Holger S. P. Müller, Oliver Zingsheim, Nadine Wehres, Jens-Uwe Grabow, Frank Lewen, and Stephan Schlemmer. Rotational Spectroscopy of the Lowest Energy Conformer of 2-Cyanobutane

Supplementary Table: Experimental Fundamental Vibrations[a] (cm^{-1}) of 2-Cyano-*anti*-butane in Comparison with Values from Quantum Chemical Calculations; Intensities (km/mol) in Parentheses.

Vibration	Exptl.[b]	B3LYP/aug-cc-pVDZ	B3LYP/aug-cc-pVTZ	MP2/aug-cc-pVTZ
ν_1	2990	3127 (18.1)	3114 (18.2)	3179 (12.5)
ν_2	2990	3119 (25.6)	3108 (25.0)	3173 (16.0)
ν_3	2990	3113 (21.9)	3101 (21.5)	3171 (14.6)
ν_4	2990	3104 (34.1)	3092 (33.3)	3163 (21.6)
ν_5	2942	3076 (6.94)	3061 (7.85)	3128 (7.32)
ν_6	2930	3044 (32.3)	3041 (24.3)	3085 (17.2)
ν_7	2880	3038 (15.1)	3032 (30.6)	3080 (7.17)
ν_8	2880	3033 (19.2)	3029 (8.49)	3076 (21.4)
ν_9	2880	3029 (2.43)	3018 (2.00)	3074 (7.01)
ν_{10}	2245	2332 (10.8)	2346 (9.75)	2190 (0.02)
ν_{11}		1483 (5.98)	1510 (6.27)	1522 (5.89)
ν_{12}	1460	1478 (7.26)	1505 (7.74)	1517 (11.8)
ν_{13}	1460	1474 (4.32)	1502 (3.77)	1515 (0.75)
ν_{14}	1448	1473 (5.55)	1498 (6.45)	1511 (7.05)
ν_{15}	1448	1464 (2.18)	1490 (1.81)	1496 (1.18)
ν_{16}	1384	1401 (6.35)	1424 (4.71)	1422 (5.39)
ν_{17}	1384	1396 (0.55)	1419 (1.80)	1415 (2.13)
ν_{18}		1357 (3.37)	1374 (4.08)	1371 (0.88)
ν_{19}	1335	1349 (3.38)	1367 (1.73)	1369 (3.53)
ν_{20}		1297 (0.05)	1315 (0.06)	1312 (0.09)
ν_{21}	1277	1269 (0.51)	1286 (0.26)	1287 (0.25)
ν_{22}		1173 (0.15)	1181 (0.12)	1196 (0.12)
ν_{23}	**1160**	1127 (0.84)	1142 (0.93)	1146 (0.86)
ν_{24}	1115	1111 (1.94)	1113 (2.37)	1134 (1.71)
ν_{25}	1094	1034 (0.41)	1027 (0.55)	1060 (0.09)
ν_{26}	1011	1017 (4.12)	1022 (4.05)	1034 (4.16)
ν_{27}	968	971 (4.16)	982 (4.31)	982 (4.39)
ν_{28}	873	892 (0.37)	892 (0.35)	910 (0.33)
ν_{29}	813	812 (1.96)	819 (2.03)	823 (1.76)
ν_{30}	**735**	741 (0.34)	746 (0.37)	758 (0.45)
ν_{31}		580 (0.19)	588 (0.18)	573 (0.24)
ν_{32}	**540**	544 (1.10)	551 (1.07)	540 (0.61)
ν_{33}	410	408 (0.52)	408 (0.53)	409 (0.38)
ν_{34}	**270**	276 (1.46)	280 (1.32)	280 (0.74)
ν_{35}		266 (0.87)	265 (0.87)	262 (0.65)
ν_{36}		223 (0.42)	225 (0.48)	234 (0.16)
ν_{37}		209 (1.44)	212 (1.31)	213 (1.87)
ν_{38}	170	162 (3.72)	163 (3.45)	159 (3.18)
ν_{39}		100 (1.55)	104 (1.62)	105 (1.58)

[a] Experimental values are anharmonic, bold ones are given as specific for the *anti* conformer; quantum chemically calculated ones harmonic and unscaled.

[b] Crowder and Carlisle, Ref. 22.