

Supporting Information for:

Generation of Singlet Oxygen Catalyzed by Room Temperature Stable Anthraquinone  
Anion Radical

Xiaowei Duan, Zhongjun Zhou\*, Xuri Huang, Zexing Qu\*

Institute of Theoretical Chemistry, College of Chemistry, Jilin University, Changchun,  
130023, China

\*Corresponding author e-mail:

zxqu@jlu.edu.cn

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Table S1: The energies for KOtBu, singlet state ( $E_s$ ) and triplet state ( $E_t$ ) AQ-(KOtBu)<sub>n</sub> (n=0, 1, 2 and 3). The complexing energy ( $E_B$ ) of AQ-(KOtBu)<sub>n</sub>. The CAM-B3LYP functional at 6-311+G(d) level was used in all the DFT calculations. The geometries were optimized by polarizable continuum model (PCM) in dimethyl sulfoxide solvent.

	$E_s$ (a.u.)	$E_t$ (a.u.)	$E_B$ (kcal/mol)
KOtBu	-832.9768114	--	--
AQ	-688.5740382	-688.4673215	-9.4
AQ-(KOtBu) <sub>1</sub>	-1521.565793	-1521.516644	2.9 <sup>a</sup> /-7.3 <sup>b</sup> /-7.5 <sup>c</sup>
AQ-(KOtBu) <sub>2</sub> <sup>a</sup>	-2354.537908	-2354.534487	-13.6
AQ-(KOtBu) <sub>2</sub> <sup>b</sup>	-2354.554236	-2354.530251	-3.3
AQ-(KOtBu) <sub>2</sub> <sup>c</sup>	-2354.554479	-2354.531034	-3.2
AQ-(KOtBu) <sub>3</sub>	-3187.525278	-3187.536339	-4.7

(AQ–KOTBu)/AQ-(KOTBu) <sub>4</sub>	-4020.498195	-4020.520596	
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The site of ligand KOTBu:

AQ-(KOTBu)<sub>1</sub>: I or II or III or IV;

AQ-(KOTBu)<sub>2</sub><sup>a</sup>: I, II or III, IV;

AQ-(KOTBu)<sub>2</sub><sup>b</sup>: I, IV or II, III;

AQ-(KOTBu)<sub>2</sub><sup>c</sup>: I, III or II, IV;

AQ-(KOTBu)<sub>3</sub>: I, II, III or I, II, IV or II, III, IV;

(AQ–KOTBu)/AQ-(KOTBu)<sub>4</sub>: I, II, III, IV.

(The site of ligand KOTBu is marked in Figure 1).

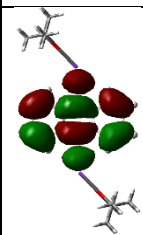
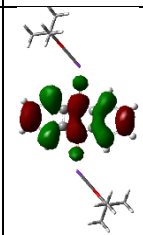
AQ-(KOTBu)<sub>m-1</sub> + KOTBu → AQ-(KOTBu)<sub>m</sub> (m=1, 2, 3 and 4)

$E_B = E[\text{AQ}-(\text{KOTBu})_m] - E[\text{AQ}-(\text{KOTBu})_{m-1}] - E[\text{KOTBu}]$

Table S2: The ESP charge for K, AQ and OtBu in AQ–KOTBu. The CAM-B3LYP functional at 6-311+G(d) level was used in all the DFT calculations.

	ESP charge (eV)
K	0.85
AQ	-0.83
OtBu	-0.64

Table S3: The UV-Vis absorption wavelength and the natural transition orbitals for ONIOM-1, ONIOM-2, ONIOM-3 and CAM-B3LYP.

		wavelength	Hole	Electron
ONIOM-1	D <sub>1</sub>	654.19 nm		

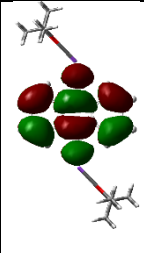
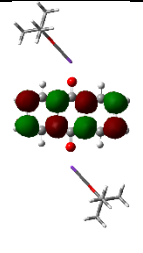
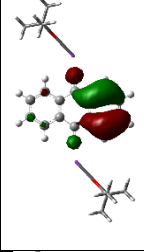
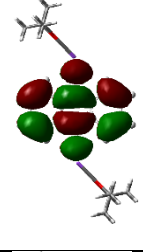
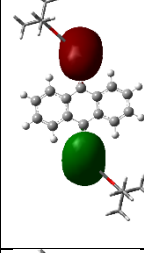
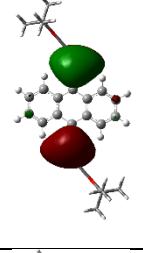
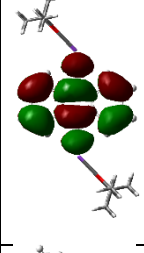
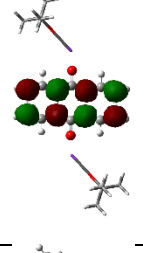
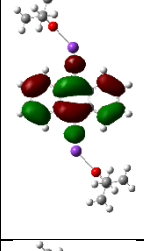
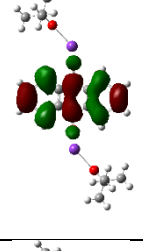
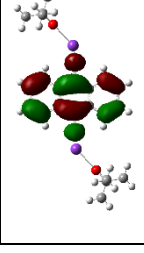
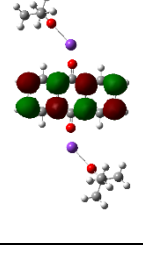
	D <sub>2</sub>	384.66 nm		
ONIOM-2	T	373.95 nm		
ONIOM-3	T <sub>1</sub>	842.76 nm		
	T <sub>2</sub>	409.16 nm		
CAM-B3	T <sub>1</sub>	652.70nm		
LYP	T <sub>2</sub>	396.97nm		

Table S4: The active orbitals of NEVPT2 (4e, 6o) of the simplified model, ( $C^M$ ).

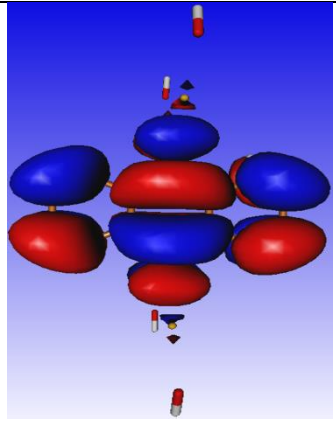
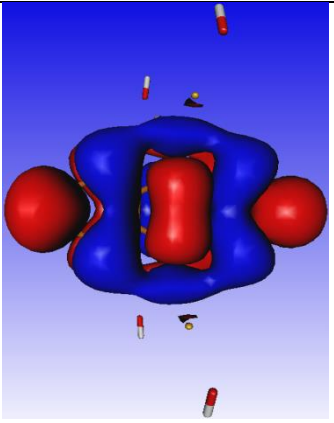
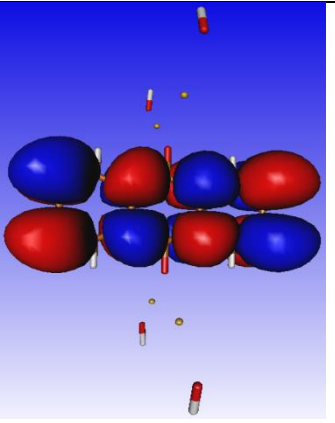
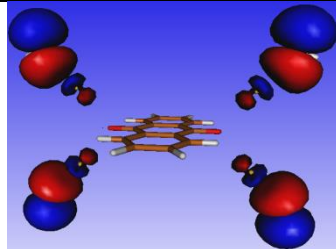
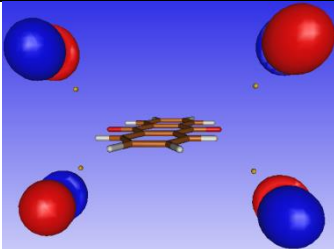
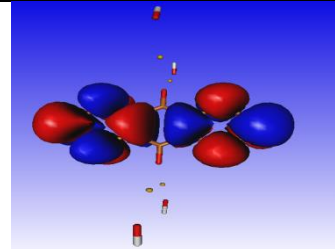
$\pi_{AQ}(b_{2g})$	$\pi_{AQ}^*(b_{3u})$	$\pi_{AN}^*(a_u)$
		
$\sigma_{OH}(a_g)$	$\pi_{OH}(a_u)$	$\pi_{AN}'(b_{1g})$
		

Table S5: The singly occupied molecular orbitals (SOMOs) and energies (E) for these transitions by means of NEVPT2 (4e/6o) at 6-311+G(d) level.

State	SOMOs	E (a.u.)
T <sub>0</sub> (B <sub>2u</sub> )	$\pi_{OH}(a_u), \pi_{AQ}(b_{2g})$	-3386.009810343247
T <sub>1</sub> (B <sub>2g</sub> )	$\sigma_{OH}(a_g), \pi_{AQ}(b_{2g})$	-3386.007405617286
T <sub>2</sub> (B <sub>3g</sub> )	$\pi_{OH}(a_u), \pi_{AQ}^*(b_{3u})$	-3385.940086643221
T <sub>3</sub> (B <sub>3u</sub> )	$\sigma_{OH}(a_g), \pi_{AQ}^*(b_{3u})$	-3385.937604322479
T <sub>4</sub> (A <sub>g</sub> )	$\pi_{OH}(a_u), \pi_{AN}^*(a_u)$	-3385.890365353002
T <sub>5</sub> (A <sub>u</sub> )	$\sigma_{OH}(a_g), \pi_{AN}^*(a_u)$	-3385.887743770551

Table S6: The ground state energy (E) for the OtBu radical. The DFT calculation for

energy is performed at 6-311+G(d) level and CAM-B3LYP functional.

	E (a.u.)
D <sub>0</sub>	-232.9402852

Table S7: The energies (E) for <sup>3</sup>O<sub>2</sub>, <sup>1</sup>O<sub>2</sub>, N<sub>2</sub>, C<sub>(1)</sub>, C<sub>(1)</sub>@N<sub>2</sub>, <sup>1</sup>[C<sub>(1)</sub>@<sup>1</sup>O<sub>2</sub>], and <sup>5</sup>[C<sub>(1)</sub>@<sup>1</sup>O<sub>2</sub>]. The geometry optimization and energy calculations were performed at 6-311+G(d) level and CAM-B3LYP functional in gas phase.

	E (a.u.)
<sup>3</sup> O <sub>2</sub>	-150.3252087
<sup>1</sup> O <sub>2</sub>	-150.3081769
N <sub>2</sub>	-109.5155007
C <sub>(1)</sub>	-4020.5386257
C <sub>(1)</sub> @N <sub>2</sub>	-4130.2018947
<sup>1</sup> [C <sub>(1)</sub> @ <sup>1</sup> O <sub>2</sub> ]	-4170.981526
<sup>5</sup> [C <sub>(1)</sub> @ <sup>1</sup> O <sub>2</sub> ]	-4170.913105

Table S8: The distance ,R(O<sub>2</sub>-AQ), between O<sub>2</sub> and [AQ·]<sup>-</sup>. The energies of the reactant (R) and the product (P<sub>1</sub><sup>OS</sup> and P<sub>1</sub><sup>CS</sup>). The diabatic couplings (V<sub>12</sub><sup>OS</sup> and V<sub>12</sub><sup>CS</sup>) between the reactant state and the product states. The superscripts OS and CS are the open-shell oxygen and the closed shell oxygen, respectively.

R(O <sub>2</sub> -AQ)	R (a.u.)	P <sub>1</sub> <sup>OS</sup> (a.u.)	P <sub>2</sub> <sup>CS</sup> (a.u.)	V <sub>12</sub> <sup>OS</sup> (eV)	V <sub>12</sub> <sup>CS</sup> (eV)
1.8 Å	-838.498643	-838.451994	-838.456947	1.11E-02	3.57E-09
1.9 Å	-838.545367	-838.499603	-838.503404	9.24E-03	5.73E-09
2.0 Å	-838.580329	-838.535440	-838.538443	7.58E-03	5.03E-09
2.1 Å	-838.606256	-838.562158	-838.564631	6.13E-03	4.59E-09
2.2 Å	-838.625338	-838.581921	-838.584053	4.89E-03	3.32E-09
2.3 Å	-838.639282	-838.596437	-838.598353	3.85E-03	2.62E-09
2.4 Å	-838.649388	-838.607012	-838.608791	2.98E-03	1.98E-09
2.5 Å	-838.656683	-838.614689	-838.616379	2.28E-03	1.42E-09
2.6 Å	-838.661900	-838.620206	-838.621838	1.72E-03	1.02E-09
2.7 Å	-838.665633	-838.624178	-838.625770	1.28E-03	7.37E-10

2.8 Å	-838.668296	-838.627024	-838.628587	9.44E-04	4.94E-10
2.9 Å	-838.670193	-838.629061	-838.630603	6.86E-04	3.62E-10
3.0 Å	-838.671549	-838.630524	-838.632049	4.92E-04	2.45E-10
3.1 Å	-838.672490	-838.631544	-838.633055	3.50E-04	1.67E-10
3.2 Å	-838.673149	-838.632262	-838.633763	2.46E-04	1.12E-10
3.3 Å	-838.673622	-838.632778	-838.634271	1.71E-04	7.46E-11
3.4 Å	-838.673945	-838.633132	-838.634617	1.18E-04	4.98E-11
3.6 Å	-838.674336	-838.633563	-838.635039	5.45E-05	2.10E-11
3.8 Å	-838.674560	-838.633808	-838.635276	2.42E-05	8.78E-12
4.0 Å	-838.674688	-838.633950	-838.635414	1.03E-05	3.49E-12
4.5 Å	-838.674852	-838.634123	-838.635581	9.58E-07	2.77E-13

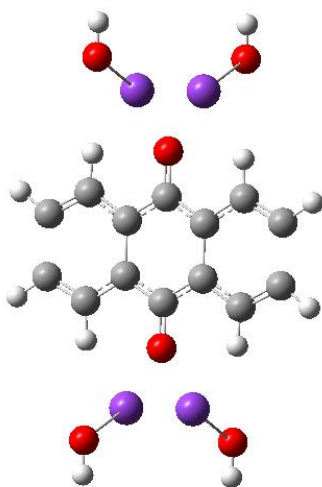


Figure S1. The simplified model ( $C^M$ ) for AQ-KOtBu

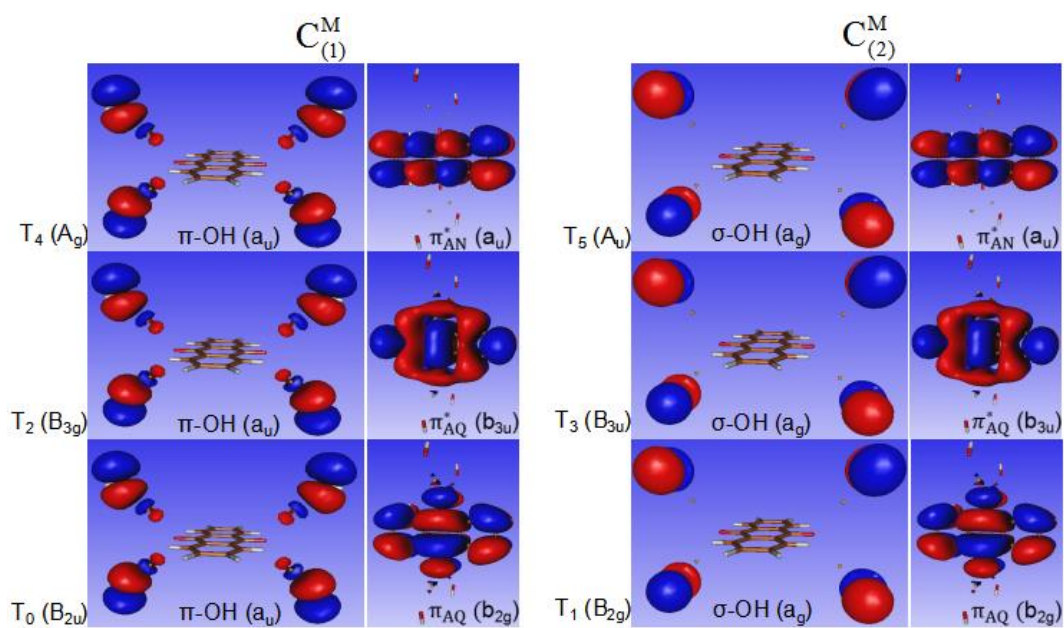


Figure S2. The single occupied molecular orbitals (SOMOs) for  $C_{(1)}^M$  and  $C_{(2)}^M$ .

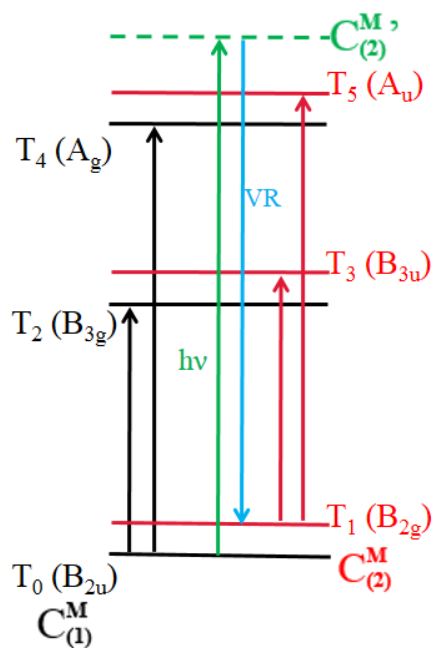


Figure S3. The excitation diagram for  $C_{(1)}^M$  (black solid) and  $C_{(2)}^M$  (red solid). The green solid represents the excited process of  $C_{(1)}^M$  with light, the blue solid is the vibrational relaxation (VR) process of  $C_{(2)}^M$ .

Cartesian Coordinates

AQ-KOtBu-triplet (PCM: DMSO) (ONIOM-1, ONIOM-2, and ONIOM-3)

K	1.32651900	4.19522400	2.04234600
C	0.48887600	1.37684000	0.00000000
C	-0.93026300	1.08163300	0.00000000
C	-1.86506600	2.13750200	0.00000000
H	-1.49230100	3.15441100	0.00000000
C	-3.21506600	1.88763500	0.00000000
H	-3.92055300	2.71110800	0.00000000
O	0.91304200	2.57037600	0.00000000
C	-3.68567700	0.56108800	0.00000000
H	-4.75246600	0.36656600	0.00000000
C	-2.79478700	-0.48343000	0.00000000
H	-3.14454400	-1.50835400	0.00000000
C	-1.40372900	-0.25272200	0.00000000
K	1.32651900	4.19522400	-2.04234600
K	-1.32651900	-4.19522400	2.04234600
C	-0.48887600	-1.37684000	0.00000000
C	0.93026300	-1.08163300	0.00000000
C	1.86506600	-2.13750200	0.00000000
H	1.49230100	-3.15441100	0.00000000
C	3.21506600	-1.88763500	0.00000000
H	3.92055300	-2.71110800	0.00000000
O	-0.91304200	-2.57037600	0.00000000
C	3.68567700	-0.56108800	0.00000000
H	4.75246600	-0.36656600	0.00000000
C	2.79478700	0.48343000	0.00000000
H	3.14454400	1.50835400	0.00000000
C	1.40372900	0.25272200	0.00000000
K	-1.32651900	-4.19522400	-2.04234600
O	0.31316400	6.44517000	2.24561000
O	0.31316400	6.44517000	-2.24561000
O	-0.31316400	-6.44517000	-2.24561000
O	-0.31316400	-6.44517000	2.24561000
C	-0.20997500	7.61370900	2.75480400
C	0.65614500	8.82124800	2.35699200
C	-1.64585700	7.83538000	2.24818900
C	-0.24539600	7.52190000	4.29678700
H	1.67832900	8.68868800	2.72167700
H	0.69583300	8.90955200	1.26794400
H	0.26856800	9.76184700	2.76086200
H	-2.28205200	6.99487400	2.53782700
H	-2.08912100	8.75319900	2.64717800



H	-1.65003400	7.90131400	1.15732500
H	-0.65486000	8.43156300	4.74715000
H	-0.86299300	6.67590700	4.60854800
H	0.76386200	7.36982500	4.68734300
C	-0.20997500	7.61370900	-2.75480400
C	-1.64585700	7.83538000	-2.24818900
C	0.65614500	8.82124800	-2.35699200
C	-0.24539600	7.52190000	-4.29678700
H	-2.28205200	6.99487400	-2.53782700
H	-1.65003400	7.90131400	-1.15732500
H	-2.08912100	8.75319900	-2.64717800
H	1.67832900	8.68868800	-2.72167700
H	0.26856800	9.76184700	-2.76086200
H	0.69583300	8.90955200	-1.26794400
H	-0.65486000	8.43156300	-4.74715000
H	0.76386200	7.36982500	-4.68734300
H	-0.86299300	6.67590700	-4.60854800
C	0.20997500	-7.61370900	-2.75480400
C	1.64585700	-7.83538000	-2.24818900
C	-0.65614500	-8.82124800	-2.35699200
C	0.24539600	-7.52190000	-4.29678700
H	2.28205200	-6.99487400	-2.53782700
H	1.65003400	-7.90131400	-1.15732500
H	2.08912100	-8.75319900	-2.64717800
H	-1.67832900	-8.68868800	-2.72167700
H	-0.26856800	-9.76184700	-2.76086200
H	-0.69583300	-8.90955200	-1.26794400
H	0.65486000	-8.43156300	-4.74715000
H	-0.76386200	-7.36982500	-4.68734300
H	0.86299300	-6.67590700	-4.60854800
C	0.20997500	-7.61370900	2.75480400
C	-0.65614500	-8.82124800	2.35699200
C	1.64585700	-7.83538000	2.24818900
C	0.24539600	-7.52190000	4.29678700
H	-1.67832900	-8.68868800	2.72167700
H	-0.69583300	-8.90955200	1.26794400
H	-0.26856800	-9.76184700	2.76086200
H	2.28205200	-6.99487400	2.53782700
H	2.08912100	-8.75319900	2.64717800
H	1.65003400	-7.90131400	1.15732500
H	0.65486000	-8.43156300	4.74715000
H	0.86299300	-6.67590700	4.60854800
H	-0.76386200	-7.36982500	4.68734300

## AQ-KOtBu-singlet (PCM: DMSO)

K	1.16192800	4.36924400	2.10909100
C	0.41949300	1.40090200	0.00000000
C	-1.01700800	1.03650300	0.00000000
C	-1.97565300	2.04352600	0.00000000
H	-1.65588400	3.07777200	0.00000000
C	-3.32460700	1.72089800	0.00000000
H	-4.06740400	2.50952600	0.00000000
O	0.77126200	2.57252200	0.00000000
C	-3.72290800	0.38927000	0.00000000
H	-4.77685900	0.13839200	0.00000000
C	-2.77278600	-0.62110800	0.00000000
H	-3.07256200	-1.66121300	0.00000000
C	-1.41865000	-0.30627800	0.00000000
K	1.16192800	4.36924400	-2.10909100
K	-1.16192800	-4.36924400	2.10909100
C	-0.41949300	-1.40090200	0.00000000
C	1.01700800	-1.03650300	0.00000000
C	1.97565300	-2.04352600	0.00000000
H	1.65588400	-3.07777200	0.00000000
C	3.32460700	-1.72089800	0.00000000
H	4.06740400	-2.50952600	0.00000000
O	-0.77126200	-2.57252200	0.00000000
C	3.72290800	-0.38927000	0.00000000
H	4.77685900	-0.13839200	0.00000000
C	2.77278600	0.62110800	0.00000000
H	3.07256200	1.66121300	0.00000000
C	1.41865000	0.30627800	0.00000000
K	-1.16192800	-4.36924400	-2.10909100
O	0.30420600	6.53027100	2.74656700
O	0.30420600	6.53027100	-2.74656700
O	-0.30420600	-6.53027100	-2.74656700
O	-0.30420600	-6.53027100	2.74656700
C	-0.18381800	7.76931400	3.11094200
C	0.67789700	8.89482100	2.50584600
C	-1.63215600	7.95518600	2.61643200
C	-0.17671700	7.92995200	4.64364400
H	1.71192800	8.79896600	2.85060600
H	0.68119600	8.81861200	1.41424700
H	0.32158900	9.89537500	2.77515700
H	-2.27525600	7.17759400	3.03964800
H	-2.05273100	8.92916400	2.89023400
H	-1.67039600	7.86426000	1.52678700
H	-0.56694700	8.89985200	4.97163600

H	-0.78580800	7.14616500	5.10404300
H	0.84354600	7.82903600	5.02573900
C	-0.18381800	7.76931400	-3.11094200
C	-1.63215600	7.95518600	-2.61643200
C	0.67789700	8.89482100	-2.50584600
C	-0.17671700	7.92995200	-4.64364400
H	-2.27525600	7.17759400	-3.03964800
H	-1.67039600	7.86426000	-1.52678700
H	-2.05273100	8.92916400	-2.89023400
H	1.71192800	8.79896600	-2.85060600
H	0.32158900	9.89537500	-2.77515700
H	0.68119600	8.81861200	-1.41424700
H	-0.56694700	8.89985200	-4.97163600
H	0.84354600	7.82903600	-5.02573900
H	-0.78580800	7.14616500	-5.10404300
C	0.18381800	-7.76931400	-3.11094200
C	1.63215600	-7.95518600	-2.61643200
C	-0.67789700	-8.89482100	-2.50584600
C	0.17671700	-7.92995200	-4.64364400
H	2.27525600	-7.17759400	-3.03964800
H	1.67039600	-7.86426000	-1.52678700
H	2.05273100	-8.92916400	-2.89023400
H	-1.71192800	-8.79896600	-2.85060600
H	-0.32158900	-9.89537500	-2.77515700
H	-0.68119600	-8.81861200	-1.41424700
H	0.56694700	-8.89985200	-4.97163600
H	-0.84354600	-7.82903600	-5.02573900
H	0.78580800	-7.14616500	-5.10404300
C	0.18381800	-7.76931400	3.11094200
C	-0.67789700	-8.89482100	2.50584600
C	1.63215600	-7.95518600	2.61643200
C	0.17671700	-7.92995200	4.64364400
H	-1.71192800	-8.79896600	2.85060600
H	-0.68119600	-8.81861200	1.41424700
H	-0.32158900	-9.89537500	2.77515700
H	2.27525600	-7.17759400	3.03964800
H	2.05273100	-8.92916400	2.89023400
H	1.67039600	-7.86426000	1.52678700
H	0.56694700	-8.89985200	4.97163600
H	0.78580800	-7.14616500	5.10404300
H	-0.84354600	-7.82903600	5.02573900

AQ-(KOTBu)<sub>n</sub>, n=0 (AQ, singlet or triplet)

C	0.48887600	1.37684000	0.00000000
C	-0.93026300	1.08163300	0.00000000
C	-1.86506600	2.13750200	0.00000000
H	-1.49230100	3.15441100	0.00000000
C	-3.21506600	1.88763500	0.00000000
H	-3.92055300	2.71110800	0.00000000
O	0.91304200	2.57037600	0.00000000
C	-3.68567700	0.56108800	0.00000000
H	-4.75246600	0.36656600	0.00000000
C	-2.79478700	-0.48343000	0.00000000
H	-3.14454400	-1.50835400	0.00000000
C	-1.40372900	-0.25272200	0.00000000
C	-0.48887600	-1.37684000	0.00000000
C	0.93026300	-1.08163300	0.00000000
C	1.86506600	-2.13750200	0.00000000
H	1.49230100	-3.15441100	0.00000000
C	3.21506600	-1.88763500	0.00000000
H	3.92055300	-2.71110800	0.00000000
O	-0.91304200	-2.57037600	0.00000000
C	3.68567700	-0.56108800	0.00000000
H	4.75246600	-0.36656600	0.00000000
C	2.79478700	0.48343000	0.00000000
H	3.14454400	1.50835400	0.00000000
C	1.40372900	0.25272200	0.00000000
K	-1.32651900	-4.19522400	-2.04234600
O	-0.31316400	-6.44517000	-2.24561000
C	0.20997500	-7.61370900	-2.75480400
C	1.64585700	-7.83538000	-2.24818900
C	-0.65614500	-8.82124800	-2.35699200
C	0.24539600	-7.52190000	-4.29678700
H	2.28205200	-6.99487400	-2.53782700
H	1.65003400	-7.90131400	-1.15732500
H	2.08912100	-8.75319900	-2.64717800
H	-1.67832900	-8.68868800	-2.72167700
H	-0.26856800	-9.76184700	-2.76086200
H	-0.69583300	-8.90955200	-1.26794400
H	0.65486000	-8.43156300	-4.74715000
H	-0.76386200	-7.36982500	-4.68734300
H	0.86299300	-6.67590700	-4.60854800

n=1 (AQ-(KOTBu)<sub>1</sub>, singlet or triplet)

C	0.48887600	1.37684000	0.00000000
C	-0.93026300	1.08163300	0.00000000

C	-1.86506600	2.13750200	0.00000000
H	-1.49230100	3.15441100	0.00000000
C	-3.21506600	1.88763500	0.00000000
H	-3.92055300	2.71110800	0.00000000
O	0.91304200	2.57037600	0.00000000
C	-3.68567700	0.56108800	0.00000000
H	-4.75246600	0.36656600	0.00000000
C	-2.79478700	-0.48343000	0.00000000
H	-3.14454400	-1.50835400	0.00000000
C	-1.40372900	-0.25272200	0.00000000
C	-0.48887600	-1.37684000	0.00000000
C	0.93026300	-1.08163300	0.00000000
C	1.86506600	-2.13750200	0.00000000
H	1.49230100	-3.15441100	0.00000000
C	3.21506600	-1.88763500	0.00000000
H	3.92055300	-2.71110800	0.00000000
O	-0.91304200	-2.57037600	0.00000000
C	3.68567700	-0.56108800	0.00000000
H	4.75246600	-0.36656600	0.00000000
C	2.79478700	0.48343000	0.00000000
H	3.14454400	1.50835400	0.00000000
C	1.40372900	0.25272200	0.00000000
K	-1.32651900	-4.19522400	-2.04234600
O	-0.31316400	-6.44517000	-2.24561000
C	0.20997500	-7.61370900	-2.75480400
C	1.64585700	-7.83538000	-2.24818900
C	-0.65614500	-8.82124800	-2.35699200
C	0.24539600	-7.52190000	-4.29678700
H	2.28205200	-6.99487400	-2.53782700
H	1.65003400	-7.90131400	-1.15732500
H	2.08912100	-8.75319900	-2.64717800
H	-1.67832900	-8.68868800	-2.72167700
H	-0.26856800	-9.76184700	-2.76086200
H	-0.69583300	-8.90955200	-1.26794400
H	0.65486000	-8.43156300	-4.74715000
H	-0.76386200	-7.36982500	-4.68734300
H	0.86299300	-6.67590700	-4.60854800

n=2 (AQ-(KOTu)<sub>2</sub><sup>a</sup>, singlet or triplet)

C	0.48887600	1.37684000	0.00000000
C	-0.93026300	1.08163300	0.00000000
C	-1.86506600	2.13750200	0.00000000
H	-1.49230100	3.15441100	0.00000000

C	-3.21506600	1.88763500	0.00000000
H	-3.92055300	2.71110800	0.00000000
O	0.91304200	2.57037600	0.00000000
C	-3.68567700	0.56108800	0.00000000
H	-4.75246600	0.36656600	0.00000000
C	-2.79478700	-0.48343000	0.00000000
H	-3.14454400	-1.50835400	0.00000000
C	-1.40372900	-0.25272200	0.00000000
K	-1.32651900	-4.19522400	2.04234600
C	-0.48887600	-1.37684000	0.00000000
C	0.93026300	-1.08163300	0.00000000
C	1.86506600	-2.13750200	0.00000000
H	1.49230100	-3.15441100	0.00000000
C	3.21506600	-1.88763500	0.00000000
H	3.92055300	-2.71110800	0.00000000
O	-0.91304200	-2.57037600	0.00000000
C	3.68567700	-0.56108800	0.00000000
H	4.75246600	-0.36656600	0.00000000
C	2.79478700	0.48343000	0.00000000
H	3.14454400	1.50835400	0.00000000
C	1.40372900	0.25272200	0.00000000
K	-1.32651900	-4.19522400	-2.04234600
O	-0.31316400	-6.44517000	-2.24561000
O	-0.31316400	-6.44517000	2.24561000
C	0.20997500	-7.61370900	-2.75480400
C	1.64585700	-7.83538000	-2.24818900
C	-0.65614500	-8.82124800	-2.35699200
C	0.24539600	-7.52190000	-4.29678700
H	2.28205200	-6.99487400	-2.53782700
H	1.65003400	-7.90131400	-1.15732500
H	2.08912100	-8.75319900	-2.64717800
H	-1.67832900	-8.68868800	-2.72167700
H	-0.26856800	-9.76184700	-2.76086200
H	-0.69583300	-8.90955200	-1.26794400
H	0.65486000	-8.43156300	-4.74715000
H	-0.76386200	-7.36982500	-4.68734300
H	0.86299300	-6.67590700	-4.60854800
C	0.20997500	-7.61370900	2.75480400
C	-0.65614500	-8.82124800	2.35699200
C	1.64585700	-7.83538000	2.24818900
C	0.24539600	-7.52190000	4.29678700
H	-1.67832900	-8.68868800	2.72167700
H	-0.69583300	-8.90955200	1.26794400
H	-0.26856800	-9.76184700	2.76086200

H	2.28205200	-6.99487400	2.53782700
H	2.08912100	-8.75319900	2.64717800
H	1.65003400	-7.90131400	1.15732500
H	0.65486000	-8.43156300	4.74715000
H	0.86299300	-6.67590700	4.60854800
H	-0.76386200	-7.36982500	4.68734300

n=2 (AQ-(KOTu)<sub>2</sub><sup>b</sup>, singlet or triplet)

C	0.48887600	1.37684000	0.00000000
C	-0.93026300	1.08163300	0.00000000
C	-1.86506600	2.13750200	0.00000000
H	-1.49230100	3.15441100	0.00000000
C	-3.21506600	1.88763500	0.00000000
H	-3.92055300	2.71110800	0.00000000
O	0.91304200	2.57037600	0.00000000
C	-3.68567700	0.56108800	0.00000000
H	-4.75246600	0.36656600	0.00000000
C	-2.79478700	-0.48343000	0.00000000
H	-3.14454400	-1.50835400	0.00000000
C	-1.40372900	-0.25272200	0.00000000
K	1.32651900	4.19522400	-2.04234600
C	-0.48887600	-1.37684000	0.00000000
C	0.93026300	-1.08163300	0.00000000
C	1.86506600	-2.13750200	0.00000000
H	1.49230100	-3.15441100	0.00000000
C	3.21506600	-1.88763500	0.00000000
H	3.92055300	-2.71110800	0.00000000
O	-0.91304200	-2.57037600	0.00000000
C	3.68567700	-0.56108800	0.00000000
H	4.75246600	-0.36656600	0.00000000
C	2.79478700	0.48343000	0.00000000
H	3.14454400	1.50835400	0.00000000
C	1.40372900	0.25272200	0.00000000
K	-1.32651900	-4.19522400	-2.04234600
O	0.31316400	6.44517000	-2.24561000
O	-0.31316400	-6.44517000	-2.24561000
C	-0.20997500	7.61370900	-2.75480400
C	-1.64585700	7.83538000	-2.24818900
C	0.65614500	8.82124800	-2.35699200
C	-0.24539600	7.52190000	-4.29678700
H	-2.28205200	6.99487400	-2.53782700
H	-1.65003400	7.90131400	-1.15732500
H	-2.08912100	8.75319900	-2.64717800

H	1.67832900	8.68868800	-2.72167700
H	0.26856800	9.76184700	-2.76086200
H	0.69583300	8.90955200	-1.26794400
H	-0.65486000	8.43156300	-4.74715000
H	0.76386200	7.36982500	-4.68734300
H	-0.86299300	6.67590700	-4.60854800
C	0.20997500	-7.61370900	-2.75480400
C	1.64585700	-7.83538000	-2.24818900
C	-0.65614500	-8.82124800	-2.35699200
C	0.24539600	-7.52190000	-4.29678700
H	2.28205200	-6.99487400	-2.53782700
H	1.65003400	-7.90131400	-1.15732500
H	2.08912100	-8.75319900	-2.64717800
H	-1.67832900	-8.68868800	-2.72167700
H	-0.26856800	-9.76184700	-2.76086200
H	-0.69583300	-8.90955200	-1.26794400
H	0.65486000	-8.43156300	-4.74715000
H	-0.76386200	-7.36982500	-4.68734300
H	0.86299300	-6.67590700	-4.60854800

n=2 (AQ-(KOtBu)<sub>2</sub>)<sup>c</sup>, singlet or triplet)

K	1.32651900	4.19522400	2.04234600
C	0.48887600	1.37684000	0.00000000
C	-0.93026300	1.08163300	0.00000000
C	-1.86506600	2.13750200	0.00000000
H	-1.49230100	3.15441100	0.00000000
C	-3.21506600	1.88763500	0.00000000
H	-3.92055300	2.71110800	0.00000000
O	0.91304200	2.57037600	0.00000000
C	-3.68567700	0.56108800	0.00000000
H	-4.75246600	0.36656600	0.00000000
C	-2.79478700	-0.48343000	0.00000000
H	-3.14454400	-1.50835400	0.00000000
C	-1.40372900	-0.25272200	0.00000000
C	-0.48887600	-1.37684000	0.00000000
C	0.93026300	-1.08163300	0.00000000
C	1.86506600	-2.13750200	0.00000000
H	1.49230100	-3.15441100	0.00000000
C	3.21506600	-1.88763500	0.00000000
H	3.92055300	-2.71110800	0.00000000
O	-0.91304200	-2.57037600	0.00000000
C	3.68567700	-0.56108800	0.00000000
H	4.75246600	-0.36656600	0.00000000



C	2.79478700	0.48343000	0.00000000
H	3.14454400	1.50835400	0.00000000
C	1.40372900	0.25272200	0.00000000
K	-1.32651900	-4.19522400	-2.04234600
O	0.31316400	6.44517000	2.24561000
O	-0.31316400	-6.44517000	-2.24561000
C	-0.20997500	7.61370900	2.75480400
C	0.65614500	8.82124800	2.35699200
C	-1.64585700	7.83538000	2.24818900
C	-0.24539600	7.52190000	4.29678700
H	1.67832900	8.68868800	2.72167700
H	0.69583300	8.90955200	1.26794400
H	0.26856800	9.76184700	2.76086200
H	-2.28205200	6.99487400	2.53782700
H	-2.08912100	8.75319900	2.64717800
H	-1.65003400	7.90131400	1.15732500
H	-0.65486000	8.43156300	4.74715000
H	-0.86299300	6.67590700	4.60854800
H	0.76386200	7.36982500	4.68734300
C	0.20997500	-7.61370900	-2.75480400
C	1.64585700	-7.83538000	-2.24818900
C	-0.65614500	-8.82124800	-2.35699200
C	0.24539600	-7.52190000	-4.29678700
H	2.28205200	-6.99487400	-2.53782700
H	1.65003400	-7.90131400	-1.15732500
H	2.08912100	-8.75319900	-2.64717800
H	-1.67832900	-8.68868800	-2.72167700
H	-0.26856800	-9.76184700	-2.76086200
H	-0.69583300	-8.90955200	-1.26794400
H	0.65486000	-8.43156300	-4.74715000
H	-0.76386200	-7.36982500	-4.68734300
H	0.86299300	-6.67590700	-4.60854800

n=3 (AQ-(KOBu)<sub>3</sub>, singlet or triplet)

K	1.32651900	4.19522400	2.04234600
C	0.48887600	1.37684000	0.00000000
C	-0.93026300	1.08163300	0.00000000
C	-1.86506600	2.13750200	0.00000000
H	-1.49230100	3.15441100	0.00000000
C	-3.21506600	1.88763500	0.00000000
H	-3.92055300	2.71110800	0.00000000
O	0.91304200	2.57037600	0.00000000
C	-3.68567700	0.56108800	0.00000000

H	-4.75246600	0.36656600	0.00000000
C	-2.79478700	-0.48343000	0.00000000
H	-3.14454400	-1.50835400	0.00000000
C	-1.40372900	-0.25272200	0.00000000
K	-1.32651900	-4.19522400	2.04234600
C	-0.48887600	-1.37684000	0.00000000
C	0.93026300	-1.08163300	0.00000000
C	1.86506600	-2.13750200	0.00000000
H	1.49230100	-3.15441100	0.00000000
C	3.21506600	-1.88763500	0.00000000
H	3.92055300	-2.71110800	0.00000000
O	-0.91304200	-2.57037600	0.00000000
C	3.68567700	-0.56108800	0.00000000
H	4.75246600	-0.36656600	0.00000000
C	2.79478700	0.48343000	0.00000000
H	3.14454400	1.50835400	0.00000000
C	1.40372900	0.25272200	0.00000000
K	-1.32651900	-4.19522400	-2.04234600
O	0.31316400	6.44517000	2.24561000
O	-0.31316400	-6.44517000	-2.24561000
O	-0.31316400	-6.44517000	2.24561000
C	-0.20997500	7.61370900	2.75480400
C	0.65614500	8.82124800	2.35699200
C	-1.64585700	7.83538000	2.24818900
C	-0.24539600	7.52190000	4.29678700
H	1.67832900	8.68868800	2.72167700
H	0.69583300	8.90955200	1.26794400
H	0.26856800	9.76184700	2.76086200
H	-2.28205200	6.99487400	2.53782700
H	-2.08912100	8.75319900	2.64717800
H	-1.65003400	7.90131400	1.15732500
H	-0.65486000	8.43156300	4.74715000
H	-0.86299300	6.67590700	4.60854800
H	0.76386200	7.36982500	4.68734300
C	0.20997500	-7.61370900	-2.75480400
C	1.64585700	-7.83538000	-2.24818900
C	-0.65614500	-8.82124800	-2.35699200
C	0.24539600	-7.52190000	-4.29678700
H	2.28205200	-6.99487400	-2.53782700
H	1.65003400	-7.90131400	-1.15732500
H	2.08912100	-8.75319900	-2.64717800
H	-1.67832900	-8.68868800	-2.72167700
H	-0.26856800	-9.76184700	-2.76086200
H	-0.69583300	-8.90955200	-1.26794400

H	0.65486000	-8.43156300	-4.74715000
H	-0.76386200	-7.36982500	-4.68734300
H	0.86299300	-6.67590700	-4.60854800
C	0.20997500	-7.61370900	2.75480400
C	-0.65614500	-8.82124800	2.35699200
C	1.64585700	-7.83538000	2.24818900
C	0.24539600	-7.52190000	4.29678700
H	-1.67832900	-8.68868800	2.72167700
H	-0.69583300	-8.90955200	1.26794400
H	-0.26856800	-9.76184700	2.76086200
H	2.28205200	-6.99487400	2.53782700
H	2.08912100	-8.75319900	2.64717800
H	1.65003400	-7.90131400	1.15732500
H	0.65486000	-8.43156300	4.74715000
H	0.86299300	-6.67590700	4.60854800
H	-0.76386200	-7.36982500	4.68734300

n=4 (AQ-KOtBu/AQ-(KOtBu)<sub>4</sub>, singlet or triplet)

K	1.32651900	4.19522400	2.04234600
C	0.48887600	1.37684000	0.00000000
C	-0.93026300	1.08163300	0.00000000
C	-1.86506600	2.13750200	0.00000000
H	-1.49230100	3.15441100	0.00000000
C	-3.21506600	1.88763500	0.00000000
H	-3.92055300	2.71110800	0.00000000
O	0.91304200	2.57037600	0.00000000
C	-3.68567700	0.56108800	0.00000000
H	-4.75246600	0.36656600	0.00000000
C	-2.79478700	-0.48343000	0.00000000
H	-3.14454400	-1.50835400	0.00000000
C	-1.40372900	-0.25272200	0.00000000
K	1.32651900	4.19522400	-2.04234600
K	-1.32651900	-4.19522400	2.04234600
C	-0.48887600	-1.37684000	0.00000000
C	0.93026300	-1.08163300	0.00000000
C	1.86506600	-2.13750200	0.00000000
H	1.49230100	-3.15441100	0.00000000
C	3.21506600	-1.88763500	0.00000000
H	3.92055300	-2.71110800	0.00000000
O	-0.91304200	-2.57037600	0.00000000
C	3.68567700	-0.56108800	0.00000000
H	4.75246600	-0.36656600	0.00000000
C	2.79478700	0.48343000	0.00000000

H	3.14454400	1.50835400	0.00000000
C	1.40372900	0.25272200	0.00000000
K	-1.32651900	-4.19522400	-2.04234600
O	0.31316400	6.44517000	2.24561000
O	0.31316400	6.44517000	-2.24561000
O	-0.31316400	-6.44517000	-2.24561000
O	-0.31316400	-6.44517000	2.24561000
C	-0.20997500	7.61370900	2.75480400
C	0.65614500	8.82124800	2.35699200
C	-1.64585700	7.83538000	2.24818900
C	-0.24539600	7.52190000	4.29678700
H	1.67832900	8.68868800	2.72167700
H	0.69583300	8.90955200	1.26794400
H	0.26856800	9.76184700	2.76086200
H	-2.28205200	6.99487400	2.53782700
H	-2.08912100	8.75319900	2.64717800
H	-1.65003400	7.90131400	1.15732500
H	-0.65486000	8.43156300	4.74715000
H	-0.86299300	6.67590700	4.60854800
H	0.76386200	7.36982500	4.68734300
C	-0.20997500	7.61370900	-2.75480400
C	-1.64585700	7.83538000	-2.24818900
C	0.65614500	8.82124800	-2.35699200
C	-0.24539600	7.52190000	-4.29678700
H	-2.28205200	6.99487400	-2.53782700
H	-1.65003400	7.90131400	-1.15732500
H	-2.08912100	8.75319900	-2.64717800
H	1.67832900	8.68868800	-2.72167700
H	0.26856800	9.76184700	-2.76086200
H	0.69583300	8.90955200	-1.26794400
H	-0.65486000	8.43156300	-4.74715000
H	0.76386200	7.36982500	-4.68734300
H	-0.86299300	6.67590700	-4.60854800
C	0.20997500	-7.61370900	-2.75480400
C	1.64585700	-7.83538000	-2.24818900
C	-0.65614500	-8.82124800	-2.35699200
C	0.24539600	-7.52190000	-4.29678700
H	2.28205200	-6.99487400	-2.53782700
H	1.65003400	-7.90131400	-1.15732500
H	2.08912100	-8.75319900	-2.64717800
H	-1.67832900	-8.68868800	-2.72167700
H	-0.26856800	-9.76184700	-2.76086200
H	-0.69583300	-8.90955200	-1.26794400
H	0.65486000	-8.43156300	-4.74715000

H	-0.76386200	-7.36982500	-4.68734300
H	0.86299300	-6.67590700	-4.60854800
C	0.20997500	-7.61370900	2.75480400
C	-0.65614500	-8.82124800	2.35699200
C	1.64585700	-7.83538000	2.24818900
C	0.24539600	-7.52190000	4.29678700
H	-1.67832900	-8.68868800	2.72167700
H	-0.69583300	-8.90955200	1.26794400
H	-0.26856800	-9.76184700	2.76086200
H	2.28205200	-6.99487400	2.53782700
H	2.08912100	-8.75319900	2.64717800
H	1.65003400	-7.90131400	1.15732500
H	0.65486000	-8.43156300	4.74715000
H	0.86299300	-6.67590700	4.60854800
H	-0.76386200	-7.36982500	4.68734300

KOtBu

K	1.32651900	4.19522400	-2.04234600
O	0.31316400	6.44517000	-2.24561000
C	-0.20997500	7.61370900	-2.75480400
C	-1.64585700	7.83538000	-2.24818900
C	0.65614500	8.82124800	-2.35699200
C	-0.24539600	7.52190000	-4.29678700
H	-2.28205200	6.99487400	-2.53782700
H	-1.65003400	7.90131400	-1.15732500
H	-2.08912100	8.75319900	-2.64717800
H	1.67832900	8.68868800	-2.72167700
H	0.26856800	9.76184700	-2.76086200
H	0.69583300	8.90955200	-1.26794400
H	-0.65486000	8.43156300	-4.74715000
H	0.76386200	7.36982500	-4.68734300
H	-0.86299300	6.67590700	-4.60854800

C<sup>M</sup>

K	2.04818183	0.00000000	4.39722172
C	-0.00000000	0.00000000	1.46105712
C	0.00000000	-1.23878279	0.70762729
C	0.00000000	-2.47321505	1.38945792
H	0.00000000	-2.46253894	2.47248316
C	0.00000000	-3.66157689	0.70190454
H	0.00000000	-4.60210584	1.24155717
O	-0.00000000	0.00000000	2.72772400

C	0.00000000	-3.66157689	-0.70190454
H	0.00000000	-4.60210584	-1.24155717
C	0.00000000	-2.47321505	-1.38945792
H	0.00000000	-2.46253894	-2.47248316
C	0.00000000	-1.23878279	-0.70762729
K	-2.04818183	-0.00000000	4.39722172
K	2.04818183	0.00000000	-4.39722172
C	-0.00000000	0.00000000	-1.46105712
C	0.00000000	1.23878279	-0.70762729
C	0.00000000	2.47321505	-1.38945792
H	0.00000000	2.46253894	-2.47248316
C	0.00000000	3.66157689	-0.70190454
H	0.00000000	4.60210584	-1.24155717
O	-0.00000000	0.00000000	-2.72772400
C	-0.00000000	3.66157689	0.70190454
H	-0.00000000	4.60210584	1.24155717
C	-0.00000000	2.47321505	1.38945792
H	-0.00000000	2.46253894	2.47248316
C	-0.00000000	1.23878279	0.70762729
K	-2.04818183	-0.00000000	-4.39722172
O	3.96738425	0.00000000	-5.96158678
H	3.64402691	-0.00000012	-6.86548945
O	-3.96738425	-0.00000000	-5.96158678
H	-3.64402691	-0.00000012	-6.86548945
O	-3.96738425	-0.00000000	5.96158678
H	-3.64402691	-0.00000012	6.86548945
O	3.96738425	0.00000000	5.96158678
H	3.64402691	-0.00000012	6.86548945

The OtBu radical (D<sub>0</sub>)

O	0.00000000	0.25884100	1.42557100
C	0.00000000	-0.02498000	0.07603000
C	0.00000000	1.38001500	-0.57341700
C	-1.26861800	-0.78755100	-0.31328800
C	1.26861800	-0.78755100	-0.31328800
H	0.88712700	1.94145800	-0.28077800
H	-0.88712700	1.94145800	-0.28077800
H	0.00000000	1.26012200	-1.65851000
H	-1.30050900	-1.75412200	0.19356900
H	-1.30381700	-0.96953900	-1.38990500
H	-2.15603400	-0.22302300	-0.02402500
H	1.30381700	-0.96953900	-1.38990500
H	1.30050900	-1.75412200	0.19356900

H	2.15603400	-0.22302300	-0.02402500
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The OtBu radical (the lowest second excited state, D<sub>2</sub>)

O	0.14958100	1.46742000	0.00000000
C	0.14604100	0.09927600	0.00000000
C	-1.60048600	-0.31469000	0.00000000
C	0.66679800	-0.50309700	1.26097100
C	0.66679800	-0.50309700	-1.26097100
H	-1.76093000	0.24703600	-0.92165800
H	-1.76093000	0.24703600	0.92165800
H	-2.07949200	-1.29442400	0.00000000
H	1.69154900	-0.08851800	1.33469500
H	0.73003800	-1.59334000	1.27257200
H	0.14331000	-0.12282100	2.13744200
H	0.73003800	-1.59334000	-1.27257200
H	1.69154900	-0.08851800	-1.33469500
H	0.14331000	-0.12282100	-2.13744200

The OtBu radical (D<sub>1</sub>)

O	1.55776400	-0.00302300	0.00000000
C	-0.10031200	-0.00062500	0.00000000
C	-0.40687700	1.46260300	0.00000000
C	-0.40687700	-0.73013400	1.26755200
C	-0.40687700	-0.73013400	-1.26755200
H	-0.00581100	1.94676600	-0.88763400
H	-0.00581100	1.94676600	0.88763400
H	-1.49923600	1.58600000	0.00000000
H	-0.01390300	-1.74397000	1.24234300
H	-1.49940000	-0.78286300	1.37867700
H	0.00051000	-0.20596800	2.12931700
H	-1.49940000	-0.78286300	-1.37867700
H	-0.01390300	-1.74397000	-1.24234300
H	0.00051000	-0.20596800	-2.12931700

The complex, C<sub>(1)</sub>, catalyzing triplet oxygen to generate singlet oxygen.

C<sub>(1)</sub>

K	1.74529700	3.56776900	2.23210600
C	0.86416900	1.17150300	0.00000000
C	-0.57783200	1.30810300	0.00000000
C	-1.17059700	2.58794500	0.00000000
H	-0.54108800	3.46949200	0.00000000
C	-2.53530100	2.73493000	0.00000000

H	-2.96759500	3.72859900	0.00000000
O	1.62337900	2.19546500	0.00000000
C	-3.36529600	1.60172300	0.00000000
H	-4.44283100	1.72291100	0.00000000
C	-2.81352300	0.34448600	0.00000000
H	-3.44155400	-0.53780700	0.00000000
C	-1.41639900	0.16568200	0.00000000
K	1.74529700	3.56776900	-2.23210600
K	-1.74529700	-3.56776900	2.23210600
C	-0.86416900	-1.17150300	0.00000000
C	0.57783200	-1.30810300	0.00000000
C	1.17059700	-2.58794500	0.00000000
H	0.54108800	-3.46949200	0.00000000
C	2.53530100	-2.73493000	0.00000000
H	2.96759500	-3.72859900	0.00000000
O	-1.62337900	-2.19546500	0.00000000
C	3.36529600	-1.60172300	0.00000000
H	4.44283100	-1.72291100	0.00000000
C	2.81352300	-0.34448600	0.00000000
H	3.44155400	0.53780700	0.00000000
C	1.41639900	-0.16568200	0.00000000
K	-1.74529700	-3.56776900	-2.23210600
O	0.50409900	5.47345300	2.68970700
O	0.50409900	5.47345300	-2.68970700
O	-0.50409900	-5.47345300	-2.68970700
O	-0.50409900	-5.47345300	2.68970700
C	-0.23067500	6.60278700	2.96047900
C	0.47912000	7.84807200	2.40589100
C	-1.63220300	6.48816600	2.33861500
C	-0.37555000	6.74974100	4.49070300
H	1.47457000	7.93736200	2.84820600
H	0.59779600	7.75620600	1.32353800
H	-0.07362600	8.76975800	2.61280700
H	-2.13901700	5.60071200	2.72642100
H	-2.25521300	7.36275600	2.55027300
H	-1.54739000	6.38453700	1.25397800
H	-0.95532500	7.63822900	4.75949900
H	-0.87669800	5.87094400	4.90328100
H	0.61165900	6.82810500	4.95195100
C	-0.23067500	6.60278700	-2.96047900
C	-1.63220300	6.48816600	-2.33861500
C	0.47912000	7.84807200	-2.40589100
C	-0.37555000	6.74974100	-4.49070300
H	-2.13901700	5.60071200	-2.72642100



H	-1.54739000	6.38453700	-1.25397800
H	-2.25521300	7.36275600	-2.55027300
H	1.47457000	7.93736200	-2.84820600
H	-0.07362600	8.76975800	-2.61280700
H	0.59779600	7.75620600	-1.32353800
H	-0.95532500	7.63822900	-4.75949900
H	0.61165900	6.82810500	-4.95195100
H	-0.87669800	5.87094400	-4.90328100
C	0.23067500	-6.60278700	-2.96047900
C	1.63220300	-6.48816600	-2.33861500
C	-0.47912000	-7.84807200	-2.40589100
C	0.37555000	-6.74974100	-4.49070300
H	2.13901700	-5.60071200	-2.72642100
H	1.54739000	-6.38453700	-1.25397800
H	2.25521300	-7.36275600	-2.55027300
H	-1.47457000	-7.93736200	-2.84820600
H	0.07362600	-8.76975800	-2.61280700
H	-0.59779600	-7.75620600	-1.32353800
H	0.95532500	-7.63822900	-4.75949900
H	-0.61165900	-6.82810500	-4.95195100
H	0.87669800	-5.87094400	-4.90328100
C	0.23067500	-6.60278700	2.96047900
C	-0.47912000	-7.84807200	2.40589100
C	1.63220300	-6.48816600	2.33861500
C	0.37555000	-6.74974100	4.49070300
H	-1.47457000	-7.93736200	2.84820600
H	-0.59779600	-7.75620600	1.32353800
H	0.07362600	-8.76975800	2.61280700
H	2.13901700	-5.60071200	2.72642100
H	2.25521300	-7.36275600	2.55027300
H	1.54739000	-6.38453700	1.25397800
H	0.95532500	-7.63822900	4.75949900
H	0.87669800	-5.87094400	4.90328100
H	-0.61165900	-6.82810500	4.95195100

C<sub>(1)</sub>@<sup>1</sup>O<sub>2</sub>

K	1.95953373	4.08710968	-0.39541897
C	0.78929674	1.23304591	-2.23307197
C	1.44641269	-0.09765301	-2.24640997
C	2.83447536	-0.16372977	-2.26110097
H	3.39889972	0.75895934	-2.29863897
C	3.47328512	-1.39230614	-2.21567097
H	4.55643403	-1.43884736	-2.22603397
O	1.45134278	2.25672683	-2.24661297

C	2.72621009	-2.56201832	-2.13886797
H	3.21986493	-3.52488115	-2.07948897
C	1.34048572	-2.50821349	-2.13444897
H	0.76467995	-3.42058474	-2.03935597
C	0.69440783	-1.27778590	-2.20422597
K	-0.73490602	3.13446477	1.59194203
K	-1.95953373	-4.08710968	-0.39541897
C	-0.78929674	-1.23304591	-2.23307197
C	-1.44641269	0.09765301	-2.24640997
C	-2.83447536	0.16372977	-2.26110097
H	-3.39889972	-0.75895934	-2.29863897
C	-3.47328512	1.39230614	-2.21567097
H	-4.55643403	1.43884736	-2.22603397
O	-1.45134278	-2.25672683	-2.24661297
C	-2.72621009	2.56201832	-2.13886797
H	-3.21986493	3.52488115	-2.07948897
C	-1.34048572	2.50821349	-2.13444897
H	-0.76467995	3.42058474	-2.03935597
C	-0.69440783	1.27778590	-2.20422597
K	0.73490602	-3.13446477	1.59194203
O	-0.33911039	5.00492607	-0.00097597
O	1.63579996	2.34448876	1.43243703
O	-1.63579996	-2.34448876	1.43243703
O	0.33911039	-5.00492607	-0.00097597
C	-0.80529728	6.29247309	-0.18921297
C	-1.96352839	6.30843747	-1.20233897
C	-1.31208209	6.88143960	1.14022003
C	0.31922983	7.20109032	-0.72325897
H	-1.62881219	5.90130768	-2.16071497
H	-2.78221129	5.68231743	-0.83583997
H	-2.36016707	7.31330224	-1.38093497
H	-0.50707340	6.87519689	1.88080103
H	-1.67753992	7.90912312	1.04404903
H	-2.13506312	6.27245159	1.52896503
H	-0.00322224	8.23386180	-0.88901797
H	1.15110030	7.22527543	-0.01107097
H	0.69149674	6.81383794	-1.67768697
C	2.59922918	1.80872316	2.27274003
C	3.62859475	2.89339604	2.64098003
C	1.96192786	1.28822753	3.57334903
C	3.34005180	0.65352234	1.57518303
H	4.13896216	3.25695513	1.74216603
H	3.12770967	3.74201976	3.11466703
H	4.39878580	2.52632945	3.32704703

H	1.21267519	0.52604180	3.35159403
H	2.69822059	0.85753079	4.25965903
H	1.46233017	2.10885749	4.09788003
H	4.09920046	0.19315767	2.21637703
H	2.63442133	-0.11960276	1.26583603
H	3.83594915	1.01897273	0.67168103
C	-2.59922918	-1.80872316	2.27274003
C	-3.62859475	-2.89339604	2.64098003
C	-1.96192786	-1.28822753	3.57334903
C	-3.34005180	-0.65352234	1.57518303
H	-4.13896216	-3.25695513	1.74216603
H	-3.12770967	-3.74201976	3.11466703
H	-4.39878580	-2.52632945	3.32704703
H	-1.21267519	-0.52604180	3.35159403
H	-2.69822059	-0.85753079	4.25965903
H	-1.46233017	-2.10885749	4.09788003
H	-4.09920046	-0.19315767	2.21637703
H	-2.63442133	0.11960276	1.26583603
H	-3.83594915	-1.01897273	0.67168103
C	0.80529728	-6.29247309	-0.18921297
C	1.96352839	-6.30843747	-1.20233897
C	1.31208209	-6.88143960	1.14022003
C	-0.31922983	-7.20109032	-0.72325897
H	1.62881219	-5.90130768	-2.16071497
H	2.78221129	-5.68231743	-0.83583997
H	2.36016707	-7.31330224	-1.38093497
H	0.50707340	-6.87519689	1.88080103
H	1.67753992	-7.90912312	1.04404903
H	2.13506312	-6.27245159	1.52896503
H	0.00322224	-8.23386180	-0.88901797
H	-1.15110030	-7.22527543	-0.01107097
H	-0.69149674	-6.81383794	-1.67768697
O	-0.17102512	0.58512241	1.12026903
O	0.17102512	-0.58512241	1.12026903

C<sub>(1)</sub>@N<sub>2</sub>

K	1.56571200	4.70906800	-0.74529900
C	0.62557000	1.32386100	-1.95162100
C	1.44612900	0.08661700	-1.89665800
C	2.83004400	0.20153900	-1.84547800
H	3.27214000	1.18880800	-1.87389700
C	3.61801200	-0.93383800	-1.74252200
H	4.69714400	-0.83931800	-1.69810100
O	1.15161500	2.41837100	-2.04946700

C	3.02436100	-2.18857900	-1.67979600
H	3.63434000	-3.07886000	-1.58270700
C	1.64387000	-2.32019500	-1.74048100
H	1.19941400	-3.30892000	-1.65320000
C	0.84994000	-1.18204700	-1.85997500
K	-0.71159400	3.73890600	1.67457500
K	-1.56571200	-4.70906800	-0.74529900
C	-0.62557000	-1.32386100	-1.95162100
C	-1.44612900	-0.08661700	-1.89665800
C	-2.83004400	-0.20153900	-1.84547800
H	-3.27214000	-1.18880800	-1.87389700
C	-3.61801200	0.93383800	-1.74252200
H	-4.69714400	0.83931800	-1.69810100
O	-1.15161500	-2.41837100	-2.04946700
C	-3.02436100	2.18857900	-1.67979600
H	-3.63434000	3.07886000	-1.58270700
C	-1.64387000	2.32019500	-1.74048100
H	-1.19941400	3.30892000	-1.65320000
C	-0.84994000	1.18204700	-1.85997500
K	0.71159400	-3.73890600	1.67457500
O	-0.90255700	5.16529400	-0.35466700
O	1.73962300	3.58431100	1.48501200
O	-1.73962300	-3.58431100	1.48501200
O	0.90255700	-5.16529400	-0.35466700
C	-1.55739300	6.34055400	-0.67687700
C	-2.79169000	6.05619900	-1.55019200
C	-2.02103700	7.06584600	0.60001500
C	-0.62059000	7.28496700	-1.45560300
H	-2.49330300	5.53517800	-2.46409000
H	-3.48893700	5.41321700	-1.00520600
H	-3.32837000	6.96622200	-1.83760700
H	-1.16087400	7.28003900	1.24140800
H	-2.53401800	8.01129600	0.39578400
H	-2.71368900	6.42878900	1.16030000
H	-1.09941200	8.22693900	-1.74040500
H	0.25473300	7.53478300	-0.84570100
H	-0.27735900	6.79730000	-2.37400200
C	2.79169000	3.26736400	2.32202400
C	3.77114100	4.45081400	2.42788200
C	2.27637200	2.94038900	3.73697200
C	3.55860400	2.04460400	1.78691800
H	4.18383900	4.68607700	1.44101600
H	3.24428900	5.33728700	2.79108800
H	4.61291800	4.25302200	3.09988200

H	1.57963500	2.09685800	3.69578300
H	3.07593300	2.67877700	4.43769000
H	1.74271200	3.80346300	4.14761500
H	4.39791000	1.75300000	2.42753300
H	2.88272400	1.19045400	1.69505700
H	3.95298400	2.26032000	0.78950100
C	-2.79169000	-3.26736400	2.32202400
C	-3.77114100	-4.45081400	2.42788200
C	-2.27637200	-2.94038900	3.73697200
C	-3.55860400	-2.04460400	1.78691800
H	-4.18383900	-4.68607700	1.44101600
H	-3.24428900	-5.33728700	2.79108800
H	-4.61291800	-4.25302200	3.09988200
H	-1.57963500	-2.09685800	3.69578300
H	-3.07593300	-2.67877700	4.43769000
H	-1.74271200	-3.80346300	4.14761500
H	-4.39791000	-1.75300000	2.42753300
H	-2.88272400	-1.19045400	1.69505700
H	-3.95298400	-2.26032000	0.78950100
C	1.55739300	-6.34055400	-0.67687700
C	2.79169000	-6.05619900	-1.55019200
C	2.02103700	-7.06584600	0.60001500
C	0.62059000	-7.28496700	-1.45560300
H	2.49330300	-5.53517800	-2.46409000
H	3.48893700	-5.41321700	-1.00520600
H	3.32837000	-6.96622200	-1.83760700
H	1.16087400	-7.28003900	1.24140800
H	2.53401800	-8.01129600	0.39578400
H	2.71368900	-6.42878900	1.16030000
H	1.09941200	-8.22693900	-1.74040500
H	-0.25473300	-7.53478300	-0.84570100
H	0.27735900	-6.79730000	-2.37400200
N	0.28136800	-0.46688900	1.80019400
N	-0.28136800	0.46688900	1.80019400
<sup>3</sup> O <sub>2</sub>			
O	0.00000000	0.00000000	0.59801900
O	0.00000000	0.00000000	-0.59801900
<sup>1</sup> O <sub>2</sub>			
O	0.00000000	0.00000000	0.59800500
O	0.00000000	0.00000000	-0.59800500

N <sub>2</sub>			
N	0.00000000	0.00000000	0.54536100
N	0.00000000	0.00000000	-0.54536100

<sup>3</sup>O<sub>2</sub>@[AQ ·]<sup>-</sup> (<sup>1</sup>O<sub>2</sub>(CS)@[AQ ·]<sup>-</sup>, <sup>1</sup>O<sub>2</sub>(OS)@[AQ ·]<sup>-</sup>) (MSDFT)

O	0.00000000	-0.60268071	1.80000000
O	0.00000000	0.60268071	1.80000000
C	-3.69271292	-0.69896583	0.00000000
C	-2.49017772	-1.39591661	0.00000000
C	-1.27524444	-0.70320798	0.00000000
C	-1.27524444	0.70320798	0.00000000
C	-2.49017772	1.39591661	0.00000000
C	-3.69271292	0.69896583	0.00000000
C	0.00000000	-1.47816607	0.00000000
C	0.00000000	1.47816607	0.00000000
C	1.27524444	0.70320798	0.00000000
C	1.27524444	-0.70320798	0.00000000
C	2.49017772	-1.39591661	0.00000000
C	3.69271292	-0.69896583	0.00000000
C	3.69271292	0.69896583	0.00000000
C	2.49017772	1.39591661	0.00000000
O	0.00000000	2.69827166	0.00000000
O	0.00000000	-2.69827166	0.00000000
H	2.46836053	-2.47935825	0.00000000
H	-4.63231729	-1.24171212	0.00000000
H	-2.46836053	-2.47935825	0.00000000
H	-2.46836053	2.47935825	0.00000000
H	-4.63231729	1.24171212	0.00000000
H	4.63231729	-1.24171212	0.00000000
H	4.63231729	1.24171212	0.00000000
H	2.46836053	2.47935825	0.00000000