TABLE I: Phonon modes of the guanine monohydrate crystal. Abbreviations are: str, stretching; bend, bending; sci, scissoring; rock, rocking; wag, wagging; twis, twisting; def, deformation; breath, breathing; a, asymmetric; s, symmetric; ip, in plane; op, out of plane; T, translation; R, rotation

mode description	C_2	C_S	C_{2h}
NH_2 a str	3273.1, 3259.0, 3247.3	3272.0,3248.4	3255.7, 3236.9
NH_2 a str, OH str	3267.2	3263.3, 3263.1	3264.3, 3260.5
CH str	3163.7, 3163.5, 3152.5, 3152.0	3163.5, 3163.0, 3152.8, 3151.8	3158.2, 3157.8, 3157.6, 3157.4
NH_2 s str, OH str	3112.6, 3097.9, 3072.0	3112.1	3115.5, 3058.2
NH_2: NH str, OH str		3112.1, 3099.7	3099.3, 3077.7
NH_2 s str	3056.1	3057.2	
OH str, NH_2: NH str	3017.0, 3012.8, 2993.8	3017.4, 3007.5, 3000.1	3029.6, 3029.5, 3020.4
OH str, NH_2 s str			2998.1
H_2O s str, NH_2 s str	2982.0	2982.1	
H_2O a str, NH str	2785.7	2783.9	
H_2O a str	2754.1	2752.0	
NH str	2609.6, 2587.8, 2504.9, 2504.1	2610.0, 2588.6, 2504.2, 2503.4	2619.8, 2580.7, 2496.9, 2495.9
	2349.4, 2263.8, 2257.7, 2208.8	2345.0, 2271.0, 2236.7, 2227.1	2350.0, 2274.6, 2245.5, 2236.4
OH str	2309.8, 2309.4	2306.0, 2305.6	1942.4, 1932.2
HOH sci			1751.2, 1750.6
CO str, NH ip bend, CC str	1734.0	1734.0	1734.2
CO str, NH_2 sci, CC str	1708.3	1708.6	1708.9
H_2O sci, NH ip bend, NH_2 sci	1705.3	1705.3	
H_2O sci, NH_2 sci	1700.7	1701.2	
CN str, NH ip bend, H_2O sci	1680.2	1680.3	
CN str, NH ip bend	1679.1	1679.2	1687.2, 1684.2
CO str, CC str, H_2O sci	1671.3	1670.8	
CN str, CC str	1668.1	1669.2	1668.3
NH ip bend, CN str	1666.8	1666.7	1666.4, 1658.8
NH ip bend, CC str	1665.1	1664.7	1658.5
NH_2 sci	1639.3	1639.4	1646.4, 1644.9, 1639.8
CC str, CN str, NH ip bend	1632.9	1632.5	1632.1
H_2O sci, NH_2 sci, CN str	1630.6, 1630.1	1631.8, 1629.8	
NH ip bend, CC str, CN str	1627.3	1627.3	1628.3
NH_2 sci, CC str, NH ip bend	1612.6, 1598.9	1612.8, 1598.9	1613.1, 1598.8
NH_2 sci, CC str	1589.3	1589.5	1599.7
HOH sci			1569.0, 1569.0
CO str, CN str, NH_2 sci	1550.5	1550.2	1549.2
CO str, CN str	1549.2	1549.6	1548.8
CN str, CO str	1537.5	1537.4	1537.4
CC str, CN str	1529.4	1529.3	1529.4
H_2O sci	1521.9, 1521.4	1522.7, 1522.0	
NH ip bend	1505.1, 1498.7	1505.2, 1498.9	1503.8, 1497.4
CN str, NH ip bend, CH ip bend	1496.4	1496.4	1495.2
NH ip bend	1486.9	1487.2	1485.9
NH ip bend, CO str, CN str	1485.7	1485.7	1486.0
CN str, CH ip bend	1484.0	1483.9	1482.5
CN str, NH ip bend, CO str	1478.5	1478.5	1479.2
NH ip bend, CN str	1474.9	1474.8	1474.7
CN str, NH ip bend, CH ip bend	1467.8	1467.8	1467.3
NH ip bend, HOH sci			1467.2

mode description	C_2	C_S	C_{2h}
NH ip bend	1464.8	1464.9	1458.8
CN str, NH ip bend	1459.7	1459.5	
CN str, NH ip bend, CH ip bend	1455.9	1456.1	1455.5
HOH bend, NH ip bend			1454.3
HOH bend			1446.6
CC str, CN str	1420.0, 1416.6	1419.9, 1416.8	1419.3, 1416.4
CN str, CC str, CO ip bend	1412.7, 1411.6	1412.1, 1412.1	1411.8, 1411.7
CN str, CC str	1395.5, 1391.0		
CN str	1394.0, 1392.0	1396.0, 1393.0, 1392.8, 1390.6	1394.9, 1391.7, 1390.4, 1387.7
H_2O: OH bend	1344.4, 1342.7	1345.0, 1343.2	
CN str, CO ip bend	1319.5, 1317.3, 1307.7, 1306.8	1319.4, 1317.5, 1307.6, 1306.9	1319.9, 1319.4, 1307.7, 1307.0
CN str	1247.2, 1243.2, 1242.8, 1235.1	1247.2, 1244.3, 1241.8, 1235.1	1247.2, 1243.7, 1242.8, 1235.2
	1216.3, 1207.5, 1206.1, 1200.3	1216.3, 1207.6, 1206.1, 1200.3	1214.5, 1207.5, 1206.0, 1200.4
CH ip bend, HOH bend			1129.2, 1125.9, 1116.4, 1114.8
CH ip bend	1125.6, 1123.6, 1117.0, 1115.3	1125.6, 1123.6, 1116.9, 1115.3	1113.7, 1112.5
NH_2 rock	1105.7, 1098.4, 1086.4	1105.7, 1098.3, 1086.7	1104.7,1093.1
NH_2 rock, NH op bend	1098.6	1098.5	
OH bend, NH op bend			1094.1
NH op bend	1085.0, 1079.4	1083.4, 1081.4	
NH op bend, NH_2rock	1078.4, 1073.2	1076.6, 1075.2	1081.3, 1080.6, 1072.7
			1071.8, 1058.6
NH_2 rock, NH op bend			1074.6
NH op bend	1066.6	1061.4	
NH op bend, OH bend	1055.9	1065.9	1055.4
NH op bend, NH_2 rock	1058.5	1053.4, 1052.8	
NH_2 rock, NH op bend	1052.2		1047.2, 1046.0
H_2O: OH bend	1028.5	1029.6, 1029.3	
H_2O: OH bend, NH_2 rock	1028.9		
NH op bend	1008.4, 1004.7, 997.2, 996.5	1008.4, 1004.9, 996.7, 996.4	1008.6, 1006.1, 999.1, 999.1
HOH rock			1003.1, 1002.5
HOH bend			981.2, 980.9
NCN bend 5-ring def	959.4, 955.9, 937.7	958.6, 956.8, 937.7	956.9, 955.1, 937.3, 936.2
H_2O: OH bend	945.1, 937.4, 929.9	945.4, 936.2, 930.9	
H_2O rock, CH op bend	861.1, 860.7	860.6, 860.4	
HOH rock, CH op bend			884.2, 882.9
CH op bend, H_2O: OH bend	848.0	847.7	
CH op bend, HOH bend			837.5, 836.7
H_2O twist/rock, CH op bend	840.7, 840.5	840.6, 840.2	
CNC bend, 6-ring, 5-ring def	837.8	838.0	843.6, 837.4
CH op bend	831.1, 830.8	831.6, 830.6	833.4, 832.7
CNC bend, 6-ring, 5-ring def	825.2, 820.8	825.2, 820.9	824.8, 820.7
H_2O wag, NH_2 twis	799.6	800.1	
H_2O wag, NH_2 twis, CH op bend	799.5	800.0	
HOH bend			790.8
HOH bend, CH op bend			790.7
op bend, CO op bend	778.5, 778.4, 777.1, 776.8	778.4, 778.1, 777.5, 776.7	778.4, 778.1, 777.2
op bend, CO op bend, HOH bend			773.7
NH_2 twis	771.3, 768.8	770.9, 769.2	773.0, 770.2, 769.3, 767.5
NH_2: NH op bend	762.7, 760.8	763.0, 760.8	
H_2O twis/rock, NH_2 wag	749.2, 743.4	747.6, 744.2	
NH_2: NH op bend, op bend			733.8, 733.8, 724.5, 721.9
op bend, NH_2: NH op bend, H_2O rock	722.5, 721.6	724.1, 720.8	

mode description	C_2	C_S	C_{2h}
NCN op bend	717.5, 712.9	717.0, 712.7	
C-NH_2 ip bend, CO ip bend	710.6	709.5	710.6, 710.6, 698.6
C-NH_2 ip bend, CO ip bend, H_2O rock	706.8	708.4	
NH_2 wag	701.7, 698.9, 698.6, 694.7	700.7, 700.6, 697.2, 695.0	706.3, 705.0, 701.3
			691.0, 689.2
CO op bend, ring op bend	679.4, 679.2, 678.6, 675.1	679.3, 678.9, 678.9, 675.2	679.8, 679.3, 676.6, 674.8
ip bend ring def, NH_2: NH op bend	669.9	670.0	
NH_2: NH op bend	668.1	668.1	
6-ring breath	664.6	664.0	666.6, 665.8
6-ring breath, NH_2: NH op bend	664.6	664.9	
6-ring breath	661.5, 657.7	661.6, 657.7	663.3, 658.4
OH str			643.3, 643.1
5-ring op bend	633.3, 632.7, 630.6, 630.4	633.5, 631.9, 631.1, 630.2	632.2, 631.3, 629.2, 629.0
OH bend			607.6, 607.6
ip bend 6-ring def	574.9, 551.5, 550.2, 538.3	574.9, 551.6, 550.1, 538.3	574.4, 551.6, 549.7, 536.9
	528.3, 524.5, 518.8, 513.3	528.3, 524.5, 518.7, 513.2	527.6, 524.0, 517.6, 512.8
H_2O: T_c	441.7, 439.4	441.6, 440.7	
C-NH_2 ip bend	425.7, 421.8, 411.4, 408.5	425.8, 421.7, 411.3, 408.6	425.0, 423.7, 409.4, 409.2
ip bend; H_2O: T_a	384.0, 372.7	383.2, 372.9	
ip bend; OH: T_a			376.0, 368.1
op bend	368.5, 366.3	368.4, 366.4	368.7, 366.5
ip bend; H_2Ocol:T_a	359.9, 358.6	359.8, 358.5	359.1, 357.8
op bend	355.5, 352.8	355.4, 352.7	355.5, 352.1
H_2O: T_a; ip bend	323.0, 311.5	322.9, 311.5	
OH: T_a; ip bend			319.1, 303.0
H_2O: $T_{b/a}$	296.1, 291.1	296.2, 291.0	
H_2Ocol: T_a	283.9, 276.9	283.9, 276.9	274.9
H_2Ocol: T_a; op bend			270.1, 259.0
op bend	262.2, 257.9, 257.8	262.1, 257.8, 257.5	257.6, 255.5, 252.8
	252.3, 234.0, 231.6	252.2, 234.0, 231.6	234.5, 231.1
op bend; H_2Ocol: T_a	217.1, 214.9	217.0, 214.9	214.4, 214.1
T_b	187.2	187.0	187.7
T_a	184.6	184.6	186.5
R_c, T_a	179.6	179.7	180.3
butterfly	176.2, 170.5, 168.1, 161.2	176.2, 170.3, 168.8, 160.9	176.4, 169.1, 168.7, 160.5
T_b	170.0	168.5	168.2
R_c	156.5, 152.2	156.5, 152.1	156.7, 152.2
R_L, T_a	148.4	149.1	148.6
R_c; H_2Ocol: T_b	142.9	142.6	143.8
R_c	137.6	137.5	138.0
R_L, T_a	125.0	125.1	124.6
R_L	122.1	122.1	122.4
H_2Ocol: $T_{b/a}$; T_b	120.4	119.4	116.3
H_2Ocol: $T_{b/a}$	115.9	115.4	115.2
R_L; H_2Ocol: $T_{a/b/c}$	107.2	107.3	106.8
R_L	103.6	103.8	103.4
R_S; H_2Ocol: T_c	99.2	98.6	94.7
T_c	84.9	84.9	85.6
R_S	85.1	85.0	85.1
H_2Ocol: T_c; R_S	74.6	75.0	
H_2Ocol: T_c			73.3
T_b, R_S; H_2Ocol: T_c	73.0	69.6	

mode description	C_2	C_S	C_{2h}
T_b			71.0
H_2Ocol: T_c; T_c, R_s		69.9	
H_2Ocol: T_c; R_S, T_c	68.8		
H_2Ocol: T_c; T_c			67.2
T_c	57.7	57.8	58.0
R_S; H_2Ocol: T_c	57.7	56.2	57.0
T_c, R_S	49.7	48.7	48.2
R_S	46.0	45.3	43.9