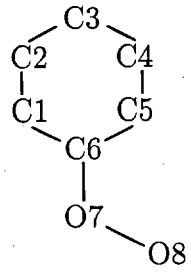
TABLES

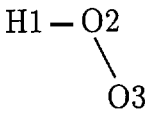
TABLE I. BLYP Geometry of Ground State Phenyl Peroxy Radical



	6-31G*	6-311G*	6-31G**	6-31+G*	6-31+G	aug-cc-pVDZ	aug-cc-pVTZ
				Bond Lengths(Å)			
C1-C2	1.403	1.400	1.402	1.404	1.409	1.404	1.397
C2-C3	1.408	1.405	1.408	1.410	1.415	1.410	1.403
C3-C4	1.410	1.407	1.410	1.412	1.416	1.412	1.404
C4-C5	1.402	1.400	1.402	1.404	1.409	1.405	1.396
C5-C6	1.404	1.401	1.404	1.407	1.408	1.407	1.399
C6-O7	1.409	1.410	1.410	1.408	1.438	1.411	1.406
O7-O8	1.358	1.355	1.358	1.362	1.427	1.355	1.356
C1-H	1.092	1.091	1.092	1.093	1.091	1.096	1.087
C2-H	1.093	1.091	1.092	1.094	1.092	1.097	1.088
C3-H	1.093	1.091	1.092	1.094	1.092	1.097	1.087
C4-H	1.094	1.092	1.093	1.094	1.093	1.097	1.087
C5-H	1.090	1.088	1.089	1.091	1.089	1.093	1.085
				Angles(deg)			
1-2-3	120.2	120.1	120.2	120.1	120.1	120.1	120.2
2-3-4	120.1	120.1	120.1	120.1	120.2	120.1	120.2
3-4-5	120.7	120.7	120.7	120.8	120.6	120.8	120.6
4-5-6	118.1	118.2	118.0	118.0	117.9	117.9	118.1
5-6-7	123.2	123.2	123.1	123.4	123.3	123.4	123.1

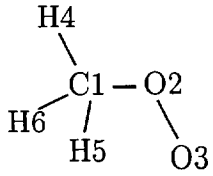
6-7-8	115.1	115.6	115.1	115.6	115.4	115.5	115.5

TABLE II. Geometry of Ground State Hydrogen Peroxy Radical at BLYP/6-31G*



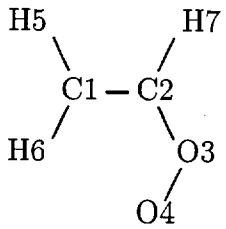
Bond Lengths (Å)			Angle (deg)
H1-O2	0.9979	1-2-3	104.6
O2-O3	1.3583		

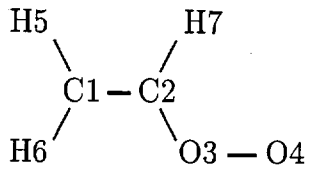
TABLE III. Geometry of Ground State Methyl Peroxy Radical at BLYP/6-31G*



Bond Lengths (Å)		Angles (deg)		Torsion Angles (deg)	
C1-O2	1.472	1-2-3	110.4	3-2-1-4	180.0
O2-O3	1.349	2-1-4	105.3	3-2-1-5	60.4
C1-H4	1.010	2-1-5	108.9	3-2-1-6	299.6
C1-H5	1.100	2-1-6	108.9		
C1-H6	1.100				

TABLE IV. Geometry of Ground State Vinyl Peroxy Radicals at BLYP/6-31G*





	cis-vinyl peroxy radical	*trans*-vinyl peroxy radical
	Bond Lengths (Å)	
C1-C2	1.344	1.345
C2-O3	1.402	1.393
O3-O4	1.357	1.363
C1-H5	1.091	1.091
C1-H6	1.090	1.092
C2-H7	1.092	1.092
	Angles (deg)	
1-2-3	125.6	119.2
2-3-4	115.1	112.6
5-1-2	119.8	120.0
6-1-2	120.7	121.5
1-2-7	126.3	127.5

TABLE V. Beta MO Eigenvalues for the Peroxy Radicals

	HO_2	CH_3O_2	*trans*-$C_2H_3O_2$	*cis*-$C_2H_3O_2$	$C_6H_5O_2$
a″(SOMO)	-0.182	-0.168	-0.173	-0.179	-0.168
a′ (HOMO)	-0.234	-0.218	-0.223	-0.222	-0.216
a″(2HOMO)	-0.378	-0.329	-0.262	-0.258	-0.242

BLYP/6-31+G*//BLYP/6-31G* beta orbital eigenvalues in au.

TABLE VI. Methane and Peroxy Substituent Beta MO Eigenvalues

HO_2		CH_4		CH_3O_2	
a″(SOMO)[a]	-0.182	a_1(LUMO)	+0.003	a″(SOMO)[a]	-0.168
a′ (HOMO)	-0.234	a_1(HOMO)	-0.342	a′(HOMO)	-0.218
a″(2HOMO)[a]	-0.378	e	-0.342	a″(2HOMO)[a]	-0.329

BLYP/6-31+G*//BLYP/6-31G* beta orbital eigenvalues in au.

[a] π-type orbital.

TABLE VII. Ethene and Peroxy Substituent Beta MO Eigenvalues

HO_2		C_2H_4		*trans/cis*-$C_2H_3O_2$	
a″(SOMO[a])	-0.182	b_{2g}(LUMO)[a]	-0.033	a″(SOMO)[a]	-0.173/-0.179
a′ (HOMO)	-0.234	b_{1u}(HOMO)[a]	-0.237	a′(HOMO)	-0.223/-0.222
a″(2HOMO)[a]	-0.378	b_{1g}	-0.312	a″(2HOMO)[a]	-0.262/-0.258

BLYP/6-31+G*//BLYP/6-31G* beta orbital eigenvalues in au.

[a] π-type orbital.

TABLE VIII. Benzene and Peroxy Substituent Beta MO Eigenvalues

HO_2		C_6H_6		$C_6H_5O_2$	
a″(SOMO)[a]	-0.182	e_{2u}(LUMO)[a]	-0.037	a″(SOMO)[a]	-0.168
a′ (HOMO)	-0.234	e_{1g}(HOMO)[a]	-0.221	a′(HOMO)	-0.216
a″(2HOMO)[a]	-0.378	e_{2g}	-0.300	a″(2HOMO)[a]	-0.242

BLYP/6-31+G*//BLYP/6-31G* beta orbital eigenvalues in au.

[a] π-type orbital.

TABLE IX. Benzene and CH_3NH Substituent Beta MO Eigenvalues

CH_3NH		C_6H_6		C_7H_8N	
a(SOMO)	-0.138	e_{2u}(LUMO)[a]	-0.037	a(SOMO)	-0.140
a(HOMO)	-0.226	e_{1g}(HOMO)[a]	-0.221	a(HOMO)	-0.216
a(2HOMO)	-0.353	e_{2g}	-0.300	a(2HOMO)	-0.230

BLYP/6-31+G*//BLYP/6-31G* beta orbital eigenvalues in au.

[a] π-type orbital.

TABLE X. Benzene and CH_3CH_2 Substituent Beta MO Eigenvalues

CH_3CH_2		C_6H_6		C_8H_9	
a(SOMO)	-0.086	e_{2u}(LUMO)[a]	-0.037	a(SOMO)	-0.093
a(HOMO)	-0.309	e_{1g}(HOMO)[a]	-0.221	a(HOMO)	-0.214
a(2HOMO)	-0.337	e_{2g}	-0.300	a(2HOMO)	-0.220

BLYP/6-31+G*//BLYP/6-31G* beta orbital eigenvalues in au.

[a] π-type orbital.