Vibrational Spectroscopy of Methyl benzoate

Kiran Sankar Maiti[†]

1 Supplementary information

Table 1 Strongly coupled modes with C–D vibrational mode for anti-o-deutero-methyl-benzoate. Although the frequency differ a little amount, but the qualitative result does not depend upon the isotopomers.

Coupled modes	SCF	V-MP2	VC-MP2
all decoupled	2316.4	2316.4	2316.4
17	2287.4	2295.9	2295.9
19	2294.8	2294.7	2294.7
17,19	2265.6	2274.7	2274.5
12,17,19	2243.1	2258.9	2258.7
12,14,17,19	2232.3	2249.8	2249.5
12,14,15,17,19	2226.4	2244.3	2243.9
12,14,15,17,19,21	2219.9	2238.8	2238.5
12,14,15,17,19,21,24	2215.6	2234.1	2233.8
12,13,14,15,17,19,21,24	2211.4	2230.3	2229.9
12,13,14,15,16,17,19,21,24	2204.5	2224.8	2224.4
12,13,14,15,16,17,18,19,21,24	2199.2	2220.2	2219.8
8,12,13,14,15,16,17,18,19,21,24	2192.3	2214.1	2213.6
7,8,12,13,14,15,16,17,18,19,21,24	2187.9	2209.9	2209.5
7,8,12,13,14,15,16,17,18,19,21,24,30	2183.8	2205.9	2205.5
7,8,9,12,13,14,15,16,17,18,19,21,24,30	2180.1	2202.7	2202.2

Table 2 Strongly coupled PM3 triple contributions for C–D vibrational mode of anti-o-deutero-methyl-benzoate. Although the frequency differ a little amount, but the qualitative result does not depend upon the isotopomers.

Triple coupled modes		SCF	V-MP2	VC-MP2
No triples		2003.2	2038.9	2038.3
17,j,40	19	2167.9	2192.1	2191.5
17,j,40	12,19	2168.4	2192.4	2191.8
17,j,40	12,14,19	2168.0	2192.0	2191.4
17,j,40	12,14,15,19	2172.6	2196.7	2196.1
17,j,40	12,14,15,19,21	2172.2	2196.2	2195.6
17,j,40	12,14,15,19,21,24	2173.9	2198.9	2198.3
17,j,40	12,13,14,15,19,21,24	2173.1	2198.6	2198.0
17,j,40	12,13,14,15,16,19,21,24	2172.5	2198.0	2197.4
17,j,40	12,13,14,15,16,18,19,21,24	2171.6	2197.2	2196.6

[†] *Physikalische Chemie, Universität Bayreuth, Universitätsstraße 30, D-95447 Bayreuth, Germany. E-mail: kiran.maiti@ch.tum.de*