Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPORTING INFORMATION

Computational predictions on Brønsted acidic ionic liquid catalyzed carbon dioxide conversion to five-membered heterocyclic carbonyl derivatives

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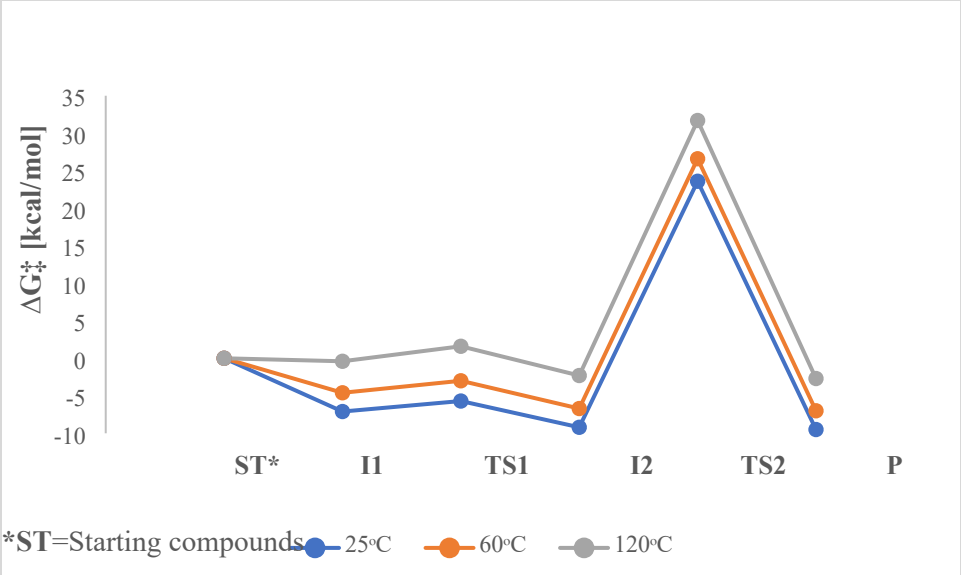

Figure S1. The calculated EDA+CO_2 reaction profile in different temperatures.

Table S1. Relative energies (kcal/mol) for EDA+ CO_2 cyclocondensation in gas phase at 298.15 K.

	Energies in gas phase				Relative energies			
Structure	**(E+ZPC)**	**Etot**	**H**	**G**	**ΔE**	**Δ(E+ZPC)**	**ΔH**	**ΔG**
CO2	-188.495463	-188.492845	-188.491901	-188.51616				
EDA	-190.291824	-190.287271	-190.286327	-190.318806				
[Et2NH2][HSO4]	-913.576638	-913.563678	-913.562733	-913.617485				
SUM	**-1292.363925**	**-1292.343794**	**-1292.340961**	**-1292.452451**				
$I1_{EDA}$	-1292.408494	-1292.386910	-1292.385965	-1292.463699				
	-0.044569	-0.043116	-0.045004	-0.011248	-28.0	-27.1	-28.2	-7.1
$TS1_{EDA}$	-1292.408306	-1292.387815	-1292.386871	-1292.461551				
	-0.044381	-0.044021	-0.045910	-0.009100	-27.8	-27.6	-28.8	-5.7
$I2_{EDA}$	-1292.413135	-1292.39176	-1292.390816	-1292.467181				
	-0.049210	-0.047966	-0.049855	-0.014730	-30.9	-30.1	-31.3	-9.2
$TS2_{EDA}$	-1292.364827	-1292.345092	-1292.344148	-1292.41484				
	-0.000902	-0.001298	-0.003187	0.037611	-0.6	-0.8	-2.0	23.6
P_{EDA}	-1292.413637	-1292.391592	-1292.390648	-1292.467612				
	-0.049712	-0.047798	-0.049687	-0.015161	-31.2	-30.0	-31.2	-9.5

Table S2. Relative energies (kcal/mol) for EDA+CO_2 cyclocondensation in the presence of n-hexane at 298.15 K.

	Energies in solvent (n-hexane)				Relative energies			
Structure	**(E+ZPC)**	**Etot**	**H**	**G**	**ΔE**	**Δ(E+ZPC)**	**ΔH**	**ΔG**
CO2	-188.496425	-188.493319	-188.492238	-188.520664				
EDA	-190.294548	-190.288895	-190.287815	-190.326308				
[Et2NH2][HSO4]	-913.586907	-913.570719	-913.569639	-913.636279				
SUM	**-1292.377880**	**-1292.352933**	**-1292.349692**	**-1292.483251**				
$I1_{EDA}$	-1292.421984	-1292.395046	-1292.393965	-1292.488656				
	-0.044104	-0.042113	-0.044273	-0.005405	-27.7	-26.4	-27.8	-3.4
$TS1_{EDA}$	-1292.418437	-1292.393069	-1292.391988	-1292.481637				
	-0.040557	-0.040136	-0.042296	0.001614	-25.4	-25.2	-26.5	1.0
$I2_{EDA}$	-1292.425678	-1292.398717	-1292.397637	-1292.491991				
	-0.047798	-0.045784	-0.047945	-0.008740	-30.0	-28.7	-30.1	-5.5
$TS2_{EDA}$	-1292.37713	-1292.352233	-1292.351153	-1292.437762				
	0.000750	0.000700	-0.001461	0.045489	0.5	0.4	-0.9	28.5
P_{EDA}	-1292.425763	-1292.398094	-1292.397013	-1292.4919				
	-0.047883	-0.045161	-0.047321	-0.008649	-30.0	-28.3	-29.7	-5.4

Table S3. Relative energies (kcal/mol) for EDA+CO_2 cyclocondensation in the presence of THF at 298.15 K.

	Energies in solvent (THF)				Relative energies			
Structure	**(E+ZPC)**	**Etot**	**H**	**G**	**ΔE**	**Δ(E+ZPC)**	**ΔH**	**ΔG**
CO2	-188.497632	-188.494416	-188.493308	-188.522625				
EDA	-190.298267	-190.292383	-190.291274	-190.33103				
[Et2NH2][HSO4]	-913.600555	-913.583635	-913.582526	-913.652024				
SUM	**-1292.396454**	**-1292.370434**	**-1292.367108**	**-1292.505679**				
$I1_{EDA}$	-1292.440265	-1292.412049	-1292.410940	-1292.510020				
	-0.043811	-0.041615	-0.043832	-0.004341	-27.5	-26.1	-27.5	-2.7
$TS1_{EDA}$	-1292.437270	-1292.410307	-1292.409198	-1292.503992				
	-0.040816	-0.039873	-0.042090	0.001687	-25.6	-25.0	-26.4	1.1
$I2_{EDA}$	-1292.442282	-1292.413859	-1292.41275	-1292.513177				
	-0.045828	-0.043425	-0.045642	-0.007498	-28.8	-27.2	-28.6	-4.7
$TS2_{EDA}$	-1292.394757	-1292.368535	-1292.367426	-1292.458383				
	0.001697	0.001899	-0.000318	0.047296	1.1	1.2	-0.2	29.7
P_{EDA}	-1292.442432	-1292.413189	-1292.41208	-1292.512364				
	-0.045978	-0.042755	-0.044972	-0.006685	-28.9	-26.8	-28.2	-4.2

Table S4. Relative energies (kcal/mol) for EDA+CO_2 cyclocondensation in the presence of acetonitrile at 298.15 K.

	Energies in solvent (Acetonitrile)				Relative energies			
Structure	**(E+ZPC)**	**Etot**	**H**	**G**	**ΔE**	**Δ(E+ZPC)**	**ΔH**	**ΔG**
CO2	-188.498054	-188.494778	-188.493654	-188.523467				
EDA	-190.299684	-190.293669	-190.292544	-190.333005				
[Et2NH2][HSO4]	-913.605673	-913.588389	-913.587264	-913.656987				
SUM	**-1292.403411**	**-1292.376836**	**-1292.373462**	**-1292.513459**				
$I1_{EDA}$	-1292.447615	-1292.418467	-1292.417342	-1292.519996				
	-0.044204	-0.041631	-0.043880	-0.006537	-27.7	-26.1	-27.5	-4.1
$TS1_{EDA}$	-1292.443919	-1292.416218	-1292.415093	-1292.511830				
	-0.040508	-0.039382	-0.041631	0.001629	-25.4	-24.7	-26.1	1.0
$I2_{EDA}$	-1292.448404	-1292.419305	-1292.41818	-1292.520241				
	-0.044993	-0.042469	-0.044718	-0.006782	-28.2	-26.6	-28.1	-4.3
$TS2_{EDA}$	-1292.402339	-1292.383122	-1292.382177	-1292.452013				
	0.001072	-0.006286	-0.008715	0.061446	0.7	-3.9	-5.5	38.6
P_{EDA}	-1292.453651	-1292.424336	-1292.423211	-1292.523746				
	-0.050240	-0.047500	-0.049749	-0.010287	-31.5	-29.8	-31.2	-6.5

Table S5. Relative energies (kcal/mol) for EDA+CO_2 cyclocondensation in the presence of methanol at 298.15 K.

	Energies in solvent (methanol)				Relative energies			
Structure	**(E+ZPC)**	**Etot**	**H**	**G**	**ΔE**	**Δ(E+ZPC)**	**ΔH**	**ΔG**
CO2	-188.498043	-188.494827	-188.493718	-188.523036				
EDA	-190.299642	-190.293763	-190.292654	-190.332402				
[Et2NH2][HSO4]	-913.600554	-913.583635	-913.582526	-913.652023				
SUM	**-1292.398239**	**-1292.372225**	**-1292.368898**	**-1292.507461**				
$I1_{EDA}$	-1292.447431	-1292.418945	-1292.417837	-1292.518802				
	-0.049192	-0.046720	-0.048939	-0.011341	-30.9	-29.3	-30.7	-7.1
$TS1_{EDA}$	-1292.443741	-1292.416700	-1292.415591	-1292.510296				
	-0.045502	-0.044475	-0.046693	-0.002835	-28.6	-27.9	-29.3	-1.8
$I2_{EDA}$	-1292.448224	-1292.419814	-1292.418705	-1292.518437				
	-0.049985	-0.047589	-0.049807	-0.010976	-31.4	-29.9	-31.3	-6.9
$TS2_{EDA}$	-1292.40213	-1292.381984	-1292.38104	-1292.455615				
	-0.003891	-0.009759	-0.012142	0.051846	-2.4	-6.1	-7.6	32.5
P_{EDA}	-1292.453464	-1292.431568	-1292.430624	-1292.508041				
	-0.055225	-0.059343	-0.061726	-0.000580	-34.7	-37.2	-38.7	-0.4

Table S6. Relative energies (kcal/mol) for $(CH_3)_2$N-EDA+CO_2 cyclocondensation in gas phase at 298.15 K.

	Energies in gas phase				Relative energies			
Structure	**(E+ZPC)**	**Etot**	**H**	**G**	**ΔE**	**Δ(E+ZPC)**	**ΔH**	**ΔG**
CO2	-188.495463	-188.492845	-188.491901	-188.51616				
(CH3)2N-EDA	-324.128747	-324.114379	-324.113134	-324.175834				
[Et2NH2][HSO4]	-913.576638	-913.563678	-913.562733	-913.617485				
SUM	**-1426.200848**	**-1426.170902**	**-1426.167768**	**-1426.309479**				
$I1_{Me2N-EDA}$	-1426.237417	-1426.212180	-1426.211236	-1426.297204				
	-0.036569	-0.041278	-0.043468	0.012275	-22.9	-25.9	-27.3	7.7
$TS1_{Me2N-EDA}$	-1426.232271	-1426.207585	-1426.206641	-1426.291536				
	-0.031423	-0.036683	-0.038873	0.017943	-19.7	-23.0	-24.4	11.3
$I2_{Me2N-EDA}$	-1426.242576	-1426.217313	-1426.216369	-1426.302177				
	-0.041728	-0.046411	-0.048601	0.007302	-26.2	-29.1	-30.5	4.6
$TS2_{Me2N-EDA}$	-1426.18904	-1426.165744	-1426.1648	-1426.242285				
	0.011808	0.005158	0.002968	0.067194	7.4	3.2	1.9	42.2
$P_{Me2N-EDA}$	-1426.257242	-1426.231693	-1426.230749	-1426.314097				
	-0.056394	-0.060791	-0.062981	-0.004618	-35.4	-38.1	-39.5	-2.9

Table S7. Relative energies (kcal/mol) for HO-EDA+CO_2 cyclocondensation in gas phase at 298.15 K.

	Energies in gas phase				Relative energies			
Structure	**(E+ZPC)**	**Etot**	**H**	**G**	**ΔE**	**Δ(E+ZPC)**	**ΔH**	**ΔG**
CO2	-188.495463	-188.492845	-188.491901	-188.51616				
OH-EDA	-265.489745	-265.479693	-265.478448	-265.530799				
[Et2NH2][HSO4]	-913.576638	-913.563678	-913.562733	-913.617485				
SUM	**-1367.561846**	**-1367.536216**	**-1367.533082**	**-1367.664444**				
$I1_{HO-EDA}$	-1367.598295	-1367.575551	-1367.574607	-1367.655242				
	-0.036449	-0.039335	-0.041525	0.009202	-22.9	-24.7	-26.1	5.8
$TS1_{HO-EDA}$	-1367.597992	-1367.575689	-1367.574745	-1367.654548				
	-0.036146	-0.039473	-0.041663	0.009896	-22.7	-24.8	-26.1	6.2
$I2_{HO-EDA}$	-1367.603767	-1367.581239	-1367.580294	-1367.659896				
	-0.041921	-0.045023	-0.047212	0.004548	-26.3	-28.3	-29.6	2.9
$TS2_{HO-EDA}$	-1367.550655	-1367.529825	-1367.528881	-1367.60212				
	0.011191	0.006391	0.004201	0.062324	7.0	4.0	2.6	39.1
P_{HO-EDA}	-1367.623541	-1367.601373	-1367.600428	-1367.675281				
	-0.061695	-0.065157	-0.067346	-0.010837	-38.7	-40.9	-42.3	-6.8

Table S8. Relative energies (kcal/mol) for NO2-EDA+CO_2 cyclocondensation in gas phase at 298.15 K.

	Energies in gas phase				Relative energies			
Structure	**(E+ZPC)**	**Etot**	**H**	**G**	**ΔE**	**Δ(E+ZPC)**	**ΔH**	**ΔG**
CO2	-188.495463	-188.492845	-188.491901	-188.51616				
NO2-EDA	-394.729017	-394.721645	-394.720701	-394.761362				
[Et2NH2][HSO4]	-913.576638	-913.563678	-913.562733	-913.617485				
SUM	**-1496.801118**	**-1496.778168**	**-1496.775335**	**-1496.895007**				
$I1_{NO2-EDA}$	-1496.833823	-1496.809642	-1496.808698	-1496.893917				
	-0.032705	-0.031474	-0.033363	0.001090	-20.5	-19.8	-20.9	0.7
$TS1_{NO2-EDA}$	-1496.833368	-1496.810356	-1496.809412	-1496.890966				
	-0.032250	-0.032188	-0.034077	0.004041	-20.2	-20.2	-21.4	2.5
$I2_{NO2-EDA}$	-1496.842234	-1496.818237	-1496.817293	-1496.90164				
	-0.041116	-0.040069	-0.041958	-0.006633	-25.8	-25.1	-26.3	-4.2
$TS2_{NO2-EDA}$	-1496.783721	-1496.761545	-1496.760601	-1496.837609				
	0.017397	0.016623	0.014734	0.057398	10.9	10.4	9.2	36.0
$P_{NO2-EDA}$	-1496.843551	-1496.818924	-1496.81798	-1496.901931				
	-0.042433	-0.040756	-0.042645	-0.006924	-26.6	-25.6	-26.8	-4.3

Table S9. Relative energies (kcal/mol) for ETA+CO_2 cyclocondensation in gas phase at 298.15 K.

	Energies in gas phase				Relative energies			
Structure	**(E+ZPC)**	**Etot**	**H**	**G**	**ΔE**	**Δ(E+ZPC)**	**ΔH**	**ΔG**
CO2	-188.495463	-188.492845	-188.491901	-188.51616				
ETA	-210.168228	-210.160614	-210.159369	-210.206344				
water	-76.350722	-76.346972	-76.345727	-76.375382				
[Et2NH2][HSO4]	-913.576638	-913.563678	-913.562733	-913.617485				
SUM	**-1312.240329**	**-1312.217137**	**-1312.214003**	**-1312.339989**				
$I1_{ETA}$	-1312.279811	-1312.245786	-1312.244541	-1312.361439				
	-0.039482	-0.028649	-0.030538	-0.021450	-24.8	-18.0	-19.2	-13.5
$TS1_{EYA}$	-1312.279303	-1312.246812	-1312.245567	-1312.358045				
	-0.038974	-0.029675	-0.031564	-0.018056	-24.5	-18.6	-19.8	-11.3
$I2_{ETA}$	-1312.285932	-1312.252112	-1312.250867	-1312.366293				
	-0.045603	-0.034975	-0.036864	-0.026304	-28.6	-21.9	-23.1	-16.5
$TS2_{ETA}$	-1312.223859	-1312.191657	-1312.190412	-1312.299366				
	0.016470	0.025480	0.023591	0.040623	10.3	16.0	14.8	25.5
P_{ETA}	-1312.305933	-1312.271588	-1312.270343	-1312.38575				
	-0.065604	-0.054451	-0.056340	-0.045761	-41.2	-34.2	-35.4	-28.7

Table S10. Relative energies (kcal/mol) for EG+CO_2 cyclocondensation in gas phase at 298.15 K.

	Energies in gas phase				Relative energies			
Structure	**(E+ZPC)**	**Etot**	**H**	**G**	**ΔE**	**Δ(E+ZPC)**	**ΔH**	**ΔG**
CO2	-188.495463	-188.492845	-188.491901	-188.51616				
EG	-230.043156	-230.035057	-230.033812	-230.081803				
water	-76.350722	-76.346972	-76.345727	-76.375382				
[Et2NH2][HSO4]	-913.576638	-913.563678	-913.562733	-913.617485				
SUM	**-1332.115257**	**-1332.091580**	**-1332.088446**	**-1332.215448**				
$I1_{EG}$	-1332.157933	-1332.122131	-1332.120886	-1332.242955				
	-0.042676	-0.030551	-0.032440	-0.027507	-26.8	-19.2	-20.4	-17.3
$TS1_{EG}$	-1332.141007	-1332.108263	-1332.107018	-1332.220894				
	-0.025750	-0.016683	-0.018572	-0.005446	-16.2	-10.5	-11.7	-3.4
$I2_{EG}$	-1332.165151	-1332.131975	-1332.13073	-1332.24207				
	-0.049894	-0.040395	-0.042284	-0.026622	-31.3	-25.3	-26.5	-16.7
$TS2_{EG}$	-1332.104095	-1332.072983	-1332.071738	-1332.177164				
	0.011162	0.018597	0.016708	0.038284	7.0	11.7	10.5	24.0
P_{EG}	-1332.165233	-1332.131705	-1332.13046	-1332.24417				
	-0.049976	-0.040125	-0.042014	-0.028722	-31.4	-25.2	-26.4	-18.0

Table S11. Relative energies (kcal/mol) for ME+CO_2 cyclocondensation in gas phase at 298.15 K.

	Energies in gas phase				Relative energies			
Structure	**(E+ZPC)**	**Etot**	**H**	**G**	**ΔE**	**Δ(E+ZPC)**	**ΔH**	**ΔG**
CO2	-188.495463	-188.492845	-188.491901	-188.51616				
ME	-553.01644	-553.008464	-553.007219	-553.056196				
Water	-76.350722	-76.346972	-76.345727	-76.375382				
[Et2NH2][HSO4]	-913.576638	-913.563678	-913.562733	-913.617485				
SUM	**-1655.088541**	**-1655.064987**	**-1655.061853**	**-1655.189841**				
$I1_{ME}$	-1655.128938	-1655.093715	-1655.092470	-1655.210658				
	-0.040397	-0.028728	-0.030617	-0.020817	-25.3	-18.0	-19.2	-13.1
$TS1_{ME}$	-1655.109460	-1655.075853	-1655.074608	-1655.191240				
	-0.020919	-0.010866	-0.012755	-0.001399	-13.1	-6.8	-8.0	-0.9
$I2_{ME}$	-1655.13364	-1655.099268	-1655.098022	-1655.214769				
	-0.045099	-0.034281	-0.036169	-0.024928	-28.3	-21.5	-22.7	-15.6
$TS2_{ME}$	-1655.066276	-1655.033801	-1655.032556	-1655.14256				
	0.022265	0.031186	0.029297	0.047281	14.0	19.6	18.4	29.7
P_{ME}	-1655.121107	-1655.086451	-1655.085206	-1655.201979				
	-0.032566	-0.021464	-0.023353	-0.012138	-20.4	-13.5	-14.7	-7.6

Table S12. Relative energies (kcal/mol) for EDT+CO_2 cyclocondensation in gas phase at 298.15 K.

	Energies in gas phase				Relative energies			
Structure	**(E+ZPC)**	**Etot**	**H**	**G**	**ΔE**	**Δ(E+ZPC)**	**ΔH**	**ΔG**
CO2	-188.495463	-188.492845	-188.491901	-188.51616				
EDT	-875.988779	-875.980021	-875.978776	-876.030832				
water	-76.350722	-76.346972	-76.345727	-76.375382				
[Et2NH2][HSO4]	-913.576638	-913.563678	-913.562733	-913.617485				
SUM	**-1978.060880**	**-1978.036544**	**-1978.033410**	**-1978.164477**				
	-1978.100559	-1978.063072	-1978.061827	-1978.184853				
$I1_{EDT}$	-0.039679	-0.026528	-0.028417	-0.020376	-24.9	-16.6	-17.8	-12.8
	-1978.064791	-1978.029491	-1978.028246	-1978.149388				
$TS1_{EDT}$	-0.003911	0.007053	0.005164	0.015089	-2.5	4.4	3.2	9.5
$I2_{EDT}$	-1978.086552	-1978.050839	-1978.049594	-1978.171001				
	-0.025672	-0.014295	-0.016184	-0.006524	-16.1	-9.0	-10.2	-4.1
$TS2_{EDT}$	-1978.023896	-1977.990061	-1977.988816	-1978.102145				
	0.036984	0.046483	0.044594	0.062332	23.2	29.2	28.0	39.1
P_{EDT}	-1978.082951	-1978.047448	-1978.046203	-1978.163666				
	-0.022071	-0.010904	-0.012793	0.000811	-13.8	-6.8	-8.0	0.5

Table S13. Relative energies (kcal/mol) for intermediates and TSs of [Et_2NH_2][$HSeO_4$] catalyzed EDA+CO_2 cyclocondensation reaction.

	Energies in gas phase				Relative energies			
Structure	**(E+ZPC)**	**Etot**	**H**	**G**	**ΔE**	**Δ(E+ZPC)**	**ΔH**	**ΔG**
CO_2	-188.495463	-188.492845	-188.491901	-188.516159				
EDA	-190.295679	-190.290188	-190.289243	-190.323354				
[Et_2NH_2][$HSeO_4$]	-2914.322913	-2914.309427	-2914.308482	-2914.364299				
SUM	**-3293.114055**	**-3293.092460**	**-3293.089626**	**-3293.203812**				
	-3293.156281	-3293.134309	-3293.133365	-3293.210686				
$I1_{EDA}$	-0.042226	-0.041849	-0.043739	-0.006874	-26.5	-26.3	-27.4	-4.3
	-3293.156365	-3293.135383	-3293.134439	-3293.209394				
$TS1_{EDA}$	-0.042310	-0.042923	-0.044813	-0.005582	-26.5	-26.9	-28.1	-3.5
	-3293.162055	-3293.140021	-3293.139077	-3293.217375				
$I2_{EDA}$	-0.048000	-0.047561	-0.049451	-0.013563	-30.1	-29.8	-31.0	-8.5
	-3293.11271	-3293.092512	-3293.091567	-3293.162663				
$TS2_{EDA}$	0.001345	-0.000052	-0.001941	0.041149	0.8	0.0	-1.2	25.8
	-3293.174182	-3293.152207	-3293.151263	-3293.227255				
P_{EDA}	-0.060127	-0.059747	-0.061637	-0.023443	-37.7	-37.5	-38.7	-14.7

Table S14. Relative energies (kcal/mol) for intermediates and TSs of $[Et_2NH_2][H_2PO_4]$ catalyzed EDA+CO_2 cyclocondensation reaction.

	Energies in gas phase				Relative energies			
Structure	**(E+ZPC)**	**Etot**	**H**	**G**	**ΔE**	**Δ(E+ZPC)**	**ΔH**	**ΔG**
CO_2	-188.495463	-188.492845	-188.491901	-188.516159				
EDA	-190.295679	-190.290188	-190.289243	-190.323354				
$[Et_2NH_2][H_2PO_4]$	-857.481182	-857.467426	-857.466481	-857.523252				
SUM	**-1236.272324**	**-1236.250459**	**-1236.247625**	**-1236.362765**				
	-1236.332742	-1236.310925	-1236.309981	-1236.384639				
$I1_{EDA}$	-0.060418	-0.060466	-0.062356	-0.021874	-37.91	-37.94	-39.13	-13.73
	-1236.316013	-1236.294796	-1236.293852	-1236.368215				
$TS1_{EDA}$	-0.043689	-0.044337	-0.046227	-0.005450	-27.42	-27.82	-29.01	-3.42
	-1236.322392	-1236.300287	-1236.299343	-1236.376003				
$I2_{EDA}$	-0.050068	-0.049828	-0.051718	-0.013238	-31.42	-31.27	-32.45	-8.31
	-1236.265727	-1236.245039	-1236.244095	-1236.317347				
$TS2_{EDA}$	0.006597	0.005420	0.003530	0.045418	4.14	3.40	2.22	28.50
	-1236.33405	-1236.312332	-1236.311388	-1236.386556				
P_{EDA}	-0.061726	-0.061873	-0.063763	-0.023791	-38.73	-38.83	-40.01	-14.93

Table S15. Relative energies (kcal/mol) for intermediates and TSs of $[Et_2NH_2][H_2AsO_4]$ catalyzed EDA+CO_2 cyclocondensation reaction.

	Energies in gas phase				Relative energies			
Structure	**(E+ZPC)**	**Etot**	**H**	**G**	**ΔE**	**Δ(E+ZPC)**	**ΔH**	**ΔG**
CO2	-188.495463	-188.492845	-188.491901	-188.516159				
EDA	-190.295679	-190.290188	-190.289243	-190.323354				
water	-76.350722	-76.347887	-76.346943	-76.368377				
$[Et_2NH_2][H_2AsO_4]$	-2749.512517	-2749.497929	-2749.496985	-2749.555589				
SUM	**-3128.303659**	**-3128.280962**	**-3128.278129**	**-3128.395102**				
	-3128.368154	-3128.345498	-3128.344554	-3128.421683				
$I1_{EDA}$	-0.064495	-0.064536	-0.066425	-0.026581	-40.47	-40.50	-41.68	-16.68
	-3128.350709	-3128.328756	-3128.327812	-3128.403917				
$TS1_{EDA}$	-0.047050	-0.047794	-0.049683	-0.008815	-29.52	-29.99	-31.18	-5.53
	-3128.350375	-3128.327347	-3128.326403	-3128.40673				
$I2_{EDA}$	-0.046716	-0.046385	-0.048274	-0.011628	-29.31	-29.11	-30.29	-7.30
	-3128.299719	-3128.278456	-3128.277512	-3128.350766				
$TS2_{EDA}$	0.003940	0.002506	0.000617	0.044336	2.47	1.57	0.39	27.82
	-3128.368329	-3128.345948	-3128.345004	-3128.421248				
P_{EDA}	-0.064670	-0.064986	-0.066875	-0.026146	-40.58	-40.78	-41.96	-16.41

Table S16. Natural charges of the crucial atoms involved in TS1EDA and the original location in substrate.

Natural charges of the crucial atoms in substrates		Natural charges of the same atoms in $TS1_{EDA}$
CO_2	1C +1.09	1C +1.02
	1O -0.54	1O -0.74
EDA	1N -0.93	1N -0.78
	2H +0.38	2H +0.51
HSO_4^-	2O -0.98	2O -1.03
	3O -0.97	3O -1.06
	1H +0.52	1H +0.54

$I1_{EDA}$

Symbol	X	Y	Z
C	2.878922	0.684437	-1.317984
O	1.857318	1.376439	-1.342611
N	-3.814288	0.211977	0.110809
H	-3.11387	0.185497	-0.673478
H	-3.177996	-0.142377	0.867159
C	-4.208986	1.614193	0.394611
H	-4.850229	1.602878	1.280781
H	-4.802014	1.967513	-0.453855
C	-4.902335	-0.763009	-0.142235
H	-5.482233	-0.396751	-0.994187
H	-5.552094	-0.769794	0.737676
C	-4.294031	-2.131194	-0.413231
H	-3.631839	-2.093083	-1.282467
H	-3.700703	-2.465481	0.442245
H	-5.08436	-2.860769	-0.601984
C	-2.957289	2.453839	0.605007
H	-2.326122	2.442264	-0.287783
H	-3.235771	3.4864	0.826604
H	-2.358249	2.062466	1.432013
S	-0.703042	-0.462358	0.084154
O	-1.572156	-0.686595	1.262536
O	-1.497265	-0.186742	-1.140856
O	0.318589	-1.501455	-0.114184
H	0.70124	1.138467	-0.311589
O	0.065916	0.888216	0.445199
N	2.826816	-0.320205	-0.044015
H	1.946185	-0.872651	-0.117019
H	2.743854	0.260429	0.803829
O	3.887903	0.562877	-1.969694
C	4.019771	-1.16994	0.119877
H	3.751948	-2.01291	0.765072
H	4.310847	-1.53623	-0.864619
C	5.130634	-0.330267	0.741689
H	6.015244	-0.962036	0.899288
H	5.397694	0.450784	0.025783
N	4.615574	0.30477	1.955645
H	4.638604	-0.341479	2.740479
H	5.179282	1.108534	2.212988

$TS1_{EDA}$

Symbol	X	Y	Z
C	2.89639	0.714695	-1.213296
O	1.900548	1.505356	-1.331888
N	-3.738855	0.152686	0.187286
H	-3.057384	0.177521	-0.625244
H	-3.058501	-0.220927	0.895873
C	-4.148507	1.530298	0.549963
H	-4.764485	1.467994	1.452265
H	-4.771415	1.91385	-0.263611
C	-4.813686	-0.831875	-0.070902
H	-5.435387	-0.439154	-0.880897
H	-5.429712	-0.899971	0.830823
C	-4.185704	-2.169426	-0.435334
H	-3.557356	-2.068117	-1.324305
H	-3.55064	-2.530475	0.378262
H	-4.96486	-2.908986	-0.632122
C	-2.905731	2.383081	0.764612
H	-2.293402	2.41357	-0.1407
H	-3.1958	3.401619	1.032297
H	-2.2813	1.969464	1.5613
S	-0.622156	-0.338688	-0.059369
O	-1.41085	-0.697451	1.150868
O	-1.525181	-0.068375	-1.218669
O	0.375853	-1.40399	-0.405048
H	1.042077	1.275564	-0.642059
O	0.172621	0.935119	0.260916
N	2.685628	-0.300521	-0.100539
H	1.739371	-0.837739	-0.276447
H	2.534261	0.216074	0.78328
O	3.929046	0.665446	-1.826288
C	3.823279	-1.216005	0.11821
H	3.431825	-2.080657	0.662486
H	4.200104	-1.534771	-0.853061
C	4.895184	-0.490158	0.926105
H	5.712263	-1.189122	1.149631
H	5.301524	0.313152	0.306417
N	4.263896	0.104115	2.104059
H	4.147318	-0.584834	2.842813
H	4.827658	0.858498	2.481976

$I2_{EDA}$

Symbol	X	Y	Z
C	2.860022	-0.629586	1.283808
O	2.069115	-1.696597	1.282621
N	-3.768135	0.2524	0.084805
H	-2.99287	-0.095831	0.704827
H	-3.220422	0.298801	-0.80577
C	-4.83876	-0.768795	-0.020864
H	-5.573795	-0.404559	-0.744237
H	-5.32406	-0.838903	0.956615
C	-4.170069	1.620333	0.500674
H	-4.661583	1.535499	1.473966

$TS2_{EDA}$

Symbol	X	Y	Z
C	3.29309	-0.288715	0.371172
O	2.718373	-1.374308	-0.934302
N	-3.163267	-0.041078	0.439469
H	-2.838729	-0.249988	-0.551801
H	-2.219548	0.251629	0.801383
C	-4.100601	1.103904	0.442181
H	-4.325055	1.353385	1.483805
H	-5.027461	0.774895	-0.036941
C	-3.609867	-1.287157	1.105008
H	-4.53746	-1.605529	0.61991

H	-4.903985	1.982809	-0.224825
C	-2.936508	2.509999	0.560365
H	-2.209134	2.120348	1.277898
H	-2.441977	2.558487	-0.413878
H	-3.222694	3.520046	0.861481
C	-4.224508	-2.093696	-0.447806
H	-3.478537	-2.425176	0.279689
H	-5.001276	-2.856867	-0.528818
H	-3.726265	-1.994759	-1.416227
S	-0.650601	-0.228211	-0.433985
O	-1.61271	0.087496	-1.509701
O	-1.340127	-0.542942	0.843524
O	0.138217	1.142197	-0.194218
H	1.420152	-1.672011	0.537954
O	0.364673	-1.232682	-0.794872
N	2.69009	0.221607	0.161648
H	1.080264	0.911701	0.076539
H	2.565145	-0.315098	-0.701323
O	3.634686	-0.384973	2.174388
C	3.741167	1.223782	-0.016762
H	3.350802	1.996556	-0.689092
H	3.946842	1.675931	0.953974
C	5.003363	0.598711	-0.603299
H	5.783836	1.368591	-0.700504
H	5.367395	-0.152372	0.104199
N	4.657217	-0.072116	-1.856509
H	4.574326	0.606774	-2.609597
H	5.384177	-0.726314	-2.129364

H	-3.835589	-1.047082	2.148669
C	-2.517096	-2.340081	0.984567
H	-2.288353	-2.547845	-0.064235
H	-1.590621	-1.995051	1.451604
H	-2.836287	-3.264644	1.470896
C	-3.464074	2.270344	-0.299837
H	-3.227741	1.986117	-1.328712
H	-4.144219	3.124771	-0.311824
H	-2.528677	2.566414	0.182611
S	-0.336822	-0.156932	-0.986325
O	0.610641	0.668041	-1.779536
O	-1.650455	-0.319911	-1.67746
O	-0.554076	0.46883	0.376999
H	1.652457	-1.520158	-0.933922
O	0.276588	-1.531948	-0.746103
N	2.275169	-0.402558	1.364188
H	3.169685	-2.21006	-0.733717
H	1.391187	-0.71653	0.960307
O	4.474243	-0.44669	0.529844
C	2.114514	0.96058	1.863813
H	1.143469	1.058897	2.346847
H	2.910257	1.174438	2.582144
C	2.216162	1.906814	0.632089
H	1.224507	2.159737	0.256977
H	2.800802	2.805427	0.829144
N	2.884616	1.07369	-0.403378
H	2.183167	0.866352	-1.156532
H	3.742442	1.469104	-0.786876

P_{EDA}

Symbol	X	Y	Z
C	-3.554939	0.871944	-0.391139
O	-2.743246	-0.516686	2.07151
N	3.439633	0.342481	-0.243114
H	3.014059	0.101366	0.685775
H	2.596345	0.137573	-0.834204
C	3.754714	1.792575	-0.29073
H	4.107088	2.020351	-1.300845
H	4.576033	1.973696	0.408396
C	4.535794	-0.602848	-0.567277
H	5.355078	-0.410276	0.131103
H	4.8843	-0.370862	-1.577689
C	4.015318	-2.028274	-0.456275
H	3.656046	-2.230553	0.556482
H	3.181017	-2.189193	-1.144533
H	4.81136	-2.736437	-0.69537
C	2.509458	2.58786	0.073957
H	2.158193	2.327334	1.076136
H	2.728711	3.657221	0.042364
H	1.694396	2.373301	-0.622673
S	0.463267	-0.500859	0.558502
O	-0.375939	0.836553	0.840873
O	1.585316	-0.409119	1.518501

$I1_{HO-EDA}$

Symbol	X	Y	Z
C	-2.449925	0.993133	1.303022
O	-1.40947	1.645441	1.204618
N	4.163454	0.098089	-0.136954
H	3.453108	0.178074	0.633088
H	3.526647	-0.297948	-0.868761
C	4.623738	1.450082	-0.543525
H	5.280155	1.327215	-1.40976
H	5.215255	1.857005	0.281525
C	5.205382	-0.892881	0.227866
H	5.78622	-0.470545	1.052667
H	5.867631	-1.008481	-0.634866
C	4.538014	-2.204401	0.6148
H	3.863518	-2.05922	1.46309
H	3.947732	-2.598636	-0.216943
H	5.295972	-2.941191	0.889086
C	3.413992	2.31709	-0.860568
H	2.764403	2.414008	0.013695
H	3.741521	3.312598	-1.167923
H	2.817306	1.877053	-1.664537
S	1.015175	-0.433788	-0.087747
O	1.881948	-0.806972	-1.227943
O	1.80675	-0.057691	1.111964

O	0.932013	-0.384236	-0.85373
H	-1.940727	-1.027806	1.865822
O	-0.443376	-1.629459	0.766526
N	-4.191997	-0.344348	-0.43117
H	-2.407493	0.369382	2.265699
H	-4.70639	-0.54064	0.419794
O	-3.918646	1.895358	0.138358
C	-3.276885	-1.3753	-0.910143
H	-2.724876	-1.832137	-0.084011
H	-3.804564	-2.143708	-1.478747
C	-2.325664	-0.558957	-1.79548
H	-1.320956	-0.982659	-1.834577
H	-2.729249	-0.451149	-2.80903
N	-2.324977	0.732764	-1.094653
H	-1.140589	0.834472	0.183902
H	-2.094405	1.556887	-1.64105

O	-0.042049	-1.413789	0.206393
H	-0.303883	1.259277	0.149011
O	0.292086	0.898255	-0.59162
N	-2.501773	-0.13434	0.122217
H	-1.637089	-0.711111	0.20665
H	-2.441325	0.357565	-0.779593
O	-3.425593	0.962006	2.012814
C	-3.725343	-0.951371	0.117428
H	-3.560607	-1.85219	-0.482383
H	-3.946765	-1.227517	1.148995
C	-4.87026	-0.1409	-0.486975
H	-5.022535	0.759881	0.118429
N	-4.482729	0.265989	-1.811252
H	-4.514019	-0.546042	-2.427314
H	-5.145947	0.94251	-2.17921
O	-6.043882	-0.929834	-0.533843
H	-6.374672	-1.043702	0.369577

TS1 $_{\text{HO-EDA}}$

Symbol	X	Y	Z
C	-2.465091	1.007022	1.283303
O	-1.413158	1.644754	1.198297
N	4.164712	0.097425	-0.137777
H	3.455701	0.179966	0.633545
H	3.525163	-0.300387	-0.866684
C	4.624498	1.447898	-0.549332
H	5.27899	1.322396	-1.416675
H	5.217953	1.857249	0.273149
C	5.206664	-0.893186	0.227306
H	5.789815	-0.469203	1.049653
H	5.866892	-1.011781	-0.636595
C	4.539021	-2.203104	0.619291
H	3.866578	-2.054997	1.468705
H	3.946301	-2.59882	-0.210011
H	5.296869	-2.939958	0.893732
C	3.4142	2.314234	-0.866338
H	2.766404	2.413695	0.008962
H	3.741197	3.308772	-1.177413
H	2.81571	1.871709	-1.667595
S	1.017367	-0.433214	-0.081247
O	1.88282	-0.80826	-1.222413
O	1.811939	-0.051754	1.115178
O	-0.035826	-1.415478	0.218846
H	-0.310973	1.254149	0.15234
O	0.290154	0.894746	-0.587198
N	-2.502161	-0.143063	0.133041
H	-1.635695	-0.714303	0.230969
H	-2.441025	0.337595	-0.774799
O	-3.459127	1.012064	1.968788
C	-3.722649	-0.966749	0.131164
H	-3.549556	-1.867914	-0.466107
H	-3.95355	-1.243406	1.159021
C	-4.875177	-0.170866	-0.472636

I2 $_{\text{HO-EDA}}$

Symbol	X	Y	Z
C	2.42273	-0.942902	1.282779
O	1.567576	-1.951259	1.154041
N	-4.059983	0.336848	0.106078
H	-3.27012	-0.070103	0.669643
H	-3.547608	0.446413	-0.796661
C	-5.151692	-0.658212	-0.037036
H	-5.908354	-0.226475	-0.698194
H	-5.597963	-0.798289	0.95136
C	-4.424425	1.672987	0.644044
H	-4.876278	1.516046	1.627428
H	-5.18218	2.099682	-0.019233
C	-3.17675	2.540965	0.72192
H	-2.425736	2.086143	1.3738
H	-2.724276	2.665024	-0.266002
H	-3.435077	3.525981	1.116504
C	-4.579852	-1.954501	-0.591459
H	-3.809356	-2.353034	0.07428
H	-5.373384	-2.697394	-0.695468
H	-4.12343	-1.789608	-1.571472
S	-0.959966	-0.189057	-0.519072
O	-1.927899	0.243239	-1.545013
O	-1.631284	-0.565262	0.752849
O	-0.107427	1.1278	-0.204943
H	0.959673	-1.823364	0.386698
O	0.002619	-1.210707	-0.968218
N	2.36313	0.00719	0.230655
H	0.797609	0.83087	0.114899
H	2.238726	-0.448973	-0.67633
O	3.167562	-0.826189	2.222819
C	3.475145	0.951418	0.185931
H	3.202086	1.784558	-0.471544
H	3.65061	1.336044	1.189895
C	4.746119	0.298615	-0.346395

H	-5.073609	0.692518	0.168732
N	-4.459485	0.316637	-1.768941
H	-4.466812	-0.461465	-2.427839
H	-5.118187	1.005877	-2.121066
O	-5.992887	-1.037695	-0.53829
H	-6.717616	-0.66577	-0.020528

TS2 $_{HO\text{-}EDA}$

Symbol	X	Y	Z
C	3.327475	-0.303813	0.208752
O	2.786483	-1.518583	-0.865441
N	-3.246387	0.290321	0.246198
H	-2.844659	-0.401518	-0.462572
H	-2.370063	0.466586	0.773884
C	-3.686094	1.525781	-0.450174
H	-4.033655	2.233131	0.308864
H	-4.538162	1.251803	-1.078628
C	-4.248267	-0.389753	1.101583
H	-5.105317	-0.629696	0.466104
H	-4.577123	0.320219	1.866375
C	-3.629656	-1.640794	1.70747
H	-3.269809	-2.310587	0.921811
H	-2.778129	-1.384849	2.34408
H	-4.370556	-2.167776	2.312484
C	-2.538832	2.089865	-1.276257
H	-2.16764	1.348613	-1.989915
H	-2.883379	2.966539	-1.829486
H	-1.700457	2.393681	-0.643223
S	-0.397975	-0.857024	-0.710209
O	0.304601	-0.029378	-1.722796
O	-1.738522	-1.31198	-1.178592
O	-0.570819	-0.032344	0.562058
H	1.760747	-1.841487	-0.696927
O	0.456181	-2.05903	-0.357811
N	2.483766	-0.448844	1.357542
H	3.412526	-2.244852	-0.7049
H	1.587186	-0.876185	1.124325
O	4.533712	-0.259065	0.229542
C	2.28027	0.921353	1.812715
H	1.388391	0.988845	2.436918
H	3.151258	1.241162	2.390547
C	2.111699	1.834981	0.557293
H	2.748741	2.719397	0.607721
N	2.631311	0.952929	-0.558385
H	1.8228	0.642255	-1.148576
H	3.344053	1.393831	-1.140192
O	0.825645	2.254273	0.311194
H	0.232187	1.465552	0.393639

I1$_{ME2N\text{-}EDA}$

Symbol	X	Y	Z
C	1.720795	0.945585	-1.487877
O	0.661396	1.576958	-1.423993

H	5.033922	-0.511933	0.334794
N	4.465826	-0.287332	-1.639263
H	4.403835	0.454496	-2.33478
H	5.198507	-0.926873	-1.933183
O	5.717969	1.326341	-0.36097
H	6.584861	0.926836	-0.516801

P$_{HO\text{-}EDA}$

Symbol	X	Y	Z
C	-1.183982	1.50583	0.90858
O	-1.62084	-2.115167	2.224906
N	2.247193	0.782599	0.465119
H	1.491535	1.117898	1.099216
H	1.693126	0.292417	-0.256638
C	2.935298	1.950889	-0.14983
H	3.718379	1.56088	-0.804162
H	3.410323	2.506503	0.662844
C	3.151486	-0.198487	1.142144
H	2.526979	-0.765798	1.829826
H	3.88392	0.383675	1.708687
C	3.801849	-1.12772	0.13164
H	3.037444	-1.700207	-0.403733
H	4.422878	-0.588881	-0.589982
H	4.445604	-1.836902	0.657222
C	1.947497	2.81534	-0.916378
H	1.177132	3.192947	-0.240397
H	2.473322	3.658881	-1.369342
H	1.472034	2.23663	-1.714287
S	0.024915	-1.678187	-0.681402
O	0.288515	-0.22623	-1.427657
O	0.589704	-1.437031	0.663815
O	0.751503	-2.650825	-1.471962
H	-1.932953	-2.337461	1.330207
O	-1.45139	-1.821362	-0.66783
N	-2.008855	0.533024	1.347033
H	-0.659478	-2.09441	2.073333
H	-1.709017	-0.266311	1.914666
O	-0.087708	1.842614	1.362825
C	-3.213735	0.455865	0.544366
H	-3.460214	-0.578756	0.294718
H	-4.064313	0.912109	1.062231
C	-2.842256	1.276619	-0.705342
H	-3.676545	1.862132	-1.095543
N	-1.821006	2.137703	-0.153984
H	-0.579774	0.193631	-1.649951
H	-1.258194	2.716582	-0.762515
O	-2.340236	0.483523	-1.769374
H	-2.345476	-0.46203	-1.500006

TS1$_{ME2N\text{-}EDA}$

Symbol	X	Y	Z
C	1.725844	1.438654	-1.057748
O	0.65389	1.991928	-0.796737

N	-4.798058	0.025401	0.149087
H	-4.077293	0.022419	-0.617395
H	-4.158059	-0.241439	0.934689
C	-5.311075	1.40273	0.357935
H	-5.977115	1.378129	1.225295
H	-5.902583	1.669575	-0.522485
C	-5.798464	-1.044135	-0.085325
H	-6.380438	-0.762142	-0.967311
H	-6.470274	-1.063822	0.777625
C	-5.078851	-2.370789	-0.279158
H	-4.396059	-2.318652	-1.131594
H	-4.488115	-2.623475	0.605628
H	-5.805421	-3.166486	-0.456782
C	-4.137222	2.348987	0.564481
H	-3.478821	2.349121	-0.308562
H	-4.503987	3.364459	0.729238
H	-3.537126	2.044949	1.426727
S	-1.636175	-0.395953	0.186667
O	-2.498266	-0.630584	1.367085
O	-2.434273	-0.221141	-1.055776
O	-0.550874	-1.377625	0.034773
H	-0.378306	1.291354	-0.301555
O	-0.957434	1.014116	0.492652
N	1.860827	-0.016533	-0.191022
H	1.018459	-0.629118	-0.161054
H	1.827755	0.585885	0.645159
O	2.662337	0.863182	-2.238982
C	3.114067	-0.784534	-0.131686
H	2.988267	-1.624325	0.560178
H	3.313023	-1.148405	-1.138262
C	4.23305	0.138711	0.370499
H	4.393921	0.910853	-0.401989
N	3.734598	0.810061	1.563194
H	3.879349	0.20427	2.370077
H	4.218189	1.685095	1.735308
N	5.453378	-0.625994	0.6268
C	6.546832	0.26311	0.994726
H	7.436296	-0.331889	1.216542
H	6.798902	0.979567	0.191575
H	6.293221	0.827258	1.895027
C	5.851482	-1.437617	-0.519114
H	6.818336	-1.899108	-0.303506
H	5.136129	-2.24419	-0.691638
H	5.948556	-0.846716	-1.446979

N	-4.81676	-0.030065	0.171007
H	-4.113876	0.253733	-0.557784
H	-4.160684	-0.566372	0.78789
C	-5.319168	1.16991	0.886256
H	-5.964363	0.822773	1.698479
H	-5.930494	1.740328	0.1812
C	-5.826897	-0.941325	-0.419854
H	-6.427087	-0.355875	-1.122074
H	-6.479416	-1.281049	0.389572
C	-5.117872	-2.099939	-1.105672
H	-4.454111	-1.734479	-1.893975
H	-4.508724	-2.658871	-0.390011
H	-5.851973	-2.776793	-1.547898
C	-4.137101	1.978646	1.400643
H	-3.499476	2.305316	0.574574
H	-4.495865	2.859229	1.937938
H	-3.518057	1.380301	2.075024
S	-1.656631	-0.4328	-0.01107
O	-2.499441	-1.087633	1.015344
O	-2.47474	0.189499	-1.085026
O	-0.579809	-1.287506	-0.533778
H	-0.393075	1.314162	0.140757
O	-0.964066	0.764771	0.78385
N	1.839593	0.04755	-0.225054
H	0.998428	-0.523927	-0.450618
H	1.771278	0.282513	0.774627
O	2.694572	1.654772	-1.745062
C	3.100363	-0.686954	-0.43544
H	2.971511	-1.726169	-0.113868
H	3.339499	-0.659856	-1.497743
C	4.215145	-0.023577	0.369525
H	4.274387	1.021285	0.044206
N	3.79683	0.008139	1.760633
H	3.80518	-0.920412	2.176009
H	4.397349	0.605623	2.320727
N	5.48236	-0.696034	0.027028
C	6.176343	-1.357683	1.110861
H	7.039479	-1.885819	0.695937
H	6.547486	-0.673054	1.89531
H	5.538807	-2.110292	1.584369
C	6.362674	0.172771	-0.735507
H	7.189529	-0.412572	-1.148645
H	5.808113	0.614079	-1.568618
H	6.788854	0.994202	-0.130662

$I2_{ME2N\text{-}EDA}$

Symbol	X	Y	Z
C	1.684614	-1.416778	1.193256
O	0.781425	-2.333302	0.860973
N	-4.652656	0.470281	0.115889
H	-3.906597	-0.078783	0.615337
H	-4.108252	0.695064	-0.74603
C	-5.802138	-0.408817	-0.21265

$TS2_{ME2N\text{-}EDA}$

Symbol	X	Y	Z
C	3.013146	-0.984524	0.445104
O	2.422123	-2.317145	-0.602773
N	-3.218551	0.369715	0.222164
H	-3.135396	-0.265502	-0.605655
H	-2.249243	0.164173	0.62241
C	-3.287198	1.784329	-0.212564

H	-6.510331	0.179094	-0.803357
H	-6.284303	-0.682506	0.729859
C	-4.944617	1.718873	0.866207
H	-5.439577	1.431184	1.797945
H	-5.648722	2.305113	0.268891
C	-3.644784	2.468867	1.119601
H	-2.950996	1.859072	1.704901
H	-3.1483	2.720504	0.178132
H	-3.85047	3.391367	1.666789
C	-5.300471	-1.629489	-0.969669
H	-4.57621	-2.186313	-0.368763
H	-6.137356	-2.28803	-1.211223
H	-4.807332	-1.333905	-1.899941
S	-1.575152	-0.144075	-0.534123
O	-2.483365	0.523828	-1.48624
O	-2.306985	-0.688754	0.640055
O	-0.651087	1.037822	0.021281
H	0.212863	-2.035258	0.111207
O	-0.666227	-1.13467	-1.13702
N	1.720952	-0.297629	0.321989
H	0.221395	0.62549	0.306533
H	1.616575	-0.582421	-0.655427
O	2.392551	-1.510769	2.163493
C	2.884602	0.574925	0.474929
H	2.639027	1.527914	-0.006892
H	3.057966	0.746069	1.537121
C	4.129078	-0.05419	-0.155625
H	4.271528	-1.020105	0.341471
N	3.823535	-0.338342	-1.557848
H	3.801801	0.519437	-2.10631
H	4.517707	-0.95166	-1.975343
N	5.323128	0.733976	0.140104
C	6.541005	-0.002296	-0.145521
H	7.403253	0.562684	0.220982
H	6.520011	-0.965551	0.372259
H	6.696234	-0.187208	-1.224963
C	5.358682	2.037057	-0.498964
H	6.230369	2.587543	-0.133559
H	5.439832	1.985039	-1.6008
H	4.471275	2.621208	-0.243515

H	-3.283154	2.403776	0.68966
H	-4.243021	1.933615	-0.724221
C	-4.279824	-0.113695	1.133895
H	-5.242303	0.02148	0.631075
H	-4.267196	0.523797	2.02304
C	-4.018101	-1.572608	1.479602
H	-3.996854	-2.186799	0.575498
H	-3.049003	-1.682065	1.973867
H	-4.799729	-1.945569	2.145081
C	-2.09733	2.089835	-1.112797
H	-2.1132	1.458747	-2.006559
H	-2.130867	3.1378	-1.423868
H	-1.152851	1.892391	-0.591887
S	-0.67587	-1.252605	-0.743604
O	0.215341	-0.475823	-1.671373
O	-2.02861	-1.433123	-1.327813
O	-0.775343	-0.500869	0.573614
H	1.372045	-2.505055	-0.577294
O	-0.028203	-2.5853	-0.450087
N	2.06033	-0.937601	1.509135
H	2.901176	-3.088825	-0.259423
H	1.162079	-1.325519	1.218055
O	4.207207	-1.076163	0.556559
C	1.877616	0.49394	1.767183
H	0.827092	0.670126	1.999828
H	2.515245	0.818572	2.592937
C	2.258253	1.271323	0.460224
H	3.221561	1.798182	0.588063
N	2.498279	0.180658	-0.511031
H	1.578078	-0.09588	-1.003824
H	3.230283	0.381938	-1.192876
N	1.216292	2.170063	0.011464
C	1.457339	2.667022	-1.336373
H	1.356311	1.852319	-2.058014
H	0.693302	3.411188	-1.576961
H	2.448365	3.146075	-1.443748
C	1.085707	3.272817	0.951601
H	0.8754	2.894544	1.955314
H	1.995298	3.899226	0.999729
H	0.248293	3.905845	0.645047

$P_{ME2N-EDA}$

Symbol	X	Y	Z
C	-1.539943	1.071835	1.635136
O	-0.074002	-2.703438	2.077199
N	3.26361	0.741885	-0.174345
H	2.500901	0.274606	0.400952
H	2.940259	0.478219	-1.12191
C	3.227044	2.215358	0.026553
H	3.949083	2.658074	-0.666422
H	3.573463	2.400915	1.046963
C	4.568107	0.083389	0.10088
H	4.826277	0.317264	1.137391

$I1_{ETA}$

Symbol	X	Y	Z
C	2.830861	0.58747	-1.324673
O	1.84548	1.327797	-1.32314
N	-3.830679	0.191074	0.056819
H	-3.093978	0.14544	-0.691279
H	-3.228313	-0.113522	0.858297
C	-4.264887	1.596925	0.255868
H	-4.94842	1.612129	1.109646
H	-4.821668	1.897879	-0.636099
C	-4.888096	-0.816166	-0.20364
H	-5.429536	-0.500076	-1.099731

H	5.315833	0.546331	-0.549985
C	4.46197	-1.416481	-0.127094
H	3.680505	-1.845905	0.504832
H	4.20518	-1.640764	-1.16469
H	5.415751	-1.890332	0.116004
C	1.817782	2.74359	-0.186776
H	1.109882	2.303409	0.523865
H	1.818815	3.827996	-0.05002
H	1.465324	2.520277	-1.197864
S	0.592134	-0.902316	-0.699504
O	-0.21855	0.410917	-1.064589
O	1.180776	-0.661347	0.663894
O	1.672557	-0.973931	-1.699803
H	-0.349381	-2.833179	1.151944
O	-0.374395	-2.009664	-0.695063
N	-1.62919	-0.271936	1.801683
H	0.725074	-2.167929	1.941954
H	-0.870089	-0.874412	2.108863
O	-0.665037	1.838906	1.988222
C	-2.82568	-0.824366	1.21489
H	-2.59666	-1.741526	0.672293
H	-3.59216	-1.03619	1.970371
C	-3.308547	0.322753	0.29935
H	-4.406666	0.389417	0.264716
N	-2.727524	1.451728	0.977297
H	-1.244211	0.216882	-1.034113
H	-2.738856	2.380164	0.581727
N	-2.799001	0.180459	-1.089854
C	-3.127432	1.362548	-1.890485
H	-2.629221	2.244888	-1.484268
H	-2.756861	1.215162	-2.906983
H	-4.213556	1.539514	-1.92877
C	-3.31239	-1.022753	-1.751982
H	-2.950059	-1.033234	-2.781932
H	-2.930865	-1.918892	-1.265634
H	-4.413442	-1.035423	-1.762396
H	-5.581058	-0.79405	0.642283
C	-4.2458	-2.184256	-0.379923
H	-3.540465	-2.175226	-1.215417
H	-3.693944	-2.471543	0.519318
H	-5.014821	-2.934495	-0.575626
C	-3.041251	2.471728	0.486862
H	-2.3684	2.435087	-0.374286
H	-3.350431	3.506728	0.648026
H	-2.476232	2.131108	1.359107
S	-0.699933	-0.427187	0.186631
O	-1.609093	-0.593992	1.342583
O	-1.445466	-0.196311	-1.077743
O	0.316994	-1.483284	0.067346
H	0.699774	1.154986	-0.253954
O	0.071809	0.932369	0.514103
N	2.833056	-0.317457	0.036305
H	1.951813	-0.875041	0.02953
H	2.761688	0.322353	0.83586
O	3.777543	0.354705	-2.034671
C	4.029179	-1.162034	0.21366
H	3.812698	-1.906299	0.984513
H	4.238254	-1.651031	-0.73771
C	5.191801	-0.283618	0.634253
H	6.065773	-0.913192	0.844578
H	5.43361	0.40248	-0.184627
O	4.760222	0.412412	1.79296
H	5.355194	1.156092	1.95366

$TS1_{ETA}$

Symbol	X	Y	Z
C	2.87096	0.569799	-1.251817
O	1.89155	1.370718	-1.415513
N	-3.759452	0.151089	0.15264
H	-3.068259	0.135953	-0.646973
H	-3.088561	-0.160008	0.897703
C	-4.199801	1.542787	0.415719
H	-4.828853	1.527788	1.310768
H	-4.815964	1.858712	-0.431174
C	-4.814037	-0.867865	-0.056544
H	-5.425079	-0.541701	-0.90319
H	-5.445844	-0.882052	0.836491
C	-4.161111	-2.21805	-0.314582
H	-3.516165	-2.171533	-1.196268
H	-3.539952	-2.515082	0.534867

$I2_{ETA}$

Symbol	X	Y	Z
C	2.783619	-0.598927	1.267499
O	1.979573	-1.656678	1.250867
N	-3.756249	0.221567	0.127435
H	-2.939392	-0.083406	0.713988
H	-3.261777	0.267978	-0.79132
C	-4.793469	-0.839773	0.102912
H	-5.579088	-0.518069	-0.5865
H	-5.221313	-0.902322	1.10727
C	-4.18702	1.583937	0.535302
H	-4.619798	1.503212	1.536304
H	-4.97336	1.900682	-0.155664
C	-2.987545	2.520171	0.506137
H	-2.207034	2.175258	1.190063
H	-2.551398	2.565909	-0.49576

H	-4.927309	-2.979547	-0.475351
C	-2.976455	2.431498	0.592195
H	-2.353379	2.418604	-0.306255
H	-3.289536	3.458729	0.791848
H	-2.356503	2.081183	1.422145
S	-0.619836	-0.318999	0.008451
O	-1.431605	-0.579376	1.227137
O	-1.494453	-0.117668	-1.184613
O	0.368093	-1.420975	-0.242541
H	1.040034	1.219646	-0.685879
O	0.192184	0.964119	0.251617
N	2.683045	-0.314664	-0.02278
H	1.736975	-0.873898	-0.141788
H	2.509289	0.289945	0.792418
O	3.874405	0.417036	-1.894663
C	3.82753	-1.199965	0.278536
H	3.468335	-1.95242	0.984515
H	4.144901	-1.675235	-0.648887
C	4.949183	-0.38354	0.893331
H	5.751596	-1.058434	1.217349
H	5.347074	0.308321	0.142753
O	4.36979	0.305115	1.988159
H	4.972107	1.000312	2.282989

H	-3.295455	3.525329	0.801986
C	-4.157668	-2.153279	-0.327396
H	-3.360527	-2.441735	0.363268
H	-4.910852	-2.94371	-0.344492
H	-3.720516	-2.064292	-1.325847
S	-0.643797	-0.184627	-0.528432
O	-1.657697	0.096065	-1.562561
O	-1.261659	-0.47756	0.790764
O	0.137422	1.202698	-0.361304
H	1.359815	-1.636417	0.482822
O	0.366981	-1.187661	-0.909122
N	2.679372	0.234844	0.126964
H	1.06051	0.990421	-0.032836
H	2.53253	-0.300238	-0.730687
O	3.521976	-0.347665	2.186741
C	3.76076	1.208567	-0.031596
H	3.444624	1.935936	-0.785146
H	3.904361	1.716493	0.922531
C	5.048131	0.538758	-0.477441
H	5.835947	1.294581	-0.604707
H	5.365717	-0.171449	0.296614
O	4.752127	-0.114213	-1.699636
H	5.465276	-0.731616	-1.906257

$TS2_{ETA}$

Symbol	X	Y	Z
C	3.384727	-0.194287	0.323189
O	2.821053	-1.331994	-1.027315
N	-3.230233	0.047154	0.357548
H	-2.857962	-0.255005	-0.584665
H	-2.304692	0.31559	0.77201
C	-4.101718	1.236342	0.210551
H	-4.381563	1.571704	1.213607
H	-5.00966	0.917116	-0.309091
C	-3.793097	-1.121678	1.077526
H	-4.707281	-1.418983	0.555633
H	-4.065438	-0.791745	2.084498
C	-2.763772	-2.242889	1.101711
H	-2.492829	-2.545227	0.086426
H	-1.846429	-1.919422	1.601333
H	-3.168988	-3.107079	1.632682
C	-3.354975	2.312394	-0.564002
H	-3.064937	1.945215	-1.552213
H	-3.987785	3.194144	-0.685063
H	-2.441918	2.603086	-0.037228
S	-0.296738	-0.318694	-0.832565
O	0.665143	0.524972	-1.639451
O	-1.55613	-0.511087	-1.600938
O	-0.575406	0.367917	0.480612
H	1.833544	-1.593384	-0.949933
O	0.36133	-1.64309	-0.534364
N	2.451015	-0.407113	1.345925
H	3.377966	-2.119852	-0.924706

P_{ETA}

Symbol	X	Y	Z
C	-1.496082	1.618829	0.038271
O	-2.388291	-2.35982	0.558156
N	2.127674	1.001169	0.068689
H	2.316048	-0.021651	-0.027373
H	1.088518	1.116026	0.077918
C	2.646751	1.478892	1.379778
H	2.387647	2.538872	1.450942
H	3.73619	1.385538	1.347379
C	2.653381	1.760669	-1.096922
H	3.740972	1.644267	-1.096257
H	2.416526	2.812369	-0.912525
C	2.030742	1.273318	-2.393081
H	2.229496	0.212073	-2.556042
H	0.946363	1.406952	-2.367803
H	2.438232	1.849471	-3.227609
C	2.041372	0.679305	2.519838
H	2.236779	-0.388758	2.39423
H	2.471524	1.015504	3.46653
H	0.95928	0.823613	2.548384
S	0.683381	-1.893926	-0.225369
O	0.005476	-1.123054	1.041496
O	2.120028	-1.792116	0.080646
O	0.306734	-1.07524	-1.400757
H	-1.747653	-2.919881	0.067962
O	0.109705	-3.242489	-0.227859
H	-2.627986	-2.893687	1.329175
O	-0.37054	2.051079	0.247033

H	1.597118	-0.836806	0.983877
O	4.563497	-0.187799	0.325997
C	2.162126	0.93079	1.868898
H	1.201385	0.908225	2.380761
H	2.950326	1.214189	2.570035
C	2.134306	1.889804	0.640533
H	1.111024	2.15338	0.370027
H	2.739542	2.783067	0.798016
O	2.703313	1.145553	-0.442888
H	1.852927	0.821973	-1.05294

$I1_{EG}$

Symbol	X	Y	Z
C	2.081034	-1.923868	-1.237772
O	1.514871	-1.189913	-1.94229
N	-3.622352	0.390989	-0.04296
H	-2.940108	-0.195601	-0.584523
H	-2.98639	0.649362	0.746514
C	-3.972984	1.605227	-0.824351
H	-4.607846	2.231178	-0.190835
H	-4.561278	1.279968	-1.686988
C	-4.744336	-0.446042	0.448916
H	-5.325778	-0.760149	-0.422361
H	-5.378738	0.187486	1.07521
C	-4.186211	-1.633423	1.219139
H	-3.536603	-2.238277	0.58054
H	-3.594857	-1.296953	2.075191
H	-5.003847	-2.259512	1.582407
C	-2.696389	2.321287	-1.240835
H	-2.067402	1.672317	-1.856598
H	-2.944829	3.217288	-1.813726
H	-2.10893	2.614155	-0.366074
S	-0.493966	-0.193958	0.356918
O	-1.330353	0.506295	1.355663
O	-1.324527	-0.816163	-0.70315
O	0.515724	-1.101098	0.913695
H	1.224641	0.701228	-0.555928
O	0.314691	1.009437	-0.353665
H	2.278104	-0.405114	0.951527
O	2.670179	-2.676611	-0.575453
C	4.223436	-0.070646	0.634687
H	4.400095	-0.152771	1.713574
H	4.568357	-0.990525	0.145294
C	4.948356	1.148158	0.098774
H	6.022616	1.062938	0.285237
H	4.793068	1.20477	-0.990248
O	4.495451	2.313625	0.743825
H	3.526861	2.252172	0.74172
O	2.842131	0.152963	0.38247

$I2_{EG}$

Symbol	X	Y	Z
C	3.438358	-0.773549	0.194409

C	-3.734864	1.398059	0.313818
H	-3.960864	0.875468	1.248238
H	-4.576539	2.031233	0.03425
C	-3.300371	0.417518	-0.789792
H	-3.62509	-0.604913	-0.590017
H	-3.646703	0.730225	-1.781643
N	-1.863076	0.538597	-0.67057
H	-0.961404	-1.334662	1.017167
H	-1.164536	-0.072347	-1.106369
O	-2.594193	2.23654	0.535169

$TS1_{EG}$

Symbol	X	Y	Z
C	2.927892	1.171394	-0.991531
O	1.879392	1.824498	-0.888074
N	-3.767433	0.008824	0.093523
H	-3.083343	0.243695	-0.661477
H	-3.109894	-0.448264	0.762651
C	-4.298751	1.262984	0.693567
H	-4.941814	0.976166	1.530105
H	-4.916611	1.749518	-0.066038
C	-4.762987	-0.975717	-0.403526
H	-5.37591	-0.469246	-1.153947
H	-5.404326	-1.246618	0.439537
C	-4.036424	-2.181499	-0.979503
H	-3.386759	-1.88484	-1.807567
H	-3.414449	-2.660899	-0.218413
H	-4.761022	-2.910622	-1.347791
C	-3.139606	2.14301	1.137446
H	-2.498576	2.403545	0.290581
H	-3.524921	3.063916	1.580137
H	-2.518924	1.631083	1.878228
S	-0.564842	-0.213592	0.011332
O	-1.376985	-0.834736	1.070076
O	-1.37305	0.223268	-1.145284
O	0.560383	-1.119554	-0.436762
H	0.865736	1.424326	0.002137
O	0.121809	1.030292	0.657941
H	1.694585	-0.617828	-0.33687
O	4.00683	1.291727	-1.495705
C	3.814575	-1.127766	-0.321588
H	3.342395	-2.104145	-0.185667
H	4.272905	-1.048639	-1.30867
C	4.801151	-0.846232	0.793479
H	5.607672	-1.584016	0.761082
H	5.238547	0.148945	0.634631
O	4.187811	-0.960571	2.055711
H	3.454669	-0.327142	2.072567
O	2.748116	-0.162459	-0.226808

$TS2_{EG}$

Symbol	X	Y	Z
C	3.260112	-0.252628	0.223519

O	3.152935	-1.858003	-0.490589
N	-3.157228	0.394718	0.232866
H	-2.247859	0.324197	0.75164
H	-2.888039	-0.199976	-0.589427
C	-4.245462	-0.260045	0.999982
H	-5.144318	-0.241572	0.377231
H	-4.432206	0.346655	1.890653
C	-3.380084	1.797113	-0.200062
H	-3.582855	2.389874	0.696526
H	-4.274889	1.808455	-0.828818
C	-2.152536	2.296884	-0.94897
H	-1.264761	2.276813	-0.309607
H	-1.946726	1.668614	-1.820572
H	-2.320913	3.32226	-1.286232
C	-3.826958	-1.679415	1.354215
H	-2.918154	-1.67467	1.962493
H	-4.622509	-2.172585	1.916654
H	-3.620155	-2.259861	0.45113
S	-0.382333	-0.957994	-0.576054
O	-1.65116	-1.192248	-1.301666
O	-0.604353	-0.250717	0.716373
O	0.388056	0.106783	-1.502346
H	2.171742	-2.014641	-0.490587
O	0.456467	-2.153052	-0.472552
H	0.914537	0.711399	-0.92291
O	4.541644	-0.329694	0.383153
C	2.469816	0.983503	1.440938
H	1.528112	1.096884	1.981543
H	3.305027	0.868097	2.135963
C	2.707982	2.169339	0.532172
H	2.821369	3.0805	1.132855
H	3.622729	2.002253	-0.045504
O	1.571159	2.275601	-0.324303
H	1.799895	2.823451	-1.088013
O	2.301653	-0.19795	0.67139

O	2.726587	-1.264185	-0.813093
N	-3.223886	-0.00609	0.390475
H	-2.927018	-0.241889	-0.583512
H	-2.292769	0.288045	0.765029
C	-4.162426	1.14467	0.377156
H	-4.381185	1.401429	1.417261
H	-5.088454	0.806573	-0.095732
C	-3.676307	-1.239836	1.089068
H	-4.608449	-1.558484	0.614429
H	-3.893214	-0.96529	2.125087
C	-2.592781	-2.304069	0.994037
H	-2.377734	-2.553636	-0.048791
H	-1.660498	-1.95929	1.450376
H	-2.920765	-3.209222	1.50962
C	-3.527678	2.303571	-0.376342
H	-3.297826	2.017946	-1.406568
H	-4.210472	3.155518	-0.393178
H	-2.594151	2.612131	0.102249
S	-0.302327	-0.240284	-0.886717
O	0.685111	0.614638	-1.708982
O	-1.533849	-0.402379	-1.678312
O	-0.553287	0.427656	0.415884
H	1.577284	-1.517317	-0.694806
O	0.353815	-1.594966	-0.67641
H	3.352752	-2.006174	-0.778781
O	4.454561	-0.328656	0.414857
C	2.212265	0.921159	1.833005
H	1.248809	0.992219	2.337621
H	3.031018	1.08507	2.542172
C	2.318857	1.880299	0.619163
H	1.350038	2.315799	0.359219
H	3.056147	2.67077	0.773069
O	2.734102	1.041539	-0.453939
H	1.644411	0.790258	-1.182423
O	2.308493	-0.363182	1.260517

P_{EG}

Symbol	X	Y	Z
C	2.503955	0.686139	1.007941
O	2.845145	-2.21148	-0.369123
N	-2.766671	0.31459	0.289338
H	-2.654363	-0.385498	-0.479516
H	-1.743468	0.474371	0.483497
C	-3.381867	1.553847	-0.245736
H	-3.357778	2.302156	0.551612
H	-4.427879	1.33264	-0.47592
C	-3.419083	-0.30487	1.472111
H	-4.451995	-0.533497	1.194351
H	-3.43474	0.447606	2.26569
C	-2.647933	-1.550132	1.883475
H	-2.623165	-2.284101	1.073058
H	-1.611745	-1.307772	2.135319
H	-3.124012	-2.006563	2.754105

$I1_{ME}$

Symbol	X	Y	Z
C	1.214897	1.799507	-1.454955
O	0.987016	2.699161	-0.74467
N	-2.898045	-1.222328	-0.409039
H	-2.01387	-0.763411	-0.726182
H	-2.983193	-0.745757	0.520253
C	-4.028421	-0.830908	-1.288953
H	-4.938821	-1.259633	-0.861268
H	-3.85872	-1.288651	-2.267442
C	-2.667028	-2.676767	-0.208431
H	-2.481094	-3.117789	-1.191637
H	-3.591583	-3.102446	0.191129
C	-1.492868	-2.875581	0.738913
H	-0.586288	-2.414723	0.335795
H	-1.69638	-2.419925	1.711919
H	-1.308887	-3.942256	0.882754

C	-2.61365	2.007131	-1.478452
H	-3.032839	2.941355	-1.857901
H	-1.558567	2.163166	-1.235473
H	-2.658394	1.250092	-2.265362
S	-0.148439	-1.130979	-0.707305
O	1.014108	-1.003779	-1.778031
O	-1.40274	-1.167173	-1.492777
O	-0.094159	0.128004	0.114853
H	2.104269	-2.700464	0.034709
O	0.102922	-2.330755	0.0958
H	3.137466	-1.607532	0.340725
O	2.889981	-0.223627	1.688862
C	1.453501	2.589154	0.374142
H	0.363723	2.625836	0.35103
H	1.862101	3.588774	0.536408
C	2.037438	1.883846	-0.865458
H	1.269884	1.500438	-1.537687
H	2.758609	2.4968	-1.408865
O	2.729219	0.770096	-0.311152
H	1.858271	-1.380143	-1.348186
O	1.849546	1.761862	1.463042

$TS1_{ME}$

Symbol	X	Y	Z
C	2.556968	1.463033	-0.996267
O	1.511909	2.03765	-0.666767
N	-4.012612	-0.046065	0.166364
H	-3.357085	0.321432	-0.56053
H	-3.328819	-0.605477	0.722823
C	-4.526705	1.080482	0.992141
H	-5.135198	0.646791	1.790463
H	-5.176415	1.682456	0.350962
C	-5.022114	-0.940256	-0.456662
H	-5.66346	-0.318935	-1.087595
H	-5.631818	-1.356858	0.349708
C	-4.313548	-2.023752	-1.255102
H	-3.69622	-1.584565	-2.043615
H	-3.661748	-2.618877	-0.609452
H	-5.049039	-2.686777	-1.715356
C	-3.355964	1.885114	1.536807
H	-2.750127	2.29525	0.72399
H	-3.728711	2.711421	2.145799
H	-2.703115	1.261558	2.154146
S	-0.817619	-0.219357	-0.049546
O	-1.593418	-1.036216	0.897263
O	-1.66084	0.389134	-1.099473
O	0.318148	-1.005049	-0.665684
H	0.559056	1.437029	0.205265
O	-0.151674	0.913763	0.792696
H	1.43919	-0.473191	-0.574108
O	3.575217	1.722237	-1.573429
C	3.554078	-0.872716	-0.904864
H	3.152252	-1.88692	-0.830938

C	-4.098341	0.686668	-1.371711
H	-3.179199	1.095054	-1.800842
H	-4.93958	0.986676	-1.999965
H	-4.228084	1.125264	-0.378152
S	-0.99928	0.871065	1.129386
O	-2.265542	0.345008	1.673331
O	-0.717795	0.35311	-0.242524
O	0.152844	0.762788	2.021677
H	-0.534019	2.845562	0.52182
O	-1.323235	2.437273	0.931123
H	1.755643	0.667946	1.103135
O	1.423965	0.980024	-2.249666
C	2.303146	-0.870957	0.051644
H	2.266475	-1.500055	0.952179
H	1.398071	-1.057244	-0.546249
C	3.519449	-1.237318	-0.776375
H	3.482997	-2.29852	-1.033795
H	3.526077	-0.643809	-1.693587
O	2.40356	0.491034	0.394397
S	5.036495	-0.891735	0.193527
H	5.809827	-1.794305	-0.433328

$I2_{ME}$

Symbol	X	Y	Z
C	-2.48133	1.762559	0.651386
O	-1.69883	2.425597	-0.176305
N	3.587118	-0.058167	0.369648
H	2.680499	0.340897	0.715247
H	3.232463	-0.458564	-0.528294
C	4.560942	1.02982	0.10242
H	5.453362	0.573046	-0.334419
H	4.835142	1.468142	1.065933
C	4.026632	-1.155933	1.269978
H	4.304173	-0.702563	2.225623
H	4.92118	-1.604025	0.828418
C	2.897688	-2.165025	1.423431
H	2.006446	-1.691595	1.844887
H	2.619489	-2.591298	0.455438
H	3.212765	-2.974084	2.085882
C	3.929123	2.053122	-0.829259
H	3.028916	2.482176	-0.380518
H	4.637004	2.859438	-1.031893
H	3.644417	1.590557	-1.778402
S	0.581909	-0.235276	-0.762268
O	1.766408	-0.72623	-1.496059
O	0.970487	0.52471	0.451007
O	-0.136436	-1.577681	-0.236046
H	-1.083904	1.798046	-0.629476
O	-0.408457	0.469461	-1.58986
H	-1.099832	-1.524085	-0.429257
O	-3.442817	2.215116	1.213976
C	-2.964298	-0.400404	1.445594
H	-2.357131	-1.252829	1.75875

H	3.824547	-0.642577	-1.937722
C	4.754576	-0.685086	0.000654
H	5.523565	-1.403821	-0.292929
H	5.139307	0.328781	-0.120185
O	2.489828	-0.001029	-0.504123
S	4.25713	-0.98247	1.737904
H	5.50284	-1.159871	2.206886

H	-3.395391	0.098473	2.317185
C	-4.05988	-0.830653	0.482023
H	-4.669933	-1.619959	0.928438
H	-4.712563	0.013465	0.248324
O	-2.060268	0.475174	0.785261
S	-3.384861	-1.529112	-1.067567
H	-2.893646	-0.37796	-1.561277

$TS2_{ME}$

Symbol	X	Y	Z
C	3.139787	-0.619965	0.266039
O	2.583556	-1.349707	-0.948755
N	-3.380139	-0.037725	0.439891
H	-3.110553	-0.188771	-0.558133
H	-2.444675	0.221666	0.819559
C	-4.318194	1.110029	0.547859
H	-4.510306	1.277091	1.611117
H	-5.255312	0.810378	0.071219
C	-3.819386	-1.328376	1.039327
H	-4.758906	-1.606669	0.554373
H	-4.01902	-1.14264	2.098174
C	-2.73772	-2.379256	0.836335
H	-2.53965	-2.53901	-0.227362
H	-1.799101	-2.075344	1.308498
H	-3.05885	-3.325585	1.276685
C	-3.702288	2.329169	-0.121201
H	-3.497748	2.131972	-1.177215
H	-4.386277	3.177302	-0.050576
H	-2.758524	2.601713	0.359431
S	-0.507826	-0.169096	-0.986411
O	0.403641	0.809005	-1.783007
O	-1.772315	-0.274839	-1.728925
O	-0.686308	0.344309	0.387977
H	1.375446	-1.475397	-0.929049
O	0.185131	-1.521588	-0.986359
H	3.099327	-2.174941	-0.989633
O	4.255021	-0.971439	0.589509
C	2.124412	0.461364	2.019481
H	1.253906	0.400508	2.673809
H	3.044994	0.390233	2.610199
C	2.112487	1.757078	1.183427
H	1.084929	2.067006	0.981187
H	2.638255	2.560353	1.703214
H	1.32457	1.014357	-1.300736
O	2.043941	-0.635545	1.137029
S	2.950485	1.353973	-0.381174

P_{ME}

Symbol	X	Y	Z
C	2.497781	0.410419	1.147381
O	2.335645	-2.59566	-0.172055
N	-2.886305	0.565121	0.259013
H	-2.782027	-0.101474	-0.546983
H	-1.879834	0.591434	0.54987
C	-3.312569	1.893961	-0.243856
H	-3.33398	2.579405	0.608229
H	-4.332149	1.789089	-0.624862
C	-3.71434	-0.043978	1.332817
H	-4.733808	-0.132328	0.946828
H	-3.724058	0.655481	2.173653
C	-3.131708	-1.394523	1.721101
H	-3.112709	-2.077119	0.867002
H	-2.103736	-1.291999	2.079892
H	-3.736745	-1.841206	2.513181
C	-2.348959	2.356678	-1.326296
H	-2.660682	3.328557	-1.714552
H	-1.335724	2.446185	-0.92404
H	-2.315167	1.637155	-2.148773
S	-0.478911	-1.22371	-0.713117
O	0.721455	-1.223442	-1.757592
O	-1.696143	-1.032122	-1.538277
O	-0.2578	-0.036823	0.173728
H	1.508164	-2.999252	0.150552
O	-0.438788	-2.492572	0.020123
H	2.647372	-2.053896	0.576449
O	2.736404	-0.548073	1.831515
C	1.599571	2.481928	0.60338
H	0.577969	2.854749	0.698312
H	2.306406	3.276744	0.863008
C	1.878142	1.933658	-0.79669
H	1.000938	1.452616	-1.231492
H	2.267693	2.709084	-1.457165
H	1.5036	-1.666554	-1.297061
O	1.743458	1.435577	1.559535
S	3.133989	0.661431	-0.503007

$I1_{EDT}$

Symbol	X	Y	Z
C	-2.38998	-0.736992	1.568473
O	-2.629784	-1.802264	1.161968
N	2.421996	0.385103	-0.240928
H	2.452546	-0.65005	-0.394173

$TS1_{EDT}$

Symbol	X	Y	Z
C	-1.333668	-1.364864	1.271593
O	-0.504585	-2.263277	1.282917
N	3.295095	1.042446	0.511367
H	3.47464	0.487351	-0.346213

H	1.455197	0.514084	0.107792
C	3.358194	0.792845	0.840163
H	3.236788	1.871322	0.977276
H	4.370668	0.598574	0.476284
C	2.583446	1.102333	-1.537617
H	3.656441	1.164458	-1.739199
H	2.198941	2.114556	-1.38148
C	1.849389	0.365094	-2.647201
H	2.293039	-0.61724	-2.826337
H	0.79664	0.202606	-2.39796
H	1.903326	0.95017	-3.568335
C	3.053821	0.015624	2.110441
H	3.114597	-1.061711	1.931951
H	3.772637	0.285611	2.88714
H	2.045657	0.232863	2.471899
S	0.225667	-1.929345	-0.256937
O	0.153964	-0.893809	0.815135
O	1.621119	-2.196603	-0.653103
O	-0.704279	-1.657593	-1.353943
H	-1.192831	-3.232692	0.609514
O	-0.237224	-3.313405	0.428053
H	-2.604116	-0.251006	-1.843982
O	-2.204531	0.320382	2.013225
C	-1.322121	1.486799	-0.914359
H	-0.861596	0.600112	-0.48053
H	-0.723597	1.815421	-1.769519
C	-1.387631	2.59762	0.125296
H	-1.519602	3.580203	-0.33397
H	-2.204766	2.438106	0.830047
S	0.169898	2.684993	1.089263
H	-0.06608	1.553049	1.778691
S	-2.991983	0.981991	-1.47048

H	2.256406	0.943046	0.576635
C	3.923868	0.385949	1.693165
H	3.675533	0.996424	2.565164
H	5.006521	0.418031	1.544693
C	3.655271	2.466078	0.265184
H	4.739493	2.509803	0.132296
H	3.394972	3.02338	1.168683
C	2.905529	2.976486	-0.955426
H	3.159126	2.392875	-1.844461
H	1.824618	2.908008	-0.803643
H	3.165045	4.021404	-1.137099
C	3.402596	-1.03653	1.828755
H	3.63283	-1.628759	0.93816
H	3.871044	-1.515355	2.691253
H	2.317966	-1.050164	1.971972
S	1.173064	-0.71202	-1.13638
O	0.77823	0.178422	-0.022356
O	2.464799	-0.392996	-1.738817
O	0.06297	-0.779655	-2.161701
H	0.587354	-2.309888	0.155253
O	1.314718	-2.166331	-0.543365
H	-0.989415	-1.052461	-1.568037
O	-1.810207	-0.511085	1.954393
C	-2.908692	0.365246	-0.559455
H	-2.158941	0.957754	-0.028839
H	-3.01258	0.74851	-1.577562
C	-4.241653	0.407981	0.172172
H	-5.008343	-0.123954	-0.397398
H	-4.153591	-0.063654	1.152227
S	-4.867085	2.112592	0.371589
H	-3.925883	2.500589	1.249204
S	-2.292813	-1.349495	-0.640607

$I2_{EDT}$

Symbol	X	Y	Z
C	3.210643	-1.449896	-0.352947
O	2.462352	-2.353608	-0.950983
N	-3.745195	0.444779	0.153558
H	-2.90465	0.431706	0.773158
H	-3.360297	-0.143065	-0.626524
C	-4.879109	-0.25631	0.807745
H	-5.70234	-0.287565	0.088727
H	-5.191609	0.349595	1.662783
C	-3.992465	1.826373	-0.333988
H	-4.334038	2.420469	0.518263
H	-4.804156	1.773421	-1.064735
C	-2.712886	2.381666	-0.942556
H	-1.915382	2.427314	-0.195262
H	-2.363724	1.74866	-1.763502
H	-2.892296	3.388583	-1.325621
C	-4.435582	-1.650077	1.226472
H	-3.599927	-1.59726	1.929915
H	-5.264031	-2.174796	1.706801

$TS2_{EDT}$

Symbol	X	Y	Z
C	3.173078	-0.43163	-0.332807
O	2.329276	-0.62466	-1.59802
N	-3.516576	-0.317978	0.440634
H	-3.360907	-0.091104	-0.562181
H	-2.575404	-0.074986	0.820097
C	-4.550428	0.588126	1.009053
H	-4.631168	0.359169	2.074858
H	-5.500705	0.338727	0.529673
C	-3.745427	-1.782921	0.598543
H	-4.701465	-2.013667	0.121027
H	-3.837825	-1.97841	1.670114
C	-2.590683	-2.552608	-0.024809
H	-2.501477	-2.333793	-1.092918
H	-1.638868	-2.296103	0.449816
H	-2.760841	-3.624763	0.09442
C	-4.147405	2.033754	0.763562
H	-4.047234	2.23533	-0.306512
H	-4.904333	2.704363	1.175265

H	-4.107772	-2.229834	0.359267	H	-3.188757	2.256887	1.240155
S	-0.867292	-0.862245	-0.385916	S	-0.766869	0.383824	-1.052497
O	-2.034928	-1.053128	-1.271486	O	0.132188	1.579314	-1.481419
O	-1.214867	-0.159374	0.871855	O	-2.052769	0.50949	-1.74243
O	0.044425	0.173889	-1.221635	O	-0.883692	0.382191	0.418147
H	1.513754	-2.322637	-0.658988	H	1.076689	-0.818296	-1.546588
O	-0.081586	-2.083496	-0.174267	O	-0.065755	-0.883153	-1.546398
H	0.685484	0.603344	-0.6097	H	2.884199	-1.163416	-2.188544
O	4.340414	-1.193306	-0.671944	O	4.35498	-0.630587	-0.520843
C	3.636796	0.6876	1.286629	C	2.635047	-0.141493	2.263013
H	3.410551	1.134689	2.25922	H	2.165497	-0.437617	3.204632
H	4.619112	0.213157	1.335658	H	3.720128	-0.109252	2.401672
C	3.649663	1.738229	0.183052	C	2.100598	1.214356	1.797333
H	4.428078	2.474875	0.397165	H	1.008555	1.212103	1.827084
H	3.864503	1.257633	-0.772686	H	2.485681	2.014216	2.436246
S	2.027807	2.590286	0.100047	H	1.011875	1.604186	-0.908522
H	2.266375	3.262407	-1.036954	S	2.666706	1.513305	0.093127
S	2.394478	-0.612884	1.038953	S	2.23453	-1.383629	1.00938

P_{EDT}

Symbol	X	Y	Z
C	-2.258983	-0.13986	1.137443
O	-1.400285	3.06432	0.542059
N	2.603416	-1.098927	0.136056
H	2.699605	-0.444781	-0.675224
H	1.669204	-0.766915	0.484661
C	2.494955	-2.495225	-0.353094
H	2.335341	-3.136686	0.518097
H	3.452213	-2.762132	-0.809348
C	3.658027	-0.826071	1.147872
H	4.615316	-1.120982	0.708653
H	3.458223	-1.474217	2.005749
C	3.633926	0.646276	1.52872
H	3.817855	1.283146	0.658992
H	2.662419	0.930588	1.942118
H	4.405151	0.84425	2.276434
C	1.341753	-2.586062	-1.339792
H	1.244941	-3.608056	-1.71317
H	0.411819	-2.295572	-0.841872
H	1.497262	-1.909342	-2.184974
S	0.906111	1.435419	-0.675376
O	-0.317792	1.864629	-1.608608
O	1.908949	0.873283	-1.606812
O	0.36462	0.370881	0.227893
H	-0.476683	3.299328	0.747474
O	1.346945	2.62238	0.062291
H	-1.62838	2.37062	1.187073
O	-2.141949	0.597618	2.077856
C	-2.382511	-2.272262	-0.479033
H	-1.772492	-3.085419	-0.882135
H	-3.420368	-2.607612	-0.41046
C	-2.268212	-1.021412	-1.344229
H	-1.227383	-0.765613	-1.56353

H	-2.825238	-1.137104	-2.276508
H	-0.958886	2.327016	-0.992619
S	-2.990456	0.355156	-0.414261
S	-1.764497	-1.867151	1.184851