.000031	1.254586	-0.000044	C	-2.363783	-2.407161	-0.712908
2-ts				C	-2.809921	-1.903557	0.675501
Cartesian coordinates				H	-0.905796	-1.900480	1.790606
C	1.926090	-1.777376	-1.025477	H	-1.759622	-0.315976	1.802734
O	1.044089	-1.510078	0.075709	H	-2.038590	-0.429582	-1.607273
				H	-0.682084	-1.579272	-1.902285

H	-3.210353	-2.581690	-1.380274
H	-1.793797	-3.336871	-0.627208
H	-3.615953	-1.172813	0.570869
H	-3.155417	-2.714646	1.319632
C	4.250184	-0.460616	0.022353
C	3.773965	0.854292	-0.014708
C	2.410508	1.131279	-0.019428
C	1.451536	0.084794	0.014291
C	1.951277	-1.241057	0.052729
C	3.319961	-1.501547	0.056145
H	4.477270	1.683499	-0.041022
H	2.056389	2.153780	-0.049071
H	1.257685	-2.075291	0.082885
H	3.659703	-2.534125	0.086555
C	0.035651	0.360931	0.006802
C	-0.647233	1.593247	-0.020851
O	-0.148088	2.725815	-0.047235
O	-2.035405	1.433037	-0.007431
C	-2.779675	2.654288	-0.030239
H	-2.562032	3.236223	-0.930127
H	-2.557151	3.272193	0.844186
H	5.316205	-0.666917	0.025540
H	-3.830625	2.361393	-0.021267

4-ts

Cartesian coordinates

C	-0.617769	1.707822	-0.477683
O	1.203510	1.771457	0.045638
C	1.416247	3.048281	0.702646
C	0.347083	3.926904	0.073094
C	-0.949923	3.086982	0.018047
H	-0.364447	1.563320	-1.517818
H	-0.791464	0.835599	0.125125
H	1.273126	2.924029	1.777359
H	2.436873	3.378667	0.490589
H	0.197891	4.844836	0.648147
H	0.650033	4.212823	-0.940174
H	-1.396321	3.015810	1.013328
H	-1.677642	3.550690	-0.650696
C	4.826074	-1.132834	-1.934113
C	4.431923	-1.775315	-0.756376
C	3.436419	-1.243234	0.059241
C	2.786292	-0.026297	-0.275328
C	3.201986	0.611264	-1.471462
C	4.197880	0.066917	-2.278520
H	4.908841	-2.707950	-0.463379
H	3.146349	-1.752467	0.969215

H	2.730422	1.543759	-1.760974
H	4.485561	0.589161	-3.188022
C	1.756051	0.567992	0.556990
C	1.136673	0.000794	1.673546
O	1.276232	-1.182565	2.103068
O	0.261400	0.857540	2.323928
C	-0.610208	0.263895	3.291432
H	-0.064491	-0.398905	3.965211
H	-1.412072	-0.293132	2.795311
N	-4.295427	-0.313966	-1.029558
C	-4.894620	-1.532800	-0.524398
H	-5.868285	-1.324944	-0.059246
H	-4.232418	-1.970781	0.219198
C	-5.088338	0.448904	-1.974306
H	-5.330711	-0.154858	-2.860165
H	-4.523960	1.325695	-2.283474
H	-1.218094	-1.715360	0.252828
N	-0.486335	-2.468960	0.407371
C	0.138661	-2.817963	-0.895469
H	0.599669	-1.922617	-1.311170
H	-0.629727	-3.192825	-1.573218
C	-1.135715	-3.618499	1.089469
H	-0.395047	-4.397409	1.276119
H	-1.933734	-4.009923	0.457374
H	0.241139	-2.057856	1.050498
C	-3.037111	0.107046	-0.621170
O	-2.609219	1.207469	-1.108825
O	-2.409474	-0.621843	0.219401
H	5.602711	-1.554939	-2.564964
H	-5.061645	-2.259723	-1.332587
H	-6.036969	0.772432	-1.522846
H	0.902302	-3.581199	-0.741494
H	-1.552180	-3.272656	2.035547
H	-1.042610	1.095580	3.850170

5

Cartesian coordinates

C	-1.844876	1.359835	-0.417708
O	0.972516	1.089466	-0.146970
C	0.931001	2.412347	0.409371
C	-0.127358	3.226930	-0.331418
C	-1.587646	2.814879	-0.061944
H	-1.537865	1.149054	-1.447096
H	-1.304765	0.702110	0.258252
H	0.692986	2.352819	1.478752
H	1.916785	2.886907	0.302911
H	-0.005584	4.279113	-0.048387

H	0.080623	3.168554	-1.407933	Cartesian coordinates			
H	-1.831768	2.975605	0.995263	C	0.926438	2.416379	0.065807
H	-2.256648	3.457934	-0.646367	O	0.886706	1.034924	-0.312966
C	5.786149	-0.145262	-1.161950	C	-1.876711	1.261241	-0.560790
C	5.448878	-0.861757	-0.008417	C	-1.614234	2.746001	-0.355584
C	4.179955	-0.770050	0.557273	C	-0.167691	3.144297	-0.713573
C	3.176190	0.056821	-0.014691	H	0.760030	2.514604	1.145190
C	3.538051	0.772602	-1.185650	H	1.910698	2.845276	-0.170582
C	4.811636	0.672688	-1.740708	H	-1.560215	0.938897	-1.557573
H	6.189405	-1.504449	0.463470	H	-1.345673	0.671347	0.179169
H	3.938195	-1.326436	1.453608	H	-2.305347	3.325995	-0.979249
H	2.795164	1.406590	-1.657122	H	-1.827606	3.010501	0.687445
H	5.044138	1.242538	-2.638001	H	0.001798	2.978348	-1.785542
C	1.824782	0.169580	0.517486	H	-0.048733	4.220912	-0.542916
C	1.394872	-0.359211	1.763790	C	5.717339	-0.206305	-1.172181
O	2.007523	-1.114086	2.538369	C	5.395559	-0.808229	0.047134
O	0.074643	0.005856	2.070510	C	4.112942	-0.706703	0.584891
C	-0.420645	-0.518078	3.301145	C	3.096823	0.015150	-0.082294
H	0.181948	-0.186212	4.152134	C	3.438246	0.609099	-1.317898
H	-0.433672	-1.612758	3.299692	C	4.722704	0.502334	-1.849444
H	6.778964	-0.221996	-1.595878	H	6.153493	-1.366451	0.591894
H	-1.439017	-0.137010	3.399364	H	3.883623	-1.174071	1.533400
N	-4.937574	-0.430075	-0.342212	H	2.674865	1.153859	-1.861813
C	-5.460918	-1.783057	-0.474237	H	4.945776	0.978234	-2.801474
H	-4.644069	-2.463702	-0.702528	C	1.696647	0.110280	0.406590
H	-6.203942	-1.822950	-1.278739	C	1.377345	-0.072694	1.815944
C	-5.913313	0.613681	-0.049403	O	2.036769	-0.684578	2.657895
H	-6.410283	0.408598	0.906000	O	0.123851	0.407484	2.135164
H	-6.677093	0.639902	-0.834784	C	-0.304654	0.147861	3.476607
H	0.660800	-1.135937	-0.342597	H	0.372490	0.604474	4.203356
N	-0.035051	-1.680003	-0.930272	H	-0.355667	-0.926229	3.675780
C	-0.035038	-3.103565	-0.495068	N	-4.967703	-0.512669	-0.305402
H	-0.294710	-3.142890	0.562599	C	-5.488389	-1.872031	-0.302129
H	0.958770	-3.524851	-0.647221	H	-6.178409	-2.018437	-1.141680
C	0.315953	-1.482042	-2.363719	H	-6.033138	-2.068524	0.628718
H	-0.431898	-1.970014	-2.989630	C	-5.951632	0.556437	-0.191092
H	1.300419	-1.911022	-2.550755	H	-6.653840	0.516568	-1.032461
H	-0.983758	-1.288650	-0.759983	H	-5.457655	1.523878	-0.186174
C	-3.606187	-0.207657	-0.461911	H	0.913657	-1.058306	-0.127478
O	-3.266145	1.086329	-0.301046	N	0.128986	-1.851081	-0.680960
O	-2.781345	-1.102571	-0.702486	C	0.244729	-3.174454	-0.033022
H	-5.424851	1.582401	0.004546	H	0.006104	-3.072950	1.026927
H	-5.944788	-2.096385	0.458216	H	1.270716	-3.534541	-0.134456
H	-0.770851	-3.657010	-1.078980	C	0.419542	-1.873543	-2.130768
H	0.339266	-0.411359	-2.561890	H	-0.268178	-2.542999	-2.655858
				H	1.445307	-2.213826	-2.284714
				H	-0.825917	-1.491146	-0.542823

6-ts

C	-3.630270	-0.305470	-0.427765
O	-3.299199	1.004925	-0.428521
O	-2.799634	-1.215598	-0.530833
H	0.318405	-0.860708	-2.521537
H	-0.438656	-3.895012	-0.491414
H	-6.523680	0.441928	0.737109
H	-4.660501	-2.571924	-0.390237
H	6.718448	-0.289787	-1.585350
H	-1.297528	0.591175	3.560371

HNMe₂

Cartesian coordinates

N	-0.028001	0.589319	0.000000
H	0.805497	1.172636	0.000000
C	-0.028001	-0.222490	1.213340
H	0.040284	0.425067	2.092843
H	-0.970427	-0.778561	1.280783
H	0.793409	-0.960497	1.265384
C	-0.028001	-0.222490	-1.213340
H	-0.970427	-0.778561	-1.280783
H	0.040284	0.425067	-2.092843
H	0.793409	-0.960497	-1.265384

P1

Cartesian coordinates

C	0.990988	-1.621742	-0.658623
O	0.889275	-0.801421	0.514312
C	-2.078512	-1.094883	0.102019
C	-1.550511	-2.078601	-0.933708
C	-0.149187	-2.633372	-0.630403
H	0.936356	-1.004395	-1.562882
H	1.954276	-2.147976	-0.659347
H	-2.039262	-1.514019	1.112607
H	-1.518061	-0.160008	0.101135
H	-2.252237	-2.919206	-0.995492
H	-1.551597	-1.595905	-1.918938
H	-0.143915	-3.134075	0.346272
H	0.081096	-3.404766	-1.374921
C	5.933670	-0.798887	0.181166
C	5.242509	-0.285151	-0.917640
C	3.903825	0.089489	-0.790907
C	3.241250	-0.041656	0.436274
C	3.942961	-0.560593	1.532165
C	5.280296	-0.936991	1.407965
H	5.744086	-0.175057	-1.874448
H	3.378596	0.488589	-1.654488
H	3.437016	-0.667829	2.487995

H	5.812368	-1.332403	2.268059
C	1.767433	0.308235	0.611242
C	1.309218	1.464766	-0.291328
O	0.441047	1.400717	-1.137176
O	1.983007	2.586894	0.011092
C	1.623215	3.763886	-0.742687
H	0.568355	4.002924	-0.593445
H	1.811697	3.607161	-1.806821
N	-5.418682	0.201276	0.192629
C	-6.238526	1.166651	0.908280
H	-6.459210	2.039035	0.279173
H	-5.704189	1.494189	1.797648
C	-6.001076	-0.381278	-1.008424
H	-6.996625	-0.774505	-0.775535
H	-5.377735	-1.193491	-1.372923
C	-4.117170	0.030202	0.569275
O	-3.459121	-0.830526	-0.247085
O	-3.593889	0.571687	1.538521
H	1.631524	0.671379	1.636275
H	6.975944	-1.087298	0.082885
H	-7.188930	0.707438	1.202696
H	-6.108492	0.369822	-1.802503
H	2.254869	4.562227	-0.356717

7-ts

Cartesian coordinates

C	-4.280601	0.765347	-0.941688
C	-3.935395	0.352026	0.351757
C	-2.784688	-0.398376	0.552080
C	-1.967303	-0.784653	-0.543801
C	-2.355579	-0.371302	-1.842824
C	-3.487465	0.410120	-2.038592
H	-4.561771	0.628443	1.194239
H	-2.515175	-0.725516	1.551251
H	-1.735011	-0.673993	-2.679372
H	-3.766022	0.731608	-3.037143
C	-0.789285	-1.588676	-0.416032
C	-0.364271	-2.100786	0.852376
O	-0.986072	-3.065629	1.314089
O	0.771994	-1.619546	1.398061
H	-5.174879	1.362633	-1.094246
C	1.247397	-2.334855	2.553874
H	2.164867	-1.827818	2.850677
H	0.516802	-2.298579	3.365513
H	1.454609	-3.378823	2.307092
N	2.792644	-0.346485	-1.340401
C	4.238200	-0.179565	-1.387825

H	4.563926	0.477781	-0.585605
H	4.561152	0.245469	-2.348529
C	2.223986	-1.343114	-2.235706
H	2.791255	-2.275496	-2.143858
H	2.276725	-1.015756	-3.284058
H	1.401464	3.769786	1.779150
N	0.913621	3.010356	1.308460
C	-0.035704	3.574881	0.337589
H	0.494679	4.256752	-0.332237
H	-0.858701	4.122116	0.819030
C	0.259388	2.161633	2.315210
H	-0.138785	1.275492	1.815660
H	-0.559473	2.677278	2.837051
H	1.939722	2.062799	0.500727
C	1.971044	0.524886	-0.685742
O	0.730532	0.460744	-0.727150
O	2.621526	1.462146	0.004925
H	1.184962	-1.528708	-1.962328
H	4.722618	-1.155019	-1.270379
H	-0.447742	2.755504	-0.255660
H	0.998730	1.839840	3.053148

8

Cartesian coordinates

C	-4.620521	0.783569	-0.392551
C	-4.279274	0.007747	0.723593
C	-2.960823	-0.340037	0.991965
C	-1.898333	0.082344	0.142130
C	-2.265688	0.868207	-0.985285
C	-3.594093	1.205657	-1.239771
H	-5.059629	-0.335898	1.399666
H	-2.715255	-0.942007	1.857430
H	-1.490765	1.220480	-1.657712
H	-3.825585	1.810123	-2.114383
C	-0.525160	-0.259217	0.391040
C	0.000771	-0.963160	1.489413
O	-0.624735	-1.538714	2.398962
O	1.403003	-1.001078	1.486368
H	-5.654600	1.047793	-0.593352
C	1.979603	-1.790507	2.523154
H	3.060194	-1.735586	2.375405
H	1.721193	-1.407057	3.515148
H	1.652247	-2.833500	2.465758
N	1.124423	-1.513669	-1.699010
C	2.238174	-2.290317	-2.236748
H	3.173016	-1.930888	-1.812075
H	2.287595	-2.207835	-3.329321

C	-0.209514	-2.060532	-1.941053
H	-0.466361	-2.833492	-1.210035
H	-0.214418	-2.505371	-2.941543
H	3.530577	2.811367	0.196776
N	2.563769	2.479958	0.195195
C	1.713575	3.444463	-0.560891
H	2.131387	3.568918	-1.559822
H	1.693409	4.401716	-0.039609
C	2.116160	2.260212	1.601929
H	1.104022	1.860332	1.578706
H	2.147490	3.207764	2.140706
H	2.553321	1.547428	-0.340101
C	1.378576	-0.307021	-1.154798
O	0.416988	0.376994	-0.500218
O	2.490599	0.251143	-1.269772
H	-0.963224	-1.277609	-1.907740
H	2.099295	-3.343028	-1.973074
H	0.711384	3.023314	-0.627810
H	2.779810	1.533788	2.068191

9-ts

Cartesian coordinates

C	-4.069563	-1.642830	0.168366
C	-3.548666	-1.065598	1.329879
C	-2.276310	-0.497271	1.344643
C	-1.467898	-0.494719	0.184833
C	-2.011010	-1.077276	-0.982634
C	-3.287003	-1.641731	-0.986941
H	-4.139500	-1.057849	2.242563
H	-1.886276	-0.060727	2.254297
H	-1.420013	-1.084594	-1.891566
H	-3.667835	-2.084163	-1.903997
C	-0.149579	0.174949	0.126561
C	0.648756	0.466076	1.304121
O	0.267621	0.455516	2.474320
O	1.908475	0.909906	0.978833
H	-5.062544	-2.082510	0.165184
C	2.738550	1.270228	2.090156
H	3.694026	1.568633	1.658349
H	2.303575	2.100010	2.653495
H	2.879742	0.423195	2.766354
N	2.058619	-1.786372	-0.501660
C	3.421285	-2.305012	-0.508608
H	4.100555	-1.531494	-0.860521
H	3.511775	-3.180586	-1.164763
C	1.067241	-2.629890	0.154378
H	1.069202	-2.495958	1.242904

H	1.303338	-3.677330	-0.062168
H	-0.103268	2.284087	-1.884865
N	-0.558612	2.584920	-1.022584
C	-1.971438	2.931903	-1.290735
H	-2.464390	2.075152	-1.750957
H	-2.039718	3.799070	-1.953542
C	0.229184	3.673612	-0.402335
H	-0.219852	3.926288	0.560187
H	0.238677	4.560104	-1.041981
H	-0.476330	1.567478	-0.329337
C	1.795986	-0.666009	-1.232298
O	0.562931	-0.071267	-1.113756
O	2.586648	-0.177186	-2.029662
H	0.069393	-2.425090	-0.224639
H	3.702677	-2.605283	0.506278
H	-2.462487	3.160935	-0.343236
H	1.246597	3.316452	-0.242537

P2

Cartesian coordinates

C	-3.960289	-1.722982	0.131477
C	-3.669106	-1.165053	-1.114265
C	-2.444711	-0.527824	-1.326201
C	-1.506733	-0.441797	-0.292914
C	-1.805472	-0.996926	0.958945
C	-3.025280	-1.639136	1.167124
H	-4.390537	-1.228878	-1.923231
H	-2.216667	-0.099234	-2.298018
H	-1.079751	-0.923878	1.762645
H	-3.248332	-2.070879	2.138229
C	-0.187063	0.268735	-0.518131
C	-0.116845	1.545390	0.330403
O	0.377151	1.616746	1.434928
O	-0.733816	2.553271	-0.301236
H	-4.910731	-2.221830	0.295813
C	-0.809208	3.798881	0.424312
H	-1.341679	4.486518	-0.230547
H	-1.353971	3.660838	1.360501
H	0.193782	4.172837	0.638929
N	3.081256	-1.064187	-0.044223
C	4.482641	-0.725271	-0.251427
H	4.988448	-0.572510	0.709713
H	4.545224	0.188232	-0.838853
C	2.813675	-2.281672	0.712361
H	3.153081	-2.175703	1.750295
H	3.355301	-3.118353	0.258284
C	2.125897	-0.188904	-0.446777

O	0.865434	-0.621557	-0.131215
O	2.326937	0.864393	-1.042565
H	1.750447	-2.505095	0.707666
H	4.990352	-1.536981	-0.783935
H	-0.074438	0.550760	-1.566674

10-ts

Cartesian coordinates

C	3.648808	-2.083887	0.532405
C	3.392821	-0.941892	1.306038
C	2.549660	0.042919	0.816347
C	1.951552	-0.083103	-0.471564
C	2.241803	-1.248596	-1.233220
C	3.072815	-2.241545	-0.734193
H	3.850746	-0.837245	2.284210
H	2.348519	0.931734	1.406293
H	1.785704	-1.337185	-2.213379
H	3.282809	-3.130574	-1.319476
C	1.075478	0.879008	-1.041560
C	0.783142	2.115925	-0.379984
O	1.549149	3.072918	-0.523756
O	-0.412274	2.196522	0.246437
C	-0.776043	3.506587	0.729195
H	-0.819834	4.223220	-0.093888
H	-0.060497	3.858351	1.475620
H	4.305676	-2.856055	0.921980
H	-1.760624	3.386230	1.178698
C	-1.679326	-0.954217	0.987579
C	-2.369259	-0.307810	-1.164386
C	-3.034410	-1.609465	1.223698
H	-1.691438	0.081594	1.355532
H	-0.886172	-1.503172	1.504127
C	-3.722828	-0.964711	-0.926679
H	-2.410324	0.754164	-0.884616
H	-2.076005	-0.383635	-2.215360
H	-3.325416	-1.535907	2.275892
H	-2.984779	-2.674069	0.944437
H	-4.517451	-0.420232	-1.445601
H	-3.703465	-2.001399	-1.299203
O	-1.354742	-0.968556	-0.403935
O	-4.049972	-0.952271	0.464089

11

Cartesian coordinates

C	4.221556	-1.044130	-0.000343
C	3.996408	0.336518	-0.000079
C	2.707458	0.860357	0.000304

C	1.570067	0.009268	0.000416
C	1.816912	-1.386480	0.000188
C	3.114476	-1.894856	-0.000188
H	4.840386	1.022448	-0.000188
H	2.549504	1.930959	0.000445
H	0.983961	-2.080584	0.000328
H	3.256301	-2.972881	-0.000379
C	0.231706	0.551746	0.000867
C	-0.199856	1.893113	0.000224
O	0.521415	2.900651	0.000260
O	-1.587534	2.023121	-0.000254
C	-2.070363	3.370697	-0.000815
H	-1.732827	3.912727	-0.888361
H	-1.735220	3.912606	0.887732
H	5.230968	-1.444053	-0.000631
H	-3.158262	3.294149	-0.002245
C	-1.612157	-0.658899	1.248508
C	-1.611081	-0.659187	-1.248363
C	-2.313830	-2.001090	1.166626
H	-2.302201	0.182823	1.294468
H	-0.879098	-0.613819	2.051778
C	-2.312796	-2.001361	-1.166801
H	-2.301081	0.182527	-1.295081
H	-0.877273	-0.614255	-2.050961
H	-2.973095	-2.100080	2.032938
H	-1.580175	-2.819428	1.189480
H	-2.971299	-2.100486	-2.033682
H	-1.579155	-2.819729	-1.188857
O	-0.812266	-0.475889	0.000426
O	-3.121919	-2.088772	-0.000438

12-ts

Cartesian coordinates

C	4.530050	-1.567162	-2.087944
C	4.073032	-2.273688	-0.971146
C	3.161584	-1.709810	-0.081915
C	2.662814	-0.394305	-0.275998
C	3.140858	0.306519	-1.412304
C	4.051675	-0.270644	-2.294191
H	4.433184	-3.282870	-0.784661
H	2.823823	-2.270696	0.779729
H	2.787231	1.314255	-1.597910
H	4.390485	0.303225	-3.153532
C	1.721946	0.228730	0.637414
C	1.046620	-0.369008	1.704275
O	1.072095	-1.592742	2.025969
O	0.274484	0.509581	2.448325

C	-0.638818	-0.077501	3.382305
H	-0.152430	-0.849446	3.980914
H	-1.499678	-0.503038	2.857224
N	-4.216741	-0.122568	-1.070556
C	-4.981298	-1.220416	-0.510142
H	-5.323495	-1.899522	-1.302225
H	-5.871392	-0.855759	0.023529
C	-4.922280	0.736163	-2.003988
H	-5.357933	0.136617	-2.813095
H	-4.223916	1.455308	-2.426143
H	-1.452410	-1.812133	0.225819
N	-0.817340	-2.659123	0.331404
C	-0.266086	-3.038061	-0.995351
H	0.310401	-2.200087	-1.386197
H	-1.088243	-3.274937	-1.672260
C	-1.582253	-3.745023	0.996885
H	-0.932787	-4.608123	1.150118
H	-2.429532	-4.027422	0.370597
H	-0.036985	-2.348265	0.966546
C	-2.965790	0.217704	-0.571976
O	-2.434449	1.286152	-1.032132
O	-2.435501	-0.543753	0.301052
C	-0.432503	1.650405	-0.337050
C	1.780300	2.654284	1.117753
C	-0.421088	3.070537	-0.847271
H	-0.835188	1.423261	0.635544
H	-0.233661	0.828795	-1.003279
C	1.402539	3.936296	0.399727
H	1.282480	2.573386	2.085731
H	2.863628	2.571093	1.244500
H	-1.442055	3.339806	-1.119495
H	0.213797	3.144084	-1.741117
H	1.648451	4.791530	1.035361
H	1.966723	4.026205	-0.540464
O	1.346140	1.555775	0.274922
O	0.004222	4.001659	0.140950
H	-5.742531	1.282693	-1.514628
H	-4.352810	-1.769333	0.187512
H	0.384353	-3.906638	-0.885510
H	-1.942003	-3.379711	1.958854
H	-0.972664	0.740456	4.022693
H	5.239991	-2.014398	-2.777272

13

Cartesian coordinates

C	4.697569	-0.823491	-2.206946
C	4.436823	-1.504119	-1.012807

C	3.441555	-1.076176	-0.137657	O	-1.006652	3.898987	0.341182
C	2.651172	0.071232	-0.421509	H	-4.489789	0.729887	-2.243255
C	2.933399	0.746010	-1.638457	H	-3.367914	-2.843621	-0.423066
C	3.931160	0.307591	-2.505020	H	1.311884	-3.896719	-0.294856
H	5.021582	-2.384544	-0.754225	H	-1.004176	-3.490259	2.582482
H	3.262532	-1.612219	0.785518	H	-0.877936	0.875356	4.017858
H	2.346678	1.621681	-1.891659	H	5.474678	-1.164655	-2.884755
H	4.110828	0.857147	-3.426608				
C	1.609336	0.573797	0.457048	14-ts			
C	1.164314	-0.029597	1.626671	Cartesian coordinates			
O	1.481925	-1.185324	2.079034	C	5.413774	-0.762885	-1.529514
O	0.261084	0.733746	2.357546	C	5.204437	-1.156625	-0.205245
C	-0.383993	0.083946	3.450550	C	4.005489	-0.876173	0.449714
H	0.330572	-0.441637	4.087665	C	2.962805	-0.177970	-0.201808
H	-1.141205	-0.626390	3.098972	C	3.189323	0.203421	-1.544024
N	-3.709130	-1.004021	-1.352047	C	4.390790	-0.080703	-2.192000
C	-3.694561	-2.460435	-1.387386	H	5.986046	-1.690099	0.330754
H	-3.024120	-2.836147	-2.170947	H	3.861831	-1.187125	1.476157
H	-4.704723	-2.825055	-1.593566	H	2.402693	0.724802	-2.078132
C	-4.409851	-0.334592	-2.444567	H	4.525740	0.234498	-3.223893
H	-5.414970	-0.756662	-2.538344	C	1.639069	0.098779	0.416369
H	-3.883136	-0.481775	-3.395613	C	1.452835	0.049892	1.859416
H	-0.952370	-2.190425	0.581893	O	2.086490	-0.638206	2.664782
N	-0.146402	-2.812580	0.780920	O	0.358685	0.770890	2.275974
C	0.443592	-3.271322	-0.504441	C	0.027336	0.632968	3.662709
H	0.756672	-2.396640	-1.073647	H	0.848527	0.968339	4.301679
H	-0.298443	-3.842233	-1.064751	H	-0.206507	-0.405975	3.911639
C	-0.580534	-3.918816	1.674132	N	-4.591839	-1.075397	-0.438851
H	0.286122	-4.530391	1.928018	C	-4.713873	-2.521280	-0.307940
H	-1.328765	-4.531740	1.169701	H	-4.736106	-2.995975	-1.296139
H	0.569280	-2.198537	1.308671	H	-5.643042	-2.771897	0.215349
C	-2.931231	-0.354980	-0.449502	C	-5.692945	-0.397101	-1.114319
O	-3.006127	0.985962	-0.574998	H	-6.632876	-0.605683	-0.591511
O	-2.247684	-0.919993	0.414057	H	-5.785364	-0.760353	-2.144654
C	-2.214321	1.805979	0.319446	H	-0.900419	-1.656588	-0.029800
C	1.265211	2.960486	0.634389	N	0.029945	-1.978860	-0.336196
C	-1.741309	3.007730	-0.493895	C	0.046219	-2.084564	-1.810000
H	-2.855779	2.123844	1.148210	H	-0.232135	-1.118669	-2.233375
H	-1.367352	1.244669	0.705682	H	-0.654527	-2.851001	-2.155050
C	0.381206	4.046121	0.040389	C	0.370540	-3.238168	0.358422
H	1.097180	2.892662	1.715212	H	1.371897	-3.553737	0.058334
H	2.321066	3.222227	0.459877	H	-0.345330	-4.027656	0.111677
H	-2.606383	3.549598	-0.899457	H	0.807868	-1.091056	0.039816
H	-1.132849	2.654915	-1.332450	C	-3.475866	-0.453619	0.015386
H	0.681412	5.011186	0.463864	O	-3.510173	0.882137	-0.192768
H	0.530230	4.094210	-1.047824	O	-2.538435	-1.035453	0.572668
O	0.935042	1.725658	0.005261	C	-2.384977	1.682916	0.237306

C	1.241095	2.427597	-0.082304
C	-1.866295	2.450055	-0.976468
H	-2.762162	2.384185	0.987634
H	-1.609098	1.057460	0.674983
C	0.395677	3.327619	-0.967208
H	1.107127	2.710129	0.968920
H	2.298902	2.566103	-0.349348
H	-2.710373	2.933048	-1.486819
H	-1.391345	1.759444	-1.681384
H	0.819042	4.337779	-0.931635
H	0.444654	2.978680	-2.008585
O	0.853117	1.065487	-0.278823
O	-0.960751	3.461617	-0.549437
H	-5.524097	0.675538	-1.128737
H	-3.867273	-2.903979	0.257148
H	1.053881	-2.341702	-2.141549
H	0.361655	-3.061335	1.435057
H	-0.849775	1.261283	3.820239
H	6.349778	-0.985399	-2.033577

P3

Cartesian coordinates

C	6.231914	0.027193	-0.439874
C	5.532494	-0.335792	0.712875
C	4.150692	-0.527830	0.665735
C	3.449912	-0.360560	-0.536112
C	4.161509	0.004938	-1.686657
C	5.542565	0.197304	-1.642398
H	6.062130	-0.471996	1.651068
H	3.622480	-0.824178	1.566004
H	3.627679	0.139538	-2.623874
H	6.078726	0.474963	-2.544971
C	1.935041	-0.475389	-0.635307
C	1.335476	-1.560081	0.280069
O	1.894238	-2.608742	0.534802
O	0.094883	-1.253623	0.677857
C	-0.599435	-2.259818	1.450448
H	-0.118316	-2.382899	2.423341
H	-0.590507	-3.214056	0.920215
N	-4.916553	-0.724469	-0.769866
C	-5.355237	-2.085806	-0.494547
H	-5.142594	-2.728877	-1.355374
H	-6.434718	-2.114494	-0.300896
C	-5.508023	-0.075497	-1.934298
H	-6.568020	0.152282	-1.763905
H	-5.436701	-0.748497	-2.794691
C	-4.121169	-0.089924	0.131475

O	-3.889044	1.206958	-0.220115
O	-3.658863	-0.605442	1.146966
C	-2.989564	1.949126	0.622655
C	1.493967	1.542172	0.635854
C	-1.561997	1.833554	0.100444
H	-3.336060	2.984001	0.587141
H	-3.047345	1.577435	1.646651
C	0.594026	2.770451	0.611934
H	1.278092	0.950447	1.535457
H	2.541866	1.867898	0.680614
H	-1.486340	2.276012	-0.904337
H	-1.268638	0.781024	0.032762
H	0.995707	3.502235	1.320136
H	0.622080	3.216380	-0.394202
O	1.263612	0.777488	-0.549865
O	-0.744759	2.541144	1.026321
H	-4.978838	0.845979	-2.161995
H	-4.825317	-2.461579	0.377877
H	-1.614745	-1.882527	1.559437
H	7.307379	0.172727	-0.401971
H	1.694303	-0.827065	-1.646930

THP

Cartesian coordinates

C	1.183306	-0.770495	0.201759
C	1.259112	0.697131	-0.222980
C	-1.259116	0.697125	-0.222980
C	-1.183301	-0.770501	0.201759
H	2.164855	1.153563	0.193639
H	1.216347	-0.843903	1.302607
H	2.023169	-1.346393	-0.198619
H	-2.164862	1.153552	0.193639
H	-1.343152	0.744453	-1.316218
H	-1.216343	-0.843909	1.302607
H	-2.023162	-1.346402	-0.198619
H	1.343148	0.744459	-1.316218
O	0.000003	-1.403754	-0.286619
C	-0.000003	1.449616	0.234121
H	-0.000005	2.475366	-0.150599
H	-0.000003	1.521990	1.330658

15-ts

Cartesian coordinates

C	3.588424	-2.179388	0.554423
C	3.402982	-1.010620	1.308337
C	2.605825	0.006797	0.809543
C	1.983560	-0.113866	-0.467973

C	2.202400	-1.307885	-1.209579
C	2.988054	-2.332395	-0.701133
H	3.879675	-0.911269	2.278100
H	2.458881	0.916865	1.382812
H	1.727754	-1.390836	-2.181128
H	3.143475	-3.242787	-1.270385
C	1.148141	0.877506	-1.045661
C	0.909311	2.131409	-0.394477
O	1.692232	3.068973	-0.561534
O	-0.271618	2.241474	0.258001
C	-0.600339	3.562822	0.733310
H	-0.638335	4.273423	-0.095280
H	0.132191	3.905690	1.467542
H	4.209651	-2.976952	0.951494
H	-1.581621	3.468415	1.196367
C	-1.738575	-1.048638	0.977167
C	-2.330854	-0.407808	-1.223778
C	-3.167064	-1.478237	1.318441
H	-1.577190	0.000523	1.272694
H	-1.001916	-1.664523	1.502531
C	-3.796555	-0.797724	-1.022789
H	-2.182940	0.657327	-0.986693
H	-2.012664	-0.568699	-2.258085
H	-3.352495	-1.322394	2.388151
H	-3.269694	-2.553509	1.123326
H	-4.436325	-0.153066	-1.637576
H	-3.940445	-1.828117	-1.372588
O	-1.459379	-1.201601	-0.415133
C	-4.176207	-0.697529	0.462679
H	-5.194622	-1.066030	0.629668
H	-4.167879	0.358509	0.767310

16

Cartesian coordinates

C	-4.187202	-1.113895	-0.000357
C	-3.992722	0.271482	-0.000308
C	-2.716293	0.824308	-0.000223
C	-1.560161	-0.001057	-0.000183
C	-1.775946	-1.402050	-0.000239
C	-3.061599	-1.939642	-0.000322
H	-4.851955	0.938288	-0.000334
H	-2.581919	1.898132	-0.000184
H	-0.926249	-2.075996	-0.000214
H	-3.179656	-3.020689	-0.000359
C	-0.233610	0.568496	-0.000081
C	0.167539	1.918951	0.000035
O	-0.571525	2.912579	-0.000016

O	1.555244	2.076809	0.000196
C	2.006234	3.434233	0.000302
H	1.657219	3.969606	0.887673
H	1.657364	3.969699	-0.887068
H	-5.187519	-1.536199	-0.000421
H	3.096081	3.383935	0.000389
C	1.617379	-0.612960	-1.260960
C	1.616812	-0.613318	1.261306
C	2.266059	-1.984343	-1.257112
H	2.333382	0.209772	-1.284964
H	0.872468	-0.487343	-2.044203
C	2.265488	-1.984703	1.257357
H	2.332800	0.209409	1.285870
H	0.871545	-0.487927	2.044246
H	2.876485	-2.054692	-2.164386
H	1.489861	-2.754517	-1.331264
H	2.875500	-2.055319	2.164888
H	1.489249	-2.754893	1.330932
O	0.829941	-0.434509	0.000020
C	3.116389	-2.207655	0.000283
H	3.527302	-3.221319	0.000232
H	3.968566	-1.516055	0.000576

17-ts

Cartesian coordinates

C	4.805782	-1.282352	-1.871499
C	4.335182	-2.026209	-0.785006
C	3.328137	-1.538277	0.043756
C	2.742436	-0.264351	-0.182660
C	3.236590	0.475837	-1.286694
C	4.242961	-0.025728	-2.108713
H	4.760989	-3.004697	-0.574313
H	2.981180	-2.126061	0.883666
H	2.818949	1.454796	-1.492529
H	4.590738	0.576064	-2.945180
C	1.698606	0.283073	0.665801
C	1.009495	-0.371994	1.688062
O	1.095827	-1.597812	1.996466
O	0.135553	0.440862	2.395835
C	-0.805690	-0.227208	3.243653
H	-0.318122	-0.990448	3.852376
H	-1.600776	-0.681688	2.643621
N	-4.386907	-0.146120	-0.835420
C	-5.118772	-1.285605	-0.317489
H	-5.435426	-1.963197	-1.124928
H	-6.022582	-0.953950	0.210366
C	-5.112422	0.723662	-1.741410

H	-5.397490	0.198765	-2.665701	H	2.344729	1.430868	-1.988346
H	-4.484263	1.573209	-1.999537	H	4.052735	0.525957	-3.513521
H	-1.250076	-1.865384	0.016836	C	1.635322	0.549829	0.431932
N	-0.564366	-2.678396	0.108254	C	1.190034	0.022316	1.636719
C	0.082226	-2.954044	-1.199575	O	1.456670	-1.131532	2.130039
H	0.636594	-2.069242	-1.510823	O	0.343189	0.858492	2.354816
H	-0.685117	-3.193516	-1.937519	C	-0.303909	0.281859	3.485800
C	-1.311671	-3.835258	0.663383	H	0.405448	-0.220779	4.147476
H	-0.634318	-4.679996	0.798601	H	-1.075691	-0.434744	3.181039
H	-2.114305	-4.110535	-0.022331	N	-3.792138	-1.022689	-1.268897
H	0.156134	-2.365830	0.812519	C	-3.900763	-2.471113	-1.163580
C	-3.020838	-0.005637	-0.624137	H	-3.263730	-2.977295	-1.900991
O	-2.441928	0.967005	-1.215903	H	-4.937694	-2.769386	-1.343177
O	-2.456093	-0.836815	0.160138	C	-4.413475	-0.402724	-2.435186
C	-0.515775	1.559314	-0.440817	H	-5.440703	-0.767344	-2.530519
C	1.621584	2.689995	1.174933	H	-3.870156	-0.656883	-3.354184
C	-0.597919	2.960780	-0.971003	H	-0.992808	-2.072495	0.658678
H	-0.937982	1.299955	0.516376	N	-0.194112	-2.711389	0.838483
H	-0.190969	0.747434	-1.067748	C	0.362856	-3.170667	-0.460240
C	1.250912	3.989055	0.478536	H	0.686991	-2.298325	-1.026560
H	1.086829	2.568633	2.120674	H	-0.401690	-3.719736	-1.013071
H	2.697583	2.615675	1.358392	C	-0.645340	-3.815564	1.723230
H	-1.630852	3.105398	-1.298272	H	0.206952	-4.453580	1.960912
H	0.037546	3.055158	-1.858554	H	-1.415522	-4.402952	1.220521
H	1.476718	4.812446	1.166068	H	0.544378	-2.113977	1.367331
H	1.888500	4.126164	-0.403839	C	-2.966306	-0.356597	-0.419344
O	1.263895	1.586509	0.299220	O	-2.912170	0.960988	-0.675155
H	-6.034120	1.084869	-1.267004	O	-2.349674	-0.899383	0.508901
H	-4.479673	-1.830074	0.373915	C	-2.081141	1.786582	0.190990
H	0.771299	-3.793672	-1.097618	C	1.438444	2.954235	0.491807
H	-1.735521	-3.546285	1.624991	C	-1.791718	3.075365	-0.565676
H	-1.230943	0.548770	3.882622	H	-2.645257	1.983198	1.110132
H	5.590731	-1.670607	-2.513698	H	-1.167702	1.255093	0.441272
C	-0.224338	4.037849	0.061769	C	0.602390	4.078885	-0.108875
H	-0.444703	5.019616	-0.370516	H	1.325912	2.938236	1.583253
H	-0.864582	3.934441	0.947868	H	2.503163	3.115425	0.263003
18				H	-2.748916	3.550901	-0.811598
Cartesian coordinates				H	-1.313277	2.821840	-1.518025
C	4.623556	-1.092433	-2.205511	H	1.031004	5.020760	0.258155
C	4.374663	-1.690750	-0.965739	H	0.738117	4.084440	-1.198680
C	3.411323	-1.183521	-0.097385	O	1.004693	1.709807	-0.056789
C	2.643283	-0.036157	-0.435689	H	-4.429740	0.677679	-2.320213
C	2.914358	0.555776	-1.696969	H	-3.608023	-2.783679	-0.163034
C	3.879902	0.038584	-2.556298	H	1.221143	-3.816834	-0.273273
H	4.944823	-2.567388	-0.664927	H	-1.047714	-3.387567	2.641532
H	3.242030	-1.655385	0.862164	H	-0.779358	1.112637	4.011367
				H	5.376058	-1.495051	-2.877418

C	-0.906608	4.077564	0.217420
H	-1.281258	5.085612	0.006596
H	-1.043394	3.933533	1.298081

19-ts

Cartesian coordinates

C	5.267548	-1.304256	-1.651708
C	5.192837	-1.301063	-0.256545
C	4.074728	-0.793818	0.405275
C	2.981490	-0.258408	-0.313597
C	3.071443	-0.278794	-1.724550
C	4.191977	-0.788121	-2.378421
H	6.018037	-1.697967	0.330350
H	4.034230	-0.797821	1.486735
H	2.240625	0.108107	-2.304653
H	4.222573	-0.781085	-3.465420
C	1.733244	0.238852	0.320803
C	1.680805	0.571925	1.735756
O	2.370268	0.086347	2.637380
O	0.644612	1.427195	2.042527
C	0.469223	1.688765	3.438921
H	1.367922	2.131989	3.876141
H	0.232333	0.773023	3.988508
N	-4.839783	-1.162436	-0.345286
C	-5.184411	-2.501508	0.111606
H	-5.627629	-3.074636	-0.710072
H	-5.911612	-2.455747	0.931690
C	-5.933034	-0.358912	-0.879610
H	-6.650978	-0.101422	-0.090603
H	-6.461079	-0.931742	-1.649098
H	-0.847545	-1.606485	0.385035
N	0.112666	-1.976433	0.315914
C	0.242869	-2.689186	-0.972894
H	0.017467	-1.996136	-1.784423
H	-0.447405	-3.537120	-1.017254
C	0.395502	-2.827223	1.492028
H	1.419908	-3.199316	1.426735
H	-0.296055	-3.673678	1.535228
H	0.867186	-1.004112	0.351358
C	-3.586044	-0.683609	-0.131234
O	-3.438390	0.591410	-0.538398
O	-2.677827	-1.347966	0.381047
C	-2.123117	1.185354	-0.363712
C	1.358147	2.361464	-0.775718
C	-2.240228	2.634026	-0.811108
H	-1.830390	1.110720	0.686481
H	-1.391639	0.631169	-0.952064

C	0.253091	3.158531	-1.460824
H	1.632005	2.841628	0.172842
H	2.254502	2.338200	-1.411728
H	-3.074550	3.089129	-0.263019
H	-2.514597	2.661250	-1.873767
H	0.709909	4.098104	-1.795293
H	-0.055242	2.632660	-2.374289
O	0.904300	1.027260	-0.525588
H	-5.547300	0.555754	-1.321365
H	-4.284218	-3.003330	0.459038
H	1.267208	-3.047939	-1.085667
H	0.294838	-2.226930	2.397181
H	-0.363921	2.389459	3.506074
H	6.141223	-1.701685	-2.160173
C	-0.978137	3.483669	-0.578941
H	-1.266571	4.526055	-0.755579
H	-0.690705	3.421898	0.477754

P4

Cartesian coordinates

C	-6.205804	-0.141601	0.558432
C	-5.539879	-0.405068	-0.640161
C	-4.150996	-0.542607	-0.657708
C	-3.408520	-0.419315	0.524071
C	-4.087068	-0.153501	1.720768
C	-5.475165	-0.016065	1.741698
H	-6.101439	-0.506642	-1.564157
H	-3.648316	-0.763246	-1.593524
H	-3.521140	-0.053244	2.643391
H	-5.984398	0.183987	2.679791
C	-1.886978	-0.479564	0.560358
C	-1.285322	-1.486338	-0.439854
O	-1.826714	-2.526578	-0.758256
O	-0.057349	-1.127851	-0.835279
C	0.645187	-2.067303	-1.680316
H	0.164339	-2.121878	-2.659888
H	0.642371	-3.059100	-1.223926
N	4.828016	-0.862885	0.798928
C	5.229237	-2.215994	0.443260
H	4.923641	-2.918227	1.227030
H	6.318729	-2.281104	0.329012
C	5.364648	-0.334653	2.046629
H	6.447304	-0.168617	1.972375
H	5.184766	-1.055179	2.851647
C	4.107980	-0.126892	-0.092859
O	3.906079	1.144083	0.343142
O	3.689432	-0.550143	-1.168698

C	3.068351	1.987630	-0.480504
C	-1.559490	1.622745	-0.603312
C	1.612039	1.931029	-0.033258
H	3.483122	2.992508	-0.360112
H	3.174451	1.679719	-1.522947
C	-0.749403	2.912981	-0.501872
H	-1.320162	1.089313	-1.535250
H	-2.631209	1.858624	-0.619542
H	1.543634	2.252753	1.013591
H	1.259814	0.897604	-0.076214
H	-1.240229	3.653777	-1.145249
H	-0.836247	3.290291	0.525098
O	-1.264915	0.798950	0.530555
H	4.878484	0.604193	2.297655
H	4.754397	-2.492457	-0.495546
H	1.658001	-1.675677	-1.758576
H	-7.286862	-0.039016	0.570673
H	-1.596209	-0.883818	1.539015
C	0.728197	2.823674	-0.915642
H	1.139330	3.842613	-0.922090
H	0.783361	2.470374	-1.954851

CO₂

Cartesian coordinates

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.168927
O	0.000000	0.000000	-1.168927

20

Cartesian coordinates

N	1.632717	0.235944	-0.430911
C	2.058829	1.084418	0.674418
H	1.501052	2.026442	0.655906
H	3.124291	1.327714	0.572956
C	2.273739	-1.072184	-0.397816
H	1.871652	-1.703247	-1.197290
H	2.149320	-1.616153	0.558416
H	0.617316	0.107065	-0.376934
N	-1.541057	-0.198231	-0.343276
C	-2.250951	1.079044	-0.414069
H	-1.882521	1.657992	-1.265464
H	-2.054015	1.655278	0.496494
C	-2.041749	-1.059569	0.727700
H	-3.128801	-1.243394	0.678129
H	-1.828352	-0.596400	1.697166
H	-1.654586	-0.682325	-1.230930
H	3.352718	-0.967247	-0.569373

H	1.924402	0.630597	1.675300
H	-1.528138	-2.024529	0.695459
H	-3.345155	0.973963	-0.511919

21

Cartesian coordinates

N	-0.684423	1.016956	0.180533
C	-0.780350	1.470521	1.563104
H	-0.516788	0.650217	2.237379
H	-1.811108	1.770651	1.788205
C	-0.979712	2.072169	-0.780591
H	-0.828462	1.697265	-1.797377
H	-0.361082	2.979353	-0.654128
H	0.260699	0.655540	0.009205
N	2.109086	-0.311685	-0.436668
C	2.191975	-1.511779	0.397492
H	1.255336	-2.071224	0.328291
H	2.329826	-1.216388	1.443213
C	3.346372	0.468944	-0.424819
H	4.240558	-0.112691	-0.706851
H	3.514708	0.868192	0.581181
H	1.913010	-0.595485	-1.393989
C	-2.096501	-1.240815	-0.204940
O	-2.673489	-0.836022	-1.140604
O	-1.599205	-1.783778	0.707399
H	-2.029343	2.377177	-0.691641
H	-0.129740	2.332417	1.798482
H	3.255278	1.314601	-1.112237
H	3.025319	-2.182355	0.127370

22-ts

Cartesian coordinates

N	-0.795269	0.848259	0.230730
C	-0.955048	1.142194	1.652883
H	-0.657839	0.268186	2.237530
H	-2.007050	1.356204	1.871314
C	-1.204515	1.944791	-0.642030
H	-1.053159	1.654924	-1.684689
H	-0.649379	2.877019	-0.452345
H	0.185428	0.596552	0.039354
N	2.026766	-0.215353	-0.405064
C	2.259959	-1.303186	0.548000
H	1.377809	-1.947371	0.588243
H	2.415428	-0.881155	1.546614
C	3.182263	0.673212	-0.541406
H	4.114534	0.147278	-0.806950
H	3.353368	1.194797	0.406305

H	1.821000	-0.622018	-1.315107
C	-1.787908	-1.114227	-0.316571
O	-2.232476	-0.847274	-1.380069
O	-1.514984	-1.752067	0.643270
H	-2.270608	2.152467	-0.501189
H	-0.359225	2.007106	1.984688
H	2.980276	1.425101	-1.309324
H	3.140103	-1.921415	0.305034

23

Cartesian coordinates

N	0.873929	0.603516	0.166232
C	1.173195	1.620445	-0.870953
H	0.772921	1.268379	-1.821709
H	2.255358	1.744297	-0.951591
C	1.376553	0.980572	1.502373
H	0.995837	1.966689	1.780532
H	2.466140	0.987793	1.481283
H	-0.168483	0.458048	0.195283
N	-1.890712	-0.166314	-0.030778
C	-2.856993	0.673415	-0.742933
H	-2.386153	1.103640	-1.630930
H	-3.177508	1.495221	-0.093904
C	-2.478621	-0.855142	1.121206
H	-3.365501	-1.454357	0.860966
H	-2.780390	-0.119011	1.873602
H	-1.503542	-0.857693	-0.672524
C	1.462594	-0.889301	-0.356384
O	2.502025	-1.188035	0.206796
O	0.708259	-1.343920	-1.209785
H	1.042690	0.240133	2.229939
H	0.715523	2.577030	-0.606526
H	-3.757505	0.123441	-1.059088
H	-1.734550	-1.518319	1.570555

24-ts

Cartesian coordinates

N	0.789141	0.561761	0.213038
C	0.963969	1.717827	-0.691341
H	0.563321	1.456549	-1.670783
H	2.024867	1.977651	-0.798538
C	1.350732	0.822419	1.546632
H	0.855277	1.695584	1.982154
H	2.428921	1.007689	1.495325
H	-0.574890	0.257378	0.193411
N	-1.672583	-0.207074	-0.087876
C	-2.670769	0.821633	-0.447966

H	-2.269459	1.448262	-1.245688
H	-2.878106	1.441762	0.426704
C	-2.135155	-1.150515	0.953061
H	-3.043969	-1.667400	0.633056
H	-2.340117	-0.597385	1.871919
H	-1.370909	-0.727687	-0.919796
C	1.311978	-0.734970	-0.443059
O	2.225082	-1.310803	0.157963
O	0.674857	-1.020506	-1.482150
H	1.184653	-0.044616	2.186398
H	0.431332	2.587703	-0.295088
H	-3.601295	0.357711	-0.787058
H	-1.349565	-1.883901	1.141383

25

Cartesian coordinates

N	1.036600	-0.164490	-0.457271
C	1.589857	-1.126319	0.493340
H	1.186461	-2.122093	0.287566
H	1.289786	-0.844572	1.508702
C	1.613394	1.169039	-0.304099
H	1.231293	1.828687	-1.088669
H	2.716551	1.186054	-0.344721
H	1.211820	-0.495121	-1.402802
C	-1.693113	0.039822	0.080249
O	-1.473246	0.527870	1.121495
O	-2.021037	-0.439469	-0.935809
H	1.309367	1.584753	0.662708
H	2.691968	-1.188741	0.475684

26-ts

Cartesian coordinates

N	-0.685621	0.163780	-0.408971
C	-1.279426	1.169307	0.490815
H	-0.735849	2.110147	0.384498
H	-1.180704	0.812473	1.518182
C	-1.388985	-1.128534	-0.374876
H	-0.954470	-1.796006	-1.121425
H	-2.459223	-1.008201	-0.574407
H	-0.650493	0.526207	-1.359812
C	1.147082	-0.057892	0.051118
O	1.163823	-0.649108	1.098008
O	1.773205	0.466950	-0.831510
H	-1.249650	-1.565414	0.615864
H	-2.338507	1.334312	0.265579

26-ts				H	-2.415094	-1.006683	-0.588968
Cartesian coordinates				H	-0.602666	0.485432	-1.375582
N	-0.637517	0.151995	-0.412146	C	1.083075	-0.050433	0.051121
C	-1.259884	1.185676	0.450524	O	1.119376	-0.601604	1.129646
H	-0.712893	2.123075	0.332789	O	1.759922	0.422350	-0.833753
H	-1.186153	0.851632	1.486505	H	-1.242153	-1.539816	0.656082
C	-1.356423	-1.142717	-0.352480	H	-2.307204	1.334624	0.180174
H	-0.906211	-1.833349	-1.068118				

Part 9: References

1. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, Williams, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, *Gaussian 09. Revision B.01*, Gaussian, Inc. Wallingford, CT, **2009**,
2. (a) B. Mennucci and J. Tomasi, Continuum solvation models: A new approach to the problem of solute's charge distribution and cavity boundaries, *J. Chem. Phys.*, 1997, **106**, 5151-5158; (b) V. Barone and M. Cossi, Quantum Calculation of Molecular Energies and Energy Gradients in Solution by a Conductor Solvent Model, *J. Phys. Chem. A*, 1998, **102**, 1995-2001.
3. D.-C. Fang, *THERMO*, Beijing Normal University, Beijing, China, **2013**.
4. Y. Shao, Z. Gan, E. Epifanovsky, A. T. B. Gilbert, M. Wormit, J. Kussmann, A. W. Lange, A. Behn, J. Deng, X. Feng, D. Ghosh, M. Goldey, P. R. Horn, L. D. Jacobson, I. Kaliman, R. Z. Khaliullin, T. Kuś, A. Landau, J. Liu, E. I. Proynov, Y. M. Rhee, R. M. Richard, M. A. Rohrdanz, R. P. Steele, E. Sundstrom, H. L. J.; Woodcock, P. M. Zimmerman, D. Zuev, B. Albrecht, E. Alguire, B. Austin, G. J. O. Beran, Y. A. Bernard, E. Berquist, K. Brandhorst, K. B. Bravaya, S. T. Brown, D. Casanova, C.-M. Chang, Y. Chen, S. H. Chien, K. D. Closser, D. L. Crittenden, M. Diedenhofen, R. A. DiStasio, H. Do, A. D. Dutoi, R. G. Edgar, S. Fatehi, L. Fusti-Molnar, A. Ghysels, A. Golubeva-Zadorozhnaya, J. Gomes, M. W. D. Hanson-Heine, P. H. P. Harbach, A. W. Hauser, E. G. Hohenstein, Z. C. Holden, T.-C. Jagau, H. Ji, B. Kaduk, K. Khistyayev, J. Kim, J. Kim, R. A. King, P. Klunzinger, D. Kosenkov, T. Kowalczyk, C. M. Krauter, K. U. Lao, A. D. Laurent, K. V. Lawler, S. V. Levchenko, C. Y. Lin, F. Liu, E. Livshits, R. C. Lochan, A. Luenser, P. Manohar, S. F. Manzer, S.-P. Mao, N. Mardirossian, A. V. Marenich, S. A. Maurer, N. J. Mayhall, E. Neuscamman, C. M. Oana, R. Olivares-Amaya, D. P. O'Neill, J. A. Parkhill, T. M. Perrine, R. Peverati, A. Prociuk, D. R. Rehn, E. Rosta, N. J. Russ, S. M. Sharada, S. Sharma, D. W. Small and A. Sodt, *Mol. Phys.*, **2014**, *113*, 184-215.