Excited State Structural Dynamics of Propanil in S_2 State: Resonance Raman and First-principle Investigation

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Table S1 The depolarization ratio (ρ) of parallel and vertical spectrum of propanil in H_2O/CH_3OH(4:1 by volume) solution

Mode	Frequency / cm^{-1}	ρ
ν_{51}	1659	0.20
ν_{50}	1590	0.27
ν_{49}	1534	0.19
ν_{40}	1299	0.21
ν_{37}	1249	0.50
ν_{20}	688	0.81

Table S2 The standard orientation of S_2/S_1 point at CASSCF(8,7)/6-31G(d) level

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.780519	-1.251072	0.000000
2	6	0	2.894942	-0.410009	0.000000
3	6	0	0.418955	-0.941249	0.000000
4	8	0	2.784304	0.795542	0.000000
5	6	0	0.000000	0.443549	0.000000
6	6	0	-0.530237	-1.929187	0.000000
7	6	0	5.379608	-0.001316	0.000000
8	6	0	-1.410064	0.794322	0.000000
9	6	0	-1.900661	-1.662208	0.000000
10	17	0	-1.850618	2.447519	0.000000
11	6	0	-2.383730	-0.293323	0.000000
12	17	0	-4.076013	0.008421	0.000000
13	1	0	1.982381	-2.225904	0.000000
14	1	0	0.718846	1.228800	0.000000
15	1	0	-0.219979	-2.960401	0.000000
16	1	0	6.355254	-0.466801	0.000000
17	1	0	5.308949	0.637066	0.873814
18	1	0	5.308949	0.637066	-0.873814
19	1	0	-2.610999	-2.461868	0.000000
20	6	0	4.269022	-1.058536	0.000000
21	1	0	4.372132	-1.699010	0.873262
22	1	0	4.372132	-1.699010	-0.873262

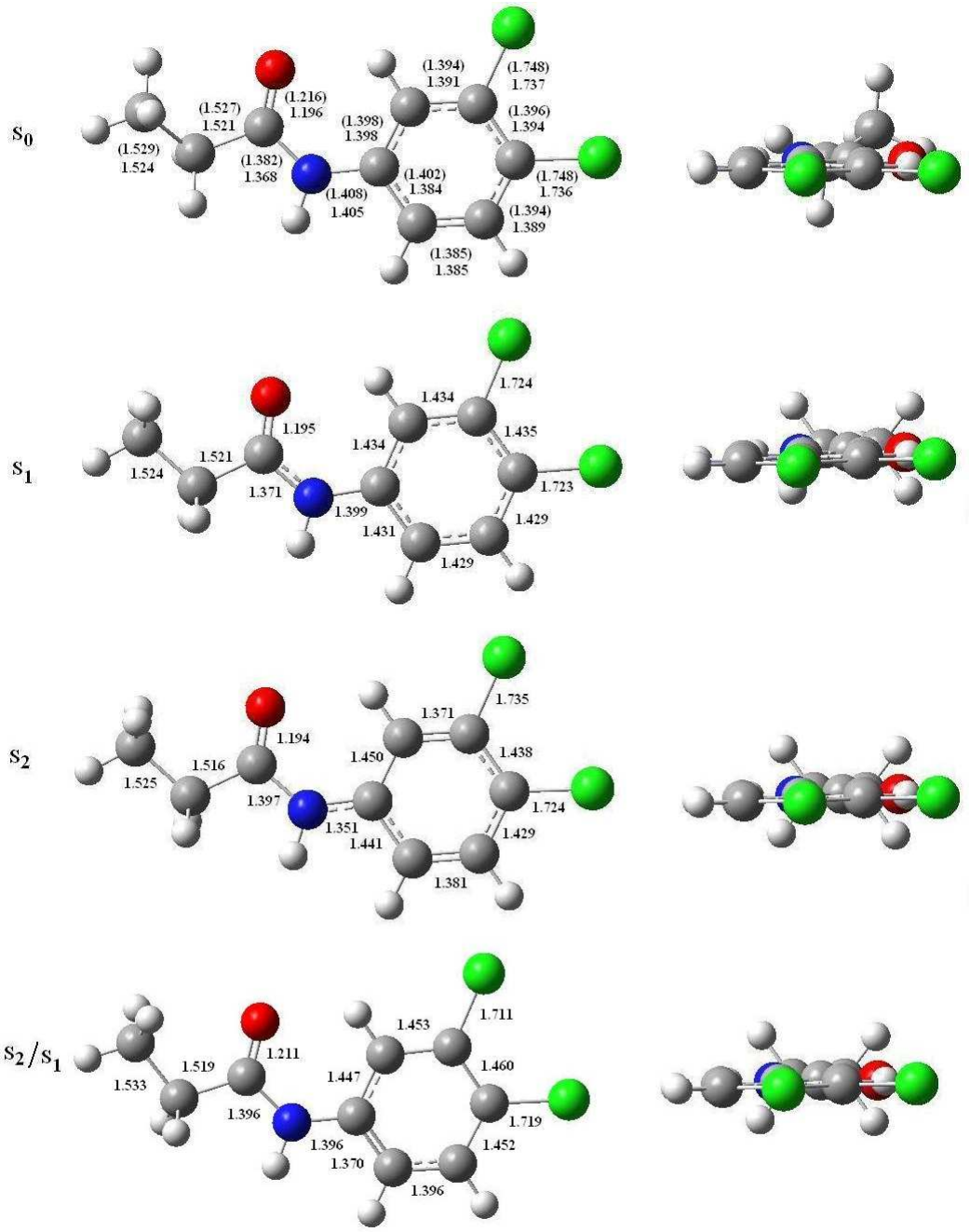

Figure S1 Two views of the S_0, S_1, S_2 and S_2/S_1 optimized structures of propanil at CASSCF (8, 7)/6-31g/G (d) level. B3LYP/6-311+G (d,p) structural parameters for S_0 state are also shown for comparison.

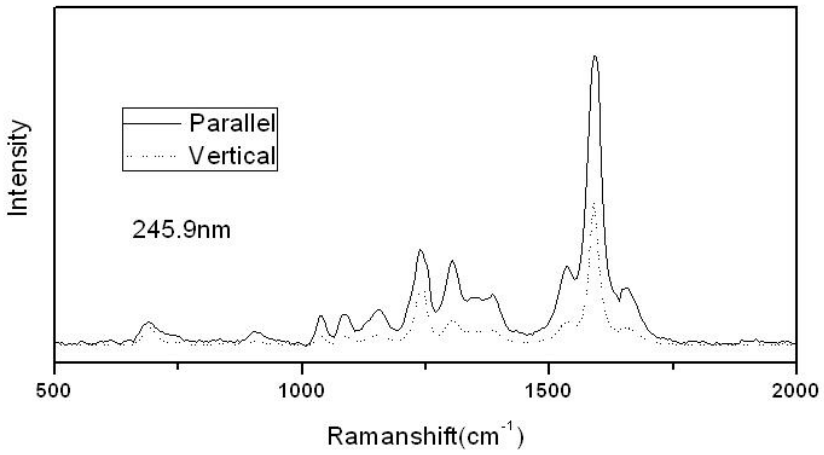

Figure S2 The depolarization spectra of propanil in water/methanol (4:1 by volume) solution excited with 245.9nm

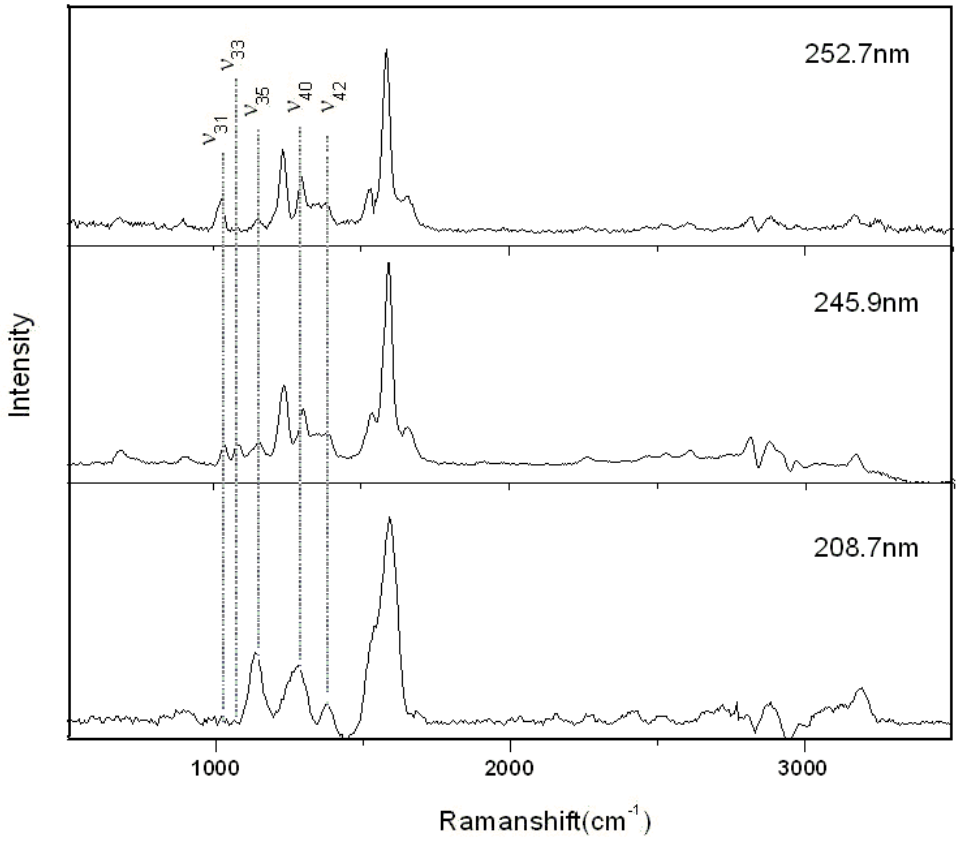

Figure S3 An overview of the 208.8, 245.9 and 252.7 nm resonance Raman spectra of propanil in water/methanol (4:1 by volume) solution.