

A Mechanistic Study of the 2-thienylmethyl + HO₂ Radical
Recombination Reaction

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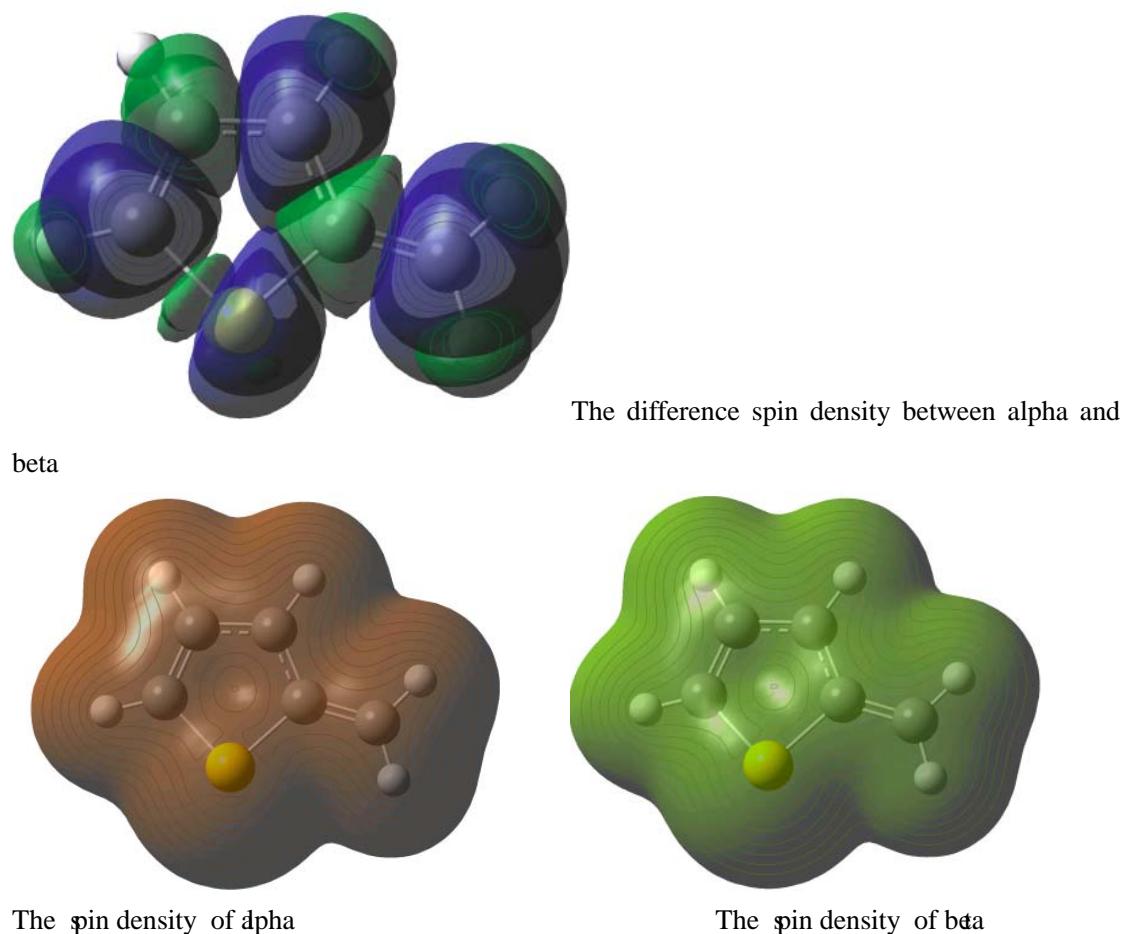


Figure S1. The spin density map of the 2-thienylmethyl radical at the UB3LYP/6-311++G(d, p) level (isovalue=0.0004)

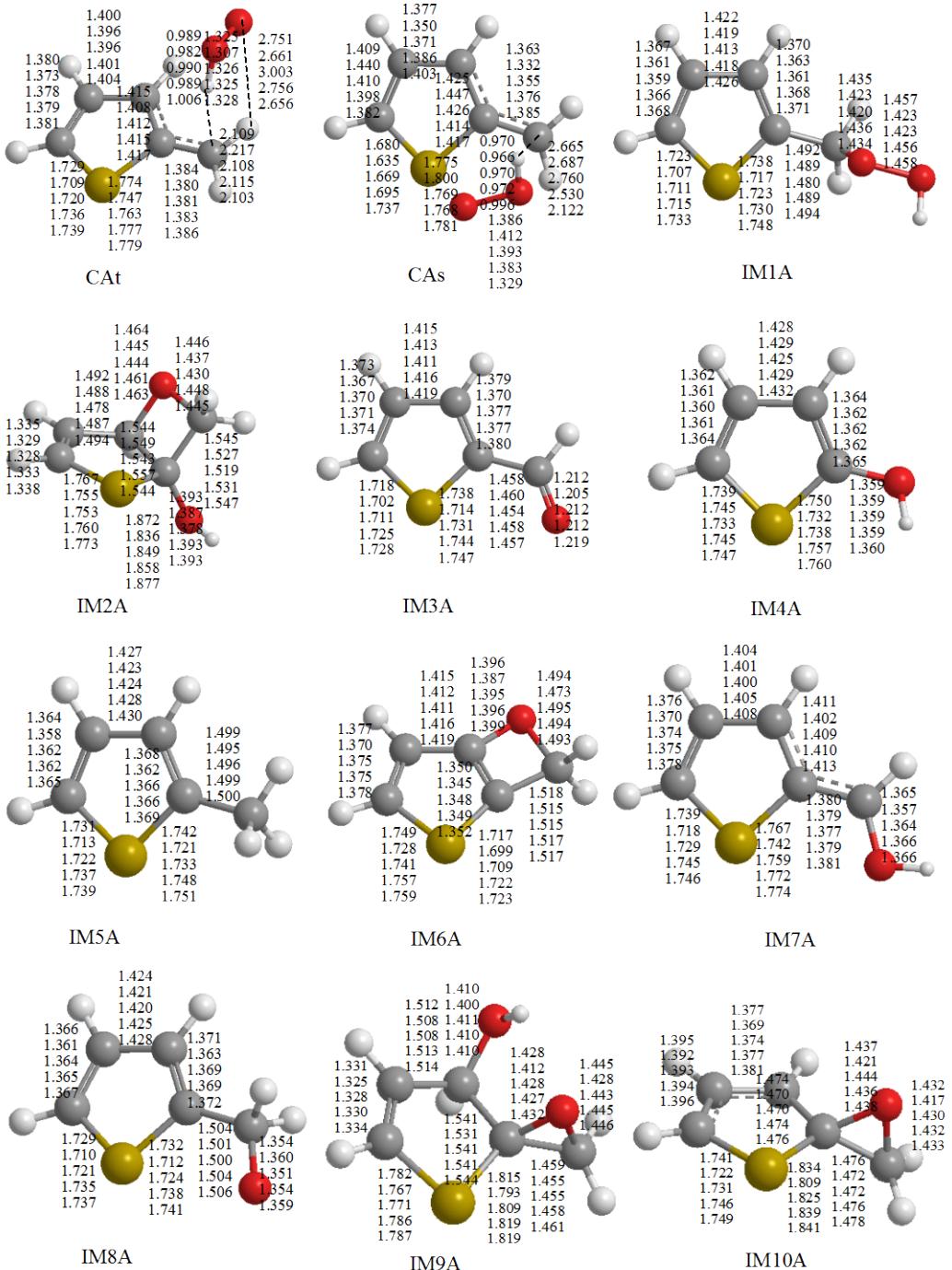


Figure S2a. Optimized geometries (\AA , degrees) of all intermediates and complexes involved in the 2-thienylmethyl (A) + HO_2 reaction at different levels of theory (From top to bottom, the methods are B3LYP/CBSB7, M06-2X/aug-cc-pV(T+d)Z, B3LYP/aug-cc-pV(T+d)Z, B3LYP/6-311G(d,p) and B3LYP/6-31G(d))

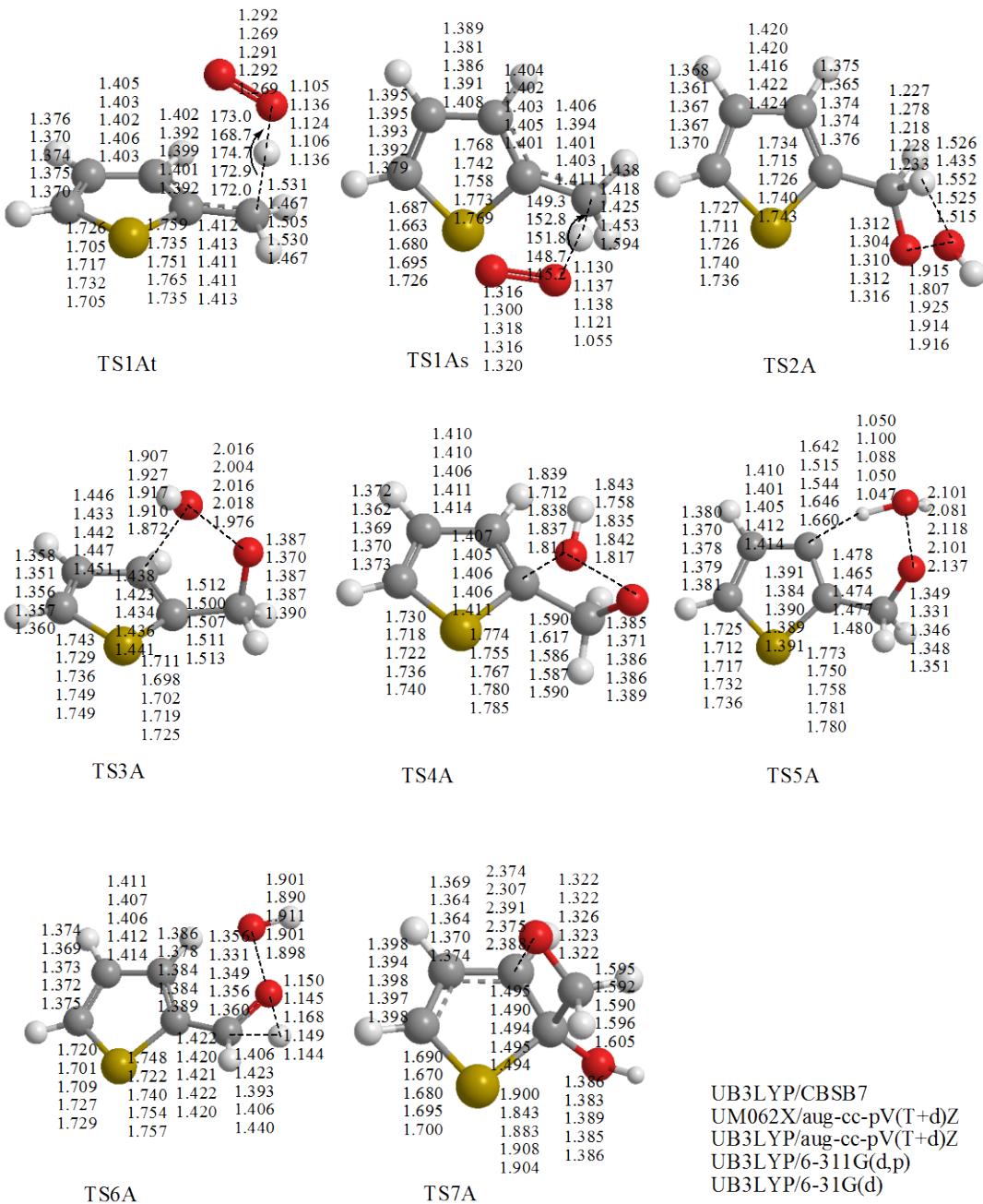


Figure S2b. Optimized geometries (Å, degrees) of all transition states involved in the 2-thienylmethyl (A) + HO₂ reaction at different levels of theory (From top to bottom, the methods are B3LYP/CBSB7, M06-2X/aug-cc-pV(T+d)Z, B3LYP/aug-cc-pV(T+d)Z, B3LYP/6-311G(d,p) and B3LYP/6-31G(d))

Table S3a. The absolute energy, zpe, lowest frequency, S^2 , and coefficient of Norm(A) values involved in the 2-thienylmethyl (A) + HO₂ reaction at the CBS-QB3 level.

Species	CBS-QB3	ZPE(scaled)	Lowest Freq	$\langle S^2 \rangle$ (CCSD(T) step)	Norm (A) coefficient
HO ₂	-150.741101	0.013984	1164.93	0.762(0.75)	0.119
2-Thienylmethyl	-590.862805	0.079868	215.87	1.130(0.843)	0.107
H ₂ O	-76.337482	0.021112	1637.92	0.000	0.103
CH ₂ O	-114.344172	0.026224	1202.13	0.000	0.106
OH	-75.649720	0.008356	3704.74	0.756(0.750)	0.102
O ₂ (T)	-150.164605	0.003702	1641.22	2.044(2.001)	0.105
O ₂ (S)	-150.119013	0.003669	1626.82	0.000	0.107
CAt	-741.611534	0.09579	28.14	2.384(2.068)	0.125
CAs	-741.608054	0.098551	65.76	0.000	0.132
IM1A	-741.691145	0.101289	32.77	0.000	0.121
IM2A	-741.736765	0.102731	73.79	0.000	0.121
IM3A	-665.453865	0.075238	133.67	0.000	0.119
IM4A	-627.407728	0.069623	151.20	0.000	0.116
IM5A	-591.498619	0.093068	83.72	0.000	0.117
IM6A	-665.37617	0.075849	46.79	0.000	0.119
IM7A	-666.009365	0.084719	137.01	1.124(0.841)	0.121
IM8A	-665.969481	0.083401	27.32	0.760(0.758)	0.119
IM9A	-741.735193	0.103546	102.38	0.000	0.121
IM10A	-665.966073	0.084434	126.91	0.951(0.760)	0.120
TS1At	-741.605745	0.092342	-1104.25	2.402(2.077)	0.126
TS1As	-741.595242	0.094024	-981.91	0.000	0.129
TS2A	-741.619784	0.093979	-1345.53	0.000	0.125
TS3A	-741.600721	0.098165	-797.23	0.000	0.126
TS4A	-741.593562	0.097453	-904.59	0.000	0.129
TS5A	-741.853147	0.092617	-434.32	0.000	0.223
TS6A	-741.606401	0.093026	-1466.35	0.000	0.128
TS7A	-741.670526	0.097981	-567.55	0.000	0.128

Table S3b. The absolute energy, zpe, lowest frequency, S^2 , T1 diagnostic and coefficient of Norm(A) values involved in the 2-thienylmethyl (A) + HO₂ reaction at the CCSD(T)/cc-pVTZ level.

Species	CCSD(T)/cc-pV TZ	ZPE(scaled)	Lowest Freq	$\langle S^2 \rangle$	T1 Diag	Norm(A)
HO ₂	-150.7122532	0.013984	1164.93	0.762(0.750)	0.027	0.107
2-Thienyl methyl	-590.8547653	0.079868	215.87	1.131(0.845)	0.034	0.121
H ₂ O	-76.3322033	0.021112	1637.92	0.000	0.007	0.103
CH ₂ O	-114.3336982	0.026224	1202.13	0.000	0.015	0.106
OH	-75.6377081	0.008356	3704.74	0.756(0.750)	0.007	0.103
O ₂ (T)	-150.1289765	0.003702	1641.23	2.042(2.001)	0.016	0.107
O ₂ (S)	-150.0809544	0.003669	1626.82	0.000	0.014	0.107
CAt	-741.5767481	0.09579	28.14	2.386(2.069)	0.034	0.127
CAs	-741.5692729	0.098551	65.76	0.000	0.045	0.132
IM1A	-741.6602218	0.101289	32.77	0.000	0.013	0.123
IM2A	-741.7080216	0.102731	73.79	0.000	0.013	0.123
IM3A	-665.4218162	0.075238	133.67	0.000	0.015	0.120
IM4A	-627.3824373	0.069623	151.20	0.000	0.013	0.118
IM5A	-591.5053963	0.093068	83.72	0.000	0.012	0.118
IM6A	-665.343309	0.075849	46.79	0.000	0.014	0.120
IM7A	-665.9821483	0.084719	137.01	1.126(0.843)	0.031	0.123
IM8A	-665.9466722	0.083401	27.32	0.760(0.750)	0.017	0.120
IM9A	-741.7063826	0.103546	102.38	0.000	0.013	0.123
IM10A	-665.9411126	0.084434	126.91	0.953(0.761)	0.026	0.122
TS1At	-741.5654585	0.092342	-1104.25	2.405(2.079)	0.037	0.128
TS1As	-741.5519611	0.094024	-981.91	0.000	0.034	0.129
TS2A	-741.5796345	0.093979	-1345.53	0.000	0.019	0.126
TS3A	-741.5603926	0.098165	-797.23	0.000	0.018	0.127
TS4A	-741.5586908	0.097453	-904.59	0.000	0.038	0.130
TS5A	-741.8905194	0.092617	-434.32	0.000	0.183	0.236
TS6A	-741.563797	0.093026	-1466.35	0.000	0.032	0.129
TS7A	-741.633347	0.097981	-567.55	0.000	0.041	0.129

Table S3c. The absolute energy, zpe, lowest frequency, and S^2 values involved in the 2-thienylmethyl (A) + HO₂ reaction at the G3B3 level.

Species	G3B3	ZPE(scaled)	Lowest	$\langle S^2 \rangle$
			Freq	QCISD(T) step
HO ₂	-150.829951	0.013472	1178.26	0.760(0.750)
2-Thienylmethyl	-591.387004	0.078000	215.69	1.158(0.859)
H ₂ O	-76.383725	0.020322	1712.80	0.000
CH ₂ O	-114.433748	0.025754	1198.76	0.000
OH	-75.696367	0.007972	3645.11	0.756(0.750)
O ₂ (T)	-150.252734	0.003628	1658.85	2.006(2.000)
O ₂ (S)	-150.206589	0.003593	1643.04	0.000
CAt	-742.224115	0.093503	33.46	2.035(2.001)
CA _s	-742.237602	0.099545	74.69	0.000
IM1A	-742.304788	0.098775	34.55	0.000
IM2A	-742.352072	0.100224	72.60	0.000
IM3A	-666.022553	0.073490	135.34	0.000
IM4A	-627.932714	0.067800	162.35	0.000
IM5A	-592.025976	0.091026	96.89	0.000
IM6A	-665.944180	0.073997	-21.26	0.000
IM7A	-666.576699	0.082527	136.64	1.148(0.853)
IM8A	-666.539890	0.081473	-22.49	0.759(0.750)
IM9A	-742.350077	0.100042	101.87	0.000
IM10A	-666.534300	0.082552	128.60	0.964(0.761)
TS1At	-742.218012	0.090328	-836.11	2.420(2.083)
TS1As	-742.102609	0.092121	-879.06	0.000
TS2A	-742.234486	0.091475	-1371.61	0.000
TS3A	-742.216837	0.095895	-841.57	0.000
TS4A	-742.211709	0.095132	-928.63	0.000
TS5A	-742.253975	0.095647	-601.31	0.000
TS6A	-742.226244	0.090444	-1460.73	0.000
TS7A	-742.254047	0.095646	-601.41	0.000

Table S3d. The absolute energy, zpe, lowest frequency, and S^2 values involved in the 2-thienylmethyl (A) + HO₂ reaction at the M06-2X/aug-cc-pV(T+d)Z level.

Species	M06-2X/aug-cc-pV(T+d)Z	ZPE (unscaled)	Lowest Freq	$\langle S^2 \rangle$
HO ₂	-150.9081075	0.014608	1256.16	0.755(0.750)
2-Thienylmethyl	-591.6628166	0.081195	218.66	0.783(0.751)
H ₂ O	-76.4300923	0.021560	1616.12	0.000
CH ₂ O	-114.4989846	0.027102	1219.91	0.000
OH	-75.733789	0.008525	3742.26	0.753(0.750)
O ₂ (T)	-150.324815	0.004005	1758.00	2.008(2.000)
O ₂ (S)	-150.2657285	0.003996	1753.84	0.000
CAt	-742.581085	0.097715	31.88	2.037(2.001)
CA _s	-742.5718331	0.100443	100.00	0.000
IM1A	-742.6656051	0.104121	35.26	0.000
IM2A	-742.7179778	0.105951	86.69	0.000
IM3A	-666.329797	0.077352	133.18	0.000
IM4A	-628.2233511	0.071229	177.16	0.000
IM5A	-592.31153	0.094513	-32.92	0.000
IM6A	-666.2545925	0.077983	73.55	0.000
IM7A	-666.894234	0.086483	142.42	0.772(0.750)
IM8A	-666.8560331	0.086052	64.65	0.755(0.750)
IM9A	-742.7160189	0.105115	97.52	0.000
IM10A	-666.8520431	0.086401	120.43	0.772(0.750)
TS1At	-742.5728398	0.094324	-1727.66	2.032
TS1As	-742.5441474	0.096051	-1046.69	0.000
TS2A	-742.5689868	0.096028	-1937.16	0.000
TS3A	-742.5366044	0.100836	-1114.72	0.000
TS4A	-742.5405519	0.099814	-1108.97	0.000
TS5A	XXX	XXX	XXX	XXX
TS6A	-742.5569841	0.095921	-1359.62	0.000
TS7A	-742.637173	0.100832	-691.96	0.000

Table S3e. The absolute energy, zpe, lowest frequency, and S^2 values involved in the 2-thienylmethyl (A) + HO₂ reaction at the M06/aug-cc-pV(T+d)Z level.

Species	M06/aug-cc-pV(T+d)Z	ZPE(unscaled)	Lowest Freq	$\langle S^2 \rangle$
HO ₂	-150.8882645	0.014321	1221.91	0.754(0.750)
2-Thienylmethyl	-591.5917358	0.07984	208.27	0.785(0.751)
H ₂ O	-76.4225491	0.021549	1611.42	0.000
CH ₂ O	-114.4799644	0.026289	1196.89	0.000
OH	-75.7248459	0.008567	3760.70	0.754(0.750)
O ₂ (T)	-150.3028101	0.003866	1696.88	2.008(2.000)
O ₂ (S)	-150.2443372	0.003883	1704.59	0.000
CAt	-742.4896203	0.096618	31.71	2.038(2.001)
CAs	xxx	xxx	xxx	xxx
IM1A	-742.5678863	0.102455	44.76	0.000
IM2A	-742.6249113	0.104352	101.43	0.000
IM3A	-666.2474952	0.075713	127.63	0.000
IM4A	-628.1526007	0.070293	164.15	0.000
IM5A	-592.2374963	0.093398	-103.16	0.000
IM6A	-666.1712741	0.076751	42.99	0.000
IM7A	-666.8128487	0.085376	145.10	0.782(0.751)
IM8A	-666.7726603	0.083767	57.90	0.756(0.750)
IM9A	-742.6222924	0.103764	100.85	0.000
IM10A	-666.7729007	0.085297	123.08	0.772(0.750)
TS1At	-742.4845162	0.093147	-1022.64	2.029
TS1As	-742.4617348	0.0948	-610.83	0.000
TS2A	-742.4861058	0.095224	-1237.90	0.000
TS3A	-742.4587453	0.098712	-884.85	0.000
TS4A	-742.459454	0.098385	-1078.53	0.000
TS5A	-742.4346061	0.09135	-1034.21	0.000
TS6A	-742.4748962	0.094246	-1334.65	0.000
TS7A	-742.5565655	0.099243	-541.50	0.000

Table S3f. The absolute energy, zpe, lowest frequency, and S^2 values involved in the 2-thienylmethyl (A) + HO₂ reaction at the B3LYP/aug-cc-pV(T+d)Z level.

Species	B3LYP/aug-cc-pV(T+d)Z	ZPE(unscaled)	Lowest Freq	$\langle S^2 \rangle$
HO ₂	-150.9733516	0.014082	1157.56	0.754(0.750)
2-Thienylmethyl	-591.7895857	0.080908	218.16	0.780(0.750)
H ₂ O	-76.4661967	0.021234	1627.23	0.000
CH ₂ O	-114.5521474	0.026498	1198.23	0.000
OH	-75.7685993	0.008421	3696.25	0.753(0.750)
O ₂ (T)	-150.3846184	0.003704	1625.75	2.009(2.000)
O ₂ (S)	-150.3233665	0.003679	1614.85	0.000
CAt	-742.7691375	0.096617	15.51	2.032(2.001)
CAs	-742.7569898	0.099481	52.39	0.000
IM1A	-742.8395955	0.102422	44.73	0.000
IM2A	-742.8817449	0.104051	91.99	0.000
IM3A	-666.4731029	0.076083	130.52	0.000
IM4A	-628.3485142	0.070331	85.27	0.000
IM5A	-592.4355391	0.094142	83.39	0.000
IM6A	-666.390212	0.076747	71.59	0.000
IM7A	-667.0424083	0.085801	143.52	0.778(0.751)
IM8A	-667.0045075	0.084202	20.97	0.755(0.750)
IM9A	-742.8767062	0.103357	93.34	0.000
IM10A	-666.995584	0.085503	130.97	0.770(0.750)
TS1At	-742.7639735	0.093114	-1337.09	2.027(2.005)
TS1As	-742.739958	0.094846	-987.69	0.000
TS2A	-742.76097	0.094936	-1294.58	0.000
TS3A	-742.7347291	0.098796	-796.10	0.000
TS4A	-742.736206	0.098478	-939.68	0.000
TS5A	-742.7095464	0.091827	-845.79	0.000
TS6A	-742.7498269	0.094114	-1455.82	0.000
TS7A	-742.8176047	0.099085	-536.44	0.000

Table S3g. The absolute energy, zpe, lowest frequency, and S^2 values involved in the 2-thienylmethyl (A) + HO₂ reaction at the B3LYP/6-311G(d,p) level.

Species	B3LYP/6-311G(d,p)	ZPE	Lowest Freq	$\langle S^2 \rangle$
HO ₂	-150.9504075	0.014136	1163.36	0.753(0.750)
2-Thienylmethyl	-591.7516999	0.080638	213.80	0.781(0.751)
H ₂ O	-76.447448	0.021314	1638.64	0.000
CH ₂ O	-114.5363413	0.026491	1201.80	0.000
OH	-75.7545274	0.00844	3704.74	0.752(0.750)
O ₂ (T)	-150.3647909	0.003739	1641.22	2.007(2.000)
O ₂ (S)	-150.3026075	0.003705	1626.33	0.000
CAt	-742.7114034	0.096717	28.37	2.031(2.000)
CAs	-742.6960006	0.099661	3.42	0.000
IM1A	-742.7793909	0.10226	32.32	0.000
IM2A	-742.8219111	0.103821	74.20	0.000
IM3A	-666.4263859	0.075965	134.04	0.000
IM4A	-628.303049	0.070306	156.79	0.000
IM5A	-592.3981701	0.093998	90.41	0.000
IM6A	-666.3415123	0.076529	8.66	0.000
IM7A	-666.9933018	0.085552	138.75	0.779(0.751)
IM8A	-666.9575511	0.0842	22.98	0.754(0.750)
IM9A	-742.8200976	0.103578	102.89	0.000
IM10A	-666.9473758	0.085276	125.57	0.770(0.750)
TS1At	-742.7074746	0.093239	-1114.68	2.025(2.000)
TS1As	-742.680631	0.094965	-950.30	0.000
TS2A	-742.7029129	0.094894	-1345.45	0.000
TS3A	-742.6778185	0.099118	-801.19	0.000
TS4A	-742.6799995	0.098487	-905.43	0.000
TS5A	-742.6519285	0.093587	-428.36	0.000
TS6A	-742.6852136	0.093912	-1466.73	0.000
TS7A	-742.757139	0.099072	-569.51	0.000

Table S2. CBS-QB3 relative energies (kcal mol⁻¹) of all the species involved in the 2-thienylmethyl + HO₂ reaction.

Species	CBS-QB3
2-thienylmethyl + HO ₂	0.00
CAt	-4.79
CAs	-2.60
IM1A	-54.75
IM2A	-83.37
IM3A + H ₂ O	-117.62
IM4A + CH ₂ O	-92.87
IM5A + O ₂ (Triplet)	-37.22
IM5A + O ₂ (Singlet)	-8.61
IM6A + H ₂ O	-68.87
IM7A + OH	-34.63
IM8A + OH	-9.60
IM9A	-82.38
TS1At	-1.15
TS1As	5.43
TS2A	-9.97
TS3A	2.00
TS4A	6.49
TS5A	-157.79
TS6A	-1.57
TS7A	-41.81
CBt	-4.89
IM1B	-37.47
IM2B + O ₂ (Triplet)	-16.04

IM3B + H ₂ O	-105.57
IM4B + H	-33.71
IM5B + OH	-34.59
IM6B + OH	8.81
TS1Bt	7.33
TS2B	7.73
TS3B	4.48
TS4B	8.55
CCt	-4.45
IM1C	-40.60
IM2C + O ₂ (Triplet)	-19.99
IM3C + H ₂ O	-112.99
IM4C + OH	-32.31
IM5C + OH	4.68
TS1Ct	6.40
TS2C	3.27
TS3C	7.48

RA	(215.87)	(-590.862805)		
C		0.00000000	0.89510700	0.00000000
C		1.32350700	0.39680000	0.00000000
C		1.40088100	-1.00246400	0.00000000
C		0.16782800	-1.61908300	0.00000000
S		-1.12936500	-0.47254300	0.00000000
H		2.18099800	1.05686900	0.00000000
H		2.33194700	-1.55452100	0.00000000
H		-0.04741400	-2.67640700	0.00000000
C		-0.42802200	2.20565000	0.00000000
H		-1.47708400	2.46840300	0.00000000
H		0.29623000	3.01029000	0.00000000
CAt	(28.14)	(-741.611534)		
C		0.24753700	-0.43265900	0.50012100
C		0.25539800	0.97125400	0.67832900
C		1.39561700	1.59552600	0.15920100
C		2.28390300	0.71477200	-0.42324900
S		1.72681300	-0.92044800	-0.34236800
H		-0.56746500	1.48550100	1.15616100
H		1.57186100	2.66223900	0.20340900
H		3.23064400	0.93780600	-0.89065500
C		-0.72756100	-1.33832700	0.87970200
H		-1.57477000	-0.99477100	1.46231800
H		-0.61398200	-2.40244300	0.72066400
O		-2.83319300	-0.11776000	-0.94881400
H		-2.05565000	-0.61215300	-0.58872400
O		-3.21043400	0.69121200	0.03007600
CAs	(65.76)	(-741.608054)		
C		0.12526800	0.84202900	0.38846300
C		1.20515600	1.31353000	-0.41311700
C		2.13604300	0.33618100	-0.68517300
C		1.81845600	-0.90648200	-0.10136400
S		0.33859300	-0.89326300	0.69422700
H		1.28292700	2.34785100	-0.72048600
H		3.03734300	0.49520800	-1.26258200
H		2.37556400	-1.82658000	-0.19168500
C		-1.02545300	1.46345700	0.77192300
H		-1.20786900	2.49132900	0.47813200
H		-1.70865900	1.02345200	1.48037200

O		-2.40325800	0.02714800	-0.57933300
H		-2.16019100	0.45157600	-1.41741200
O		-1.67091900	-1.15001300	-0.57546200
IM1A	(32.77)	(-741.691145)		
C		0.13851000	0.28796900	0.31554500
C		0.94628600	1.36904400	0.07836300
C		2.28327300	1.01351000	-0.24992700
C		2.47580300	-0.34020000	-0.26664100
S		1.02806200	-1.19218300	0.11802000
H		0.58784400	2.38894300	0.13758300
H		3.06602100	1.72932500	-0.46292500
H		3.38146300	-0.88628700	-0.48144800
C		-1.31535000	0.28706800	0.64866400
H		-1.61097500	1.26763000	1.03495000
H		-1.56914400	-0.47416600	1.39437100
O		-2.03074400	0.01386200	-0.56514100
O		-3.44386400	0.01558400	-0.21149700
H		-3.67845700	-0.89043000	-0.45377100
IM2A	(73.79)	(-741.736765)		
C		-0.45122800	0.95295400	0.60239000
C		0.95807300	1.43903700	0.55304900
C		1.82139100	0.56317300	0.03441500
S		1.15816700	-0.99083200	-0.48444400
H		-0.96128800	1.14809900	1.55069600
H		1.24535900	2.41916900	0.91158900
H		2.88520500	0.71550800	-0.09675000
C		-1.52241900	-0.00645500	-0.92298500
H		-2.55367700	-0.32084200	-0.72462000
H		-1.25926600	-0.17857400	-1.96843900
O		-1.28437500	1.36452400	-0.52836000
C		-0.53867900	-0.52123900	0.15146500
O		-1.01798500	-1.39100100	1.12844600
H		-1.07095600	-2.28305000	0.76792400
IM3A	(133.67)	(-665.453865)		
C		0.39957700	0.41548300	0.00002400
C		-0.56978800	1.39587100	0.00009300
C		-1.88427400	0.87212400	0.00005800
C		-1.89320900	-0.50065800	-0.00003500
S		-0.31088900	-1.17105100	-0.00008900
H		-0.33421000	2.45288900	0.00016400
H		-2.78173700	1.47583400	0.00009900

H	-2.75174700	-1.15551400	-0.00007500
C	1.84603000	0.59836600	0.00002700
H	2.16076100	1.66353900	0.00006400
O	2.66139400	-0.29838100	0.00002200
IM4A (151.20) (-627.407728)			
C	0.03832300	1.37454700	0.00405100
C	-1.35792300	1.07546800	0.00237800
C	-1.63098600	-0.25888200	0.00923800
S	-0.16962300	-1.20195900	-0.01265600
H	0.46197900	2.36902900	0.01051900
H	-2.12941900	1.83430800	0.01090900
H	-2.58593000	-0.75897000	0.03347400
C	0.80802100	0.24905500	0.00817800
O	2.16584700	0.21494400	-0.04865300
H	2.49595800	-0.57370500	0.39374900
IM5A (83.2) (-591.498619)			
C	0.78385501	0.22063282	0.00000000
C	0.01835994	1.35460177	0.00000000
C	-1.38536905	1.09978268	0.00000000
C	-1.67791597	-0.23222134	0.00000000
S	-0.23698091	-1.19053125	0.00000000
H	0.44874287	2.34851380	0.00000000
H	-2.13993310	1.87557064	0.00000000
H	-2.64455694	-0.71150540	0.00000000
C	2.27882501	0.10505191	0.00000000
H	2.64775207	-0.42578427	0.88272477
H	2.64775207	-0.42578427	-0.88272477
H	2.72545295	1.10147193	0.00000000
IM6A (46.79) (-665.37617)			
C	0.35723800	-0.64021900	-0.00022700
C	0.60196200	0.68788300	-0.00017100
C	-0.52229300	1.54661400	-0.00000700
C	-1.65051300	0.75730600	0.00010400
S	-1.32954500	-0.96236500	0.00001100
H	-0.53315900	2.62648400	0.00009400
H	-2.67934200	1.08315400	0.00008000
C	1.86156500	-0.84328300	0.00010200
H	2.30965300	-1.25957000	-0.90227000
H	2.30925100	-1.25939000	0.90275300
O	1.99732100	0.64466900	0.00004500

IM7A	(137.01)	(-666.009365)		
C	0.35219400	0.46966900	-0.00003900	
C	-0.70047400	1.40872000	0.00001700	
C	-1.97204300	0.81242200	-0.00000400	
C	-1.93330100	-0.56280600	0.00002800	
S	-0.30452200	-1.17064300	-0.00000300	
H	-0.52625600	2.47673300	0.00008000	
H	-2.89729200	1.37444000	-0.00005100	
H	-2.76040000	-1.25537900	0.00004900	
C	1.71072800	0.71390300	-0.00002800	
H	2.10847400	1.72170300	-0.00001600	
O	2.58937900	-0.33031000	-0.00003700	
H	3.49017700	0.00382400	0.00044000	
IM8A	(27.32)	(-665.969481)		
C	-0.34156600	0.45814700	0.00002600	
C	0.66254700	1.39142000	-0.00008200	
C	1.96258700	0.81013100	-0.00006800	
C	1.92224400	-0.55545100	-0.00001000	
S	0.29938000	-1.15088500	0.00006200	
H	0.48091200	2.45951800	-0.00012800	
H	2.88114800	1.38215400	-0.00018800	
H	2.74747500	-1.25076700	0.00003200	
C	-1.83020600	0.67437600	0.00021000	
H	-2.13213300	1.30352000	-0.86425900	
H	-2.13198500	1.30236800	0.86558700	
O	-2.61114100	-0.43179700	-0.00031200	
IM9A	(41.76)	(-741.648768)		
C	-0.30887700	-0.40016600	0.22481000	
C	1.49413200	1.18488500	0.27664800	
C	2.12986700	0.06278900	-0.06073700	
S	1.06748400	-1.34492400	-0.22028800	
H	1.98289800	2.14375800	0.39107900	
H	3.18588600	-0.07101500	-0.24734300	
C	-1.68302000	-0.96200500	0.33982600	
H	-2.03603900	-0.96810000	1.40425700	
H	-1.74871000	-2.01915600	0.03632500	
O	-2.66205100	-0.20418200	-0.27038300	
C	0.00393300	1.05765000	0.43723300	
H	-0.30634900	1.36040400	1.45500800	
O	-0.64076000	1.92915400	-0.50892800	
H	-1.55115400	1.61421400	-0.58691100	

TS1At	(-1104.25)	(-741.605745)	
C	0.11072800	-0.40302100	0.67147300
C	0.58399500	0.85136300	1.08187800
C	1.72010800	1.28461100	0.37804500
C	2.13263100	0.38761800	-0.58066000
S	1.12479500	-1.01229100	-0.63074200
H	0.09911800	1.41819200	1.86550000
H	2.22266000	2.22501000	0.56103600
H	2.97135600	0.47202400	-1.25445800
C	-1.03024600	-1.10084100	1.12341200
H	-1.44327000	-0.80588000	2.08414300
H	-1.14677800	-2.14890900	0.86619700
O	-2.80855600	0.07939400	-0.41602000
H	-2.11097500	-0.47677000	0.23583600
O	-2.15296100	1.09493100	-0.87288900
TS1As	(-981.91)	(-741.595242)	
C	0.02100600	0.81277000	0.35443000
C	0.99303200	1.31219200	-0.52998300
C	2.04117600	0.42702900	-0.74976600
C	1.89574600	-0.77618600	-0.05866700
S	0.45661800	-0.83615400	0.82006900
H	0.92770000	2.30509600	-0.95424500
H	2.89373300	0.63879500	-1.38125300
H	2.55291700	-1.63169700	-0.08290500
C	-1.19974000	1.37476900	0.76165700
H	-1.38203800	2.41019200	0.48534900
H	-1.64334100	1.05843100	1.69917400
O	-2.46104800	-0.31893700	-0.53527100
H	-2.05467500	0.66253600	-0.14963400
O	-1.42739000	-1.05210400	-0.89018300
TS2A	(-1345.53)	(-741.619784)	
C	-0.12843800	0.49208100	-0.18435800
C	-1.14533100	1.37575100	0.09183000
C	-2.39489400	0.73402900	0.30194000
C	-2.30632800	-0.62738600	0.19574400
S	-0.69895300	-1.14517900	-0.16755800
H	-1.00011800	2.44805500	0.13582100
H	-3.31597200	1.25838400	0.51927600
H	-3.09257600	-1.35884400	0.30329300
C	1.30208900	0.80316100	-0.43464700
H	1.81484800	0.89410000	0.67668100
H	1.50026100	1.80146200	-0.85903600

O	2.11355800	-0.14500900	-0.83956400
O	2.85680400	-0.19226900	0.92428700
H	3.55132100	-0.68787700	1.40406700

TS3A (-797.23) (-741.600721)

C	-0.17694400	-0.41053800	0.55535200
C	0.07689900	1.00067800	0.66393300
C	1.40726700	1.33329500	0.20479200
C	2.07713100	0.26618500	-0.30256600
S	1.14470300	-1.20196700	-0.18980800
H	-0.40939800	1.59696200	1.42657400
H	1.81359900	2.33461200	0.24840700
H	3.08418800	0.23016300	-0.68958000
C	-1.59561600	-0.93175100	0.51869200
H	-2.10036900	-0.70694700	1.47136400
H	-1.62205700	-2.02429400	0.38189000
O	-2.20953000	-0.35732000	-0.58405700
O	-1.39033500	1.48024400	-0.45582400
H	-1.01470700	1.27037300	-1.32388300

TS4A (-904.59) (-741.593562)

C	0.24147700	0.19412900	-0.20226700
C	-0.54893400	1.35719700	-0.15208400
C	-1.92987800	1.10694500	-0.01418500
C	-2.23713400	-0.22803900	0.05633800
S	-0.82077200	-1.21702000	-0.03229900
H	-0.11987500	2.34265200	-0.28261500
H	-2.67901600	1.88756700	0.01348200
H	-3.20816300	-0.68924800	0.14809500
C	1.62199100	0.07100500	-0.98082000
H	1.76542500	1.00777500	-1.53564100
H	1.57062200	-0.77048200	-1.68009700
O	2.60761400	-0.11976100	-0.02601200
O	1.32273900	0.08084400	1.28044200
H	1.47540300	0.99797300	1.57621900

TS5A (-434.32) (-741.853147)

C	0.02131200	-0.34932000	0.03571900
C	-0.02303600	1.03616900	-0.07577100
C	1.26735400	1.59083900	-0.20415700
C	2.27907200	0.65871800	-0.09037500
S	1.68745700	-0.94523600	0.14161300
H	-1.62975200	1.31488200	0.11518100
H	1.47239300	2.65198000	-0.27709900

H	3.34416900	0.84003600	-0.04002100
C	-1.16366500	-1.23068400	0.08315200
H	-1.33229200	-1.60674700	1.11380100
H	-0.97982400	-2.17895700	-0.48543500
O	-2.26614400	-0.77759500	-0.54822300
O	-2.65438900	1.12667900	0.24933300
H	-2.79595800	1.07557100	1.20747500

TS6A (-1466.35) (-741.606401)

C	-0.05671600	-0.29759800	-0.16586300
C	-0.18883500	1.06377900	-0.38951100
C	-1.51372600	1.51633400	-0.21786700
C	-2.38281000	0.50710100	0.12016400
S	-1.59237200	-1.01451700	0.26047200
H	0.67592600	1.67902400	-0.59531900
H	-1.82143900	2.54699100	-0.33224500
H	-3.44615200	0.57305300	0.29367500
C	1.15849500	-1.03537200	-0.21384700
H	2.00424900	-1.19968200	-1.32552500
H	1.25907400	-1.96335800	0.35047900
O	2.29725600	-0.38858400	-0.56538200
O	2.82111000	0.80194300	0.82080500
H	3.76090800	0.76389300	0.59954700

TS7A (-567.55) (-741.670526)

C	-0.04955500	0.70967100	1.13468000
C	1.26744700	0.99957800	0.89958600
C	1.82712000	0.19645400	-0.09842400
S	0.86665100	-1.07788400	-0.65448600
H	-0.67254200	1.17433700	1.88606700
H	1.80648900	1.81647100	1.35818100
H	2.81825100	0.33559500	-0.51220200
C	-1.43105300	0.50536300	-0.78518100
H	-2.44390900	0.46291400	-0.30217100
H	-1.55046900	-0.01596100	-1.76813800
O	-0.86437400	1.69767100	-0.86406500
C	-0.62901000	-0.37140000	0.27934000
O	-1.33868300	-1.34545100	0.96380500
H	-2.10948700	-1.58296300	0.43211400

CBt (27.11) (-741.611699)

C	-0.37221500	0.75915600	0.35622700
C	0.07395000	-0.48351000	0.87387400
C	-0.78731800	-1.55490000	0.58318500

C	-1.89197800	-1.18453900	-0.15211200
S	-1.89917100	0.50878000	-0.50703200
H	0.97669300	-0.55915000	1.46785600
H	-0.61073100	-2.57293200	0.90524300
H	-2.69682900	-1.81152700	-0.50345500
C	0.22938700	1.99653100	0.45734400
H	-0.20768800	2.88455700	0.02164000
H	1.17280900	2.09359000	0.97876100
O	2.57356500	-0.49320500	-0.96129200
H	1.63307300	-0.52804400	-0.67189400
O	3.25249200	-0.11221900	0.11169800

IM1B (57.69)	(-741.663617)		
C	0.23396300	0.88651300	-0.28188600
C	-0.65250100	-0.25501800	-0.79623400
C	0.06425000	-1.54459300	-0.51393500
C	1.26830300	-1.40703500	0.03430000
S	1.77654000	0.26141000	0.34476500
H	-0.83710900	-0.13047100	-1.87116400
H	-0.38935000	-2.49588200	-0.75771700
H	1.95564500	-2.19826000	0.30030300
C	-0.12555400	2.16977200	-0.27550200
H	0.50991600	2.95187400	0.12089100
H	-1.08653400	2.46337900	-0.68286900
O	-1.94614600	-0.36983900	1.15115600
H	-1.83756400	0.54510700	1.45231500
O	-1.98765600	-0.18217800	-0.28596200

IM2B (5846)	(-591.46486)		
C	0.89768900	0.18090700	0.00001300
C	0.04739200	1.44730700	0.00008100
C	-1.39981500	1.03476300	-0.00000100
C	-1.61228400	-0.27905900	-0.00005100
S	-0.14729600	-1.27274100	-0.00001300
H	0.28435900	2.06027900	-0.87811200
H	-2.19973500	1.76485900	-0.00000800
H	-2.56893600	-0.78314900	-0.00010300
C	2.22861700	0.12338400	-0.00002500
H	2.76867000	-0.81507900	-0.00007200
H	2.81851000	1.03301200	-0.00000600
H	0.28428300	2.06012600	0.87840400

IM3B (114.91)	(-665.434662)		
C	0.32261000	0.76537100	0.00001500

C	0.96058200	-0.61359900	-0.00012300
C	-0.09536000	-1.63114200	0.00001500
C	-1.33665400	-1.11557000	0.00009500
S	-1.44783100	0.63835900	-0.00002000
H	0.13539900	-2.68706100	0.00004600
H	-2.26409900	-1.67218300	0.00018100
C	1.03184700	1.89269300	0.00008100
H	0.58467100	2.87875500	0.00014000
H	2.11372500	1.81347400	0.00005700
O	2.16218100	-0.79165500	-0.00007500

IM4B (73.0) (-741.157804)			
C	-0.25790900	-0.37641000	0.11292600
C	-0.01108200	1.05481600	0.07831700
C	1.42657900	1.32092700	-0.06023800
C	2.16456600	0.20016700	-0.12176800
S	1.18876000	-1.27109500	-0.01806800
H	1.81722900	2.32760800	-0.11283700
H	3.23418400	0.09928900	-0.22887800
C	-1.62749200	-0.96109800	0.31262300
H	-1.64370800	-2.01808600	0.03759000
H	-1.86769400	-0.90341200	1.38765300
O	-2.60812000	-0.30742200	-0.46688400
H	-2.50955400	0.63961700	-0.28837200
O	-0.91920500	1.90268400	0.16223100

IM5B (16470) (-666.009306)			
C	-0.23964800	0.77463100	0.00009700
C	-0.87106900	-0.49765700	0.00001800
C	0.01806700	-1.58605800	-0.00000200
C	1.33853300	-1.19845700	0.00031700
S	1.51458800	0.52743000	-0.00031400
H	-2.50560900	-1.48500900	-0.00001700
H	-0.29708500	-2.62294900	-0.00000800
H	2.21248300	-1.83016100	0.00051400
C	-0.84473200	2.00799400	0.00023800
H	-0.27452800	2.92661100	0.00016100
H	-1.92437000	2.07082400	0.00042700
O	-2.23140000	-0.56261300	-0.00000700

IM6B (75.0) (-665.940144)			
C	0.28497400	0.80155500	0.08074400
C	0.96137300	-0.57180500	0.27267300
C	-0.09021600	-1.63461500	0.03293800

C	-1.32581900	-1.15906700	-0.09827200
S	-1.48165400	0.60472700	-0.01724100
H	1.22633900	-0.63539800	1.36375100
H	0.17900400	-2.68193100	0.01198100
H	-2.22992700	-1.73394000	-0.24493000
C	0.93957000	1.95288200	-0.02733600
H	0.43717500	2.89777500	-0.19088600
H	2.02169600	1.95580900	0.03059900
O	2.18161100	-0.72645600	-0.28239400

TS1Bt	(-1780.66)	(-741.592232)	
C	-0.16578200	0.74124800	0.49178100
C	0.08564800	-0.60509200	0.98707900
C	-0.96638500	-1.51440600	0.58882500
C	-1.84900900	-0.97863900	-0.28794200
S	-1.53279000	0.70355000	-0.63827500
H	0.57350500	-0.71441300	1.95378800
H	-1.01347000	-2.54373000	0.92026000
H	-2.68045300	-1.46934900	-0.77182900
C	0.53876400	1.87152100	0.75771800
H	0.29863600	2.82024900	0.29662100
H	1.37541900	1.84242600	1.44290900
O	2.20595200	-1.04440400	-0.44452800
H	1.18752500	-0.92530600	0.20118500
O	2.65955700	0.12509500	-0.68738500

TS2B	(-1790.67)	(-741.591584)	
C	-0.32335000	0.86991700	-0.08947500
C	0.61896200	-0.31040200	-0.21734300
C	-0.16035800	-1.58285800	-0.25124400
C	-1.46054000	-1.41086700	0.00645200
S	-1.96026000	0.26544100	0.25755900
H	1.21770800	-0.35048900	0.86225300
H	0.31893500	-2.53589300	-0.42809900
H	-2.21842600	-2.17873700	0.06968600
C	0.02068600	2.15356000	-0.20246900
H	-0.69610800	2.95924100	-0.11188700
H	1.05599700	2.40579200	-0.39726800
O	2.74778000	-0.08317000	0.78951400
H	3.33650100	-0.85697100	0.80708200
O	1.77436300	-0.16759300	-0.83929300

TS3B	(-523.83)	(-741.596710)	
C	0.04553500	-0.63082900	-0.47754100

C	0.35169700	0.85616300	-0.59873800
C	-0.77898400	1.57181300	0.10560800
C	-1.81526200	0.79232600	0.42743000
S	-1.57048500	-0.92242000	0.05860600
H	0.15584900	1.04874800	-1.69251800
H	-0.75422100	2.64450700	0.24615300
H	-2.76759900	1.08780100	0.84484800
C	1.10251600	-1.48039600	-0.48432000
H	1.03947700	-2.48176300	-0.07869800
H	2.00377600	-1.20357900	-1.00749300
O	2.03663900	-0.32047300	1.15381400
H	2.68320500	0.38636500	1.02782200
O	1.63014200	1.14824600	-0.41787000

TS4B (-1496.45) (-741.590276)

C	-0.27099500	0.81966700	0.21282700
C	0.47226900	-0.41768600	0.48683800
C	-0.27639300	-1.58208300	0.09450300
C	-1.55754500	-1.28788900	-0.22620900
S	-1.95817100	0.41487900	-0.18841800
H	1.15472600	-0.50949700	1.68433700
H	0.14350300	-2.57755700	0.11175800
H	-2.33531600	-1.99164600	-0.48662500
C	0.29213700	2.03235700	0.14173800
H	-0.26292700	2.91716600	-0.14158000
H	1.35659100	2.11695800	0.32325000
O	2.67131200	-0.05988600	-0.95704300
H	3.47269500	-0.53586000	-0.70204800
O	1.80926600	-0.37059200	0.70297100

CCt (25.11) (-741.610988)

C	1.84030000	0.18368300	0.18929500
C	1.16357600	1.37188000	-0.17055100
C	-0.09392900	1.15063900	-0.74795100
C	-0.42629900	-0.18877400	-0.84716000
S	0.82771600	-1.21024400	-0.22889900
H	1.59725800	2.34935600	-0.00636700
H	-0.74634800	1.94097600	-1.09734000
H	-1.32245400	-0.61737300	-1.27301800
C	3.08080200	0.04397600	0.77586600
H	3.50148500	-0.92488600	1.00778600
H	3.66647900	0.92210500	1.01607300
O	-2.87155800	0.23180300	1.02702800
H	-1.93210200	0.24951600	0.73276000

O	-3.55275100	-0.22233000	-0.01634200
IM1C (65.20) (-741.668604)			
C	1.52008500	0.10994300	0.12402700
C	0.88264700	1.39611700	-0.15075000
C	-0.36265300	1.33787200	-0.62586600
C	-0.94565700	-0.03810000	-0.78903900
S	0.41446800	-1.20838400	-0.33521300
H	1.42042900	2.31848300	0.03692000
H	-0.97156800	2.20013700	-0.87188200
H	-1.25993200	-0.25052300	-1.81534500
C	2.75266500	-0.05729000	0.61745400
H	3.17077400	-1.03535400	0.81726200
H	3.37492900	0.80419000	0.82976200
O	-2.16427200	-0.24818300	-0.09054200
O	-1.96356400	-0.00582600	1.32633100
H	-2.42594500	0.83803300	1.42542500
IM2C (110.90) (-591.471156)			
C	-0.93319900	0.17282800	-0.00002100
C	-0.12812800	1.39263900	-0.00008100
C	1.19574300	1.22068000	-0.00005500
C	1.67866800	-0.20030700	0.00003200
S	0.15941600	-1.24230800	0.00007200
H	-0.61352100	2.36173600	-0.00014300
H	1.91176600	2.03458100	-0.00009300
H	2.28056000	-0.42849100	0.88471900
C	-2.27050100	0.10665200	-0.00003200
H	-2.80647100	-0.83354000	0.00001600
H	-2.85907200	1.01627900	-0.00009100
H	2.28058400	-0.42859200	-0.88461200
IM3C (115.73) (-665.446482)			
C	1.23929500	0.07583800	0.00002900
C	0.61340700	1.39502900	0.00007000
C	-0.72683500	1.39930700	0.00007300
C	-1.34775800	0.05888800	0.00004800
S	-0.00136900	-1.19179800	-0.00012900
H	1.23047500	2.28584900	0.00011200
H	-1.36503600	2.27270000	0.00011000
C	2.56076700	-0.14166800	0.00004600
H	2.98543000	-1.13726500	-0.00002500
H	3.24971400	0.69547300	0.00011600
O	-2.51399200	-0.22154500	0.00002000

IM4C	(-37.29)	(-666.005666)	
C	-1.30897200	0.09931500	0.00000100
C	-0.72170700	1.38600300	-0.00003400
C	0.68166400	1.39036900	-0.00000700
C	1.22217000	0.12622700	0.00003100
S	-0.00723300	-1.12463600	-0.00003500
H	-1.32922600	2.28125600	-0.00001900
H	1.29974500	2.27784600	0.00002300
H	2.69660100	-1.09860600	0.00122100
C	-2.63597300	-0.25476100	0.00005400
H	-2.96131500	-1.28579300	0.00009800
H	-3.39507200	0.51710100	0.00004700
O	2.54773800	-0.14756900	-0.00013600
IM5C	(69.48)	(-665.946723)	
C	-1.27227800	0.09233200	-0.03446100
C	-0.61054600	1.39743900	-0.02002300
C	0.71653100	1.39419400	0.10481800
C	1.36087400	0.03336900	0.24560300
S	-0.06291500	-1.20779000	0.07048600
H	-1.20361500	2.30001800	-0.11592400
H	1.35335400	2.26962100	0.11629900
H	1.67105400	-0.10495300	1.31503400
C	-2.59517700	-0.10106900	-0.11618300
H	-3.03801800	-1.08828400	-0.13077600
H	-3.26555700	0.74846900	-0.17552600
O	2.48662400	-0.21222700	-0.40192600
TS1Ct	(-1728.41)	(-741.593698)	
C	-1.53726000	0.36889700	-0.15901100
C	-0.71844700	1.26389400	0.60829600
C	0.35577300	0.66852800	1.21070000
C	0.52410100	-0.71818000	0.88801200
S	-0.88568000	-1.27592200	-0.03409800
H	-0.95169900	2.31852600	0.67728000
H	1.06481000	1.19451200	1.83630300
H	0.93596500	-1.42459300	1.60407100
C	-2.64063300	0.68306600	-0.89152300
H	-3.19031100	-0.05888000	-1.45514200
H	-2.99766800	1.70495300	-0.92140500
O	2.52314000	-0.40047800	-0.72007900
H	1.59968100	-0.63910800	-0.01251400
O	2.70297200	0.86574200	-0.67015400

TS2C (-1142.16)

C	-1.71267800	0.00200000	0.09708400
C	-1.19891000	1.37154200	0.07498100
C	0.11878000	1.50859200	-0.10105300
C	0.87505600	0.22066300	-0.18969300
S	-0.40722500	-1.15825000	-0.22686400
H	-1.88278900	2.20332200	0.19720800
H	0.66554000	2.44134100	-0.14448200
H	1.34099200	0.00634100	0.89904300
C	-2.99147500	-0.34029100	0.31989200
H	-3.32416100	-1.36982200	0.33165500
H	-3.73686500	0.42888400	0.48494800
O	1.98065800	0.09859000	-0.84414000
O	2.91552500	-0.22832900	0.80073400
H	3.73878600	-0.71517700	1.00144000

TS3C (-1499.03) (-741.591974)

C	1.68870200	0.00891400	0.14226000
C	1.17645500	1.36835800	0.15849700
C	-0.12704200	1.48559500	-0.17257700
C	-0.74808400	0.23210500	-0.53719900
S	0.37056300	-1.11430500	-0.28151800
H	1.81879400	2.19600600	0.43167100
H	-0.70181100	2.40174300	-0.18126000
H	-1.60624300	0.33444300	-1.64557300
C	2.94899000	-0.37659400	0.39734900
H	3.25452500	-1.41445500	0.37560800
H	3.70348700	0.36218500	0.64008900
O	-2.07505700	0.02531100	-0.61601300
O	-2.76935900	-0.19578700	1.11874400
H	-3.27655300	-0.99751600	0.93191600