

Supplementary Materials:

Computational Study of the Dissociation Reactions of Secondary Ozonide

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Figure S2: PED for the reaction of SOZ with ammonia (Pathway **B**) at the respective levels of theory. Relative energies are in kJ mol⁻¹.

Figure S3: PED for the reaction of SOZ with ammonia (Pathway **C**) at the respective levels of theory. Relative energies are in kJ mol⁻¹.

Figure S4: PED for the reaction of SOZ with water (Pathway **D**) at the respective levels of theory. Relative energies are in kJ mol⁻¹.

Figure S5: PED for the reaction of SOZ with water (Pathway **E**) at the respective levels of theory. Relative energies are in kJ mol⁻¹.

Table S1: Barrier heights and Gibbs energies of activation (in kJ mol⁻¹) at 298.15K for Pathways **A** and **B**. Relative energies with respect to the complex reactant.

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Table S3. Barrier heights and Gibbs energies of activation (in kJ mol⁻¹) at 298.15K for Pathways **D** and **E**. Relative energies with respect to the complex reactant.

Figure S1: PED for the reaction of SOZ with ammonia (Pathway **A**) at the respective levels of theory. Relative energies are in kJ mol^{-1} .

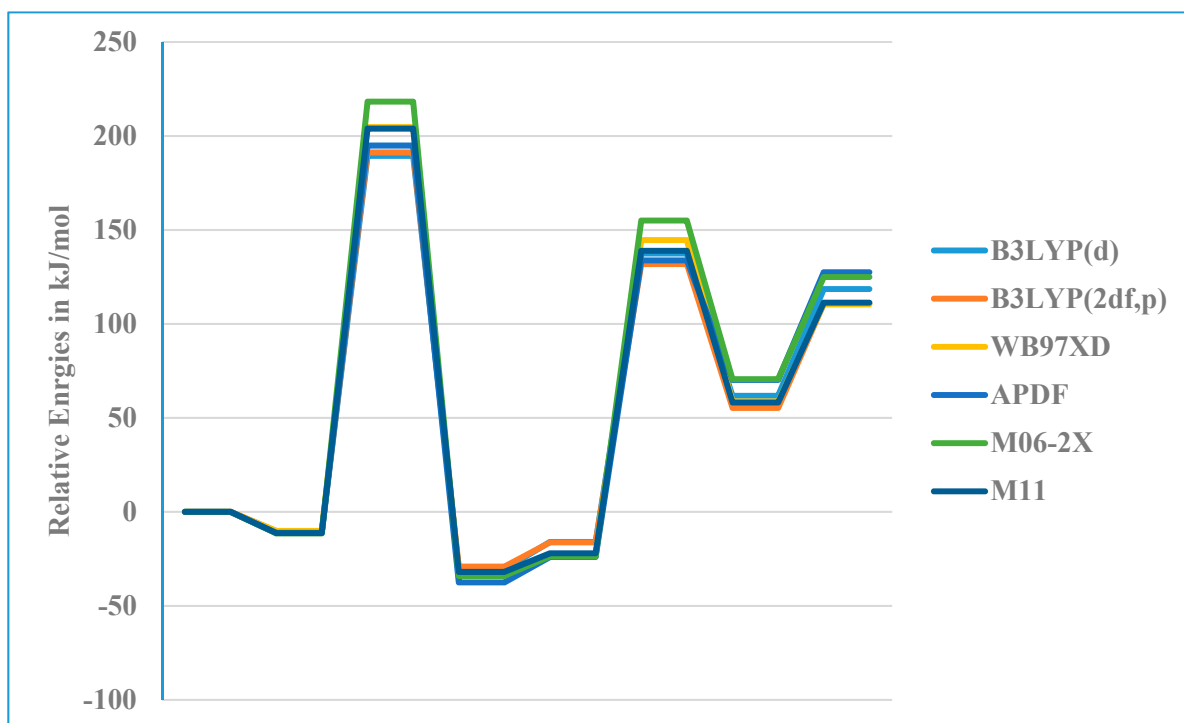


Figure S2: PED for the reaction of SOZ with ammonia (Pathway **B**) at the respective levels of theory. Relative energies are in kJ mol^{-1} .

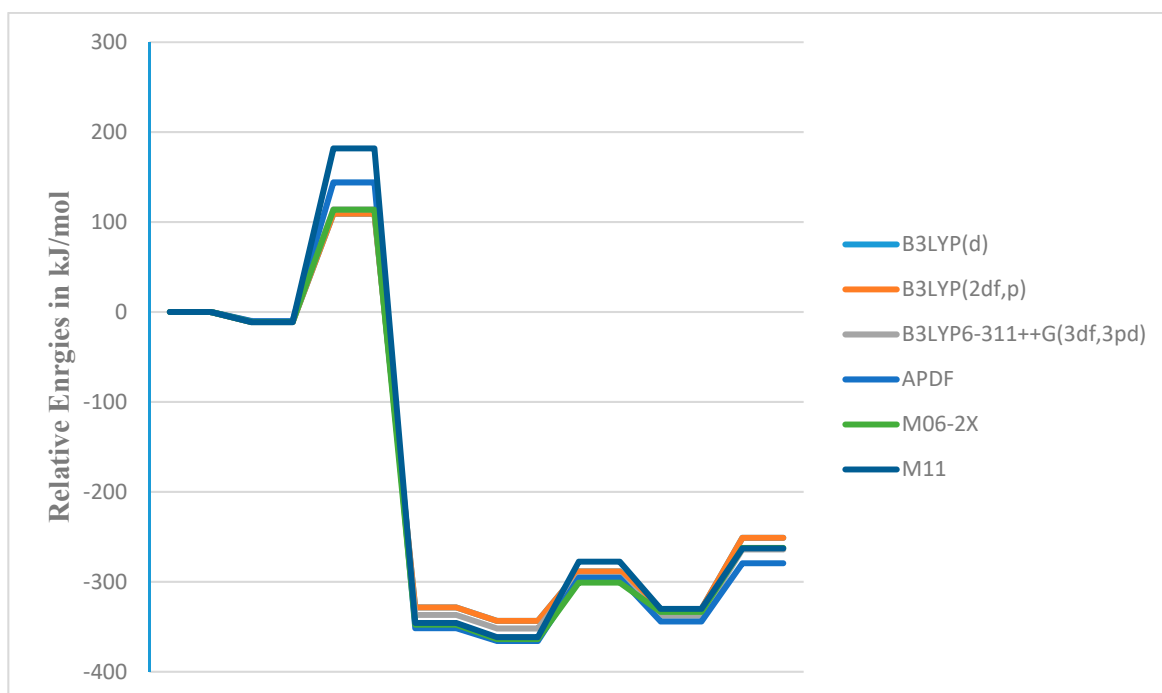


Figure S3: PED for the reaction of SOZ with ammonia (Pathway C) at the respective levels of theory. Relative energies are in kJ mol^{-1} .

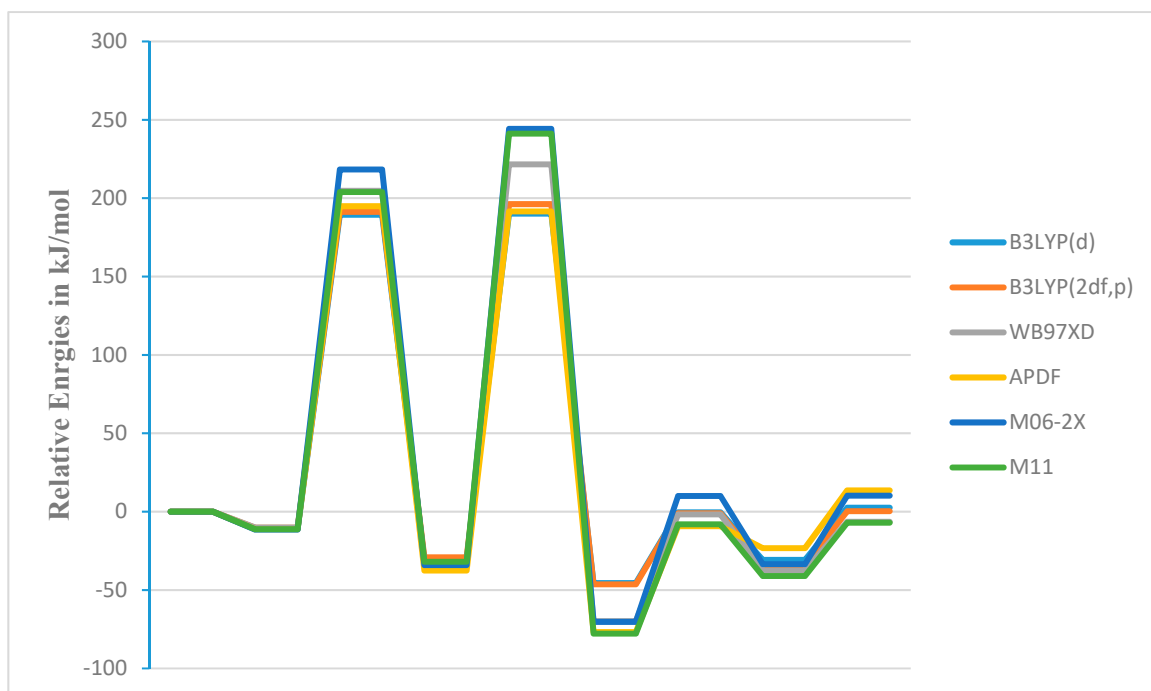


Figure S4: PED for the reaction of SOZ with water (Pathway D) at the respective levels of theory. Relative energies are in kJ mol^{-1} .

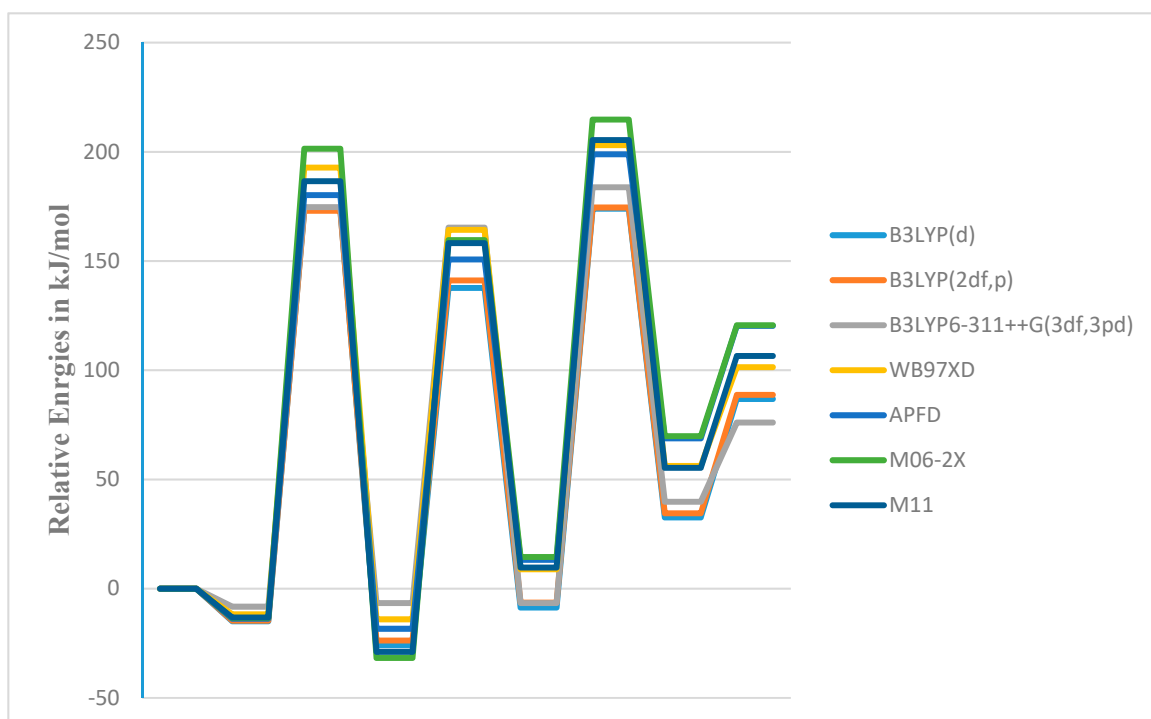


Figure S5: PED for the reaction of SOZ with water (Pathway E) at the respective levels of theory. Relative energies are in kJ mol^{-1} .

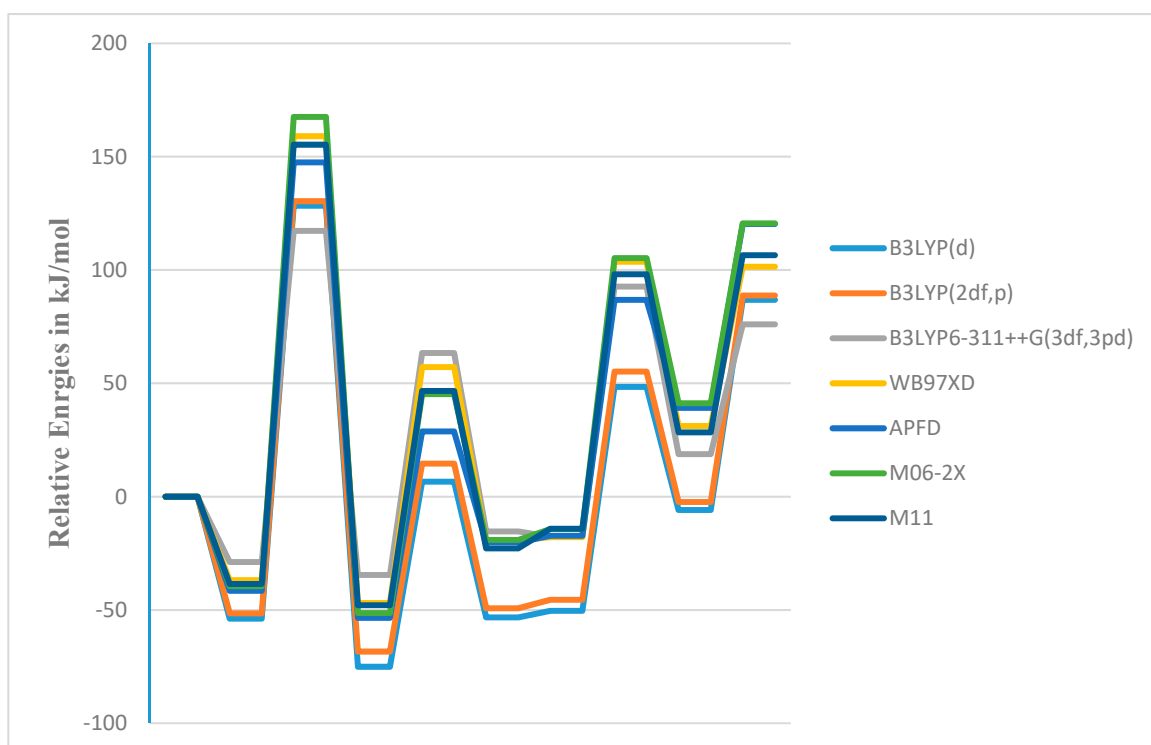


Table S1: Barrier heights and Gibbs energies of activation (in kJ mol^{-1}) at 298.15K for Pathways A and B.

Theory/Basis Set	TS1A		TS2A		TS1B		TS2B	
	E_a	$\Delta G^\ddagger$	E_a	$\Delta G^\ddagger$	E_a	$\Delta G^\ddagger$	E_a	$\Delta G^\ddagger$
B3LYP/6-31G(d)	200	211	153	151	120	129	55	58
B3LYP/6-31G(2df,p)	201	211	148	146	125	133	57	60
B3LYP/6-311++G(3df,3pd)	193	205	140	137	93	125	58	61
B97XD/6-311++G(3df,3pd)	215	223	167	164	154	163	70	73
APDF/6-311++G(3df,3pd)	206	215	158	155	125	134	63	66
M06-2X/6-311++G(3df,3pd)	230	235	179	176	193	199	84	88
M11/6-11++G(3df,3pd)	215	220	161	157	183	188	73	76
G3MP2	214	221	170	166	169	173	84	88
G4MP2	225	234	169	167	128	137	82	85
SMD ^a	158	169	136	129	96	102	26	29

^a Calculations were carried out at the B3LYP/6-311++G(3df,3pd) level of theory.

Table S2: Barrier heights and Gibbs energies of activation (in kJ mol⁻¹) at 298.15 K for Pathway C.

Theory/Basis Set	TS1C		TS2C		TS3C	
	E_a	$\Delta G^\ddagger$	E_a	$\Delta G^\ddagger$	E_a	$\Delta G^\ddagger$
B3LYP/6-31G(d)	200	211	221	223	45	42
B3LYP/6-31G(2df,p)	201	211	225	228	45	42
B3LYP/6-311++G(3df,3pd)	193	205	213	215	48	45
B97XD/6-311++G(3df,3pd)	215	223	255	257	68	63
APDF/6-311++G(3df,3pd)	206	215	229	231	68	61
M06-2X/6-311++G(3df,3pd)	230	235	278	281	80	75
M11/6-11++G(3df,3pd)	215	220	273	276	70	75
G3MP2	214	221	223	225	73	70
G4MP2	225	234	218	220	74	71
SMD ^a	158	169	179	181	77	67

^a Calculations were carried out at the B3LYP/6-311++G(3df,3pd) level of theory.

Table S3. Barrier heights and Gibbs energies of activation (in kJ mol⁻¹) at 298.15K for Pathways D and E.

Theory/Basis Set	TS1D		TS2D		TS3D		TS1E		TS2E		TS3E	
	E_a	$G^\ddagger$	E_a	$\Delta G^\ddagger$	E_a	$\Delta G^\ddagger$	E_a	$\Delta G^\ddagger$	E_a	$\Delta G^\ddagger$	E_a	$\Delta G^\ddagger$
B3LYP/6-31G(d)	189	198	164	166	183	179	182	191	82	89	99	105
B3LYP/6-31G(2df,p)	188	197	165	167	181	178	182	190	83	91	101	106
B3LYP/6-311++G(3df,3pd)	183	194	172	174	190	177	146	144	98	106	110	118
B97XD/6-1++G(3df,3pd)	204	214	178	181	194	192	196	204	104	112	122	130
APDF/6-311++G(3df,3pd)	194	204	169	172	186	183	189	198	82	90	104	110
M06-2X/6-11++G(3df,3pd)	215	223	191	193	200	196	207	214	97	105	120	126
M11/6-++G(3df,3pd)	200	205	187	189	196	191	194	197	95	102	112	120
G3MP2	175	175	179	182	197	194	173	174	113	122	127	138
G4MP2	215	224	177	180	195	182	209	217	110	118	125	131
SMD ^a	147	153	173	174	197	182	75	80	98	106	43	42

^a Calculations were carried out at the B3LYP/6-311++G(3df,3pd) level of theory.

Optimized Structures

Pathway A

RA:

Zero-point correction= 0.104518 (Hartree/Particle)
Thermal correction to Energy= 0.112939
Thermal correction to Enthalpy= 0.113883
Thermal correction to Gibbs Free Energy= 0.070293
Sum of electronic and zero-point Energies= -360.481002
Sum of electronic and thermal Energies= -360.472580
Sum of electronic and thermal Enthalpies= -360.471636
Sum of electronic and thermal Free Energies= -360.515226

0 1

O	-0.20894000	-0.99247900	0.43038600
O	-0.15421000	0.26916900	1.11147300
C	-0.35644900	1.14598400	0.02598300
H	-0.73791500	2.07788800	0.44593900
H	0.56867600	1.28093600	-0.53987900
C	-1.37642500	-0.80726300	-0.33159400
H	-1.32554400	-1.50639800	-1.16784300
H	-2.26843300	-0.96719000	0.28393000
O	-1.33462300	0.52309500	-0.78283800
N	2.73309000	-0.03935100	-0.37698400
H	2.01044300	-0.72799100	-0.20126100
H	3.15376200	0.17228100	0.51933800
H	3.44680800	-0.48467100	-0.93983900

TS1A:

Zero-point correction= 0.102269 (Hartree/Particle)
Thermal correction to Energy= 0.109429
Thermal correction to Enthalpy= 0.110373
Thermal correction to Gibbs Free Energy= 0.071532
Sum of electronic and zero-point Energies= -360.402536
Sum of electronic and thermal Energies= -360.395376
Sum of electronic and thermal Enthalpies= -360.394432
Sum of electronic and thermal Free Energies= -360.433273

0 1

O	-0.95450500	-1.02728700	-0.41439900
O	-0.10118600	-1.24451400	0.69257400
C	0.39266300	1.22130500	0.56775300
H	0.22164200	0.76452700	1.53446800
H	1.23248200	1.86979300	0.37239400

C	-1.55067800	0.14140600	-0.18595100
H	-2.26499000	0.37084500	-0.97369400
H	-1.95041800	0.23321300	0.83025600
O	-0.51856600	1.22676000	-0.31314200
N	2.20251800	-0.21229200	-0.34912300
H	2.31106000	-0.24108200	-1.35448000
H	1.48248100	-0.88880800	-0.05190500
H	3.09226100	-0.43837400	0.07574200

I1aA:

Zero-point correction= 0.108511 (Hartree/Particle)

Thermal correction to Energy= 0.114873

Thermal correction to Enthalpy= 0.115817

Thermal correction to Gibbs Free Energy= 0.078458

Sum of electronic and zero-point Energies= -360.491068

Sum of electronic and thermal Energies= -360.484706

Sum of electronic and thermal Enthalpies= -360.483762

Sum of electronic and thermal Free Energies= -360.521121

0 1

O	1.52813700	0.08533800	-0.40947100
O	1.20203700	1.26068800	0.32707700
C	-1.42460300	-0.36269100	0.33417400
H	-1.23229200	-0.24262300	1.40725000
H	-2.36935900	-0.89726500	0.20113000
C	0.87413800	-0.99708900	0.15523200
H	1.41104800	-1.87150100	-0.21294000
H	0.92205000	-0.92568900	1.24845600
O	-0.45767200	-1.17325700	-0.26158100
N	-1.43896200	0.97083500	-0.26220600
H	-1.72122600	0.91927700	-1.23403000
H	0.27662500	1.42264300	0.01850000
H	-2.09134600	1.57584200	0.22245700

I1bA:

Zero-point correction= 0.107183 (Hartree/Particle)

Thermal correction to Energy= 0.114462

Thermal correction to Enthalpy= 0.115406

Thermal correction to Gibbs Free Energy= 0.075643

Sum of electronic and zero-point Energies= -360.485902

Sum of electronic and thermal Energies= -360.478623

Sum of electronic and thermal Enthalpies= -360.477679

Sum of electronic and thermal Free Energies= -360.517442

0 1			
O	-1.76567900	0.27057500	-0.38613500
O	-1.72424500	-1.09971100	0.02129200
C	1.17872000	-0.43779800	0.16203300
H	0.76168700	-1.25811000	-0.42329400
H	0.97607900	-0.63027400	1.22147700
C	-0.74917400	0.95912000	0.29891500
H	-1.01637900	2.00663900	0.14791000
H	-0.79686800	0.69076400	1.36339900
O	0.51871900	0.78488800	-0.20738100
N	2.57835400	-0.36476000	-0.05477600
H	2.79769900	-0.25182100	-1.03522900
H	-2.57360300	-1.18231900	0.46867500
H	2.99527500	0.40448700	0.45259600

TS2A:

Zero-point correction= 0.097525 (Hartree/Particle)
 Thermal correction to Energy= 0.105546
 Thermal correction to Enthalpy= 0.106490
 Thermal correction to Gibbs Free Energy= 0.064868
 Sum of electronic and zero-point Energies= -360.425791
 Sum of electronic and thermal Energies= -360.417770
 Sum of electronic and thermal Enthalpies= -360.416826
 Sum of electronic and thermal Free Energies= -360.458448

0 1			
O	-0.91276500	-0.55688800	-0.54216500
O	-1.38728400	-1.57672600	0.33176500
C	2.61536400	-0.46248800	0.07658100
H	3.42507500	0.19786400	0.37984500
H	2.84037400	-1.50972600	-0.11042700
C	-1.24598300	1.06980500	0.17747000
H	-2.15840700	1.26220000	-0.40619100
H	-1.44833300	0.65705900	1.17914900
O	-0.24562500	1.81217700	-0.01450300
N	1.44494200	-0.03234000	-0.05778200
H	0.46787500	-0.54545900	-0.33665900
H	-2.17536000	-1.87289100	-0.13312200
H	1.08329700	0.96492800	0.10679100

PA:

Zero-point correction= 0.098784 (Hartree/Particle)

Thermal correction to Energy= 0.109533
 Thermal correction to Enthalpy= 0.110477
 Thermal correction to Gibbs Free Energy= 0.061247
 Sum of electronic and zero-point Energies= -360.450017
 Sum of electronic and thermal Energies= -360.439268
 Sum of electronic and thermal Enthalpies= -360.438324
 Sum of electronic and thermal Free Energies= -360.487554

0 1

O	0.69731100	-1.22616000	0.71417000
O	1.02766200	-1.82968200	-0.53664900
C	-2.78809000	0.07453400	-0.08172400
H	-3.44211500	0.88878400	-0.40399100
H	-3.26288200	-0.88189600	0.13494000
C	1.68124800	1.20627100	-0.10505200
H	2.46555100	1.09402600	0.66378500
H	1.74722500	0.52242100	-0.96643000
O	0.81770000	2.03748700	-0.00919600
N	-1.54092800	0.18659600	0.04857200
H	-0.18370500	-0.81866400	0.50598400
H	0.94513300	-2.76482800	-0.32541900
H	-1.18304700	1.11600200	-0.17482800

Pathway B

RB:

Zero-point correction= 0.104520 (Hartree/Particle)
 Thermal correction to Energy= 0.112940
 Thermal correction to Enthalpy= 0.113884
 Thermal correction to Gibbs Free Energy= 0.070296
 Sum of electronic and zero-point Energies= -360.481000
 Sum of electronic and thermal Energies= -360.472579
 Sum of electronic and thermal Enthalpies= -360.471635
 Sum of electronic and thermal Free Energies= -360.515224

0 1

C	-1.37546800	-0.80782200	-0.33169900
O	-1.33342200	0.52207200	-0.78423600
C	-0.35682300	1.14621200	0.02553900
H	-2.26805600	-0.96733000	0.28307800
H	-1.32353600	-1.50773000	-1.16722200
H	-0.73956900	2.07805400	0.44445500
O	-0.15539400	0.27018300	1.11188500

O	-0.20876400	-0.99201500	0.43173000
H	0.56891700	1.28151900	-0.53921500
N	2.73257300	-0.03948000	-0.37699300
H	3.44546900	-0.48677100	-0.93933100
H	3.15396600	0.17328400	0.51872300
H	2.00918200	-0.72692200	-0.19960600

TS1B:

Zero-point correction= 0.098431 (Hartree/Particle)

Thermal correction to Energy= 0.105592

Thermal correction to Enthalpy= 0.106536

Thermal correction to Gibbs Free Energy= 0.067538

Sum of electronic and zero-point Energies= -360.433436

Sum of electronic and thermal Energies= -360.426275

Sum of electronic and thermal Enthalpies= -360.425331

Sum of electronic and thermal Free Energies= -360.464329

0 1

C	-1.19293900	-0.91021500	-0.16948300
O	-0.99194300	0.28544100	-0.98274200
C	-0.17560400	1.09384100	-0.22222400
H	-2.20394700	-0.80919000	0.25901900
H	-1.19663000	-1.73924200	-0.89740900
H	-0.18904100	2.13728400	-0.58108500
O	-0.34426400	0.98737800	1.04879600
O	-0.22638900	-1.08371600	0.71030000
H	0.94898400	0.81588800	-0.48933800
N	2.28827600	-0.22471600	-0.24560800
H	2.70070200	-0.67928600	-1.04830500
H	3.01224100	0.07360900	0.39357100
H	1.62177600	-0.84062700	0.22221400

I1aB:

Zero-point correction= 0.104968 (Hartree/Particle)

Thermal correction to Energy= 0.113852

Thermal correction to Enthalpy= 0.114796

Thermal correction to Gibbs Free Energy= 0.069505

Sum of electronic and zero-point Energies= -360.609236

Sum of electronic and thermal Energies= -360.600352

Sum of electronic and thermal Enthalpies= -360.599408

Sum of electronic and thermal Free Energies= -360.644698

0 1

C	-0.07111200	0.76635000	0.65496900
O	-0.58454200	-0.59075800	0.55886700
C	-1.74243900	-0.75026300	-0.08726500
H	-0.91527500	1.44971200	0.71918400
H	0.49281700	0.74716600	1.59161200
H	-1.97728100	-1.82388600	-0.13650400
O	-2.44050100	0.10937100	-0.53756200
O	0.68767500	1.09816100	-0.42751800
H	2.61402700	-1.40434500	0.15507200
N	2.96439500	-0.52288900	-0.20060600
H	3.71463300	-0.22458700	0.41020700
H	3.37137400	-0.70691100	-1.10953300
H	1.52919300	0.59234400	-0.38231100

I1bB:

Zero-point correction= 0.105427 (Hartree/Particle)

Thermal correction to Energy= 0.113698

Thermal correction to Enthalpy= 0.114642

Thermal correction to Gibbs Free Energy= 0.072617

Sum of electronic and zero-point Energies= -360.615310

Sum of electronic and thermal Energies= -360.607040

Sum of electronic and thermal Enthalpies= -360.606095

Sum of electronic and thermal Free Energies= -360.648120

0 1

C	-0.56042700	1.16175600	0.46013600
O	-1.56092900	0.28599300	-0.15474600
C	-1.28576300	-1.00375400	-0.20607600
H	-1.14442100	2.04795700	0.70021900
H	-0.21687500	0.66058500	1.36960000
H	-2.10708700	-1.53611300	-0.70607000
O	-0.30580900	-1.55640100	0.22192700
O	0.44312500	1.48363500	-0.39228700
H	1.78737900	-1.13488900	0.21958900
N	2.41848100	-0.37583800	-0.01663900
H	3.08220500	-0.26302500	0.73842100
H	2.93722600	-0.64604900	-0.84239700
H	1.19824200	0.84857600	-0.28639700

TS2B:

Zero-point correction= 0.101632 (Hartree/Particle)

Thermal correction to Energy= 0.108925

Thermal correction to Enthalpy= 0.109869

Thermal correction to Gibbs Free Energy= 0.070088
 Sum of electronic and zero-point Energies= -360.591414
 Sum of electronic and thermal Energies= -360.584121
 Sum of electronic and thermal Enthalpies= -360.583177
 Sum of electronic and thermal Free Energies= -360.622959

0 1

C	-0.59676300	-1.42219000	0.42310100
O	1.20399200	-0.96259600	-0.23882400
C	1.69174200	0.18577600	-0.11954300
H	-0.28173000	-2.46770300	0.38285300
H	-0.37097400	-0.89978600	1.36391700
H	2.77079500	0.25800100	-0.35019200
O	1.12765100	1.24913600	0.22323700
O	-1.50044800	-1.02106600	-0.32500000
H	-0.31925400	1.46620300	0.10870400
N	-1.40798900	1.50695300	-0.04340600
H	-1.63586800	2.03061100	-0.87906300
H	-1.88135600	1.91635700	0.75155300
H	-1.64511400	0.44234100	-0.17057500

PB:

Zero-point correction= 0.100595 (Hartree/Particle)
 Thermal correction to Energy= 0.110596
 Thermal correction to Enthalpy= 0.111540
 Thermal correction to Gibbs Free Energy= 0.063951
 Sum of electronic and zero-point Energies= -360.603796
 Sum of electronic and thermal Energies= -360.593795
 Sum of electronic and thermal Enthalpies= -360.592851
 Sum of electronic and thermal Free Energies= -360.640440

0 1

C	-1.97543900	-0.96763200	0.16646400
O	0.65997300	-1.37087600	0.12204800
C	1.73880200	-0.85616700	-0.05825000
H	-2.00543800	-1.90619300	-0.41111500
H	-1.66896200	-1.05883700	1.22065200
H	2.65492400	-1.45327500	-0.18611600
O	2.00276100	0.42292500	-0.12865600
O	-2.27497900	0.08774600	-0.32494500
H	1.16591800	1.00023200	-0.01616700
N	-0.09451400	2.05678700	0.13198400
H	-0.09743100	2.75362700	-0.60315500

H	-0.10117400	2.55465900	1.01383700
H	-0.96845600	1.53672000	0.06132600

Pathway C

RC:

Zero-point correction= 0.104518 (Hartree/Particle)
 Thermal correction to Energy= 0.112939
 Thermal correction to Enthalpy= 0.113883
 Thermal correction to Gibbs Free Energy= 0.070293
 Sum of electronic and zero-point Energies= -360.481002
 Sum of electronic and thermal Energies= -360.472580
 Sum of electronic and thermal Enthalpies= -360.471636
 Sum of electronic and thermal Free Energies= -360.515226

0 1

O	-0.20894000	-0.99247900	0.43038600
O	-0.15421000	0.26916900	1.11147300
C	-0.35644900	1.14598400	0.02598300
H	-0.73791500	2.07788800	0.44593900
H	0.56867600	1.28093600	-0.53987900
C	-1.37642500	-0.80726300	-0.33159400
H	-1.32554400	-1.50639800	-1.16784300
H	-2.26843300	-0.96719000	0.28393000
O	-1.33462300	0.52309500	-0.78283800
N	2.73309000	-0.03935100	-0.37698400
H	2.01044300	-0.72799100	-0.20126100
H	3.15376200	0.17228100	0.51933800
H	3.44680800	-0.48467100	-0.93983900

TS1C:

Zero-point correction= 0.102269 (Hartree/Particle)
 Thermal correction to Energy= 0.109429
 Thermal correction to Enthalpy= 0.110373
 Thermal correction to Gibbs Free Energy= 0.071532
 Sum of electronic and zero-point Energies= -360.402536
 Sum of electronic and thermal Energies= -360.395376
 Sum of electronic and thermal Enthalpies= -360.394432
 Sum of electronic and thermal Free Energies= -360.433273

0 1

O	-0.95450500	-1.02728700	-0.41439900
O	-0.10118600	-1.24451400	0.69257400
C	0.39266300	1.22130500	0.56775300

H	0.22164200	0.76452700	1.53446800
H	1.23248200	1.86979300	0.37239400
C	-1.55067800	0.14140600	-0.18595100
H	-2.26499000	0.37084500	-0.97369400
H	-1.95041800	0.23321300	0.83025600
O	-0.51856600	1.22676000	-0.31314200
N	2.20251800	-0.21229200	-0.34912300
H	2.31106000	-0.24108200	-1.35448000
H	1.48248100	-0.88880800	-0.05190500
H	3.09226100	-0.43837400	0.07574200

I1C:

Zero-point correction= 0.108511 (Hartree/Particle)

Thermal correction to Energy= 0.114873

Thermal correction to Enthalpy= 0.115817

Thermal correction to Gibbs Free Energy= 0.078457

Sum of electronic and zero-point Energies= -360.491068

Sum of electronic and thermal Energies= -360.484706

Sum of electronic and thermal Enthalpies= -360.483762

Sum of electronic and thermal Free Energies= -360.521122

0 1

O	1.52824300	0.08529100	-0.40942400
O	1.20207500	1.26072500	0.32697000
C	-1.42466400	-0.36275800	0.33407800
H	-1.23247000	-0.24281300	1.40718700
H	-2.36936000	-0.89739600	0.20087700
C	0.87413200	-0.99706100	0.15532000
H	1.41108200	-1.87152200	-0.21267800
H	0.92191600	-0.92552400	1.24853900
O	-0.45760900	-1.17321700	-0.26165800
N	-1.43907000	0.97082600	-0.26212000
H	-1.72168800	0.91950700	-1.23384900
H	0.27667300	1.42260700	0.01837600
H	-2.09114200	1.57588500	0.22289200

TS2C:

Zero-point correction= 0.104415 (Hartree/Particle)

Thermal correction to Energy= 0.110498

Thermal correction to Enthalpy= 0.111442

Thermal correction to Gibbs Free Energy= 0.075134

Sum of electronic and zero-point Energies= -360.403793

Sum of electronic and thermal Energies= -360.397710

Sum of electronic and thermal Enthalpies= -360.396766
 Sum of electronic and thermal Free Energies= -360.433074

0 1

O	1.75905800	0.63111600	-0.12261200
O	-0.08673100	1.35552100	0.14290600
C	-1.09603400	-0.85788500	0.20802200
H	-0.97539600	-0.90277900	1.29562000
H	-1.78996100	-1.63744600	-0.11792600
C	1.34280900	-0.57322100	0.23555600
H	2.07602900	-1.32760000	-0.08127900
H	1.12110400	-0.68255300	1.31261500
O	0.09872400	-1.06270900	-0.44869700
N	-1.69868700	0.46002800	-0.07717500
H	-2.08934700	0.57845400	-1.00287000
H	0.18579100	1.09833300	-0.74551200
H	-2.28647700	0.84861200	0.64533400

I2C:

Zero-point correction= 0.109733 (Hartree/Particle)
 Thermal correction to Energy= 0.115745
 Thermal correction to Enthalpy= 0.116689
 Thermal correction to Gibbs Free Energy= 0.079936
 Sum of electronic and zero-point Energies= -360.506020
 Sum of electronic and thermal Energies= -360.500008
 Sum of electronic and thermal Enthalpies= -360.499064
 Sum of electronic and thermal Free Energies= -360.535817

0 1

O	-1.30141600	-1.12304100	-0.28883500
O	1.19619100	-1.20730500	0.33126100
C	0.62440000	1.13822400	0.22407700
H	0.67090500	1.03261700	1.31319000
H	1.11842900	2.05509400	-0.10958300
C	-1.51574300	0.10522900	0.25661300
H	-2.51554300	0.44596200	-0.00612900
H	-1.38062800	0.11671700	1.34879800
O	-0.64277800	1.12704100	-0.27985400
N	1.44677500	-0.02982600	-0.29040700
H	1.25450900	-0.09206900	-1.30037000
H	-0.38195500	-1.39877600	-0.00747200
H	2.43894100	0.21495500	-0.19029500

TS3C:

Zero-point correction= 0.102578 (Hartree/Particle)
 Thermal correction to Energy= 0.110334
 Thermal correction to Enthalpy= 0.111279
 Thermal correction to Gibbs Free Energy= 0.070355
 Sum of electronic and zero-point Energies= -360.480298
 Sum of electronic and thermal Energies= -360.472541
 Sum of electronic and thermal Enthalpies= -360.471597
 Sum of electronic and thermal Free Energies= -360.512521

0 1

O	-1.20243000	-1.27365100	-0.23767800
O	1.36013300	-1.26726600	0.29345300
C	0.39520600	1.45249100	0.34544000
H	0.42704000	1.00934900	1.35585300
H	1.16582500	2.22098500	0.16571600
C	-1.84018700	-0.32509000	0.18099000
H	-2.66671400	0.10579700	-0.39810700
H	-1.74625600	0.02299000	1.22110000
O	-0.64870500	1.46760200	-0.31460600
N	1.58018500	-0.02827100	-0.31031000
H	1.41040000	-0.10810700	-1.31299200
H	0.37914500	-1.39280800	0.22180900
H	2.56716600	0.16180900	-0.16913400

PC:

Zero-point correction= 0.099771 (Hartree/Particle)
 Thermal correction to Energy= 0.110070
 Thermal correction to Enthalpy= 0.111014
 Thermal correction to Gibbs Free Energy= 0.063227
 Sum of electronic and zero-point Energies= -360.485646
 Sum of electronic and thermal Energies= -360.475347
 Sum of electronic and thermal Enthalpies= -360.474403
 Sum of electronic and thermal Free Energies= -360.522190

0 1

O	-0.71281200	-1.66358400	-0.31440000
O	1.89358500	-0.89268700	0.19298700
C	-0.46648900	1.80816400	0.25780300
H	-0.16477600	1.43608800	1.25179500
H	0.12352900	2.65148700	-0.13855200
C	-1.64612200	-1.17607700	0.26561000
H	-2.65921800	-1.17895200	-0.16608100

H	-1.54319300	-0.72968900	1.26857400
O	-1.41326000	1.36235800	-0.33357800
N	1.85779400	0.47502800	-0.16643200
H	2.28045400	0.53451200	-1.09009500
H	0.97663200	-1.19444500	0.07123000
H	2.51758300	0.91458200	0.46760300

Pathway D

RD:

Zero-point correction= 0.092093 (Hartree/Particle)
 Thermal correction to Energy= 0.100120
 Thermal correction to Enthalpy= 0.101065
 Thermal correction to Gibbs Free Energy= 0.058181
 Sum of electronic and zero-point Energies= -380.360978
 Sum of electronic and thermal Energies= -380.352950
 Sum of electronic and thermal Enthalpies= -380.352006
 Sum of electronic and thermal Free Energies= -380.394890

0 1

O	-0.35989000	-1.11050600	-0.00492200
O	0.19842600	-0.07555300	0.81919300
C	-0.19239900	1.06467200	0.07971400
H	-0.18446400	1.90580600	0.77357800
H	0.47856300	1.21941700	-0.76952100
C	-1.65602300	-0.59912300	-0.18963300
H	-2.05529900	-1.06712400	-1.09045600
H	-2.28116700	-0.79323700	0.68831900
O	-1.49863900	0.78868100	-0.36752600
O	2.88583600	0.01994800	-0.25798800
H	3.21367300	-0.76869300	-0.69148400
H	2.11336000	-0.27002500	0.23902600

TS1D:

Zero-point correction= 0.089547 (Hartree/Particle)
 Thermal correction to Energy= 0.096235
 Thermal correction to Enthalpy= 0.097179
 Thermal correction to Gibbs Free Energy= 0.059279
 Sum of electronic and zero-point Energies= -380.287087
 Sum of electronic and thermal Energies= -380.280399
 Sum of electronic and thermal Enthalpies= -380.279455
 Sum of electronic and thermal Free Energies= -380.317355

0 1			
O	-0.97732800	-1.02256200	-0.38870000
O	0.00513400	-1.25516700	0.60342000
C	0.45611500	1.24588000	0.48967000
H	0.36315800	0.80638200	1.47643300
H	1.29246800	1.87038000	0.20773600
C	-1.54058900	0.13964500	-0.07821600
H	-2.33658900	0.38267400	-0.77771100
H	-1.81502400	0.23116900	0.97828600
O	-0.51076400	1.22807700	-0.31596700
O	2.08324800	-0.23649900	-0.43799800
H	2.86556900	-0.48633200	0.05757300
H	1.33493900	-0.82821300	-0.09708100

I1D:

Zero-point correction= 0.095211 (Hartree/Particle)
 Thermal correction to Energy= 0.101753
 Thermal correction to Enthalpy= 0.102698
 Thermal correction to Gibbs Free Energy= 0.064835
 Sum of electronic and zero-point Energies= -380.362717
 Sum of electronic and thermal Energies= -380.356175
 Sum of electronic and thermal Enthalpies= -380.355231
 Sum of electronic and thermal Free Energies= -380.393094

0 1			
O	1.53900800	0.04782600	-0.38824300
O	1.20667300	1.24102900	0.31374800
C	-1.42935000	-0.31936600	0.30933600
H	-1.22666800	-0.19440600	1.38273400
H	-2.40070300	-0.79564000	0.15747600
C	0.83944500	-1.00775900	0.17161300
H	1.35557600	-1.90065300	-0.17996700
H	0.86377600	-0.93045300	1.26483900
O	-0.48929700	-1.13702000	-0.27478800
O	-1.41577000	0.95172200	-0.33404700
H	-2.11703800	1.49615100	0.03199400
H	0.33957100	1.45929800	-0.07613800

TS2D:

Zero-point correction= 0.089864 (Hartree/Particle)
 Thermal correction to Energy= 0.095708
 Thermal correction to Enthalpy= 0.096652
 Thermal correction to Gibbs Free Energy= 0.060475

Sum of electronic and zero-point Energies= -380.298332
 Sum of electronic and thermal Energies= -380.292488
 Sum of electronic and thermal Enthalpies= -380.291544
 Sum of electronic and thermal Free Energies= -380.327721

0 1

O	-1.50020400	-0.08496300	-0.37738600
O	-1.09337400	-1.24399100	0.34771600
C	1.48832400	0.04719300	0.48595300
H	1.03208500	-0.19634400	1.45442200
H	2.41571900	0.62230500	0.58802900
C	-0.88541400	1.01732600	0.15932400
H	-1.38022800	1.87856400	-0.28876400
H	-0.93939600	1.03454100	1.24854300
O	0.50843500	1.10628200	-0.21370500
O	1.42555100	-0.84643100	-0.48756500
H	0.74612300	0.25719200	-0.95642300
H	-0.21503100	-1.43054900	-0.06994000

I2D:

Zero-point correction= 0.090493 (Hartree/Particle)
 Thermal correction to Energy= 0.099050
 Thermal correction to Enthalpy= 0.099994
 Thermal correction to Gibbs Free Energy= 0.056640
 Sum of electronic and zero-point Energies= -380.350712
 Sum of electronic and thermal Energies= -380.342155
 Sum of electronic and thermal Enthalpies= -380.341211
 Sum of electronic and thermal Free Energies= -380.384565

0 1

O	-1.42535300	-0.73047000	-0.38216800
O	-0.43229200	-1.40261100	0.38626800
C	2.20225500	0.40323600	0.35420700
H	1.54820600	0.49068900	1.23508800
H	3.06053500	1.09483800	0.29243700
C	-1.63088500	0.52700600	0.17463200
H	-2.57091100	0.85644000	-0.28170500
H	-1.72925100	0.45570300	1.25842700
O	-0.58810700	1.43030600	-0.06516000
O	1.99501700	-0.40574000	-0.51043200
H	-0.51922900	1.56246600	-1.01425200
H	0.38831800	-1.17347000	-0.09108300

TS3D:

Zero-point correction= 0.083294 (Hartree/Particle)
 Thermal correction to Energy= 0.091989
 Thermal correction to Enthalpy= 0.092933
 Thermal correction to Gibbs Free Energy= 0.048309
 Sum of electronic and zero-point Energies= -380.279985
 Sum of electronic and thermal Energies= -380.271290
 Sum of electronic and thermal Enthalpies= -380.270346
 Sum of electronic and thermal Free Energies= -380.314970

0 1

O	-0.52623500	0.03747300	-0.25076900
O	0.02871700	1.33509200	-0.17101200
C	2.55838400	-0.87543000	-0.11955600
H	1.67967500	-1.37761200	-0.55517900
H	3.48832700	-1.46198100	-0.02903500
C	-1.91789000	-0.26357000	0.67958000
H	-1.62393700	-1.09490800	1.33614200
H	-2.01779000	0.70019200	1.20011500
O	-2.61985000	-0.51291300	-0.37828200
O	2.51197100	0.26871100	0.24704300
H	-1.48649900	-0.06316300	-0.90897000
H	0.96043800	1.10457500	0.02093500

PD:

Zero-point correction= 0.086033 (Hartree/Particle)
 Thermal correction to Energy= 0.096622
 Thermal correction to Enthalpy= 0.097567
 Thermal correction to Gibbs Free Energy= 0.047846
 Sum of electronic and zero-point Energies= -380.329534
 Sum of electronic and thermal Energies= -380.318945
 Sum of electronic and thermal Enthalpies= -380.318001
 Sum of electronic and thermal Free Energies= -380.367721

0 1

O	0.01686500	0.93896100	-0.71343500
O	-0.01685300	0.93656500	0.71651000
C	-2.80472300	-0.40438100	-0.44190200
H	-2.31886000	0.27556800	-1.15892400
H	-3.73712200	-0.90613600	-0.75697400
C	2.80462900	-0.40594700	0.44063600
H	3.73700200	-0.90877800	0.75406500
H	2.31861100	0.27140500	1.16000700

O	2.33780500	-0.59963200	-0.65058600
O	-2.33770900	-0.60194500	0.64854300
H	0.79081100	0.37067000	-0.87574800
H	-0.79074000	0.36765300	0.87692500

Pathway E

RE:

Zero-point correction= 0.117206 (Hartree/Particle)
 Thermal correction to Energy= 0.128080
 Thermal correction to Enthalpy= 0.129024
 Thermal correction to Gibbs Free Energy= 0.079079
 Sum of electronic and zero-point Energies= -456.751114
 Sum of electronic and thermal Energies= -456.740240
 Sum of electronic and thermal Enthalpies= -456.739296
 Sum of electronic and thermal Free Energies= -456.789241

0 1

O	-1.35323700	1.10169800	0.19738600
O	-0.26256500	0.43943100	-0.46067800
C	-0.39656300	-0.85943900	0.08663000
H	0.12891700	-1.54281300	-0.57688400
H	0.01139900	-0.89013500	1.09990800
C	-2.37886000	0.16644400	-0.03417000
H	-3.13498000	0.33508600	0.73434000
H	-2.78759800	0.27550900	-1.04433700
O	-1.78362500	-1.10119500	0.10295200
O	2.64964900	-1.30150300	-0.09086500
H	2.71867800	-0.33988300	0.03283800
H	3.35850800	-1.67807300	0.43060400
O	2.29569400	1.44315100	0.19059800
H	2.62916800	2.03876800	-0.48197000
H	1.36111600	1.30685100	-0.02440400

TS1E:

Zero-point correction= 0.114524 (Hartree/Particle)
 Thermal correction to Energy= 0.124078
 Thermal correction to Enthalpy= 0.125022
 Thermal correction to Gibbs Free Energy= 0.079901
 Sum of electronic and zero-point Energies= -456.679127
 Sum of electronic and thermal Energies= -456.669573
 Sum of electronic and thermal Enthalpies= -456.668629
 Sum of electronic and thermal Free Energies= -456.713750

0 1			
O	-0.78298900	-1.27870000	-0.46224800
O	0.01179500	-1.16272600	0.71091800
C	-0.74792300	1.35356500	0.62610200
H	-0.56696500	0.74743800	1.50759500
H	-0.38850200	2.36832600	0.52804300
C	-1.86608900	-0.55830900	-0.24576600
H	-2.56522800	-0.64861900	-1.07335600
H	-2.30402900	-0.69677800	0.74790600
O	-1.50140200	0.93774500	-0.28469600
O	1.57230100	1.58546100	-0.21426300
H	1.98106900	0.68144100	-0.14577700
H	1.54798000	1.75714900	-1.15765200
O	2.38772100	-0.90333400	-0.16540200
H	3.01639300	-1.26953300	0.45653200
H	1.46394600	-1.13852100	0.18021400

I1E:

Zero-point correction= 0.120966 (Hartree/Particle)
Thermal correction to Energy= 0.130241
Thermal correction to Enthalpy= 0.131185
Thermal correction to Gibbs Free Energy= 0.086495
Sum of electronic and zero-point Energies= -456.755653
Sum of electronic and thermal Energies= -456.746379
Sum of electronic and thermal Enthalpies= -456.745434
Sum of electronic and thermal Free Energies= -456.790125

0 1			
O	-0.55419600	-1.48758500	-0.44780100
O	0.31963900	-1.53898800	0.68332400
C	-0.59189900	1.41895400	0.50668200
H	-0.38872700	0.85650900	1.41821600
H	-1.09665500	2.36119700	0.73786900
C	-1.61202600	-0.65786000	-0.12688100
H	-2.41449400	-0.95017300	-0.80379100
H	-1.89959800	-0.82217800	0.91667800
O	-1.41686100	0.71523900	-0.36421800
O	0.66867300	1.70093900	-0.06580800
H	1.96198600	0.50899600	-0.22659600
H	0.51818600	2.17329400	-0.88910500
O	2.49894500	-0.30114500	-0.30569800
H	3.25033400	-0.18359200	0.27718200

H	1.16291400	-1.21830400	0.29235200
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TS2E:

Zero-point correction= 0.115867 (Hartree/Particle)
 Thermal correction to Energy= 0.123244
 Thermal correction to Enthalpy= 0.124189
 Thermal correction to Gibbs Free Energy= 0.084313
 Sum of electronic and zero-point Energies= -456.724328
 Sum of electronic and thermal Energies= -456.716950
 Sum of electronic and thermal Enthalpies= -456.716006
 Sum of electronic and thermal Free Energies= -456.755882

0 1

O	1.45060900	-0.52377000	-0.45396300
O	1.49781500	0.83541600	-0.88220700
C	-0.93605400	0.97790300	0.80154900
H	-0.22189200	1.63332400	1.31592100
H	-1.86535700	0.85898900	1.37117700
C	1.10700700	-0.57061700	0.87930500
H	1.41434700	-1.55599400	1.23263800
H	1.59251800	0.23003600	1.43981500
O	-0.30278600	-0.47945300	1.10614600
O	-1.05514000	1.14965800	-0.48638300
H	-0.84986400	-1.05609600	0.23482700
H	-1.47106600	-0.15736800	-0.92994500
O	-1.49740400	-1.21832700	-0.82478300
H	-0.89501800	-1.57234700	-1.48621500
H	0.52586400	1.06754200	-0.93382000

I2aE:

Zero-point correction= 0.116709 (Hartree/Particle)
 Thermal correction to Energy= 0.127526
 Thermal correction to Enthalpy= 0.128470
 Thermal correction to Gibbs Free Energy= 0.080898
 Sum of electronic and zero-point Energies= -456.742968
 Sum of electronic and thermal Energies= -456.732151
 Sum of electronic and thermal Enthalpies= -456.731207
 Sum of electronic and thermal Free Energies= -456.778779

0 1

O	-1.44887700	-0.16807500	-0.66683100
O	-0.75828400	-1.38245000	-0.94533800
C	1.85378100	-0.78825900	0.67523100

H	1.33561700	-1.68894800	1.03466000
H	2.39065700	-0.19286000	1.43045200
C	-1.57114700	-0.02018500	0.72425100
H	-2.34832300	0.74794400	0.81375200
H	-1.90121800	-0.95837000	1.17067100
O	-0.39378400	0.35826200	1.36014300
O	1.85773400	-0.47849900	-0.49113600
H	-0.07466000	1.16348200	0.91078400
H	1.26521500	1.64134400	-0.81561700
O	0.45384200	2.11637300	-0.60622300
H	-0.21550100	1.66040000	-1.12929300
H	0.16736100	-1.08720600	-1.01721200

I2bE:

Zero-point correction= 0.115854 (Hartree/Particle)

Thermal correction to Energy= 0.127119

Thermal correction to Enthalpy= 0.128064

Thermal correction to Gibbs Free Energy= 0.078406

Sum of electronic and zero-point Energies= -456.741861

Sum of electronic and thermal Energies= -456.730596

Sum of electronic and thermal Enthalpies= -456.729652

Sum of electronic and thermal Free Energies= -456.779309

0 1

O	-1.26044300	-0.25597300	-0.82220400
O	-1.37544300	-1.42930500	-0.01064000
C	1.32962300	-1.45646900	0.55425400
H	1.25538300	-2.55240900	0.64746200
H	0.75236100	-0.85233900	1.26856000
C	-1.62061600	0.85682400	-0.02569900
H	-1.71103200	1.64315400	-0.78661900
H	-2.58738300	0.66821200	0.44559500
O	-0.71971500	1.16230500	0.96096700
O	2.01761400	-0.95527400	-0.29806000
H	0.09945400	1.50147600	0.54447300
H	1.88242700	0.80826500	-0.36817100
O	1.63808200	1.74711800	-0.24389000
H	1.69757500	2.15022600	-1.11060900
H	-2.04358300	-1.91969800	-0.50140200

TS3E:

Zero-point correction= 0.110816 (Hartree/Particle)

Thermal correction to Energy= 0.120768

Thermal correction to Enthalpy= 0.121712
 Thermal correction to Gibbs Free Energy= 0.075727
 Sum of electronic and zero-point Energies= -456.702214
 Sum of electronic and thermal Energies= -456.692262
 Sum of electronic and thermal Enthalpies= -456.691318
 Sum of electronic and thermal Free Energies= -456.737303

0 1

O	-1.35348500	0.74055200	0.58936200
O	-0.43290600	1.65121800	-0.01194500
C	2.12534600	0.15715800	-0.88122900
H	2.84493600	0.63429900	-1.56806400
H	1.13849400	-0.12766600	-1.27928000
C	-1.81956400	-0.44231400	-0.64629000
H	-2.67404500	-0.78729100	-0.03881400
H	-2.09697500	0.28890300	-1.41757900
O	-0.85991300	-1.23161800	-0.87331700
O	2.42783300	-0.04379100	0.26970100
H	-0.17001500	-1.38694600	0.46692200
H	1.07289400	-0.65423400	1.14549100
O	0.15489600	-0.95301800	1.35076100
H	-0.53337000	-0.04416000	1.16766700
H	-0.90801700	2.48128800	0.09226900

PE:

Zero-point correction= 0.111699 (Hartree/Particle)
 Thermal correction to Energy= 0.124598
 Thermal correction to Enthalpy= 0.125542
 Thermal correction to Gibbs Free Energy= 0.072224
 Sum of electronic and zero-point Energies= -456.720393
 Sum of electronic and thermal Energies= -456.707494
 Sum of electronic and thermal Enthalpies= -456.706550
 Sum of electronic and thermal Free Energies= -456.759868

0 1

O	-1.02428900	1.40873100	0.57270300
O	-0.14405000	1.70800500	-0.50947500
C	1.91334800	-0.30814700	-1.02469300
H	2.43769700	0.08924100	-1.91169600
H	0.89283800	-0.69082900	-1.17545200
C	-2.11896700	-0.66643600	-0.61649800
H	-2.90742900	-0.54150300	0.14406500
H	-2.16348500	0.01618700	-1.48015800
O	-1.27139100	-1.51576400	-0.52045200

O	2.45048900	-0.32365100	0.05249000
H	-0.19246600	-1.30592900	1.32611600
H	1.15765100	-0.58343900	1.33131300
O	0.28036800	-0.58333400	1.75377700
H	-0.49947800	0.73268400	1.07811900
H	0.17936500	2.57918600	-0.25750200