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Unifying Path-Dependent and Thermodynamic Descriptors of Asynchronicity in Double Proton Transfer reactions

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Supplementary tables

Table S1. Electronic proton affinities in the gas phase for the monomer species involved in double proton transfer (DPT): neutral monomer ($\alpha - H_a$ or $\beta - H_b$), cationic intermediate (${}^+ \alpha - H_a H_b$ or $H_a H_b - \beta^+$), and anionic intermediate (α^- or β^-). Two proton affinities are reported: $PA_{\alpha - H_a(\beta - H_b)}$, corresponding to protonation of the neutral monomer to form the cationic intermediate, and $PA_{\alpha^-(\beta^-)}$, corresponding to protonation of the anionic intermediate to regenerate the neutral monomer. Proton affinities were computed from electronic energies in the gas phase.

	<i>Neutral monomer</i> ($\alpha - H_a$ or $\beta - H_b$)	<i>Cationic intermediate</i> (${}^+ \alpha - H_a H_b$ or $H_a H_b - \beta^+$)	<i>Anionic intermediate</i> (α^- or β^-)	$PA_{\alpha - H_a(\beta - H_b)}$	$PA_{\alpha^-(\beta^-)}$
	(Hartree)	(Hartree)	(Hartree)	(kcal/mol)	(kcal/mol)
A	-477.2894628	-477.6498161	-476.7318543	226.123	349.90
B	-323.6135986	-323.9672292	-323.0489337	221.904	354.33
C	-205.7700503	-206.0018676	-205.2249844	145.466	342.03
D	-76.45853198	-76.72951226	-75.82744793	170.041	396.01
E	-399.4226462	-399.6521224	-398.8589548	143.997	353.72
F	-189.8277702	-190.1111193	-189.2727986	177.802	348.25
G	-512.776132	-513.0776877	-512.2436936	189.227	334.11
H	-835.736388	-836.051201	-835.2118041	197.546	329.18
I	-512.7796071	-513.0808314	-512.2436945	189.019	336.29
J	-229.164828	-229.4665567	-228.6024864	189.336	352.87
K	-150.0600165	-150.4350226	-149.4550384	235.317	379.63
L	-169.9548487	-170.2759687	-169.3644449	201.504	370.48
M	-379.9620789	-380.3330371	-379.3933567	232.777	356.87
N	-226.2659907	-226.618653	-225.6880431	221.297	362.66

Table S2. Concerted DPT reaction set constructed from monomers A–N, covering all analyzed monomer-pair combinations. The table reports, for each reaction, the hydrogen-bond complexation energy (ΔE_{HB}), the thermodynamic driving force (ΔE^0), activation barrier (ΔE^\ddagger), barrier width ($\Delta \xi_{TS}$), and the thermodynamic asynchronicity descriptor (η).

Reaction	ΔE_{HB} (kcal/mol)	ΔE^0 (kcal/mol)	ΔE^\ddagger (kcal/mol)	$\Delta \xi_{TS}$ (amu ^{1/2} · bohr)	η (kcal/mol)
AA	-14.6	1.3	7.4	0.63	0.0
AB	-15.3	-2.0	6.0	0.57	0.2
AD	-9.7	2.1	14.9	0.77	-10.0
AJ	-18.9	-6.2	8.8	1.11	-33.8
AK	-13.8	0.7	7.1	2.07	38.9
AL	-11.7	9.8	13.8	0.75	-4.0
AM	-13.1	7.0	11.3	1.13	13.6
AN	-13.0	0.6	10.8	0.72	7.9
BB	-15.9	-5.3	4.8	0.63	0.0
BD	-10.2	-2.1	13.4	0.77	-10.2
BE	-4.0	-2.3	8.6	3.35	-78.5
BF	-15.9	-3.0	2.8	1.41	-50.2
BI	-9.4	-5.8	2.1	3.02	-50.9
BJ	-15.8	-2.8	3.9	1.11	-34.0
BK	-14.5	-2.8	5.6	1.76	38.7
BL	-12.4	6.5	12.1	0.74	-4.2
BM	-13.9	3.8	9.7	1.09	13.4
BN	-13.7	-3.1	9.3	0.77	7.7
CC	-4.4	0.0	16.2	0.65	0.0
CD	-8.2	0.0	17.2	0.96	78.6
CE	-3.6	0.0	27.5	0.94	10.2
CF	-9.5	0.0	9.9	0.80	38.6
CG	-7.3	-1.9	12.5	0.93	35.8
CH	-5.3	0.0	16.8	1.03	39.2
CI	-7.1	1.9	14.4	0.93	37.8
CJ	-10.4	0.0	8.6	1.03	54.7
CL	-11.0	11.1	13.4	1.94	84.5
DD	-4.2	0.0	46.5	1.01	0.0
DE	-2.9	0.0	40.6	1.81	-68.3
DF	-10.3	0.0	14.8	0.84	-40.0
DG	-10.4	1.2	13.2	1.06	-42.7
DH	-6.7	0.0	11.3	1.21	-39.3
DI	-7.1	-1.2	12.1	1.06	-40.7

DJ	-10.3	0.0	14.4	0.73	-23.8
DK	-10.7	0.0	17.2	1.29	48.9
DL	-9.4	11.0	22.6	0.77	5.9
DM	-10.4	9.4	23.2	0.97	23.6
DN	-8.1	0.0	29.3	1.02	17.9
EE	-0.8	0.0	45.0	1.21	0.0
EF	-4.5	0.0	19.0	1.15	28.3
EG	-4.3	-0.9	16.9	0.93	25.6
EH	-2.6	0.0	15.4	0.92	29.0
EI	-3.0	0.9	17.8	0.93	27.6
EJ	-4.3	0.0	16.5	1.21	44.5
EL	-4.2	12.5	21.1	2.00	74.3
FF	-15.1	0.0	7.3	0.64	0.0
FG	-12.9	0.5	9.6	0.75	-2.7
FH	-8.5	0.0	11.4	0.96	0.7
FI	-10.2	-0.5	9.1	0.75	-0.7
FJ	-15.4	0.0	7.1	0.65	16.2
FL	-14.8	9.9	12.0	1.07	45.9
FM	-16.6	7.2	7.7	2.86	63.6
FN	-15.8	0.0	7.1	1.30	57.9
GG	-10.2	-0.4	12.6	0.74	0.0
GH	-6.9	-0.6	12.6	0.83	3.4
GI	-8.9	0.0	9.9	0.74	2.0
GJ	-13.5	1.1	9.1	0.93	18.9
GL	-13.0	-13.0	1.8	1.86	48.7
GN	-14.9	2.6	6.7	2.89	60.6
HH	-4.1	0.0	12.9	0.83	0.0
HI	-5.3	0.6	13.3	0.83	-1.4
HJ	-8.6	0.0	10.0	1.16	15.5
HL	-8.1	11.9	14.2	2.65	45.3
II	-6.3	0.4	13.0	0.74	0.0
IJ	-10.2	-1.1	8.0	0.93	16.9
IL	-9.6	8.7	10.3	1.96	46.7
IN	-10.2	-2.6	4.1	2.89	58.7
JJ	-15.7	0.0	7.1	0.54	0.0
JL	-14.5	9.7	12.5	0.91	29.8
JM	-16.1	7.3	8.6	2.53	47.4
JN	-15.3	0.0	8.2	1.10	41.8
KK	-13.2	0.0	13.3	0.72	0.0
KL	-13.5	9.6	12.8	1.69	-43.0

KM	-14.1	7.8	13.1	1.94	-25.3
LL	-13.2	19.4	20.5	0.82	0.0
LM	-13.6	17.2	18.2	1.26	17.7
LN	-13.3	10.3	17.0	0.90	12.0
MM	-14.1	14.5	17.5	0.87	0.0
MN	-13.9	8.1	16.2	1.20	-5.7
NN	-12.2	0.0	19.5	1.14	0.0

Table S3. Classification of reactions according to the topological features of the transition region (single minimum, double minimum with positive/negative local maximum, or shoulder-like weakly decoupled double minimum).

Reaction	<i>Transition region profile</i>
AA	Single minimum
AB	Single minimum
AD	Single minimum
AJ	Two minima + negative local maximum
AK	Two minima + positive local maximum
AL	Shoulder-like profile
AM	Two minima + positive local maximum
AN	Single minimum
BB	Single minimum
BD	Single minimum
BE	Two minima + positive local maximum
BF	Two minima + negative local maximum
BI	Two minima + positive local maximum
BJ	Two minima + negative local maximum
BK	Two minima + positive local maximum
BL	Shoulder-like profile
BM	Two minima + negative local maximum
BN	Single minimum
CC	Single minimum
CD	Shoulder-like profile
CE	Single minimum
CF	Two minima + negative local maximum
CG	Shoulder-like profile
CH	Shoulder-like profile
CI	Shoulder-like profile
CJ	Two minima + negative local maximum
CL	Two minima + positive local maximum

DD	Single minimum
DE	Two minima + negative local maximum
DF	Single minimum
DG	Two minima + negative local maximum
DH	Two minima + negative local maximum
DI	Two minima + negative local maximum
DJ	Single minimum
DK	Two minima + negative local maximum
DL	Single minimum
DM	Single minimum
DN	Single minimum
EE	Single minimum
EF	Two minima + negative local maximum
EG	Single minimum
EH	Single minimum
EI	Single minimum
EJ	Two minima + negative local maximum
EL	Two minima + positive local maximum
FF	Single minimum
FG	Single minimum
FH	Two minima + negative local maximum
FI	Single minimum
FJ	Single minimum
FL	Two minima + negative local maximum
FM	Two minima + positive local maximum
FN	Two minima + negative local maximum
GG	Single minimum
GH	Single minimum
GI	Single minimum
GJ	Two minima + negative local maximum
GL	Two minima + positive local maximum
GN	Two minima + positive local maximum
HH	Single minimum
HI	Single minimum
HJ	Two minima + negative local maximum
HL	Two minima + positive local maximum
II	Single minimum
IJ	Two minima + negative local maximum
IL	Two minima + positive local maximum
IN	Two minima + positive local maximum

JJ	Single minimum
JL	Two minima + negative local maximum
JM	Two minima + positive local maximum
JN	Two minima + negative local maximum
KK	Single minimum
KL	Two minima + negative local maximum
KM	Two minima + positive local maximum
LL	Single minimum
LM	Two minima + positive local maximum
LN	Shoulder-like profile
MM	Two minima + negative local maximum
MN	Two minima + negative local maximum
NN	Two minima + negative local maximum

Table S4. Selected proton-transfer distances (Å) for reactants (R), transition states (TS), and products (P) for each reaction. Reactions are labeled as **AA**, **AB**, **AC**, ..., where the first letter denotes the left monomer and the second letter denotes the right monomer, indicated with a prime (') in atom labels. *Z/Z'* are the proton donors and *X/X'* are the proton acceptors (see Figure 2). XH_a_R and $X'H_b_R$ are the donor–H distances in the left and right monomers in R, respectively. In the TS, XH_a_TS and $X'H_b_TS$ are the donor–H distances, while $H_aX'_TS$ and H_bX_TS are the distances between each transferring proton and the acceptor atom in the opposite monomer. In the products, $H_aX'_P$ and H_bX_P are the newly formed H–acceptor distances in the right and left monomers, respectively.

REACTION	ZH _a _R	Z'H _b _R	ZH _a _TS	H _a X'_TS	H _b X_TS	Z'H _b _TS	H _a X'_P	H _b X_P
AA	0.97	0.97	1.23	1.26	1.26	1.23	1.01	1.01
AB	0.97	0.97	1.22	1.27	1.28	1.21	1.01	1.01
AD	0.97	0.96	1.19	1.24	1.22	1.29	0.96	1.01
AJ	0.97	0.97	1.06	1.44	1.23	1.26	0.97	1.01
AK	0.97	1.01	1.53	1.08	1.39	1.21	1.01	1.01
AL	0.97	1.01	1.18	1.23	1.19	1.41	0.97	1.01
AM	0.97	1.01	1.43	1.11	1.32	1.26	1.01	1.01
AN	0.97	1.01	1.26	1.23	1.32	1.26	1.01	1.01
BB	0.97	0.97	1.19	1.30	1.30	1.20	1.01	1.01
BD	0.97	0.96	1.18	1.26	1.24	1.27	0.96	1.01
BE	0.97	1.35	1.02	2.12	1.22	1.74	1.35	1.01
BF	0.97	0.97	1.04	1.46	1.20	1.30	0.97	1.01

BI	0.97	1.35	1.00	1.61	1.38	1.59	0.97	1.01
BJ	0.97	0.97	1.07	1.41	1.19	1.32	0.97	1.01
BK	0.97	1.01	1.50	1.09	1.45	1.17	1.01	1.01
BL	0.97	1.01	1.17	1.25	1.21	1.37	0.97	1.01
BM	0.97	1.01	1.42	1.12	1.36	1.23	1.01	1.01
BN	0.97	1.01	1.25	1.24	1.34	1.24	1.01	1.01
CC	0.98	0.98	1.22	1.22	1.22	1.22	0.98	0.98
CD	0.98	0.96	1.37	1.11	1.37	1.11	0.96	0.98
CE	0.98	1.35	1.25	1.64	1.25	1.64	1.35	0.98
CF	0.98	0.97	1.32	1.13	1.32	1.13	0.97	0.98
CG	0.98	0.97	1.38	1.54	1.30	1.14	1.35	0.98
CH	0.98	1.35	1.38	1.54	1.38	1.54	1.35	0.98
CI	0.98	1.35	1.30	1.14	1.38	1.54	0.97	0.98
CJ	0.98	0.97	1.36	1.11	1.36	1.11	0.97	0.98
CL	0.98	1.01	1.24	1.27	1.60	1.02	0.97	0.98
DD	0.96	0.96	1.25	1.25	1.25	1.25	0.96	0.96
DE	0.96	1.35	1.08	1.97	1.08	1.97	1.35	0.96
DF	0.96	0.97	1.15	1.31	1.15	1.31	0.97	0.96
DG	0.96	0.97	1.17	1.72	1.08	1.40	1.35	0.96
DH	0.96	1.35	1.11	1.80	1.11	1.80	1.35	0.96
DI	0.96	1.35	1.08	1.40	1.17	1.72	0.97	0.96
DJ	0.96	0.97	1.17	1.27	1.17	1.27	0.97	0.96
DK	0.96	1.01	1.42	1.14	1.42	1.14	1.01	0.96
DL	0.96	1.01	1.25	1.19	1.21	1.29	0.97	0.96
DM	0.96	1.01	1.35	1.19	1.29	1.23	1.01	0.96
DN	0.96	1.01	1.24	1.29	1.24	1.29	1.01	0.96
EE	1.35	1.35	1.70	1.70	1.70	1.70	1.35	1.35
EF	1.35	0.97	1.76	1.15	1.76	1.15	0.97	1.35
EG	1.35	0.97	1.75	1.59	1.65	1.22	1.35	1.35
EH	1.35	1.35	1.67	1.65	1.67	1.65	1.35	1.35
EI	1.35	1.35	1.65	1.22	1.75	1.59	0.97	1.35
EJ	1.35	0.97	1.80	1.12	1.80	1.12	0.97	1.35
EL	1.35	1.01	2.07	1.03	1.70	1.26	0.97	1.35
FF	0.97	0.97	1.21	1.21	1.21	1.21	0.97	0.97
FG	0.97	0.97	1.22	1.65	1.13	1.29	1.35	0.97
FH	0.97	1.35	1.15	1.74	1.15	1.74	1.35	0.97
FI	0.97	1.35	1.13	1.29	1.22	1.65	0.97	0.97
FJ	0.97	0.97	1.24	1.17	1.24	1.17	0.97	0.97
FL	0.97	1.01	1.45	1.06	1.24	1.26	0.97	0.97
FM	0.97	1.01	1.65	1.05	1.20	1.30	1.01	0.97

FN	0.97	1.01	1.45	1.12	1.45	1.12	1.01	0.97
GG	0.97	0.97	1.28	1.59	1.59	1.28	1.35	1.35
GH	0.97	1.35	1.22	1.65	1.60	1.74	1.35	1.35
GI	0.97	1.35	1.20	1.20	1.67	1.67	0.97	1.35
GJ	0.97	0.97	1.35	1.09	1.68	1.19	0.97	1.35
GL	0.97	1.01	1.57	1.02	1.57	1.40	0.97	1.35
GN	0.97	1.01	1.69	1.05	1.66	1.29	1.01	1.35
HH	1.35	1.35	1.66	1.66	1.66	1.66	1.35	1.35
HI	1.35	1.35	1.65	1.22	1.74	1.60	0.97	1.35
HJ	1.35	0.97	1.80	1.12	1.80	1.12	0.97	1.35
HL	1.35	1.01	2.07	1.02	1.59	1.38	0.97	1.35
II	1.35	1.35	1.59	1.28	1.28	1.59	0.97	0.97
IJ	1.35	0.97	1.68	1.19	1.35	1.09	0.97	0.97
IL	1.35	1.01	2.00	1.03	1.24	1.25	0.97	0.97
IN	1.35	1.01	1.66	1.29	1.69	1.05	1.01	0.97
JJ	0.97	0.97	1.21	1.21	1.21	1.21	0.97	0.97
JL	0.97	1.01	1.40	1.08	1.24	1.25	0.97	0.97
JM	0.97	1.01	1.59	1.07	1.23	1.26	1.01	0.97
JN	0.97	1.01	1.41	1.13	1.41	1.13	1.01	0.97
KK	1.01	1.01	1.29	1.29	1.29	1.29	1.01	1.01
KL	1.01	1.01	1.18	1.32	1.08	1.65	0.97	1.01
KM	1.01	1.01	1.21	1.38	1.09	1.62	1.01	1.01
LL	1.01	1.01	1.38	1.13	1.13	1.38	0.97	0.97
LM	1.01	1.01	1.60	1.10	1.20	1.29	1.01	0.97
LN	1.01	1.01	1.43	1.17	1.29	1.21	1.01	0.97
MM	1.01	1.01	1.31	1.27	1.17	1.44	1.01	1.01
MN	1.01	1.01	1.21	1.38	1.13	1.52	1.01	1.01
NN	1.01	1.01	1.43	1.18	1.43	1.18	1.01	1.01

Supplementary Figures

Figure S1. Comparison of the transition region for the **AD** pair calculated at the B3LYP and M06-2X levels of theory. The M06-2X profile is shown in orange and the B3LYP profile in blue.

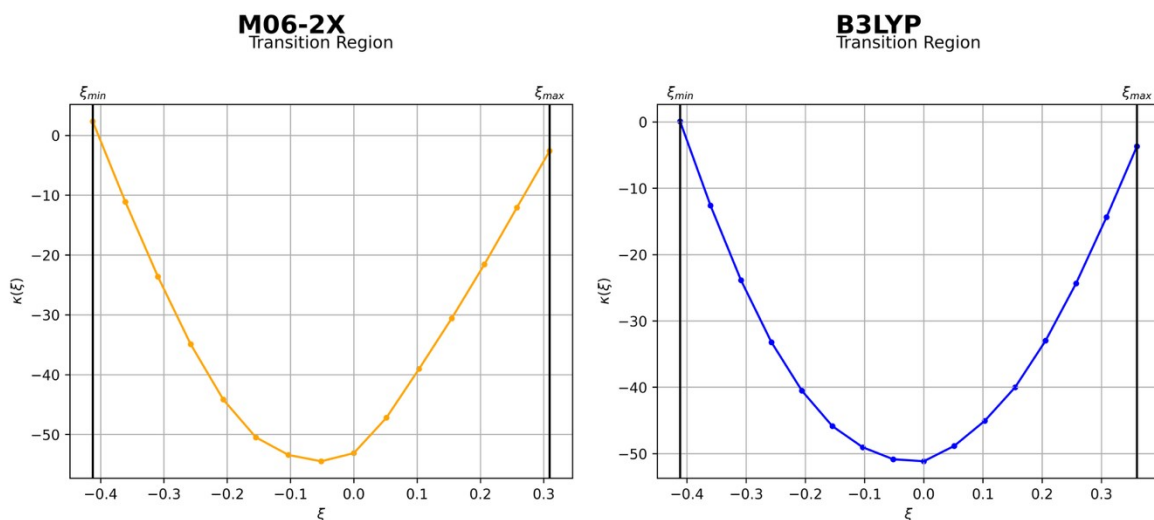


Figure S2. Comparison of the transition region for the **BD** pair calculated at the B3LYP and M06-2X levels of theory. The M06-2X profile is shown in orange and the B3LYP profile in blue.

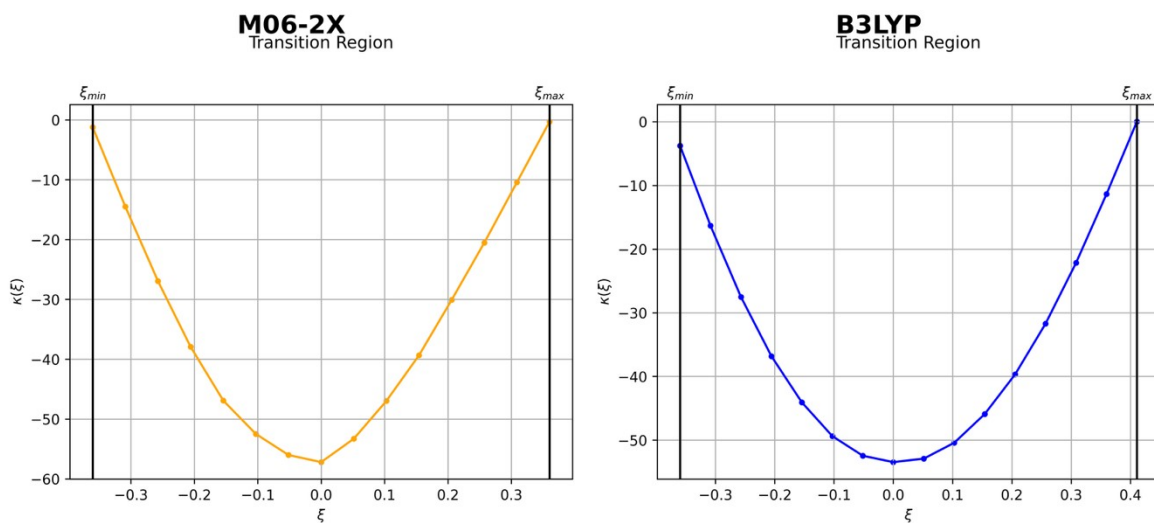


Figure S3. Comparison of the transition region for the **DG** pair calculated at the B3LYP and M06-2X levels of theory. The M06-2X profile is shown in orange and the B3LYP profile in blue.

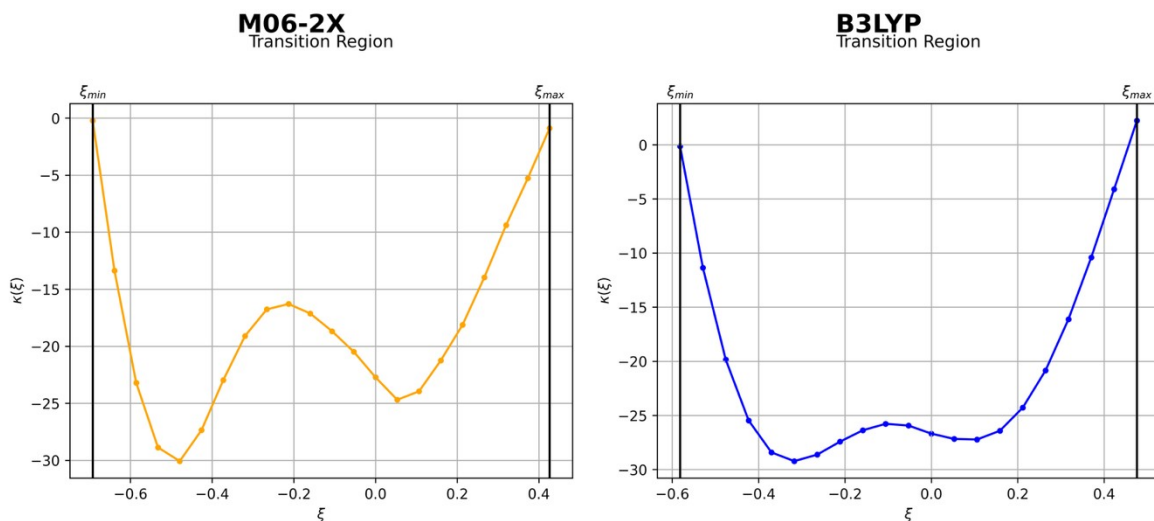


Figure S4. Comparison of the transition region for the **DI** pair calculated at the B3LYP and M06-2X levels of theory. The M06-2X profile is shown in orange and the B3LYP profile in blue.

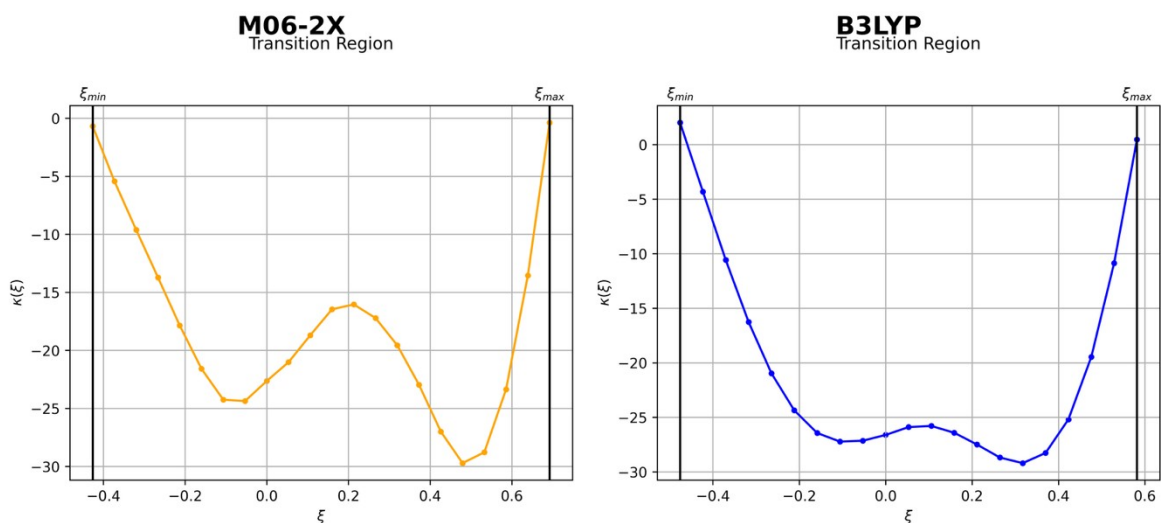


Figure S5. Comparison of the transition region for the **DL** pair calculated at the B3LYP and M06-2X levels of theory. The M06-2X profile is shown in orange and the B3LYP profile in blue.

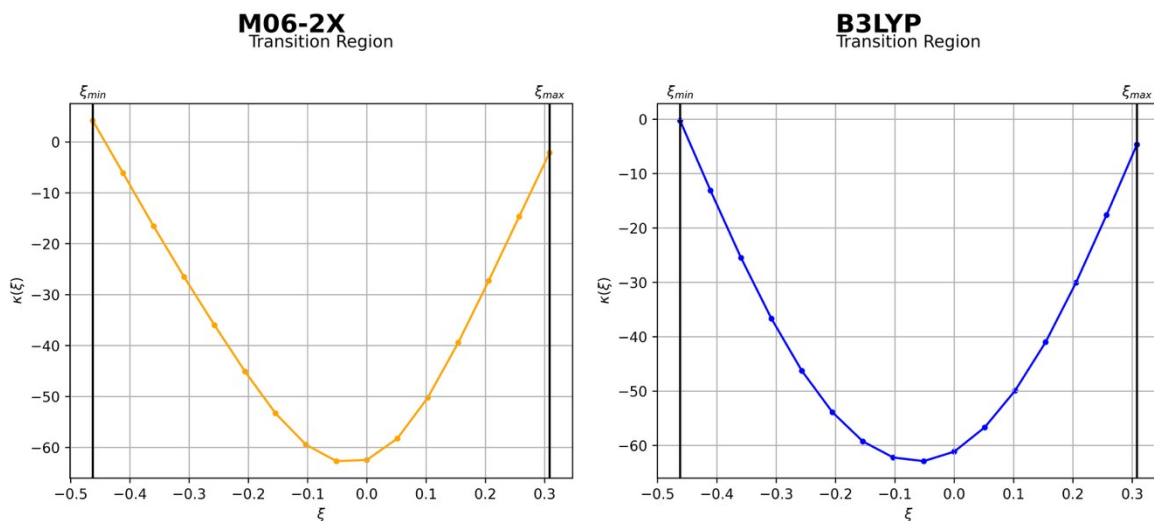


Figure S6. Comparison of the transition region for the **DM** pair calculated at the B3LYP and M06-2X levels of theory. The M06-2X profile is shown in orange and the B3LYP profile in blue.

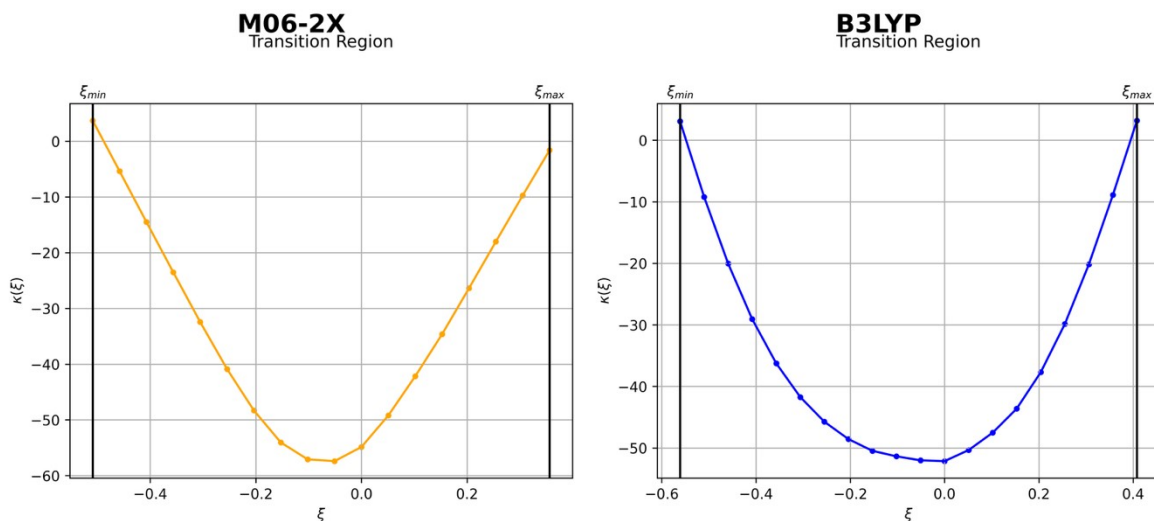


Figure S7. Comparison of the transition region for the **EG** pair calculated at the B3LYP and M06-2X levels of theory. The M06-2X profile is shown in orange and the B3LYP profile in blue.

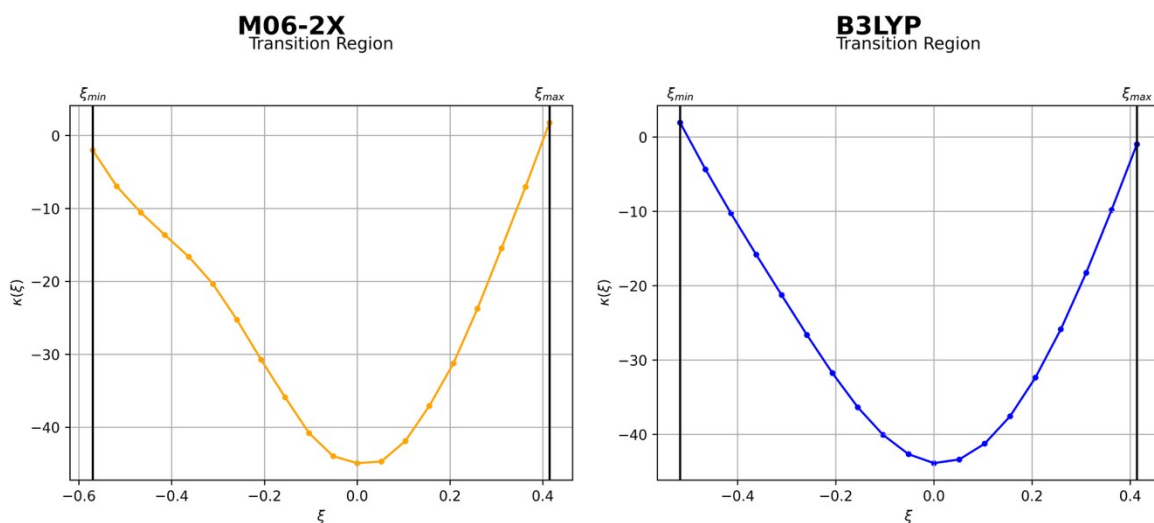


Figure S8. Comparison of the transition region for the **EI** pair calculated at the B3LYP and M06-2X levels of theory. The M06-2X profile is shown in orange and the B3LYP profile in blue.

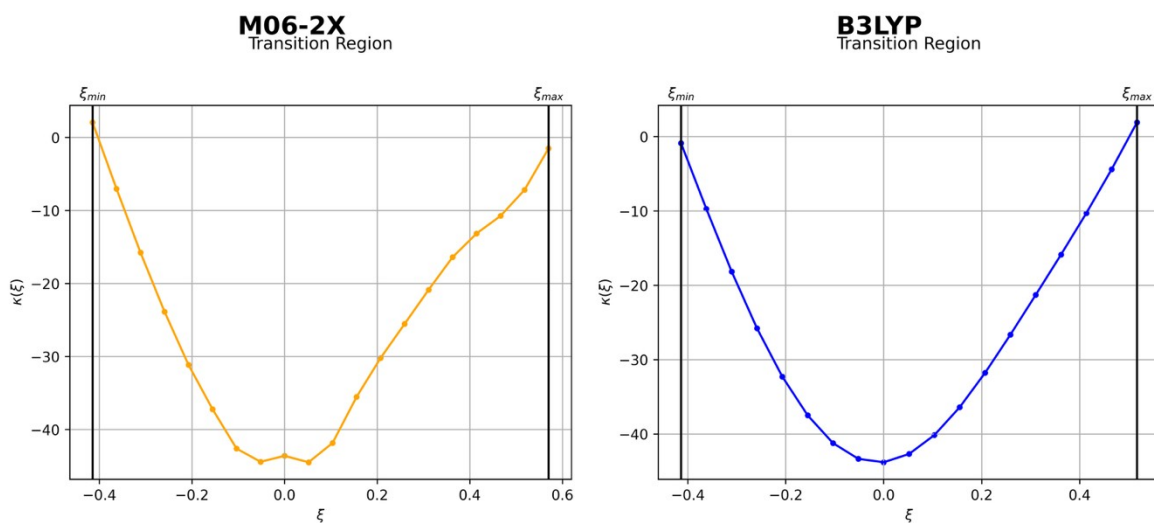


Figure S9. Comparison of the transition region for the **EL** pair calculated at the B3LYP and M06-2X levels of theory. The M06-2X profile is shown in orange and the B3LYP profile in blue.

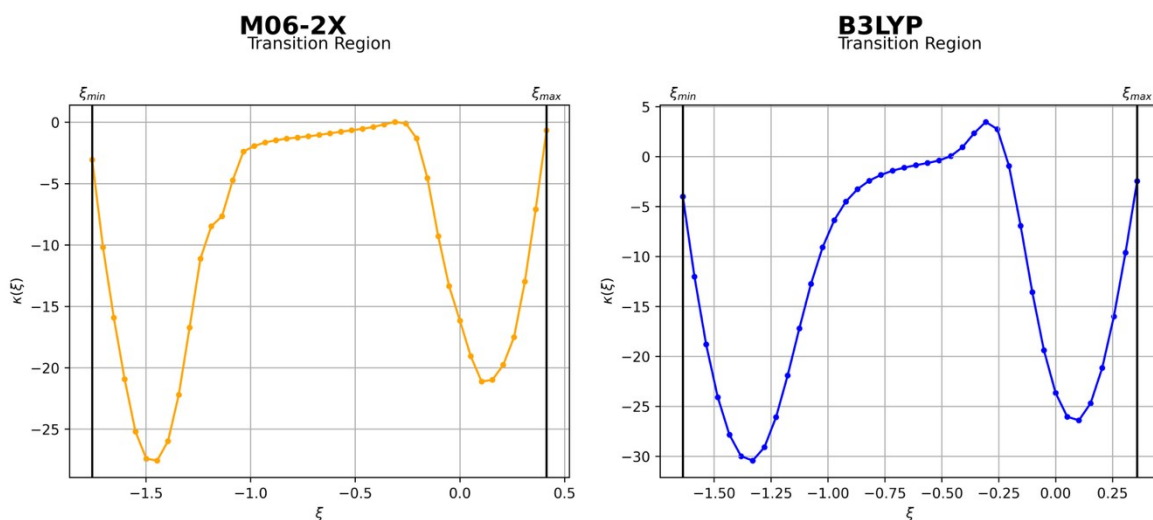


Figure S10. Bell–Evans–Polanyi diagram for the subset of double proton transfer reactions proceeding through six-membered transition states, comparing results obtained at the B3LYP and M06-2X levels of theory. Linear regressions are shown for both methods, with B3LYP in blue and M06-2X in orange.

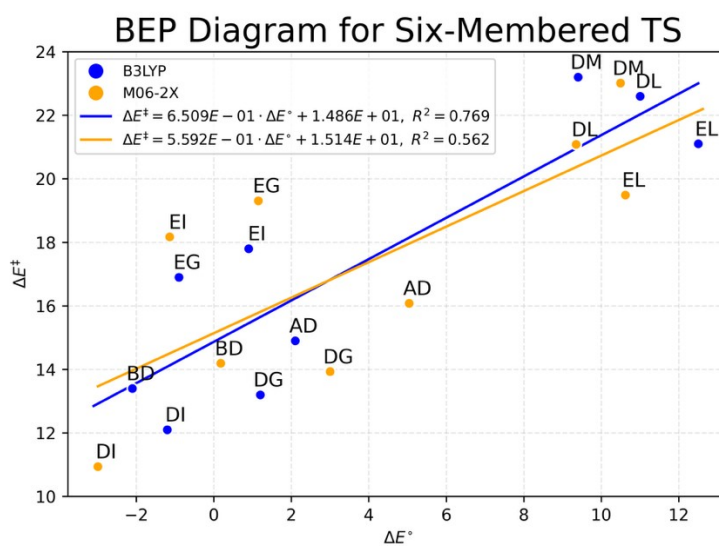


Figure S11. Comparison of proton affinity values associated with the neutral-to-anionic process for the monomers, calculated at the B3LYP and M06-2X levels of theory. B3LYP results are shown in blue and M06-2X results in orange.

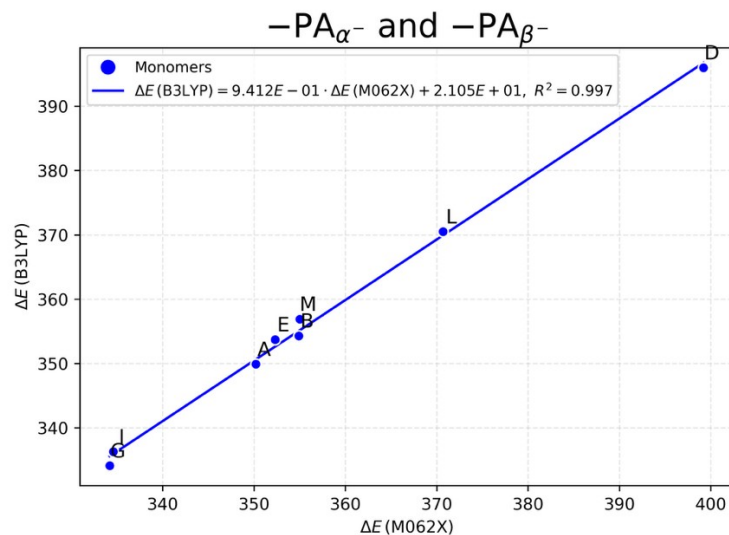
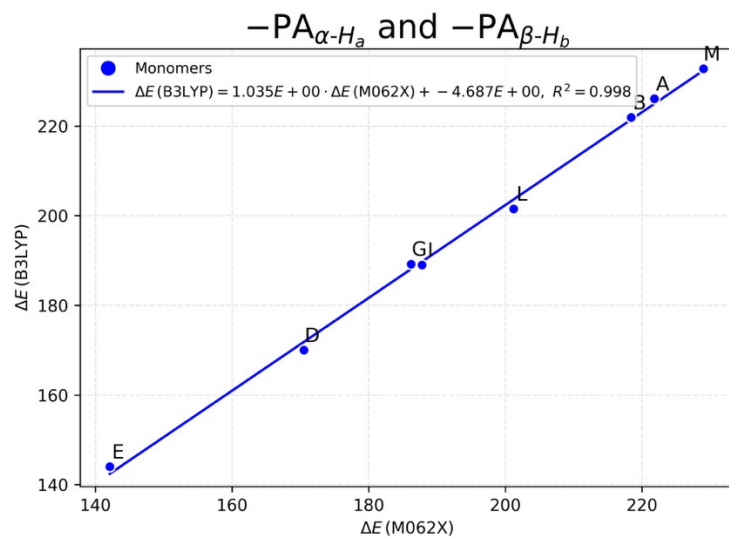


Figure S12. Comparison of proton affinity values associated with the cationic-to-neutral process for the monomers, calculated at the B3LYP and M06-2X levels of theory. B3LYP results are shown in blue and M06-2X results in orange.



Transition state coordinates

AA

C	6.39092	0.92881	0.00056
C	5.14508	1.49638	0.00044
C	3.98319	0.67503	0.00019
C	4.10914	-0.75550	0.00000
C	5.42627	-1.30688	0.00014
C	6.52449	-0.48824	0.00041
H	2.51386	2.27206	0.00017
H	7.27831	1.55044	0.00077
H	5.02643	2.57495	0.00056
C	2.68554	1.19957	0.00005
C	2.94717	-1.53741	-0.00027
H	5.54220	-2.38504	0.00002
H	7.51789	-0.92359	0.00051
C	1.68079	-0.94309	-0.00037
H	3.00172	-2.61861	-0.00043
C	-1.68080	0.94305	-0.00049
C	-2.94712	1.53739	-0.00035
C	-4.10909	0.75547	-0.00003
C	-3.98317	-0.67506	0.00012
C	-2.68557	-1.19965	-0.00008
H	-5.54210	2.38505	0.00006
H	-3.00165	2.61858	-0.00049
C	-5.42619	1.30689	0.00016
C	-5.14508	-1.49640	0.00046
H	-2.51376	-2.27210	-0.00000
C	-6.39089	-0.92879	0.00064
C	-6.52443	0.48828	0.00050
H	-5.02647	-2.57497	0.00056

H	-7.27830	-1.55038	0.00090
H	-7.51782	0.92363	0.00066
N	1.60062	0.43691	-0.00020
N	-1.60069	-0.43688	-0.00038
O	-0.58284	1.62376	-0.00069
H	0.47312	0.99636	-0.00044
O	0.58283	-1.62375	-0.00066
H	-0.47430	-0.99575	-0.00053

E = -954.590482600

Sum of electronic and zero-point Energies=	-954.318110
Sum of electronic and thermal Energies=	-954.301543
Sum of electronic and thermal Enthalpies=	-954.300598
Sum of electronic and thermal Free Energies=	-954.363908

AB

C	5.19789	0.80319	0.00132
C	5.33750	-0.59778	0.00078
H	3.72803	2.38403	0.00120
C	3.92173	1.31696	0.00085
C	4.22484	-1.40685	-0.00016
C	2.93002	-0.82315	-0.00059
H	4.29423	-2.48654	-0.00058
N	2.82498	0.53195	-0.00009
O	1.86315	-1.55010	-0.00146
H	0.81160	-0.95599	-0.00097
H	6.05629	1.46097	0.00207
H	6.32670	-1.04296	0.00112
C	-0.46126	0.96992	-0.00066
C	-1.74007	1.53621	-0.00053

C	-2.88433	0.72846	-0.00010
C	-2.72533	-0.69846	0.00021
C	-1.41532	-1.19257	0.00002
H	-4.35427	2.32480	-0.00017
H	-1.81863	2.61594	-0.00076
C	-4.21362	1.24958	0.00006
C	-3.86784	-1.54632	0.00066
H	-1.22133	-2.26147	0.00019
C	-5.12656	-1.00763	0.00081
C	-5.29280	0.40587	0.00050
H	-3.72444	-2.62191	0.00089
H	-5.99936	-1.64959	0.00115
H	-6.29597	0.81823	0.00062
N	-0.34693	-0.40717	-0.00040
O	0.61985	1.67948	-0.00102
H	1.67775	1.08152	-0.00059

E = -800.917768885

Sum of electronic and zero-point Energies= -800.691579
Sum of electronic and thermal Energies= -800.677731
Sum of electronic and thermal Enthalpies= -800.676787
Sum of electronic and thermal Free Energies= -800.733775

AD

O	-3.92320	-0.78984	-0.07304
H	-2.66459	-1.05908	0.00250
H	-4.48052	-1.04564	0.66781
C	-1.53962	0.71094	-0.00415
C	-0.32919	1.40450	0.00248
C	0.88785	0.70854	0.00330

C	0.87506	-0.72918	-0.00206
C	-0.37446	-1.35984	-0.00713
H	2.18835	2.44458	0.01242
H	-0.35573	2.48654	0.00383
C	2.15766	1.36078	0.00846
C	2.09895	-1.45588	-0.00322
H	-0.45866	-2.44204	-0.01384
C	3.29553	-0.79171	0.00164
C	3.31689	0.63134	0.00769
H	2.06634	-2.54040	-0.00846
H	4.22913	-1.34134	0.00064
H	4.27269	1.14373	0.01137
N	-1.50845	-0.67575	-0.00592
O	-2.71032	1.26751	-0.00896
H	-3.50170	0.38552	-0.02088

E = -553.739700121

Sum of electronic and zero-point Energies=	-553.581155
Sum of electronic and thermal Energies=	-553.571946
Sum of electronic and thermal Enthalpies=	-553.571001
Sum of electronic and thermal Free Energies=	-553.615622

AJ

O	-2.23300	1.09183	0.00988
C	-2.55796	-0.11982	-0.01150
O	-1.72166	-1.08822	-0.03351
H	-0.51498	-0.71088	-0.02886
C	1.04176	0.88417	-0.00176
C	2.43799	1.23902	0.00119
C	3.40120	0.19459	-0.02202

C	2.94305	-1.15797	-0.04717
C	1.60653	-1.40278	-0.04814
H	1.19426	-2.40402	-0.06661
N	0.67535	-0.39834	-0.02577
O	0.14871	1.83117	0.01930
H	-0.85124	1.48879	0.01476
C	-4.02159	-0.49334	-0.00223
H	-4.23167	-1.17966	-0.82514
H	-4.24913	-1.02215	0.92710
H	-4.64624	0.39444	-0.08059
H	3.65068	-1.97686	-0.06525
C	2.85021	2.58799	0.02629
C	4.19358	2.89655	0.02839
C	5.15645	1.86651	0.00553
C	4.77179	0.54304	-0.01917
H	5.51589	-0.24554	-0.03669
H	6.21060	2.12051	0.00743
H	4.51333	3.93171	0.04763
H	2.09534	3.36332	0.04356

E = -706.480055133

Sum of electronic and zero-point Energies=	-706.282295
Sum of electronic and thermal Energies=	-706.269348
Sum of electronic and thermal Enthalpies=	-706.268404
Sum of electronic and thermal Free Energies=	-706.324296

AK

C	4.29723	-0.68627	0.00031
C	0.75855	0.97406	-0.00006
C	-0.53976	1.53122	0.00012

C	-1.68204	0.72880	0.00009
C	-1.52838	-0.70051	-0.00013
C	-0.21604	-1.19201	-0.00025
H	-3.15548	2.32460	0.00040
H	-0.62041	2.61144	0.00026
C	-3.01554	1.24895	0.00024
C	-2.67234	-1.54509	-0.00019
H	-0.04185	-2.26737	-0.00039
C	-3.93222	-1.00766	-0.00004
C	-4.09552	0.40768	0.00017
H	-2.53029	-2.62160	-0.00036
H	-4.80564	-1.64905	-0.00009
H	-5.09821	0.82205	0.00029
N	0.85998	-0.42112	-0.00021
O	1.82494	1.66400	-0.00011
H	3.25096	1.10569	-0.00046
H	2.12427	-0.99880	0.00002
H	5.29170	-1.13316	0.00085
N	3.24206	-1.46111	0.00033
H	3.42264	-2.45422	0.00106
N	4.21935	0.62875	-0.00044
H	5.06944	1.16784	-0.00000

E = -627.360182075

Sum of electronic and zero-point Energies= -627.165984
Sum of electronic and thermal Energies= -627.154129
Sum of electronic and thermal Enthalpies= -627.153185
Sum of electronic and thermal Free Energies= -627.204955

AL

C	4.24095	-0.58770	-0.00019
C	0.79046	0.92802	-0.00044
C	-0.48374	1.50908	-0.00024
C	-1.63811	0.71920	0.00009
C	-1.50473	-0.71235	0.00023
C	-0.20739	-1.22772	0.00003
H	-3.08028	2.34093	0.00019
H	-0.54485	2.58971	-0.00033
C	-2.95895	1.26355	0.00030
C	-2.66358	-1.54043	0.00058
H	-0.02486	-2.29835	0.00012
C	-3.91060	-0.97843	0.00077
C	-4.05166	0.43913	0.00063
H	-2.54026	-2.61840	0.00069
H	-4.79519	-1.60389	0.00104
H	-5.04747	0.86863	0.00079
N	0.87120	-0.45217	-0.00032
O	1.87221	1.62622	-0.00076
H	2.92916	1.10227	-0.00034
H	1.94569	-0.95956	-0.00047
H	5.28174	-0.93820	-0.00014
O	4.08707	0.67519	0.00012
N	3.26399	-1.45513	-0.00056
H	3.57976	-2.41750	-0.00083

E = -647.240884492

Sum of electronic and zero-point Energies=	-647.060658
Sum of electronic and thermal Energies=	-647.049273
Sum of electronic and thermal Enthalpies=	-647.048329
Sum of electronic and thermal Free Energies=	-647.099122

AM

C	4.03099	0.85841	0.00001
C	2.74589	0.22454	-0.00001
C	3.68506	-1.89725	0.00003
C	4.96675	-1.35589	0.00005
C	5.15181	0.03128	0.00004
C	3.74405	2.25836	-0.00001
C	2.36972	2.36386	-0.00004
H	3.50112	-2.96333	0.00003
H	5.81620	-2.02600	0.00007
H	6.15436	0.44513	0.00005
H	4.45075	3.07304	-0.00001
H	1.77293	3.26434	-0.00006
N	1.75010	1.12949	-0.00003
H	0.54681	0.75331	-0.00004
N	2.59496	-1.11183	0.00000
C	-0.85455	-1.13381	-0.00008
C	-2.17694	-1.61964	-0.00007
C	-3.27455	-0.75526	-0.00002
C	-3.04211	0.66278	0.00004
C	-1.70739	1.08277	0.00003
H	-1.46811	2.14423	0.00007
N	-0.67642	0.24951	-0.00003
O	0.17110	-1.89397	-0.00013
H	1.54792	-1.49326	-0.00005
C	-4.63282	-1.20348	-0.00001
C	-4.13870	1.56927	0.00010
H	-3.93867	2.63618	0.00013
C	-5.42462	1.09972	0.00010
H	-6.26216	1.78716	0.00014

C	-5.66514	-0.30444	0.00005
H	-4.83059	-2.26983	-0.00005
H	-6.68889	-0.66309	0.00007
H	-2.31551	-2.69369	-0.00012

E = -857.254499019

Sum of electronic and zero-point Energies=	-857.002059
Sum of electronic and thermal Energies=	-856.987250
Sum of electronic and thermal Enthalpies=	-856.986306
Sum of electronic and thermal Free Energies=	-857.045373

AN

C	4.55634	0.61442	-0.00037
C	5.03364	-0.69872	-0.00034
C	3.88543	-1.49296	0.00002
H	6.06029	-1.02591	-0.00055
H	3.78384	-2.56706	0.00019
N	2.80699	-0.69622	0.00021
H	1.54909	-0.68563	0.00033
C	0.09076	1.09885	0.00021
C	-1.22906	1.57108	0.00006
C	-2.31441	0.68843	-0.00002
C	-2.05969	-0.72514	0.00007
C	-0.71948	-1.12782	0.00023
H	-3.89006	2.18123	-0.00025
H	-1.38248	2.64280	-0.00002
C	-3.67718	1.11793	-0.00018
C	-3.14287	-1.64820	-0.00001
H	-0.46174	-2.18395	0.00030
C	-4.43488	-1.19623	-0.00017

C	-4.69641	0.20359	-0.00026
H	-2.92762	-2.71193	0.00005
H	-5.26238	-1.89565	-0.00023
H	-5.72524	0.54700	-0.00038
N	0.29666	-0.27528	0.00031
O	1.11335	1.88377	0.00028
H	2.25095	1.34062	0.00009
N	3.21837	0.58662	-0.00004
H	5.09125	1.55116	-0.00060

E = -703.558907760

Sum of electronic and zero-point Energies= -703.354944
Sum of electronic and thermal Energies= -703.342670
Sum of electronic and thermal Enthalpies= -703.341726
Sum of electronic and thermal Free Energies= -703.394575

BB

C	-3.91106	-0.95058	-0.00348
C	-4.12736	0.44031	-0.00185
H	-2.35846	-2.44882	-0.00301
C	-2.60819	-1.39326	-0.00216
C	-3.06000	1.30843	0.00080
C	-1.73604	0.79513	0.00174
H	-3.18756	2.38281	0.00213
C	1.73599	-0.79511	0.00197
C	3.06002	-1.30849	0.00063
C	4.12746	-0.44049	-0.00206
C	3.91124	0.95042	-0.00352
C	2.60832	1.39311	-0.00195
H	3.18751	-2.38289	0.00173

H	2.35889	2.44876	-0.00279
N	-1.55466	-0.55126	0.00045
N	1.55462	0.55137	0.00085
O	0.71152	-1.58293	0.00422
H	-0.35959	-1.05160	0.00250
O	-0.71160	1.58316	0.00378
H	0.35751	1.05279	0.00260
H	5.13938	-0.83127	-0.00312
H	4.73218	1.65445	-0.00570
H	-4.73198	-1.65464	-0.00559
H	-5.13931	0.83102	-0.00268

E = -647.244983021

Sum of electronic and zero-point Energies=	-647.064953
Sum of electronic and thermal Energies=	-647.053805
Sum of electronic and thermal Enthalpies=	-647.052860
Sum of electronic and thermal Free Energies=	-647.103539

BD

O	-2.72895	-0.64809	-0.07887
H	-1.51238	-0.99847	-0.00446
H	-3.29582	-0.88194	0.66209
C	-0.26470	0.67686	-0.00236
C	1.00129	1.31214	0.00986
C	2.14045	0.53901	0.01187
C	2.05558	-0.86739	0.00335
C	0.80276	-1.43664	-0.00681
H	1.03326	2.39340	0.01409
H	0.65390	-2.51026	-0.01634
N	-0.31534	-0.68692	-0.00723

O	-1.38436	1.32596	-0.00864
H	-2.23153	0.50877	-0.02151
H	2.94089	-1.48832	0.00233
H	3.11327	1.01850	0.01902

E = -400.066975537

Sum of electronic and zero-point Energies=	-399.954754
Sum of electronic and thermal Energies=	-399.948158
Sum of electronic and thermal Enthalpies=	-399.947214
Sum of electronic and thermal Free Energies=	-399.985581

BE

H	-1.19425	-0.68956	-0.01733
S	-2.89811	-0.36642	-0.07439
H	-3.06397	-0.42912	1.26410
C	0.34198	0.80067	-0.00217
C	1.69444	1.18604	0.00855
C	2.66105	0.20105	0.01088
C	2.29855	-1.15738	0.00245
C	0.95747	-1.46833	-0.00835
H	1.93609	2.24030	0.01342
H	0.58593	-2.48641	-0.01686
N	0.01684	-0.50550	-0.00844
O	-0.61995	1.70168	-0.00782
H	-1.52546	1.24198	-0.02049
H	3.04345	-1.94141	0.00237
H	3.70864	0.47970	0.01852

E = -723.028961399

Sum of electronic and zero-point Energies=	-722.920990
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Sum of electronic and thermal Energies= -722.913401
Sum of electronic and thermal Enthalpies= -722.912457
Sum of electronic and thermal Free Energies= -722.953675

BF

O	-2.76215	0.81015	0.00011
C	-2.98599	-0.41765	0.00005
O	-2.11313	-1.34245	-0.00020
H	-0.89704	-0.87974	-0.00007
H	-4.03563	-0.75066	0.00024
C	0.54161	0.81340	-0.00003
C	1.89494	1.21775	-0.00006
C	2.88448	0.26047	-0.00000
C	2.55162	-1.10658	0.00007
C	1.21926	-1.44225	0.00006
H	2.11025	2.27759	-0.00012
H	0.87161	-2.46847	0.00010
N	0.24597	-0.50509	0.00002
O	-0.40814	1.70768	-0.00003
H	-1.37544	1.31503	0.00005
H	3.31106	-1.87617	0.00011
H	3.92524	0.56414	-0.00001

E = -513.462255012

Sum of electronic and zero-point Energies= -513.338218
Sum of electronic and thermal Energies= -513.329707
Sum of electronic and thermal Enthalpies= -513.328762
Sum of electronic and thermal Free Energies= -513.372663

BI

H	0.81922	-0.75231	0.00056
C	3.01395	0.31801	-0.00061
O	2.41121	1.38952	-0.00033
H	4.11491	0.32233	-0.00137
S	2.32153	-1.27178	0.00005
C	-0.98225	0.86840	0.00034
C	-2.37037	1.11237	-0.00032
C	-3.23667	0.03952	-0.00060
C	-2.73369	-1.27164	-0.00026
C	-1.36570	-1.43269	0.00034
H	-2.71440	2.13797	-0.00057
H	-0.89874	-2.41261	0.00057
N	-0.51376	-0.38988	0.00064
O	-0.15388	1.89363	0.00066
H	0.81663	1.63348	0.00108
H	-4.30698	0.21178	-0.00109
H	-3.38896	-2.13209	-0.00047

E = -836.404789196

Sum of electronic and zero-point Energies=	-836.284742
Sum of electronic and thermal Energies=	-836.275522
Sum of electronic and thermal Enthalpies=	-836.274577
Sum of electronic and thermal Free Energies=	-836.320934

BJ

O	-2.21205	1.08274	0.01168
C	-2.56655	-0.12499	0.01090
O	-1.75757	-1.11046	0.01175
H	-0.48590	-0.75325	0.00655

C	1.05391	0.81905	-0.00078
C	2.43562	1.12183	-0.00473
C	3.35263	0.09573	-0.00545
C	2.92272	-1.24494	-0.00200
C	1.57016	-1.48402	0.00193
H	2.72769	2.16316	-0.00720
H	1.14888	-2.48222	0.00486
N	0.66795	-0.47832	0.00248
O	0.16886	1.76987	-0.00024
H	-0.84795	1.44081	0.00476
C	-4.04281	-0.44835	-0.01432
H	-4.31101	-0.77785	-1.02244
H	-4.25933	-1.27164	0.66793
H	-4.63409	0.42961	0.24028
H	3.62523	-2.06679	-0.00241
H	4.41272	0.32331	-0.00853

E = -552.797463821

Sum of electronic and zero-point Energies= -552.646438
Sum of electronic and thermal Energies= -552.636182
Sum of electronic and thermal Enthalpies= -552.635238
Sum of electronic and thermal Free Energies= -552.684523

BK

C	-3.11266	0.43174	-0.00018
C	0.57572	-0.80438	0.00018
C	1.94085	-1.24271	-0.00015
C	2.96631	-0.32960	-0.00028
C	2.68552	1.05221	-0.00012
C	1.35893	1.42438	0.00016

H	2.12162	-2.31022	-0.00028
H	1.07785	2.47544	0.00029
N	0.33617	0.54897	0.00032
O	-0.39470	-1.62715	0.00037
H	-1.83642	-1.21894	0.00004
H	-1.03898	1.02221	0.00017
H	-4.15365	0.75479	-0.00030
N	-2.16399	1.33642	-0.00004
H	-2.45598	2.30189	-0.00001
N	-2.86742	-0.85990	-0.00020
H	3.47092	1.79631	-0.00021
H	3.99618	-0.67307	-0.00053
H	-3.64521	-1.49949	-0.00036

E = -473.687806206

Sum of electronic and zero-point Energies=	-473.539554
Sum of electronic and thermal Energies=	-473.530501
Sum of electronic and thermal Enthalpies=	-473.529557
Sum of electronic and thermal Free Energies=	-473.574784

BL

C	-3.04595	0.35626	-0.00022
C	0.52512	-0.78054	0.00020
C	1.86936	-1.24473	0.00035
C	2.90558	-0.34237	0.00033
C	2.64591	1.04347	0.00017
C	1.33256	1.44411	0.00006
H	2.03156	-2.31426	0.00044
H	1.04555	2.49015	-0.00006
N	0.30965	0.56317	0.00012

O	-0.46144	-1.60531	0.00016
H	-1.55869	-1.19782	-0.00043
H	-0.83273	0.97400	-0.00006
H	-4.11608	0.60305	0.00036
O	-2.76486	-0.88304	-0.00088
N	-2.16145	1.31892	-0.00027
H	-2.56626	2.24701	0.00073
H	3.44455	1.77239	0.00013
H	3.92961	-0.69961	0.00043

E = -493.568869414

Sum of electronic and zero-point Energies=	-493.435026
Sum of electronic and thermal Energies=	-493.426303
Sum of electronic and thermal Enthalpies=	-493.425359
Sum of electronic and thermal Free Energies=	-493.469729

BM

C	-2.90667	0.72172	-0.00009
C	-1.57763	0.18741	0.00021
C	-2.34954	-1.99868	0.00024
C	-3.66938	-1.55771	0.00009
C	-3.96079	-0.18912	-0.00012
C	-2.72833	2.13989	-0.00032
C	-1.36670	2.35215	-0.00012
H	-2.08475	-3.04769	0.00025
H	-4.46469	-2.29127	0.00008
H	-4.99217	0.14646	-0.00032
H	-3.49585	2.89748	-0.00051
H	-0.83943	3.29481	-0.00011
N	-0.65618	1.16830	0.00024

H	0.54436	0.89528	0.00003
N	-1.32259	-1.13258	0.00028
C	2.09641	-0.88881	-0.00016
C	3.46757	-1.29704	-0.00023
C	4.47263	-0.36135	-0.00007
C	4.16200	1.01378	0.00018
C	2.83031	1.35970	0.00023
H	3.67079	-2.36020	-0.00041
H	2.52008	2.40113	0.00044
N	1.82944	0.45655	0.00001
O	1.14621	-1.74118	-0.00031
H	-0.24295	-1.43576	0.00015
H	5.50937	-0.68231	-0.00013
H	4.93152	1.77395	0.00036

E = -703.582357022

Sum of electronic and zero-point Energies=	-703.376297
Sum of electronic and thermal Energies=	-703.364182
Sum of electronic and thermal Enthalpies=	-703.363237
Sum of electronic and thermal Free Energies=	-703.415971

BN

C	3.22760	-0.87427	0.00040
C	3.85642	0.37368	-0.00017
C	2.81017	1.29776	-0.00042
H	4.91444	0.57773	-0.00032
H	2.83461	2.37632	-0.00083
N	1.64651	0.63201	0.00006
H	0.41567	0.77898	-0.00008
C	-1.24962	-0.81233	-0.00015

C	-2.63374	-1.14459	-0.00015
C	-3.58009	-0.14780	0.00005
C	-3.18680	1.20493	0.00020
C	-1.83783	1.47447	0.00013
H	-2.89972	-2.19341	-0.00031
H	-1.46265	2.49309	0.00016
N	-0.89694	0.50800	-0.00002
O	-0.34339	-1.72731	-0.00045
H	0.84195	-1.32782	0.00077
N	1.90202	-0.69060	0.00050
H	3.64914	-1.86721	0.00058
H	-3.91014	2.00901	0.00034
H	-4.63401	-0.40513	0.00009

E = -549.886606765

Sum of electronic and zero-point Energies=	-549.728794
Sum of electronic and thermal Energies=	-549.719233
Sum of electronic and thermal Enthalpies=	-549.718289
Sum of electronic and thermal Free Energies=	-549.764758

CC

N	-1.89090	-0.00022	-0.00009
O	-1.22248	1.06729	0.00031
O	-1.22182	-1.06758	-0.00031
H	0.00027	-0.99531	-0.00005
N	1.89089	0.00026	-0.00027
O	1.22248	-1.06728	0.00042
O	1.22184	1.06754	-0.00010
H	-0.00027	0.99530	0.00005

E = -411.521262613

Sum of electronic and zero-point Energies= -411.484312
Sum of electronic and thermal Energies= -411.478544
Sum of electronic and thermal Enthalpies= -411.477600
Sum of electronic and thermal Free Energies= -411.514493

CD

H	-0.80777	-0.76082	-0.03685
O	-1.61911	-0.00012	-0.09543
H	-2.19256	0.00022	0.68260
N	1.19704	0.00003	0.02547
O	0.52394	-1.07211	-0.00147
O	0.52384	1.07215	-0.00150
H	-0.80833	0.76102	-0.03689

E = -282.214239874

Sum of electronic and zero-point Energies= -282.172962
Sum of electronic and thermal Energies= -282.168833
Sum of electronic and thermal Enthalpies= -282.167889
Sum of electronic and thermal Free Energies= -282.199539

CE

H	0.21896	-0.85970	-0.03102
S	1.61666	0.00001	-0.07979
H	1.74610	-0.00026	1.26413
N	-1.68506	0.00002	0.01161
O	-1.01596	-1.07390	-0.00045
O	-1.01595	1.07388	-0.00042
H	0.21908	0.85976	-0.03093

E = -605.154670725

Sum of electronic and zero-point Energies= -605.122119
Sum of electronic and thermal Energies= -605.117383
Sum of electronic and thermal Enthalpies= -605.116439
Sum of electronic and thermal Free Energies= -605.150074

CF

O	1.21228	-1.12475	0.00148
H	0.08500	-1.06387	-0.00003
C	1.78449	0.00053	0.00022
O	1.21091	1.12492	-0.00194
O	-1.23816	1.06827	0.00196
H	0.08303	1.06320	-0.00001
O	-1.23771	-1.06853	-0.00164
H	2.87696	0.00102	0.00106
N	-1.90437	-0.00040	-0.00017

E = -395.597218703

Sum of electronic and zero-point Energies= -395.546070
Sum of electronic and thermal Energies= -395.540329
Sum of electronic and thermal Enthalpies= -395.539385
Sum of electronic and thermal Free Energies= -395.576112

CG

H	0.03696	-1.00668	-0.00002
H	0.44386	1.17243	0.00006
C	-1.57391	0.76736	0.00016
H	-2.57376	1.20828	0.00045

O	1.40219	-1.19464	0.00036
O	-0.61762	1.58777	0.00004
S	-1.50054	-0.92456	-0.00015
N	2.21501	-0.24047	-0.00019
O	1.72043	0.91912	-0.00013

E = -718.537931037

Sum of electronic and zero-point Energies=	-718.491984
Sum of electronic and thermal Energies=	-718.485655
Sum of electronic and thermal Enthalpies=	-718.484711
Sum of electronic and thermal Free Energies=	-718.523687

CH

H	-0.43023	1.14920	-0.01120
C	1.74573	-0.00157	-0.00057
O	-1.81182	-1.06634	0.05179
H	-0.43370	-1.14829	0.01045
O	-1.80853	1.06864	-0.05313
H	2.83399	-0.00281	-0.00198
N	-2.46918	0.00230	0.00105
S	1.05817	1.53163	0.01908
S	1.05449	-1.53309	-0.01848

E = -1041.48815261

Sum of electronic and zero-point Energies=	-1041.446838
Sum of electronic and thermal Energies=	-1041.440799
Sum of electronic and thermal Enthalpies=	-1041.439855
Sum of electronic and thermal Free Energies=	-1041.478003

CI

H	0.03833	-1.00648	0.00057
H	0.44331	1.17293	0.00012
C	-1.57412	0.76702	0.00032
H	-2.57408	1.20766	0.00042
O	1.40225	-1.19459	0.00143
O	-0.61813	1.58788	0.00092
S	-1.50005	-0.92480	-0.00060
N	2.21486	-0.24007	-0.00034
O	1.72012	0.91933	-0.00122

E = -718.537931049

Sum of electronic and zero-point Energies=	-718.491983
Sum of electronic and thermal Energies=	-718.485654
Sum of electronic and thermal Enthalpies=	-718.484710
Sum of electronic and thermal Free Energies=	-718.523680

CJ

O	0.71337	-1.12102	0.01725
H	-0.39245	-1.05332	0.00701
C	1.31392	0.00001	0.01620
O	0.71357	1.12117	0.01763
O	-1.74756	1.06675	-0.00553
H	-0.39219	1.05332	0.00706
O	-1.74773	-1.06678	-0.00513
N	-2.41600	0.00005	-0.01001
C	2.80722	-0.00014	-0.01516
H	3.19594	0.89952	0.45893
H	3.19589	-0.89934	0.45986
H	3.12478	-0.00070	-1.06275

E = -434.937736033

Sum of electronic and zero-point Energies= -434.858770
Sum of electronic and thermal Energies= -434.851270
Sum of electronic and thermal Enthalpies= -434.850326
Sum of electronic and thermal Free Energies= -434.892026

CL

H	0.36529	-1.14304	0.00010
H	-0.14423	1.05305	-0.00010
C	1.85418	0.05721	-0.00004
H	2.94301	0.10547	-0.00016
N	1.12019	1.11579	-0.00025
H	1.61825	1.99727	-0.00057
O	1.38218	-1.15105	0.00036
O	-1.38852	1.04658	0.00037
O	-1.23264	-1.08354	-0.00042
N	-1.97670	-0.09465	0.00003

E = -375.721170917

Sum of electronic and zero-point Energies= -375.656490
Sum of electronic and thermal Energies= -375.650217
Sum of electronic and thermal Enthalpies= -375.649273
Sum of electronic and thermal Free Energies= -375.687084

DD

O	1.09063	-0.08828	-0.00003
H	-0.00002	-0.02027	0.60464
H	1.60430	0.72655	0.00011

O	-1.09062	-0.08829	0.00003
H	-0.00012	-0.02032	-0.60463
H	-1.60420	0.72661	-0.00014

E = -152.849628804

Sum of electronic and zero-point Energies=	-152.808729
Sum of electronic and thermal Energies=	-152.805227
Sum of electronic and thermal Enthalpies=	-152.804283
Sum of electronic and thermal Free Energies=	-152.832013

DE

H	-0.84125	-0.05595	0.69207
H	-0.84149	-0.05594	-0.69225
S	1.00336	-0.07359	0.00000
H	-2.14945	0.75694	0.00008
H	1.17279	1.26648	-0.00004
O	-1.67430	-0.09175	0.00001

E = -475.821050295

Sum of electronic and zero-point Energies=	-475.783430
Sum of electronic and thermal Energies=	-475.779489
Sum of electronic and thermal Enthalpies=	-475.778545
Sum of electronic and thermal Free Energies=	-475.808381

DF

O	-0.49336	1.12031	0.00213
H	0.76724	0.78419	-0.03005
C	-1.08314	-0.00000	0.01391
O	-0.49337	-1.12031	0.00213

H	0.76724	-0.78419	-0.03005
H	2.18752	-0.00000	0.67292
H	-2.17886	0.00000	0.03846
O	1.60619	-0.00000	-0.09610

E = -266.279248028

Sum of electronic and zero-point Energies=	-266.224972
Sum of electronic and thermal Energies=	-266.220882
Sum of electronic and thermal Enthalpies=	-266.219938
Sum of electronic and thermal Free Energies=	-266.251513

DG

H	-0.60394	-1.05581	-0.04612
C	0.62290	0.95515	0.01556
O	-0.54431	1.40774	-0.00280
H	-1.43271	0.32464	-0.04564
H	-2.19883	-0.97253	0.70843
H	1.44589	1.67864	0.04333
O	-1.72495	-0.71729	-0.09452
S	1.07539	-0.70185	0.00158

E = -589.230162272

Sum of electronic and zero-point Energies=	-589.179408
Sum of electronic and thermal Energies=	-589.174870
Sum of electronic and thermal Enthalpies=	-589.173926
Sum of electronic and thermal Free Energies=	-589.207129

DH

H	-0.81783	1.26533	-0.05650
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C	-0.00018	-1.09334	0.02266
H	0.81831	1.26442	-0.05679
H	0.00034	2.52867	0.72988
H	-0.00026	-2.18165	0.05519
O	0.00030	2.01408	-0.09090
S	-1.53588	-0.38826	-0.00252
S	1.53576	-0.38858	-0.00251

E = -912.187552864

Sum of electronic and zero-point Energies=	-912.139818
Sum of electronic and thermal Energies=	-912.134904
Sum of electronic and thermal Enthalpies=	-912.133960
Sum of electronic and thermal Free Energies=	-912.168603

DI

H	1.43229	0.32453	-0.04525
C	-0.62216	0.95545	0.01565
H	0.60352	-1.05610	-0.04664
H	2.19736	-0.97478	0.70830
H	-1.44455	1.67959	0.04346
O	1.72408	-0.71796	-0.09448
S	-1.07570	-0.70129	0.00155
O	0.54537	1.40730	-0.00285

E = -589.230162197

Sum of electronic and zero-point Energies=	-589.179408
Sum of electronic and thermal Energies=	-589.174871
Sum of electronic and thermal Enthalpies=	-589.173927
Sum of electronic and thermal Free Energies=	-589.207128

DJ

O	0.04700	1.11561	0.00498
H	1.27240	0.78541	-0.02788
C	-0.56866	-0.00001	0.01414
O	0.04701	-1.11562	0.00498
H	1.27243	-0.78542	-0.02787
H	2.71994	0.00004	0.67168
O	2.14084	0.00001	-0.09799
C	-2.06971	0.00001	0.00883
H	-2.40860	0.00008	-1.03165
H	-2.45237	-0.89867	0.49098
H	-2.45241	0.89860	0.49110

E = -305.616744977

Sum of electronic and zero-point Energies=	-305.535201
Sum of electronic and thermal Energies=	-305.529417
Sum of electronic and thermal Enthalpies=	-305.528473
Sum of electronic and thermal Free Energies=	-305.564860

DK

H	0.65775	0.94929	0.00217
C	-1.12841	-0.00028	0.01055
H	0.65821	-0.94846	0.00210
H	2.46491	0.00017	0.51360
H	-2.21687	-0.00055	0.02496
O	1.71101	0.00033	-0.08137
N	-0.46698	1.13756	0.00217
N	-0.46628	-1.13765	0.00220
H	-0.97352	-2.00742	0.00707

H	-0.97531	2.00668	0.00723
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E = -226.508152715

Sum of electronic and zero-point Energies=	-226.430447
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Sum of electronic and thermal Energies=	-226.425412
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Sum of electronic and thermal Enthalpies=	-226.424468
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Sum of electronic and thermal Free Energies=	-226.457681
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DL

O	0.38112	-1.17831	0.00240
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H	-0.74095	-0.77587	-0.02348
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C	1.09396	-0.11184	0.01256
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H	-0.72603	0.88636	-0.01808
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H	-2.24785	0.10587	0.65036
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H	2.17872	-0.24591	0.03025
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O	-1.64010	0.09085	-0.09574
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N	0.55234	1.07587	0.00424
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H	1.17774	1.86921	0.00272
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E = -246.392309978

Sum of electronic and zero-point Energies=	-246.326818
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Sum of electronic and thermal Energies=	-246.322471
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Sum of electronic and thermal Enthalpies=	-246.321527
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Sum of electronic and thermal Free Energies=	-246.353513
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DM

H	1.10684	-1.80108	-0.00373
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C	-0.79493	1.01500	0.00564
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C	0.23530	0.02870	0.00394
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C	-1.23974	-1.74047	-0.00193
C	-2.31450	-0.85010	0.00195
C	-2.10486	0.53523	0.00516
C	-0.08984	2.26098	0.00260
C	1.25601	1.94407	-0.00176
H	-1.38032	-2.81357	-0.00829
H	-3.31993	-1.25071	-0.00023
H	-2.95420	1.20987	0.00532
H	-0.51086	3.25410	0.00222
H	2.09874	2.61934	-0.00698
N	1.46271	0.58107	0.00087
H	2.27117	-0.34700	-0.01177
N	0.02713	-1.29854	-0.00056
O	2.44627	-1.62426	-0.08336
H	3.00482	-2.01496	0.59460

E = -456.400141912

Sum of electronic and zero-point Energies=	-456.264251
Sum of electronic and thermal Energies=	-456.256570
Sum of electronic and thermal Enthalpies=	-456.255626
Sum of electronic and thermal Free Energies=	-456.296464

DN

C	1.03205	-1.10901	0.00151
C	1.88372	0.00001	-0.00981
C	1.03201	1.10901	0.00154
N	-0.23511	0.67855	0.02489
H	-1.52053	0.77928	-0.02245
H	1.26450	-2.16244	-0.00507
H	2.96150	0.00002	-0.02441

H	1.26446	2.16244	-0.00508
N	-0.23505	-0.67851	0.02495
H	-1.52022	-0.77960	-0.02252
O	-2.47603	-0.00002	-0.11230
H	-3.03708	0.00005	0.66958

E = -302.690774302

Sum of electronic and zero-point Energies=	-302.601462
Sum of electronic and thermal Energies=	-302.596249
Sum of electronic and thermal Enthalpies=	-302.595305
Sum of electronic and thermal Free Energies=	-302.630228

EE

H	-0.00088	0.06600	-0.74217
H	-0.00094	0.06606	0.74230
S	-1.52501	0.07535	-0.00012
S	1.52505	0.07541	0.00011
H	-1.60336	-1.27212	0.00174
H	1.60461	-1.27200	-0.00171

E = -798.774938185

Sum of electronic and zero-point Energies=	-798.746709
Sum of electronic and thermal Energies=	-798.742479
Sum of electronic and thermal Enthalpies=	-798.741534
Sum of electronic and thermal Free Energies=	-798.772890

EF

O	-0.99903	1.12422	0.00081
H	0.13315	0.92983	-0.01888

C	-1.58183	0.00003	0.00806
O	-0.99915	-1.12420	0.00083
H	0.13292	-0.92965	-0.01863
H	1.80924	0.00025	1.25646
H	-2.67436	0.00007	0.02131
S	1.62971	-0.00005	-0.08136

E = -589.227315399

Sum of electronic and zero-point Energies=	-589.180095
Sum of electronic and thermal Energies=	-589.175365
Sum of electronic and thermal Enthalpies=	-589.174421
Sum of electronic and thermal Free Energies=	-589.208027

EG

H	-0.30070	-0.90791	-0.03422
C	1.32257	0.76952	0.00832
O	0.33916	1.55573	-0.00064
H	-0.72558	0.95978	-0.02546
H	-2.03957	-0.24489	1.26230
H	2.31233	1.23378	0.02166
S	1.28491	-0.93535	0.00031
S	-1.90336	-0.19613	-0.07963

E = -912.178639932

Sum of electronic and zero-point Energies=	-912.136374
Sum of electronic and thermal Energies=	-912.131213
Sum of electronic and thermal Enthalpies=	-912.130269
Sum of electronic and thermal Free Energies=	-912.165410

EH

H	0.75192	0.98966	-0.03975
C	-1.49793	-0.00001	0.01068
H	0.75195	-0.98964	-0.03974
H	2.21299	0.00003	1.26681
H	-2.58570	-0.00002	0.02593
S	-0.80263	1.53711	-0.00105
S	-0.80260	-1.53711	-0.00104
S	2.09625	0.00001	-0.07774

E = -1235.13856096

Sum of electronic and zero-point Energies= -1235.099853

Sum of electronic and thermal Energies= -1235.094248

Sum of electronic and thermal Enthalpies= -1235.093304

Sum of electronic and thermal Free Energies= -1235.129955

EI

H	0.72603	0.95960	-0.02531
C	-1.32249	0.76967	0.00853
H	0.30067	-0.90794	-0.03454
H	2.03950	-0.24556	1.26232
H	-2.31226	1.23393	0.02237
S	-1.28498	-0.93532	0.00024
O	-0.33893	1.55573	-0.00082
S	1.90325	-0.19618	-0.07959

E = -912.178639963

Sum of electronic and zero-point Energies= -912.136375

Sum of electronic and thermal Energies= -912.131215

Sum of electronic and thermal Enthalpies= -912.130271

Sum of electronic and thermal Free Energies= -912.165411

EJ

O	-0.47458	1.12005	-0.01820
H	0.62848	0.92645	-0.02141
C	-1.08487	0.00002	-0.01426
O	-0.47461	-1.12005	-0.01820
H	0.62844	-0.92649	-0.02142
H	2.34557	-0.00000	1.26815
C	-2.57686	0.00002	0.02070
H	-2.96602	-0.89880	-0.45527
H	-2.89342	-0.00113	1.06852
H	-2.96610	0.89976	-0.45345
S	2.17418	-0.00000	-0.07078

E = -628.568063590

Sum of electronic and zero-point Energies= -628.492829

Sum of electronic and thermal Energies= -628.486364

Sum of electronic and thermal Enthalpies= -628.485420

Sum of electronic and thermal Free Energies= -628.524001

EL

O	1.08865	-1.17298	0.00386
H	0.06688	-1.06165	-0.00903
C	1.64376	0.00323	0.00483
H	-0.28055	0.89702	-0.01499
H	-1.90754	0.00471	1.25338
H	2.73317	-0.01734	0.00732
N	0.96525	1.09952	0.00407

S	-1.71379	-0.00788	-0.08257
H	1.48013	1.97122	-0.00385

E = -569.350511694

Sum of electronic and zero-point Energies=	-569.289614
Sum of electronic and thermal Energies=	-569.284335
Sum of electronic and thermal Enthalpies=	-569.283391
Sum of electronic and thermal Free Energies=	-569.318107

EM

H	1.04622	-1.45132	-0.00945
C	-1.53282	0.68097	0.00445
C	-0.19686	0.15304	-0.00107
C	-0.98232	-2.05445	-0.00252
C	-2.29311	-1.60515	0.00416
C	-2.58172	-0.23055	0.00727
C	-1.34880	2.09859	0.00319
C	0.01460	2.30636	-0.00380
H	-0.71435	-3.10159	-0.00668
H	-3.09152	-2.33484	0.00538
H	-3.61384	0.10225	0.01097
H	-2.11532	2.85731	0.00550
H	0.54832	3.24521	-0.00847
N	0.72449	1.11912	-0.00551
H	1.94496	0.65864	-0.02267
N	0.04257	-1.17600	-0.00458
H	3.40320	-0.42484	1.25274
S	3.17182	-0.45284	-0.07668

E = -779.367706671

Sum of electronic and zero-point Energies= -779.235003
Sum of electronic and thermal Energies= -779.226412
Sum of electronic and thermal Enthalpies= -779.225468
Sum of electronic and thermal Free Energies= -779.269165

FF

O	-1.20874	1.12673	0.00000
H	0.00064	1.11487	-0.00000
C	-1.77600	0.00036	0.00000
O	-1.20976	-1.12636	-0.00000
O	1.20867	-1.12672	0.00000
H	-0.00039	-1.11483	-0.00000
C	1.77599	-0.00038	0.00000
O	1.20980	1.12637	-0.00000
H	2.87109	-0.00101	0.00000
H	-2.87111	0.00094	0.00000

E = -379.667895801

Sum of electronic and zero-point Energies= -379.604142
Sum of electronic and thermal Energies= -379.598407
Sum of electronic and thermal Enthalpies= -379.597463
Sum of electronic and thermal Free Energies= -379.634054

FG

H	-0.14239	-1.07938	0.00091
H	-0.60824	1.19993	-0.00019
C	1.57077	0.78123	0.00065
H	2.57953	1.20998	0.00134
O	-1.35163	-1.25376	0.00220

O	0.61964	1.59489	0.00113
S	1.50362	-0.92120	-0.00099
O	-1.72080	0.97620	-0.00152
C	-2.08681	-0.23537	-0.00044
H	-3.16827	-0.40504	-0.00191

E = -702.609159857

Sum of electronic and zero-point Energies=	-702.549740
Sum of electronic and thermal Energies=	-702.543446
Sum of electronic and thermal Enthalpies=	-702.542501
Sum of electronic and thermal Free Energies=	-702.581086

FH

O	1.79027	1.13288	0.00001
H	0.63958	1.19436	-0.00000
C	2.34380	0.00000	-0.00002
O	1.79027	-1.13288	0.00003
H	0.63958	-1.19436	0.00001
C	-1.75346	-0.00000	0.00000
H	-2.84283	0.00000	0.00001
S	-1.06440	1.53539	0.00000
S	-1.06440	-1.53539	-0.00001
H	3.43804	0.00000	-0.00010

E = -1025.55951933

Sum of electronic and zero-point Energies=	-1025.503518
Sum of electronic and thermal Energies=	-1025.496699
Sum of electronic and thermal Enthalpies=	-1025.495755
Sum of electronic and thermal Free Energies=	-1025.536355

FI

H	-0.14213	-1.07925	0.00013
H	-0.60815	1.19986	0.00004
C	1.57085	0.78101	0.00011
H	2.57972	1.20954	0.00017
O	-1.35234	-1.25378	0.00040
O	0.61989	1.59473	0.00025
S	1.50350	-0.92133	-0.00018
O	-1.72015	0.97642	-0.00034
C	-2.08689	-0.23501	-0.00005
H	-3.16839	-0.40391	-0.00022

E = -702.609159663

Sum of electronic and zero-point Energies= -702.549736

Sum of electronic and thermal Energies= -702.543440

Sum of electronic and thermal Enthalpies= -702.542496

Sum of electronic and thermal Free Energies= -702.581088

FJ

O	0.70655	-1.12290	0.01687
H	-0.46752	-1.10389	0.00581
C	1.29934	-0.00003	0.01600
O	0.70652	1.12277	0.01621
O	-1.71229	1.12514	-0.00458
H	-0.46782	1.10385	0.00576
O	-1.71220	-1.12509	-0.00525
C	2.79909	0.00007	-0.01443
H	3.18905	-0.89925	0.45974
H	3.11931	0.00144	-1.06095

H	3.18879	0.89840	0.46185
C	-2.28065	-0.00002	-0.00862
H	-3.37714	-0.00002	-0.01602

E = -419.005959598

Sum of electronic and zero-point Energies=	-418.914826
Sum of electronic and thermal Energies=	-418.907313
Sum of electronic and thermal Enthalpies=	-418.906369
Sum of electronic and thermal Free Energies=	-418.947986

FL

H	-0.25954	-1.14836	0.00007
H	0.11458	1.13563	0.00004
C	-1.82760	0.02374	-0.00022
H	-2.91876	0.03995	-0.00050
N	-1.14393	1.12209	-0.00037
H	-1.69099	1.97348	-0.00080
O	-1.31537	-1.15874	0.00027
O	1.34985	1.11087	0.00033
O	1.18989	-1.13587	-0.00011
C	1.83350	-0.06704	0.00016
H	2.93181	-0.12564	0.00024

E = -359.787075848

Sum of electronic and zero-point Energies=	-359.709835
Sum of electronic and thermal Energies=	-359.703704
Sum of electronic and thermal Enthalpies=	-359.702760
Sum of electronic and thermal Free Energies=	-359.740129

FM

H	-0.90382	-1.38875	0.00026
C	1.77463	0.64753	-0.00000
C	0.41596	0.17830	0.00009
C	1.10859	-2.05506	-0.00013
C	2.43988	-1.66600	-0.00024
C	2.78574	-0.30680	-0.00017
C	1.65839	2.07086	0.00013
C	0.30621	2.33915	0.00028
H	0.79626	-3.09011	-0.00015
H	3.20544	-2.43015	-0.00038
H	3.83043	-0.01551	-0.00023
H	2.45863	2.79365	0.00013
H	-0.18244	3.30253	0.00040
N	-0.46098	1.18958	0.00029
H	-1.75043	1.01163	-0.00026
N	0.12062	-1.13792	0.00004
O	-2.93017	0.81656	-0.00094
O	-2.55475	-1.41122	0.00075
C	-3.29094	-0.41271	-0.00006
H	-4.38302	-0.55932	-0.00005

E = -569.804094869

Sum of electronic and zero-point Energies= -569.655033

Sum of electronic and thermal Energies= -569.645515

Sum of electronic and thermal Enthalpies= -569.644571

Sum of electronic and thermal Free Energies= -569.690685

FN

C	1.76998	1.10886	0.00009
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C	2.61774	-0.00006	-0.00008
C	1.76983	-1.10887	-0.00019
N	0.50633	-0.67060	-0.00009
H	-0.53506	-1.08115	-0.00011
H	1.99151	2.16378	0.00021
H	3.69466	-0.00012	-0.00011
H	1.99127	-2.16382	-0.00033
N	0.50644	0.67067	0.00007
O	-1.98231	-1.12900	-0.00008
O	-1.98250	1.12901	0.00020
H	-0.53468	1.08150	0.00016
C	-2.54605	-0.00002	0.00006
H	-3.64768	-0.00017	0.00007

E = -416.107568483

Sum of electronic and zero-point Energies=	-416.005045
Sum of electronic and thermal Energies=	-415.998292
Sum of electronic and thermal Enthalpies=	-415.997348
Sum of electronic and thermal Free Energies=	-416.036825

GG

H	-0.35899	-1.16616	-0.00000
C	1.83355	-0.90122	-0.00000
H	0.35744	1.16618	-0.00000
C	-1.83324	0.90121	-0.00000
H	-2.80921	1.39993	0.00000
H	2.80978	-1.39952	-0.00000
O	0.83152	-1.65004	-0.00001
O	-0.83092	1.64977	-0.00001
S	-1.90678	-0.79979	0.00000

S	1.90643	0.79990	0.00000
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E = -1025.54853839

Sum of electronic and zero-point Energies= -1025.494597

Sum of electronic and thermal Energies= -1025.487673

Sum of electronic and thermal Enthalpies= -1025.486728

Sum of electronic and thermal Free Energies= -1025.527712

GH

H	0.08337	-1.34385	-0.18699
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C	-2.02939	0.17829	0.07530
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H	0.44558	1.10366	0.03010
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O	1.24511	-1.55136	-0.50670
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H	-3.10329	0.30102	0.21087
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S	-1.50199	-1.41273	0.25092
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S	-1.19979	1.59339	-0.27620
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C	2.14693	-0.73174	-0.20462
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H	3.17498	-1.09434	-0.30880
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S	1.99761	0.86716	0.34306
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E = -1348.50332527

Sum of electronic and zero-point Energies= -1348.452341

Sum of electronic and thermal Energies= -1348.444963

Sum of electronic and thermal Enthalpies= -1348.444019

Sum of electronic and thermal Free Energies= -1348.486167

GI

H	-0.00003	-1.01048	0.00001
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H	-0.00006	1.43448	-0.00002
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C	-1.99751	0.59220	-0.00001
H	-3.05907	0.86063	-0.00002
O	-1.19657	1.56109	-0.00001
S	-1.67109	-1.06969	0.00001
C	1.99749	0.59224	0.00001
H	3.05904	0.86072	0.00002
S	1.67114	-1.06966	-0.00001
O	1.19651	1.56110	0.00001

E = -1025.55429298

Sum of electronic and zero-point Energies= -1025.499294

Sum of electronic and thermal Energies= -1025.492415

Sum of electronic and thermal Enthalpies= -1025.491471

Sum of electronic and thermal Free Energies= -1025.532969

GJ

O	-1.17847	1.13257	0.01477
H	-0.09054	1.25137	0.00713
C	-1.65239	-0.05337	0.01547
O	-0.95975	-1.10918	0.02015
H	0.23102	-1.01944	0.00962
O	1.22624	1.56552	-0.00205
C	-3.14520	-0.18038	-0.01653
H	-3.47500	-0.06811	-1.05394
H	-3.45208	-1.16016	0.34368
H	-3.60384	0.61673	0.56790
C	2.11517	0.68910	-0.00683
H	3.15575	1.03738	-0.01324
S	1.91407	-1.00633	-0.00480

E = -741.947846101

Sum of electronic and zero-point Energies= -741.860552
Sum of electronic and thermal Energies= -741.852436
Sum of electronic and thermal Enthalpies= -741.851492
Sum of electronic and thermal Free Energies= -741.895286

GL

H	-0.90293	1.17889	-0.00018
H	0.07665	-1.07465	0.00015
C	-2.18495	-0.27793	-0.00000
H	-3.25866	-0.47369	-0.00000
N	-1.31635	-1.22599	0.00018
H	-1.71664	-2.15782	0.00037
O	-1.90279	0.99135	-0.00020
O	0.61125	1.57654	0.00016
C	1.60343	0.84552	0.00009
H	2.60142	1.30934	0.00020
S	1.63975	-0.88430	-0.00012

E = -682.728181319

Sum of electronic and zero-point Energies= -682.654826
Sum of electronic and thermal Energies= -682.647998
Sum of electronic and thermal Enthalpies= -682.647054
Sum of electronic and thermal Free Energies= -682.686869

GN

C	2.27936	1.02325	0.00022
C	2.98305	-0.17509	0.00025
C	2.00040	-1.17419	-0.00005

N	0.79233	-0.60645	-0.00023
H	-0.45643	-0.94027	-0.00061
H	2.61842	2.04646	0.00039
H	4.05236	-0.30389	0.00047
H	2.10100	-2.24796	-0.00010
N	0.97053	0.72261	-0.00012
O	-1.57226	1.59226	0.00019
H	0.09473	1.29413	-0.00001
C	-2.40385	0.68032	0.00038
H	-3.47400	0.93995	0.00103
S	-2.11574	-1.02909	-0.00032

E = -739.055259910

Sum of electronic and zero-point Energies=	-738.957012
Sum of electronic and thermal Energies=	-738.949369
Sum of electronic and thermal Enthalpies=	-738.948425
Sum of electronic and thermal Free Energies=	-738.990637

HH

H	0.00007	1.25224	0.00003
C	2.23239	-0.00007	-0.00014
H	-0.00007	-1.25225	0.00002
C	-2.23239	0.00006	-0.00013
H	-3.32150	0.00013	-0.00034
H	3.32151	-0.00015	-0.00036
S	-1.52918	1.38592	0.64152
S	1.52918	-1.38592	0.64152
S	1.52920	1.38595	-0.64145
S	-1.52920	-1.38596	-0.64145

E = -1671.45864416

Sum of electronic and zero-point Energies= -1671.411299

Sum of electronic and thermal Energies= -1671.403399

Sum of electronic and thermal Enthalpies= -1671.402455

Sum of electronic and thermal Free Energies= -1671.445939

HI

H 0.44571 -1.10372 -0.02975

H 0.08401 1.34383 0.18747

C 2.14699 0.73148 0.20471

H 3.17504 1.09404 0.30894

O 1.24526 1.55115 0.50701

S 1.99753 -0.86723 -0.34331

C -2.02946 -0.17815 -0.07564

H -3.10329 -0.30084 -0.21176

S -1.50178 1.41280 -0.25099

S -1.20005 -1.59324 0.27646

E = -1348.50332526

Sum of electronic and zero-point Energies= -1348.452338

Sum of electronic and thermal Energies= -1348.444961

Sum of electronic and thermal Enthalpies= -1348.444017

Sum of electronic and thermal Free Energies= -1348.486164

HJ

O 1.34632 -1.12854 0.01991

H 0.23158 -1.16999 0.01118

C 1.92946 0.00001 0.01698

O 1.34631 1.12856 0.02048

H	0.23159	1.17000	0.01144
C	3.42587	0.00002	-0.01990
H	3.81696	-0.89927	0.45300
H	3.73824	0.00008	-1.06897
H	3.81697	0.89924	0.45314
C	-2.22282	-0.00002	-0.00754
H	-3.31247	-0.00004	-0.01430
S	-1.52682	-1.53243	-0.00320
S	-1.52687	1.53242	-0.00342

E = -1064.89887649

Sum of electronic and zero-point Energies= -1064.814430

Sum of electronic and thermal Energies= -1064.805892

Sum of electronic and thermal Enthalpies= -1064.804948

Sum of electronic and thermal Free Energies= -1064.850660

HL

H	1.01057	1.17930	-0.00051
H	0.32901	-1.24403	-0.00016
C	2.45426	-0.11909	0.00017
H	3.54355	-0.18451	0.00065
N	1.70756	-1.16496	-0.00001
H	2.22081	-2.03997	0.00041
O	2.02518	1.10884	-0.00021
C	-1.81704	0.11590	0.00016
H	-2.90582	0.16464	0.00045
S	-1.24208	-1.48765	-0.00010
S	-1.01891	1.57688	0.00003

E = -1005.68157839

Sum of electronic and zero-point Energies= -1005.610900
Sum of electronic and thermal Energies= -1005.603590
Sum of electronic and thermal Enthalpies= -1005.602646
Sum of electronic and thermal Free Energies= -1005.644463

II

H	0.35845	-1.16592	0.00005
C	1.83332	0.90134	0.00007
O	0.83094	1.64985	0.00018
H	-0.35837	1.16594	0.00004
C	-1.83332	-0.90134	0.00003
O	-0.83095	-1.64984	0.00023
H	-2.80925	-1.40014	-0.00004
H	2.80925	1.40015	0.00010
S	1.90665	-0.79976	-0.00014
S	-1.90665	0.79975	-0.00012

E = -1025.54853851

Sum of electronic and zero-point Energies= -1025.494595
Sum of electronic and thermal Energies= -1025.487672
Sum of electronic and thermal Enthalpies= -1025.486728
Sum of electronic and thermal Free Energies= -1025.527710

IJ

O	-1.17847	1.13257	0.01477
H	-0.09054	1.25137	0.00714
C	-1.65239	-0.05337	0.01547
O	-0.95975	-1.10918	0.02015
H	0.23102	-1.01944	0.00962

O	1.22624	1.56552	-0.00205
C	-3.14520	-0.18038	-0.01653
H	-3.47500	-0.06811	-1.05394
H	-3.45208	-1.16016	0.34368
H	-3.60384	0.61673	0.56790
C	2.11517	0.68910	-0.00683
H	3.15575	1.03738	-0.01324
S	1.91407	-1.00633	-0.00480

E = -741.947846101

Sum of electronic and zero-point Energies=	-741.860552
Sum of electronic and thermal Energies=	-741.852436
Sum of electronic and thermal Enthalpies=	-741.851492
Sum of electronic and thermal Free Energies=	-741.895286

II

H	-0.50308	-1.15991	0.00003
H	-0.39312	1.25216	0.00005
C	-2.16880	-0.15466	-0.00001
H	-3.25335	-0.26800	-0.00004
N	-1.61993	1.01300	0.00001
H	-2.26954	1.78990	-0.00001
O	-1.53075	-1.27883	-0.00001
O	0.79543	1.60075	0.00003
C	1.68581	0.69907	-0.00004
H	2.71682	1.07066	-0.00013
S	1.48889	-0.97611	0.00001

E = -682.733384816

Sum of electronic and zero-point Energies=	-682.658917
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Sum of electronic and thermal Energies= -682.652250
Sum of electronic and thermal Enthalpies= -682.651306
Sum of electronic and thermal Free Energies= -682.690672

IN

C	2.27936	1.02325	0.00022
C	2.98305	-0.17509	0.00025
C	2.00040	-1.17419	-0.00005
N	0.79233	-0.60645	-0.00023
H	-0.45643	-0.94027	-0.00061
H	2.61842	2.04646	0.00039
H	4.05236	-0.30389	0.00047
H	2.10100	-2.24796	-0.00010
N	0.97053	0.72261	-0.00012
O	-1.57226	1.59226	0.00019
H	0.09473	1.29413	-0.00001
C	-2.40385	0.68032	0.00038
H	-3.47400	0.93995	0.00103
S	-2.11574	-1.02909	-0.00032

E = -739.055259910

Sum of electronic and zero-point Energies= -738.957012
Sum of electronic and thermal Energies= -738.949369
Sum of electronic and thermal Enthalpies= -738.948425
Sum of electronic and thermal Free Energies= -738.990637

JJ

O	1.20695	1.12123	0.01636
H	-0.00000	1.09458	-0.00000

C	1.80078	-0.00001	0.01793
O	1.20694	-1.12125	0.01635
C	3.30290	-0.00002	-0.00771
H	3.62722	0.00101	-1.05293
H	3.69183	0.89818	0.46974
H	3.69190	-0.89905	0.46811
O	-1.20695	-1.12121	-0.01635
H	0.00001	-1.09457	0.00000
C	-1.80079	0.00002	-0.01793
O	-1.20695	1.12126	-0.01636
C	-3.30290	-0.00001	0.00771
H	-3.69189	0.89905	-0.46807
H	-3.69185	-0.89819	-0.46978
H	-3.62721	-0.00108	1.05293

E = -458.343270711

Sum of electronic and zero-point Energies=	-458.224919
Sum of electronic and thermal Energies=	-458.215617
Sum of electronic and thermal Enthalpies=	-458.214673
Sum of electronic and thermal Free Energies=	-458.261328

JK

H	-0.52722	-1.13152	0.00001
C	-2.40278	-0.06037	-0.00000
O	0.80539	1.14128	-0.00011
H	-0.79900	1.23448	0.00005
O	0.82265	-1.10490	0.00009
H	-3.49049	-0.12087	-0.00004
N	-1.69541	-1.15699	-0.00004
N	-1.85912	1.14267	0.00008

H	-2.20207	-2.02951	-0.00021
H	-2.45448	1.95383	0.00015
C	1.39812	0.03604	-0.00005
C	2.91599	0.01368	0.00001
H	3.31919	1.02520	-0.00046
H	3.27169	-0.52870	0.87960
H	3.27173	-0.52970	-0.87892

E = -379.246766288

Sum of electronic and zero-point Energies=	-379.128817
Sum of electronic and thermal Energies=	-379.120507
Sum of electronic and thermal Enthalpies=	-379.119563
Sum of electronic and thermal Free Energies=	-379.163708

JL

H	-0.69650	-1.12739	0.00329
H	-0.43594	1.14539	0.00360
C	-2.33104	-0.02365	-0.00574
H	-3.42282	-0.04359	-0.01037
N	-1.68766	1.10100	-0.00411
H	-2.26307	1.93312	-0.00661
O	-1.77303	-1.18125	-0.00248
O	0.80332	1.15227	0.01189
O	0.69864	-1.08903	0.01115
C	1.34020	-0.00795	0.01139
C	2.84854	-0.05416	-0.01039
H	3.25647	0.67751	0.68845
H	3.20545	-1.05489	0.22591
H	3.19239	0.22144	-1.01156

E = -399.122825585

Sum of electronic and zero-point Energies= -399.018639

Sum of electronic and thermal Energies= -399.010764

Sum of electronic and thermal Enthalpies= -399.009820

Sum of electronic and thermal Free Energies= -399.052592

JM

H	-0.59752	-1.27113	-0.00006
C	2.24000	0.55102	0.00002
C	0.85286	0.18046	-0.00003
C	1.37315	-2.09378	-0.00003
C	2.73098	-1.80520	0.00003
C	3.17786	-0.47636	0.00005
C	2.22732	1.97954	0.00003
C	0.89852	2.34669	-0.00002
H	0.98554	-3.10319	-0.00005
H	3.43735	-2.62446	0.00005
H	4.24141	-0.26398	0.00009
H	3.07785	2.64242	0.00006
H	0.48027	3.34249	-0.00003
N	0.05255	1.25474	-0.00006
H	-1.20749	1.16036	-0.00003
N	0.45635	-1.10715	-0.00006
O	-2.42937	1.03055	-0.00000
O	-2.19013	-1.20625	-0.00001
C	-2.88853	-0.16883	0.00001
C	-4.39812	-0.28473	0.00005
H	-4.80184	0.22328	-0.87908
H	-4.70442	-1.32925	-0.00010
H	-4.80176	0.22300	0.87938

E = -609.138855629

Sum of electronic and zero-point Energies= -608.962697
Sum of electronic and thermal Energies= -608.951362
Sum of electronic and thermal Enthalpies= -608.950417
Sum of electronic and thermal Free Energies= -609.002167

JN

C	2.26803	1.10861	0.00418
C	3.11667	-0.00000	0.00861
C	2.26803	-1.10861	0.00418
N	1.00413	-0.67090	-0.00246
H	-0.05682	-1.07256	-0.00734
H	2.49031	2.16346	0.00530
H	4.19367	0.00000	0.01413
H	2.49031	-2.16347	0.00529
N	1.00412	0.67090	-0.00246
O	-1.46733	-1.12437	-0.01451
O	-1.46734	1.12439	-0.01452
H	-0.05683	1.07256	-0.00733
C	-2.05563	0.00001	-0.01474
C	-3.56812	-0.00001	0.01650
H	-3.96189	-0.89779	-0.45922
H	-3.89123	-0.00026	1.06218
H	-3.96191	0.89796	-0.45883

E = -455.442078550

Sum of electronic and zero-point Energies= -455.312895
Sum of electronic and thermal Energies= -455.304317
Sum of electronic and thermal Enthalpies= -455.303373

Sum of electronic and thermal Free Energies= -455.348075

KK

H	0.00007	-1.22609	0.00007
C	-1.91384	-0.00000	-0.00007
H	0.00003	1.22606	0.00010
C	1.91385	-0.00000	-0.00008
H	3.00975	0.00002	-0.00037
H	-3.00975	-0.00002	-0.00028
N	-1.28841	1.15911	0.00012
N	-1.28840	-1.15913	-0.00003
N	1.28841	-1.15911	0.00015
N	1.28839	1.15913	0.00001
H	-1.89587	-1.96624	-0.00016
H	1.89582	1.96627	-0.00027
H	-1.89590	1.96621	0.00001
H	1.89588	-1.96623	-0.00004

E = -300.119895476

Sum of electronic and zero-point Energies= -300.010861

Sum of electronic and thermal Energies= -300.003781

Sum of electronic and thermal Enthalpies= -300.002837

Sum of electronic and thermal Free Energies= -300.042316

KL

H	-0.02013	-1.13688	-0.00001
H	-0.29097	1.27055	0.00001
C	1.92058	-0.04364	-0.00002
H	3.02068	-0.11758	-0.00020

N	1.35096	1.13048	-0.00011
H	2.04239	1.87360	-0.00040
O	1.30440	-1.16331	0.00025
C	-1.90932	-0.04139	0.00000
H	-2.99797	-0.10358	0.00008
N	-1.36886	1.16327	0.00011
N	-1.20477	-1.14054	-0.00021
H	-1.97680	1.96557	0.00042
H	-1.72135	-2.00745	-0.00027

E = -320.016066085

Sum of electronic and zero-point Energies=	-319.914406
Sum of electronic and thermal Energies=	-319.907575
Sum of electronic and thermal Enthalpies=	-319.906631
Sum of electronic and thermal Free Energies=	-319.945532

KM

H	1.35937	-1.23895	-0.00023
C	-1.88144	0.52942	0.00024
C	-0.47233	0.21295	-0.00008
C	-0.89901	-2.05158	0.00005
C	-2.27856	-1.83605	0.00036
C	-2.78308	-0.53312	0.00046
C	-1.93094	1.95223	0.00025
C	-0.60859	2.36626	-0.00006
H	-0.49307	-3.05819	-0.00004
H	-2.94519	-2.68951	0.00053
H	-3.85504	-0.36232	0.00072
H	-2.80733	2.58236	0.00043
H	-0.24820	3.38714	-0.00015

N	0.29113	1.32752	-0.00027
H	1.90698	1.19947	-0.00056
N	-0.00438	-1.05218	-0.00018
C	3.37822	-0.30511	-0.00007
H	4.45586	-0.47455	0.00036
N	2.96766	0.94835	-0.00054
N	2.57288	-1.33671	-0.00017
H	3.66475	1.67534	0.00015
H	3.02518	-2.23961	0.00005

E = -530.023580907

Sum of electronic and zero-point Energies=	-529.851323
Sum of electronic and thermal Energies=	-529.841299
Sum of electronic and thermal Enthalpies=	-529.840355
Sum of electronic and thermal Free Energies=	-529.887499

KN

C	-1.85097	1.10014	0.00031
C	-2.71176	-0.00105	0.00089
C	-1.84905	-1.10067	-0.00006
N	-0.57411	-0.67867	-0.00122
H	0.88150	-1.15403	-0.00040
H	-2.08613	2.15501	0.00073
H	-3.79028	-0.00202	0.00181
H	-2.08223	-2.15599	-0.00011
N	-0.57525	0.68066	-0.00087
H	0.88317	1.15532	-0.00068
C	2.63497	-0.00029	0.00054
H	3.72361	-0.00035	0.00133
N	2.00483	1.15266	-0.00022

N	2.00423	-1.15274	0.00034
H	2.55696	1.99581	0.00026
H	2.55638	-1.99592	0.00080

E = -376.331142619

Sum of electronic and zero-point Energies=	-376.204369
Sum of electronic and thermal Energies=	-376.197104
Sum of electronic and thermal Enthalpies=	-376.196160
Sum of electronic and thermal Free Energies=	-376.236774

LL

H	-0.20711	-1.15807	0.00006
C	1.85561	-0.01108	0.00023
H	0.20689	1.15797	-0.00002
C	-1.85559	0.01114	0.00002
H	-2.95052	0.03099	-0.00003
H	2.95055	-0.03081	0.00112
N	1.17324	-1.11408	-0.00089
N	-1.17309	1.11405	-0.00049
H	1.74784	-1.94822	-0.00059
H	-1.74757	1.94827	-0.00084
O	-1.34158	-1.16746	0.00066
O	1.34142	1.16743	0.00039

E = -339.898045600

Sum of electronic and zero-point Energies=	-339.809692
Sum of electronic and thermal Energies=	-339.803451
Sum of electronic and thermal Enthalpies=	-339.802507
Sum of electronic and thermal Free Energies=	-339.840080

LM

H	-0.97473	-1.35778	0.00017
C	1.79856	0.62022	-0.00010
C	0.43131	0.17723	-0.00009
C	1.06860	-2.06119	-0.00012
C	2.41180	-1.70579	-0.00015
C	2.78957	-0.35651	-0.00014
C	1.71255	2.04534	-0.00004
C	0.36539	2.34233	-0.00000
H	0.73772	-3.09135	-0.00012
H	3.15902	-2.48822	-0.00018
H	3.84064	-0.08870	-0.00014
H	2.52747	2.75170	-0.00003
H	-0.10249	3.31606	0.00004
N	-0.42394	1.21044	-0.00004
H	-1.70261	1.05853	0.00001
N	0.09957	-1.12803	-0.00011
O	-2.89555	0.89513	-0.00001
C	-3.32097	-0.31557	0.00016
H	-4.41601	-0.40776	-0.00000
N	-2.57592	-1.38319	0.00053
H	-3.14345	-2.22452	0.00051

E = -549.909521681

Sum of electronic and zero-point Energies=	-549.749292
Sum of electronic and thermal Energies=	-549.739650
Sum of electronic and thermal Enthalpies=	-549.738706
Sum of electronic and thermal Free Energies=	-549.784981

LN

C	1.81524	1.10660	0.00013
C	2.63389	-0.02366	0.00058
C	1.74982	-1.10561	-0.00005
N	0.49602	-0.63841	-0.00091
H	-0.64872	-1.04249	-0.00058
H	2.06942	2.15472	0.00034
H	3.71080	-0.05443	0.00125
H	1.94490	-2.16634	-0.00000
N	0.53744	0.70549	-0.00082
O	-1.92756	-1.18072	0.00004
H	-0.55411	1.14012	-0.00042
C	-2.55497	-0.06909	0.00055
H	-3.65034	-0.14178	0.00123
N	-1.98572	1.10895	0.00028
H	-2.64950	1.87435	0.00075

E = -396.214878572

Sum of electronic and zero-point Energies=	-396.102554
Sum of electronic and thermal Energies=	-396.095533
Sum of electronic and thermal Enthalpies=	-396.094589
Sum of electronic and thermal Free Energies=	-396.134456

MM

C	3.29063	-0.59237	0.00003
C	1.89408	-0.24149	-0.00002
C	2.37916	2.01674	-0.00004
C	3.74998	1.76271	-0.00001
C	4.21895	0.44648	0.00003
C	3.30877	-2.01789	0.00007

C	1.98314	-2.40640	0.00005
H	1.99251	3.02949	-0.00006
H	4.43942	2.59729	-0.00002
H	5.28550	0.24685	0.00006
H	4.17183	-2.66544	0.00012
H	1.59713	-3.41686	0.00006
N	1.10881	-1.34163	-0.00001
H	-0.33290	-1.26465	-0.00006
N	1.46330	1.03596	-0.00004
C	-3.27994	0.60110	0.00004
C	-1.89110	0.23299	-0.00005
C	-2.40544	-2.02634	-0.00007
C	-3.76959	-1.75018	-0.00000
C	-4.22009	-0.42637	0.00006
C	-3.27992	2.02849	0.00009
C	-1.95337	2.40434	0.00002
H	-2.02385	-3.03975	-0.00012
H	-4.47128	-2.57398	0.00001
H	-5.28367	-0.21314	0.00012
H	-4.13554	2.68524	0.00015
H	-1.54958	3.40682	0.00003
N	-1.09679	1.32275	-0.00006
H	0.21067	1.25102	-0.00006
N	-1.48274	-1.05047	-0.00009

E = -759.918709771

Sum of electronic and zero-point Energies=	-759.689528
Sum of electronic and thermal Energies=	-759.676419
Sum of electronic and thermal Enthalpies=	-759.675475
Sum of electronic and thermal Free Energies=	-759.730243

MN

C	2.45898	0.48433	0.00007
C	1.05636	0.19513	-0.00002
C	1.42153	-2.09340	-0.00007
C	2.79883	-1.89565	0.00006
C	3.33181	-0.60110	0.00011
C	2.53591	1.91208	0.00007
C	1.23383	2.36448	0.00000
H	0.97713	-3.08010	-0.00015
H	3.44993	-2.75981	0.00008
H	4.40677	-0.45711	0.00018
H	3.42626	2.52067	0.00012
H	0.88002	3.38481	0.00001
N	0.32619	1.32518	-0.00003
H	-0.88263	1.22106	-0.00002
N	0.56520	-1.05765	-0.00011
H	-0.56728	-1.12966	-0.00018
C	-3.27034	-1.22477	0.00014
C	-4.20624	-0.18659	0.00025
C	-3.42729	0.97196	0.00001
N	-2.12793	0.63565	-0.00029
H	-3.43147	-2.29305	0.00030
H	-5.28169	-0.26217	0.00054
H	-3.73110	2.00846	0.00008
N	-2.02721	-0.71916	-0.00024

E = -606.224489635

Sum of electronic and zero-point Energies= -606.040825

Sum of electronic and thermal Energies= -606.030371

Sum of electronic and thermal Enthalpies= -606.029427

Sum of electronic and thermal Free Energies= -606.078015

NN

C	-2.52061	1.10851	-0.00018
C	-3.37006	0.00002	-0.00010
C	-2.52061	-1.10848	0.00006
N	-1.25468	-0.67491	0.00009
H	-0.13486	-1.03942	0.00015
H	-2.74742	2.16267	-0.00030
H	-4.44709	0.00001	-0.00013
H	-2.74745	-2.16264	0.00022
N	-1.25460	0.67488	-0.00006
C	2.52942	-1.10315	-0.00018
C	3.38676	0.00010	-0.00027
C	2.52924	1.10320	0.00009
N	1.25562	0.68273	0.00040
H	-0.13461	1.03929	-0.00022
H	2.76404	-2.15733	-0.00033
H	4.46471	0.00019	-0.00054
H	2.76369	2.15741	0.00019
N	1.25569	-0.68290	0.00021

E = -452.520426589

Sum of electronic and zero-point Energies= -452.384237

Sum of electronic and thermal Energies= -452.376208

Sum of electronic and thermal Enthalpies= -452.375264

Sum of electronic and thermal Free Energies= -452.418207