

Table 1 Harmonic vibrational frequencies of all the species

Species	Frequencies (cm ⁻¹)
C ₃ F ₇ CN	25.96, 79.79, 95.52, 148.90, 156.66, 238.30, 243.90, 289.08, 318.63, 338.20, 420.79, 438.70, 444.92, 524.62, 542.18, 563.50, 574.26, 649.90, 721.99, 762.07, 987.64, 1076.29, 1149.09, 1167.44, 1190.36, 1231.16, 1240.01, 1285.32, 1328.69, 2346.73
C ₃ NF ₄	59.47, 109.54, 161.04, 235.57, 367.41, 396.25, 438.86, 457.63, 563.93, 578.39, 647.09, 759.15, 1075.61, 1118.00, 1193.75, 1348.46, 1378.87, 2200.78
CF ₃	490.57, 492.58, 682.66, 1070.25, 1197.08, 1210.57
C ₃ F ₇	43.13, 59.93, 130.03, 164.90, 254.38, 290.12, 319.62, 346.23, 446.17, 482.77, 525.97, 536.52, 609.30, 655.18, 690.94, 767.42, 976.40, 1086.24, 1116.69, 1152.44, 1196.10, 1215.79, 1359.83, 1410.50
CN	2155.63
C ₄ NF ₆	10.34, 25.91, 122.76, 143.22, 144.85, 282.18, 303.20, 326.23, 395.28, 431.31, 485.83, 491.39, 530.51, 533.33, 580.15, 670.59, 709.51, 754.79, 987.06, 1097.37, 1136.43, 1144.27, 1153.32, 1225.58, 1317.71, 1371.30, 2159.81,
CNF	496.03, 1091.35, 2390.51
CF	1279.26
CF ₂	655.95, 1067.99, 1213.64
CF ₄	421.96, 424.02, 614.19, 617.94, 618.70, 894.91, 1230.54, 1236.53, 1248.13,