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

Supplementary Material

From electronic structure to model application for alkyl cyclohexanes combustion chemistry: H-atom abstraction reactions by $H\dot{O}_2$ radical

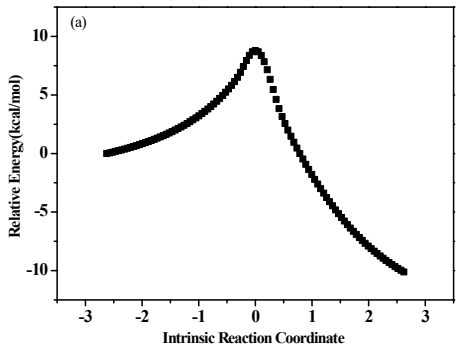
Mingxia Liu[1], Xin Hui[2], Xin Xue[2], Yuzhen Lin[2], Chong-Wen Zhou*[1,3]

[1]*School of Energy and Power Engineering, Beihang University, Beijing 100191, PR China*

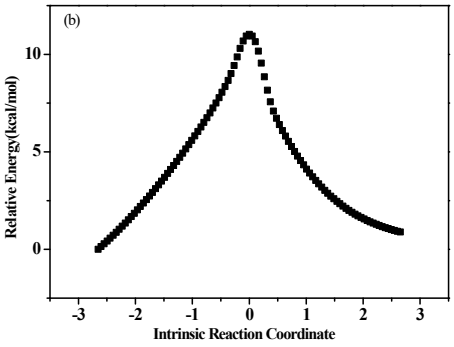
[2]*National Key Laboratory of Science and Technology on Aero-Engine Aero-thermodynamics, Research Institute of Aero-Engine, Beihang University, Beijing, 100191, PR China*

[3]*Combustion Chemistry Centre, School of Chemistry, Ryan Institute, National University of Ireland, Galway, Galway H91 TK33, Ireland.*

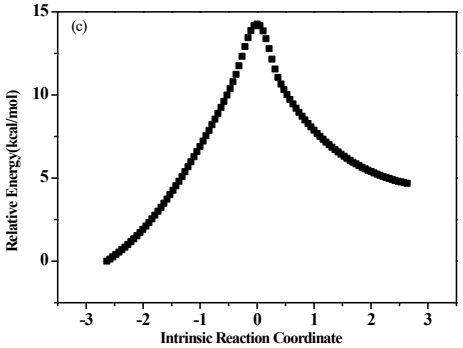
E-mail address: chongwen.zhou@universityofgalway.ie (C.-W. Zhou)



(a) MCH+HO_2→MP1+H_2O_2



(b) MCH+HO_2→MP2+H_2O_2



(c) MCH+HO_2→MP3+H_2O_2

Fig. S 1. The representative IRC profiles for reactions of MCH+HO_2→MP1+H_2O_2 (a, primary carbon site), MCH+HO_2→MP2+H_2O_2 (b, tertiary carbon site), MCH+HO_2→MP3+H_2O_2 (c, secondary carbon site).

Table S 1

Early or late transition states for these investigated reactions.

Reactions	$D_{C\text{-}H}$(R)	$D_{H\text{-}O}$(P)	$D_{C\text{-}H}$(TS)	$D_{H\text{-}O}$(TS)	γ	Type
MCH+HO_2 = MP1+H_2O_2	1.09	0.96	1.34	1.18	1.14	Late
MCH+HO_2 = MP2+H_2O_2	1.10	0.96	1.29	1.23	0.70	Early
MCH+HO_2 = MP3+H_2O_2	1.10	0.96	1.31	1.22	0.81	Early
MCH+HO_2 = MP4+H_2O_2	1.10	0.96	1.31	1.21	0.84	Early
MCH+HO_2 = MP5+H_2O_2	1.10	0.96	1.31	1.21	0.84	Early
ECH+HO_2 = EP1+ H_2O_2	1.09	0.96	1.34	1.18	1.14	Late
ECH+HO_2 = EP2+ H_2O_2	1.10	0.96	1.31	1.21	0.84	Early
ECH+HO_2 = EP3+ H_2O_2	1.10	0.96	1.29	1.24	0.68	Early
ECH+HO_2 = EP4+ H_2O_2	1.10	0.96	1.31	1.22	0.81	Early
ECH+HO_2 = EP5+ H_2O_2	1.10	0.96	1.31	1.22	0.81	Early
ECH+HO_2 = EP6+ H_2O_2	1.10	0.96	1.31	1.21	0.84	Early
nPCH+HO_2 = nP1+ H_2O_2	1.09	0.96	1.34	1.18	1.14	Late
nPCH+HO_2 = nP2+ H_2O_2	1.09	0.96	1.31	1.20	0.92	Early
nPCH+HO_2 = nP3+ H_2O_2	1.10	0.96	1.31	1.22	0.81	Early
nPCH+HO_2 = nP4+ H_2O_2	1.10	0.96	1.29	1.24	0.68	Early
nPCH+HO_2 = nP5+ H_2O_2	1.10	0.96	1.31	1.22	0.81	Early
nPCH+HO_2 = nP6+ H_2O_2	1.10	0.96	1.31	1.22	0.81	Early
nPCH+HO_2 = nP7+ H_2O_2	1.10	0.96	1.31	1.21	0.84	Early
iPCH+HO_2 = iP1+ H_2O_2	1.09	0.96	1.34	1.18	1.14	Late
iPCH+HO_2 = iP2+ H_2O_2	1.10	0.96	1.29	1.24	0.68	Early
iPCH+HO_2 = iP3+ H_2O_2	1.10	0.96	1.29	1.24	0.68	Early
iPCH+HO_2 = iP4+ H_2O_2	1.10	0.96	1.31	1.22	0.81	Early
iPCH+HO_2 = iP5+ H_2O_2	1.10	0.96	1.31	1.22	0.81	Early
iPCH+HO_2 = iP6+ H_2O_2	1.10	0.96	1.31	1.22	0.81	Early
iBCH+HO_2 = iBP1+ H_2O_2	1.09	0.96	1.33	1.19	1.04	Late
iBCH+HO_2 = iBP2+ H_2O_2	1.10	0.96	1.29	1.23	0.70	Early
iBCH+HO_2 = iBP3+ H_2O_2	1.10	0.96	1.31	1.21	0.84	Early
iBCH+HO_2 = iBP4+ H_2O_2	1.10	0.96	1.30	1.23	0.74	Early
iBCH+HO_2 = iBP5+ H_2O_2	1.10	0.96	1.31	1.22	0.81	Early
iBCH+HO_2 = iBP6+ H_2O_2	1.10	0.96	1.31	1.22	0.81	Early
iBCH+HO_2 = iBP7+ H_2O_2	1.10	0.96	1.31	1.21	0.84	Early
sBCH+HO_2= sBP1+ H_2O_2	1.09	0.96	1.33	1.19	1.04	Late
sBCH+HO_2= sBP2+ H_2O_2	1.09	0.96	1.32	1.21	0.92	Early
sBCH+HO_2= sBP3+ H_2O_2	1.09	0.96	1.34	1.19	1.09	Late
sBCH+HO_2= sBP4+ H_2O_2	1.10	0.96	1.28	1.25	0.62	Early
sBCH+HO_2= sBP5+ H_2O_2	1.10	0.96	1.30	1.24	0.71	Early
sBCH+HO_2= sBP6+ H_2O_2	1.10	0.96	1.31	1.21	0.84	Early
sBCH+HO_2= sBP7+ H_2O_2	1.10	0.96	1.30	1.22	0.77	Early
sBCH+HO_2= sBP8+ H_2O_2	1.09	0.96	1.31	1.22	0.85	Early

Table S 2

The influence of tunning effect on the rate constants at 500-2000 K.

T(K)	$MCH+HO_2 \rightarrow MP1+H_2O_2$			$MCH+HO_2 \rightarrow MP2+H_2O_2$			$MCH+HO_2 \rightarrow MP3+H_2O_2$		
	K1	K1’	K1/K1’	K2	K2’	K2/K2’	K3	K3’	K3/K3’
500	7.02E+02	2.80E+02	2.5	1.91E+05	9.39E+04	2.0	5.77E+04	2.67E+04	2.2
600	2.69E+04	1.43E+04	1.9	2.64E+06	1.62E+06	1.6	1.15E+06	6.74E+05	1.7
700	4.12E+05	2.61E+05	1.6	1.92E+07	1.34E+07	1.4	1.09E+07	7.40E+06	1.5
800	3.48E+06	2.46E+06	1.4	9.17E+07	6.98E+07	1.3	6.39E+07	4.74E+07	1.3
900	1.94E+07	1.48E+07	1.3	3.27E+08	2.64E+08	1.2	2.67E+08	2.11E+08	1.3
1000	8.04E+07	6.50E+07	1.2	9.42E+08	7.95E+08	1.2	8.75E+08	7.22E+08	1.2
1100	2.67E+08	2.23E+08	1.2	2.31E+09	2.01E+09	1.2	2.39E+09	2.05E+09	1.2
1200	7.43E+08	6.44E+08	1.2	5.03E+09	4.47E+09	1.1	5.68E+09	5.00E+09	1.1
1300	1.81E+09	1.60E+09	1.1	9.90E+09	8.97E+09	1.1	1.21E+10	1.08E+10	1.1
1400	3.96E+09	3.56E+09	1.1	1.80E+10	1.66E+10	1.1	2.34E+10	2.14E+10	1.1
1500	7.91E+09	7.22E+09	1.1	3.07E+10	2.85E+10	1.1	4.23E+10	3.91E+10	1.1
1600	1.47E+10	1.35E+10	1.1	4.96E+10	4.65E+10	1.1	7.18E+10	6.68E+10	1.1
1700	2.56E+10	2.39E+10	1.1	7.65E+10	7.22E+10	1.1	1.16E+11	1.09E+11	1.1
1800	4.25E+10	4.00E+10	1.1	1.14E+11	1.08E+11	1.0	1.79E+11	1.70E+11	1.1
1900	6.73E+10	6.38E+10	1.1	1.63E+11	1.56E+11	1.0	2.66E+11	2.53E+11	1.0
2000	1.03E+11	9.75E+10	1.1	2.27E+11	2.19E+11	1.0	3.83E+11	3.67E+11	1.0

KX(X=1-3) represents rate constants with tunneling correction.

KX’(X=1-3) represents rate constants without tunneling correction.

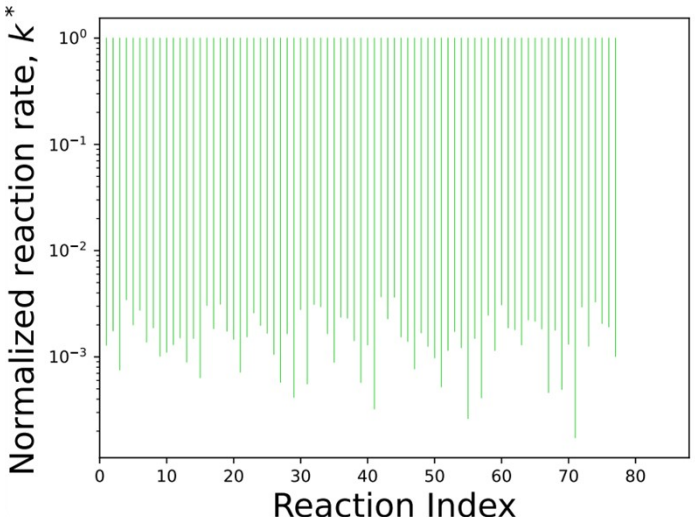


Fig. S 2. The maximum ratio of the rate coefficient to its collision limit.

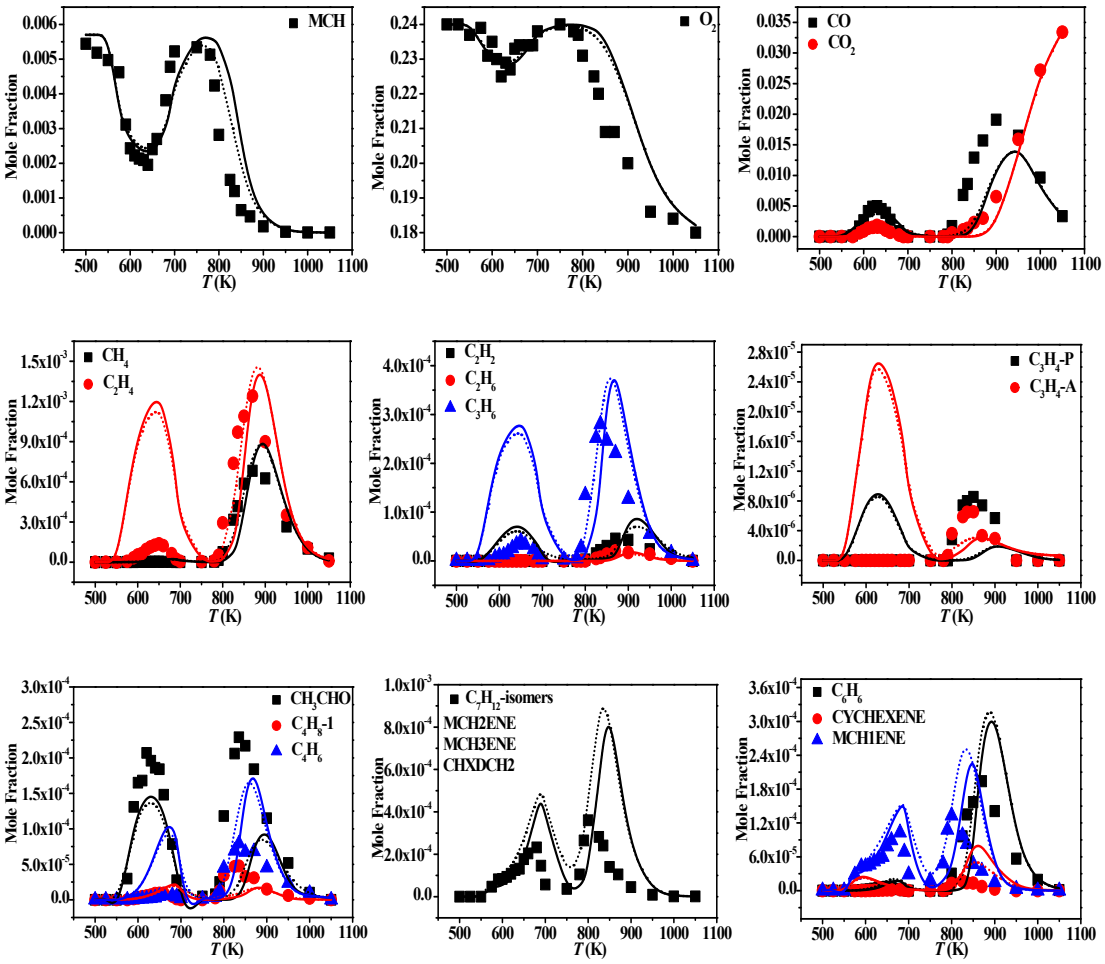


Fig. S 3. Speciation results comparison for the conditions of 0.57% MCH, 24.0% O_2, 75.43% He, φ = 0.25, p = 1.06 bar, and at a residence time of 2 s. Symbols: JSR experimental measurements [1]; Simulations from the literature [1] (Dotted lines: the previous model, Solid lines: the updated model).

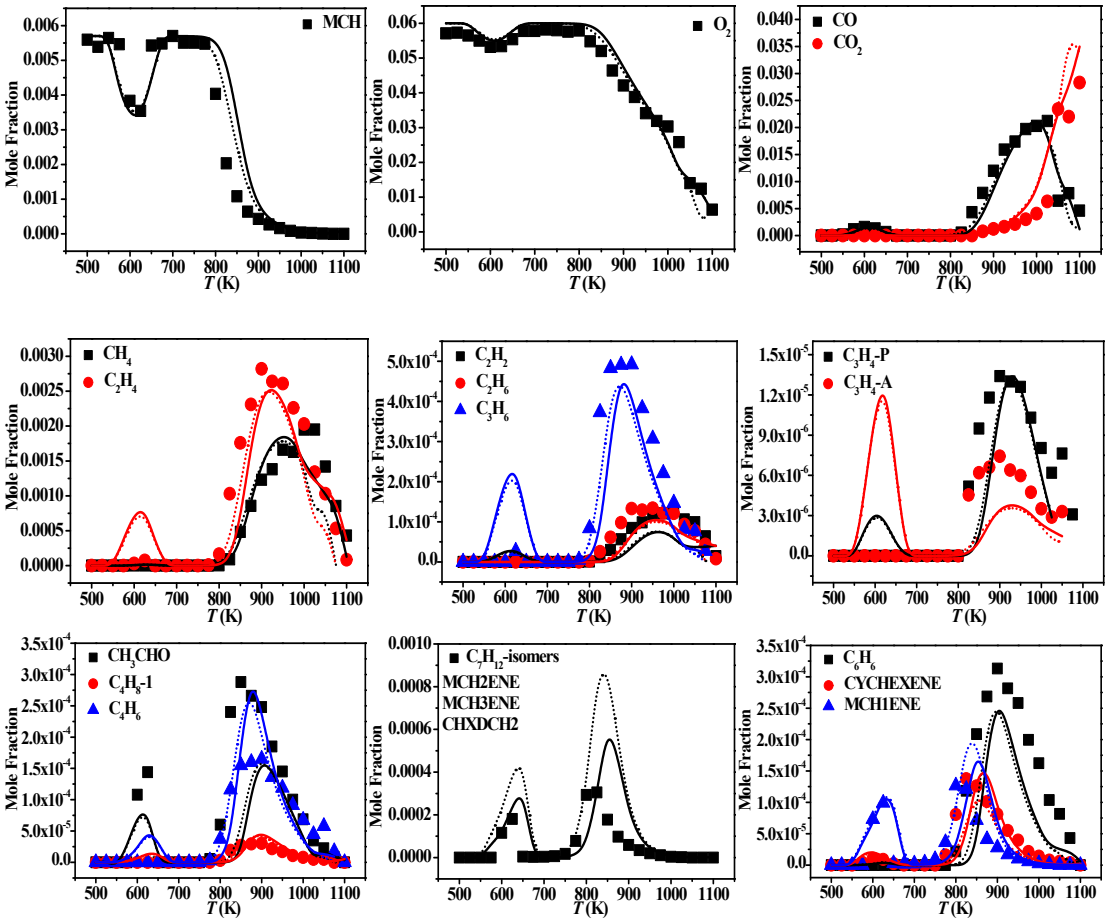


Fig. S 4. Speciation results comparison for the conditions of 0.57% MCH, 6.0% O_2, 93.43% He, φ = 1.0, p = 1.06 bar, and at a residence time of 2 s. Symbols: JSR experimental measurements [1]; Simulations from the literature [1] (Dotted lines: the previous model, Solid lines: the updated model).

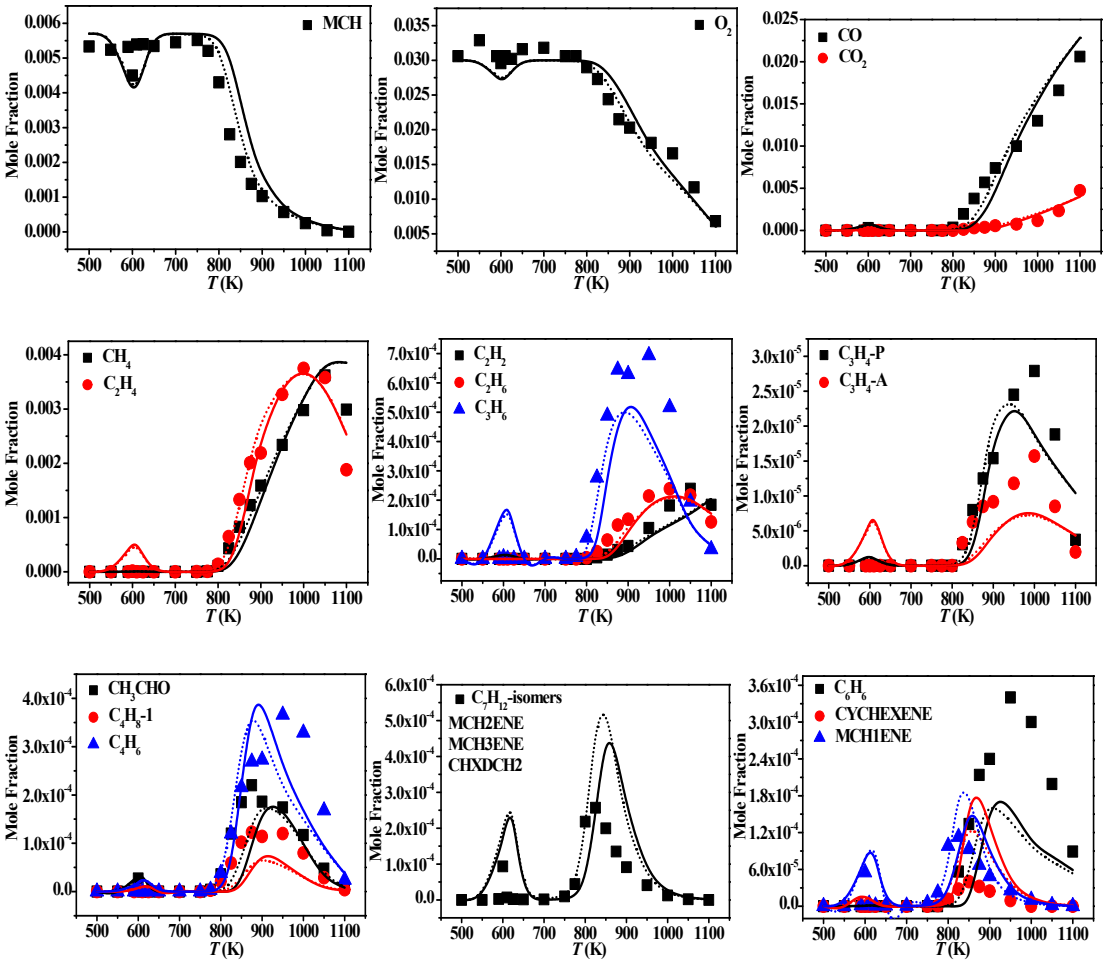


Fig. S 5. Speciation results comparison for the conditions of 0.57% MCH, 3.0% O_2, 96.43% He, $\varphi = 2.0$, $p = 1.06$ bar, and at a residence time of 2 s. Symbols: JSR experimental measurements [1]; Simulations from the literature [1] (Dotted lines: the previous model, Solid lines: the updated model).

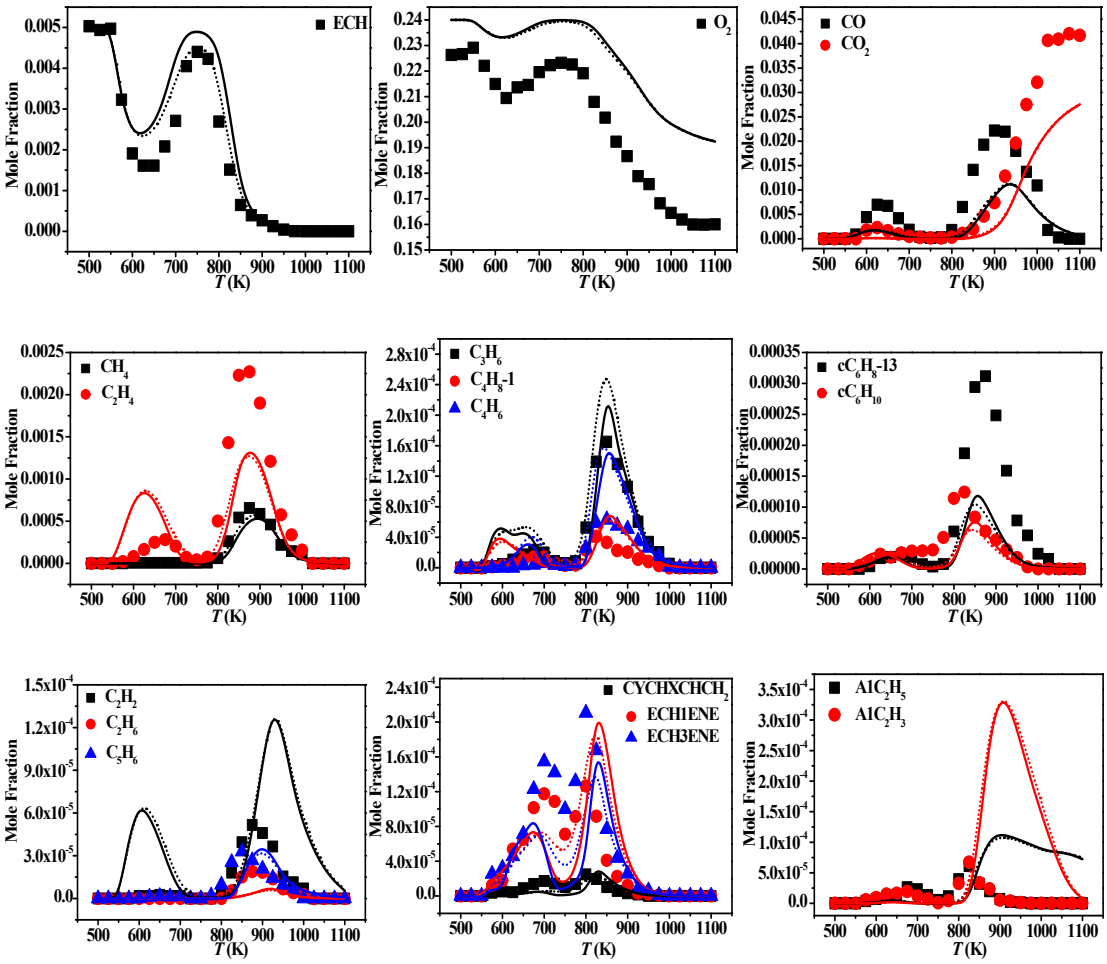


Fig. S 6. Speciation results comparison for the conditions of 0.5% ECH, 24% O_2, 75.5% He, φ = 0.25, p = 1.06 bar, and at a residence time of 2 s. Symbols: JSR experimental measurements [2]; Simulations from the literature [3] (Dotted lines: the previous model, Solid lines: the updated model).

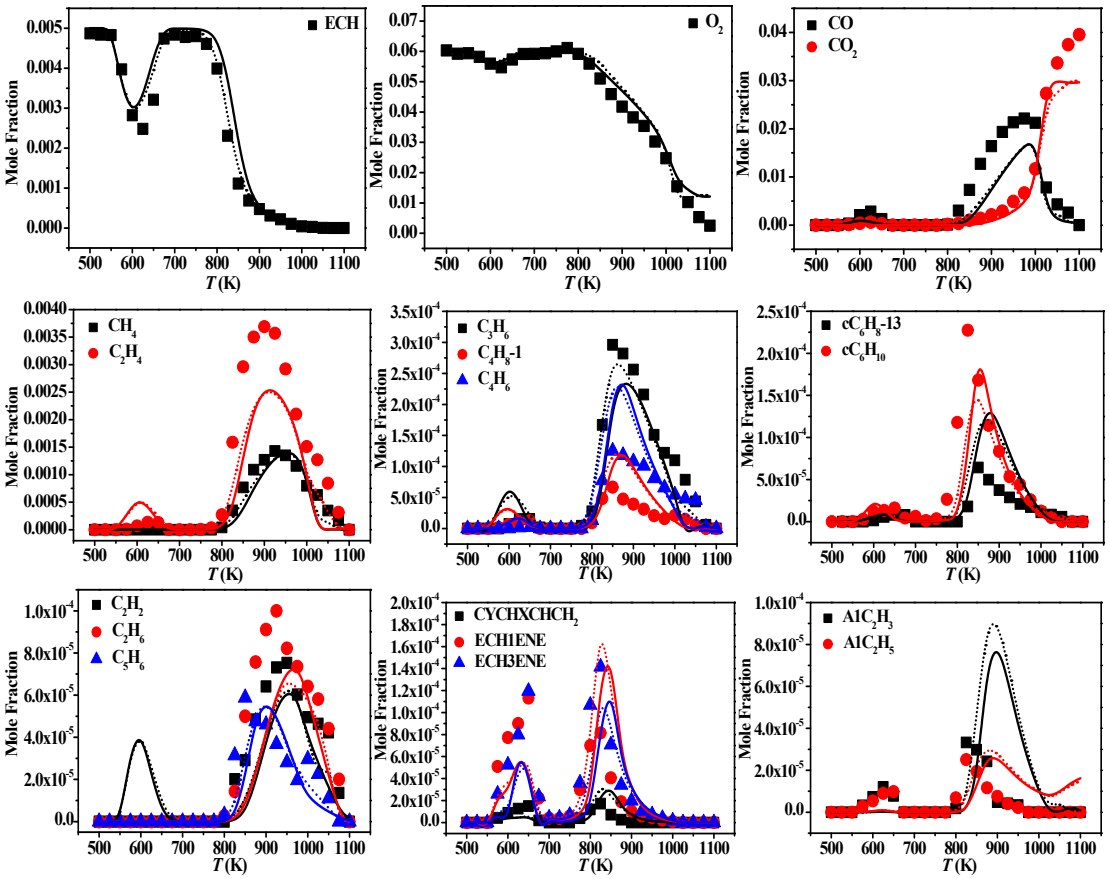


Fig. S 7. Speciation results comparison for the conditions of 0.5% ECH, 6.0% O_2, 93.5% HE, φ = 1.0, p = 1.06 bar, and at a residence time of 2 s. Symbols: JSR experimental measurements [2]; Simulations from the literature [3] (Dotted lines: the previous model, Solid lines: the updated model).

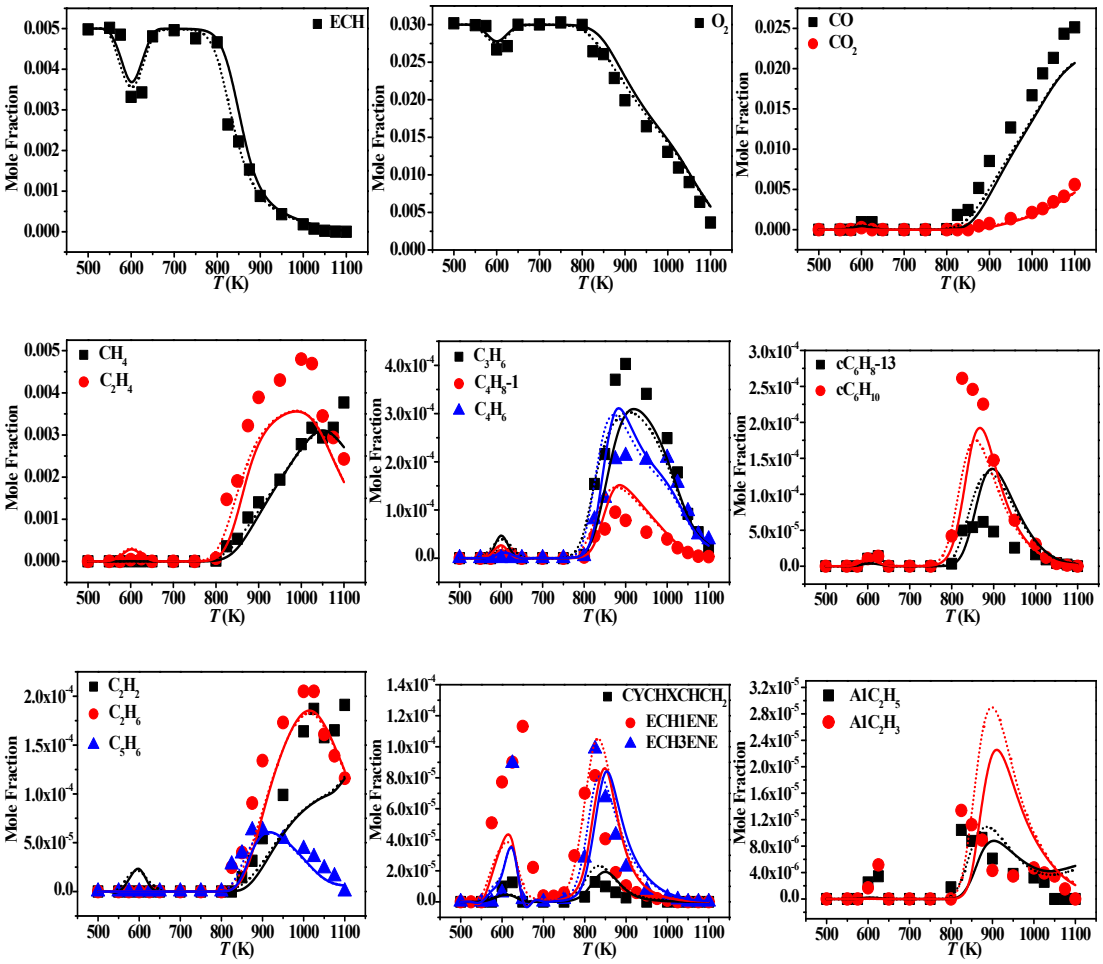


Fig. S 8. Speciation results comparison for the conditions of 0.5% ECH, 3.0% O_2, 96.5% He, φ = 2.0, p = 1.06 bar, and at a residence time of 2 s. Symbols: JSR experimental measurements [2]; Simulations from the literature [3] (Dotted lines: the previous model, Solid lines: the updated model).

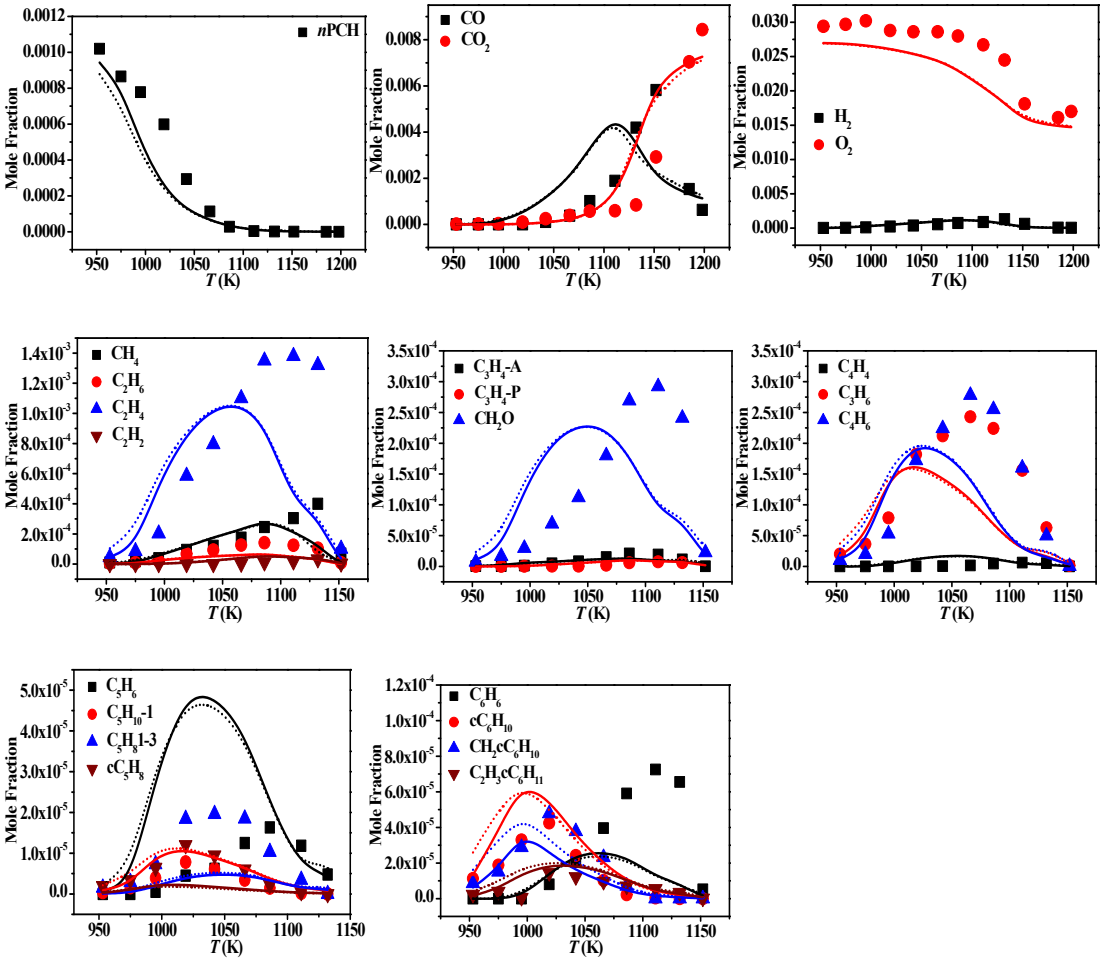


Fig. S 9. Speciation results comparison for the conditions of 0.1% *n*PCH, 2.7% O_2, 97.2% N_2, $\varphi = 0.5$, $p = 1$ bar, and at a residence time of 0.07 s. Symbols: JSR experimental measurements [4]; Simulations from the literature [5] (Dotted lines: the previous model, Solid lines: the updated model).

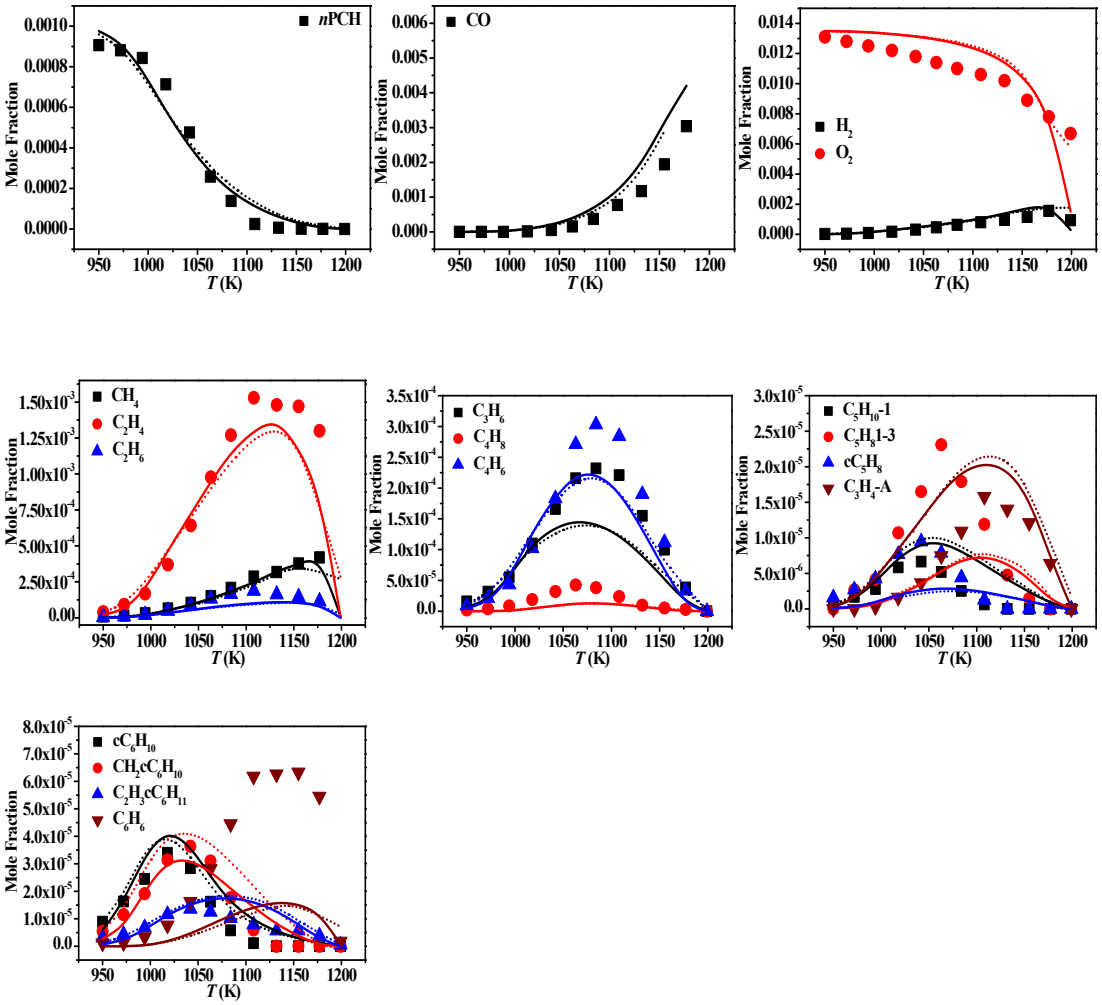


Fig. S 10. Speciation results comparison for the conditions of 0.1% *n*PCH, 1.35% O_2, 98.55% N_2, φ = 1.0, p = 1 bar, and at a residence time of 0.07 s. Symbols: JSR experimental measurements [4]; Simulations from the literature [5] (Dotted lines: the previous model, Solid lines: the updated model).

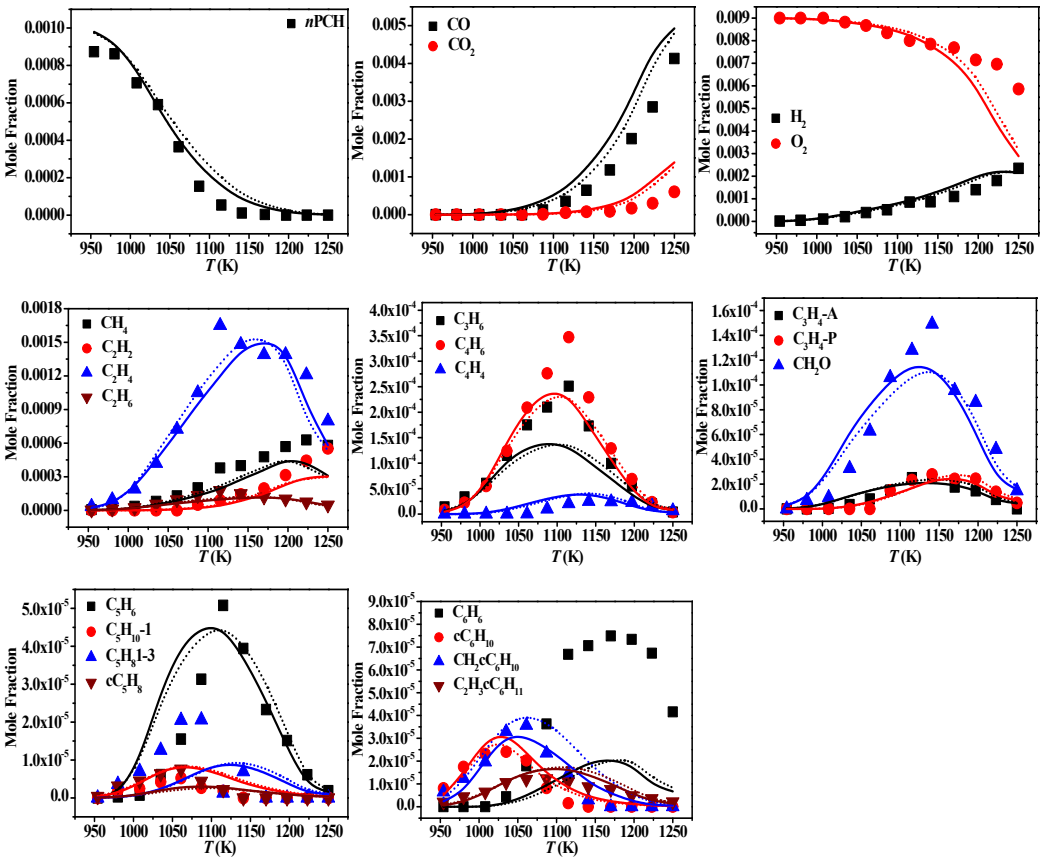
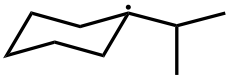
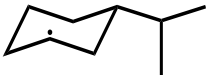
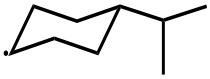
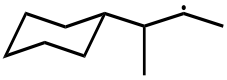
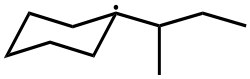
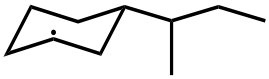
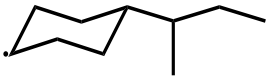
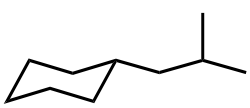
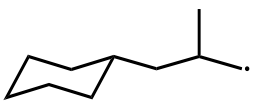


Fig. S 11. Speciation results comparison for the conditions of 0.1% *n*PCH, 0.9% O_2, 99% N_2, φ = 1.5, p = 1 bar, and at a residence time of 0.07 s. Symbols: JSR experimental measurements [4]; Simulations from the literature [5] (Dotted lines: the previous model, Solid lines: the updated model).

Table S 3

Structure and SMILES for reactants and products studied in this work.

Name	Structure	SMILES
MCH		CC1CCCCC1
MP1		[C]C1CCCCC1
MP2		C[C]1CCCCC1
MP3		CC1[C]CCCC1
MP4		CC1C[C]CCC1
MP5		CC1CC[C]CC1
ECH		CCC1CCCCC1
EP1		[C]CC1CCCCC1
EP2		C[C]C1CCCCC1
EP3		CC[C]1CCCCC1
EP4		CCC1[C]CCCC1
EP5		CCC1C[C]CCC1
EP6		CCC1CC[C]CC1
***n*PCH**		CCCC1CCCCC1
*n*P1		[C]CCC1CCCCC1
*n*P2		C[C]CC1CCCCC1
*n*P3		CC[C]C1CCCCC1
*n*P4		CCC[C]1CCCCC1
*n*P5		CCCC1[C]CCCC1

*n*P6		CCCC1C[C]CCC1
*n*P7		CCCC1CC[C]CC1
***i*PCH**		CC(C)C1CCCCC1
*i*P1		[C]C(C)C1CCCCC1
*i*P2		C[C](C)C1CCCCC1
*i*P3		CC(C)[C]1CCCCC1
*i*P4		CC(C)C1[C]CCCC1
*i*P5		CC(C)C1C[C]CCC1
*i*P6		CC(C)C1CC[C]CC1
***s*BCH**		CC(CC)C1CCCCC1
*s*BP1		CC(C[C])C1CCCCC1
*s*BP2		CC([C]C)C1CCCCC1
*s*BP3		[C]C(CC)C1CCCCC1
*s*BP4		C[C](CC)C1CCCCC1
*s*BP5		CC(CC)[C]1CCCCC1
*s*BP6		CC(CC)C1[C]CCCC1
*s*BP7		CC(CC)C1C[C]CCC1
*s*BP8		CC(CC)C1CC[C]CC1
***i*BCH**		CC(C)CC1CCCCC1
*i*BP1		[C]C(C)CC1CCCCC1

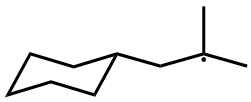
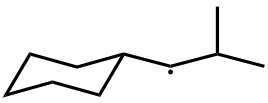
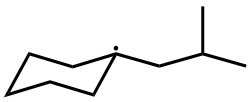
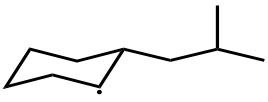
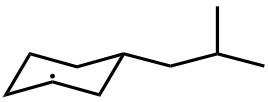
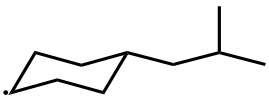
*i*BP2		C[C](C)CC1CCCCC1
*i*BP3		CC(C)[C]C1CCCCC1
*i*BP4		CC(C)C[C]1CCCCC1
*i*BP5		CC(C)CC1[C]CCCC1
*i*BP6		CC(C)CC1C[C]CCC1
*i*BP7		CC(C)CC1CC[C]CC1

Table S 4

T1 diagnostic values for reactants, transition states, and products calculated in this work.

Species	T1	Species	T1	Species	T1
MCH	0.009	**ECH**	0.009	***n*PCH**	0.009
MP1	0.017	EP1	0.016	*n*P1	0.015
MP2	0.014	EP2	0.015	*n*P2	0.014
MP3	0.015	EP3	0.013	*n*P3	0.014
MP4	0.015	EP4	0.014	*n*P4	0.013
MP5	0.015	EP5	0.014	*n*P5	0.014
$TS_a\alpha$	0.010	EP6	0.014	*n*P6	0.014
$TS_a\alpha'$	0.011	$TS_b\alpha$	0.010	*n*P7	0.014
$TS_a\beta'$	0.011	$TS_b\beta$	0.011	$TS_c\alpha$	0.010
$TS_a\gamma'$	0.011	$TS_b\alpha'$	0.011	$TS_c\beta$	0.010
$TS_a\delta'$	0.011	$TS_b\beta'$	0.011	$TS_c\gamma$	0.011
***i*PCH**	0.009	$TS_b\gamma'$	0.011	$TS_c\alpha'$	0.011
*i*P1	0.016	$TS_b\delta'$	0.011	$TS_c\beta'$	0.011
*i*P2	0.013	***s*BCH**	0.009	$TS_c\gamma'$	0.011
*i*P3	0.013	*s*BP1	0.015	$TS_c\delta'$	0.011
*i*P4	0.014	*s*BP2	0.014	***i*BCH**	0.009
*i*P5	0.014	*s*BP3	0.015	*i*BP1	0.015
*i*P6	0.014	*s*BP4	0.013	*i*BP2	0.013
$TS_d\alpha$	0.010	*s*BP5	0.013	*i*BP3	0.014
$TS_d\beta$	0.011	*s*BP6	0.014	*i*BP4	0.013
$TS_d\alpha'$	0.011	*s*BP7	0.013	*i*BP5	0.014
$TS_d\beta'$	0.011	*s*BP8	0.014	*i*BP6	0.013
$TS_d\gamma'$	0.011	$TS_e\alpha$	0.010	*i*BP7	0.014

$TS_d\delta'$	0.011	$TS_e\beta$(S)	0.011	$TS_f\alpha$	0.010
HO_2	0.036	$TS_e\beta$(P)	0.010	$TS_f\beta$	0.011
H_2O_2	0.011	$TS_e\gamma$	0.011	$TS_f\gamma$	0.011
		$TS_e\alpha'$	0.011	$TS_f\alpha'$	0.011
		$TS_e\beta'$	0.011	$TS_f\beta'$	0.011
		$TS_e\gamma'$	0.011	$TS_f\gamma'$	0.011
		$TS_e\delta'$	0.011	$TS_f\delta'$	0.011

Table S 5
The optimized Cartesian coordinate, frequencies, electronic state and point group, rotational constants, and ZPE for all species.

MCH				
optimized Cartesian coordinate	C	-0.292734000000	-1.255982000000	0.169216000000
	C	-1.011560000000	-0.000173000000	-0.335054000000
	C	-2.481170000000	-0.000012000000	0.075482000000
	C	-0.292977000000	1.255838000000	0.169168000000
	C	1.188347000000	1.260708000000	-0.214201000000
	C	1.891899000000	0.000129000000	0.293392000000
	C	1.188563000000	-1.260560000000	-0.214225000000
	H	-0.791080000000	2.149591000000	-0.219912000000
	H	-0.955070000000	-0.000193000000	-1.432716000000
	H	-0.383820000000	-1.294132000000	1.263367000000
	H	-0.790672000000	-2.149864000000	-0.219786000000
	H	1.276633000000	1.305711000000	-1.306626000000
	H	1.678374000000	2.155173000000	0.179844000000
	H	2.941421000000	0.000224000000	-0.013084000000
	H	1.880415000000	0.000114000000	1.390340000000
	H	1.276806000000	-1.305508000000	-1.306656000000
	H	1.678767000000	-2.154951000000	0.179765000000
	H	-0.384123000000	1.294022000000	1.263311000000
	H	-2.571875000000	0.000123000000	1.166314000000
	H	-2.998891000000	0.884823000000	-0.303520000000
	H	-2.999098000000	-0.884821000000	-0.303309000000
frequencies	158.2 227.8 245.0 312.2 336.7 410.3 446.4 450.6 548.0 787.0 797.0 860.2 870.7 891.0 925.2 982.1 987.6 994.4 1056.7 1082.2 1103.2 1122.2 1142.8 1189.5 1234.9 1279.0 1292.7 1297.1 1336.3 1336.4 1368.9 1383.2 1387.0 1387.8 1405.1 1411.2 1480.3 1487.5 1489.3 1494.0 1501.3 1503.8 1508.5 3014.2 3024.6 3032.2 3037.4 3041.0 3045.6 3048.2 3082.1 3085.0 3094.5 3095.8 3100.0 3117.4 3126.0				
electronic state	1-A			
point group	C1			
rotational constants	4.22239 2.19540 1.59611			
ZPE	0.199238 (Hartree/Particle)			
MP1				
optimized Cartesian coordinate	C	-0.340383000000	-1.260441000000	-0.186127000000
	C	-1.062865000000	-0.000132000000	0.312548000000
	C	-2.501170000000	-0.000011000000	-0.072937000000
	C	-0.340568000000	1.260332000000	-0.186016000000
	C	1.135611000000	-1.261397000000	0.215706000000
	C	1.843500000000	0.000105000000	-0.283934000000
	C	1.135443000000	1.261495000000	0.215753000000
	H	-0.844232000000	-2.151496000000	0.200928000000
	H	-0.988479000000	-0.000203000000	1.415618000000
	H	-0.423785000000	1.296327000000	-1.279714000000
	H	-0.844538000000	2.151266000000	0.201154000000
	H	1.211004000000	-1.306795000000	1.309105000000
	H	1.631089000000	-2.154970000000	-0.173143000000
	H	2.889491000000	0.000169000000	0.034152000000
	H	1.843962000000	0.000121000000	-1.380821000000
	H	1.210872000000	1.306877000000	1.309149000000

	H	1.630784000000	2.155147000000	-0.173091000000
	H	-0.423551000000	-1.296344000000	-1.279830000000
	H	-3.055291000000	-0.928483000000	-0.135978000000
	H	-3.054727000000	0.928689000000	-0.137485000000
frequencies	122.6	161.2	239.4	317.9
	490.6	559.7	794.5	796.3
	977.8	990.6	1054.3	1076.8
	1230.7	1247.3	1288.9	1295.3
	1385.7	1386.3	1396.9	1463.9
	1507.9	2939.1	3034.1	3037.0
	3089.9	3096.6	3097.3	3101.5
electronic state	2-A			
point group	C1			
rotational constants	4.26112	2.29808	1.63840	
ZPE	0.184119 (Hartree/Particle)			
MP2				
optimized Cartesian coordinate	C	-0.298221000000	-1.276040000000	0.210047000000
	C	-1.017007000000	0.000031000000	-0.104488000000
	C	-2.509157000000	0.000036000000	-0.105031000000
	H	-2.910594000000	-0.886921000000	-0.602096000000
	C	-0.298127000000	1.276094000000	0.209902000000
	C	1.160800000000	1.258211000000	-0.262942000000
	C	1.879499000000	-0.000101000000	0.225503000000
	C	1.160641000000	-1.258252000000	-0.263073000000
	H	-0.832057000000	2.127533000000	-0.223370000000
	H	-0.306918000000	-1.435294000000	1.304197000000
	H	-0.832267000000	-2.127461000000	-0.223126000000
	H	1.180562000000	1.278015000000	-1.358355000000
	H	1.677905000000	2.155991000000	0.085942000000
	H	2.917940000000	-0.000123000000	-0.116322000000
	H	1.904270000000	-0.000175000000	1.322697000000
	H	1.180076000000	-1.277675000000	-1.358503000000
	H	1.677752000000	-2.156202000000	0.085355000000
	H	-0.306947000000	1.435426000000	1.304046000000
	H	-2.910605000000	0.887113000000	-0.601871000000
	H	-2.909688000000	-0.000102000000	0.921898000000
frequencies	95.7	135.1	214.4	271.7
	547.8	748.0	788.7	851.5
	1000.4	1002.3	1051.8	1094.5
	1263.1	1283.4	1302.0	1314.4
	1406.4	1412.5	1466.3	1474.9
	1503.8	2940.3	2943.9	2979.1
	3077.1	3079.8	3097.5	3099.1
electronic state	2-A			
point group	C1			
rotational constants	4.25351	2.22687	1.59260	
ZPE	0.184883 (Hartree/Particle)			
MP3				
optimized Cartesian coordinate	C	-0.311456000000	-1.240400000000	-0.149845000000
	C	1.877475000000	-0.002466000000	-0.339103000000
	C	1.201808000000	1.289036000000	0.147751000000
	C	-0.273655000000	1.246469000000	-0.078896000000
	C	-1.034017000000	0.027482000000	0.337726000000
	H	2.933847000000	-0.001827000000	-0.057647000000
	H	-0.404078000000	-1.292925000000	-1.242073000000
	H	-0.809967000000	-2.124702000000	0.259278000000
	H	1.406598000000	1.393982000000	1.227131000000
	H	1.644496000000	2.162979000000	-0.335681000000
	H	-0.816804000000	2.161314000000	-0.290033000000
	H	-1.036893000000	-0.015748000000	1.442290000000
	H	1.831998000000	-0.037755000000	-1.433232000000
	C	1.169844000000	-1.232829000000	0.231010000000

	H	1.654304000000	-2.146127000000	-0.124608000000				
	H	1.262467000000	-1.229013000000	1.324397000000				
	C	-2.482927000000	0.064109000000	-0.142298000000				
	H	-2.516510000000	0.100857000000	-1.234966000000				
	H	-3.028381000000	-0.824139000000	0.185378000000				
	H	-3.003515000000	0.944696000000	0.241691000000				
frequencies	127.7	192.4	239.1	307.5	325.2	341.6	415.4	448.6
	504.3	598.2	785.7	822.2	871.2	885.2	909.2	975.5
	987.3	1001.1	1069.5	1091.9	1095.6	1117.2	1142.4	1176.0
	1231.9	1264.6	1279.8	1317.5	1326.0	1355.6	1359.1	1373.6
	1386.3	1409.0	1418.3	1473.4	1484.8	1490.4	1498.8	1502.1
	1503.9	2940.0	2962.4	3034.6	3039.5	3051.7	3052.4	3088.0
	3096.0	3098.4	3103.0	3123.9	3130.3	3188.5		
electronic state	2-A							
point group	C1							
rotational constants	4.36165	2.21154	1.60912					
ZPE	0.184562 (Hartree/Particle)							
MP4								
optimized Cartesian coordinate	C	-0.993804000000	-0.020406000000	-0.344740000000				
	C	1.248498000000	-1.201630000000	-0.229874000000				
	C	1.938103000000	0.092751000000	0.228768000000				
	C	1.143842000000	1.293499000000	-0.167134000000				
	H	1.777172000000	-2.070477000000	0.171186000000				
	H	-0.937491000000	-0.056465000000	-1.440466000000				
	H	2.032018000000	0.057154000000	1.327968000000				
	H	2.955189000000	0.149221000000	-0.165876000000				
	H	1.646043000000	2.222365000000	-0.406877000000				
	H	1.300959000000	-1.265949000000	-1.322275000000				
	C	-0.218435000000	-1.222391000000	0.202804000000				
	H	-0.697207000000	-2.150280000000	-0.125743000000				
	H	-0.275900000000	-1.207514000000	1.300170000000				
	C	-0.322726000000	1.287508000000	0.111883000000				
	H	-0.495986000000	1.383288000000	1.199491000000				
	H	-0.814607000000	2.146282000000	-0.353429000000				
	C	-2.459863000000	-0.061342000000	0.074279000000				
	H	-3.009428000000	0.796850000000	-0.321017000000				
	H	-2.948071000000	-0.970938000000	-0.284292000000				
	H	-2.546390000000	-0.041478000000	1.165244000000				
frequencies	147.5	173.9	236.8	281.8	311.2	364.5	417.3	435.3
	474.0	616.6	783.5	851.5	854.8	876.7	899.0	966.7
	985.0	993.0	1063.7	1104.1	1112.1	1117.8	1128.0	1167.6
	1237.3	1268.3	1287.8	1314.5	1333.4	1358.8	1366.4	1369.9
	1398.2	1402.3	1410.9	1468.4	1474.2	1488.5	1497.3	1501.7
	1502.8	2945.6	2960.4	3021.0	3035.2	3048.5	3051.4	3084.1
	3088.1	3099.8	3101.1	3118.0	3126.8	3205.0		
electronic state	2-A							
point group	C1							
rotational constants	4.39359	2.22106	1.61101					
ZPE	0.184368 (Hartree/Particle)							
MP5								
optimized Cartesian coordinate	C	-0.262871000000	1.255031000000	-0.209744000000				
	C	-0.959759000000	0.000105000000	0.324900000000				
	C	-2.443865000000	0.000116000000	-0.030600000000				
	H	-2.946870000000	-0.884728000000	0.367456000000				
	C	-0.263115000000	-1.254917000000	-0.209900000000				
	C	1.228195000000	-1.279992000000	0.157529000000				
	C	1.900443000000	-0.000214000000	-0.216289000000				
	C	1.228640000000	1.279822000000	0.157394000000				
	H	-0.759834000000	-2.151263000000	0.174544000000				
	H	-0.861356000000	0.000019000000	1.420042000000				
	H	-0.365631000000	1.272214000000	-1.301984000000				
	H	-0.759333000000	2.151427000000	0.174914000000				

	H	1.308194000000	-1.434970000000	1.247433000000				
	H	1.724982000000	-2.133104000000	-0.310492000000				
	H	2.946661000000	-0.000200000000	-0.496046000000				
	H	1.308922000000	1.434991000000	1.247256000000				
	H	1.725540000000	2.132718000000	-0.310897000000				
	H	-0.365698000000	-1.271870000000	-1.302157000000				
	H	-2.574670000000	0.000131000000	-1.117287000000				
	H	-2.946912000000	0.884931000000	0.367477000000				
frequencies	136.6	214.9	238.9	244.5	314.6	359.0	427.8	454.4
	459.7	637.1	783.9	793.8	879.8	900.4	932.4	962.8
	974.9	1005.1	1040.8	1100.5	1102.1	1123.1	1137.7	1172.4
	1241.0	1256.9	1293.3	1318.9	1330.4	1343.3	1371.8	1381.7
	1400.4	1404.8	1413.1	1470.7	1479.1	1482.5	1497.2	1503.0
	1503.9	2959.5	2961.9	3013.3	3036.8	3041.7	3049.4	3087.0
	3089.9	3097.4	3097.4	3118.5	3126.8	3205.4		
electronic state	2-A							
point group	C1							
rotational constants	4.25724	2.27085	1.61438					
ZPE	0.184473 (Hartree/Particle)							
$TS_a\alpha$								
optimized Cartesian coordinate	C	-1.221339000000	1.398539000000	0.152412000000				
	C	0.074768000000	0.572781000000	0.022708000000				
	C	1.187708000000	1.403101000000	-0.551895000000				
	H	2.279307000000	0.632461000000	-0.445973000000				
	O	3.130339000000	-0.157840000000	-0.246681000000				
	O	2.793802000000	-0.725666000000	0.974443000000				
	H	2.358076000000	-1.551789000000	0.725245000000				
	C	-0.188821000000	-0.683496000000	-0.815143000000				
	C	-2.355130000000	0.557015000000	0.744374000000				
	C	-2.599811000000	-0.707452000000	-0.081821000000				
	C	-1.316660000000	-1.529347000000	-0.222410000000				
	H	-1.036610000000	2.281700000000	0.770304000000				
	H	0.365365000000	0.261845000000	1.035947000000				
	H	-0.462934000000	-0.372637000000	-1.832025000000				
	H	0.730888000000	-1.269935000000	-0.913932000000				
	H	-2.091139000000	0.272761000000	1.770005000000				
	H	-3.268937000000	1.154001000000	0.806006000000				
	H	-3.389757000000	-1.310438000000	0.373362000000				
	H	-2.952693000000	-0.421772000000	-1.080249000000				
	H	-1.013140000000	-1.893851000000	0.766944000000				
	H	-1.495453000000	-2.410426000000	-0.844164000000				
	H	-1.510614000000	1.756981000000	-0.843581000000				
	H	1.478056000000	2.280324000000	0.025953000000				
	H	1.132156000000	1.591976000000	-1.625287000000				
frequencies	-1823.8	59.6	72.5	86.5	157.9	217.2	245.6	315.2
	334.9	366.0	419.5	436.8	448.3	523.4	549.9	601.5
	792.3	797.9	858.3	871.6	897.0	926.7	979.2	980.9
	1021.4	1052.8	1071.6	1079.2	1095.6	1116.7	1127.3	1174.8
	1181.9	1225.0	1278.9	1291.2	1294.7	1330.4	1340.8	1363.6
	1370.5	1385.8	1387.4	1406.1	1409.1	1454.1	1472.2	1485.5
	1487.6	1491.1	1497.4	1511.0	3022.7	3032.3	3037.4	3041.4
	3043.3	3048.5	3081.3	3093.8	3096.6	3098.4	3099.0	3103.5
	3181.6	3804.8						
electronic state	2-A							
point group	C1							
rotational constants	2.67919	0.85066	0.74417					
ZPE	0.209881 (Hartree/Particle)							
$TS_a\alpha'$								
optimized Cartesian coordinate	C	0.132043000000	-0.080399000000	1.331571000000				
	C	-0.238894000000	0.841933000000	0.187529000000				
	C	-1.205953000000	1.940840000000	0.554046000000				
	H	-2.109182000000	1.527395000000	1.009252000000				

	H	-0.939759000000	0.080819000000	-0.584628000000
	O	-1.697673000000	-0.704650000000	-1.158735000000
	O	-2.515848000000	-1.164417000000	-0.138664000000
	H	-2.116219000000	-2.008697000000	0.109867000000
	C	0.938549000000	1.263580000000	-0.670092000000
	C	1.794433000000	0.072147000000	-1.108597000000
	C	2.218250000000	-0.774039000000	0.093347000000
	C	0.995442000000	-1.259192000000	0.874146000000
	H	0.583650000000	1.827475000000	-1.537718000000
	H	0.689567000000	0.510140000000	2.075846000000
	H	-0.777024000000	-0.428081000000	1.832640000000
	H	1.212199000000	-0.549948000000	-1.797805000000
	H	2.671385000000	0.424794000000	-1.657005000000
	H	2.818682000000	-1.625621000000	-0.236565000000
	H	2.853498000000	-0.172408000000	0.755320000000
	H	0.399955000000	-1.910839000000	0.222598000000
	H	1.300954000000	-1.857055000000	1.736475000000
	H	1.556012000000	1.957142000000	-0.076888000000
	H	-1.495102000000	2.524248000000	-0.322466000000
	H	-0.743669000000	2.623954000000	1.278567000000
frequencies	-1685.6 39.6 87.8 97.9 152.7 190.9 209.6 247.5 311.8 341.0 382.3 398.6 426.8 452.2 536.0 579.1 784.7 789.2 857.6 869.8 898.2 929.6 977.8 998.8 1001.4 1054.2 1077.0 1092.8 1109.2 1125.0 1168.9 1177.1 1193.3 1271.9 1276.5 1296.1 1312.7 1350.0 1368.5 1383.1 1386.6 1398.0 1404.3 1409.9 1462.7 1467.5 1476.2 1487.0 1489.7 1492.8 1494.8 1505.6 2992.4 2998.2 3028.1 3036.2 3043.7 3054.2 3081.7 3089.0 3100.9 3101.4 3105.0 3106.7 3138.8 3806.2			
electronic state	2-A			
point group	C1			
rotational constants	1.90283 1.17881 1.01958			
ZPE	0.209534 (Hartree/Particle)			
$TS_a\beta'$				
optimized Cartesian coordinate	C	1.476941000000	0.224401000000	-0.898149000000
	C	-0.225792000000	1.874575000000	-0.048186000000
	C	-0.402811000000	1.052484000000	1.231708000000
	C	-0.005044000000	-0.390949000000	1.028811000000
	H	-0.868798000000	-0.834621000000	0.149836000000
	O	-1.707065000000	-1.115898000000	-0.683868000000
	O	-2.773709000000	-0.278612000000	-0.385327000000
	H	-3.361660000000	-0.840705000000	0.135334000000
	C	1.335985000000	-0.633236000000	0.365421000000
	H	-0.428409000000	2.928421000000	0.158263000000
	H	0.773923000000	-0.150023000000	-1.652196000000
	H	2.484330000000	0.102421000000	-1.307178000000
	H	0.230799000000	1.473814000000	2.027669000000
	H	-1.434865000000	1.114791000000	1.586764000000
	H	-0.198896000000	-1.042158000000	1.885379000000
	H	2.106247000000	-0.301995000000	1.082134000000
	H	-0.964153000000	1.540918000000	-0.784662000000
	C	1.181095000000	1.699644000000	-0.622483000000
	H	1.287400000000	2.280843000000	-1.542025000000
	H	1.918513000000	2.092146000000	0.089137000000
	C	1.553639000000	-2.115429000000	0.069033000000
	H	0.798069000000	-2.475304000000	-0.635529000000
	H	2.537363000000	-2.284321000000	-0.374863000000
	H	1.482253000000	-2.717090000000	0.978566000000
frequencies	-1748.8 59.6 83.5 95.7 147.6 201.3 234.1 266.0 314.1 344.5 393.4 417.0 444.1 479.2 555.0 599.0 780.6 796.1 866.7 869.5 889.6 922.1 981.1 986.6 1003.0 1058.8 1070.5 1096.8 1101.1 1120.3 1156.0 1170.5 1199.6 1244.2 1271.8 1289.9 1318.2 1331.3 1353.7 1366.8 1383.0 1388.1 1397.1 1406.3 1415.0 1460.2 1467.6 1487.7 1492.9 1502.4 1504.8 1507.5 2974.2 2998.8 3035.7 3046.4 3052.4 3065.1 3091.6 3094.8 3098.5 3100.2 3111.9 3124.3			

	3131.2 3820.5
electronic state	2-A
point group	C1
rotational constants	1.71520 1.31513 0.96311
ZPE	0.209676 (Hartree/Particle)
$TS_a\gamma'$	
optimized Cartesian coordinate	C 1.434209000000 -0.405498000000 -0.330459000000 C -0.139797000000 1.572659000000 -0.511872000000 C -0.708307000000 1.283284000000 0.880019000000 C -0.516699000000 -0.164626000000 1.266983000000 H -1.244050000000 -0.813989000000 0.394412000000 O -1.933613000000 -1.294027000000 -0.481803000000 O -2.897110000000 -0.324630000000 -0.724681000000 H -3.656973000000 -0.629487000000 -0.212468000000 H -0.204561000000 2.642930000000 -0.722974000000 H 0.814333000000 -0.945711000000 -1.057059000000 H -0.189640000000 1.907514000000 1.624347000000 H -1.766463000000 1.553471000000 0.924640000000 H -0.983464000000 -0.449987000000 2.211876000000 H -0.756537000000 1.058912000000 -1.256448000000 C 1.307453000000 1.091220000000 -0.629780000000 H 1.693372000000 1.298777000000 -1.632309000000 H 1.940757000000 1.647251000000 0.075227000000 C 0.880443000000 -0.708533000000 1.067842000000 H 1.542937000000 -0.241860000000 1.814834000000 H 0.904636000000 -1.785081000000 1.261954000000 C 2.876986000000 -0.883053000000 -0.459838000000 H 2.961131000000 -1.953266000000 -0.255061000000 H 3.263130000000 -0.699649000000 -1.465256000000 H 3.521452000000 -0.353292000000 0.248784000000
frequencies	-1747.7 59.5 89.5 99.8 167.3 218.2 238.5 244.7 315.5 328.9 407.3 430.5 441.4 473.2 555.1 606.8 783.1 800.4 851.5 871.7 890.2 923.9 982.8 986.1 996.2 1062.5 1072.7 1084.2 1122.8 1124.8 1154.2 1167.6 1204.4 1245.7 1279.6 1290.3 1314.8 1336.3 1357.5 1375.8 1386.0 1388.6 1406.6 1408.8 1412.7 1462.0 1464.6 1469.7 1491.1 1502.0 1503.4 1504.2 2989.2 2997.9 3023.1 3044.6 3050.7 3064.9 3083.8 3089.5 3097.7 3111.4 3111.8 3119.0 3129.5 3819.7
electronic state	2-A
point group	C1
rotational constants	2.23608 0.99617 0.90570
ZPE	0.209793 (Hartree/Particle)
$TS_a\delta'$	
optimized Cartesian coordinate	C -1.174160000000 0.799531000000 -0.893279000000 C -1.712316000000 -0.173587000000 0.160261000000 C -2.642983000000 -1.205516000000 -0.469903000000 H -3.041698000000 -1.890621000000 0.282449000000 C -0.545875000000 -0.853630000000 0.883734000000 C 0.402114000000 0.161574000000 1.528038000000 C 0.857614000000 1.207383000000 0.536894000000 H 1.548228000000 0.520697000000 -0.337126000000 O 2.136325000000 -0.233937000000 -1.084768000000 O 2.571817000000 -1.259834000000 -0.257318000000 H 3.488108000000 -1.021571000000 -0.066539000000 C -0.243948000000 1.848611000000 -0.277601000000 H -0.927229000000 -1.540142000000 1.645546000000 H -2.281386000000 0.407576000000 0.900221000000 H -0.621138000000 0.226905000000 -1.647732000000 H -2.004262000000 1.293514000000 -1.407098000000 H -0.116092000000 0.674706000000 2.353046000000 H 1.263461000000 -0.348156000000 1.967473000000

	H	1.602736000000	1.906130000000	0.922524000000
	H	-0.827155000000	2.501152000000	0.390244000000
	H	0.178990000000	2.494951000000	-1.051143000000
	H	0.017371000000	-1.456138000000	0.161302000000
	H	-2.101812000000	-1.799928000000	-1.212314000000
	H	-3.485942000000	-0.725091000000	-0.973032000000

frequencies	-1758.3	52.9	77.5	100.7	161.8	216.0	235.5	267.3
	308.0	314.9	389.3	426.8	450.9	459.9	553.0	611.5
	783.5	788.9	850.9	875.2	896.5	928.0	973.8	983.7
	994.5	1054.1	1072.3	1095.6	1112.4	1121.2	1156.2	1169.0
	1202.0	1234.5	1275.1	1298.9	1323.9	1338.6	1348.8	1369.7
	1381.0	1388.1	1405.2	1408.7	1413.8	1458.5	1464.6	1477.0
	1486.5	1500.1	1503.8	1505.2	2997.6	3002.2	3011.9	3046.2
	3049.2	3053.8	3093.5	3094.9	3096.1	3098.6	3112.4	3120.5
	3127.0	3820.8						
electronic state	2-A							
point group	C1							
rotational constants	2.04192	1.04822	0.94170					
ZPE	0.209571 (Hartree/Particle)							
ECH								

optimized Cartesian coordinate	C	-0.074986000000	1.099610000000	-0.275741000000
	C	-0.559667000000	-0.260824000000	0.238941000000
	C	0.434976000000	-1.357051000000	-0.160390000000
	C	1.858560000000	-1.047843000000	0.306795000000
	C	2.325622000000	0.308721000000	-0.223238000000
	C	1.350643000000	1.413829000000	0.185339000000
	H	0.102933000000	-2.319761000000	0.241252000000
	H	-0.585636000000	-0.213576000000	1.338278000000
	H	-0.108521000000	1.088403000000	-1.374278000000
	H	-0.750555000000	1.893490000000	0.053613000000
	H	1.882378000000	-1.032530000000	1.403344000000
	H	2.541727000000	-1.839127000000	-0.013661000000
	H	3.331972000000	0.534859000000	0.139571000000
	H	2.383183000000	0.266266000000	-1.317893000000
	H	1.358996000000	1.512468000000	1.277859000000
	H	1.673055000000	2.376493000000	-0.220762000000
	H	0.427885000000	-1.452253000000	-1.254798000000
	C	-1.967755000000	-0.605924000000	-0.253575000000
	H	-2.223529000000	-1.608439000000	0.106241000000
	H	-1.951719000000	-0.667349000000	-1.348686000000
	C	-3.049277000000	0.378089000000	0.190072000000
	H	-3.031541000000	0.511020000000	1.275609000000
	H	-2.916715000000	1.359589000000	-0.268930000000
	H	-4.042610000000	0.018810000000	-0.085971000000

frequencies	83.6	131.8	220.1	232.8	246.7	334.9	368.1	431.1
	445.1	458.5	541.5	762.5	797.4	805.8	858.8	890.2
	904.5	935.8	937.5	1003.9	1033.4	1058.4	1061.1	1081.5
	1109.4	1126.1	1145.6	1190.1	1221.2	1261.2	1290.4	1293.1
	1310.0	1320.3	1343.4	1366.9	1377.7	1385.1	1387.4	1394.1
	1407.6	1416.5	1480.3	1486.1	1489.4	1491.5	1495.1	1504.0
	1509.2	1514.8	3001.8	3023.2	3028.7	3036.6	3039.9	3041.1
	3045.3	3059.0	3075.2	3084.3	3094.0	3094.6	3097.6	3100.2
	3127.8	3138.8						
electronic state	1-A							
point group	C1							
rotational constants	3.83172	1.30285	1.05166					
ZPE	0.227885 (Hartree/Particle)							
EP1								

optimized Cartesian coordinate	C	0.369891000000	-1.357220000000	0.153849000000
	C	-0.609745000000	-0.246281000000	-0.235640000000
	C	-2.028028000000	-0.559842000000	0.260399000000
	C	-3.057149000000	0.398265000000	-0.231182000000

	C	-0.116350000000	1.104347000000	0.293942000000
	C	1.306584000000	1.415296000000	-0.174462000000
	C	2.274257000000	0.297797000000	0.220428000000
	C	1.794661000000	-1.053027000000	-0.314636000000
	H	-0.803933000000	1.898257000000	-0.012543000000
	H	-0.639790000000	-0.189854000000	-1.334053000000
	H	0.363391000000	-1.461965000000	1.247385000000
	H	0.030012000000	-2.313321000000	-0.256922000000
	H	1.309784000000	1.523893000000	-1.266048000000
	H	1.639363000000	2.371211000000	0.238981000000
	H	3.280551000000	0.516853000000	-0.146815000000
	H	2.338001000000	0.248371000000	1.314437000000
	H	1.814848000000	-1.032339000000	-1.411164000000
	H	2.473722000000	-1.850431000000	-0.000819000000
	H	-0.138741000000	1.074459000000	1.392212000000
	H	-2.284833000000	-1.582557000000	-0.060397000000
	H	-3.045477000000	0.718014000000	-1.266275000000
	H	-3.915201000000	0.666583000000	0.369337000000
	H	-2.026420000000	-0.583179000000	1.356498000000
frequencies	102.0 127.8 149.2 218.2 236.8 327.5 368.1 423.3 445.0 449.4 485.9 545.6 789.6 800.1 813.9 860.8 885.4 907.6 939.3 963.8 997.9 1056.6 1072.7 1084.6 1094.5 1118.7 1130.7 1174.5 1193.7 1239.6 1276.7 1291.1 1298.9 1312.3 1337.1 1367.0 1373.9 1383.8 1387.5 1388.9 1405.9 1464.0 1473.4 1483.3 1487.3 1489.9 1494.9 1508.8 2976.0 3006.2 3024.2 3030.5 3036.9 3041.4 3045.5 3063.1 3083.5 3091.2 3094.9 3095.4 3099.7 3167.1 3272.8			
electronic state	2-A			
point group	C1			
rotational constants	3.86881 1.34882 1.08617			
ZPE	0.212681 (Hartree/Particle)			
EP2				
optimized Cartesian coordinate	C	-0.400818000000	-1.366249000000	-0.163490000000
	C	0.588431000000	-0.260114000000	0.220780000000
	C	1.973033000000	-0.558441000000	-0.251436000000
	C	3.130730000000	0.266966000000	0.196789000000
	H	4.075266000000	-0.271275000000	0.092861000000
	C	0.086830000000	1.102161000000	-0.308218000000
	C	-1.330194000000	1.410279000000	0.180247000000
	C	-2.302138000000	0.294141000000	-0.207449000000
	C	-1.819445000000	-1.058835000000	0.319427000000
	H	0.776690000000	1.894035000000	-0.001678000000
	H	0.606880000000	-0.183798000000	1.320485000000
	H	-0.403159000000	-1.464281000000	-1.257253000000
	H	-0.055380000000	-2.322508000000	0.240200000000
	H	-1.318646000000	1.514013000000	1.272226000000
	H	-1.668004000000	2.368008000000	-0.225178000000
	H	-3.304287000000	0.514096000000	0.170379000000
	H	-2.376876000000	0.247725000000	-1.300856000000
	H	-1.829956000000	-1.041693000000	1.416154000000
	H	-2.503331000000	-1.853659000000	0.009627000000
	H	0.100276000000	1.072518000000	-1.405488000000
	H	3.228021000000	1.194999000000	-0.385682000000
	H	3.018665000000	0.563607000000	1.244530000000
	H	2.095266000000	-1.211239000000	-1.110230000000
frequencies	55.5 115.0 138.9 209.0 237.5 304.3 364.4 387.6 434.4 459.1 478.9 544.7 793.1 800.3 857.4 891.4 901.5 932.4 937.3 986.4 1012.5 1050.3 1065.3 1087.6 1104.2 1118.8 1162.3 1171.0 1214.5 1253.1 1287.1 1294.3 1308.3 1325.2 1352.3 1368.8 1379.1 1384.7 1386.6 1406.3 1430.1 1478.0 1483.4 1486.6 1489.6 1493.9 1494.7 1508.5 2979.9 2998.4 3030.6 3035.6 3037.5 3041.9 3045.8 3071.9 3090.5 3092.4 3094.3 3095.7 3100.1 3122.2 3179.5			
electronic state	2-A			
point group	C1			

rotational constants	3.93364	1.30514	1.05880	
ZPE	0.212878 (Hartree/Particle)			
EP3				
optimized Cartesian coordinate	C	-0.103490000000	1.273825000000	0.079733000000
	C	0.551130000000	0.000083000000	-0.361243000000
	C	2.012392000000	0.000235000000	-0.677810000000
	C	2.887920000000	-0.000155000000	0.590745000000
	H	2.685401000000	-0.884221000000	1.200001000000
	H	2.260829000000	-0.880436000000	-1.279713000000
	H	2.685279000000	0.883449000000	1.200630000000
	C	-0.103350000000	-1.273766000000	0.079612000000
	C	-1.616909000000	-1.260094000000	-0.175227000000
	C	-2.257591000000	-0.000106000000	0.409070000000
	C	-1.617050000000	1.260016000000	-0.175090000000
	H	0.363400000000	-2.131507000000	-0.415143000000
	H	0.059409000000	1.417000000000	1.163342000000
	H	0.363158000000	2.131659000000	-0.414952000000
	H	-1.796030000000	-1.284663000000	-1.255949000000
	H	-2.076861000000	-2.156156000000	0.250021000000
	H	-3.334285000000	-0.000157000000	0.219230000000
	H	-2.125793000000	-0.000159000000	1.498610000000
	H	-1.796184000000	1.284685000000	-1.255808000000
	H	-2.077099000000	2.155981000000	0.250260000000
	H	0.059554000000	-1.417018000000	1.163209000000
	H	3.950154000000	0.000008000000	0.336659000000
	H	2.260759000000	0.881309000000	-1.279142000000
frequencies	47.7	75.3	204.0	211.3	229.1	318.8	363.3	379.9
	444.2	468.6	584.3	739.6	784.6	792.8	855.9	856.7
	914.3	928.4	942.1	997.2	1046.4	1050.7	1051.2	1096.8
	1101.1	1105.9	1173.3	1196.1	1249.9	1263.4	1287.0	1311.9
	1328.3	1337.3	1359.7	1375.9	1376.0	1387.0	1398.0	1409.6
	1468.6	1475.9	1486.2	1487.4	1491.5	1502.5	1503.9	1509.1
	2945.4	2948.6	3035.6	3042.6	3048.3	3049.9	3057.5	3074.5
	3077.1	3083.9	3095.3	3097.6	3101.3	3132.4	3133.3	
electronic state	2-A			
point group	C1			
rotational constants	3.73696	1.33903	1.11229	
ZPE	0.213901 (Hartree/Particle)			
EP4				
optimized Cartesian coordinate	C	0.437341000000	1.339036000000	-0.064852000000
	C	1.885278000000	1.094439000000	0.204638000000
	C	2.317603000000	-0.289438000000	-0.301813000000
	C	-0.075469000000	-1.093838000000	-0.212007000000
	C	-0.564593000000	0.281260000000	0.276361000000
	H	3.344633000000	-0.499502000000	0.008472000000
	H	-0.142063000000	-1.115745000000	-1.307816000000
	H	-0.732297000000	-1.880593000000	0.168228000000
	H	2.071103000000	1.132348000000	1.291883000000
	H	2.500529000000	1.880261000000	-0.239828000000
	H	0.087567000000	2.348220000000	-0.255346000000
	H	-0.640563000000	0.217067000000	1.378860000000
	H	2.301476000000	-0.289984000000	-1.397353000000
	C	-1.953101000000	0.638159000000	-0.265336000000
	H	-1.887600000000	0.722590000000	-1.356320000000
	C	-3.046541000000	-0.357822000000	0.114749000000
	H	-3.073292000000	-0.512194000000	1.197352000000
	H	-4.028959000000	0.003106000000	-0.195598000000
	H	-2.889446000000	-1.329429000000	-0.357685000000
	C	1.367799000000	-1.370413000000	0.214110000000
	H	1.681438000000	-2.353769000000	-0.146437000000
	H	1.419740000000	-1.403035000000	1.309793000000
	H	-2.222164000000	1.632361000000	0.106704000000

frequencies	80.6	120.1	183.3	213.4	247.7	321.6	340.8	367.6
	431.0	461.0	495.0	601.1	763.0	799.7	837.5	868.4
	901.0	932.0	938.3	998.4	1020.8	1054.0	1076.4	1093.5
	1100.4	1121.6	1155.1	1176.7	1220.5	1255.1	1265.0	1294.5
	1315.6	1334.2	1349.1	1359.9	1370.6	1379.6	1387.3	1415.0
	1418.6	1472.3	1485.3	1489.9	1491.8	1500.4	1504.9	1514.3
	2924.1	2961.0	3031.2	3038.7	3044.3	3051.9	3058.2	3081.8
	3095.2	3098.1	3099.7	3102.6	3127.5	3138.3	3184.4	
electronic state	2-A							
point group	C1							
rotational constants	3.98231	1.30879	1.05640					
ZPE	0.213148 (Hartree/Particle)							
EP5								
optimized Cartesian coordinate	C	-1.334130000000	1.422789000000	-0.134260000000				
	C	0.089900000000	1.140629000000	0.215923000000				
	C	0.536258000000	-0.258228000000	-0.249355000000				
	C	-1.894369000000	-1.000061000000	-0.321539000000				
	C	-2.360675000000	0.380949000000	0.162415000000				
	H	-1.886424000000	-1.010957000000	-1.416996000000				
	H	-2.597880000000	-1.770537000000	0.005199000000				
	H	0.223157000000	1.180618000000	1.313336000000				
	H	0.742271000000	1.911225000000	-0.201072000000				
	H	-1.641132000000	2.436705000000	-0.358836000000				
	H	-2.525970000000	0.321789000000	1.252112000000				
	H	-3.323473000000	0.643359000000	-0.282109000000				
	H	0.557170000000	-0.250760000000	-1.348442000000				
	C	1.935878000000	-0.616163000000	0.255621000000				
	H	2.179997000000	-1.626240000000	-0.090465000000				
	C	3.030291000000	0.350133000000	-0.195000000000				
	H	2.904590000000	1.338560000000	0.251414000000				
	H	4.018335000000	-0.015597000000	0.091083000000				
	H	3.019224000000	0.469903000000	-1.282133000000				
	C	-0.488323000000	-1.307833000000	0.194360000000				
	H	-0.504219000000	-1.340906000000	1.292674000000				
	H	-0.168320000000	-2.297716000000	-0.146141000000				
	H	1.913686000000	-0.662742000000	1.351391000000				
frequencies	90.4	130.5	166.9	214.8	248.1	288.6	360.9	374.2
	428.8	461.1	467.6	613.0	764.7	797.2	852.7	862.1
	895.1	925.5	937.8	981.7	1030.1	1056.9	1072.5	1103.3
	1121.0	1126.8	1132.8	1162.1	1228.2	1253.2	1276.6	1305.3
	1317.8	1326.4	1358.8	1363.6	1375.5	1379.7	1402.8	1406.3
	1416.0	1468.8	1473.4	1485.4	1493.0	1498.8	1504.6	1514.7
	2939.2	2960.8	3016.2	3026.7	3040.3	3051.8	3058.9	3076.6
	3085.8	3099.6	3101.0	3102.3	3128.2	3138.0	3205.4	
electronic state	2-A							
point group	C1							
rotational constants	3.99311	1.31400	1.06124					
ZPE	0.213116 (Hartree/Particle)							
EP6								
optimized Cartesian coordinate	C	2.329726000000	0.328731000000	-0.130533000000				
	C	1.910467000000	-1.048003000000	0.265162000000				
	C	0.480068000000	-1.350189000000	-0.204165000000				
	C	-0.507939000000	-0.256257000000	0.214479000000				
	C	-1.926859000000	-0.615340000000	-0.236475000000				
	C	-3.003802000000	0.363648000000	0.228940000000				
	H	-4.001101000000	-0.007689000000	-0.014874000000				
	C	-0.047245000000	1.099538000000	-0.331735000000				
	C	1.377121000000	1.447962000000	0.129105000000				
	H	0.153049000000	-2.317432000000	0.190236000000				
	H	-0.504104000000	-0.197167000000	1.313982000000				
	H	-0.073801000000	1.060077000000	-1.428353000000				
	H	-0.731559000000	1.892437000000	-0.019292000000				

	H	1.935766000000	-1.140661000000	1.364785000000
	H	2.607310000000	-1.795447000000	-0.121494000000
	H	3.371650000000	0.540645000000	-0.336367000000
	H	1.340531000000	1.656773000000	1.212469000000
	H	1.717719000000	2.369808000000	-0.348332000000
	H	0.470674000000	-1.428045000000	-1.298516000000
	H	-2.164767000000	-1.616444000000	0.138879000000
	H	-2.956174000000	0.507099000000	1.312215000000
	H	-2.894474000000	1.341782000000	-0.243033000000
	H	-1.939944000000	-0.686270000000	-1.330966000000
frequencies	79.8 118.9 197.4 211.4 237.3 266.6 352.8 372.6 443.5 449.5 471.2 630.0 762.5 783.0 822.7 881.7 914.0 933.3 946.7 994.0 1021.5 1046.4 1064.2 1097.8 1106.6 1126.4 1148.6 1170.2 1231.3 1243.2 1293.1 1293.7 1309.3 1335.7 1345.2 1366.1 1377.6 1391.9 1401.3 1408.3 1416.9 1469.3 1477.5 1481.8 1490.6 1498.0 1504.6 1515.2 2957.7 2960.4 2999.5 3035.9 3037.2 3043.8 3059.5 3076.6 3088.8 3096.6 3097.2 3103.2 3128.2 3139.8 3203.3			
electronic state	2-A			
point group	C1			
rotational constants	3.84905 1.33778 1.06676			
ZPE	0.213072 (Hartree/Particle)			
$TS_b\beta$				
optimized Cartesian coordinate	C	0.257725000000	-0.752548000000	-0.246145000000
	C	0.398100000000	0.774533000000	-0.250213000000
	C	-0.881444000000	1.479527000000	0.205052000000
	C	-2.038299000000	1.363619000000	-0.751950000000
	H	-2.616694000000	0.168495000000	-0.570784000000
	O	-3.108413000000	-0.863597000000	-0.295292000000
	O	-2.792556000000	-1.048817000000	1.042784000000
	H	-2.006805000000	-1.611009000000	1.007654000000
	C	1.594294000000	1.184834000000	0.615439000000
	C	2.886586000000	0.500601000000	0.163880000000
	C	2.733347000000	-1.021610000000	0.148010000000
	C	1.541360000000	-1.442085000000	-0.713785000000
	H	1.713874000000	2.272502000000	0.590694000000
	H	0.608181000000	1.089232000000	-1.283186000000
	H	0.049648000000	-1.066029000000	0.788045000000
	H	-0.590008000000	-1.061494000000	-0.866253000000
	H	3.139532000000	0.846045000000	-0.845892000000
	H	3.714970000000	0.793019000000	0.814465000000
	H	3.650775000000	-1.492234000000	-0.214989000000
	H	2.577490000000	-1.378017000000	1.173714000000
	H	1.734247000000	-1.168377000000	-1.757996000000
	H	1.417066000000	-2.527938000000	-0.689904000000
	H	1.382434000000	0.913410000000	1.658549000000
	H	-1.180197000000	1.107078000000	1.194533000000
	H	-2.891746000000	2.004869000000	-0.536924000000
	H	-1.780765000000	1.340266000000	-1.811668000000
	H	-0.664270000000	2.548266000000	0.348277000000
frequencies	-1842.8 44.0 82.9 98.1 112.4 143.1 223.9 241.3 266.7 331.7 361.5 394.2 434.4 449.8 471.8 518.8 550.0 559.4 776.2 806.4 822.8 860.2 903.0 910.7 938.3 944.5 1005.9 1030.2 1058.4 1067.0 1073.9 1077.1 1104.9 1125.7 1136.0 1169.0 1186.0 1222.2 1245.3 1286.3 1291.2 1299.7 1317.6 1337.7 1366.2 1377.3 1381.7 1386.4 1390.2 1409.7 1417.4 1453.3 1462.2 1475.2 1486.9 1489.6 1492.7 1501.2 1516.9 3000.1 3006.8 3011.7 3030.3 3038.6 3044.2 3046.5 3048.5 3086.1 3088.7 3097.9 3098.3 3099.1 3102.5 3184.9 3809.2			
electronic state	2-A			
point group	C1			
rotational constants	2.05324 0.69559 0.58972			
ZPE	0.238479 (Hartree/Particle)			

$TS_b\alpha$				
optimized Cartesian coordinate	C	-1.179994000000	1.358763000000	-0.047608000000
	C	-0.051662000000	0.310589000000	0.027516000000
	C	1.191040000000	0.879267000000	0.669743000000
	C	1.903024000000	1.994475000000	-0.053337000000
	H	2.047831000000	-0.108468000000	0.612973000000
	O	2.796776000000	-1.018412000000	0.330999000000
	O	2.518819000000	-1.275394000000	-1.003231000000
	H	1.901446000000	-2.018490000000	-0.966748000000
	H	2.872950000000	2.203801000000	0.400410000000
	C	-0.548939000000	-0.940343000000	0.762466000000
	C	-1.803393000000	-1.522480000000	0.109618000000
	C	-2.917388000000	-0.476670000000	0.035276000000
	C	-2.438951000000	0.778592000000	-0.696284000000
	H	0.249710000000	-1.688163000000	0.808409000000
	H	0.202952000000	0.030880000000	-1.005700000000
	H	-1.412863000000	1.696265000000	0.970910000000
	H	-0.840171000000	2.234228000000	-0.606852000000
	H	-1.559509000000	-1.859549000000	-0.905717000000
	H	-2.142581000000	-2.402415000000	0.662432000000
	H	-3.798405000000	-0.892484000000	-0.460544000000
	H	-3.222723000000	-0.205684000000	1.053302000000
	H	-2.217726000000	0.524887000000	-1.740025000000
	H	-3.229678000000	1.533459000000	-0.714820000000
	H	-0.774627000000	-0.667750000000	1.801973000000
	H	2.064698000000	1.728143000000	-1.101187000000
	H	1.317941000000	2.920884000000	-0.024972000000
	H	1.093571000000	1.027739000000	1.749674000000
frequencies	-1770.1	42.7	59.3	83.0
	238.5	296.2	359.3	375.8
	530.1	604.9	795.3	799.6
	937.5	941.2	1002.7	1054.5
	1112.3	1122.1	1139.4	1165.6
	1295.4	1309.0	1334.2	1363.7
	1403.8	1411.2	1417.4	1468.2
	1493.4	1496.5	1510.0	3011.8
	3042.2	3047.6	3082.7	3087.7
	3110.4	3142.5	3803.8	
	121.7	137.0	185.4	215.6
	406.9	415.9	441.4	473.5
	850.1	860.9	891.5	904.1
	1058.9	1073.5	1077.6	1085.4
	1185.9	1219.1	1264.7	1291.5
	1371.4	1376.7	1386.3	1388.1
	1483.5	1487.3	1489.5	1490.5
	3030.2	3035.5	3037.9	3040.6
	3096.8	3098.1	3100.7	3103.8
electronic state	2-A			
point group	C1			
rotational constants	1.86449	0.77883	0.62313	
ZPE	0.238454 (Hartree/Particle)			
$TS_b\alpha'$				
optimized Cartesian coordinate	C	-0.579994000000	0.320382000000	1.324643000000
	C	0.287206000000	-0.428737000000	0.331531000000
	C	1.629925000000	-0.853244000000	0.891475000000
	C	2.574439000000	-1.489395000000	-0.126602000000
	H	0.615773000000	0.483281000000	-0.521270000000
	O	0.983836000000	1.464165000000	-1.177159000000
	O	1.416206000000	2.354713000000	-0.206227000000
	H	0.655747000000	2.937334000000	-0.077817000000
	H	2.695585000000	-0.834340000000	-0.993019000000
	H	2.105408000000	0.030405000000	1.330303000000
	H	2.204679000000	-2.455626000000	-0.475119000000
	C	-0.471959000000	-1.452424000000	-0.491740000000
	C	-1.750947000000	-0.872465000000	-1.103940000000
	C	-2.628975000000	-0.206719000000	-0.043587000000
	C	-1.851693000000	0.887335000000	0.689317000000
	H	0.168105000000	-1.860556000000	-1.277457000000
	H	-0.859420000000	-0.381129000000	2.126587000000
	H	0.009196000000	1.111285000000	1.800000000000
	H	-1.474562000000	-0.126988000000	-1.858433000000
	H	-2.304528000000	-1.660514000000	-1.620497000000
	H	-3.528347000000	0.209870000000	-0.504259000000

	H	-2.960688000000	-0.960890000000	0.680910000000
	H	-1.578295000000	1.667376000000	-0.032143000000
	H	-2.474806000000	1.358236000000	1.453818000000
	H	-0.730894000000	-2.293554000000	0.172063000000
	H	3.559373000000	-1.652760000000	0.313779000000
	H	1.449337000000	-1.550858000000	1.723062000000
frequencies	-1676.7 32.0 74.3 84.0 96.1 136.2 185.4 221.3 246.5 271.2 332.0 374.8 382.3 402.7 451.9 460.7 540.0 568.8 756.1 789.4 806.2 859.1 889.2 917.1 936.0 950.1 1002.5 1044.2 1057.2 1067.6 1076.8 1095.1 1117.4 1126.6 1173.5 1176.2 1185.4 1247.5 1260.1 1292.2 1300.8 1325.0 1351.4 1366.1 1379.6 1386.6 1389.1 1401.6 1408.4 1416.0 1460.1 1465.9 1472.6 1479.7 1487.7 1493.3 1505.4 1508.4 1513.6 2988.4 2997.3 3008.5 3035.8 3043.3 3052.1 3063.2 3074.1 3081.2 3099.7 3100.6 3104.1 3105.0 3137.1 3140.1 3807.1			
electronic state	2-A			
point group	C1			
rotational constants	1.45402 1.00574 0.78416			
ZPE	0.238375 (Hartree/Particle)			
$TS_b\beta'$				
optimized Cartesian coordinate	C	-0.124152000000	0.233719000000	0.874805000000
	C	1.190604000000	-0.332013000000	1.361104000000
	C	1.945322000000	-1.067403000000	0.251718000000
	H	0.223747000000	1.133713000000	-0.010058000000
	O	0.667141000000	1.916063000000	-0.828249000000
	O	1.923100000000	2.245210000000	-0.335960000000
	H	1.773972000000	3.084898000000	0.117222000000
	C	-0.210435000000	-1.445672000000	-0.987718000000
	C	-1.016408000000	-0.708334000000	0.089526000000
	H	2.840717000000	-1.540010000000	0.663127000000
	H	0.081101000000	-0.721738000000	-1.758421000000
	H	-0.852163000000	-2.189069000000	-1.470001000000
	H	0.976505000000	-1.032688000000	2.183238000000
	H	1.809416000000	0.464543000000	1.782978000000
	H	-0.648218000000	0.834373000000	1.620715000000
	H	-1.388768000000	-1.460752000000	0.807402000000
	H	2.277313000000	-0.336026000000	-0.492650000000
	C	-2.229712000000	0.000225000000	-0.523231000000
	H	-2.797341000000	-0.738174000000	-1.098739000000
	C	-3.153356000000	0.665898000000	0.495247000000
	H	-2.672984000000	1.515362000000	0.984822000000
	H	-4.058606000000	1.039414000000	0.013037000000
	H	-3.456081000000	-0.043484000000	1.270896000000
	C	1.046615000000	-2.105848000000	-0.420229000000
	H	1.591721000000	-2.618997000000	-1.216628000000
	H	0.758822000000	-2.870343000000	0.312570000000
	H	-1.871960000000	0.745367000000	-1.243172000000
frequencies	-1755.2 51.1 57.5 90.0 96.9 129.6 187.1 227.3 243.4 270.1 343.0 366.2 397.5 436.4 454.7 478.7 551.5 595.0 763.1 793.1 805.9 865.7 892.3 902.6 934.6 937.7 1001.3 1037.5 1060.6 1063.0 1070.4 1101.4 1111.2 1121.7 1157.9 1171.8 1196.3 1231.8 1257.2 1289.5 1299.0 1303.7 1335.7 1361.8 1367.1 1382.5 1387.7 1391.7 1399.3 1406.9 1418.0 1454.1 1464.8 1485.2 1493.2 1496.6 1503.9 1506.8 1516.1 2959.2 2998.5 3035.2 3044.8 3048.8 3058.3 3062.3 3084.6 3092.8 3095.3 3099.2 3109.6 3114.7 3128.7 3138.4 3822.2			
electronic state	2-A			
point group	C1			
rotational constants	1.34537 1.01477 0.72676			
ZPE	0.238317 (Hartree/Particle)			

$TS_b\gamma'$				
optimized Cartesian coordinate	C	-1.283353000000	0.099798000000	1.094825000000
	C	0.222824000000	-0.021799000000	1.109640000000
	C	0.783420000000	-0.513382000000	-0.231253000000
	H	-1.494555000000	1.040366000000	0.209121000000
	O	-1.538854000000	1.910220000000	-0.638755000000
	O	-0.350016000000	2.607962000000	-0.474251000000
	H	-0.607524000000	3.367626000000	0.063773000000
	C	-1.455261000000	-1.573996000000	-0.773627000000
	C	-2.033134000000	-1.100930000000	0.562876000000
	H	-1.658572000000	-0.816419000000	-1.537994000000
	H	-1.952518000000	-2.494660000000	-1.089017000000
	H	0.509606000000	-0.738242000000	1.898222000000
	H	0.668066000000	0.938617000000	1.380956000000
	H	-1.710472000000	0.537980000000	1.999159000000
	H	-1.944773000000	-1.912552000000	1.301546000000
	H	-3.099264000000	-0.877319000000	0.471754000000
	H	0.581233000000	0.267499000000	-0.976467000000
	C	2.296142000000	-0.734198000000	-0.173115000000
	H	2.624791000000	-1.110879000000	-1.147505000000
	C	3.092220000000	0.523223000000	0.174982000000
	H	2.923294000000	0.835666000000	1.207588000000
	H	4.164286000000	0.354830000000	0.055703000000
	H	2.803736000000	1.353073000000	-0.476105000000
	C	0.055523000000	-1.787793000000	-0.670020000000
	H	0.264035000000	-2.586042000000	0.055986000000
	H	0.454667000000	-2.123677000000	-1.632001000000
	H	2.514632000000	-1.526853000000	0.553485000000
frequencies	-1765.6	56.1	70.6	88.0
	240.8	278.3	315.3	372.5
	554.6	602.6	764.1	796.9
	936.1	939.4	1000.5	1035.1
	1125.6	1132.9	1157.5	1163.3
	1306.7	1320.7	1333.2	1350.4
	1406.4	1412.3	1416.1	1460.7
	1500.6	1503.0	1515.3	2979.2
	3057.7	3059.4	3076.6	3088.0
	3130.3	3135.4	3820.7	
	104.5	149.5	202.0	220.9
	399.9	432.2	461.6	468.1
	803.5	859.7	889.9	901.5
	1060.9	1062.9	1070.9	1088.4
	1203.8	1234.0	1260.6	1285.3
	1373.8	1378.6	1388.8	1395.2
	1463.3	1472.8	1487.1	1494.4
	3001.1	3021.2	3033.1	3047.0
	3095.1	3101.0	3106.3	3111.5
electronic state	2-A			
point group	C1			
rotational constants	1.31487	1.06534	0.72108	
ZPE	0.238372 (Hartree/Particle)			
$TS_b\delta'$				
optimized Cartesian coordinate	C	1.422438000000	1.210469000000	0.361907000000
	C	1.017305000000	0.311577000000	1.506106000000
	C	-0.077074000000	-0.673356000000	1.086947000000
	C	-1.275527000000	0.025683000000	0.435954000000
	C	-2.345754000000	-0.999263000000	0.050710000000
	C	-3.626520000000	-0.389171000000	-0.516870000000
	H	1.939112000000	0.382673000000	-0.510616000000
	O	2.373095000000	-0.488475000000	-1.235539000000
	O	2.838630000000	-1.458936000000	-0.358782000000
	H	3.785928000000	-1.278531000000	-0.305724000000
	H	-4.394218000000	-1.152572000000	-0.657366000000
	C	-0.804561000000	0.852106000000	-0.766225000000
	C	0.276216000000	1.864967000000	-0.374820000000
	H	-0.409752000000	-1.248476000000	1.956277000000
	H	-1.713607000000	0.716925000000	1.172697000000
	H	-0.401552000000	0.168074000000	-1.523603000000
	H	-1.644593000000	1.382140000000	-1.221582000000
	H	0.645976000000	0.946657000000	2.325446000000
	H	1.884936000000	-0.227721000000	1.894926000000
	H	2.262998000000	1.873389000000	0.576889000000
	H	-0.166348000000	2.623649000000	0.289026000000
	H	0.641925000000	2.399403000000	-1.255530000000

	H	0.347766000000	-1.388560000000	0.372767000000				
	H	-2.591994000000	-1.591011000000	0.938897000000				
	H	-4.029535000000	0.369178000000	0.160670000000				
	H	-3.455503000000	0.084455000000	-1.485405000000				
	H	-1.914487000000	-1.698452000000	-0.675460000000				
frequencies	-1752.8	47.8	69.6	83.1	108.7	140.3	212.2	226.2
	246.8	268.6	314.9	365.1	405.9	440.1	458.0	470.9
	549.2	608.3	763.6	785.4	810.4	852.3	892.4	917.8
	935.6	937.5	994.9	1034.4	1057.4	1061.7	1073.6	1100.8
	1113.2	1129.6	1158.8	1171.2	1200.3	1223.8	1258.9	1296.6
	1302.6	1314.8	1340.3	1352.5	1370.4	1379.0	1384.6	1395.8
	1407.4	1412.0	1416.0	1459.1	1464.8	1475.4	1486.3	1492.3
	1501.7	1506.3	1515.2	2997.0	2997.9	3001.9	3042.1	3046.5
	3053.7	3058.4	3079.6	3093.5	3096.1	3098.7	3107.3	3110.4
	3127.0	3138.9	3821.4					
electronic state	2-A							
point group	C1							
rotational constants	1.89814	0.71392	0.66667					
ZPE	0.238371 (Hartree/Particle)							
*n*PCH								
optimized Cartesian coordinate	C	-0.457552000000	1.114257000000	0.255287000000				
	C	0.042493000000	-0.236934000000	-0.269808000000				
	C	-0.920285000000	-1.353391000000	0.151451000000				
	C	-2.360140000000	-1.073379000000	-0.282230000000				
	C	-2.842075000000	0.272815000000	0.260748000000				
	C	-1.900530000000	1.398131000000	-0.170441000000				
	H	-0.577664000000	-2.308933000000	-0.258289000000				
	H	0.042498000000	-0.190171000000	-1.369366000000				
	H	-0.396078000000	1.105683000000	1.352650000000				
	H	0.193012000000	1.921234000000	-0.092053000000				
	H	-2.409956000000	-1.057484000000	-1.377916000000				
	H	-3.019295000000	-1.878807000000	0.053022000000				
	H	-3.861525000000	0.478468000000	-0.076841000000				
	H	-2.871641000000	0.228291000000	1.356454000000				
	H	-1.937683000000	1.496789000000	-1.262383000000				
	H	-2.232994000000	2.353813000000	0.244011000000				
	H	-0.886098000000	-1.448608000000	1.245349000000				
	C	1.467070000000	-0.554088000000	0.191447000000				
	H	1.738902000000	-1.551436000000	-0.176199000000				
	H	1.479536000000	-0.618838000000	1.287835000000				
	C	2.531631000000	0.442909000000	-0.265573000000				
	H	2.352680000000	1.418095000000	0.196039000000				
	H	2.445800000000	0.590476000000	-1.348233000000				
	C	3.943575000000	-0.025176000000	0.080504000000				
	H	4.696662000000	0.699961000000	-0.234231000000				
	H	4.049702000000	-0.172129000000	1.158682000000				
	H	4.169024000000	-0.977278000000	-0.406849000000				
frequencies	70.4	77.6	129.1	184.2	232.6	248.6	296.0	328.7
	358.7	442.9	445.5	472.7	571.5	741.3	793.8	802.5
	848.8	861.0	901.0	913.6	917.8	943.4	989.6	1039.8
	1058.5	1060.6	1079.5	1089.6	1115.1	1129.3	1143.7	1190.1
	1218.7	1247.4	1284.3	1291.0	1298.1	1307.0	1326.2	1339.4
	1353.6	1367.9	1382.7	1386.0	1389.5	1403.1	1411.7	1414.1
	1479.2	1485.5	1488.3	1489.7	1494.0	1497.5	1504.9	1508.4
	1512.4	3002.9	3022.2	3022.9	3031.2	3036.6	3040.5	3045.0
	3049.1	3055.7	3060.0	3083.2	3090.7	3093.6	3094.6	3098.7
	3101.9	3126.3	3132.1					
electronic state	1-A							
point group	C1							
rotational constants	3.74039	0.77496	0.67882					
ZPE	0.256397 (Hartree/Particle)							
*n*P1								

optimized Cartesian coordinate	C	0.202686000000	0.986567000000	-0.518677000000
	C	-0.222132000000	-0.350625000000	0.098255000000
	C	-1.521826000000	-0.889049000000	-0.508423000000
	C	-2.714874000000	0.073818000000	-0.438176000000
	C	-3.031115000000	0.514745000000	0.949173000000
	C	0.899546000000	-1.384726000000	-0.048350000000
	C	2.222394000000	-0.889750000000	0.538062000000
	C	2.637065000000	0.437416000000	-0.099792000000
	C	1.531660000000	1.482756000000	0.057189000000
	H	0.599009000000	-2.324577000000	0.426120000000
	H	-0.386928000000	-0.180329000000	1.171862000000
	H	0.298398000000	0.860026000000	-1.606405000000
	H	-0.572385000000	1.739826000000	-0.349981000000
	H	2.107521000000	-0.748585000000	1.619711000000
	H	3.003562000000	-1.641860000000	0.397620000000
	H	3.569056000000	0.799602000000	0.342640000000
	H	2.832152000000	0.276806000000	-1.167360000000
	H	1.396204000000	1.702337000000	1.123349000000
	H	1.822648000000	2.420697000000	-0.423644000000
	H	1.039413000000	-1.600924000000	-1.116340000000
	H	-1.788348000000	-1.820146000000	0.006077000000
	H	-1.339887000000	-1.154423000000	-1.556725000000
	H	-3.587438000000	-0.433668000000	-0.877846000000
	H	-2.536439000000	0.944946000000	-1.075623000000
	H	-2.960326000000	-0.188745000000	1.770208000000
	H	-3.516635000000	1.462107000000	1.140768000000
frequencies	62.2	96.3	146.7	176.5	229.4	237.0	310.4	336.0
	398.3	437.2	444.7	464.8	504.2	547.3	764.4	798.0
	830.8	856.3	865.5	907.9	911.6	924.1	944.7	991.6
	1038.7	1059.3	1080.2	1088.7	1102.3	1127.1	1139.1	1172.8
	1189.9	1237.6	1241.6	1291.1	1292.3	1304.5	1323.0	1342.2
	1365.8	1373.7	1380.9	1386.0	1388.3	1398.1	1410.8	1465.6
	1478.2	1480.7	1487.4	1489.9	1493.3	1495.4	1508.7	2987.3
	3013.2	3021.7	3029.4	3036.3	3037.7	3041.1	3045.0	3069.5
	3080.7	3087.3	3093.5	3094.3	3095.4	3099.2	3163.6	3268.0
electronic state	2-A							
point group	C1							
rotational constants	3.09872	0.93739	0.82111					
ZPE	0.241673 (Hartree/Particle)							
*n*P2								
optimized Cartesian coordinate	C	-0.333155000000	1.073807000000	0.239858000000
	C	0.063899000000	-0.307684000000	-0.292185000000
	C	1.484291000000	-0.687405000000	0.136792000000
	C	2.545224000000	0.206202000000	-0.411744000000
	C	3.910631000000	0.220176000000	0.184515000000
	C	-0.953796000000	-1.358979000000	0.160817000000
	C	-2.380941000000	-0.986262000000	-0.246413000000
	C	-2.763886000000	0.395436000000	0.288033000000
	C	-1.757840000000	1.454152000000	-0.167978000000
	H	-0.684444000000	-2.337643000000	-0.249104000000
	H	0.040921000000	-0.267244000000	-1.391526000000
	H	-0.261899000000	1.055218000000	1.336317000000
	H	0.379984000000	1.826976000000	-0.107771000000
	H	-2.451132000000	-0.979406000000	-1.341077000000
	H	-3.085635000000	-1.742086000000	0.110890000000
	H	-3.773178000000	0.662827000000	-0.036582000000
	H	-2.779515000000	0.364394000000	1.384485000000
	H	-1.805746000000	1.548032000000	-1.259897000000
	H	-2.020281000000	2.431976000000	0.244925000000
	H	-0.901364000000	-1.448265000000	1.254492000000
	H	1.677781000000	-1.730341000000	-0.168682000000
	H	1.538419000000	-0.691930000000	1.234996000000
	H	2.404416000000	0.609479000000	-1.409759000000
	H	4.518864000000	1.036825000000	-0.207597000000
	H	3.863347000000	0.320387000000	1.273872000000
	H	4.452902000000	-0.715848000000	-0.018145000000

frequencies	47.1	83.0	104.2	157.1	190.0	237.6	307.8	326.6
	355.8	428.5	447.8	455.9	471.2	568.6	790.8	799.4
	840.3	861.3	903.2	916.4	924.3	946.9	987.7	993.1
	1056.3	1070.7	1075.1	1093.3	1118.0	1130.9	1147.9	1173.2
	1198.4	1229.0	1275.5	1290.3	1296.4	1299.7	1336.1	1346.5
	1368.9	1383.5	1387.2	1388.5	1401.4	1409.9	1429.8	1468.4
	1481.7	1482.8	1487.9	1489.4	1491.4	1494.5	1508.6	2958.7
	2992.7	3004.8	3023.1	3024.9	3033.6	3037.0	3040.6	3045.3
	3068.8	3083.4	3091.1	3094.5	3095.1	3099.4	3129.8	3176.3
electronic state	2-A							
point group	C1							
rotational constants	3.70566	0.79848	0.69836					
ZPE	0.241383 (Hartree/Particle)							
*n*P3								
optimized Cartesian coordinate	C	-0.842099000000	-1.353224000000	-0.173493000000				
	C	0.078779000000	-0.189638000000	0.211054000000				
	C	1.476601000000	-0.399252000000	-0.268437000000				
	C	2.592414000000	0.494192000000	0.159805000000				
	C	3.962396000000	-0.179641000000	0.059303000000				
	H	4.157651000000	-0.500570000000	-0.966902000000				
	C	-0.510471000000	1.141548000000	-0.306995000000				
	C	-1.940236000000	1.357390000000	0.193565000000				
	C	-2.843609000000	0.184833000000	-0.193527000000				
	C	-2.273231000000	-1.138401000000	0.321542000000				
	H	0.130951000000	1.973279000000	-0.000841000000				
	H	0.098109000000	-0.117990000000	1.311086000000				
	H	-0.846523000000	-1.444365000000	-1.267835000000				
	H	-0.434352000000	-2.288452000000	0.221273000000				
	H	-1.926730000000	1.455591000000	1.286033000000				
	H	-2.340363000000	2.294366000000	-0.203516000000				
	H	-3.854583000000	0.339832000000	0.192888000000				
	H	-2.923645000000	0.139804000000	-1.286622000000				
	H	-2.276452000000	-1.128185000000	1.418397000000				
	H	-2.908374000000	-1.972668000000	0.011673000000				
	H	-0.503216000000	1.118380000000	-1.404470000000				
	H	1.640515000000	-1.051784000000	-1.122812000000				
	H	2.602961000000	1.411050000000	-0.450767000000				
	H	4.763686000000	0.498828000000	0.358256000000				
	H	4.004282000000	-1.063892000000	0.698828000000				
	H	2.412823000000	0.829931000000	1.188428000000				
frequencies	47.3	55.9	113.4	189.2	239.3	241.5	282.1	310.6
	362.1	394.7	446.3	467.2	491.2	585.8	770.5	796.7
	807.0	859.1	897.5	903.7	917.7	940.5	994.4	1041.4
	1052.0	1062.4	1072.2	1091.1	1117.2	1124.0	1163.5	1170.3
	1213.7	1243.5	1277.7	1286.3	1293.4	1300.1	1324.8	1338.4
	1357.8	1370.1	1385.3	1387.8	1394.1	1410.7	1438.2	1477.8
	1482.7	1486.7	1489.7	1494.6	1501.6	1507.7	1508.5	2978.7
	2981.4	3030.7	3035.7	3037.6	3042.0	3045.9	3050.9	3060.4
	3090.8	3092.3	3094.8	3095.5	3100.2	3131.2	3137.7	3158.0
electronic state	2-A							
point group	C1							
rotational constants	3.80446	0.77578	0.68024					
ZPE	0.241812 (Hartree/Particle)							
*n*P4								
optimized Cartesian coordinate	C	-0.575844000000	-1.061454000000	-0.921993000000				
	C	0.173126000000	0.195647000000	-0.608397000000				
	C	1.608266000000	0.368588000000	-0.995908000000				
	C	2.546075000000	0.467727000000	0.222872000000				
	C	2.561207000000	-0.817473000000	1.046686000000				
	H	3.234929000000	-0.737003000000	1.902057000000				
	C	-0.636385000000	1.399541000000	-0.238393000000				
	C	-1.722971000000	1.071113000000	0.794415000000				

	C	-2.554665000000	-0.131854000000	0.346087000000
	C	-1.666607000000	-1.356263000000	0.117865000000
	H	0.014744000000	2.198453000000	0.130477000000
	H	-1.060316000000	-0.967635000000	-1.910763000000
	H	0.116673000000	-1.905258000000	-0.999441000000
	H	-1.243761000000	0.838087000000	1.752356000000
	H	-2.364314000000	1.941805000000	0.955867000000
	H	-3.325272000000	-0.357139000000	1.088184000000
	H	-3.074424000000	0.116844000000	-0.587946000000
	H	-1.189079000000	-1.632400000000	1.065147000000
	H	-2.267876000000	-2.211514000000	-0.202220000000
	H	-1.129033000000	1.798953000000	-1.143263000000
	H	1.724848000000	1.278224000000	-1.600940000000
	H	1.933789000000	-0.471306000000	-1.620413000000
	H	2.225380000000	1.305337000000	0.851414000000
	H	3.558187000000	0.702127000000	-0.121119000000
	H	1.561044000000	-1.047050000000	1.423825000000
	H	2.891260000000	-1.663958000000	0.437378000000
frequencies	35.5 46.3 107.4 180.3 217.2 255.0 295.3 360.2 374.6 406.1 442.0 467.6 545.7 727.2 790.8 796.0 851.7 854.3 865.2 890.4 924.0 930.7 985.6 1038.2 1051.9 1061.9 1082.0 1096.6 1103.5 1109.8 1173.3 1192.8 1226.2 1255.6 1282.7 1285.2 1307.8 1317.7 1355.2 1359.7 1364.0 1375.5 1380.3 1387.1 1409.3 1415.4 1466.3 1474.5 1484.2 1486.4 1490.9 1491.0 1502.6 1504.8 1508.5 2945.1 2948.1 3013.4 3035.2 3046.2 3048.3 3050.4 3052.8 3068.9 3076.9 3080.6 3090.2 3095.9 3096.9 3100.4 3122.2 3132.6		
electronic state	2-A		
point group	C1		
rotational constants	2.60410 1.00754 0.92530		
ZPE	0.242382 (Hartree/Particle)		
*n*P5			
optimized Cartesian coordinate	C	0.455933000000	1.075456000000	-0.205759000000
	C	1.858835000000	1.449896000000	0.140089000000
	C	2.833237000000	0.332993000000	-0.286945000000
	C	0.949794000000	-1.352364000000	-0.158668000000
	C	-0.045518000000	-0.251634000000	0.268339000000
	H	3.846300000000	0.567583000000	0.051820000000
	H	0.909874000000	-1.452302000000	-1.250716000000
	H	0.637263000000	-2.311876000000	0.266108000000
	H	1.949711000000	1.575279000000	1.229615000000
	H	2.140371000000	2.401142000000	-0.315637000000
	H	-0.091066000000	1.621402000000	-0.966143000000
	H	-0.047953000000	-0.245529000000	1.372414000000
	H	2.858570000000	0.282195000000	-1.381171000000
	C	2.380067000000	-1.017758000000	0.271015000000
	H	3.063427000000	-1.807466000000	-0.052991000000
	H	2.427544000000	-0.987666000000	1.366769000000
	C	-1.464417000000	-0.556355000000	-0.210495000000
	H	-1.722981000000	-1.585960000000	0.064379000000
	H	-1.483089000000	-0.514355000000	-1.307547000000
	C	-2.520481000000	0.391309000000	0.355623000000
	H	-2.268600000000	1.422683000000	0.089644000000
	H	-2.492235000000	0.341810000000	1.449718000000
	C	-3.925648000000	0.059062000000	-0.140349000000
	H	-4.207757000000	-0.959062000000	0.140859000000
	H	-4.670507000000	0.740189000000	0.275810000000
	H	-3.979682000000	0.128302000000	-1.230032000000
frequencies	57.3 76.8 92.7 146.4 192.7 246.2 274.5 299.2 328.1 356.2 450.3 466.7 511.5 588.2 741.8 801.9 837.9 857.7 874.8 904.6 921.8 945.2 973.4 1038.8 1048.4 1065.6 1075.4 1100.0 1108.6 1143.2 1152.9 1163.0 1215.4 1243.8 1261.7 1287.1 1294.6 1314.0 1331.0 1340.6 1346.5 1354.7 1368.0 1384.5 1402.7 1413.6 1424.2 1479.6 1482.4 1488.9 1490.9 1496.9 1501.2 1504.6 1512.0 2962.1 2999.5 3027.6 3035.3 3039.2 3049.5 3051.2 3055.6 3064.1		

	3085.4	3091.2	3094.8	3099.7	3110.0	3124.7	3132.9	3190.0
electronic state	2-A							
point group	C1							
rotational constants	3.82023	0.77981	0.68530					
ZPE	0.241472 (Hartree/Particle)							
*n*P6								
optimized Cartesian coordinate	C	1.581136000000	1.478020000000	-0.015119000000				
	C	0.245790000000	1.023312000000	-0.504675000000				
	C	-0.157207000000	-0.340994000000	0.083946000000				
	C	2.282756000000	-0.842655000000	0.579406000000				
	C	2.712564000000	0.504351000000	-0.021135000000				
	H	2.115517000000	-0.717767000000	1.654880000000				
	H	3.081573000000	-1.579361000000	0.459066000000				
	H	0.264504000000	0.915024000000	-1.605441000000				
	H	-0.515171000000	1.777149000000	-0.286122000000				
	H	1.779670000000	2.536450000000	0.099046000000				
	H	3.041341000000	0.324109000000	-1.059291000000				
	H	3.577551000000	0.908033000000	0.510264000000				
	H	-0.325192000000	-0.202496000000	1.160150000000				
	C	0.993881000000	-1.339970000000	-0.075337000000				
	H	1.171716000000	-1.505621000000	-1.146978000000				
	H	0.701001000000	-2.305772000000	0.348695000000				
	C	-1.438156000000	-0.887910000000	-0.552533000000				
	H	-1.228306000000	-1.130595000000	-1.601674000000				
	H	-1.691527000000	-1.834866000000	-0.060303000000				
	C	-2.651953000000	0.043871000000	-0.487325000000				
	H	-2.472453000000	0.932051000000	-1.101177000000				
	H	-3.505956000000	-0.467931000000	-0.940719000000				
	C	-3.014008000000	0.467049000000	0.935624000000				
	H	-2.232637000000	1.087603000000	1.381072000000				
	H	-3.942299000000	1.041407000000	0.953021000000				
	H	-3.148150000000	-0.407870000000	1.578394000000				
frequencies	78.4	91.1	162.3	178.8	202.9	267.7	296.7	312.8
	370.6	405.5	429.8	467.0	501.3	615.2	747.9	800.5
	844.6	854.1	866.9	892.7	922.7	940.2	967.3	1017.8
	1049.6	1067.8	1084.2	1106.8	1125.1	1127.4	1136.1	1165.8
	1214.4	1241.1	1273.5	1289.4	1302.4	1324.0	1330.5	1360.0
	1365.6	1369.2	1380.2	1389.8	1403.2	1409.4	1417.3	1467.3
	1473.0	1482.1	1491.7	1498.2	1500.1	1507.5	1515.2	2939.1
	2959.9	3021.2	3029.7	3036.7	3051.2	3055.5	3058.6	3072.8
	3084.5	3090.6	3096.6	3098.7	3100.6	3125.3	3133.8	3205.4
electronic state	2-A							
point group	C1							
rotational constants	3.15993	0.91640	0.81109					
ZPE	0.242085 (Hartree/Particle)							
*n*P7								
optimized Cartesian coordinate	C	2.853708000000	0.284427000000	-0.155833000000				
	C	2.407210000000	-1.080874000000	0.249418000000				
	C	0.963227000000	-1.347379000000	-0.199537000000				
	C	0.008390000000	-0.229548000000	0.234128000000				
	C	-1.424166000000	-0.553899000000	-0.197692000000				
	C	-2.483623000000	0.442161000000	0.273220000000				
	C	-3.900014000000	-0.037067000000	-0.037687000000				
	H	-4.109577000000	-0.985427000000	0.463804000000				
	C	0.494535000000	1.115778000000	-0.316631000000				
	C	1.934809000000	1.427269000000	0.120609000000				
	H	0.617782000000	-2.306572000000	0.198742000000				
	H	0.029491000000	-0.172867000000	1.333422000000				
	H	0.448074000000	1.080091000000	-1.412725000000				
	H	-0.164324000000	1.924607000000	0.009379000000				
	H	2.445677000000	-1.172063000000	1.348763000000				
	H	3.079658000000	-1.845993000000	-0.145700000000				

	H	3.896884000000	0.470374000000	-0.379641000000				
	H	1.921662000000	1.635615000000	1.204645000000				
	H	2.290598000000	2.340721000000	-0.361822000000				
	H	0.936481000000	-1.423621000000	-1.293684000000				
	H	-1.685176000000	-1.549295000000	0.182517000000				
	H	-1.457176000000	-0.626849000000	-1.293025000000				
	H	-2.320825000000	1.413903000000	-0.201269000000				
	H	-2.375132000000	0.600236000000	1.352342000000				
	H	-4.650080000000	0.687169000000	0.286110000000				
	H	-4.028472000000	-0.195239000000	-1.111822000000				
frequencies	66.8	74.1	125.6	161.1	211.7	242.3	252.3	296.5
	351.6	358.9	446.8	449.2	517.1	637.8	741.5	781.8
	808.4	864.1	897.7	907.9	920.0	954.7	979.8	1029.7
	1043.8	1062.7	1080.0	1106.3	1111.2	1129.1	1149.0	1166.8
	1229.7	1235.9	1276.4	1287.0	1303.6	1317.9	1330.1	1342.9
	1350.6	1372.6	1380.8	1400.8	1403.5	1412.0	1414.2	1469.5
	1477.6	1480.6	1487.7	1495.2	1499.4	1505.0	1512.3	2956.9
	2960.2	3000.4	3024.3	3035.9	3041.6	3049.2	3055.8	3061.1
	3087.6	3092.9	3096.9	3097.7	3105.7	3126.4	3132.6	3203.8
electronic state	2-A							
point group	C1							
rotational constants	3.76228	0.79112	0.68784					
ZPE	0.241578 (Hartree/Particle)							
$TS_c\gamma$								
optimized Cartesian coordinate	C	1.509919000000	1.227803000000	0.207666000000				
	C	0.649951000000	-0.022055000000	-0.014419000000				
	C	-0.681171000000	0.293822000000	-0.697650000000				
	C	-1.574598000000	1.260214000000	0.082009000000				
	C	-2.960150000000	1.355658000000	-0.493545000000				
	H	-3.457351000000	0.125147000000	-0.344174000000				
	O	-3.747573000000	-0.997531000000	-0.106221000000				
	O	-2.954941000000	-1.335219000000	0.983600000000				
	H	-3.551072000000	-1.226734000000	1.735782000000				
	C	1.432323000000	-1.063039000000	-0.822960000000				
	C	2.774797000000	-1.407419000000	-0.176027000000				
	C	3.621847000000	-0.150306000000	0.028481000000				
	C	2.858088000000	0.889596000000	0.849701000000				
	H	0.824051000000	-1.964370000000	-0.945405000000				
	H	0.425858000000	-0.459875000000	0.969806000000				
	H	1.680307000000	1.711412000000	-0.764613000000				
	H	0.978217000000	1.951071000000	0.832629000000				
	H	2.594577000000	-1.881770000000	0.796389000000				
	H	3.313594000000	-2.135606000000	-0.788325000000				
	H	4.567414000000	-0.401240000000	0.516816000000				
	H	3.872010000000	0.277337000000	-0.950304000000				
	H	2.683311000000	0.491616000000	1.856896000000				
	H	3.456355000000	1.797200000000	0.968154000000				
	H	1.610763000000	-0.661385000000	-1.829836000000				
	H	-1.229204000000	-0.642390000000	-0.846738000000				
	H	-0.484883000000	0.708227000000	-1.695420000000				
	H	-1.132313000000	2.266235000000	0.090716000000				
	H	-1.629687000000	0.943222000000	1.129852000000				
	H	-3.671644000000	1.980262000000	0.044939000000				
	H	-3.016229000000	1.477998000000	-1.575741000000				
frequencies	-1816.7	24.2	43.7	75.1	96.5	132.4	176.0	200.0
	233.7	249.5	320.5	332.0	360.6	391.5	445.2	445.7
	477.2	513.7	567.0	581.2	738.7	795.3	804.3	857.7
	872.6	899.0	911.0	932.5	946.2	990.9	1037.5	1058.4
	1066.2	1071.2	1088.2	1093.8	1110.1	1126.0	1135.2	1167.7
	1184.4	1216.1	1230.1	1274.0	1291.7	1296.1	1303.6	1323.3
	1343.4	1351.8	1369.0	1384.9	1387.0	1391.4	1406.1	1406.9
	1413.2	1456.0	1464.8	1470.6	1481.1	1486.1	1489.5	1492.9
	1496.7	1509.0	3007.0	3016.4	3022.0	3026.7	3035.5	3037.0
	3041.1	3045.5	3066.4	3087.4	3091.9	3093.7	3094.2	3095.4
	3099.5	3100.7	3185.7	3822.1				

electronic state	2-A			
point group	C1			
rotational constants	1.97828	0.45552	0.40999	
ZPE	0.267129 (Hartree/Particle)			
$TS_c\beta$				
optimized Cartesian coordinate	C	1.714482000000	-1.288955000000	0.626426000000
	C	0.589213000000	-0.677542000000	-0.216195000000
	C	-0.781235000000	-1.131374000000	0.290872000000
	C	-1.943701000000	-0.857198000000	-0.632354000000
	C	-3.266609000000	-1.446952000000	-0.210492000000
	H	-2.192545000000	0.431095000000	-0.569560000000
	O	-2.516759000000	1.563789000000	-0.317390000000
	O	-2.277536000000	1.682521000000	1.042852000000
	H	-1.389750000000	2.064331000000	1.080126000000
	C	0.730052000000	0.849805000000	-0.236619000000
	C	2.107358000000	1.288493000000	-0.739372000000
	C	3.223354000000	0.667372000000	0.102184000000
	C	3.097658000000	-0.856985000000	0.135059000000
	H	-0.058497000000	1.300776000000	-0.846106000000
	H	0.708300000000	-1.039834000000	-1.247994000000
	H	1.582865000000	-0.971963000000	1.669994000000
	H	1.633170000000	-2.380378000000	0.616043000000
	H	2.223085000000	0.973584000000	-1.783436000000
	H	2.182495000000	2.379062000000	-0.728834000000
	H	4.202141000000	0.960160000000	-0.286747000000
	H	3.158921000000	1.055443000000	1.126243000000
	H	3.257451000000	-1.251818000000	-0.875697000000
	H	3.875413000000	-1.289738000000	0.769817000000
	H	0.603229000000	1.212184000000	0.795226000000
	H	-0.984163000000	-0.681097000000	1.272943000000
	H	-0.750795000000	-2.217846000000	0.468085000000
	H	-1.708382000000	-0.983053000000	-1.692924000000
	H	-4.075730000000	-1.134413000000	-0.871737000000
	H	-3.220434000000	-2.542595000000	-0.223048000000
	H	-3.515847000000	-1.134354000000	0.806860000000
frequencies	-1793.8	34.5	67.2	83.5
	214.3	242.9	279.4	315.6
	459.6	478.5	566.0	575.3
	865.6	908.2	918.8	921.9
	1068.4	1075.2	1085.0	1094.6
	1186.9	1215.3	1242.7	1284.9
	1343.9	1368.1	1382.1	1387.7
	1417.5	1464.6	1470.0	1486.5
	1500.5	1514.8	2994.9	2998.4
	3042.3	3043.4	3047.7	3085.8
	3101.9	3109.3	3146.5	3801.5
	109.2	123.5	153.8	195.2
	337.3	376.2	428.4	450.8
	787.0	805.1	817.2	859.0
	949.6	992.4	1048.6	1059.2
	1119.2	1133.6	1146.8	1162.6
	1291.1	1297.0	1301.0	1338.3
	1390.1	1395.7	1409.0	1413.7
	1488.8	1489.1	1492.3	1494.6
	3012.5	3029.1	3036.8	3038.0
	3093.3	3096.8	3097.3	3098.3
electronic state	2-A			
point group	C1			
rotational constants	1.66998	0.57221	0.47281	
ZPE	0.267114 (Hartree/Particle)			
$TS_c\alpha$				
optimized Cartesian coordinate	C	-1.259334000000	-1.372567000000	0.192595000000
	C	-0.395641000000	-0.109155000000	0.008275000000
	C	0.948571000000	-0.438897000000	-0.597401000000
	C	1.869752000000	-1.355874000000	0.169494000000
	C	3.284908000000	-1.394643000000	-0.406850000000
	H	1.563437000000	0.716089000000	-0.562701000000
	H	3.734441000000	-0.398185000000	-0.407746000000
	O	2.119063000000	1.753092000000	-0.255496000000
	O	2.201243000000	1.682508000000	1.127693000000
	H	3.098997000000	1.360481000000	1.284892000000
	C	-1.146600000000	0.928267000000	-0.834810000000

	C	-2.513118000000	1.265624000000	-0.237110000000
	C	-3.363519000000	0.006337000000	-0.062999000000
	C	-2.628621000000	-1.031873000000	0.786125000000
	H	-0.534763000000	1.829455000000	-0.929338000000
	H	-0.214657000000	0.321544000000	1.004296000000
	H	-1.392604000000	-1.852354000000	-0.786316000000
	H	-0.743111000000	-2.090936000000	0.835159000000
	H	-2.369337000000	1.742520000000	0.739812000000
	H	-3.030559000000	1.991263000000	-0.870082000000
	H	-4.326314000000	0.254588000000	0.391533000000
	H	-3.577849000000	-0.422519000000	-1.049705000000
	H	-2.488804000000	-0.634199000000	1.798532000000
	H	-3.228402000000	-1.941139000000	0.882638000000
	H	-1.285054000000	0.522555000000	-1.846270000000
	H	0.913403000000	-0.646323000000	-1.672886000000
	H	1.450672000000	-2.370840000000	0.164376000000
	H	1.889410000000	-1.041901000000	1.219472000000
	H	3.929387000000	-2.064351000000	0.165043000000
	H	3.270871000000	-1.743853000000	-1.442202000000
frequencies	-1758.1	39.1	42.3	79.6
	230.5	234.3	293.4	306.6
	457.3	468.7	541.7	620.6
	886.7	902.5	914.8	935.1
	1059.0	1073.7	1081.0	1093.8
	1183.8	1219.6	1247.2	1289.0
	1348.8	1365.1	1371.5	1386.7
	1419.7	1471.1	1478.9	1482.8
	1508.5	1511.8	3013.3	3025.5
	3048.5	3059.4	3065.0	3080.4
	3103.6	3127.3	3140.0	3806.3
electronic state	2-A			
point group	C1			
rotational constants	1.61163	0.58977	0.48739	
ZPE	0.267210 (Hartree/Particle)			
$TS_c\alpha'$				
optimized Cartesian coordinate	C	-1.071221000000	0.172735000000	1.384310000000
	C	-0.132520000000	-0.296061000000	0.289023000000
	C	1.273060000000	-0.590797000000	0.767846000000
	C	2.289947000000	-0.882016000000	-0.337866000000
	C	3.720962000000	-0.897872000000	0.194248000000
	H	0.026106000000	0.765515000000	-0.430945000000
	O	0.296257000000	1.826125000000	-1.003255000000
	O	1.218599000000	2.428124000000	-0.161008000000
	H	2.071334000000	2.185777000000	-0.547102000000
	H	3.835013000000	-1.651416000000	0.977844000000
	C	-0.750195000000	-1.300372000000	-0.666121000000
	C	-2.116679000000	-0.841364000000	-1.183935000000
	C	-3.054329000000	-0.475882000000	-0.032676000000
	C	-2.433060000000	0.613026000000	0.842688000000
	H	-0.076157000000	-1.495047000000	-1.504157000000
	H	-1.210896000000	-0.661317000000	2.090650000000
	H	-0.597811000000	0.984838000000	1.944716000000
	H	-1.975912000000	0.037479000000	-1.823916000000
	H	-2.557653000000	-1.623420000000	-1.807177000000
	H	-4.019521000000	-0.143361000000	-0.423207000000
	H	-3.246153000000	-1.368341000000	0.576328000000
	H	-2.297762000000	1.522206000000	0.246803000000
	H	-3.098197000000	0.866480000000	1.671950000000
	H	-0.865018000000	-2.253705000000	-0.124751000000
	H	1.235487000000	-1.445095000000	1.461681000000
	H	1.619187000000	0.263383000000	1.362134000000
	H	2.188697000000	-0.128833000000	-1.128963000000
	H	2.066119000000	-1.843801000000	-0.807554000000
	H	4.441021000000	-1.123207000000	-0.594522000000
	H	3.987482000000	0.069495000000	0.629193000000

frequencies	-1681.0	34.2	62.8	73.7	96.0	112.8	137.9	184.9
	205.6	239.7	255.8	297.9	328.8	361.7	384.4	398.1
	449.8	477.0	546.2	599.1	743.8	788.4	801.2	848.9
	860.6	904.0	916.7	922.5	942.2	989.1	1051.0	1061.1
	1067.1	1075.9	1087.8	1090.5	1117.7	1131.4	1169.0	1177.3
	1189.1	1243.4	1249.7	1285.9	1293.9	1310.1	1324.7	1339.2
	1355.6	1368.7	1384.6	1388.1	1399.0	1407.0	1410.5	1417.0
	1460.6	1464.4	1472.5	1478.7	1490.8	1493.1	1500.6	1504.0
	1507.3	1515.7	2989.0	2993.1	3001.8	3036.8	3044.3	3051.0
	3055.0	3057.7	3060.8	3086.6	3090.7	3099.0	3102.1	3102.6
	3107.4	3124.0	3135.9	3801.8				
electronic state	2-A							
point group	C1							
rotational constants	1.45168	0.66211	0.56522					
ZPE	0.266970 (Hartree/Particle)							
TS$_c\beta'$								
optimized Cartesian coordinate	C	0.289289000000	0.161750000000	0.897053000000				
	C	1.700383000000	-0.149875000000	1.340540000000				
	C	2.547207000000	-0.722323000000	0.201746000000				
	H	0.433903000000	1.118480000000	0.015382000000				
	O	0.691385000000	1.977377000000	-0.805383000000				
	O	1.877415000000	2.537425000000	-0.349286000000				
	H	1.586197000000	3.329679000000	0.119979000000				
	C	0.466441000000	-1.491184000000	-0.983014000000				
	C	-0.433455000000	-0.923906000000	0.122951000000				
	H	3.527509000000	-1.020087000000	0.582124000000				
	H	0.595981000000	-0.721049000000	-1.753165000000				
	H	-0.038081000000	-2.338693000000	-1.456535000000				
	H	1.646077000000	-0.883673000000	2.159828000000				
	H	2.170103000000	0.746380000000	1.754821000000				
	H	-0.316373000000	0.646519000000	1.665133000000				
	H	-0.640226000000	-1.737775000000	0.840337000000				
	H	2.712938000000	0.063158000000	-0.543025000000				
	C	1.840174000000	-1.907356000000	-0.456346000000				
	H	2.448716000000	-2.305342000000	-1.272449000000				
	H	1.721475000000	-2.715755000000	0.276217000000				
	C	-1.771790000000	-0.449008000000	-0.452485000000				
	H	-2.212898000000	-1.277676000000	-1.019182000000				
	H	-1.579700000000	0.352052000000	-1.177675000000				
	C	-2.786890000000	0.035827000000	0.581827000000				
	H	-2.421777000000	0.946360000000	1.065796000000				
	H	-2.890563000000	-0.718554000000	1.370301000000				
	C	-4.150717000000	0.317660000000	-0.045121000000				
	H	-4.565325000000	-0.586472000000	-0.498203000000				
	H	-4.866063000000	0.681170000000	0.695109000000				
	H	-4.066151000000	1.073345000000	-0.830349000000				
frequencies	-1746.5	43.6	55.3	66.3	90.9	102.7	133.4	167.7
	205.5	249.2	262.8	298.1	343.4	354.0	398.7	444.1
	472.5	484.0	574.1	597.2	742.7	788.5	800.9	853.0
	867.1	902.0	911.3	920.8	944.0	986.1	1042.3	1061.2
	1063.1	1071.0	1083.4	1102.4	1117.1	1127.7	1159.5	1170.1
	1195.4	1228.1	1248.0	1279.8	1292.2	1295.6	1322.7	1335.6
	1341.9	1365.4	1368.6	1386.5	1390.0	1398.5	1406.0	1410.2
	1414.7	1454.9	1465.4	1483.2	1492.1	1493.6	1498.4	1505.1
	1506.3	1512.8	2961.7	2998.2	3032.3	3036.0	3046.2	3048.0
	3056.8	3063.2	3068.2	3091.3	3092.5	3095.3	3098.4	3110.4
	3117.3	3127.8	3134.4	3820.7				
electronic state	2-A							
point group	C1							
rotational constants	1.29885	0.65251	0.51427					
ZPE	0.266882 (Hartree/Particle)							
TS$_c\gamma'$								

optimized Cartesian coordinate	C	-1.712919000000	0.144231000000	1.095695000000
	C	-0.212414000000	-0.034832000000	1.110821000000
	C	0.329487000000	-0.547351000000	-0.230379000000
	H	-1.887344000000	1.093835000000	0.212266000000
	O	-1.895912000000	1.964546000000	-0.637360000000
	O	-0.679257000000	2.612452000000	-0.474060000000
	H	-0.904195000000	3.381608000000	0.065137000000
	C	-1.949200000000	-1.518282000000	-0.775150000000
	C	-2.508704000000	-1.025486000000	0.561978000000
	H	-2.121792000000	-0.751665000000	-1.538066000000
	H	-2.482045000000	-2.418038000000	-1.092782000000
	H	0.047151000000	-0.761531000000	1.899411000000
	H	0.268905000000	0.907929000000	1.382337000000
	H	-2.122711000000	0.596628000000	2.001094000000
	H	-2.452048000000	-1.841187000000	1.299256000000
	H	-3.565326000000	-0.760391000000	0.471188000000
	H	0.158120000000	0.240829000000	-0.975445000000
	C	-0.448209000000	-1.791784000000	-0.670591000000
	H	-0.272156000000	-2.598096000000	0.055066000000
	H	-0.061728000000	-2.142570000000	-1.632398000000
	C	1.831581000000	-0.828672000000	-0.172323000000
	H	2.022189000000	-1.633007000000	0.551433000000
	H	2.149001000000	-1.214215000000	-1.148927000000
	C	2.692138000000	0.385180000000	0.178774000000
	H	2.398575000000	1.227087000000	-0.458008000000
	H	2.497400000000	0.693966000000	1.210158000000
	C	4.183274000000	0.100012000000	0.014191000000
	H	4.417214000000	-0.163038000000	-1.020620000000
	H	4.791088000000	0.965336000000	0.285915000000
	H	4.490863000000	-0.737560000000	0.646242000000
frequencies	-1761.1	47.2	65.9	73.2
	201.6	251.0	265.5	310.8
	466.6	490.8	567.3	613.6
	863.0	897.4	914.5	918.7
	1064.2	1072.1	1080.6	1100.3
	1204.7	1230.0	1247.7	1283.0
	1340.4	1364.0	1375.1	1386.6
	1416.6	1461.0	1463.5	1473.3
	1505.1	1512.7	2979.1	3000.7
	3055.6	3057.6	3061.8	3086.6
	3111.7	3125.2	3132.7	3820.5
	93.4	102.9	146.1	187.5
	313.9	356.4	397.6	437.7
	743.4	793.5	798.9	848.4
	943.8	987.9	1040.6	1060.7
	1130.2	1132.8	1158.4	1165.4
	1295.0	1302.2	1326.0	1335.0
	1390.8	1402.5	1405.8	1414.2
	1484.3	1492.1	1497.9	1500.4
	3020.3	3022.2	3045.1	3052.0
	3091.3	3094.0	3103.5	3106.2
electronic state	2-A			
point group	C1			
rotational constants	1.30198	0.65990	0.50900	
ZPE	0.266955 (Hartree/Particle)			
$TS_c\delta'$				
optimized Cartesian coordinate	C	2.049714000000	1.119500000000	0.162051000000
	C	1.592891000000	0.446362000000	1.434606000000
	C	0.352095000000	-0.418204000000	1.198213000000
	C	-0.776409000000	0.355170000000	0.506744000000
	C	-1.996462000000	-0.547951000000	0.310455000000
	C	-3.223437000000	0.142599000000	-0.284369000000
	C	-4.449419000000	-0.768134000000	-0.285704000000
	H	2.394588000000	0.118660000000	-0.607834000000
	O	2.660106000000	-0.894099000000	-1.221789000000
	O	3.041811000000	-1.796482000000	-0.238351000000
	H	4.006323000000	-1.748751000000	-0.251207000000
	H	-4.713861000000	-1.067015000000	0.731918000000
	C	-0.269642000000	0.944103000000	-0.814823000000
	C	0.962794000000	1.831035000000	-0.610801000000
	H	-0.004243000000	-0.822422000000	2.150437000000
	H	-1.070922000000	1.190835000000	1.160360000000
	H	-0.012729000000	0.117568000000	-1.489227000000
	H	-1.054424000000	1.528155000000	-1.301518000000
	H	1.359820000000	1.230043000000	2.172192000000
	H	2.400011000000	-0.155685000000	1.859983000000

	H	2.984921000000	1.676260000000	0.249405000000
	H	0.670428000000	2.726374000000	-0.040635000000
	H	1.345215000000	2.186841000000	-1.571119000000
	H	0.632497000000	-1.273056000000	0.571681000000
	H	-2.271500000000	-0.976809000000	1.282010000000
	H	-1.710965000000	-1.394364000000	-0.327886000000
	H	-3.012698000000	0.462454000000	-1.308750000000
	H	-3.438950000000	1.052017000000	0.288386000000
	H	-5.317292000000	-0.274420000000	-0.727323000000
	H	-4.254302000000	-1.678916000000	-0.857990000000
frequencies	-1754.9 40.7 61.3 64.6 93.9 107.6 133.7 184.9 219.8 250.6 263.0 298.4 312.8 352.8 406.6 442.2 458.7 501.3 562.1 613.7 741.2 784.6 802.5 848.2 860.0 905.5 917.6 922.6 943.9 982.4 1037.6 1057.9 1063.5 1072.2 1084.3 1101.2 1125.7 1128.5 1159.4 1168.7 1201.0 1223.3 1246.5 1286.6 1290.5 1308.3 1323.6 1332.2 1349.4 1356.3 1371.5 1384.1 1388.9 1405.1 1406.6 1413.6 1414.5 1458.6 1464.5 1475.6 1483.2 1490.1 1496.3 1503.0 1506.2 1512.4 2996.4 2997.0 3001.7 3026.8 3045.9 3047.8 3053.0 3055.9 3063.0 3091.9 3092.5 3094.9 3098.4 3109.4 3110.5 3126.9 3132.5 3820.9			
electronic state	2-A			
point group	C1			
rotational constants	1.72090 0.49229 0.46122			
ZPE	0.266850 (Hartree/Particle)			
*i*PCH				
optimized Cartesian coordinate	C	-0.246231000000	1.087398000000	0.423905000000
	C	0.273294000000	-0.074340000000	-0.433224000000
	C	1.775943000000	-0.367791000000	-0.248847000000
	C	2.170607000000	-0.650655000000	1.203311000000
	C	2.647495000000	0.754952000000	-0.816650000000
	C	-0.598558000000	-1.314731000000	-0.200052000000
	C	-2.072104000000	-1.030506000000	-0.502390000000
	C	-2.586802000000	0.144775000000	0.331163000000
	C	-1.717649000000	1.386303000000	0.121909000000
	H	-0.236831000000	-2.142916000000	-0.818280000000
	H	0.139737000000	0.214895000000	-1.486639000000
	H	-0.151159000000	0.823691000000	1.484503000000
	H	0.356883000000	1.985463000000	0.262603000000
	H	-2.180463000000	-0.790798000000	-1.567224000000
	H	-2.676043000000	-1.922659000000	-0.315458000000
	H	-3.628840000000	0.362198000000	0.081256000000
	H	-2.565001000000	-0.132203000000	1.392405000000
	H	-1.810529000000	1.719739000000	-0.918909000000
	H	-2.072115000000	2.207903000000	0.750381000000
	H	-0.508695000000	-1.634237000000	0.845367000000
	H	1.984823000000	-1.273021000000	-0.833284000000
	H	1.566513000000	-1.443466000000	1.649404000000
	H	2.063382000000	0.246153000000	1.819670000000
	H	2.386341000000	0.974431000000	-1.855154000000
	H	2.534912000000	1.675598000000	-0.237663000000
	H	3.704135000000	0.477717000000	-0.785317000000
	H	3.216980000000	-0.960914000000	1.257594000000
frequencies	38.7 121.2 210.7 228.2 246.2 255.9 282.2 312.4 369.2 421.4 446.9 470.3 504.8 577.4 783.4 800.9 848.0 868.3 904.5 907.7 928.9 938.1 972.1 974.3 1041.3 1054.6 1060.7 1087.0 1100.5 1119.2 1152.6 1185.0 1212.3 1225.3 1270.5 1295.4 1301.6 1325.0 1328.1 1354.8 1366.9 1371.5 1386.7 1387.7 1400.3 1405.4 1411.3 1425.2 1483.2 1487.1 1490.0 1491.7 1495.7 1503.0 1509.3 1514.0 1515.9 3002.0 3030.8 3036.6 3037.4 3041.4 3043.3 3046.1 3052.8 3059.5 3084.8 3093.5 3094.6 3096.6 3100.6 3122.9 3126.2 3127.0 3135.6			
electronic state	1-A			
point group	C1			

rotational constants	2.84446	1.01329	0.90793					
ZPE	0.256299 (Hartree/Particle)							
*i*P1								
optimized Cartesian coordinate	C	-0.197246000000	1.101857000000	0.396748000000				
	C	0.307966000000	-0.075040000000	-0.445346000000				
	C	1.813653000000	-0.389078000000	-0.224877000000				
	C	2.127508000000	-0.797393000000	1.177761000000				
	C	2.705593000000	0.776959000000	-0.662016000000				
	H	3.754950000000	0.475269000000	-0.670964000000				
	C	-0.569039000000	-1.307498000000	-0.200940000000				
	C	-2.043470000000	-1.018962000000	-0.491426000000				
	C	-2.542858000000	0.159082000000	0.347213000000				
	C	-1.673992000000	1.396967000000	0.118221000000				
	H	-0.214805000000	-2.142530000000	-0.814848000000				
	H	0.201826000000	0.201673000000	-1.504976000000				
	H	-0.069781000000	0.856523000000	1.459066000000				
	H	0.399677000000	1.996864000000	0.201234000000				
	H	-2.162565000000	-0.779896000000	-1.555312000000				
	H	-2.648201000000	-1.908943000000	-0.296939000000				
	H	-3.588120000000	0.378742000000	0.113346000000				
	H	-2.504062000000	-0.115177000000	1.408588000000				
	H	-1.784063000000	1.724332000000	-0.923036000000				
	H	-2.016494000000	2.223649000000	0.746692000000				
	H	-0.467558000000	-1.615072000000	0.847304000000				
	H	2.029362000000	-1.243824000000	-0.881210000000				
	H	1.881850000000	-1.784349000000	1.546127000000				
	H	2.439461000000	1.122624000000	-1.664236000000				
	H	2.611763000000	1.622161000000	0.024410000000				
	H	2.568069000000	-0.093418000000	1.872733000000				
frequencies	44.2	75.8	120.1	208.5	234.5	254.4	275.8	315.7
	367.0	416.4	439.0	446.5	469.6	511.5	616.4	785.2
	800.3	852.2	872.1	901.7	906.6	926.6	938.6	970.5
	1026.4	1044.9	1058.6	1075.0	1095.2	1118.2	1149.3	1164.8
	1195.5	1216.1	1252.8	1292.8	1299.7	1303.5	1321.4	1342.5
	1368.0	1371.5	1386.6	1387.9	1395.4	1407.0	1410.3	1469.8
	1484.1	1488.2	1490.8	1495.4	1498.8	1509.7	1511.5	3005.0
	3014.8	3033.8	3036.9	3039.6	3041.6	3045.4	3057.8	3082.6
	3093.3	3095.0	3097.6	3100.7	3130.1	3134.7	3165.4	3270.2
electronic state	2-A							
point group	C1							
rotational constants	2.88844	1.04776	0.91857					
ZPE	0.241089 (Hartree/Particle)							
*i*P2								
optimized Cartesian coordinate	C	-0.291047000000	1.108289000000	0.502970000000				
	C	0.299091000000	0.024417000000	-0.428785000000				
	C	1.773361000000	-0.152031000000	-0.199451000000				
	C	2.259526000000	-1.080965000000	0.868110000000				
	C	2.679623000000	0.962760000000	-0.615166000000				
	H	3.349352000000	-1.153620000000	0.854937000000				
	H	3.678445000000	0.591794000000	-0.864003000000				
	C	-0.510956000000	-1.270074000000	-0.286323000000				
	C	-1.993881000000	-1.037797000000	-0.583009000000				
	C	-2.574312000000	0.039356000000	0.335924000000				
	C	-1.778031000000	1.340935000000	0.225165000000				
	H	-0.099627000000	-2.037924000000	-0.949086000000				
	H	0.163870000000	0.388494000000	-1.458989000000				
	H	-0.158267000000	0.785186000000	1.543762000000				
	H	0.266439000000	2.042094000000	0.383718000000				
	H	-2.108757000000	-0.721819000000	-1.627058000000				
	H	-2.551102000000	-1.971967000000	-0.471927000000				
	H	-3.626897000000	0.216546000000	0.099026000000				
	H	-2.536817000000	-0.317154000000	1.372701000000				
	H	-1.891663000000	1.745777000000	-0.787973000000				

	H	-2.177528000000		2.091808000000		0.912584000000		
	H	-0.412017000000		-1.646101000000		0.739537000000		
	H	1.852844000000		-2.089529000000		0.756550000000		
	H	1.972159000000		-0.733993000000		1.873724000000		
	H	2.285890000000		1.497774000000		-1.483409000000		
	H	2.813426000000		1.703296000000		0.189290000000		
frequencies	57.1	102.0	136.5	152.9	170.3	242.1	259.8	309.6
	365.6	395.8	437.2	451.8	494.7	544.0	773.9	798.3
	837.0	864.3	900.0	906.9	934.3	938.8	980.3	989.7
	1046.8	1048.9	1051.0	1070.9	1093.9	1117.9	1147.0	1197.8
	1231.4	1283.0	1288.6	1293.0	1317.3	1325.6	1344.1	1358.7
	1367.7	1384.4	1385.3	1401.9	1410.6	1414.8	1476.2	1478.0
	1482.5	1487.1	1488.4	1495.0	1497.4	1497.9	1509.6	2981.1
	2984.8	2996.6	3032.8	3036.9	3039.8	3041.8	3045.5	3071.0
	3082.3	3089.1	3091.1	3093.8	3095.0	3100.0	3118.9	3127.4
electronic state	2-A							
point group	C1							
rotational constants	2.86462	1.03742	0.88588					
ZPE	0.241631 (Hartree/Particle)							
*i*P3								
optimized Cartesian coordinate	C	0.587075000000		-1.338954000000		-0.171750000000		
	C	-0.275098000000		-0.111995000000		-0.180661000000		
	C	-1.759895000000		-0.291489000000		-0.340079000000		
	C	-2.484051000000		0.977199000000		-0.798797000000		
	C	-2.389098000000		-0.818010000000		0.965012000000		
	H	-1.998141000000		1.414373000000		-1.674461000000		
	H	-3.462266000000		-0.985338000000		0.839591000000		
	H	-1.910189000000		-1.059915000000		-1.108849000000		
	H	-2.504665000000		1.731132000000		-0.007586000000		
	C	0.282584000000		1.084266000000		0.531798000000		
	C	1.737399000000		1.365102000000		0.128273000000		
	C	2.602023000000		0.111929000000		0.266091000000		
	C	2.035868000000		-1.033227000000		-0.574034000000		
	H	-0.330670000000		1.970583000000		0.352612000000		
	H	0.600328000000		-1.771463000000		0.845158000000		
	H	0.159850000000		-2.106980000000		-0.824510000000		
	H	1.756562000000		1.700043000000		-0.914986000000		
	H	2.141842000000		2.178571000000		0.736654000000		
	H	3.632036000000		0.327593000000		-0.030490000000		
	H	2.630410000000		-0.193242000000		1.319856000000		
	H	2.059772000000		-0.748264000000		-1.631822000000		
	H	2.651953000000		-1.929957000000		-0.465848000000		
	H	0.257255000000		0.905777000000		1.622265000000		
	H	-3.520375000000		0.749175000000		-1.059017000000		
	H	-1.931675000000		-1.760222000000		1.275329000000		
	H	-2.252881000000		-0.090800000000		1.770982000000		
frequencies	26.9	68.6	186.8	211.9	227.4	269.1	273.9	295.8
	354.1	406.1	441.5	447.0	492.3	585.2	731.4	790.3
	849.2	856.6	886.8	918.1	926.5	931.4	965.4	978.3
	1048.0	1062.8	1089.9	1095.3	1100.8	1121.9	1153.7	1174.1
	1215.4	1260.2	1271.5	1290.6	1318.5	1328.5	1353.6	1360.5
	1372.6	1384.2	1388.4	1397.6	1410.4	1415.1	1468.2	1475.7
	1487.4	1490.3	1490.9	1496.4	1503.7	1509.4	1515.6	2944.5
	2949.2	3030.7	3036.1	3048.4	3048.8	3050.6	3055.1	3076.2
	3095.5	3097.6	3101.5	3102.7	3119.1	3128.0	3129.8	3130.9
electronic state	2-A							
point group	C1							
rotational constants	2.85092	1.03020	0.89088					
ZPE	0.242208 (Hartree/Particle)							
*i*P4								
optimized Cartesian	C	0.585857000000		-1.241934000000		-0.374052000000		
	C	2.069559000000		-1.085458000000		-0.444769000000		

coordinate	C	2.552529000000	0.086298000000	0.421005000000
	C	0.251822000000	1.117811000000	0.360370000000
	C	-0.287020000000	-0.032818000000	-0.509072000000
	H	3.618799000000	0.261256000000	0.254992000000
	H	0.102427000000	0.872685000000	1.417932000000
	H	-0.307150000000	2.034842000000	0.155295000000
	H	2.368376000000	-0.884730000000	-1.488364000000
	H	2.570548000000	-2.013063000000	-0.156919000000
	H	0.147131000000	-2.219539000000	-0.548463000000
	H	-0.214241000000	0.315375000000	-1.557446000000
	H	2.426031000000	-0.173982000000	1.477852000000
	C	-1.772193000000	-0.367262000000	-0.261347000000
	H	-2.008263000000	-1.202887000000	-0.932464000000
	C	-2.693248000000	0.796700000000	-0.629164000000
	H	-3.740991000000	0.491395000000	-0.574200000000
	H	-2.561501000000	1.636574000000	0.058368000000
	H	-2.498024000000	1.155201000000	-1.643449000000
	C	-2.043798000000	-0.830867000000	1.171991000000
	H	-1.934885000000	-0.004419000000	1.879411000000
	H	-3.065497000000	-1.207282000000	1.264348000000
	H	-1.357904000000	-1.626146000000	1.473970000000
	C	1.745283000000	1.348714000000	0.117728000000
	H	2.099395000000	2.180745000000	0.732289000000
	H	1.902997000000	1.636885000000	-0.929296000000
frequencies	58.2	98.5	192.5	213.1	235.1	258.3	275.0	316.0
	340.1	401.9	419.4	459.2	481.0	571.2	609.4	776.6
	829.9	853.7	887.3	909.3	932.2	934.0	969.0	972.3
	1035.0	1046.1	1065.0	1083.6	1107.9	1127.1	1143.4	1178.5
	1213.4	1227.3	1261.5	1272.0	1310.2	1320.9	1348.7	1362.1
	1364.2	1375.5	1382.9	1387.1	1403.6	1414.3	1422.1	1472.2
	1485.8	1488.4	1491.3	1500.7	1501.9	1510.0	1516.2	2923.0
	2958.2	3032.0	3036.8	3050.1	3051.6	3052.0	3058.6	3092.5
	3095.5	3100.2	3104.0	3123.8	3125.3	3127.7	3130.8	3173.0
electronic state	2-A							
point group	C1							
rotational constants	2.89589	1.03611	0.91531					
ZPE	0.241593 (Hartree/Particle)							
*i*P5								
optimized Cartesian coordinate	C	-1.913008000000	1.276487000000	-0.197316000000
	C	-0.463959000000	1.301434000000	0.160166000000
	C	0.273769000000	0.000635000000	-0.219841000000
	C	-1.971552000000	-1.205990000000	-0.273948000000
	C	-2.713706000000	0.067669000000	0.150270000000
	H	-1.947884000000	-1.257004000000	-1.368162000000
	H	-2.507466000000	-2.091109000000	0.079430000000
	H	-0.350244000000	1.436612000000	1.252446000000
	H	0.016348000000	2.163587000000	-0.306037000000
	H	-2.411674000000	2.199563000000	-0.465822000000
	H	-2.871148000000	0.024595000000	1.241900000000
	H	-3.706249000000	0.110340000000	-0.304177000000
	H	0.328419000000	-0.041936000000	-1.318248000000
	C	1.716720000000	-0.014721000000	0.321339000000
	H	1.654820000000	-0.009014000000	1.418471000000
	C	2.475519000000	-1.274093000000	-0.108165000000
	H	2.470175000000	-1.368730000000	-1.199315000000
	H	3.517654000000	-1.221723000000	0.215424000000
	H	2.047618000000	-2.184558000000	0.312628000000
	C	2.504267000000	1.223793000000	-0.117258000000
	H	2.490385000000	1.318219000000	-1.208485000000
	H	2.102060000000	2.144492000000	0.307234000000
	H	3.547663000000	1.145257000000	0.196627000000
	C	-0.537452000000	-1.211865000000	0.257901000000
	H	-0.556131000000	-1.210650000000	1.357141000000
	H	-0.047929000000	-2.138046000000	-0.049943000000
frequencies	54.7	109.1	159.6	183.0	230.0	263.3	273.3	340.2
	361.3	386.5	411.5	445.9	472.1	497.8	611.4	785.8

	853.4	860.1	876.7	906.2	930.0	935.1	964.1	977.4
	994.1	1067.6	1087.6	1108.9	1111.1	1138.1	1145.3	1168.2
	1195.0	1233.7	1255.4	1277.0	1307.8	1331.1	1348.6	1354.6
	1365.6	1369.4	1373.4	1402.0	1404.0	1407.2	1421.8	1469.7
	1474.4	1487.7	1490.6	1497.1	1505.6	1508.1	1526.9	2936.2
	2960.5	3004.2	3020.1	3029.0	3049.1	3051.3	3053.2	3098.5
	3099.4	3107.6	3109.8	3116.3	3122.8	3144.0	3146.0	3200.8
electronic state	2-A							
point group	C1							
rotational constants	2.95086	1.05995	0.82878					
ZPE	0.241406 (Hartree/Particle)							
*i*P6								
optimized Cartesian coordinate	C	-2.600160000000	0.178889000000	0.244418000000				
	C	-2.117698000000	-1.058589000000	-0.437830000000				
	C	-0.635386000000	-1.323430000000	-0.131965000000				
	C	0.221750000000	-0.081189000000	-0.403565000000				
	C	1.730365000000	-0.367767000000	-0.261027000000				
	C	2.164810000000	-0.642906000000	1.181097000000				
	C	2.581028000000	0.755635000000	-0.858313000000				
	H	3.215197000000	-0.942803000000	1.209285000000				
	H	3.638741000000	0.480857000000	-0.857889000000				
	C	-0.275103000000	1.080499000000	0.465969000000				
	C	-1.748371000000	1.402719000000	0.168927000000				
	H	-0.274644000000	-2.165467000000	-0.731487000000				
	H	0.054959000000	0.201256000000	-1.454578000000				
	H	-0.182394000000	0.804486000000	1.522303000000				
	H	0.334483000000	1.974497000000	0.307562000000				
	H	-2.225691000000	-0.944752000000	-1.530413000000				
	H	-2.728235000000	-1.920525000000	-0.158003000000				
	H	-3.639671000000	0.262954000000	0.536923000000				
	H	-1.805359000000	1.832350000000	-0.846221000000				
	H	-2.116400000000	2.174614000000	0.849186000000				
	H	-0.540778000000	-1.609303000000	0.921372000000				
	H	1.926318000000	-1.274513000000	-0.847417000000				
	H	1.579613000000	-1.440184000000	1.644072000000				
	H	2.064137000000	0.254482000000	1.797765000000				
	H	2.288302000000	0.970789000000	-1.889292000000				
	H	2.484016000000	1.678095000000	-0.279440000000				
frequencies	39.6	113.3	200.8	213.2	235.6	239.7	255.5	295.6
	340.2	375.6	431.9	452.1	473.5	549.0	638.2	786.9
	799.3	853.5	897.8	914.9	927.2	948.2	966.3	971.4
	1035.1	1041.1	1055.0	1086.3	1110.3	1129.2	1140.9	1174.4
	1212.6	1232.6	1245.9	1294.4	1310.2	1320.6	1344.5	1351.7
	1360.4	1378.3	1395.7	1401.7	1404.0	1411.1	1424.5	1470.9
	1478.4	1484.0	1490.3	1497.8	1504.0	1512.9	1515.4	2958.3
	2960.7	2998.2	3031.9	3046.5	3051.7	3053.4	3060.3	3091.5
	3095.8	3096.3	3101.8	3123.7	3126.6	3127.6	3136.2	3200.6
electronic state	2-A							
point group	C1							
rotational constants	2.86041	1.03749	0.91984					
ZPE	0.241474 (Hartree/Particle)							
$TS_d\beta$								
optimized Cartesian coordinate	C	0.360877000000	0.635138000000	0.598773000000				
	C	0.545728000000	-0.850955000000	0.263370000000				
	C	-0.772387000000	-1.576869000000	-0.064767000000				
	C	-1.605910000000	-0.878405000000	-1.114008000000				
	C	-1.610131000000	-1.854317000000	1.189432000000				
	H	-2.253274000000	0.127038000000	-0.513916000000				
	O	-2.839382000000	0.991908000000	0.041535000000				
	O	-2.380974000000	2.169906000000	-0.528033000000				
	H	-1.699080000000	2.464806000000	0.090820000000				
	H	-2.517128000000	-2.408017000000	0.935100000000				

	C	1.586905000000	-0.996785000000	-0.853546000000
	C	2.919163000000	-0.348546000000	-0.467398000000
	C	2.733729000000	1.123966000000	-0.095938000000
	C	1.686315000000	1.282429000000	1.007913000000
	H	1.736053000000	-2.056575000000	-1.083525000000
	H	0.960336000000	-1.340818000000	1.156274000000
	H	-0.016696000000	1.144712000000	-0.297986000000
	H	-0.389566000000	0.759830000000	1.386491000000
	H	3.340679000000	-0.884820000000	0.391490000000
	H	3.637778000000	-0.446775000000	-1.285317000000
	H	3.686206000000	1.559990000000	0.216606000000
	H	2.405159000000	1.679440000000	-0.982955000000
	H	2.051319000000	0.806738000000	1.926029000000
	H	1.536824000000	2.340895000000	1.239195000000
	H	1.210259000000	-0.522977000000	-1.769162000000
	H	-0.492707000000	-2.555013000000	-0.488272000000
	H	-1.078819000000	-0.359784000000	-1.914957000000
	H	-1.042073000000	-2.444977000000	1.911395000000
	H	-1.917938000000	-0.922056000000	1.668465000000
	H	-2.460220000000	-1.450081000000	-1.476779000000
frequencies	-1869.3 55.7 77.8 87.8 119.4 124.3 182.5 207.8 239.5 247.2 282.4 305.0 373.6 411.4 436.5 446.9 482.1 502.3 535.4 596.0 642.2 787.3 806.1 849.8 871.9 902.7 906.7 930.2 940.3 965.9 979.8 1037.2 1048.3 1057.4 1072.0 1081.0 1096.1 1116.2 1137.3 1153.9 1191.2 1215.8 1232.3 1268.3 1293.0 1301.0 1310.2 1324.6 1347.0 1354.4 1369.7 1384.4 1387.4 1394.5 1406.3 1410.2 1415.4 1455.1 1467.5 1485.5 1489.8 1492.0 1500.6 1501.6 1509.6 1516.3 2980.8 3012.5 3029.4 3036.8 3038.7 3043.1 3046.8 3060.0 3085.3 3087.4 3093.5 3098.2 3101.2 3102.6 3132.0 3139.4 3183.4 3802.8		
electronic state	2-A		
point group	C1		
rotational constants	1.34545 0.69370 0.55259		
ZPE	0.266988 (Hartree/Particle)		
$TS_d\alpha$			
optimized Cartesian coordinate	C	1.221274000000	-1.264492000000	-0.461099000000
	C	0.148928000000	-0.197322000000	-0.165784000000
	C	-1.202559000000	-0.804560000000	0.181428000000
	C	-1.332942000000	-1.463982000000	1.538482000000
	C	-1.851615000000	-1.580668000000	-0.944358000000
	H	-1.950602000000	0.238977000000	0.264375000000
	O	-2.600052000000	1.291638000000	0.204467000000
	O	-2.111996000000	1.916942000000	-0.931156000000
	H	-1.449620000000	2.531363000000	-0.586480000000
	H	-2.357433000000	-1.804517000000	1.702321000000
	H	-2.909638000000	-1.753937000000	-0.736313000000
	C	0.670840000000	0.773934000000	0.900440000000
	C	1.970014000000	1.443595000000	0.448263000000
	C	3.038905000000	0.393442000000	0.137580000000
	C	2.536298000000	-0.613198000000	-0.899049000000
	H	-0.096645000000	1.519295000000	1.137746000000
	H	0.005038000000	0.373106000000	-1.095223000000
	H	1.393046000000	-1.859791000000	0.444484000000
	H	0.869083000000	-1.949223000000	-1.237020000000
	H	1.778165000000	2.040225000000	-0.452490000000
	H	2.327743000000	2.133976000000	1.216662000000
	H	3.955431000000	0.873997000000	-0.214622000000
	H	3.293878000000	-0.139162000000	1.061931000000
	H	2.376032000000	-0.097088000000	-1.853280000000
	H	3.292408000000	-1.382323000000	-1.078694000000
	H	0.866421000000	0.223661000000	1.828525000000
	H	-1.064662000000	-0.790441000000	2.353808000000
	H	-0.680572000000	-2.344656000000	1.599421000000
	H	-1.771072000000	-1.041210000000	-1.891063000000
	H	-1.375478000000	-2.561391000000	-1.065997000000

frequencies	-1692.0	35.4	54.3	76.2	113.4	131.7	192.1	198.5
	218.5	226.2	248.6	285.7	313.6	372.1	393.7	405.8
	435.6	446.7	490.4	527.6	647.7	781.7	802.1	846.5
	866.2	907.4	912.2	935.6	942.5	975.2	991.1	1045.8
	1054.6	1068.6	1080.7	1090.9	1104.3	1125.4	1160.8	1164.0
	1200.1	1236.0	1272.9	1280.0	1294.1	1302.9	1332.5	1347.3
	1365.7	1371.4	1385.1	1387.5	1398.4	1406.8	1408.5	1414.0
	1463.4	1479.0	1485.1	1486.5	1488.6	1491.0	1497.4	1499.8
	1507.7	1512.1	3013.4	3031.5	3035.1	3035.5	3038.1	3042.0
	3043.9	3048.0	3082.0	3095.9	3097.7	3100.2	3103.5	3108.8
	3111.8	3137.6	3145.8	3800.4				
electronic state	2-A							
point group	C1							
rotational constants	1.38353	0.71086	0.59144					
ZPE	0.266670 (Hartree/Particle)							
$TS_d\alpha'$								
optimized Cartesian coordinate	C	-0.697974000000	-0.184120000000	1.331103000000				
	C	0.139727000000	-0.280328000000	0.069003000000				
	C	1.610832000000	-0.605362000000	0.297771000000				
	C	2.460198000000	-0.424249000000	-0.963515000000				
	C	1.801879000000	-2.021044000000	0.865020000000				
	H	0.186820000000	0.947233000000	-0.322801000000				
	O	0.332316000000	2.152680000000	-0.573677000000				
	O	1.186065000000	2.591646000000	0.426424000000				
	H	2.059413000000	2.552559000000	0.013600000000				
	H	2.253383000000	0.532621000000	-1.451630000000				
	H	2.863607000000	-2.218970000000	1.030940000000				
	H	1.967464000000	0.103919000000	1.055188000000				
	H	2.263036000000	-1.216469000000	-1.690385000000				
	C	-0.565703000000	-0.989355000000	-1.073418000000				
	C	-1.961909000000	-0.408734000000	-1.325555000000				
	C	-2.799294000000	-0.398620000000	-0.045987000000				
	C	-2.092293000000	0.387998000000	1.058718000000				
	H	0.032747000000	-0.939460000000	-1.986490000000				
	H	-0.806048000000	-1.193649000000	1.755999000000				
	H	-0.169517000000	0.420930000000	2.074853000000				
	H	-1.857818000000	0.618191000000	-1.694297000000				
	H	-2.464444000000	-0.981505000000	-2.109111000000				
	H	-3.785167000000	0.029722000000	-0.244302000000				
	H	-2.960953000000	-1.431178000000	0.288658000000				
	H	-1.991153000000	1.434125000000	0.751372000000				
	H	-2.684051000000	0.375200000000	1.977434000000				
	H	-0.662741000000	-2.055010000000	-0.813399000000				
	H	3.523427000000	-0.466979000000	-0.716126000000				
	H	1.283552000000	-2.150905000000	1.816473000000				
	H	1.428623000000	-2.772108000000	0.163207000000				
frequencies	-1680.3	28.8	63.4	74.5	106.1	129.6	190.5	208.0
	235.4	250.5	274.1	278.7	324.1	364.9	406.0	410.1
	429.7	454.0	489.9	537.9	615.1	790.0	794.0	853.6
	873.1	908.1	918.2	934.1	938.0	972.8	974.9	1051.7
	1058.3	1073.1	1078.6	1097.5	1102.4	1128.7	1158.3	1176.4
	1194.3	1212.1	1255.6	1270.9	1296.8	1315.0	1344.4	1350.5
	1365.4	1378.2	1388.0	1389.8	1398.4	1401.0	1408.8	1420.5
	1459.5	1467.6	1476.1	1493.4	1493.6	1493.8	1499.7	1509.1
	1511.9	1520.0	2999.6	3005.5	3036.5	3037.2	3052.3	3053.2
	3058.3	3060.2	3084.5	3098.5	3101.9	3103.3	3109.3	3124.8
	3125.9	3130.6	3142.3	3803.1				
electronic state	2-A							
point group	C1							
rotational constants	1.17857	0.85289	0.67145					
ZPE	0.266989 (Hartree/Particle)							
$TS_d\beta'$								

optimized Cartesian coordinate	C	0.114896000000	0.081332000000	0.949527000000
	C	1.455706000000	-0.517905000000	1.314096000000
	C	2.174050000000	-1.090516000000	0.088062000000
	H	0.445859000000	1.075326000000	0.156733000000
	O	0.895451000000	1.961399000000	-0.544397000000
	O	2.166380000000	2.199973000000	-0.038653000000
	H	2.039481000000	2.966639000000	0.534770000000
	C	-0.036326000000	-1.347362000000	-1.097420000000
	C	-0.791315000000	-0.818247000000	0.130570000000
	H	3.087570000000	-1.602641000000	0.400705000000
	H	0.199323000000	-0.513722000000	-1.768094000000
	H	-0.682791000000	-2.037017000000	-1.648681000000
	H	1.281561000000	-1.321911000000	2.045849000000
	H	2.083971000000	0.226870000000	1.809029000000
	H	-0.379098000000	0.605091000000	1.771279000000
	H	-1.002095000000	-1.693914000000	0.770408000000
	H	2.474530000000	-0.261392000000	-0.560232000000
	C	-2.156094000000	-0.195866000000	-0.222665000000
	H	-2.648010000000	-0.909781000000	-0.894848000000
	C	-2.037964000000	1.140930000000	-0.959128000000
	H	-3.021079000000	1.469018000000	-1.305051000000
	H	-1.643590000000	1.918964000000	-0.299351000000
	H	-1.378783000000	1.079875000000	-1.827275000000
	C	-3.045026000000	-0.040075000000	1.013240000000
	H	-2.630315000000	0.692931000000	1.711022000000
	H	-4.040441000000	0.310315000000	0.729899000000
	H	-3.159014000000	-0.987991000000	1.545592000000
	C	1.265728000000	-2.042051000000	-0.692229000000
	H	1.785287000000	-2.412737000000	-1.579642000000
	H	1.031060000000	-2.916333000000	-0.072034000000
frequencies	-1782.3	54.3	80.5	92.3
	230.2	264.2	282.7	285.7
	460.3	481.3	522.8	587.5
	874.8	902.9	907.6	929.6
	1058.0	1061.0	1066.9	1098.5
	1196.9	1212.8	1232.1	1264.8
	1359.3	1368.0	1378.4	1388.7
	1426.9	1462.1	1469.5	1486.6
	1513.0	1516.1	2957.3	2999.9
	3060.5	3067.5	3096.0	3098.1
	3126.4	3128.3	3141.4	3820.1
	113.4	142.6	196.4	217.5
	322.4	358.2	402.3	427.3
	596.1	776.4	801.4	847.6
	937.8	971.6	973.8	1038.6
	1103.3	1130.6	1156.6	1168.8
	1288.4	1310.5	1322.9	1344.6
	1392.0	1397.9	1407.2	1409.8
	1492.3	1494.1	1502.6	1507.4
	3036.5	3037.2	3051.8	3053.0
	3100.4	3107.6	3113.4	3122.5
electronic state	2-A			
point group	C1			
rotational constants	1.22978	0.82334	0.63277	
ZPE	0.266971 (Hartree/Particle)			
$TS_d\gamma'$				
optimized Cartesian coordinate	C	-1.482034000000	-0.312830000000	1.108294000000
	C	-0.010789000000	0.034441000000	1.075328000000
	C	0.590889000000	-0.179156000000	-0.321100000000
	H	-2.015302000000	0.567495000000	0.298714000000
	O	-2.370979000000	1.432477000000	-0.477512000000
	O	-1.434135000000	2.444198000000	-0.313597000000
	H	-1.868131000000	3.056970000000	0.293904000000
	C	-1.211335000000	-1.865878000000	-0.855938000000
	C	-1.852712000000	-1.655405000000	0.518814000000
	H	-1.668158000000	-1.175851000000	-1.573311000000
	H	-1.413422000000	-2.880677000000	-1.207752000000
	H	0.507972000000	-0.607272000000	1.804742000000
	H	0.132170000000	1.067175000000	1.403366000000
	H	-1.979760000000	-0.081100000000	2.052270000000
	H	-1.494463000000	-2.437774000000	1.205675000000
	H	-2.939239000000	-1.763024000000	0.464892000000
	H	0.062464000000	0.503829000000	-0.999054000000
	C	2.083766000000	0.188548000000	-0.415986000000
	H	2.361887000000	0.038578000000	-1.466918000000
	C	2.318479000000	1.664543000000	-0.083629000000

	H	2.208610000000	1.849373000000	0.988799000000
	H	3.330547000000	1.967196000000	-0.363112000000
	H	1.607292000000	2.305710000000	-0.610853000000
	C	2.998156000000	-0.697710000000	0.433454000000
	H	2.769075000000	-0.597731000000	1.498437000000
	H	2.916383000000	-1.752826000000	0.164919000000
	H	4.041520000000	-0.402015000000	0.297592000000
	C	0.295516000000	-1.605811000000	-0.797357000000
	H	0.755481000000	-2.329361000000	-0.112613000000
	H	0.746369000000	-1.766535000000	-1.782105000000
frequencies	-1752.2 39.0 65.1 77.6 101.6 143.6 189.5 219.0 241.7 256.5 266.6 283.8 317.9 359.6 408.7 423.6 461.9 474.8 518.1 573.4 606.4 775.7 804.5 848.0 865.9 902.0 908.4 929.8 940.0 970.6 976.4 1039.6 1053.9 1063.6 1071.0 1088.9 1110.4 1137.4 1159.9 1168.2 1202.9 1214.3 1237.7 1271.6 1290.5 1312.1 1331.2 1347.8 1357.7 1370.4 1376.2 1388.7 1402.6 1405.0 1407.1 1412.4 1425.5 1460.6 1463.3 1473.1 1490.2 1492.9 1501.3 1503.2 1513.4 1516.8 2997.2 3001.2 3030.8 3035.0 3048.9 3051.7 3057.0 3058.0 3086.6 3094.4 3100.3 3107.3 3110.8 3119.7 3123.8 3129.7 3135.4 3817.3			
electronic state	2-A			
point group	C1			
rotational constants	1.21954 0.83074 0.59213			
ZPE	0.266811 (Hartree/Particle)			
$TS_d\delta'$				
optimized Cartesian coordinate	C	-1.752352000000	-1.277073000000	0.047630000000
	C	-1.287795000000	-0.757858000000	1.388306000000
	C	-0.103821000000	0.202773000000	1.242781000000
	C	1.032815000000	-0.420746000000	0.423630000000
	C	2.283043000000	0.480472000000	0.383820000000
	C	2.085340000000	1.758939000000	-0.435443000000
	C	3.514120000000	-0.278007000000	-0.117587000000
	H	-2.186800000000	-0.203784000000	-0.561078000000
	O	-2.520127000000	0.869092000000	-1.024372000000
	O	-2.890381000000	1.618575000000	0.083662000000
	H	-3.851755000000	1.528711000000	0.105557000000
	H	2.952265000000	2.415139000000	-0.326408000000
	H	4.410344000000	0.341482000000	-0.032431000000
	C	0.506493000000	-0.808725000000	-0.964009000000
	C	-0.658660000000	-1.798320000000	-0.857632000000
	H	0.263323000000	0.488088000000	2.233492000000
	H	1.331240000000	-1.349341000000	0.934555000000
	H	0.154722000000	0.090834000000	-1.480468000000
	H	1.301206000000	-1.246349000000	-1.574080000000
	H	-0.986971000000	-1.619606000000	2.004179000000
	H	-2.112233000000	-0.268824000000	1.913947000000
	H	-2.647398000000	-1.901333000000	0.085531000000
	H	-0.290573000000	-2.747741000000	-0.439384000000
	H	-1.061296000000	-2.030234000000	-1.847262000000
	H	-0.457879000000	1.115754000000	0.753521000000
	H	2.480068000000	0.775851000000	1.422305000000
	H	1.201520000000	2.318798000000	-0.123238000000
	H	1.980667000000	1.529331000000	-1.499359000000
	H	3.679931000000	-1.192727000000	0.457624000000
	H	3.408589000000	-0.554122000000	-1.170303000000
frequencies	-1755.3 35.1 49.5 71.9 104.3 139.5 199.7 219.3 237.1 254.1 266.2 284.5 310.5 349.2 402.0 436.4 457.0 472.8 523.2 572.5 614.1 785.8 788.1 847.4 863.1 906.6 917.0 930.0 937.3 968.7 972.7 1036.2 1055.3 1059.7 1073.2 1095.5 1102.7 1135.1 1158.5 1173.3 1200.0 1213.6 1226.2 1267.2 1302.3 1316.9 1327.5 1349.7 1353.8 1365.8 1373.5 1384.2 1401.7 1406.2 1406.8 1414.6 1426.8 1457.1 1463.8 1476.7 1487.0 1491.1 1501.6 1506.5 1513.6 1516.0 2996.4 2997.7 3003.0 3031.5 3052.3 3057.8 3059.3 3063.3 3092.0 3094.5 3105.4 3108.3 3112.0 3123.6			

	3125.8 3127.4 3138.5 3819.6
electronic state	2-A
point group	C1
rotational constants	1.55237 0.63788 0.56760
ZPE	0.266691 (Hartree/Particle)
*s*BCH	
optimized Cartesian coordinate	C -0.428754000000 -0.672422000000 -0.934536000000 C 0.043681000000 0.091735000000 0.309433000000 C 1.454733000000 0.700997000000 0.179430000000 C -1.010136000000 1.133955000000 0.704875000000 C -2.370122000000 0.481982000000 0.964261000000 C -2.840495000000 -0.296533000000 -0.266242000000 C -1.793853000000 -1.325975000000 -0.696641000000 H -0.673045000000 1.686173000000 1.588916000000 H 0.086502000000 -0.633141000000 1.134399000000 H -0.506134000000 0.020088000000 -1.781949000000 H 0.299995000000 -1.438013000000 -1.216434000000 H -2.286638000000 -0.204158000000 1.815884000000 H -3.108261000000 1.240543000000 1.238916000000 H -3.796718000000 -0.787484000000 -0.065696000000 H -3.010759000000 0.407268000000 -1.090328000000 H -1.692650000000 -2.084534000000 0.089600000000 H -2.123844000000 -1.848475000000 -1.598759000000 H -1.123774000000 1.865295000000 -0.104105000000 H 1.700418000000 1.112438000000 1.168772000000 C 1.531083000000 1.848992000000 -0.831208000000 H 1.241798000000 1.514953000000 -1.831721000000 H 0.888455000000 2.686199000000 -0.553941000000 H 2.554736000000 2.226490000000 -0.896243000000 C 2.530251000000 -0.345045000000 -0.151520000000 H 3.504802000000 0.152353000000 -0.109282000000 H 2.409155000000 -0.675818000000 -1.189316000000 C 2.546320000000 -1.556620000000 0.778551000000 H 3.417498000000 -2.185705000000 0.585361000000 H 2.585589000000 -1.242983000000 1.825911000000 H 1.656617000000 -2.177880000000 0.651595000000
frequencies	65.6 97.7 152.8 205.7 207.3 235.5 245.9 288.2 296.4 349.5 397.5 433.1 447.4 478.3 510.1 580.7 769.0 800.0 805.5 836.6 864.0 897.3 908.2 938.0 947.2 977.7 1011.5 1030.7 1054.9 1061.3 1081.1 1090.1 1101.3 1117.4 1153.5 1181.2 1206.9 1222.2 1269.4 1290.4 1296.3 1302.0 1320.4 1333.2 1344.8 1361.5 1371.6 1385.6 1386.8 1390.4 1402.0 1408.0 1415.7 1419.7 1483.5 1487.6 1490.6 1494.7 1496.1 1504.5 1506.8 1510.6 1511.8 1515.0 3011.1 3022.8 3034.7 3037.7 3040.8 3043.0 3045.1 3048.6 3055.7 3060.4 3080.8 3084.6 3092.7 3094.3 3095.8 3100.0 3122.7 3124.3 3132.2 3140.3
electronic state	1-A
point group	C1
rotational constants	2.02031 0.83501 0.72728
ZPE	0.285257 (Hartree/Particle)
*s*BP1	
optimized Cartesian coordinate	C -0.402126000000 -0.727807000000 -0.897523000000 C 0.072380000000 0.076265000000 0.319820000000 C 1.496468000000 0.653736000000 0.182156000000 C 2.544922000000 -0.436808000000 -0.108496000000 C 2.533730000000 -1.567784000000 0.859608000000 C -0.961343000000 1.154583000000 0.666448000000 C -2.339170000000 0.544384000000 0.932773000000 C -2.813180000000 -0.265656000000 -0.275635000000 C -1.787012000000 -1.335549000000 -0.652482000000 H -0.621207000000 1.731016000000 1.533833000000

	H	0.100992000000	-0.624761000000	1.166166000000
	H	-0.447425000000	-0.074422000000	-1.777921000000
	H	0.308956000000	-1.527456000000	-1.124094000000
	H	-2.281491000000	-0.113282000000	1.808566000000
	H	-3.061678000000	1.329569000000	1.171853000000
	H	-3.783942000000	-0.725416000000	-0.070971000000
	H	-2.955071000000	0.412123000000	-1.126553000000
	H	-1.713577000000	-2.064889000000	0.163528000000
	H	-2.118455000000	-1.884665000000	-1.538110000000
	H	-1.049882000000	1.858843000000	-0.169480000000
	H	1.747561000000	1.088957000000	1.159485000000
	H	3.533928000000	0.048439000000	-0.101901000000
	H	2.414218000000	-0.811159000000	-1.129451000000
	H	2.427629000000	-1.371579000000	1.919877000000
	H	2.818168000000	-2.567605000000	0.561217000000
	C	1.610684000000	1.763648000000	-0.865601000000
	H	0.985589000000	2.623922000000	-0.621642000000
	H	2.643231000000	2.115306000000	-0.934319000000
	H	1.320336000000	1.402987000000	-1.856482000000
frequencies	46.9 101.5 111.8 150.4 205.4 224.8 233.7 255.8 294.2 346.6 396.7 433.9 445.9 458.0 498.9 513.8 578.6 776.9 800.4 822.9 848.6 867.2 901.8 915.2 941.9 948.6 970.8 1016.5 1049.8 1057.7 1079.7 1095.2 1104.8 1115.4 1137.2 1178.0 1185.5 1202.7 1247.3 1270.1 1294.7 1301.6 1312.7 1330.7 1340.2 1358.1 1369.7 1384.6 1385.3 1387.3 1398.2 1409.3 1419.6 1465.4 1480.2 1483.6 1487.2 1490.4 1494.9 1505.0 1509.6 1510.6 2982.7 3013.0 3022.8 3035.3 3036.7 3040.7 3042.2 3045.2 3059.9 3073.6 3083.0 3093.8 3094.3 3097.5 3100.9 3123.3 3141.7 3164.0 3268.2			
electronic state	2-A			
point group	C1			
rotational constants	2.06261 0.84742 0.73970			
ZPE	0.269893 (Hartree/Particle)			
*s*BP2				
optimized Cartesian coordinate	C	1.053694000000	1.252312000000	-0.237748000000
	C	0.106946000000	0.149347000000	0.252047000000
	C	-1.347578000000	0.356333000000	-0.210405000000
	C	-2.257341000000	-0.677092000000	0.380155000000
	C	-3.598846000000	-0.952072000000	-0.209335000000
	C	0.630166000000	-1.222420000000	-0.197090000000
	C	2.074290000000	-1.469722000000	0.241753000000
	C	2.999847000000	-0.365139000000	-0.268290000000
	C	2.501846000000	1.004195000000	0.193032000000
	H	-0.022921000000	-2.013059000000	0.182080000000
	H	0.108180000000	0.171700000000	1.353577000000
	H	1.001918000000	1.297824000000	-1.334803000000
	H	0.729859000000	2.226502000000	0.135881000000
	H	2.118488000000	-1.497819000000	1.337536000000
	H	2.412302000000	-2.447120000000	-0.113338000000
	H	4.024535000000	-0.533834000000	0.073972000000
	H	3.020716000000	-0.390965000000	-1.364777000000
	H	2.560912000000	1.055311000000	1.287321000000
	H	3.147202000000	1.797207000000	-0.194703000000
	H	0.574092000000	-1.268840000000	-1.293611000000
	H	-1.367619000000	0.242802000000	-1.305443000000
	H	-2.064260000000	-0.995381000000	1.401083000000
	H	-3.983369000000	-1.925971000000	0.101269000000
	H	-4.347770000000	-0.205352000000	0.093902000000
	H	-3.558646000000	-0.932537000000	-1.302706000000
	C	-1.878963000000	1.767277000000	0.113490000000
	H	-1.763662000000	1.980011000000	1.180905000000
	H	-1.353898000000	2.539951000000	-0.451206000000
	H	-2.940420000000	1.841449000000	-0.132587000000
frequencies	39.7 67.2 108.4 125.1 182.5 232.5 240.2 277.7 319.5 321.4 371.2 394.5 441.7 456.1 480.3 527.6			

	569.6	797.3	803.8	848.7	870.7	896.6	906.7	938.3
	948.6	974.4	998.4	1024.1	1050.9	1061.9	1075.8	1094.4
	1110.3	1130.2	1136.7	1173.6	1189.6	1224.3	1243.9	1289.3
	1293.6	1298.3	1314.4	1336.8	1353.4	1367.5	1380.0	1386.4
	1387.9	1393.3	1403.8	1408.8	1423.3	1478.9	1482.2	1487.5
	1489.2	1493.4	1494.6	1498.0	1508.1	1515.9	2991.4	2996.0
	3003.2	3021.0	3028.5	3036.7	3039.7	3045.0	3052.4	3075.0
	3092.5	3093.9	3096.1	3098.4	3103.5	3123.2	3126.2	3136.1
	3166.9							
electronic state	2-A							
point group	C1							
rotational constants	2.50374	0.74272	0.60678					
ZPE	0.269882 (Hartree/Particle)							
*s*BP3								
optimized Cartesian coordinate	C	0.990568000000		1.324479000000		-0.116762000000		
	C	-0.027642000000		0.191663000000		0.080078000000		
	C	-1.384517000000		0.571506000000		-0.543348000000		
	C	-1.966051000000		1.780372000000		0.117237000000		
	C	-2.416279000000		-0.584675000000		-0.548159000000		
	C	0.539947000000		-1.116417000000		-0.484594000000		
	C	1.910006000000		-1.453202000000		0.110183000000		
	C	2.907029000000		-0.312369000000		-0.092693000000		
	C	2.355888000000		0.990787000000		0.486267000000		
	H	-0.147637000000		-1.945650000000		-0.299670000000		
	H	-0.175449000000		0.058482000000		1.162538000000		
	H	1.105828000000		1.499955000000		-1.195302000000		
	H	0.605095000000		2.254423000000		0.309999000000		
	H	1.794755000000		-1.640316000000		1.185115000000		
	H	2.291601000000		-2.377845000000		-0.331401000000		
	H	3.868427000000		-0.559943000000		0.365459000000		
	H	3.089478000000		-0.179774000000		-1.166231000000		
	H	2.254363000000		0.886692000000		1.573579000000		
	H	3.054848000000		1.813205000000		0.311171000000		
	H	0.629788000000		-1.017016000000		-1.575459000000		
	H	-1.197093000000		0.815347000000		-1.600295000000		
	H	-1.694847000000		2.050897000000		1.130208000000		
	H	-3.339813000000		-0.205775000000		-0.996680000000		
	H	-2.062843000000		-1.383956000000		-1.205886000000		
	H	-2.785757000000		2.315944000000		-0.345231000000		
	C	-2.722312000000		-1.145081000000		0.839600000000		
	H	-3.501286000000		-1.908298000000		0.788175000000		
	H	-1.839434000000		-1.603309000000		1.292395000000		
	H	-3.069851000000		-0.355448000000		1.510657000000		
frequencies	80.1	95.5	142.9	152.2	200.1	237.9	252.1	263.2
	327.0	335.4	401.9	420.0	440.9	449.8	474.7	537.2
	596.9	789.8	796.3	802.5	849.3	874.8	891.1	909.6
	937.0	945.9	992.4	1012.1	1043.9	1061.5	1069.7	1082.1
	1098.1	1125.9	1135.5	1157.0	1192.4	1222.0	1248.2	1278.4
	1290.7	1295.4	1302.5	1317.9	1339.2	1367.3	1369.2	1379.4
	1383.6	1386.3	1389.1	1411.2	1417.1	1465.8	1481.8	1487.1
	1488.6	1494.2	1502.0	1505.3	1508.4	1515.3	2995.1	3009.1
	3023.2	3031.3	3036.7	3040.1	3045.4	3059.1	3062.4	3093.1
	3093.8	3094.9	3096.9	3099.4	3103.9	3129.0	3132.9	3159.9
	3263.2							
electronic state	2-A							
point group	C2							
rotational constants	2.25234	0.83905	0.68430					
ZPE	0.270169 (Hartree/Particle)							
*s*BP4								
optimized Cartesian coordinate	C	-0.532708000000		0.880074000000		0.763078000000		
	C	0.009147000000		-0.109109000000		-0.288718000000		
	C	1.379531000000		-0.623398000000		0.053953000000		

	C	2.544772000000	-0.182140000000	-0.775933000000
	C	2.937109000000	1.283937000000	-0.509765000000
	H	3.191571000000	1.431549000000	0.542726000000
	C	-1.004497000000	-1.251193000000	-0.495506000000
	C	-2.389424000000	-0.720101000000	-0.872830000000
	C	-2.907939000000	0.269153000000	0.172639000000
	C	-1.914808000000	1.413866000000	0.380756000000
	H	-0.630514000000	-1.932210000000	-1.265411000000
	H	0.081199000000	0.434807000000	-1.242098000000
	H	-0.601343000000	0.365552000000	1.729840000000
	H	0.175651000000	1.704271000000	0.893745000000
	H	-2.327053000000	-0.214820000000	-1.844505000000
	H	-3.091054000000	-1.550194000000	-0.992814000000
	H	-3.884249000000	0.661011000000	-0.125216000000
	H	-3.052532000000	-0.257022000000	1.124315000000
	H	-1.833217000000	1.992736000000	-0.547472000000
	H	-2.279841000000	2.099750000000	1.150299000000
	H	-1.080624000000	-1.831540000000	0.432477000000
	H	2.303717000000	-0.290549000000	-1.840014000000
	H	3.408578000000	-0.824912000000	-0.578069000000
	H	3.798683000000	1.579289000000	-1.113120000000
	H	2.108866000000	1.954414000000	-0.752880000000
	C	1.639810000000	-1.183340000000	1.416680000000
	H	2.472280000000	-1.892404000000	1.398272000000
	H	1.908222000000	-0.397671000000	2.140538000000
	H	0.765699000000	-1.698552000000	1.823252000000
frequencies	50.8 65.0 110.7 127.1 164.1 227.7 239.1 255.8 283.0 312.1 370.6 435.8 441.2 481.7 518.7 536.6 773.5 786.2 796.5 828.1 864.1 900.7 903.5 935.7 943.9 991.3 998.0 1022.6 1052.5 1055.7 1068.7 1076.1 1092.0 1116.2 1144.7 1201.8 1222.8 1253.8 1283.8 1290.6 1297.6 1327.2 1330.8 1354.7 1360.8 1365.6 1372.2 1385.9 1386.5 1397.4 1406.0 1415.8 1477.4 1481.4 1485.8 1487.9 1489.8 1493.0 1496.0 1502.8 1506.8 1510.3 2984.3 3009.9 3036.0 3036.3 3036.5 3041.9 3042.0 3045.8 3054.0 3075.3 3081.3 3088.4 3092.9 3094.3 3094.8 3099.8 3121.5 3128.3 3130.1		
electronic state	2-A		
point group	C1		
rotational constants	2.24046 0.76597 0.71023		
ZPE	0.270756 (Hartree/Particle)		
*s*BP5			
optimized Cartesian coordinate	C	0.950306000000	-1.150873000000	-0.805950000000
	C	-0.047726000000	-0.302240000000	-0.078085000000
	C	-1.510739000000	-0.621505000000	-0.215780000000
	C	-2.428730000000	0.585513000000	0.025888000000
	C	-2.071755000000	1.793799000000	-0.836024000000
	H	-2.059171000000	1.520906000000	-1.895024000000
	C	0.464459000000	0.411454000000	1.137822000000
	C	1.779292000000	1.151837000000	0.852602000000
	C	2.808217000000	0.219660000000	0.212113000000
	C	2.259227000000	-0.395776000000	-1.075609000000
	H	-0.281294000000	1.108606000000	1.529609000000
	H	1.189853000000	-2.043058000000	-0.199356000000
	H	0.521591000000	-1.522564000000	-1.741826000000
	H	1.576420000000	1.984886000000	0.169567000000
	H	2.174282000000	1.580906000000	1.777413000000
	H	3.735503000000	0.761865000000	0.008260000000
	H	3.056445000000	-0.582837000000	0.918293000000
	H	2.065400000000	0.402631000000	-1.800818000000
	H	2.995383000000	-1.069039000000	-1.523114000000
	H	0.651535000000	-0.322476000000	1.941958000000
	H	-1.674857000000	-0.952734000000	-1.250062000000
	H	-2.405470000000	0.859964000000	1.086217000000
	H	-3.458265000000	0.275424000000	-0.180586000000
	H	-2.792186000000	2.603708000000	-0.704429000000

	H	-1.079116000000		2.176900000000		-0.586346000000		
	C	-1.903478000000		-1.784835000000		0.714798000000		
	H	-2.955965000000		-2.050860000000		0.584120000000		
	H	-1.300016000000		-2.673288000000		0.514717000000		
	H	-1.754515000000		-1.501133000000		1.760769000000		
frequencies	39.9	57.0	128.2	188.1	193.1	223.9	229.7	247.5
	282.2	318.8	381.8	427.9	439.7	478.4	491.1	583.6
	724.1	791.3	802.7	843.0	856.7	872.0	917.6	930.7
	957.3	979.6	1007.9	1028.9	1048.6	1077.1	1090.8	1095.1
	1100.1	1116.8	1154.3	1173.4	1213.5	1253.9	1264.9	1288.5
	1297.9	1311.9	1319.8	1353.3	1359.9	1365.3	1376.6	1386.2
	1397.0	1400.2	1410.3	1415.3	1468.6	1476.7	1486.3	1490.3
	1495.1	1499.5	1502.1	1503.7	1504.0	1508.5	2946.2	2952.4
	3023.3	3035.8	3046.7	3048.2	3049.3	3053.2	3056.7	3078.8
	3083.7	3095.4	3097.3	3097.7	3101.0	3120.2	3125.2	3128.8
	3133.5							
electronic state	2-A							
point group	C1							
rotational constants	1.93965	0.86254	0.76179					
ZPE	0.270877 (Hartree/Particle)							
*s*BP6								
optimized Cartesian coordinate	C	-0.426139000000		-0.689604000000		-0.858627000000		
	C	-1.791288000000		-1.294500000000		-0.804251000000		
	C	-2.835470000000		-0.274689000000		-0.321738000000		
	C	-1.019723000000		1.090450000000		0.768892000000		
	C	0.054282000000		0.074346000000		0.334952000000		
	H	-3.799872000000		-0.767692000000		-0.172682000000		
	H	-1.126422000000		1.861296000000		-0.001631000000		
	H	-0.698508000000		1.589556000000		1.689351000000		
	H	-1.790060000000		-2.139829000000		-0.094907000000		
	H	-2.075164000000		-1.706513000000		-1.775280000000		
	H	0.263226000000		-0.986064000000		-1.639571000000		
	H	0.133870000000		-0.636877000000		1.176864000000		
	H	-2.974961000000		0.485431000000		-1.098487000000		
	C	-2.374943000000		0.408413000000		0.967366000000		
	H	-3.120207000000		1.139250000000		1.292898000000		
	H	-2.292580000000		-0.339939000000		1.765510000000		
	C	1.445467000000		0.711915000000		0.155423000000		
	H	1.706976000000		1.158880000000		1.124380000000		
	C	2.534688000000		-0.321008000000		-0.174627000000		
	H	3.500458000000		0.194133000000		-0.147041000000		
	H	2.411358000000		-0.664914000000		-1.207708000000		
	C	2.577918000000		-1.525661000000		0.763161000000		
	H	1.698868000000		-2.162360000000		0.638150000000		
	H	3.459901000000		-2.139026000000		0.568709000000		
	H	2.616002000000		-1.206889000000		1.809044000000		
	C	1.452682000000		1.822114000000		-0.898638000000		
	H	2.469993000000		2.187227000000		-1.060898000000		
	H	1.073390000000		1.449209000000		-1.855041000000		
	H	0.838888000000		2.674473000000		-0.603142000000		
frequencies	59.1	92.6	126.2	178.5	200.9	213.6	229.8	286.1
	287.1	309.5	346.2	403.0	436.1	464.6	480.9	579.7
	588.8	766.6	801.4	827.8	849.1	879.4	906.8	939.1
	944.4	978.8	1003.9	1028.1	1055.1	1071.4	1075.8	1083.8
	1120.0	1123.7	1136.6	1170.9	1203.7	1219.1	1263.1	1271.7
	1291.1	1310.9	1322.3	1334.1	1352.0	1357.1	1372.5	1378.9
	1389.1	1391.6	1411.9	1414.0	1424.2	1473.6	1486.5	1490.7
	1493.8	1501.1	1502.8	1504.2	1511.3	1515.4	2945.8	2964.3
	3022.2	3037.8	3047.1	3049.9	3050.1	3055.0	3055.7	3082.7
	3090.7	3096.6	3100.2	3102.3	3120.4	3124.4	3133.1	3139.7
	3206.7							
electronic state	2-A							
point group	C1							
rotational constants	2.06265	0.83338	0.73690					

ZPE	0.270320 (Hartree/Particle)			
*s*BP7				
optimized Cartesian coordinate	C	-1.799929000000	-1.286009000000	-0.763684000000
	C	-0.422041000000	-0.731457000000	-0.932465000000
	C	0.020503000000	0.065594000000	0.309785000000
	C	-2.397694000000	0.415748000000	0.967020000000
	C	-2.876458000000	-0.386523000000	-0.252482000000
	H	-2.280069000000	-0.261861000000	1.819692000000
	H	-3.149711000000	1.159266000000	1.244504000000
	H	-0.399489000000	-0.056632000000	-1.805670000000
	H	0.283885000000	-1.537366000000	-1.149201000000
	H	-2.062428000000	-2.219930000000	-1.245454000000
	H	-3.162880000000	0.332372000000	-1.039720000000
	H	-3.778095000000	-0.955399000000	-0.013351000000
	H	0.064131000000	-0.646382000000	1.144303000000
	C	-1.058750000000	1.093173000000	0.670975000000
	H	-1.195974000000	1.791586000000	-0.163724000000
	H	-0.730717000000	1.685625000000	1.532002000000
	C	1.421591000000	0.697417000000	0.181381000000
	H	1.661029000000	1.104210000000	1.174150000000
	C	2.509921000000	-0.332189000000	-0.156823000000
	H	2.377437000000	-0.675223000000	-1.189427000000
	H	3.476541000000	0.181665000000	-0.135028000000
	C	2.560975000000	-1.532729000000	0.786405000000
	H	1.675598000000	-2.165167000000	0.689410000000
	H	3.434447000000	-2.154428000000	0.580193000000
	H	2.621938000000	-1.205398000000	1.828474000000
	C	1.481673000000	1.856888000000	-0.817171000000
	H	0.821570000000	2.678429000000	-0.533950000000
	H	2.498464000000	2.254144000000	-0.870834000000
	H	1.205569000000	1.531016000000	-1.824012000000
frequencies	72.4 98.0 148.6 182.8 205.7 208.7 239.3 272.2 296.7 318.8 370.7 398.8 427.6 470.5 480.4 547.7 615.0 768.2 803.1 836.9 856.4 864.8 904.6 930.0 946.9 977.2 990.4 1028.9 1049.9 1070.4 1074.7 1105.7 1110.2 1131.4 1136.5 1171.4 1205.6 1226.3 1252.5 1286.5 1292.9 1313.0 1331.1 1337.5 1359.2 1360.8 1368.9 1389.4 1389.9 1404.3 1407.2 1416.1 1419.1 1469.5 1473.8 1490.5 1496.0 1499.3 1505.9 1506.8 1512.2 1515.0 2958.7 2965.4 3012.9 3032.6 3040.8 3047.9 3050.7 3056.6 3060.0 3080.9 3084.2 3097.0 3097.3 3100.4 3122.7 3124.9 3133.8 3140.3 3200.5						
electronic state	2-A			
point group	C1			
rotational constants	2.06913 0.83686 0.73301			
ZPE	0.270529 (Hartree/Particle)			
*s*BP8				
optimized Cartesian coordinate	C	-2.829311000000	-0.372717000000	0.195876000000
	C	-1.820221000000	-1.330378000000	0.737801000000
	C	-0.458506000000	-0.654924000000	0.969491000000
	C	-0.005882000000	0.109406000000	-0.280946000000
	C	1.415836000000	0.698624000000	-0.178818000000
	C	2.486529000000	-0.364551000000	0.110680000000
	C	2.457295000000	-1.568674000000	-0.828655000000
	H	2.465772000000	-1.247375000000	-1.874383000000
	C	-1.052583000000	1.172126000000	-0.636367000000
	C	-2.419226000000	0.531242000000	-0.919785000000
	H	0.277530000000	-1.413440000000	1.250707000000
	H	0.006291000000	-0.608440000000	-1.113662000000
	H	-1.163021000000	1.870483000000	0.200035000000
	H	-0.719462000000	1.752275000000	-1.503663000000
	H	-1.669705000000	-2.154029000000	0.017769000000
	H	-2.180453000000	-1.793515000000	1.659670000000
	H	-3.880656000000	-0.521850000000	0.409890000000

	H	-2.340645000000	-0.046194000000	-1.857127000000
	H	-3.176414000000	1.299376000000	-1.095168000000
	H	-0.544868000000	0.041404000000	1.811165000000
	H	1.641098000000	1.120193000000	-1.168664000000
	H	2.393413000000	-0.702118000000	1.149116000000
	H	3.465718000000	0.120601000000	0.042258000000
	H	3.326585000000	-2.209608000000	-0.669015000000
	H	1.564695000000	-2.180393000000	-0.676982000000
	C	1.530057000000	1.831540000000	0.844989000000
	H	0.884946000000	2.676545000000	0.598736000000
	H	1.267482000000	1.484637000000	1.848473000000
	H	2.557773000000	2.201288000000	0.885244000000
frequencies	66.0 92.6 142.9 202.8 205.9 221.4 223.8 261.3 290.3 305.1 372.8 406.8 433.4 453.4 485.4 555.8 638.4 778.8 787.1 809.8 841.8 888.1 917.8 940.9 951.7 977.2 1004.9 1022.6 1042.7 1063.7 1077.2 1091.2 1114.7 1129.5 1135.9 1175.0 1204.3 1231.8 1245.1 1290.3 1298.8 1315.4 1319.9 1336.9 1345.6 1363.4 1377.6 1388.5 1398.6 1403.9 1408.1 1415.6 1420.8 1470.9 1478.5 1484.3 1496.2 1497.4 1506.1 1507.7 1510.1 1515.0 2953.1 2961.2 3011.6 3021.6 3046.4 3048.7 3051.6 3055.9 3060.8 3081.5 3091.6 3095.0 3095.8 3101.7 3122.9 3124.4 3132.1 3139.6 3202.0			
electronic state	2-A			
point group	C1			
rotational constants	2.01356 0.85656 0.74076			
ZPE	0.270504 (Hartree/Particle)			
$TS_e\gamma$				
optimized Cartesian coordinate	C	-0.592007000000	-0.350972000000	-0.984319000000
	C	-0.446856000000	0.533086000000	0.260509000000
	C	0.553096000000	1.693028000000	0.087416000000
	C	2.002380000000	1.203774000000	-0.045473000000
	C	2.505867000000	0.396892000000	1.121873000000
	H	2.060824000000	-0.838633000000	0.937100000000
	O	1.740627000000	-1.934734000000	0.598596000000
	O	2.261989000000	-2.061818000000	-0.681257000000
	H	3.082661000000	-2.552574000000	-0.543688000000
	C	-1.830288000000	1.012049000000	0.717759000000
	C	-2.749702000000	-0.175275000000	1.016751000000
	C	-2.872743000000	-1.096777000000	-0.199470000000
	C	-1.496505000000	-1.550469000000	-0.692105000000
	H	-1.731738000000	1.648527000000	1.603893000000
	H	-0.062560000000	-0.109522000000	1.064572000000
	H	-1.034364000000	0.240137000000	-1.796560000000
	H	0.382986000000	-0.702607000000	-1.329756000000
	H	-2.335745000000	-0.744584000000	1.857821000000
	H	-3.736848000000	0.178351000000	1.327542000000
	H	-3.496186000000	-1.961979000000	0.042773000000
	H	-3.381274000000	-0.554801000000	-1.006751000000
	H	-1.013870000000	-2.171185000000	0.071733000000
	H	-1.600279000000	-2.170202000000	-1.586981000000
	H	-2.289144000000	1.625295000000	-0.067343000000
	H	0.501122000000	2.292694000000	1.007072000000
	H	2.656272000000	2.079639000000	-0.165365000000
	H	2.124820000000	0.623779000000	-0.969418000000
	H	3.581375000000	0.221288000000	1.144069000000
	H	2.100926000000	0.658979000000	2.100431000000
	C	0.218434000000	2.611637000000	-1.090593000000
	H	-0.808470000000	2.978487000000	-1.042993000000
	H	0.881161000000	3.480668000000	-1.098951000000
	H	0.347343000000	2.088804000000	-2.042018000000
frequencies	-1823.8 49.0 75.3 79.1 104.8 127.5 145.5 203.3 218.6 242.2 253.3 270.5 287.2 346.9 397.3 402.6 446.5 451.6 465.9 514.4 567.8 575.6 582.0 773.5 803.2 825.0 847.6 863.8 897.6 909.1 939.8 949.3 984.4 1009.3 1022.9 1053.1 1057.8 1071.0 1084.4 1086.0			

	1100.2	1117.5	1141.3	1176.4	1182.8	1204.4	1215.5	1264.6
	1270.6	1293.5	1303.6	1318.1	1330.5	1346.4	1359.6	1371.1
	1384.4	1385.5	1389.5	1401.9	1406.4	1412.8	1423.7	1454.8
	1470.3	1476.7	1484.9	1489.5	1492.5	1498.1	1506.2	1508.3
	1512.7	3011.0	3014.9	3028.7	3035.0	3035.4	3041.9	3042.8
	3051.5	3055.1	3059.6	3082.0	3092.0	3094.2	3094.7	3100.4
	3118.0	3124.2	3140.6	3176.8	3818.9			
electronic state	2-A							
point group	C1							
rotational constants	1.01051	0.68664	0.50025					
ZPE	0.295927 (Hartree/Particle)							
TS$_e\beta$(S)								
optimized Cartesian coordinate	C	0.965908000000	0.861060000000	0.775422000000				
	C	0.616999000000	-0.607932000000	0.498286000000				
	C	-0.896222000000	-0.908606000000	0.586335000000				
	C	-1.701599000000	-0.523031000000	-0.639915000000				
	C	-3.204032000000	-0.616897000000	-0.520539000000				
	H	-1.552571000000	0.769986000000	-0.828959000000				
	O	-1.646070000000	1.972957000000	-0.837243000000				
	O	-2.026378000000	2.279423000000	0.460299000000				
	H	-1.184754000000	2.443761000000	0.908888000000				
	C	1.265417000000	-1.046698000000	-0.820900000000				
	C	2.783795000000	-0.855684000000	-0.778850000000				
	C	3.142297000000	0.600786000000	-0.476232000000				
	C	2.482382000000	1.071191000000	0.821832000000				
	H	1.020985000000	-2.090328000000	-1.042561000000				
	H	1.090265000000	-1.193257000000	1.299923000000				
	H	0.545105000000	1.490559000000	-0.018257000000				
	H	0.519754000000	1.166496000000	1.729872000000				
	H	3.208118000000	-1.502609000000	-0.001492000000				
	H	3.228886000000	-1.165906000000	-1.727936000000				
	H	4.227087000000	0.721841000000	-0.415558000000				
	H	2.796497000000	1.232965000000	-1.302973000000				
	H	2.897504000000	0.503564000000	1.663473000000				
	H	2.712895000000	2.124159000000	1.004639000000				
	H	0.860851000000	-0.439908000000	-1.640165000000				
	H	-1.297388000000	-0.335733000000	1.434005000000				
	H	-1.311190000000	-0.932219000000	-1.574951000000				
	H	-3.692739000000	-0.150486000000	-1.377342000000				
	H	-3.534839000000	-1.660345000000	-0.477826000000				
	H	-3.548618000000	-0.111030000000	0.385136000000				
	C	-1.129944000000	-2.400498000000	0.897936000000				
	H	-0.809603000000	-3.030117000000	0.063273000000				
	H	-0.563127000000	-2.695163000000	1.784086000000				
	H	-2.183539000000	-2.607408000000	1.090025000000				
frequencies	-1800.6	29.3	70.0	86.4	104.2	116.5	161.8	180.8
	198.1	202.4	244.0	256.4	299.2	314.0	362.4	370.9
	412.1	427.2	456.5	484.3	513.5	593.4	623.8	785.2
	811.1	846.3	865.9	871.1	908.5	916.8	940.8	956.7
	980.2	1024.5	1033.2	1055.5	1065.9	1070.4	1087.4	1091.4
	1107.7	1127.3	1146.1	1165.0	1185.1	1193.3	1218.5	1270.2
	1294.1	1296.8	1310.6	1320.4	1335.9	1350.1	1369.3	1385.3
	1387.7	1390.6	1399.8	1401.6	1409.1	1421.4	1423.1	1467.9
	1487.1	1488.5	1490.1	1491.9	1494.3	1501.0	1503.8	1513.2
	1525.0	3009.2	3023.0	3028.3	3039.0	3039.3	3043.2	3044.8
	3047.5	3059.2	3079.8	3090.6	3097.5	3098.0	3102.5	3105.5
	3114.8	3129.6	3142.6	3146.1	3793.1			
electronic state	2-A							
point group	C1							
rotational constants	1.14444	0.60582	0.47236					
ZPE	0.295987 (Hartree/Particle)							
TS$_e\beta$(P)								

optimized Cartesian coordinate	C	0.533861000000	-0.533951000000	-0.739692000000
	C	0.511566000000	0.722359000000	0.140307000000
	C	-0.879672000000	1.038088000000	0.718947000000
	C	-1.481623000000	-0.111164000000	1.494467000000
	C	-1.890364000000	1.540679000000	-0.329782000000
	H	-2.008300000000	-0.966152000000	0.613593000000
	O	-2.500801000000	-1.702172000000	-0.175172000000
	O	-1.799886000000	-2.892396000000	-0.055237000000
	H	-1.155497000000	-2.843633000000	-0.774321000000
	C	1.586284000000	0.607337000000	1.229381000000
	C	2.974167000000	0.391007000000	0.620391000000
	C	2.994899000000	-0.842574000000	-0.284576000000
	C	1.914651000000	-0.750038000000	-1.364427000000
	H	1.581333000000	1.509510000000	1.849568000000
	H	0.800933000000	1.572927000000	-0.490086000000
	H	0.294070000000	-1.398869000000	-0.106547000000
	H	-0.236213000000	-0.473671000000	-1.516033000000
	H	3.247822000000	1.274336000000	0.030639000000
	H	3.722723000000	0.294213000000	1.411226000000
	H	3.980749000000	-0.962763000000	-0.741428000000
	H	2.815425000000	-1.736956000000	0.324741000000
	H	2.141672000000	0.088875000000	-2.033336000000
	H	1.916405000000	-1.653595000000	-1.980646000000
	H	1.354770000000	-0.235525000000	1.892330000000
	H	-0.737734000000	1.864522000000	1.436245000000
	H	-0.804366000000	-0.759242000000	2.050091000000
	H	-2.834575000000	1.737133000000	0.188943000000
	H	-2.379838000000	0.137690000000	2.059849000000
	C	-1.455106000000	2.801587000000	-1.073353000000
	H	-2.279239000000	3.201782000000	-1.666778000000
	H	-1.136974000000	3.580549000000	-0.374254000000
	H	-0.626940000000	2.607115000000	-1.757660000000
	H	-2.102706000000	0.738307000000	-1.042847000000
frequencies	-1872.7	33.9	58.9	74.1	95.7	102.3	128.9	181.5
	199.2	227.6	239.2	268.4	281.2	350.2	392.9	417.1
	441.7	445.9	474.6	508.9	532.4	599.3	639.5	772.7
	802.2	809.7	840.5	864.9	899.7	908.3	937.0	945.4
	962.8	1016.0	1027.9	1052.6	1057.3	1069.6	1079.4	1085.4
	1095.8	1114.8	1144.4	1153.0	1193.6	1214.3	1224.0	1263.5
	1281.0	1292.1	1300.9	1305.7	1331.5	1346.2	1359.9	1371.9
	1381.9	1385.9	1388.7	1395.7	1405.8	1410.3	1419.8	1455.1
	1467.2	1485.7	1489.0	1492.6	1497.7	1501.4	1504.8	1513.7
	1516.9	2968.0	3027.2	3035.1	3037.8	3042.5	3044.3	3047.0
	3056.9	3058.9	3084.7	3087.9	3093.4	3097.1	3097.5	3101.4
	3104.7	3128.3	3136.3	3185.8	3806.2			
electronic state	2-A							
point group	C1							
rotational constants	0.92142	0.64290	0.47986					
ZPE	0.295639 (Hartree/Particle)							
$TS_e\alpha$								
optimized Cartesian coordinate	C	-1.488949000000	1.068822000000	0.558813000000
	C	-0.511350000000	0.070550000000	-0.091185000000
	C	0.889607000000	0.176229000000	0.496696000000
	C	1.596486000000	1.510095000000	0.320588000000
	C	1.489026000000	2.114323000000	-1.077623000000
	H	1.576109000000	-0.588126000000	-0.267453000000
	H	0.464990000000	2.409286000000	-1.318734000000
	O	2.389781000000	-1.270569000000	-0.917247000000
	O	3.599668000000	-1.010460000000	-0.292749000000
	H	3.709462000000	-1.758672000000	0.308444000000
	C	-1.093124000000	-1.346730000000	-0.021869000000
	C	-2.457799000000	-1.414233000000	-0.710339000000
	C	-3.433761000000	-0.416289000000	-0.083066000000
	C	-2.863770000000	1.003300000000	-0.111951000000
	H	-0.393264000000	-2.056282000000	-0.475199000000
	H	-0.439443000000	0.336196000000	-1.154415000000

	H	-1.591343000000	0.827201000000	1.624271000000
	H	-1.089677000000	2.085411000000	0.497510000000
	H	-2.337189000000	-1.183134000000	-1.775453000000
	H	-2.860866000000	-2.428580000000	-0.649882000000
	H	-4.396822000000	-0.448066000000	-0.599437000000
	H	-3.621384000000	-0.706030000000	0.958208000000
	H	-2.765939000000	1.330623000000	-1.154263000000
	H	-3.551818000000	1.699722000000	0.375169000000
	H	-1.216389000000	-1.639744000000	1.027670000000
	H	2.652572000000	1.360139000000	0.568398000000
	H	1.207402000000	2.214889000000	1.070007000000
	H	2.117436000000	3.002691000000	-1.159672000000
	H	1.822952000000	1.393443000000	-1.828322000000
	C	1.096758000000	-0.419062000000	1.873896000000
	H	2.141504000000	-0.315102000000	2.177708000000
	H	0.487702000000	0.107005000000	2.619864000000
	H	0.829663000000	-1.476668000000	1.911793000000
frequencies	-1651.4 24.6 60.0 65.8 98.7 107.6 156.3 183.5 187.8 211.5 229.6 247.4 291.2 296.2 350.5 383.4 403.6 420.9 446.1 461.5 502.0 526.8 644.6 765.8 801.5 805.3 837.1 864.4 905.0 908.8 940.6 952.1 984.5 1016.3 1033.3 1054.7 1068.4 1081.1 1088.0 1095.7 1111.9 1122.7 1155.4 1165.6 1199.3 1229.4 1252.9 1274.8 1294.3 1299.7 1302.4 1334.6 1349.7 1364.4 1373.4 1382.2 1385.0 1388.5 1401.7 1406.7 1409.0 1418.2 1466.9 1474.8 1484.7 1487.6 1490.6 1491.0 1496.8 1505.0 1507.6 1510.8 1513.0 3012.8 3029.5 3035.3 3037.1 3039.0 3043.3 3046.3 3049.0 3060.6 3076.7 3090.1 3094.1 3097.2 3098.9 3103.0 3104.4 3131.2 3138.9 3139.3 3816.4			
electronic state	2-A			
point group	C1			
rotational constants	1.35136 0.52236 0.45906			
ZPE	0.295697 (Hartree/Particle)			
$TS_e\alpha'$				
optimized Cartesian coordinate	C	1.002265000000	-0.375975000000	-1.243505000000
	C	-0.056968000000	-0.328448000000	-0.154506000000
	C	-1.488668000000	-0.529251000000	-0.650347000000
	C	-2.551791000000	-0.477639000000	0.454948000000
	C	-2.575845000000	0.815053000000	1.266948000000
	H	-0.007861000000	0.921090000000	0.185956000000
	O	0.130755000000	2.144172000000	0.339358000000
	O	0.303544000000	2.626829000000	-0.948919000000
	H	-0.583317000000	2.913328000000	-1.203911000000
	H	-2.691035000000	1.684186000000	0.613745000000
	C	0.358642000000	-1.070831000000	1.104915000000
	C	1.745529000000	-0.636714000000	1.593322000000
	C	2.792364000000	-0.761884000000	0.486026000000
	C	2.383770000000	0.053268000000	-0.741767000000
	H	-0.377445000000	-0.934558000000	1.900461000000
	H	1.069786000000	-1.411693000000	-1.608606000000
	H	0.691000000000	0.241648000000	-2.091841000000
	H	1.693623000000	0.407822000000	1.919979000000
	H	2.032591000000	-1.233796000000	2.462702000000
	H	3.768306000000	-0.432423000000	0.851795000000
	H	2.896289000000	-1.817611000000	0.204587000000
	H	2.357579000000	1.116393000000	-0.484774000000
	H	3.117799000000	-0.068368000000	-1.542447000000
	H	0.378046000000	-2.148464000000	0.876995000000
	H	-1.696674000000	0.290491000000	-1.354434000000
	H	-2.419555000000	-1.337726000000	1.121034000000
	H	-3.528139000000	-0.617628000000	-0.020061000000
	H	-3.409616000000	0.810942000000	1.971923000000
	H	-1.655567000000	0.965204000000	1.834492000000
	C	-1.626120000000	-1.848222000000	-1.430926000000
	H	-2.664775000000	-1.997064000000	-1.735140000000
	H	-1.008686000000	-1.857379000000	-2.329767000000

	H	-1.335820000000		-2.698555000000		-0.806844000000		
frequencies	-1713.1	44.1	64.8	102.1	107.0	140.7	146.9	200.5
	220.5	230.2	237.3	263.4	301.6	303.6	339.3	389.7
	404.1	420.6	456.9	470.6	486.0	535.1	613.5	780.7
	792.4	802.9	844.1	866.7	898.6	919.1	938.4	955.4
	979.5	1010.1	1034.9	1056.2	1071.0	1074.7	1088.8	1095.3
	1106.4	1127.7	1165.8	1173.1	1187.0	1210.2	1242.7	1270.5
	1292.9	1301.3	1312.9	1322.1	1350.2	1365.9	1370.7	1386.3
	1389.2	1391.7	1399.5	1406.0	1406.4	1421.5	1462.9	1469.1
	1476.6	1490.7	1492.0	1494.3	1502.5	1506.1	1508.9	1510.9
	1512.5	2996.2	3003.5	3008.4	3034.1	3050.1	3055.7	3059.2
	3062.1	3069.3	3083.7	3087.8	3097.9	3104.0	3108.4	3116.1
	3126.4	3129.6	3141.2	3148.0	3811.8			
electronic state	2-A							
point group	C1							
rotational constants	1.01184	0.70447	0.59966					
ZPE	0.296178 (Hartree/Particle)							
TS$_{\mathscr{B}}\beta'$								
optimized Cartesian coordinate	C	-0.235702000000		0.011224000000		-0.847352000000		
	C	-1.418717000000		-0.793635000000		-1.339764000000		
	C	-2.279437000000		-1.309548000000		-0.182459000000		
	H	-0.803545000000		1.044546000000		-0.268929000000		
	O	-1.464468000000		1.938813000000		0.219883000000		
	O	-2.625150000000		1.974503000000		-0.541488000000		
	H	-2.459584000000		2.688573000000		-1.170300000000		
	C	-0.310429000000		-1.129915000000		1.376394000000		
	C	0.595511000000		-0.661784000000		0.228230000000		
	H	-3.061580000000		-1.968179000000		-0.568369000000		
	H	-0.762682000000		-0.259780000000		1.863382000000		
	H	0.294462000000		-1.648012000000		2.127536000000		
	H	-1.030192000000		-1.647322000000		-1.916784000000		
	H	-2.024179000000		-0.198677000000		-2.028131000000		
	H	0.340622000000		0.485974000000		-1.644902000000		
	H	0.995736000000		-1.578555000000		-0.237327000000		
	H	-2.778536000000		-0.456454000000		0.288408000000		
	C	-1.428721000000		-2.037835000000		0.860204000000		
	H	-2.057310000000		-2.369307000000		1.690805000000		
	H	-0.989854000000		-2.938568000000		0.412933000000		
	C	1.810573000000		0.155752000000		0.707843000000		
	H	2.365397000000		-0.506240000000		1.387117000000		
	C	2.767550000000		0.534479000000		-0.433152000000		
	H	3.653207000000		0.994643000000		0.016587000000		
	H	2.309533000000		1.317143000000		-1.048810000000		
	C	3.203747000000		-0.631959000000		-1.318119000000		
	H	2.377754000000		-1.017008000000		-1.921163000000		
	H	3.995762000000		-0.325924000000		-2.004299000000		
	H	3.586977000000		-1.458762000000		-0.712817000000		
	C	1.423474000000		1.414145000000		1.489051000000		
	H	2.322761000000		1.939066000000		1.821342000000		
	H	0.847518000000		2.105803000000		0.867675000000		
	H	0.827583000000		1.184971000000		2.373632000000		
frequencies	-1745.8	40.8	83.6	84.4	109.7	118.2	148.7	195.9
	216.9	220.9	259.5	264.8	290.7	309.3	351.1	390.1
	410.7	434.5	469.3	480.8	524.5	593.3	601.6	763.1
	798.4	807.4	835.5	870.2	901.6	906.4	940.4	947.1
	975.9	1007.5	1032.3	1059.5	1064.8	1069.9	1080.1	1100.0
	1105.8	1135.8	1153.1	1169.3	1194.9	1208.1	1227.9	1266.2
	1286.3	1294.0	1314.4	1326.3	1335.0	1353.8	1363.4	1378.8
	1388.6	1390.0	1395.0	1398.0	1408.1	1416.7	1420.3	1460.2
	1466.1	1491.2	1493.7	1498.4	1504.6	1507.0	1507.8	1514.7
	1517.1	2973.4	2998.3	3019.6	3036.6	3048.9	3054.0	3054.6
	3060.8	3065.3	3081.5	3095.8	3098.2	3102.3	3109.7	3111.8
	3122.1	3125.0	3132.7	3146.3	3821.1			
electronic state	2-A							
point group	C1							

rotational constants	1.06876	0.62289	0.53373					
ZPE	0.295951 (Hartree/Particle)							
$TS_e\gamma'$								
optimized Cartesian coordinate	C	-1.700328000000	-0.233173000000	1.075515000000				
	C	-0.188744000000	-0.162873000000	1.087982000000				
	C	0.421662000000	-0.461161000000	-0.289717000000				
	H	-2.057739000000	0.751470000000	0.301845000000				
	O	-2.288649000000	1.693728000000	-0.434431000000				
	O	-1.346449000000	2.642667000000	-0.064100000000				
	H	-1.826098000000	3.213057000000	0.550585000000				
	C	-1.684494000000	-1.697375000000	-0.963930000000				
	C	-2.307505000000	-1.448713000000	0.412001000000				
	H	-1.966577000000	-0.882738000000	-1.639470000000				
	H	-2.078461000000	-2.623777000000	-1.389327000000				
	H	0.179235000000	-0.894852000000	1.823926000000				
	H	0.126903000000	0.823162000000	1.441954000000				
	H	-2.167429000000	0.046145000000	2.022456000000				
	H	-2.120736000000	-2.322652000000	1.054812000000				
	H	-3.392971000000	-1.340425000000	0.340025000000				
	H	0.098482000000	0.346845000000	-0.959191000000				
	C	-0.161094000000	-1.763992000000	-0.852031000000				
	H	0.103303000000	-2.601329000000	-0.194805000000				
	H	0.286223000000	-1.972830000000	-1.829500000000				
	C	1.965747000000	-0.467529000000	-0.292372000000				
	H	2.263222000000	-0.554054000000	-1.346834000000				
	C	2.574802000000	0.838043000000	0.238722000000				
	H	2.383228000000	0.917180000000	1.315475000000				
	H	3.662493000000	0.764011000000	0.135448000000				
	C	2.085719000000	2.097400000000	-0.473309000000				
	H	1.026358000000	2.286704000000	-0.291875000000				
	H	2.645081000000	2.974083000000	-0.139504000000				
	H	2.225459000000	2.006652000000	-1.554751000000				
	C	2.572526000000	-1.658625000000	0.455848000000				
	H	2.286344000000	-2.614849000000	0.014983000000				
	H	3.663465000000	-1.599226000000	0.432102000000				
	H	2.271248000000	-1.665745000000	1.507647000000				
frequencies	-1738.4	29.3	52.2	85.8	98.1	117.9	154.7	196.4
	204.7	211.7	238.5	262.2	280.9	310.8	336.5	399.9
	403.3	429.6	469.2	479.8	519.9	577.7	605.2	765.1
	801.3	804.6	836.8	864.5	895.4	905.4	937.4	949.5
	978.1	1007.8	1031.0	1057.7	1061.8	1075.7	1081.9	1089.6
	1112.3	1135.9	1154.1	1170.9	1201.2	1207.5	1232.2	1267.8
	1292.1	1293.5	1314.9	1334.0	1337.9	1357.5	1366.1	1376.0
	1387.5	1391.1	1404.0	1408.4	1409.9	1417.6	1423.6	1459.3
	1463.0	1472.9	1491.4	1497.1	1500.7	1506.3	1508.1	1513.8
	1523.1	2998.9	3003.0	3016.6	3035.5	3044.2	3046.2	3057.3
	3057.8	3058.7	3077.8	3087.0	3091.5	3094.1	3107.5	3108.2
	3120.9	3123.0	3140.5	3148.9	3818.0			
electronic state	2-A							
point group	C1							
rotational constants	0.98211	0.72789	0.49094					
ZPE	0.295650 (Hartree/Particle)							
$TS_e\delta'$								
optimized Cartesian coordinate	C	2.016754000000	-1.279456000000	0.012527000000				
	C	1.126904000000	-1.083093000000	-1.192429000000				
	C	0.006100000000	-0.073688000000	-0.920183000000				
	C	-0.775753000000	-0.435541000000	0.349131000000				
	C	-1.984174000000	0.483078000000	0.621904000000				
	C	-2.986508000000	0.514213000000	-0.541961000000				
	C	-3.445289000000	-0.860794000000	-1.023906000000				
	H	2.572375000000	-0.105963000000	0.173196000000				
	O	2.985675000000	1.035728000000	0.225786000000				
	O	2.955026000000	1.469901000000	-1.092133000000				

	H	3.863888000000	1.341937000000	-1.392813000000
	H	-3.805691000000	-1.466634000000	-0.187199000000
	C	0.185529000000	-0.495335000000	1.542741000000
	C	1.291751000000	-1.529499000000	1.316213000000
	H	-0.658550000000	-0.036876000000	-1.787569000000
	H	-1.172385000000	-1.451878000000	0.211957000000
	H	0.652708000000	0.484321000000	1.685565000000
	H	-0.366944000000	-0.730344000000	2.458384000000
	H	0.683411000000	-2.057343000000	-1.451820000000
	H	1.718726000000	-0.768331000000	-2.055935000000
	H	2.880737000000	-1.924513000000	-0.159819000000
	H	0.848007000000	-2.536050000000	1.275586000000
	H	1.997601000000	-1.533713000000	2.151076000000
	H	0.451076000000	0.920964000000	-0.811938000000
	H	-2.507838000000	0.048467000000	1.485282000000
	H	-2.555630000000	1.076303000000	-1.378167000000
	H	-3.859269000000	1.088923000000	-0.215295000000
	H	-4.259605000000	-0.770074000000	-1.745479000000
	H	-2.636152000000	-1.412589000000	-1.508490000000
	C	-1.585026000000	1.914509000000	0.991815000000
	H	-0.995142000000	1.954955000000	1.908763000000
	H	-1.000792000000	2.381366000000	0.194093000000
	H	-2.477881000000	2.525678000000	1.146287000000
frequencies	-1759.6	48.8	49.2	70.3	107.8	117.2	160.8	205.4
	209.0	226.1	238.3	272.4	291.8	295.5	325.9	387.0
	414.1	431.6	460.1	483.8	525.1	575.9	614.5	769.7
	789.0	805.4	838.3	856.5	900.5	920.3	937.0	946.1
	977.6	1005.3	1028.3	1055.5	1062.6	1073.3	1079.0	1098.8
	1104.8	1137.0	1156.3	1173.3	1197.1	1207.9	1225.9	1266.9
	1289.7	1305.3	1320.0	1325.8	1342.6	1351.7	1361.4	1375.5
	1385.2	1390.5	1404.3	1407.0	1411.2	1416.6	1421.3	1458.8
	1464.1	1478.1	1489.2	1496.7	1500.1	1507.2	1509.7	1511.9
	1515.5	2994.9	3002.4	3009.3	3019.3	3049.4	3053.7	3055.0
	3059.9	3068.1	3082.7	3092.1	3095.1	3101.6	3110.8	3111.2
	3122.8	3125.8	3132.6	3143.2	3821.0			
electronic state	2-A							
point group	C1							
rotational constants	1.27548	0.51065	0.48543					
ZPE	0.295736 (Hartree/Particle)							
*i*BCH								
optimized Cartesian coordinate	C	-0.684308000000	-0.944049000000	-0.600034000000
	C	-0.222712000000	0.268536000000	0.216424000000
	C	-1.262956000000	1.391626000000	0.123724000000
	C	-2.656912000000	0.925315000000	0.546627000000
	C	-3.103844000000	-0.279125000000	-0.283704000000
	C	-2.082069000000	-1.413110000000	-0.187803000000
	H	-0.942373000000	2.241427000000	0.734938000000
	H	-0.164079000000	-0.037228000000	1.270542000000
	H	-0.689476000000	-0.667913000000	-1.663839000000
	H	0.026595000000	-1.768528000000	-0.492511000000
	H	-2.637232000000	0.644166000000	1.606699000000
	H	-3.375381000000	1.743813000000	0.449361000000
	H	-4.088351000000	-0.624947000000	0.042880000000
	H	-3.204728000000	0.026078000000	-1.332583000000
	H	-2.045674000000	-1.774956000000	0.847308000000
	H	-2.392350000000	-2.259367000000	-0.806832000000
	H	-1.302567000000	1.746900000000	-0.914938000000
	C	1.151355000000	0.782760000000	-0.222702000000
	H	1.431138000000	1.625922000000	0.423714000000
	H	1.060523000000	1.191701000000	-1.237789000000
	C	2.298656000000	-0.235093000000	-0.206749000000
	H	2.084728000000	-1.011674000000	-0.950163000000
	C	3.604919000000	0.449951000000	-0.610304000000
	H	4.428123000000	-0.266621000000	-0.664681000000
	H	3.513036000000	0.936465000000	-1.584704000000
	H	3.875621000000	1.216501000000	0.122897000000

	C	2.448667000000	-0.904625000000	1.159687000000
	H	2.587267000000	-0.148640000000	1.940128000000
	H	1.571688000000	-1.500524000000	1.422577000000
	H	3.318709000000	-1.565699000000	1.175995000000

frequencies	72.1	81.8	132.6	174.9	233.9	239.0	264.6	294.1
	313.0	338.6	405.1	430.2	445.0	457.4	481.9	577.9
	791.8	798.8	829.5	850.3	865.2	908.5	922.0	935.0
	942.0	963.8	979.2	1001.8	1054.2	1061.1	1079.5	1100.4
	1119.3	1132.5	1154.2	1187.4	1202.1	1222.7	1248.0	1289.2
	1292.1	1305.0	1312.6	1334.9	1353.6	1367.0	1372.1	1381.8
	1386.3	1388.5	1400.2	1404.9	1411.7	1421.9	1477.4	1481.9
	1488.7	1489.2	1493.5	1494.7	1498.2	1508.1	1509.8	1516.3
	3015.9	3017.1	3023.9	3032.2	3036.2	3040.4	3043.0	3044.8
	3045.4	3049.7	3064.0	3083.8	3092.7	3093.8	3095.1	3099.1
	3113.4	3119.1	3127.7	3130.2				
electronic state	1-A							
point group	C1							
rotational constants	2.75943	0.65169	0.59780					
ZPE	0.284858 (Hartree/Particle)							
*i*BP1								
optimized Cartesian coordinate	C	0.650542000000	0.978405000000	-0.546908000000				
	C	0.193344000000	-0.268530000000	0.218266000000				
	C	-1.186086000000	-0.759757000000	-0.229664000000				
	C	-2.319406000000	0.272743000000	-0.147598000000				
	C	-2.443972000000	0.847773000000	1.224650000000				
	C	1.228511000000	-1.389932000000	0.071566000000				
	C	2.627688000000	-0.945973000000	0.501240000000				
	C	3.070983000000	0.289916000000	-0.283483000000				
	C	2.054712000000	1.422203000000	-0.128557000000				
	H	0.910306000000	-2.263505000000	0.649782000000				
	H	0.136109000000	0.000772000000	1.282576000000				
	H	0.641623000000	0.755523000000	-1.623281000000				
	H	-0.055063000000	1.798018000000	-0.383079000000				
	H	2.617944000000	-0.707752000000	1.571872000000				
	H	3.342142000000	-1.762344000000	0.364502000000				
	H	4.060288000000	0.618275000000	0.046650000000				
	H	3.159578000000	0.027898000000	-1.345112000000				
	H	2.028748000000	1.738012000000	0.921629000000				
	H	2.362519000000	2.293878000000	-0.712560000000				
	H	1.259324000000	-1.702511000000	-0.981172000000				
	H	-1.466463000000	-1.627924000000	0.381909000000				
	H	-1.115205000000	-1.120835000000	-1.263786000000				
	H	-2.107336000000	1.085804000000	-0.850794000000				
	H	-2.872412000000	1.829417000000	1.381553000000				
	H	-2.334209000000	0.203355000000	2.089963000000				
	C	-3.647836000000	-0.372383000000	-0.587096000000				
	H	-3.911723000000	-1.192625000000	0.086107000000				
	H	-4.462509000000	0.354368000000	-0.570529000000				
	H	-3.564542000000	-0.774614000000	-1.600727000000				

frequencies	56.7	80.7	133.4	176.9	183.9	233.8	249.3	278.1
	309.4	336.6	377.5	422.8	443.8	450.5	475.8	549.3
	582.3	791.2	799.0	842.6	852.6	871.4	908.7	914.0
	940.4	948.6	966.5	997.9	1053.2	1056.1	1059.5	1084.7
	1103.5	1125.0	1140.2	1165.0	1185.9	1220.9	1246.1	1284.9
	1292.2	1304.5	1309.5	1325.5	1346.9	1366.7	1370.6	1380.4
	1386.0	1388.3	1392.6	1401.8	1411.5	1462.7	1479.1	1483.4
	1488.4	1488.8	1494.0	1498.2	1502.5	1508.3	3014.3	3021.4
	3021.7	3031.4	3036.8	3041.2	3045.2	3048.9	3051.5	3068.7
	3083.1	3093.7	3094.3	3095.3	3099.4	3122.8	3134.3	3155.0
	3259.8							
electronic state	2-A							
point group	C1							
rotational constants	2.81588	0.66026	0.60506					
ZPE	0.269962 (Hartree/Particle)							

*i*BP2				
optimized Cartesian coordinate	C	-1.359072000000	-1.321002000000	-0.407578000000
	C	-0.176800000000	-0.491044000000	0.101683000000
	C	1.142718000000	-0.974090000000	-0.535550000000
	C	2.359509000000	-0.235340000000	-0.073930000000
	C	2.987857000000	0.822848000000	-0.920268000000
	C	-0.419373000000	0.999316000000	-0.155626000000
	C	-1.750818000000	1.472012000000	0.433071000000
	C	-2.918864000000	0.633775000000	-0.089545000000
	C	-2.688323000000	-0.853025000000	0.188259000000
	H	0.403872000000	1.588796000000	0.259473000000
	H	-0.104089000000	-0.637424000000	1.189304000000
	H	-1.403507000000	-1.230423000000	-1.501460000000
	H	-1.191489000000	-2.379707000000	-0.185361000000
	H	-1.709133000000	1.384754000000	1.525838000000
	H	-1.908900000000	2.529918000000	0.206516000000
	H	-3.857628000000	0.965218000000	0.362432000000
	H	-3.014836000000	0.785842000000	-1.171708000000
	H	-2.675375000000	-1.018051000000	1.272571000000
	H	-3.513008000000	-1.448542000000	-0.212819000000
	H	-0.416259000000	1.172702000000	-1.241036000000
	H	1.048194000000	-0.896973000000	-1.625195000000
	H	1.250703000000	-2.042951000000	-0.301178000000
	H	2.801484000000	0.652489000000	-1.982966000000
	H	2.602732000000	1.826953000000	-0.680986000000
	H	4.071147000000	0.863817000000	-0.764360000000
	C	2.699160000000	-0.270067000000	1.380639000000
	H	2.163624000000	0.510852000000	1.944641000000
	H	2.429685000000	-1.228814000000	1.833001000000
	H	3.766827000000	-0.098761000000	1.546364000000
frequencies	54.0 68.6 109.2 119.5 151.0 163.9 235.8 255.8 309.1 330.3 385.6 408.9 439.0 446.8 486.8 556.5 781.5 793.9 800.8 849.7 865.1 910.3 931.8 943.8 949.1 974.3 987.8 1019.1 1038.5 1056.2 1074.7 1087.0 1098.3 1124.6 1131.7 1194.1 1212.4 1275.9 1286.1 1294.1 1297.5 1319.2 1324.5 1340.4 1367.5 1373.1 1385.2 1387.7 1390.8 1402.4 1406.5 1417.7 1472.5 1474.1 1478.2 1484.1 1487.5 1488.7 1490.1 1494.3 1502.1 1508.7 2977.3 2981.5 3006.3 3012.1 3022.1 3030.3 3037.0 3040.3 3045.3 3063.1 3068.3 3069.2 3084.5 3090.1 3093.8 3095.3 3099.5 3115.8 3122.7						
electronic state	2-A			
point group	C1			
rotational constants	2.49628 0.71104 0.65365			
ZPE	0.270075 (Hartree/Particle)			
*i*BP3				
optimized Cartesian coordinate	C	-0.864312000000	1.045901000000	0.604827000000
	C	-0.204487000000	-0.151190000000	-0.110002000000
	C	1.151950000000	-0.446188000000	0.440354000000
	C	2.406100000000	-0.177536000000	-0.329051000000
	C	3.631595000000	-0.759213000000	0.374648000000
	H	3.522966000000	-1.835124000000	0.528226000000
	C	-1.127487000000	-1.380373000000	-0.017627000000
	C	-2.526564000000	-1.089124000000	-0.564335000000
	C	-3.162135000000	0.105269000000	0.149616000000
	C	-2.262313000000	1.338779000000	0.055575000000
	H	-0.671824000000	-2.219479000000	-0.551182000000
	H	-0.101095000000	0.110574000000	-1.173572000000
	H	-0.933159000000	0.811378000000	1.674966000000
	H	-0.221690000000	1.926649000000	0.515799000000
	H	-2.454378000000	-0.869772000000	-1.636712000000
	H	-3.160643000000	-1.974403000000	-0.464852000000
	H	-4.148131000000	0.319981000000	-0.271254000000
	H	-3.314683000000	-0.147585000000	1.206054000000

	H	-2.178941000000	1.643837000000	-0.994891000000
	H	-2.709150000000	2.178949000000	0.594253000000
	H	-1.201070000000	-1.677416000000	1.036719000000
	H	1.223417000000	-0.764421000000	1.477972000000
	H	2.309622000000	-0.657690000000	-1.314601000000
	H	4.540225000000	-0.584358000000	-0.206061000000
	H	3.762268000000	-0.288484000000	1.353859000000
	C	2.592985000000	1.330138000000	-0.580202000000
	H	1.730608000000	1.756736000000	-1.098119000000
	H	2.712227000000	1.857206000000	0.370991000000
	H	3.481441000000	1.514647000000	-1.190414000000
frequencies	41.7 51.7 92.8 209.3 234.9 238.1 247.8 264.9 287.0 314.5 362.8 394.8 437.7 461.0 484.1 522.6 568.9 795.6 807.5 840.5 864.1 899.1 907.3 928.3 936.5 954.9 972.9 1007.4 1052.5 1061.1 1091.6 1109.8 1115.1 1116.7 1151.9 1187.8 1200.8 1203.2 1243.8 1288.7 1291.6 1298.6 1321.8 1325.7 1345.2 1357.9 1371.2 1383.8 1384.8 1386.7 1396.5 1414.7 1439.8 1480.8 1485.7 1488.5 1491.0 1492.7 1494.6 1506.0 1507.7 1515.0 2994.4 3010.2 3032.1 3036.0 3039.4 3041.4 3045.8 3046.6 3052.4 3091.6 3093.6 3094.3 3095.2 3099.9 3119.1 3123.6 3127.6 3134.4 3157.9			
electronic state	2-A			
point group	C1			
rotational constants	2.80875 0.64603 0.57102			
ZPE	0.270117 (Hartree/Particle)			
*i*BP4				
optimized Cartesian coordinate	C	1.031858000000	1.002786000000	-0.966614000000
	C	0.220698000000	-0.192408000000	-0.574317000000
	C	-1.234587000000	-0.287529000000	-0.903249000000
	C	-2.152005000000	-0.181153000000	0.334551000000
	C	-1.996249000000	1.180016000000	1.011018000000
	H	-2.289989000000	1.980712000000	0.323436000000
	C	0.965957000000	-1.423796000000	-0.162511000000
	C	2.099936000000	-1.110872000000	0.823054000000
	C	2.988369000000	0.015118000000	0.291406000000
	C	2.169064000000	1.279602000000	0.027270000000
	H	0.277257000000	-2.159273000000	0.265499000000
	H	1.479593000000	0.835492000000	-1.962848000000
	H	0.387070000000	1.881632000000	-1.064891000000
	H	1.663687000000	-0.800872000000	1.779745000000
	H	2.692619000000	-2.009882000000	1.012766000000
	H	3.794073000000	0.227930000000	0.999107000000
	H	3.462607000000	-0.310115000000	-0.643342000000
	H	1.738324000000	1.629296000000	0.972778000000
	H	2.810564000000	2.080142000000	-0.350922000000
	H	1.407128000000	-1.900346000000	-1.056521000000
	H	-1.444453000000	-1.244004000000	-1.402490000000
	H	-1.519846000000	0.505753000000	-1.606430000000
	H	-1.840722000000	-0.957401000000	1.044884000000
	H	-2.628702000000	1.253403000000	1.899169000000
	H	-0.960891000000	1.356132000000	1.313513000000
	C	-3.607473000000	-0.431538000000	-0.055282000000
	H	-4.265567000000	-0.375898000000	0.815325000000
	H	-3.942706000000	0.321160000000	-0.776224000000
	H	-3.733449000000	-1.415204000000	-0.514504000000
frequencies	35.9 45.6 67.8 169.9 216.0 225.7 256.4 279.0 323.1 349.7 373.0 409.4 423.8 445.2 478.0 567.2 767.2 792.1 821.3 852.8 859.1 872.7 925.3 930.5 932.6 957.4 973.0 995.1 1047.2 1076.8 1088.8 1098.7 1111.3 1141.0 1173.9 1193.9 1195.6 1236.2 1255.9 1285.5 1295.2 1319.5 1327.2 1357.1 1360.8 1365.8 1372.8 1379.4 1387.2 1402.8 1411.0 1418.1 1468.2 1475.1 1479.4 1487.6 1490.4 1491.8 1496.7 1503.9 1506.3 1513.6 2946.6 2949.5 3007.5 3033.6 3035.1 3043.6 3044.9 3047.5 3048.0 3059.9 3076.2 3079.9 3096.3 3096.8 3100.3 3112.3 3118.0 3127.4			

	3128.9							
electronic state	2-A							
point group	C1							
rotational constants	2.49867	0.70800	0.65751					
ZPE	0.270446 (Hartree/Particle)							
*i*BP5								
optimized Cartesian coordinate	C	0.695336000000	0.913114000000	-0.567789000000				
	C	2.047344000000	1.447522000000	-0.226834000000				
	C	3.099519000000	0.320749000000	-0.304710000000				
	C	1.284609000000	-1.392712000000	0.116393000000				
	C	0.219478000000	-0.276702000000	0.202836000000				
	H	4.072750000000	0.691271000000	0.029454000000				
	H	1.327867000000	-1.756037000000	-0.918006000000				
	H	0.980883000000	-2.237304000000	0.743720000000				
	H	2.042231000000	1.832062000000	0.803506000000				
	H	2.324860000000	2.277947000000	-0.878918000000				
	H	0.243260000000	1.147368000000	-1.525719000000				
	H	0.161889000000	0.003973000000	1.266728000000				
	H	3.210471000000	0.010090000000	-1.349621000000				
	C	2.665111000000	-0.882004000000	0.536233000000				
	H	3.403305000000	-1.684434000000	0.453725000000				
	H	2.632836000000	-0.588714000000	1.592895000000				
	C	-1.151790000000	-0.780114000000	-0.248170000000				
	H	-1.436294000000	-1.636854000000	0.377072000000				
	H	-1.063158000000	-1.160577000000	-1.274092000000				
	C	-2.282197000000	0.255664000000	-0.199883000000				
	H	-2.044995000000	1.056194000000	-0.910175000000				
	C	-2.422016000000	0.884266000000	1.186783000000				
	H	-2.561023000000	0.108530000000	1.947699000000				
	H	-1.539848000000	1.470419000000	1.453921000000				
	H	-3.288244000000	1.549357000000	1.225045000000				
	C	-3.598639000000	-0.390544000000	-0.632121000000				
	H	-3.511490000000	-0.846885000000	-1.621522000000				
	H	-3.888237000000	-1.175024000000	0.074543000000				
	H	-4.407596000000	0.343173000000	-0.666685000000				
frequencies	55.7	89.8	107.0	166.4	203.1	237.5	264.5	291.6
	312.9	316.8	340.8	407.3	437.3	452.4	475.6	532.2
	596.2	802.3	821.9	846.4	856.2	879.1	929.0	934.2
	937.7	964.3	978.3	985.7	1042.8	1068.4	1076.3	1103.4
	1116.2	1145.8	1161.7	1167.0	1203.4	1218.6	1245.8	1266.2
	1291.7	1304.8	1316.6	1341.8	1343.4	1351.9	1368.3	1371.5
	1384.7	1395.5	1403.9	1420.4	1427.3	1477.4	1482.4	1487.3
	1490.4	1493.5	1498.3	1502.0	1508.0	1518.0	2987.3	3008.6
	3022.6	3035.9	3040.0	3043.0	3045.3	3048.5	3050.3	3067.3
	3085.2	3094.3	3099.1	3110.1	3113.4	3118.7	3127.8	3131.2
	3187.8							
electronic state	2-A							
point group	C1							
rotational constants	2.80423	0.65537	0.60380					
ZPE	0.270267 (Hartree/Particle)							
*i*BP6								
optimized Cartesian coordinate	C	2.088685000000	1.404674000000	-0.240071000000				
	C	0.686695000000	1.002811000000	-0.560807000000				
	C	0.249378000000	-0.253007000000	0.215303000000				
	C	2.686071000000	-0.885089000000	0.554628000000				
	C	3.147374000000	0.352499000000	-0.229749000000				
	H	2.628790000000	-0.633061000000	1.619242000000				
	H	3.418855000000	-1.689836000000	0.451126000000				
	H	0.597555000000	0.771505000000	-1.638840000000				
	H	0.001080000000	1.832591000000	-0.369879000000				
	H	2.366253000000	2.451154000000	-0.266432000000				
	H	3.366326000000	0.036799000000	-1.264535000000				

	H	4.082647000000	0.743807000000	0.177271000000
	H	0.194022000000	0.013824000000	1.278755000000
	C	1.311290000000	-1.349136000000	0.073225000000
	H	1.376864000000	-1.641843000000	-0.983870000000
	H	0.995260000000	-2.238518000000	0.627670000000
	C	-1.117800000000	-0.767974000000	-0.241111000000
	H	-1.022901000000	-1.142117000000	-1.269198000000
	H	-1.388646000000	-1.634155000000	0.377804000000
	C	-2.273582000000	0.238967000000	-0.191018000000
	H	-2.060512000000	1.047537000000	-0.900064000000
	C	-2.437945000000	0.849436000000	1.201306000000
	H	-1.566176000000	1.437242000000	1.497393000000
	H	-3.311250000000	1.505321000000	1.237947000000
	H	-2.579872000000	0.060368000000	1.947582000000
	C	-3.571514000000	-0.438729000000	-0.631984000000
	H	-3.470030000000	-0.881576000000	-1.626031000000
	H	-3.839763000000	-1.238483000000	0.065763000000
	H	-4.400404000000	0.272727000000	-0.660040000000
frequencies	72.6 84.0 133.8 166.3 190.9 235.3 262.0 287.7 300.7 317.4 379.4 405.5 425.5 448.2 468.2 516.0 631.2 792.2 823.5 849.0 854.7 868.4 920.8 936.1 942.7 958.7 977.8 991.3 1043.6 1070.4 1096.4 1110.5 1125.9 1136.2 1137.3 1172.7 1201.8 1222.9 1245.2 1274.1 1300.1 1306.9 1330.2 1342.9 1362.7 1366.8 1367.8 1378.5 1391.2 1403.5 1406.9 1411.2 1422.5 1468.4 1473.4 1478.5 1490.8 1493.5 1497.8 1499.0 1508.8 1516.4 2939.4 2959.4 3018.2 3023.0 3035.5 3044.1 3046.2 3050.4 3051.9 3065.3 3085.4 3095.4 3098.8 3101.2 3114.3 3119.9 3128.2 3131.2 3204.5			
electronic state	2-A			
point group	C1			
rotational constants	2.84080 0.65427 0.60339			
ZPE	0.270206 (Hartree/Particle)			
*i*BP7				
optimized Cartesian coordinate	C	-3.103977000000	0.318673000000	-0.185230000000
	C	-2.112055000000	1.432781000000	-0.231295000000
	C	-0.718456000000	0.937689000000	-0.649257000000
	C	-0.271907000000	-0.272025000000	0.178532000000
	C	1.111496000000	-0.784239000000	-0.234118000000
	C	2.257677000000	0.234356000000	-0.195160000000
	C	2.375536000000	0.908950000000	1.171938000000
	H	2.494173000000	0.155833000000	1.958413000000
	C	-1.306305000000	-1.397223000000	0.059790000000
	C	-2.704052000000	-0.943465000000	0.504197000000
	H	-0.000111000000	1.756596000000	-0.552005000000
	H	-0.235046000000	0.032809000000	1.234323000000
	H	-1.351496000000	-1.721658000000	-0.987195000000
	H	-0.985588000000	-2.260690000000	0.651181000000
	H	-2.022116000000	1.886750000000	0.771215000000
	H	-2.450094000000	2.229783000000	-0.897832000000
	H	-4.148599000000	0.515705000000	-0.392417000000
	H	-2.679769000000	-0.778272000000	1.595256000000
	H	-3.438190000000	-1.733656000000	0.329803000000
	H	-0.736947000000	0.648459000000	-1.707967000000
	H	1.040817000000	-1.193767000000	-1.250470000000
	H	1.378998000000	-1.626678000000	0.418217000000
	H	2.061801000000	1.007964000000	-0.946506000000
	H	3.245928000000	1.568807000000	1.206649000000
	H	1.493438000000	1.507224000000	1.411501000000
	C	3.572939000000	-0.452316000000	-0.565392000000
	H	3.827343000000	-1.214777000000	0.177817000000
	H	3.503308000000	-0.943967000000	-1.539037000000
	H	4.396776000000	0.264449000000	-0.604971000000
frequencies	68.4 80.3 130.7 153.9 215.7 231.0 247.1 267.6 294.5 312.8 360.0 407.9 430.9 449.3 459.8 527.1 640.0 782.0 798.1 838.1 863.4 904.7 918.7 933.3			

	950.5 963.5 977.5 992.9 1042.3 1056.8 1085.2 1103.2 1118.0 1135.7 1153.0 1173.2 1201.8 1231.3 1233.0 1283.3 1291.2 1306.9 1321.4 1342.8 1351.0 1370.0 1370.5 1379.4 1399.6 1400.7 1405.0 1411.3 1421.9 1469.1 1477.0 1479.0 1483.2 1493.2 1497.8 1498.6 1509.2 1515.9 2954.2 2960.6 3015.1 3018.6 3036.2 3041.8 3043.6 3045.5 3050.0 3065.1 3089.1 3096.9 3097.1 3098.5 3113.6 3119.4 3127.9 3129.7 3203.0
electronic state	2-A
point group	C1
rotational constants	2.76774 0.66629 0.60695
ZPE	0.270001 (Hartree/Particle)
TS_{f}'	
optimized Cartesian coordinate	C 0.865919000000 0.314486000000 -0.967439000000 C 0.540892000000 -0.654474000000 0.174850000000 C -0.684629000000 -1.518302000000 -0.129689000000 C -2.011647000000 -0.765735000000 -0.280444000000 C -2.379807000000 -0.009562000000 0.973157000000 H -1.638052000000 1.093456000000 0.996702000000 O -1.076561000000 2.132214000000 0.872236000000 O -1.521441000000 2.613281000000 -0.351717000000 H -2.213704000000 3.241793000000 -0.109152000000 C 1.761031000000 -1.532743000000 0.475267000000 C 2.998595000000 -0.692800000000 0.799327000000 C 3.309797000000 0.290805000000 -0.330781000000 C 2.094851000000 1.165853000000 -0.644614000000 H 1.535803000000 -2.211442000000 1.304618000000 H 0.339079000000 -0.054309000000 1.072944000000 H 1.055701000000 -0.273811000000 -1.876829000000 H 0.016856000000 0.968058000000 -1.176018000000 H 2.816013000000 -0.130526000000 1.723173000000 H 3.857912000000 -1.342457000000 0.987867000000 H 4.170858000000 0.911243000000 -0.067144000000 H 3.587523000000 -0.273614000000 -1.229794000000 H 1.861568000000 1.797732000000 0.220703000000 H 2.315222000000 1.838473000000 -1.477976000000 H 1.967967000000 -2.161550000000 -0.401620000000 H -0.806957000000 -2.263014000000 0.668825000000 H -0.494447000000 -2.083498000000 -1.051047000000 H -1.931876000000 -0.045779000000 -1.104129000000 H -3.380546000000 0.425270000000 0.978267000000 H -2.127637000000 -0.498470000000 1.916396000000 C -3.141665000000 -1.748093000000 -0.632507000000 H -3.279016000000 -2.477921000000 0.170530000000 H -4.089235000000 -1.227133000000 -0.785129000000 H -2.899037000000 -2.293066000000 -1.548100000000
frequencies	-1828.2 43.3 62.3 77.3 93.7 118.1 135.5 180.8 203.2 244.1 250.2 279.4 321.7 334.4 378.2 406.3 419.0 448.2 462.6 481.6 576.8 579.4 595.1 794.9 801.9 841.2 857.3 871.5 909.8 925.7 940.0 954.6 964.1 979.3 1004.2 1056.2 1061.9 1068.2 1076.2 1097.3 1108.0 1130.3 1141.3 1164.2 1183.9 1194.5 1222.4 1248.0 1289.1 1292.2 1305.6 1309.3 1332.1 1345.8 1366.0 1370.8 1378.2 1386.5 1389.1 1396.8 1402.5 1405.9 1418.0 1452.8 1471.9 1481.1 1487.1 1489.8 1490.5 1496.3 1500.1 1503.4 1510.1 3016.0 3019.4 3022.1 3033.8 3035.8 3041.9 3044.6 3048.1 3051.9 3065.8 3080.1 3083.3 3091.5 3093.7 3098.7 3124.8 3127.5 3133.6 3167.0 3818.5
electronic state	2-A
point group	C1
rotational constants	1.11751 0.58792 0.44416
ZPE	0.295610 (Hartree/Particle)

$TS_f\beta$				
optimized Cartesian coordinate	C	-1.851573000000	-1.075935000000	-0.971849000000
	C	-0.716138000000	-0.657199000000	-0.029998000000
	C	0.644275000000	-0.926927000000	-0.674867000000
	C	1.877755000000	-0.739511000000	0.191396000000
	C	3.156372000000	-1.113042000000	-0.527306000000
	H	2.036590000000	0.536998000000	0.325722000000
	O	2.288062000000	1.738402000000	0.311412000000
	O	1.967656000000	2.124175000000	-0.979949000000
	H	1.061849000000	2.451902000000	-0.896763000000
	C	-0.894182000000	0.812142000000	0.370570000000
	C	-2.264097000000	1.066409000000	1.003447000000
	C	-3.392442000000	0.635119000000	0.064903000000
	C	-3.228071000000	-0.827894000000	-0.351484000000
	H	-0.094797000000	1.131466000000	1.045419000000
	H	-0.803824000000	-1.269587000000	0.877956000000
	H	-1.764099000000	-0.503291000000	-1.905166000000
	H	-1.741046000000	-2.131721000000	-1.238639000000
	H	-2.335331000000	0.499211000000	1.939575000000
	H	-2.368229000000	2.122454000000	1.266193000000
	H	-4.364321000000	0.788459000000	0.541347000000
	H	-3.374401000000	1.267547000000	-0.831304000000
	H	-3.343065000000	-1.467603000000	0.532022000000
	H	-4.015463000000	-1.114515000000	-1.053642000000
	H	-0.812545000000	1.420166000000	-0.543544000000
	H	0.749575000000	-0.305288000000	-1.574512000000
	H	0.659971000000	-1.969156000000	-1.032661000000
	H	4.035059000000	-0.837255000000	0.058846000000
	H	3.188975000000	-2.196525000000	-0.700446000000
	H	3.218458000000	-0.612670000000	-1.496468000000
	C	1.787706000000	-1.256940000000	1.610497000000
	H	0.975771000000	-0.789263000000	2.170971000000
	H	1.606282000000	-2.340379000000	1.603661000000
	H	2.721212000000	-1.078896000000	2.147878000000
frequencies	-1735.0	37.2	57.8	78.4
	211.3	221.5	229.1	248.1
	404.7	431.3	450.7	457.5
	803.4	821.5	846.8	865.3
	970.8	992.8	1006.7	1057.0
	1125.6	1132.4	1153.3	1172.6
	1292.2	1293.3	1301.4	1322.0
	1387.9	1392.1	1397.6	1408.6
	1477.3	1486.0	1487.7	1489.1
	1512.8	2990.5	3000.3	3022.0
	3042.2	3046.7	3050.8	3085.4
	3107.3	3109.2	3140.7	3143.1
	99.0	118.4	147.7	171.8
	289.4	306.3	338.6	354.1
	487.6	576.6	581.9	792.6
	911.6	920.6	941.3	950.4
	1066.7	1075.4	1083.3	1104.4
	1206.2	1225.6	1256.3	1273.1
	1340.5	1368.3	1380.3	1384.7
	1412.3	1416.7	1460.5	1461.5
	1491.5	1494.3	1499.4	1509.7
	3024.1	3030.3	3031.9	3037.8
	3096.7	3097.4	3099.9	3101.8
	3805.0			
electronic state	2-A			
point group	C1			
rotational constants	1.30820	0.51445	0.44640	
ZPE	0.295218 (Hartree/Particle)			
$TS_f\alpha$				
optimized Cartesian coordinate	C	1.499095000000	0.116563000000	1.375572000000
	C	0.547919000000	-0.572049000000	0.386781000000
	C	-0.894175000000	-0.274546000000	0.737990000000
	C	-2.006811000000	-0.750345000000	-0.171921000000
	C	-3.367566000000	-0.332020000000	0.387434000000
	H	-0.976258000000	1.033560000000	0.654199000000
	H	-3.402171000000	0.742763000000	0.586916000000
	O	-1.077540000000	2.220731000000	0.420677000000
	O	-1.489266000000	2.285085000000	-0.903177000000
	H	-2.446489000000	2.401481000000	-0.837640000000
	C	0.901368000000	-0.182738000000	-1.055079000000
	C	2.369384000000	-0.477088000000	-1.371663000000
	C	3.303554000000	0.218148000000	-0.380141000000
	C	2.964521000000	-0.182746000000	1.056614000000

	H	0.257021000000	-0.713697000000	-1.762046000000
	H	0.696264000000	-1.661072000000	0.490756000000
	H	1.328263000000	1.198875000000	1.321821000000
	H	1.258028000000	-0.196575000000	2.396535000000
	H	2.538588000000	-1.560322000000	-1.324221000000
	H	2.599004000000	-0.165722000000	-2.394068000000
	H	4.345941000000	-0.021307000000	-0.607000000000
	H	3.193569000000	1.304106000000	-0.484838000000
	H	3.151820000000	-1.256146000000	1.184839000000
	H	3.615926000000	0.339155000000	1.762570000000
	H	0.699888000000	0.887550000000	-1.185870000000
	H	-1.116870000000	-0.434600000000	1.799592000000
	H	-1.873985000000	-0.278368000000	-1.152180000000
	H	-4.173805000000	-0.583613000000	-0.305266000000
	H	-3.564949000000	-0.845105000000	1.333645000000
	C	-1.947430000000	-2.273425000000	-0.363799000000
	H	-1.017070000000	-2.582252000000	-0.844660000000
	H	-2.017373000000	-2.782855000000	0.602123000000
	H	-2.780054000000	-2.610905000000	-0.985930000000
frequencies	-1761.8 60.3 69.3 90.9 97.9 111.2 140.3 158.6 224.7 234.0 239.6 274.8 291.5 335.9 366.6 402.2 408.4 424.0 447.1 453.3 492.1 587.9 604.1 793.3 800.5 848.5 861.6 872.3 909.6 926.5 939.4 946.7 965.3 985.2 1012.2 1058.8 1067.1 1072.2 1083.7 1101.4 1113.4 1128.8 1152.4 1172.5 1194.3 1201.1 1223.1 1261.3 1286.6 1304.2 1309.1 1319.7 1334.0 1348.9 1367.2 1379.5 1387.3 1389.9 1395.1 1404.4 1407.3 1412.4 1418.8 1459.8 1483.4 1488.3 1489.9 1491.6 1494.7 1496.9 1507.3 1509.5 1515.8 2967.6 3035.2 3037.1 3042.6 3047.1 3048.9 3049.2 3051.0 3055.6 3070.8 3088.9 3096.0 3097.1 3098.3 3102.4 3116.2 3123.3 3131.3 3136.2 3810.2		
electronic state	2-A		
point group	C1		
rotational constants	1.20472 0.55437 0.47786		
ZPE	0.295735 (Hartree/Particle)		
$TS_f\alpha'$			
optimized Cartesian coordinate	C	-1.305232000000	-0.095030000000	1.407492000000
	C	-0.274063000000	-0.293523000000	0.308971000000
	C	1.125783000000	-0.508031000000	0.855114000000
	C	2.242610000000	-0.816310000000	-0.147975000000
	C	2.499799000000	0.354700000000	-1.097547000000
	H	-0.274340000000	0.874960000000	-0.252371000000
	O	-0.308817000000	2.037874000000	-0.652949000000
	O	0.499419000000	2.717449000000	0.244914000000
	H	1.362913000000	2.719862000000	-0.190184000000
	H	2.896326000000	1.205392000000	-0.529839000000
	C	-0.731066000000	-1.223554000000	-0.800070000000
	C	-2.129318000000	-0.868201000000	-1.314951000000
	C	-3.142037000000	-0.788148000000	-0.172365000000
	C	-2.696806000000	0.240431000000	0.867397000000
	H	-0.015408000000	-1.216096000000	-1.626538000000
	H	-1.357133000000	-1.028237000000	1.990625000000
	H	-0.957631000000	0.685289000000	2.091944000000
	H	-2.084134000000	0.103296000000	-1.820919000000
	H	-2.444974000000	-1.602668000000	-2.060234000000
	H	-4.130363000000	-0.530874000000	-0.561811000000
	H	-3.231781000000	-1.773366000000	0.302606000000
	H	-2.667752000000	1.232780000000	0.405854000000
	H	-3.411541000000	0.287361000000	1.692855000000
	H	-0.736763000000	-2.250786000000	-0.399720000000
	H	1.065491000000	-1.340340000000	1.574048000000
	H	1.408203000000	0.373048000000	1.448365000000
	H	1.944813000000	-1.686805000000	-0.742735000000
	H	3.250195000000	0.092714000000	-1.847135000000
	H	1.593990000000	0.673576000000	-1.618803000000
	C	3.526624000000	-1.179271000000	0.599328000000

	H	4.337075000000	-1.404991000000	-0.097666000000
	H	3.849923000000	-0.345438000000	1.230373000000
	H	3.380299000000	-2.049629000000	1.243205000000

frequencies	-1716.8	53.0	54.9	73.9	101.4	126.4	154.4	155.4
	205.4	239.0	245.2	282.5	307.2	311.5	330.0	380.1
	411.9	423.1	436.4	454.1	485.4	532.0	621.2	784.8
	792.3	830.1	851.6	864.3	916.6	920.7	938.4	940.4
	963.5	981.0	1001.3	1056.8	1069.7	1080.0	1095.2	1101.4
	1120.6	1149.4	1165.8	1177.0	1192.1	1207.3	1246.6	1253.8
	1291.4	1300.0	1316.3	1328.7	1354.5	1367.9	1369.8	1385.7
	1388.9	1398.6	1401.1	1405.7	1412.2	1421.6	1457.6	1460.0
	1468.5	1477.0	1493.0	1493.5	1495.7	1499.7	1509.1	1512.5
	1522.6	2987.8	2991.8	2998.9	3033.2	3036.2	3038.4	3049.8
	3050.8	3061.0	3062.8	3085.5	3096.9	3100.1	3101.9	3108.1
	3110.3	3121.4	3131.5	3134.8	3805.5			
electronic state	2-A							
point group	C1							
rotational constants	1.19664	0.58438	0.49720					
ZPE	0.295532 (Hartree/Particle)							
$TS_{\beta'}$								

optimized Cartesian coordinate	C	0.935064000000	0.152455000000	1.081992000000
	C	2.157848000000	-0.733618000000	1.123033000000
	C	2.450828000000	-1.353090000000	-0.245838000000
	H	1.278798000000	1.120555000000	0.273374000000
	O	1.700618000000	1.943304000000	-0.518673000000
	O	3.073180000000	1.939462000000	-0.308900000000
	H	3.213330000000	2.694490000000	0.276780000000
	C	0.034624000000	-1.068515000000	-0.916525000000
	C	-0.307325000000	-0.429778000000	0.436089000000
	H	3.280135000000	-2.060062000000	-0.163609000000
	H	0.289797000000	-0.269465000000	-1.624037000000
	H	-0.843081000000	-1.584457000000	-1.315378000000
	H	1.977705000000	-1.534802000000	1.856544000000
	H	3.022505000000	-0.168572000000	1.481222000000
	H	0.733506000000	0.693604000000	2.010483000000
	H	-0.658101000000	-1.231041000000	1.108059000000
	H	2.767743000000	-0.559576000000	-0.930460000000
	C	1.208159000000	-2.044444000000	-0.806944000000
	H	1.426355000000	-2.475269000000	-1.787528000000
	H	0.925883000000	-2.877164000000	-0.150013000000
	C	-1.403289000000	0.637058000000	0.329999000000
	H	-1.007217000000	1.482457000000	-0.246896000000
	H	-1.616556000000	1.021032000000	1.336977000000
	C	-2.724323000000	0.184135000000	-0.302820000000
	H	-2.533485000000	-0.082739000000	-1.348434000000
	C	-3.724674000000	1.340662000000	-0.290334000000
	H	-3.317435000000	2.221945000000	-0.791967000000
	H	-4.655430000000	1.063867000000	-0.791234000000
	H	-3.968818000000	1.622550000000	0.738944000000
	C	-3.311022000000	-1.035613000000	0.408389000000
	H	-2.669850000000	-1.915113000000	0.313518000000
	H	-3.441595000000	-0.827683000000	1.475899000000
	H	-4.289913000000	-1.292193000000	-0.003901000000

frequencies	-1745.6	50.3	54.6	75.1	97.1	100.8	134.3	163.9
	201.6	237.7	253.7	265.3	300.7	317.3	343.6	403.2
	407.8	427.3	455.5	481.7	492.8	577.8	603.6	790.2
	796.8	829.4	849.9	871.1	906.6	922.8	933.9	942.8
	965.1	980.2	999.1	1056.0	1062.6	1070.8	1081.5	1103.5
	1127.2	1141.1	1166.7	1172.2	1197.4	1202.4	1230.2	1246.0
	1284.4	1292.6	1315.0	1331.4	1337.7	1357.1	1365.9	1373.8
	1384.0	1390.0	1398.3	1401.6	1406.5	1409.7	1422.7	1461.0
	1463.9	1480.8	1489.1	1493.3	1493.5	1498.6	1506.4	1509.5
	1516.5	2977.2	2998.8	3021.0	3033.4	3044.7	3045.6	3046.6
	3053.0	3064.3	3069.8	3091.5	3097.2	3099.5	3100.9	3111.3
	3114.4	3120.1	3128.3	3130.0	3820.2			

electronic state	2-A			
point group	C1			
rotational constants	1.27538	0.50605	0.41510	
ZPE	0.295347 (Hartree/Particle)			
$TS_{f}\gamma'$				
optimized Cartesian coordinate	C	-1.908144000000	0.073690000000	1.123770000000
	C	-0.416593000000	-0.172235000000	1.112668000000
	C	0.096903000000	-0.640132000000	-0.255546000000
	H	-2.059610000000	1.076384000000	0.302280000000
	O	-2.069363000000	1.996875000000	-0.494581000000
	O	-0.855364000000	2.635891000000	-0.285124000000
	H	-1.082461000000	3.368912000000	0.301721000000
	C	-2.237988000000	-1.449581000000	-0.845157000000
	C	-2.762092000000	-1.022734000000	0.528355000000
	H	-2.375515000000	-0.624702000000	-1.552300000000
	H	-2.817863000000	-2.297320000000	-1.218556000000
	H	-0.184485000000	-0.947032000000	1.863009000000
	H	0.108906000000	0.733833000000	1.428120000000
	H	-2.288112000000	0.487692000000	2.060076000000
	H	-2.734946000000	-1.887142000000	1.209591000000
	H	-3.806251000000	-0.704633000000	0.469163000000
	H	-0.024250000000	0.194960000000	-0.957213000000
	C	-0.753596000000	-1.807351000000	-0.770172000000
	H	-0.620071000000	-2.667281000000	-0.099128000000
	H	-0.388878000000	-2.116344000000	-1.754554000000
	C	1.573508000000	-1.042720000000	-0.205109000000
	H	1.666492000000	-1.945592000000	0.413724000000
	H	1.889033000000	-1.330417000000	-1.217048000000
	C	2.551432000000	0.015524000000	0.319407000000
	H	2.305053000000	0.228061000000	1.366676000000
	C	2.455514000000	1.318742000000	-0.474328000000
	H	1.468144000000	1.777972000000	-0.394242000000
	H	3.197746000000	2.040951000000	-0.124269000000
	H	2.650803000000	1.128570000000	-1.535404000000
	C	3.978319000000	-0.533122000000	0.280211000000
	H	4.277644000000	-0.740159000000	-0.752096000000
	H	4.689415000000	0.184480000000	0.696483000000
	H	4.063444000000	-1.463801000000	0.847013000000
frequencies	-1741.1	53.1	68.9	88.9
	203.3	233.0	259.9	276.4
	409.2	426.2	450.0	470.9
	799.1	827.3	850.3	866.1
	963.9	981.6	1000.0	1054.0
	1128.4	1136.6	1160.3	1172.4
	1285.0	1301.4	1308.1	1333.1
	1385.9	1389.6	1401.2	1406.0
	1462.5	1472.4	1478.9	1491.6
	1521.5	2979.1	3001.3	3017.3
	3050.1	3059.1	3065.5	3088.7
	3112.0	3118.9	3127.1	3142.0
	94.8	105.1	140.6	176.7
	304.2	316.2	324.4	401.8
	498.6	571.9	615.1	788.8
	903.8	920.7	935.7	945.0
	1065.1	1075.4	1082.9	1111.6
	1202.6	1205.0	1232.4	1250.0
	1339.5	1361.7	1369.6	1376.1
	1408.5	1414.2	1424.2	1459.5
	1495.8	1498.5	1500.7	1510.0
	3022.3	3037.4	3045.6	3048.1
	3092.0	3094.3	3107.4	3110.6
	3818.2			
electronic state	2-A			
point group	C1			
rotational constants	1.16184	0.57553	0.44435	
ZPE	0.295433 (Hartree/Particle)			
$TS_{f}\delta'$				
optimized Cartesian coordinate	C	-2.377723000000	-0.947422000000	0.455992000000
	C	-1.448991000000	-0.325462000000	1.471652000000
	C	-0.213581000000	0.298845000000	0.815763000000
	C	0.499888000000	-0.682783000000	-0.119953000000
	C	1.716688000000	-0.053409000000	-0.804617000000
	C	2.781542000000	0.552158000000	0.118155000000
	C	3.277168000000	-0.454621000000	1.156861000000

	H	-2.778056000000	0.074930000000	-0.256234000000
	O	-3.045350000000	1.102440000000	-0.846024000000
	O	-2.948763000000	2.087648000000	0.126964000000
	H	-3.863320000000	2.215548000000	0.409845000000
	H	3.656652000000	-1.355407000000	0.662432000000
	C	-0.482630000000	-1.203908000000	-1.175505000000
	C	-1.710568000000	-1.864574000000	-0.544097000000
	H	0.466996000000	0.647469000000	1.597196000000
	H	0.835652000000	-1.543799000000	0.475832000000
	H	-0.810529000000	-0.360676000000	-1.795188000000
	H	0.023506000000	-1.913084000000	-1.837464000000
	H	-1.129842000000	-1.114971000000	2.170106000000
	H	-1.979421000000	0.422714000000	2.066406000000
	H	-3.315877000000	-1.325497000000	0.867199000000
	H	-1.399706000000	-2.778891000000	-0.015622000000
	H	-2.422294000000	-2.176627000000	-1.312934000000
	H	-0.520563000000	1.180590000000	0.240131000000
	H	1.361669000000	0.727180000000	-1.489858000000
	H	2.198413000000	-0.817206000000	-1.430323000000
	H	2.339493000000	1.404774000000	0.646109000000
	H	4.090655000000	-0.031828000000	1.751612000000
	H	2.484535000000	-0.758718000000	1.844497000000
	C	3.951447000000	1.075979000000	-0.715713000000
	H	4.445162000000	0.251549000000	-1.240166000000
	H	3.612672000000	1.795075000000	-1.465716000000
	H	4.697671000000	1.567350000000	-0.086611000000
frequencies	-1753.3 44.3 58.7 67.3 97.6 119.5 134.6 178.0 224.2 236.5 259.2 275.4 296.3 310.5 318.3 401.4 419.7 429.8 450.7 463.9 507.9 565.9 618.3 784.5 797.1 830.9 853.7 859.5 919.5 923.1 934.2 943.0 961.6 978.1 997.5 1054.3 1061.1 1072.8 1093.5 1102.0 1129.8 1140.3 1162.8 1172.1 1200.1 1202.8 1227.5 1247.8 1291.3 1298.8 1312.1 1328.8 1348.0 1358.5 1367.6 1374.9 1384.5 1387.7 1403.2 1405.0 1407.4 1414.3 1421.8 1459.2 1464.4 1476.7 1479.1 1487.4 1494.1 1498.5 1503.1 1509.5 1516.8 2995.5 3002.1 3015.0 3019.8 3044.2 3046.0 3047.2 3051.4 3055.7 3068.1 3092.8 3095.5 3095.9 3105.8 3111.9 3113.7 3119.8 3127.7 3129.4 3820.3			
electronic state	2-A			
point group	C1			
rotational constants	1.39548 0.43790 0.40569			
ZPE	0.295428 (Hartree/Particle)			

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