Laboratory blueprints for interstellar searches of aromatic chiral molecules: rotational signatures of styrene oxide†

- SUPPLEMENTARY MATERIAL -

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1 Rotational Analysis of the Vibrationally Excited States of Styrene Oxide

Table 1: Ground state prediction and experimental values from Table 2 (main script) of styrene oxide. Theoretical values are calculated with Gaussian 09 with the B3LYP/aug-cc-pVTZ and B3LYP/def2-TZVP level of theory (anharmonic frequency calculations)

Ground State	E_{harm} /cm^{-1}	E_{anharm} /cm^{-1}	A /MHz	B /MHz	C /MHz
Experiment	-	-	4348.86	1124.88	951.23
B3LYP/aug-cc-pVTZ	30421.650	30075.203	4361.78	1116.87	945.91
Experiment-Prediction	-	-	−12.92	8.01	5.32
B3LYP/def2-TZVP	30394.107	30185.962	4359.15	1117.78	946.51
Experiment-Prediction	-	-	−10.29	7.10	4.72

Table 2: The three lowest energy vibrational modes v and corresponding rotational constants A, B, C of styrene oxide calculated with Gaussian 09 with the B3LYP/aug-cc-pVTZ and B3LYP/def2-TZVP level of theory (anharmonic frequency calculations). Additionally, the experimentally adjusted corrections for the predictions (subscript *adj*) are given with the corrections obtained from the difference of the ground state rotational constants and the calculated ground state constants from Tables 2 (main script) and S1

v	A /MHz	B /MHz	C /MHz	A_{adj} /MHz	B_{adj} /MHz	C_{adj} /MHz
B3LYP/aug-cc-pVTZ						
43	4380.63	1116.04	944.92	4367.71	1124.05	950.23
44	4348.01	1117.48	946.56	4335.09	1125.49	951.88
45	4357.12	1116.37	945.85	4344.21	1124.38	951.16
B3LYP/def2-TZVP						
43	4376.85	1116.97	945.61	4366.56	1124.10	950.32
44	4345.97	1118.41	947.22	4335.68	1125.50	951.94
45	4355.12	1117.30	946.38	4344.83	1124.39	951.10

Table 3: Harmonic and anharmonic vibrational energies in units of cm^{-1} of the three lowest normal modes υ_{45}, υ_{44}, and υ_{43} of SO with respect to the ground state calculated at B3LYP/aug-cc-pVTZ and B3LYP/def2-TZVP levels of theory

	B3LYP/aug-cc-pVTZ		B3LYP/def2-TZVP	
	E_{harm}	E_{anharm}	E_{harm}	E_{anharm}
υ_{45}	58.74	56.40	55.05	71.93
υ_{44}	148.56	146.68	145.26	152.89
υ_{43}	193.76	191.13	195.20	195.38

2 Rotational Partition Functions of Styrene Oxide

Table 4: Rotational partition function Q of $C_6H_5C_2H_3O$ for different temperatures T calculated by PGOPHER with J_{max}=120

Temperature T /K	Q	$\log_{10}$(Q)
1.6	159.672	2.2032
10	2475.157	3.3936
30	12849.097	4.1089
50	27642.954	4.4416
100	78186.156	4.8931
150	143651.857	5.1573
200	221194.877	5.3310
250	309172.207	5.4616
270	347025.170	5.5404
300	406476.183	5.6090
330	468988.808	5.6712
360	534421.420	5.7279