

Supplementary Material S1: Vibrational band centers (in cm^{-1}) for $^{32}\text{SF}_6$ up to 3000 cm^{-1} . Vibrational sublevels are specified with symmetry “Sym” and “Eig” corresponds to the maximum contribution in the wave number decomposition.

Band, Sym, Eig	Band center	Band, Sym, Eig	Band center
ν_6, F_{2u} (0.98)	347.737	$2\nu_5 + 4\nu_6, E_g$ (0.67)	2427.833
ν_5, F_{2g} (-0.97)	523.449	$\nu_1 + \nu_4 + 3\nu_6, F_{1g}$ (-0.79)	2427.966
ν_4, F_{1u} (-0.98)	614.982	$\nu_3 + \nu_4 + \nu_5 + \nu_6, F_{2u}$ (0.76)	2427.993
ν_2, E_g (-0.97)	643.373	$\nu_3 + \nu_4 + \nu_5 + \nu_6, E_u$ (-0.94)	2428.001
$2\nu_6, A_{1g}$ (0.98)	693.730	$\nu_3 + \nu_4 + \nu_5 + \nu_6, F_{2u}$ (-0.65)	2428.091
$2\nu_6, F_{2g}$ (0.97)	695.383	$\nu_3 + \nu_4 + \nu_5 + \nu_6, F_{1u}$ (0.74)	2428.443
$2\nu_6, E_g$ (-0.97)	697.312	$2\nu_5 + 4\nu_6, F_{1g}$ (-0.52)	2428.502
ν_1, A_{1g} (0.93)	774.545	$\nu_3 + \nu_4 + \nu_5 + \nu_6, F_{2u}$ (0.56)	2428.638
$\nu_5 + \nu_6, A_{1u}$ (-0.97)	868.860	$2\nu_5 + 4\nu_6, F_{2g}$ (-0.63)	2428.660
$\nu_5 + \nu_6, F_{1u}$ (0.97)	869.762	$\nu_1 + \nu_4 + 3\nu_6, A_{2g}$ (-0.84)	2428.915
$\nu_5 + \nu_6, E_u$ (0.98)	870.801	$2\nu_5 + 4\nu_6, F_{2g}$ (0.75)	2429.035
$\nu_5 + \nu_6, F_{2u}$ (-0.97)	871.052	$\nu_1 + \nu_4 + 3\nu_6, F_{1g}$ (0.92)	2430.001
ν_3, F_{1u} (-0.96)	948.102	$\nu_3 + \nu_4 + \nu_5 + \nu_6, A_{1u}$ (-0.85)	2430.048
$\nu_4 + \nu_6, E_g$ (-0.97)	962.243	$\nu_3 + \nu_4 + \nu_5 + \nu_6, E_u$ (0.81)	2430.161
$\nu_4 + \nu_6, F_{2g}$ (-0.97)	962.617	$\nu_3 + \nu_4 + \nu_5 + \nu_6, F_{2u}$ (-0.78)	2430.424
$\nu_4 + \nu_6, F_{1g}$ (0.98)	962.622	$\nu_3 + \nu_4 + \nu_5 + \nu_6, F_{1u}$ (-0.74)	2430.488
$\nu_4 + \nu_6, A_{2g}$ (-0.98)	963.463	$\nu_3 + \nu_4 + \nu_5 + \nu_6, A_{2u}$ (-0.70)	2430.632
$\nu_2 + \nu_6, F_{2u}$ (0.96)	989.165	$2\nu_5 + 4\nu_6, E_g$ (0.50)	2430.651
$\nu_2 + \nu_6, F_{1u}$ (0.96)	991.307	$\nu_1 + \nu_4 + 2\nu_5, F_{1u}$ (-0.51)	2430.776
$3\nu_6, F_{2u}$ (-0.81)	1040.635	$\nu_3 + \nu_4 + \nu_5 + \nu_6, E_u$ (-0.74)	2430.859
$3\nu_6, A_{1u}$ (0.97)	1042.950	$\nu_1 + \nu_4 + 2\nu_5, F_{2u}$ (0.47)	2430.959
$3\nu_6, F_{1u}$ (-0.97)	1044.839	$2\nu_5 + 4\nu_6, A_{2g}$ (-0.80)	2431.105
$2\nu_5, F_{2g}$ (-0.97)	1046.335	$\nu_3 + \nu_4 + \nu_5 + \nu_6, F_{1u}$ (0.57)	2431.176
$3\nu_6, F_{2u}$ (0.81)	1046.930	$\nu_3 + \nu_4 + \nu_5 + \nu_6, F_{2u}$ (0.55)	2431.279
$2\nu_5, A_{1g}$ (0.97)	1047.322	$2\nu_5 + 4\nu_6, F_{2g}$ (-0.54)	2431.327
$2\nu_5, E_g$ (-0.97)	1047.626	$2\nu_5 + 4\nu_6, F_{2g}$ (0.54)	2431.504
$\nu_1 + \nu_6, F_{2u}$ (0.93)	1121.916	$\nu_1 + \nu_4 + 2\nu_5, E_u$ (-0.53)	2431.518
$\nu_4 + \nu_5, A_{2u}$ (-0.97)	1137.590	$\nu_1 + \nu_4 + 3\nu_6, A_{1g}$ (0.96)	2431.560
$\nu_4 + \nu_5, F_{2u}$ (-0.97)	1138.054	$\nu_1 + \nu_4 + 3\nu_6, F_{2g}$ (0.95)	2431.579
$\nu_4 + \nu_5, E_u$ (0.97)	1138.072	$2\nu_5 + 4\nu_6, F_{1g}$ (0.55)	2431.720
$\nu_4 + \nu_5, F_{1u}$ (-0.97)	1138.209	$\nu_3 + \nu_4 + \nu_5 + \nu_6, A_{1u}$ (0.77)	2431.814
$\nu_2 + \nu_5, F_{1g}$ (-0.96)	1164.600	$\nu_1 + \nu_4 + 3\nu_6, E_g$ (0.91)	2431.890
$\nu_2 + \nu_5, F_{2g}$ (0.96)	1166.643	$\nu_1 + \nu_4 + 2\nu_5, F_{1u}$ (-0.69)	2432.037
$\nu_5 + 2\nu_6, F_{2g}$ (-0.88)	1215.353	$\nu_1 + \nu_4 + 2\nu_5, F_{2u}$ (0.81)	2432.385
$\nu_5 + 2\nu_6, F_{2g}$ (0.80)	1215.724	$\nu_1 + \nu_4 + 3\nu_6, F_{1g}$ (-0.92)	2432.496
$\nu_5 + 2\nu_6, E_g$ (-0.95)	1216.660	$\nu_1 + \nu_4 + 2\nu_5, A_{2u}$ (0.86)	2432.497
$\nu_5 + 2\nu_6, F_{1g}$ (0.88)	1217.238	$\nu_1 + \nu_4 + 2\nu_5, E_u$ (-0.69)	2432.578
$\nu_5 + 2\nu_6, A_{1g}$ (-0.95)	1218.488	$2\nu_5 + 4\nu_6, E_g$ (0.71)	2432.759
$\nu_5 + 2\nu_6, F_{2g}$ (-0.87)	1219.640	$\nu_1 + \nu_4 + 2\nu_5, F_{1u}$ (-0.85)	2432.834
$\nu_5 + 2\nu_6, F_{1g}$ (-0.87)	1219.649	$2\nu_5 + 4\nu_6, F_{1g}$ (0.47)	2432.957
$2\nu_4, A_{1g}$ (0.97)	1229.496	$4\nu_5 + \nu_6, A_{1u}$ (0.97)	2432.963
$2\nu_4, E_g$ (0.97)	1229.640	$\nu_1 + \nu_4 + 2\nu_5, F_{1u}$ (-0.84)	2433.219
$2\nu_4, F_{2g}$ (-0.97)	1229.774	$7\nu_6, F_{1u}$ (-0.69)	2433.339
$\nu_2 + \nu_4, F_{1u}$ (0.96)	1257.019	$\nu_1 + \nu_4 + 2\nu_5, F_{2u}$ (-0.94)	2433.344
$\nu_2 + \nu_4, F_{2u}$ (0.96)	1257.312	$\nu_1 + \nu_4 + 3\nu_6, A_{2g}$ (-0.84)	2433.363
$2\nu_2, E_g$ (-0.91)	1285.598	$2\nu_5 + 4\nu_6, A_{1g}$ (-0.72)	2433.536
$2\nu_2, A_{1g}$ (-0.95)	1286.204	$2\nu_5 + 4\nu_6, E_g$ (-0.54)	2433.613
$\nu_3 + \nu_6, A_{2g}$ (0.95)	1294.260	$2\nu_5 + 4\nu_6, F_{2g}$ (-0.46)	2433.760
$\nu_3 + \nu_6, F_{2g}$ (-0.91)	1294.497	$4\nu_5 + \nu_6, F_{1u}$ (0.80)	2433.794
$\nu_3 + \nu_6, E_g$ (-0.92)	1294.505	$\nu_1 + \nu_4 + 3\nu_6, F_{2g}$ (-0.81)	2433.980

Table 1 – continued

Band, Sym, Eig	Band center	Band, Sym, Eig	Band center
$\nu_3 + \nu_6, F_{1g}$ (0.96)	1295.287	$\nu_1 + \nu_4 + 3\nu_6, F_{1g}$ (0.77)	2434.269
$\nu_1 + \nu_5, F_{2g}$ (0.88)	1297.083	$4\nu_5 + \nu_6, F_{2u}$ (0.53)	2434.520
$\nu_4 + 2\nu_6, F_{1u}$ (0.95)	1308.436	$2\nu_5 + 4\nu_6, E_g$ (0.56)	2434.616
$\nu_4 + 2\nu_6, F_{2u}$ (-0.97)	1309.792	$\nu_1 + \nu_4 + 3\nu_6, E_g$ (-0.76)	2434.794
$\nu_4 + 2\nu_6, A_{2u}$ (0.97)	1310.167	$2\nu_5 + 4\nu_6, F_{1g}$ (-0.60)	2434.800
$\nu_4 + 2\nu_6, E_u$ (-0.97)	1310.173	$2\nu_5 + 4\nu_6, F_{2g}$ (-0.75)	2435.183
$\nu_4 + 2\nu_6, F_{1u}$ (0.88)	1310.430	$2\nu_5 + 4\nu_6, A_{1g}$ (0.70)	2435.308
$\nu_4 + 2\nu_6, F_{2u}$ (0.97)	1312.086	$2\nu_5 + 4\nu_6, A_{2g}$ (0.78)	2435.511
$\nu_4 + 2\nu_6, F_{1u}$ (-0.91)	1312.366	$2\nu_5 + 4\nu_6, F_{2g}$ (-0.56)	2435.768
$\nu_2 + 2\nu_6, E_g$ (0.87)	1334.482	$7\nu_6, F_{2u}$ (-0.66)	2435.846
$\nu_2 + 2\nu_6, F_{1g}$ (0.95)	1336.030	$4\nu_5 + \nu_6, F_{2u}$ (-0.56)	2436.103
$\nu_2 + 2\nu_6, A_{1g}$ (-0.94)	1337.012	$4\nu_5 + \nu_6, E_u$ (-0.87)	2436.207
$\nu_2 + 2\nu_6, F_{2g}$ (0.95)	1338.041	$4\nu_5 + \nu_6, F_{1u}$ (-0.67)	2436.499
$\nu_2 + 2\nu_6, E_g$ (-0.86)	1339.851	$2\nu_5 + 4\nu_6, F_{1g}$ (-0.70)	2437.237
$\nu_2 + 2\nu_6, A_{2g}$ (0.96)	1340.996	$4\nu_5 + \nu_6, F_{2u}$ (-0.69)	2437.288
$4\nu_6, A_{1g}$ (0.80)	1385.897	$2\nu_5 + 4\nu_6, F_{2g}$ (0.53)	2437.664
$4\nu_6, F_{2g}$ (0.78)	1387.122	$2\nu_5 + 4\nu_6, F_{1g}$ (-0.85)	2437.761
$\nu_1 + \nu_4, F_{1u}$ (0.92)	1388.319	$4\nu_5 + \nu_6, E_u$ (0.82)	2437.956
$2\nu_5 + \nu_6, F_{2u}$ (-0.83)	1390.690	$4\nu_5 + \nu_6, F_{1u}$ (-0.91)	2437.988
$4\nu_6, E_g$ (-0.76)	1390.870	$4\nu_5 + \nu_6, A_{2u}$ (0.99)	2438.312
$2\nu_5 + \nu_6, E_u$ (0.96)	1391.853	$7\nu_6, E_u$ (0.69)	2438.561
$2\nu_5 + \nu_6, F_{1u}$ (-0.82)	1392.348	$2\nu_5 + 4\nu_6, E_g$ (-0.74)	2438.624
$4\nu_6, F_{2g}$ (0.78)	1393.138	$2\nu_5 + 4\nu_6, F_{1g}$ (-0.65)	2438.899
$2\nu_5 + \nu_6, F_{2u}$ (-0.94)	1393.307	$4\nu_5 + \nu_6, F_{2u}$ (0.62)	2439.124
$2\nu_5 + \nu_6, A_{1u}$ (-0.96)	1393.811	$4\nu_5 + \nu_6, F_{2u}$ (-0.72)	2439.227
$2\nu_5 + \nu_6, F_{1u}$ (-0.81)	1394.357	$4\nu_5 + \nu_6, A_{1u}$ (-0.97)	2439.435
$2\nu_5 + \nu_6, F_{2u}$ (-0.83)	1394.418	$2\nu_5 + 4\nu_6, A_{1g}$ (-0.67)	2439.664
$4\nu_6, F_{1g}$ (0.96)	1395.997	$2\nu_5 + 4\nu_6, E_g$ (-0.64)	2440.042
$4\nu_6, E_g$ (0.76)	1396.725	$4\nu_5 + \nu_6, F_{1u}$ (-0.74)	2440.299
$4\nu_6, A_{1g}$ (0.80)	1398.244	$4\nu_5 + \nu_6, E_u$ (0.79)	2440.419
$\nu_1 + \nu_2, E_g$ (0.90)	1415.516	$2\nu_5 + 4\nu_6, F_{1g}$ (-0.48)	2440.904
$\nu_1 + 2\nu_6, A_{1g}$ (-0.92)	1467.550	$2\nu_5 + 4\nu_6, A_{1g}$ (0.47)	2441.209
$\nu_3 + \nu_5, F_{1u}$ (-0.95)	1468.719	$2\nu_5 + 4\nu_6, F_{2g}$ (0.57)	2441.285
$\nu_3 + \nu_5, F_{2u}$ (-0.95)	1468.792	$7\nu_6, F_{2u}$ (0.60)	2442.025
$\nu_1 + 2\nu_6, F_{2g}$ (0.92)	1469.180	$4\nu_5 + \nu_6, F_{2u}$ (0.85)	2442.181
$\nu_1 + 2\nu_6, E_g$ (-0.92)	1471.135	$2\nu_5 + 4\nu_6, A_{2g}$ (0.61)	2442.229
$\nu_3 + \nu_5, A_{2u}$ (0.95)	1472.144	$2\nu_5 + 4\nu_6, F_{2g}$ (0.65)	2442.482
$\nu_3 + \nu_5, E_u$ (-0.95)	1472.375	$4\nu_5 + \nu_6, F_{1u}$ (0.92)	2442.685
$\nu_4 + \nu_5 + \nu_6, F_{1g}$ (-0.90)	1483.235	$4\nu_5 + \nu_6, F_{2u}$ (0.85)	2442.739
$\nu_4 + \nu_5 + \nu_6, F_{2g}$ (0.95)	1484.098	$2\nu_5 + 4\nu_6, E_g$ (-0.60)	2442.877
$\nu_4 + \nu_5 + \nu_6, F_{1g}$ (0.82)	1484.253	$2\nu_4 + \nu_5 + 2\nu_6, F_{2g}$ (-0.52)	2443.159
$\nu_4 + \nu_5 + \nu_6, A_{1g}$ (0.96)	1484.271	$2\nu_4 + \nu_5 + 2\nu_6, F_{2g}$ (0.69)	2443.424
$\nu_4 + \nu_5 + \nu_6, E_g$ (-0.96)	1484.379	$2\nu_4 + \nu_5 + 2\nu_6, F_{1g}$ (0.66)	2443.522
$\nu_4 + \nu_5 + \nu_6, F_{1g}$ (0.84)	1485.255	$2\nu_4 + \nu_5 + 2\nu_6, F_{1g}$ (-0.61)	2443.771
$\nu_4 + \nu_5 + \nu_6, F_{2g}$ (0.80)	1485.368	$2\nu_4 + \nu_5 + 2\nu_6, A_{1g}$ (-0.84)	2443.790
$\nu_4 + \nu_5 + \nu_6, F_{2g}$ (0.79)	1485.450	$2\nu_4 + \nu_5 + 2\nu_6, F_{2g}$ (0.77)	2443.902
$\nu_4 + \nu_5 + \nu_6, E_g$ (-0.96)	1485.600	$2\nu_4 + \nu_5 + 2\nu_6, E_g$ (0.89)	2443.978
$\nu_4 + \nu_5 + \nu_6, A_{2g}$ (-0.97)	1485.723	$2\nu_4 + \nu_5 + 2\nu_6, F_{2g}$ (0.63)	2443.989
$\nu_4 + \nu_5 + \nu_6, F_{1g}$ (-0.81)	1485.924	$3\nu_2 + \nu_5, F_{1g}$ (0.63)	2444.102
$\nu_2 + \nu_5 + \nu_6, F_{2u}$ (-0.78)	1509.780	$2\nu_4 + \nu_5 + 2\nu_6, E_g$ (0.72)	2444.177
$\nu_2 + \nu_5 + \nu_6, F_{1u}$ (-0.77)	1509.814	$2\nu_4 + \nu_5 + 2\nu_6, F_{1g}$ (0.78)	2444.200
$\nu_2 + \nu_5 + \nu_6, E_u$ (0.95)	1510.174	$2\nu_4 + \nu_5 + 2\nu_6, A_{1g}$ (0.90)	2444.277
$\nu_2 + \nu_5 + \nu_6, A_{1u}$ (-0.96)	1512.076	$7\nu_6, F_{1u}$ (-0.57)	2444.384
$\nu_2 + \nu_5 + \nu_6, E_u$ (0.96)	1512.122	$2\nu_4 + \nu_5 + 2\nu_6, F_{2g}$ (-0.59)	2444.401
$\nu_2 + \nu_5 + \nu_6, A_{2u}$ (0.96)	1512.189	$2\nu_4 + \nu_5 + 2\nu_6, F_{1g}$ (-0.52)	2444.529

Table 1 – continued

Band, Sym, Eig	Band center	Band, Sym, Eig	Band center
$\nu_2 + \nu_5 + \nu_6, F_{2u}$ (0.78)	1513.584	$2\nu_4 + \nu_5 + 2\nu_6, E_g$ (-0.81)	2444.908
$\nu_2 + \nu_5 + \nu_6, F_{1u}$ (0.77)	1513.619	$2\nu_4 + \nu_5 + 2\nu_6, A_{2g}$ (-0.88)	2445.041
$2\nu_1, A_{1g}$ (0.86)	1547.375	$2\nu_4 + \nu_5 + 2\nu_6, F_{2g}$ (0.70)	2445.164
$\nu_5 + 3\nu_6, A_{1u}$ (-0.71)	1560.175	$2\nu_4 + \nu_5 + 2\nu_6, F_{1g}$ (-0.66)	2445.324
$\nu_3 + \nu_4, E_g$ (-0.95)	1560.810	$2\nu_4 + \nu_5 + 2\nu_6, A_{1g}$ (-0.85)	2445.340
$\nu_3 + \nu_4, F_{1g}$ (-0.96)	1561.070	$2\nu_4 + \nu_5 + 2\nu_6, E_g$ (-0.72)	2445.352
$\nu_5 + 3\nu_6, F_{1u}$ (0.77)	1561.120	$2\nu_4 + \nu_5 + 2\nu_6, F_{1g}$ (-0.64)	2445.464
$\nu_3 + \nu_4, F_{2g}$ (-0.96)	1561.399	$2\nu_4 + \nu_5 + 2\nu_6, F_{2g}$ (-0.69)	2445.584
$\nu_5 + 3\nu_6, F_{2u}$ (0.79)	1561.656	$2\nu_4 + \nu_5 + 2\nu_6, F_{2g}$ (-0.62)	2445.795
$\nu_5 + 3\nu_6, E_u$ (0.84)	1561.725	$2\nu_4 + \nu_5 + 2\nu_6, F_{1g}$ (-0.50)	2445.901
$\nu_3 + \nu_4, A_{1g}$ (-0.95)	1561.842	$3\nu_2 + \nu_5, F_{2g}$ (0.79)	2446.142
$\nu_5 + 3\nu_6, F_{2u}$ (-0.74)	1562.869	$2\nu_4 + \nu_5 + 2\nu_6, F_{1g}$ (0.55)	2446.256
$\nu_5 + 3\nu_6, E_u$ (-0.69)	1564.544	$2\nu_4 + \nu_5 + 2\nu_6, E_g$ (-0.62)	2446.403
$\nu_5 + 3\nu_6, A_{2u}$ (-0.96)	1565.058	$7\nu_6, F_{2u}$ (0.55)	2446.489
$\nu_5 + 3\nu_6, F_{1u}$ (0.90)	1565.722	$2\nu_4 + \nu_5 + 2\nu_6, F_{2g}$ (0.58)	2446.549
$\nu_5 + 3\nu_6, F_{2u}$ (0.60)	1565.920	$2\nu_4 + \nu_5 + 2\nu_6, A_{2g}$ (0.92)	2446.674
$\nu_5 + 3\nu_6, F_{2u}$ (0.66)	1568.080	$2\nu_4 + \nu_5 + 2\nu_6, E_g$ (-0.93)	2446.959
$\nu_5 + 3\nu_6, E_u$ (0.63)	1568.476	$2\nu_4 + \nu_5 + 2\nu_6, A_{1g}$ (-0.92)	2446.962
$3\nu_5, A_{1g}$ (0.96)	1568.663	$2\nu_4 + \nu_5 + 2\nu_6, F_{2g}$ (-0.88)	2447.020
$\nu_5 + 3\nu_6, F_{1u}$ (-0.73)	1569.193	$3\nu_2 + \nu_5, F_{1g}$ (-0.70)	2447.396
$\nu_5 + 3\nu_6, A_{1u}$ (0.74)	1569.239	$2\nu_4 + \nu_5 + 2\nu_6, F_{2g}$ (0.70)	2447.979
$3\nu_5, F_{2g}$ (0.96)	1569.725	$2\nu_4 + \nu_5 + 2\nu_6, F_{1g}$ (0.76)	2447.984
$3\nu_5, F_{1g}$ (0.96)	1569.951	$2\nu_4 + \nu_5 + 2\nu_6, F_{1g}$ (0.74)	2448.061
$3\nu_5, F_{2g}$ (-0.96)	1572.225	$2\nu_4 + \nu_5 + 2\nu_6, F_{2g}$ (-0.68)	2448.159
$2\nu_4 + \nu_6, F_{2u}$ (0.58)	1576.605	$2\nu_4 + \nu_5 + 2\nu_6, A_{2g}$ (-0.95)	2448.282
$2\nu_4 + \nu_6, F_{1u}$ (0.97)	1576.935	$2\nu_4 + \nu_5 + 2\nu_6, F_{2g}$ (0.70)	2448.316
$2\nu_4 + \nu_6, F_{2u}$ (-0.74)	1577.090	$2\nu_4 + \nu_5 + 2\nu_6, E_g$ (-0.86)	2448.369
$2\nu_4 + \nu_6, F_{1u}$ (0.97)	1577.181	$2\nu_4 + \nu_5 + 2\nu_6, F_{1g}$ (0.78)	2448.393
$2\nu_4 + \nu_6, A_{1u}$ (-0.97)	1577.309	$2\nu_4 + \nu_5 + 2\nu_6, F_{2g}$ (0.52)	2448.500
$2\nu_4 + \nu_6, E_u$ (-0.97)	1577.315	$2\nu_4 + \nu_5 + 2\nu_6, F_{1g}$ (-0.61)	2448.730
$2\nu_4 + \nu_6, F_{2u}$ (-0.79)	1578.311	$2\nu_4 + \nu_5 + 2\nu_6, F_{1g}$ (0.68)	2448.897
$\nu_2 + \nu_3, F_{1u}$ (0.93)	1587.909	$2\nu_4 + \nu_5 + 2\nu_6, A_{1g}$ (-0.82)	2448.911
$\nu_2 + \nu_3, F_{2u}$ (-0.94)	1591.091	$2\nu_4 + \nu_5 + 2\nu_6, E_g$ (0.77)	2449.134
$\nu_2 + \nu_4 + \nu_6, A_{2g}$ (0.96)	1602.402	$2\nu_4 + \nu_5 + 2\nu_6, F_{2g}$ (-0.51)	2449.197
$\nu_2 + \nu_4 + \nu_6, E_g$ (-0.81)	1602.836	$3\nu_2 + \nu_5, F_{2g}$ (-0.46)	2449.223
$\nu_2 + \nu_4 + \nu_6, F_{2g}$ (0.86)	1602.931	$7\nu_6, E_u$ (-0.68)	2450.056
$\nu_2 + \nu_4 + \nu_6, F_{1g}$ (-0.85)	1602.949	$7\nu_6, F_{1u}$ (0.75)	2450.928
$\nu_2 + \nu_4 + \nu_6, A_{1g}$ (-0.95)	1604.821	$\nu_2 + \nu_3 + \nu_5 + \nu_6, E_g$ (-0.70)	2451.255
$\nu_2 + \nu_4 + \nu_6, F_{1g}$ (0.85)	1604.933	$\nu_2 + \nu_3 + \nu_5 + \nu_6, F_{1g}$ (-0.81)	2451.606
$\nu_2 + \nu_4 + \nu_6, F_{2g}$ (-0.86)	1604.940	$\nu_1 + \nu_2 + 3\nu_6, F_{2u}$ (-0.67)	2451.607
$\nu_2 + \nu_4 + \nu_6, E_g$ (0.82)	1605.491	$3\nu_2 + \nu_5, F_{2g}$ (-0.70)	2451.742
$2\nu_2 + \nu_6, F_{2u}$ (0.69)	1629.779	$\nu_2 + \nu_3 + \nu_5 + \nu_6, A_{1g}$ (0.91)	2451.852
$2\nu_2 + \nu_6, F_{1u}$ (0.89)	1631.343	$7\nu_6, A_{1u}$ (0.77)	2451.920
$2\nu_2 + \nu_6, F_{2u}$ (0.70)	1634.023	$\nu_2 + \nu_3 + \nu_5 + \nu_6, A_{2g}$ (0.81)	2451.927
$\nu_3 + 2\nu_6, F_{1u}$ (-0.89)	1639.582	$\nu_2 + \nu_3 + \nu_5 + \nu_6, F_{1g}$ (0.47)	2452.350
$\nu_3 + 2\nu_6, F_{1u}$ (-0.87)	1640.967	$\nu_2 + \nu_3 + \nu_5 + \nu_6, E_g$ (0.62)	2452.562
$\nu_3 + 2\nu_6, F_{2u}$ (-0.88)	1641.092	$7\nu_6, F_{2u}$ (0.60)	2452.893
$\nu_3 + 2\nu_6, E_u$ (-0.90)	1641.218	$\nu_1 + \nu_2 + 3\nu_6, F_{1u}$ (0.82)	2453.002
$\nu_1 + \nu_5 + \nu_6, A_{1u}$ (0.91)	1641.942	$\nu_2 + \nu_3 + \nu_5 + \nu_6, F_{2g}$ (-0.94)	2453.071
$\nu_3 + 2\nu_6, A_{2u}$ (-0.96)	1642.411	$\nu_2 + \nu_3 + \nu_5 + \nu_6, F_{2g}$ (-0.88)	2454.811
$\nu_1 + \nu_5 + \nu_6, F_{1u}$ (0.61)	1642.649	$\nu_1 + \nu_2 + 3\nu_6, E_u$ (0.94)	2455.209
$\nu_3 + 2\nu_6, F_{2u}$ (0.74)	1643.345	$7\nu_6, F_{1u}$ (-0.59)	2455.942
$\nu_3 + 2\nu_6, F_{1u}$ (0.66)	1643.484	$\nu_2 + \nu_3 + \nu_5 + \nu_6, E_g$ (0.60)	2456.025
$\nu_1 + \nu_5 + \nu_6, E_u$ (-0.87)	1644.153	$\nu_1 + \nu_2 + 2\nu_5, F_{2g}$ (0.73)	2456.027
$\nu_1 + \nu_5 + \nu_6, F_{2u}$ (-0.73)	1644.694	$\nu_2 + \nu_3 + \nu_5 + \nu_6, F_{1g}$ (0.89)	2456.037

Table 1 – continued

Band, Sym, Eig	Band center	Band, Sym, Eig	Band center
$\nu_4 + 3\nu_6, E_g$ (0.80)	1654.825	$\nu_2 + \nu_3 + \nu_5 + \nu_6, F_{1g}$ (0.69)	2456.297
$\nu_4 + 3\nu_6, F_{2g}$ (-0.82)	1655.094	$\nu_1 + \nu_2 + 3\nu_6, F_{2u}$ (-0.66)	2456.383
$\nu_4 + 3\nu_6, F_{1g}$ (-0.79)	1655.503	$\nu_2 + \nu_3 + \nu_5 + \nu_6, F_{1g}$ (0.80)	2456.408
$\nu_4 + 3\nu_6, A_{2g}$ (-0.84)	1656.444	$\nu_2 + \nu_3 + \nu_5 + \nu_6, A_{2g}$ (-0.83)	2456.628
$\nu_4 + 3\nu_6, F_{1g}$ (0.92)	1657.593	$\nu_1 + \nu_2 + 2\nu_5, E_g$ (-0.67)	2456.650
$\nu_4 + 3\nu_6, A_{1g}$ (-0.96)	1659.154	$\nu_2 + \nu_3 + \nu_5 + \nu_6, A_{1g}$ (0.89)	2456.798
$\nu_4 + 3\nu_6, F_{2g}$ (-0.95)	1659.166	$\nu_1 + \nu_2 + 2\nu_5, A_{2g}$ (-0.91)	2456.847
$\nu_4 + 3\nu_6, E_g$ (0.91)	1659.469	$\nu_2 + \nu_3 + \nu_5 + \nu_6, F_{2g}$ (-0.70)	2457.271
$\nu_4 + 3\nu_6, F_{1g}$ (-0.92)	1660.071	$\nu_2 + \nu_3 + \nu_5 + \nu_6, E_g$ (0.69)	2457.390
$\nu_4 + 2\nu_5, F_{1u}$ (-0.93)	1660.248	$\nu_2 + \nu_3 + \nu_5 + \nu_6, F_{1g}$ (-0.82)	2457.508
$\nu_4 + 2\nu_5, E_u$ (0.96)	1660.643	$\nu_1 + \nu_2 + 3\nu_6, F_{1u}$ (-0.87)	2457.546
$\nu_4 + 2\nu_5, F_{2u}$ (-0.96)	1660.653	$7\nu_6, F_{2u}$ (0.54)	2457.578
$\nu_4 + 2\nu_5, A_{2u}$ (0.96)	1660.876	$4\nu_4, A_{1g}$ (0.94)	2457.660
$\nu_4 + 3\nu_6, A_{2g}$ (-0.83)	1660.916	$4\nu_4, E_g$ (-0.99)	2457.726
$\nu_4 + 2\nu_5, F_{1u}$ (-0.85)	1661.465	$\nu_2 + \nu_3 + \nu_5 + \nu_6, F_{2g}$ (0.71)	2458.066
$\nu_4 + 3\nu_6, F_{2g}$ (0.81)	1661.528	$4\nu_4, F_{2g}$ (-0.97)	2458.103
$\nu_4 + 3\nu_6, F_{1g}$ (0.77)	1661.825	$\nu_1 + \nu_2 + 2\nu_5, F_{1g}$ (-0.69)	2458.207
$\nu_4 + 2\nu_5, F_{1u}$ (-0.84)	1661.866	$4\nu_4, F_{1g}$ (-1.00)	2458.430
$\nu_4 + 2\nu_5, F_{2u}$ (0.96)	1662.004	$4\nu_4, A_{1g}$ (-0.94)	2458.440
$\nu_4 + 3\nu_6, E_g$ (-0.76)	1662.336	$4\nu_4, E_g$ (0.99)	2458.532
$\nu_2 + 3\nu_6, F_{2u}$ (-0.66)	1680.134	$\nu_1 + \nu_2 + 3\nu_6, F_{2u}$ (-0.61)	2458.600
$\nu_2 + 3\nu_6, F_{1u}$ (-0.82)	1681.563	$4\nu_4, F_{2g}$ (-0.97)	2458.658
$\nu_2 + 3\nu_6, E_u$ (0.94)	1683.821	$\nu_2 + \nu_3 + \nu_5 + \nu_6, F_{2g}$ (-0.55)	2458.753
$\nu_2 + 3\nu_6, F_{2u}$ (0.66)	1684.934	$\nu_2 + \nu_3 + \nu_5 + \nu_6, F_{2g}$ (0.65)	2459.278
$\nu_2 + 3\nu_6, F_{1u}$ (0.87)	1686.146	$\nu_2 + \nu_3 + \nu_5 + \nu_6, F_{1g}$ (0.60)	2459.476
$\nu_2 + 2\nu_5, F_{2g}$ (-0.95)	1686.291	$\nu_1 + \nu_2 + 2\nu_5, E_g$ (0.68)	2460.727
$\nu_2 + 2\nu_5, E_g$ (-0.70)	1686.420	$\nu_1 + \nu_2 + 2\nu_5, A_{1g}$ (-0.93)	2460.889
$\nu_2 + 2\nu_5, A_{2g}$ (-0.95)	1686.574	$\nu_1 + \nu_2 + 3\nu_6, F_{1u}$ (-0.84)	2461.537
$\nu_2 + 3\nu_6, F_{2u}$ (-0.62)	1687.169	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, E_u$ (0.77)	2467.462
$\nu_2 + 2\nu_5, F_{1g}$ (-0.95)	1688.343	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, F_{2u}$ (-0.73)	2467.505
$\nu_2 + 3\nu_6, F_{1u}$ (-0.84)	1690.140	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, F_{1u}$ (0.69)	2467.604
$\nu_2 + 2\nu_5, E_g$ (-0.70)	1690.492	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, A_{1u}$ (0.91)	2467.800
$\nu_2 + 2\nu_5, A_{1g}$ (0.95)	1690.636	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, A_{2u}$ (0.78)	2467.927
$\nu_1 + \nu_3, F_{1u}$ (-0.89)	1719.823	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, F_{2u}$ (0.56)	2468.254
$5\nu_6, F_{2u}$ (-0.62)	1731.769	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, E_u$ (0.58)	2468.365
$5\nu_6, A_{1u}$ (0.94)	1733.198	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, F_{1u}$ (0.62)	2468.507
$\nu_1 + \nu_4 + \nu_6, E_g$ (-0.92)	1735.211	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, F_{2u}$ (0.53)	2468.805
$2\nu_5 + 2\nu_6, A_{1g}$ (0.82)	1735.251	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, E_u$ (0.49)	2469.017
$\nu_1 + \nu_4 + \nu_6, F_{2g}$ (-0.92)	1735.587	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, F_{1u}$ (-0.42)	2469.080
$\nu_1 + \nu_4 + \nu_6, F_{1g}$ (-0.92)	1735.614	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, F_{2u}$ (0.53)	2469.081
$2\nu_5 + 2\nu_6, F_{1g}$ (-0.58)	1736.195	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, A_{2u}$ (0.71)	2469.196
$\nu_1 + \nu_4 + \nu_6, A_{2g}$ (-0.92)	1736.469	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, F_{2u}$ (0.52)	2469.309
$2\nu_5 + 2\nu_6, F_{2g}$ (0.93)	1736.538	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, F_{1u}$ (-0.50)	2469.728
$5\nu_6, F_{1u}$ (0.67)	1737.074	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, E_u$ (0.76)	2470.114
$2\nu_5 + 2\nu_6, F_{2g}$ (-0.72)	1737.297	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, A_{1u}$ (0.78)	2470.166
$2\nu_5 + 2\nu_6, E_g$ (0.71)	1737.443	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, F_{1u}$ (-0.73)	2470.256
$2\nu_5 + 2\nu_6, A_{1g}$ (0.94)	1737.583	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, F_{2u}$ (0.61)	2470.336
$2\nu_5 + 2\nu_6, E_g$ (0.82)	1737.921	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, F_{1u}$ (-0.75)	2470.545
$2\nu_5 + 2\nu_6, F_{1g}$ (0.74)	1738.780	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, A_{2u}$ (0.56)	2470.557
$2\nu_5 + 2\nu_6, F_{2g}$ (0.92)	1739.275	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, A_{1u}$ (-0.92)	2470.560
$5\nu_6, F_{2u}$ (-0.64)	1740.022	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, F_{2u}$ (0.56)	2470.563
$2\nu_5 + 2\nu_6, F_{2g}$ (0.69)	1740.068	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, F_{1u}$ (-0.45)	2470.933
$2\nu_5 + 2\nu_6, E_g$ (0.93)	1741.257	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, E_u$ (-0.52)	2471.012
$2\nu_5 + 2\nu_6, A_{2g}$ (0.95)	1741.842	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, E_u$ (0.80)	2471.131
$2\nu_5 + 2\nu_6, F_{2g}$ (0.64)	1741.869	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, F_{2u}$ (-0.50)	2471.329

Table 1 – continued

Band, Sym, Eig	Band center	Band, Sym, Eig	Band center
$2\nu_5 + 2\nu_6, F_{1g}$ (0.72)	1742.343	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, F_{1u}$ (0.66)	2472.438
$2\nu_5 + 2\nu_6, E_g$ (-0.82)	1742.846	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, E_u$ (0.62)	2472.735
$2\nu_5 + 2\nu_6, A_{1g}$ (-0.85)	1742.868	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, F_{1u}$ (-0.70)	2472.748
$5\nu_6, E_u$ (-0.94)	1743.366	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, F_{2u}$ (-0.79)	2472.770
$5\nu_6, F_{2u}$ (-0.69)	1744.735	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, A_{2u}$ (0.90)	2473.492
$5\nu_6, F_{1u}$ (0.67)	1746.671	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, F_{1u}$ (0.79)	2473.503
$5\nu_6, F_{2u}$ (0.66)	1748.850	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, F_{2u}$ (-0.56)	2473.605
$2\nu_4 + \nu_5, F_{2g}$ (-0.65)	1751.775	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, F_{1u}$ (0.67)	2473.754
$2\nu_4 + \nu_5, F_{2g}$ (-0.82)	1752.293	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, E_u$ (0.62)	2473.848
$2\nu_4 + \nu_5, F_{1g}$ (-0.78)	1752.410	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, F_{2u}$ (-0.61)	2473.968
$2\nu_4 + \nu_5, E_g$ (0.96)	1752.527	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, A_{1u}$ (0.72)	2474.067
$2\nu_4 + \nu_5, F_{2g}$ (0.69)	1752.565	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, E_u$ (0.55)	2474.468
$2\nu_4 + \nu_5, F_{1g}$ (-0.78)	1752.646	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, A_{2u}$ (0.76)	2474.555
$2\nu_4 + \nu_5, A_{1g}$ (-0.96)	1752.762	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, F_{2u}$ (0.67)	2474.835
$\nu_1 + \nu_2 + \nu_6, F_{2u}$ (0.90)	1760.978	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, F_{1u}$ (0.61)	2474.853
$\nu_1 + \nu_2 + \nu_6, F_{1u}$ (0.90)	1763.110	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, A_{1u}$ (-0.88)	2475.368
$\nu_2 + \nu_4 + \nu_5, E_u$ (-0.76)	1777.899	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, E_u$ (0.66)	2475.585
$\nu_2 + \nu_4 + \nu_5, F_{2u}$ (-0.82)	1777.985	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, F_{1u}$ (0.71)	2475.978
$\nu_2 + \nu_4 + \nu_5, F_{1u}$ (-0.78)	1778.051	$\nu_2 + \nu_4 + \nu_5 + 2\nu_6, F_{2u}$ (0.77)	2475.991
$\nu_2 + \nu_4 + \nu_5, A_{1u}$ (-0.96)	1778.215	$\nu_2 + 3\nu_4, F_{1u}$ (-0.98)	2483.266
$\nu_2 + \nu_4 + \nu_5, E_u$ (0.76)	1779.743	$\nu_2 + 3\nu_4, F_{2u}$ (0.76)	2483.795
$\nu_2 + \nu_4 + \nu_5, A_{2u}$ (-0.96)	1779.933	$\nu_2 + 3\nu_4, F_{1u}$ (0.75)	2483.827
$\nu_2 + \nu_4 + \nu_5, F_{1u}$ (0.78)	1780.195	$\nu_2 + 3\nu_4, F_{2u}$ (0.91)	2484.144
$\nu_2 + \nu_4 + \nu_5, F_{2u}$ (-0.82)	1780.254	$\nu_2 + 3\nu_4, E_u$ (-1.00)	2484.251
$2\nu_2 + \nu_5, F_{2g}$ (0.70)	1804.942	$\nu_2 + 3\nu_4, F_{1u}$ (0.76)	2484.344
$2\nu_2 + \nu_5, F_{1g}$ (0.91)	1806.682	$\nu_2 + 3\nu_4, F_{2u}$ (-0.68)	2484.366
$2\nu_2 + \nu_5, F_{2g}$ (0.71)	1808.833	$2\nu_1 + \nu_3, F_{1u}$ (0.81)	2489.876
$\nu_3 + \nu_5 + \nu_6, F_{1g}$ (0.85)	1813.722	$2\nu_2 + \nu_5 + 2\nu_6, F_{2g}$ (-0.63)	2492.029
$\nu_3 + \nu_5 + \nu_6, A_{1g}$ (-0.93)	1813.842	$2\nu_2 + \nu_5 + 2\nu_6, F_{1g}$ (-0.68)	2493.318
$\nu_1 + 3\nu_6, F_{2u}$ (0.77)	1814.121	$2\nu_2 + \nu_5 + 2\nu_6, E_g$ (-0.68)	2493.394
$\nu_3 + \nu_5 + \nu_6, F_{1g}$ (-0.72)	1814.206	$2\nu_2 + \nu_5 + 2\nu_6, A_{1g}$ (0.78)	2493.707
$\nu_3 + \nu_5 + \nu_6, E_g$ (0.89)	1814.257	$2\nu_2 + \nu_5 + 2\nu_6, F_{2g}$ (-0.59)	2494.031
$\nu_3 + \nu_5 + \nu_6, F_{2g}$ (0.72)	1814.511	$2\nu_2 + \nu_5 + 2\nu_6, F_{1g}$ (0.77)	2495.366
$\nu_3 + \nu_5 + \nu_6, F_{2g}$ (-0.91)	1815.112	$2\nu_2 + \nu_5 + 2\nu_6, F_{2g}$ (0.57)	2495.561
$\nu_3 + \nu_5 + \nu_6, E_g$ (0.89)	1815.407	$2\nu_2 + \nu_5 + 2\nu_6, F_{1g}$ (0.70)	2495.843
$\nu_3 + \nu_5 + \nu_6, A_{2g}$ (-0.95)	1815.801	$2\nu_2 + \nu_5 + 2\nu_6, F_{1g}$ (0.50)	2496.685
$\nu_1 + 3\nu_6, A_{1u}$ (-0.91)	1816.401	$2\nu_2 + \nu_5 + 2\nu_6, A_{2g}$ (-0.95)	2496.692
$\nu_3 + \nu_5 + \nu_6, F_{1g}$ (-0.85)	1817.664	$2\nu_2 + \nu_5 + 2\nu_6, F_{2g}$ (-0.81)	2497.112
$\nu_1 + 2\nu_5, F_{2g}$ (0.58)	1818.022	$2\nu_2 + \nu_5 + 2\nu_6, E_g$ (0.66)	2497.559
$\nu_1 + 3\nu_6, F_{1u}$ (-0.91)	1818.309	$2\nu_2 + \nu_5 + 2\nu_6, F_{2g}$ (-0.63)	2497.908
$\nu_3 + \nu_5 + \nu_6, F_{1g}$ (0.75)	1818.513	$2\nu_2 + \nu_5 + 2\nu_6, F_{2g}$ (0.58)	2498.763
$\nu_1 + 2\nu_5, F_{2g}$ (-0.67)	1819.371	$2\nu_2 + \nu_5 + 2\nu_6, F_{1g}$ (0.76)	2499.319
$\nu_1 + 2\nu_5, A_{1g}$ (-0.89)	1819.783	$2\nu_2 + \nu_5 + 2\nu_6, F_{1g}$ (0.70)	2500.122
$\nu_1 + 2\nu_5, E_g$ (0.89)	1820.106	$2\nu_3 + \nu_4, F_{1u}$ (0.93)	2500.597
$\nu_1 + 3\nu_6, F_{2u}$ (-0.77)	1820.439	$2\nu_2 + \nu_5 + 2\nu_6, E_g$ (-0.62)	2500.832
$\nu_4 + \nu_5 + 2\nu_6, A_{2u}$ (0.95)	1829.322	$2\nu_2 + \nu_5 + 2\nu_6, F_{2g}$ (-0.62)	2501.137
$\nu_4 + \nu_5 + 2\nu_6, E_u$ (-0.64)	1829.426	$2\nu_2 + \nu_5 + 2\nu_6, A_{1g}$ (0.70)	2501.255
$\nu_4 + \nu_5 + 2\nu_6, F_{2u}$ (-0.86)	1829.679	$2\nu_2 + \nu_5 + 2\nu_6, F_{2g}$ (-0.51)	2502.845
$\nu_4 + \nu_5 + 2\nu_6, F_{1u}$ (-0.78)	1829.753	$\nu_3 + \nu_5 + 3\nu_6, F_{1g}$ (0.64)	2503.134
$\nu_4 + \nu_5 + 2\nu_6, F_{1u}$ (0.88)	1829.952	$2\nu_3 + \nu_4, F_{1u}$ (0.92)	2503.192
$\nu_4 + \nu_5 + 2\nu_6, E_u$ (0.74)	1830.080	$2\nu_3 + \nu_4, F_{2u}$ (0.93)	2503.346
$\nu_4 + \nu_5 + 2\nu_6, F_{2u}$ (0.71)	1830.231	$\nu_3 + \nu_5 + 3\nu_6, F_{1g}$ (0.57)	2503.661
$\nu_4 + \nu_5 + 2\nu_6, F_{1u}$ (-0.89)	1831.032	$\nu_3 + \nu_5 + 3\nu_6, A_{1g}$ (-0.61)	2503.767
$\nu_4 + \nu_5 + 2\nu_6, A_{2u}$ (-0.87)	1831.133	$\nu_3 + \nu_5 + 3\nu_6, E_g$ (-0.73)	2503.861
$\nu_4 + \nu_5 + 2\nu_6, F_{2u}$ (-0.74)	1831.168	$\nu_3 + \nu_5 + 3\nu_6, F_{2g}$ (-0.57)	2504.127

Table 1 – continued

Band, Sym, Eig	Band center	Band, Sym, Eig	Band center
$\nu_4 + \nu_5 + 2\nu_6, A_{1u}$ (0.89)	1831.377	$\nu_3 + \nu_5 + 3\nu_6, F_{2g}$ (-0.57)	2504.283
$\nu_4 + \nu_5 + 2\nu_6, F_{1u}$ (-0.81)	1831.506	$2\nu_2 + \nu_5 + 2\nu_6, F_{1g}$ (-0.69)	2504.315
$\nu_4 + \nu_5 + 2\nu_6, E_u$ (-0.79)	1831.749	$\nu_3 + \nu_5 + 3\nu_6, E_g$ (0.76)	2504.527
$\nu_4 + \nu_5 + 2\nu_6, F_{2u}$ (0.83)	1832.137	$\nu_3 + \nu_5 + 3\nu_6, A_{2g}$ (-0.89)	2504.730
$\nu_4 + \nu_5 + 2\nu_6, F_{1u}$ (-0.91)	1832.844	$\nu_3 + \nu_5 + 3\nu_6, F_{1g}$ (0.76)	2505.211
$\nu_4 + \nu_5 + 2\nu_6, A_{2u}$ (-0.89)	1833.745	$\nu_3 + \nu_5 + 3\nu_6, F_{2g}$ (-0.74)	2505.312
$\nu_4 + \nu_5 + 2\nu_6, F_{2u}$ (-0.75)	1833.931	$\nu_3 + \nu_5 + 3\nu_6, F_{1g}$ (0.64)	2506.356
$\nu_4 + \nu_5 + 2\nu_6, E_u$ (0.82)	1833.935	$\nu_3 + \nu_5 + 3\nu_6, E_g$ (-0.70)	2506.396
$\nu_4 + \nu_5 + 2\nu_6, A_{1u}$ (0.89)	1834.030	$2\nu_1 + \nu_4 + \nu_6, E_g$ (0.93)	2506.571
$\nu_4 + \nu_5 + 2\nu_6, F_{2u}$ (-0.71)	1834.134	$\nu_1 + 5\nu_6, F_{2u}$ (-0.62)	2506.785
$\nu_4 + \nu_5 + 2\nu_6, F_{1u}$ (0.73)	1834.188	$2\nu_1 + \nu_4 + \nu_6, F_{2g}$ (-0.92)	2506.953
$\nu_4 + \nu_5 + 2\nu_6, E_u$ (0.77)	1834.349	$2\nu_1 + \nu_4 + \nu_6, F_{1g}$ (0.88)	2506.999
$\nu_4 + \nu_5 + 2\nu_6, F_{1u}$ (0.69)	1834.588	$\nu_3 + \nu_5 + 3\nu_6, F_{1g}$ (0.60)	2507.024
$3\nu_4, F_{1u}$ (-0.92)	1843.793	$\nu_3 + \nu_5 + 3\nu_6, F_{2g}$ (-0.58)	2507.063
$3\nu_4, F_{1u}$ (-0.91)	1844.186	$\nu_1 + 2\nu_5 + 2\nu_6, A_{1g}$ (0.82)	2507.220
$3\nu_4, F_{2u}$ (-0.97)	1844.246	$\nu_3 + \nu_5 + 3\nu_6, A_{2g}$ (0.82)	2507.235
$3\nu_4, A_{2u}$ (0.97)	1844.371	$\nu_3 + \nu_5 + 3\nu_6, F_{2g}$ (0.64)	2507.342
$\nu_2 + \nu_5 + 2\nu_6, F_{1g}$ (-0.86)	1854.239	$2\nu_3 + \nu_4, F_{2u}$ (-0.94)	2507.442
$\nu_2 + \nu_5 + 2\nu_6, F_{2g}$ (0.71)	1855.067	$\nu_3 + \nu_5 + 3\nu_6, F_{1g}$ (0.62)	2507.542
$\nu_2 + \nu_5 + 2\nu_6, A_{2g}$ (0.93)	1855.174	$\nu_3 + \nu_5 + 3\nu_6, E_g$ (-0.77)	2507.571
$\nu_2 + \nu_5 + 2\nu_6, F_{2g}$ (-0.62)	1855.786	$2\nu_3 + \nu_4, E_u$ (0.94)	2507.639
$\nu_2 + \nu_5 + 2\nu_6, E_g$ (-0.78)	1855.876	$2\nu_1 + \nu_4 + \nu_6, A_{2g}$ (-0.93)	2507.865
$\nu_2 + \nu_5 + 2\nu_6, F_{1g}$ (-0.77)	1856.994	$2\nu_3 + \nu_4, A_{2u}$ (0.94)	2508.128
$\nu_2 + \nu_5 + 2\nu_6, F_{1g}$ (0.68)	1857.122	$\nu_1 + 5\nu_6, A_{1u}$ (-0.94)	2508.136
$\nu_2 + \nu_5 + 2\nu_6, F_{2g}$ (-0.59)	1857.557	$\nu_1 + 2\nu_5 + 2\nu_6, F_{2g}$ (0.43)	2508.150
$\nu_2 + \nu_5 + 2\nu_6, A_{1g}$ (0.93)	1859.055	$2\nu_3 + \nu_4, F_{1u}$ (-0.93)	2508.164
$\nu_2 + \nu_5 + 2\nu_6, F_{2g}$ (0.86)	1859.481	$\nu_3 + \nu_5 + 3\nu_6, A_{1g}$ (0.85)	2508.247
$\nu_2 + \nu_5 + 2\nu_6, E_g$ (0.78)	1860.268	$\nu_1 + 2\nu_5 + 2\nu_6, F_{1g}$ (-0.54)	2508.421
$\nu_2 + \nu_5 + 2\nu_6, F_{1g}$ (0.74)	1860.411	$\nu_3 + \nu_5 + 3\nu_6, F_{2g}$ (0.56)	2508.495
$\nu_2 + \nu_5 + 2\nu_6, F_{2g}$ (-0.71)	1861.272	$\nu_1 + 2\nu_5 + 2\nu_6, F_{2g}$ (-0.67)	2508.634
$\nu_2 + \nu_5 + 2\nu_6, F_{1g}$ (-0.87)	1862.390	$\nu_3 + \nu_5 + 3\nu_6, F_{1g}$ (-0.58)	2508.835
$\nu_2 + 2\nu_4, E_g$ (0.75)	1870.275	$\nu_1 + 2\nu_5 + 2\nu_6, E_g$ (0.54)	2509.401
$\nu_2 + 2\nu_4, A_{1g}$ (-0.96)	1870.351	$\nu_3 + \nu_5 + 3\nu_6, F_{2g}$ (-0.55)	2509.478
$\nu_2 + 2\nu_4, F_{1g}$ (-0.96)	1870.629	$\nu_3 + \nu_5 + 3\nu_6, A_{2g}$ (0.79)	2509.539
$\nu_2 + 2\nu_4, E_g$ (-0.75)	1870.873	$\nu_3 + 3\nu_5, F_{1u}$ (-0.71)	2509.627
$\nu_2 + 2\nu_4, F_{2g}$ (-0.96)	1870.929	$\nu_3 + 3\nu_5, F_{2u}$ (-0.70)	2509.674
$\nu_2 + 2\nu_4, A_{2g}$ (-0.96)	1870.936	$\nu_3 + \nu_5 + 3\nu_6, F_{1g}$ (-0.56)	2509.691
$2\nu_3, A_{1g}$ (-0.93)	1889.355	$\nu_1 + 2\nu_5 + 2\nu_6, A_{1g}$ (-0.91)	2509.817
$2\nu_3, E_g$ (0.93)	1892.005	$\nu_1 + 2\nu_5 + 2\nu_6, E_g$ (0.63)	2510.011
$2\nu_1 + \nu_6, F_{2u}$ (0.86)	1894.402	$\nu_1 + 2\nu_5 + 2\nu_6, F_{2g}$ (-0.50)	2510.045
$2\nu_3, F_{2g}$ (-0.94)	1896.537	$2\nu_2 + 2\nu_4, E_g$ (-0.68)	2510.261
$2\nu_2 + \nu_4, F_{1u}$ (0.85)	1898.139	$2\nu_2 + 2\nu_4, A_{1g}$ (-0.80)	2510.281
$2\nu_2 + \nu_4, F_{2u}$ (0.91)	1898.277	$\nu_3 + \nu_5 + 3\nu_6, E_g$ (0.55)	2510.284
$2\nu_2 + \nu_4, F_{1u}$ (-0.88)	1898.950	$\nu_3 + \nu_5 + 3\nu_6, A_{2g}$ (-0.75)	2510.462
$\nu_5 + 4\nu_6, F_{2g}$ (-0.67)	1905.731	$2\nu_2 + 2\nu_4, E_g$ (0.75)	2510.646
$\nu_5 + 4\nu_6, F_{2g}$ (-0.66)	1906.220	$2\nu_2 + 2\nu_4, A_{2g}$ (-0.97)	2510.704
$\nu_5 + 4\nu_6, E_g$ (-0.78)	1906.924	$\nu_1 + 2\nu_5 + 2\nu_6, F_{1g}$ (0.60)	2510.704
$\nu_3 + \nu_4 + \nu_6, F_{2u}$ (-0.81)	1907.012	$2\nu_2 + 2\nu_4, F_{2g}$ (0.89)	2510.704
$\nu_3 + \nu_4 + \nu_6, F_{1u}$ (-0.64)	1907.189	$2\nu_2 + 2\nu_4, F_{1g}$ (-0.97)	2510.803
$\nu_3 + \nu_4 + \nu_6, A_{2u}$ (0.91)	1907.388	$\nu_3 + \nu_5 + 3\nu_6, E_g$ (-0.46)	2511.084
$\nu_3 + \nu_4 + \nu_6, F_{2u}$ (-0.75)	1907.406	$\nu_3 + \nu_5 + 3\nu_6, F_{1g}$ (0.48)	2511.301
$\nu_5 + 4\nu_6, F_{1g}$ (0.74)	1907.433	$\nu_1 + 2\nu_5 + 2\nu_6, F_{2g}$ (0.86)	2511.471
$\nu_3 + \nu_4 + \nu_6, F_{1u}$ (-0.86)	1907.527	$2\nu_2 + 2\nu_4, A_{1g}$ (-0.83)	2511.474
$\nu_3 + \nu_4 + \nu_6, E_u$ (-0.88)	1907.628	$2\nu_2 + 2\nu_4, F_{2g}$ (-0.92)	2511.492
$\nu_5 + 4\nu_6, A_{1g}$ (-0.77)	1907.724	$2\nu_2 + 2\nu_4, E_g$ (0.86)	2511.552

Table 1 – continued

Band, Sym, Eig	Band center	Band, Sym, Eig	Band center
$\nu_3 + \nu_4 + \nu_6, F_{1u}$ (0.70)	1907.953	$\nu_1 + 2\nu_5 + 2\nu_6, F_{2g}$ (-0.47)	2511.804
$\nu_3 + \nu_4 + \nu_6, F_{2u}$ (0.62)	1907.964	$\nu_3 + \nu_5 + 3\nu_6, A_{1g}$ (-0.74)	2511.882
$\nu_3 + \nu_4 + \nu_6, E_u$ (0.91)	1908.279	$\nu_1 + 5\nu_6, F_{1u}$ (-0.67)	2511.914
$\nu_3 + \nu_4 + \nu_6, A_{1u}$ (0.96)	1908.483	$\nu_3 + 3\nu_5, F_{1u}$ (0.97)	2512.001
$\nu_3 + \nu_4 + \nu_6, F_{2u}$ (0.75)	1908.987	$\nu_3 + 3\nu_5, F_{1u}$ (0.97)	2512.053
$\nu_1 + \nu_4 + \nu_5, A_{2u}$ (0.87)	1910.013	$\nu_3 + 3\nu_5, F_{2u}$ (0.98)	2512.062
$\nu_1 + \nu_4 + \nu_5, F_{2u}$ (-0.87)	1910.482	$\nu_3 + \nu_5 + 3\nu_6, E_g$ (-0.59)	2512.171
$\nu_1 + \nu_4 + \nu_5, E_u$ (0.88)	1910.500	$\nu_3 + \nu_5 + 3\nu_6, F_{2g}$ (-0.52)	2512.273
$\nu_1 + \nu_4 + \nu_5, F_{1u}$ (-0.88)	1910.588	$\nu_1 + 2\nu_5 + 2\nu_6, F_{2g}$ (-0.56)	2512.549
$\nu_5 + 4\nu_6, F_{1g}$ (-0.71)	1910.596	$\nu_3 + \nu_5 + 3\nu_6, F_{1g}$ (-0.54)	2512.813
$\nu_5 + 4\nu_6, A_{1g}$ (0.78)	1911.033	$\nu_3 + 3\nu_5, A_{2u}$ (-0.98)	2512.927
$\nu_5 + 4\nu_6, F_{2g}$ (-0.73)	1911.188	$\nu_3 + 3\nu_5, E_u$ (-0.98)	2513.193
$\nu_5 + 4\nu_6, F_{1g}$ (0.69)	1911.740	$\nu_3 + 3\nu_5, E_u$ (0.98)	2513.230
$3\nu_5 + \nu_6, F_{2u}$ (-0.64)	1912.062	$\nu_3 + \nu_5 + 3\nu_6, F_{1g}$ (0.56)	2513.366
$3\nu_5 + \nu_6, E_u$ (0.67)	1912.834	$\nu_3 + 3\nu_5, A_{1u}$ (-0.98)	2513.464
$\nu_5 + 4\nu_6, F_{2g}$ (-0.51)	1913.285	$\nu_1 + 2\nu_5 + 2\nu_6, E_g$ (-0.89)	2513.520
$\nu_5 + 4\nu_6, E_g$ (-0.72)	1913.960	$\nu_1 + 2\nu_5 + 2\nu_6, F_{2g}$ (-0.45)	2513.774
$3\nu_5 + \nu_6, F_{2u}$ (0.76)	1914.298	$\nu_1 + 2\nu_5 + 2\nu_6, A_{2g}$ (-0.91)	2514.208
$3\nu_5 + \nu_6, A_{1u}$ (0.77)	1914.326	$\nu_3 + \nu_5 + 3\nu_6, F_{1g}$ (0.47)	2514.672
$3\nu_5 + \nu_6, A_{2u}$ (-0.96)	1914.505	$\nu_1 + 5\nu_6, F_{2u}$ (0.65)	2514.773
$3\nu_5 + \nu_6, F_{1u}$ (0.77)	1914.555	$\nu_1 + 2\nu_5 + 2\nu_6, F_{1g}$ (0.49)	2514.862
$\nu_5 + 4\nu_6, F_{2g}$ (0.59)	1915.171	$\nu_1 + 2\nu_5 + 2\nu_6, A_{1g}$ (-0.79)	2515.205
$\nu_5 + 4\nu_6, F_{1g}$ (-0.67)	1915.237	$\nu_1 + 2\nu_5 + 2\nu_6, E_g$ (-0.77)	2515.238
$3\nu_5 + \nu_6, F_{1u}$ (-0.73)	1915.377	$\nu_3 + \nu_5 + 3\nu_6, F_{2g}$ (0.51)	2515.479
$\nu_5 + 4\nu_6, A_{2g}$ (-0.94)	1915.881	$\nu_3 + 3\nu_5, F_{1u}$ (0.70)	2516.585
$3\nu_5 + \nu_6, E_u$ (-0.65)	1916.291	$\nu_3 + 3\nu_5, F_{2u}$ (0.70)	2516.871
$3\nu_5 + \nu_6, F_{2u}$ (0.66)	1916.607	$\nu_1 + 5\nu_6, E_u$ (0.94)	2517.966
$\nu_5 + 4\nu_6, E_g$ (0.84)	1917.428	$\nu_3 + 2\nu_4 + \nu_6, A_{2g}$ (-0.72)	2519.214
$\nu_5 + 4\nu_6, F_{2g}$ (-0.64)	1917.710	$\nu_1 + 5\nu_6, F_{2u}$ (0.70)	2519.365
$3\nu_5 + \nu_6, E_u$ (0.76)	1917.783	$\nu_3 + 2\nu_4 + \nu_6, E_g$ (-0.60)	2519.577
$3\nu_5 + \nu_6, F_{2u}$ (-0.89)	1917.886	$\nu_3 + 2\nu_4 + \nu_6, F_{1g}$ (0.59)	2519.578
$3\nu_5 + \nu_6, A_{1u}$ (-0.79)	1918.175	$\nu_3 + 2\nu_4 + \nu_6, A_{1g}$ (-0.91)	2519.708
$3\nu_5 + \nu_6, F_{1u}$ (0.82)	1918.345	$\nu_3 + 2\nu_4 + \nu_6, F_{2g}$ (0.65)	2519.756
$\nu_5 + 4\nu_6, F_{1g}$ (0.64)	1918.740	$\nu_3 + 2\nu_4 + \nu_6, F_{1g}$ (-0.57)	2519.952
$\nu_5 + 4\nu_6, F_{2g}$ (0.68)	1919.634	$\nu_3 + 2\nu_4 + \nu_6, F_{2g}$ (-0.55)	2520.024
$2\nu_4 + 2\nu_6, A_{1g}$ (0.93)	1922.603	$\nu_3 + 2\nu_4 + \nu_6, E_g$ (0.68)	2520.029
$2\nu_4 + 2\nu_6, F_{2g}$ (-0.93)	1922.906	$\nu_3 + 2\nu_4 + \nu_6, A_{2g}$ (0.75)	2520.123
$2\nu_4 + 2\nu_6, E_g$ (-0.95)	1922.909	$\nu_3 + 2\nu_4 + \nu_6, E_g$ (-0.78)	2520.264
$2\nu_4 + 2\nu_6, F_{2g}$ (0.67)	1924.155	$\nu_3 + 2\nu_4 + \nu_6, F_{1g}$ (0.80)	2520.301
$2\nu_4 + 2\nu_6, F_{1g}$ (0.79)	1924.177	$\nu_3 + 2\nu_4 + \nu_6, F_{2g}$ (-0.69)	2520.337
$2\nu_4 + 2\nu_6, E_g$ (-0.91)	1924.363	$\nu_3 + 2\nu_4 + \nu_6, A_{1g}$ (-0.90)	2520.381
$2\nu_4 + 2\nu_6, F_{2g}$ (0.82)	1924.621	$\nu_3 + 2\nu_4 + \nu_6, F_{2g}$ (0.66)	2520.605
$2\nu_4 + 2\nu_6, F_{1g}$ (0.75)	1924.853	$\nu_3 + 2\nu_4 + \nu_6, F_{1g}$ (0.58)	2520.702
$2\nu_4 + 2\nu_6, A_{1g}$ (0.74)	1924.936	$\nu_3 + 2\nu_4 + \nu_6, F_{2g}$ (-0.59)	2520.915
$2\nu_4 + 2\nu_6, F_{2g}$ (-0.67)	1925.295	$\nu_3 + 2\nu_4 + \nu_6, E_g$ (-0.68)	2520.951
$3\nu_2, A_{2g}$ (-0.76)	1925.865	$\nu_3 + 2\nu_4 + \nu_6, F_{1g}$ (0.70)	2520.960
$2\nu_4 + 2\nu_6, E_g$ (0.85)	1926.478	$\nu_3 + 2\nu_4 + \nu_6, F_{1g}$ (0.60)	2521.204
$2\nu_4 + 2\nu_6, A_{2g}$ (-0.99)	1926.569	$\nu_1 + 5\nu_6, F_{1u}$ (-0.67)	2521.249
$2\nu_4 + 2\nu_6, E_g$ (0.84)	1926.752	$\nu_3 + 2\nu_4 + \nu_6, E_g$ (-0.61)	2521.262
$2\nu_4 + 2\nu_6, F_{2g}$ (0.93)	1926.916	$\nu_3 + 2\nu_4 + \nu_6, F_{2g}$ (-0.61)	2521.947
$3\nu_2, A_{1g}$ (0.86)	1927.053	$\nu_3 + 2\nu_4 + \nu_6, F_{1g}$ (-0.68)	2522.146
$2\nu_4 + 2\nu_6, F_{1g}$ (-0.88)	1927.221	$\nu_3 + 3\nu_5, E_u$ (-0.98)	2522.565
$2\nu_4 + 2\nu_6, A_{1g}$ (0.80)	1927.565	$\nu_3 + 3\nu_5, A_{2u}$ (-0.98)	2522.579
$3\nu_2, E_g$ (0.85)	1927.634	$\nu_3 + 2\nu_4 + \nu_6, A_{2g}$ (0.87)	2522.669
$\nu_2 + \nu_3 + \nu_6, E_g$ (0.66)	1932.514	$\nu_1 + 2\nu_4 + \nu_5, F_{2g}$ (-0.61)	2523.064

Table 1 – continued

Band, Sym, Eig	Band center	Band, Sym, Eig	Band center
$\nu_2 + \nu_3 + \nu_6, F_{1g}$ (-0.87)	1933.657	$\nu_1 + 5\nu_6, F_{2u}$ (0.66)	2523.430
$\nu_2 + \nu_3 + \nu_6, F_{2g}$ (0.91)	1934.435	$\nu_1 + 2\nu_4 + \nu_5, F_{2g}$ (0.82)	2523.594
$\nu_2 + \nu_3 + \nu_6, A_{2g}$ (0.76)	1934.659	$\nu_1 + 2\nu_4 + \nu_5, F_{1g}$ (-0.82)	2523.703
$\nu_1 + \nu_2 + \nu_5, F_{1g}$ (-0.83)	1935.910	$\nu_1 + 2\nu_4 + \nu_5, E_g$ (0.94)	2523.798
$\nu_2 + \nu_3 + \nu_6, F_{2g}$ (0.79)	1936.379	$\nu_1 + 2\nu_4 + \nu_5, F_{2g}$ (0.68)	2523.820
$\nu_2 + \nu_3 + \nu_6, F_{1g}$ (-0.93)	1937.229	$\nu_1 + 2\nu_4 + \nu_5, F_{1g}$ (0.82)	2523.892
$\nu_2 + \nu_3 + \nu_6, E_g$ (-0.65)	1937.558	$\nu_1 + 2\nu_4 + \nu_5, A_{1g}$ (-0.95)	2523.991
$\nu_1 + \nu_2 + \nu_5, F_{2g}$ (-0.78)	1938.063	$\nu_4 + 3\nu_5 + \nu_6, F_{1g}$ (-0.61)	2525.388
$\nu_2 + \nu_3 + \nu_6, A_{1g}$ (0.86)	1938.577	$\nu_4 + 3\nu_5 + \nu_6, E_g$ (-0.75)	2525.667
$\nu_2 + \nu_4 + 2\nu_6, F_{1u}$ (0.86)	1947.946	$\nu_4 + 3\nu_5 + \nu_6, F_{2g}$ (0.60)	2526.080
$\nu_2 + \nu_4 + 2\nu_6, F_{2u}$ (-0.89)	1948.247	$\nu_4 + 3\nu_5 + \nu_6, A_{2g}$ (0.68)	2526.670
$\nu_2 + \nu_4 + 2\nu_6, F_{2u}$ (0.87)	1949.425	$\nu_4 + 3\nu_5 + \nu_6, F_{1g}$ (0.64)	2526.701
$\nu_2 + \nu_4 + 2\nu_6, F_{1u}$ (0.66)	1949.719	$\nu_2 + 2\nu_3, E_g$ (-0.73)	2526.792
$\nu_2 + \nu_4 + 2\nu_6, E_u$ (-0.70)	1949.827	$\nu_4 + 3\nu_5 + \nu_6, F_{2g}$ (0.65)	2526.839
$\nu_2 + \nu_4 + 2\nu_6, A_{1u}$ (-0.98)	1949.844	$\nu_4 + 3\nu_5 + \nu_6, F_{2g}$ (-0.63)	2527.696
$\nu_2 + \nu_4 + 2\nu_6, F_{1u}$ (0.64)	1950.704	$\nu_4 + 3\nu_5 + \nu_6, E_g$ (0.60)	2527.862
$\nu_2 + \nu_4 + 2\nu_6, E_u$ (-0.70)	1951.540	$\nu_4 + 3\nu_5 + \nu_6, F_{1g}$ (0.69)	2528.001
$\nu_2 + \nu_4 + 2\nu_6, A_{2u}$ (0.97)	1951.573	$\nu_2 + 2\nu_3, A_{1g}$ (0.88)	2528.030
$\nu_2 + \nu_4 + 2\nu_6, F_{1u}$ (0.68)	1951.801	$\nu_4 + 3\nu_5 + \nu_6, F_{1g}$ (-0.73)	2528.286
$\nu_2 + \nu_4 + 2\nu_6, F_{2u}$ (0.83)	1951.830	$\nu_4 + 3\nu_5 + \nu_6, F_{2g}$ (0.72)	2528.332
$\nu_2 + \nu_4 + 2\nu_6, F_{1u}$ (-0.64)	1953.496	$\nu_4 + 3\nu_5 + \nu_6, E_g$ (0.57)	2528.383
$\nu_2 + \nu_4 + 2\nu_6, F_{2u}$ (-0.75)	1953.638	$\nu_4 + 3\nu_5 + \nu_6, A_{2g}$ (0.83)	2528.394
$\nu_2 + \nu_4 + 2\nu_6, F_{2u}$ (-0.80)	1954.750	$\nu_4 + 3\nu_5 + \nu_6, A_{1g}$ (0.82)	2528.539
$2\nu_2 + 2\nu_6, A_{1g}$ (-0.79)	1973.805	$\nu_4 + 3\nu_5 + \nu_6, F_{2g}$ (0.70)	2528.597
$2\nu_2 + 2\nu_6, E_g$ (-0.78)	1974.181	$\nu_4 + 3\nu_5 + \nu_6, F_{1g}$ (-0.74)	2528.755
$2\nu_2 + 2\nu_6, F_{2g}$ (0.72)	1975.735	$\nu_4 + 3\nu_5 + \nu_6, F_{1g}$ (0.58)	2529.062
$2\nu_2 + 2\nu_6, F_{1g}$ (-0.92)	1977.576	$\nu_4 + 3\nu_5 + \nu_6, F_{2g}$ (0.74)	2529.263
$2\nu_2 + 2\nu_6, E_g$ (-0.71)	1977.794	$\nu_4 + 3\nu_5 + \nu_6, A_{1g}$ (-0.79)	2529.408
$2\nu_2 + 2\nu_6, A_{2g}$ (-0.89)	1979.141	$\nu_4 + 3\nu_5 + \nu_6, E_g$ (0.69)	2529.457
$2\nu_2 + 2\nu_6, F_{2g}$ (0.74)	1979.675	$\nu_4 + 3\nu_5 + \nu_6, A_{2g}$ (-0.69)	2530.101
$2\nu_2 + 2\nu_6, A_{1g}$ (-0.74)	1982.289	$\nu_4 + 3\nu_5 + \nu_6, F_{2g}$ (-0.65)	2530.149
$2\nu_2 + 2\nu_6, E_g$ (0.70)	1983.250	$\nu_4 + 3\nu_5 + \nu_6, F_{1g}$ (0.62)	2530.219
$\nu_3 + 3\nu_6, E_g$ (-0.68)	1985.196	$\nu_4 + 3\nu_5 + \nu_6, E_g$ (-0.69)	2530.499
$\nu_3 + 3\nu_6, F_{2g}$ (0.71)	1985.263	$\nu_4 + 3\nu_5 + \nu_6, F_{2g}$ (0.69)	2530.570
$\nu_3 + 3\nu_6, A_{2g}$ (-0.73)	1985.410	$\nu_4 + 3\nu_5 + \nu_6, F_{1g}$ (0.58)	2530.577
$\nu_3 + 3\nu_6, F_{1g}$ (0.79)	1985.983	$2\nu_1 + \nu_2 + \nu_6, F_{2u}$ (0.92)	2531.337
$\nu_3 + 3\nu_6, F_{1g}$ (-0.84)	1987.639	$\nu_4 + 3\nu_5 + \nu_6, F_{2g}$ (-0.89)	2531.405
$\nu_1 + \nu_5 + 2\nu_6, F_{2g}$ (-0.66)	1988.219	$\nu_4 + 3\nu_5 + \nu_6, F_{1g}$ (0.51)	2531.418
$\nu_1 + \nu_5 + 2\nu_6, F_{2g}$ (0.60)	1988.603	$\nu_4 + 3\nu_5 + \nu_6, F_{2g}$ (-0.76)	2531.704
$\nu_3 + 2\nu_5, A_{2u}$ (-0.95)	1988.795	$\nu_4 + 3\nu_5 + \nu_6, F_{1g}$ (-0.60)	2531.723
$\nu_3 + 2\nu_5, E_u$ (0.95)	1988.884	$\nu_4 + 3\nu_5 + \nu_6, A_{2g}$ (0.96)	2531.914
$\nu_3 + 3\nu_6, A_{1g}$ (-0.82)	1989.050	$\nu_4 + 3\nu_5 + \nu_6, E_g$ (0.93)	2531.958
$\nu_1 + \nu_5 + 2\nu_6, E_g$ (-0.73)	1989.069	$\nu_4 + 3\nu_5 + \nu_6, F_{2g}$ (0.77)	2532.037
$\nu_3 + 3\nu_6, F_{1g}$ (-0.64)	1989.451	$\nu_4 + 3\nu_5 + \nu_6, F_{1g}$ (0.74)	2532.153
$\nu_3 + 3\nu_6, F_{2g}$ (-0.84)	1989.664	$\nu_4 + 3\nu_5 + \nu_6, A_{1g}$ (-0.87)	2532.409
$\nu_3 + 2\nu_5, F_{1u}$ (-0.78)	1989.958	$\nu_4 + 3\nu_5 + \nu_6, E_g$ (0.86)	2532.446
$\nu_3 + 2\nu_5, F_{2u}$ (-0.95)	1990.160	$\nu_4 + 3\nu_5 + \nu_6, F_{1g}$ (-0.74)	2532.566
$\nu_3 + 3\nu_6, E_g$ (-0.80)	1990.328	$2\nu_1 + \nu_2 + \nu_6, F_{1u}$ (0.92)	2533.454
$\nu_1 + \nu_5 + 2\nu_6, F_{1g}$ (-0.70)	1990.632	$\nu_2 + 2\nu_3, E_g$ (-0.75)	2533.601
$\nu_3 + 3\nu_6, E_g$ (0.67)	1991.206	$\nu_2 + 2\nu_3, F_{1g}$ (-0.92)	2534.499
$\nu_3 + 3\nu_6, A_{2g}$ (0.68)	1991.402	$\nu_2 + 2\nu_3, A_{2g}$ (-0.92)	2534.699
$\nu_1 + \nu_5 + 2\nu_6, F_{1g}$ (-0.56)	1991.591	$\nu_2 + 2\nu_3, F_{2g}$ (0.91)	2537.470
$\nu_1 + \nu_5 + 2\nu_6, A_{1g}$ (-0.81)	1991.706	$3\nu_2 + \nu_4, F_{2u}$ (-0.83)	2537.592
$\nu_3 + 3\nu_6, F_{2g}$ (-0.58)	1992.033	$3\nu_2 + \nu_4, F_{1u}$ (0.83)	2538.564
$\nu_3 + 2\nu_5, F_{1u}$ (0.95)	1992.317	$3\nu_2 + \nu_4, F_{1u}$ (-0.83)	2539.177

Table 1 – continued

Band, Sym, Eig	Band center	Band, Sym, Eig	Band center
$\nu_3 + 2\nu_5$, F_{2u} (-0.95)	1992.482	$3\nu_2 + \nu_4$, F_{2u} (0.91)	2539.565
$\nu_3 + 3\nu_6$, F_{2g} (0.58)	1993.230	$\nu_2 + \nu_3 + \nu_4 + \nu_6$, F_{2u} (0.73)	2544.286
$\nu_1 + \nu_5 + 2\nu_6$, F_{1g} (0.59)	1993.325	$\nu_2 + \nu_3 + \nu_4 + \nu_6$, F_{1u} (-0.58)	2544.487
$\nu_3 + 2\nu_5$, F_{1u} (0.78)	1997.119	$\nu_2 + \nu_3 + \nu_4 + \nu_6$, F_{1u} (-0.64)	2545.489
$\nu_4 + 4\nu_6$, F_{1u} (0.78)	2000.322	$\nu_2 + \nu_3 + \nu_4 + \nu_6$, F_{2u} (0.44)	2545.718
$\nu_4 + 4\nu_6$, F_{2u} (-0.80)	2001.265	$\nu_2 + \nu_3 + \nu_4 + \nu_6$, E_u (-0.69)	2545.770
$\nu_4 + 4\nu_6$, E_u (0.77)	2001.574	$\nu_2 + \nu_3 + \nu_4 + \nu_6$, A_{1u} (-0.89)	2545.848
$\nu_1 + 2\nu_4$, A_{1g} (-0.91)	2001.649	$\nu_2 + \nu_3 + \nu_4 + \nu_6$, F_{1u} (-0.63)	2546.138
$\nu_1 + 2\nu_4$, E_g (-0.91)	2001.780	$\nu_2 + \nu_3 + \nu_4 + \nu_6$, F_{2u} (0.48)	2546.371
$\nu_1 + 2\nu_4$, F_{2g} (0.91)	2001.915	$\nu_2 + \nu_3 + \nu_4 + \nu_6$, E_u (-0.63)	2546.524
$\nu_4 + 4\nu_6$, A_{2u} (0.86)	2002.108	$\nu_2 + \nu_3 + \nu_4 + \nu_6$, A_{2u} (0.90)	2546.524
$\nu_4 + 4\nu_6$, F_{1u} (-0.75)	2002.400	$\nu_2 + \nu_3 + \nu_4 + \nu_6$, F_{2u} (0.64)	2546.696
$\nu_4 + 2\nu_5 + \nu_6$, A_{2g} (0.81)	2004.221	$\nu_1 + \nu_2 + \nu_4 + \nu_5$, E_u (-0.77)	2548.096
$\nu_4 + 2\nu_5 + \nu_6$, F_{2g} (0.83)	2004.538	$\nu_1 + \nu_2 + \nu_4 + \nu_5$, F_{2u} (0.80)	2548.161
$\nu_4 + 2\nu_5 + \nu_6$, E_g (-0.83)	2004.982	$\nu_1 + \nu_2 + \nu_4 + \nu_5$, F_{1u} (0.70)	2548.174
$\nu_4 + 2\nu_5 + \nu_6$, F_{1g} (-0.80)	2005.059	$\nu_2 + \nu_3 + \nu_4 + \nu_6$, A_{2u} (-0.83)	2548.285
$\nu_4 + 4\nu_6$, F_{2u} (-0.77)	2005.347	$\nu_2 + \nu_3 + \nu_4 + \nu_6$, E_u (0.61)	2548.286
$\nu_4 + 4\nu_6$, F_{1u} (-0.76)	2005.648	$\nu_2 + \nu_3 + \nu_4 + \nu_6$, F_{2u} (-0.63)	2548.379
$\nu_4 + 2\nu_5 + \nu_6$, F_{2g} (-0.88)	2005.870	$\nu_1 + \nu_2 + \nu_4 + \nu_5$, A_{1u} (-0.89)	2548.384
$\nu_4 + 2\nu_5 + \nu_6$, F_{1g} (0.86)	2006.099	$\nu_2 + \nu_3 + \nu_4 + \nu_6$, F_{1u} (-0.43)	2548.668
$\nu_4 + 2\nu_5 + \nu_6$, E_g (-0.82)	2006.320	$\nu_2 + \nu_3 + \nu_4 + \nu_6$, F_{1u} (0.75)	2548.917
$\nu_4 + 2\nu_5 + \nu_6$, F_{2g} (-0.76)	2006.405	$\nu_2 + \nu_3 + \nu_4 + \nu_6$, E_u (0.72)	2549.053
$\nu_4 + 2\nu_5 + \nu_6$, A_{1g} (0.79)	2006.589	$\nu_2 + \nu_3 + \nu_4 + \nu_6$, A_{1u} (0.93)	2549.063
$\nu_4 + 2\nu_5 + \nu_6$, F_{1g} (-0.71)	2006.792	$\nu_2 + \nu_3 + \nu_4 + \nu_6$, F_{2u} (-0.56)	2549.146
$\nu_4 + 2\nu_5 + \nu_6$, E_g (0.93)	2007.056	$\nu_2 + \nu_3 + \nu_4 + \nu_6$, F_{2u} (0.62)	2549.457
$\nu_4 + 4\nu_6$, E_u (-0.77)	2007.254	$\nu_2 + \nu_3 + \nu_4 + \nu_6$, F_{1u} (0.55)	2549.911
$\nu_4 + 4\nu_6$, F_{1u} (0.79)	2007.345	$\nu_1 + \nu_2 + \nu_4 + \nu_5$, E_u (0.69)	2550.017
$\nu_4 + 2\nu_5 + \nu_6$, F_{1g} (-0.95)	2007.470	$\nu_2 + 3\nu_5 + \nu_6$, A_{2u} (0.58)	2550.127
$\nu_4 + 2\nu_5 + \nu_6$, F_{2g} (-0.96)	2007.486	$\nu_2 + 3\nu_5 + \nu_6$, F_{2u} (-0.65)	2550.182
$\nu_4 + 2\nu_5 + \nu_6$, F_{1g} (-0.95)	2008.032	$\nu_1 + \nu_2 + \nu_4 + \nu_5$, A_{2u} (-0.69)	2550.219
$\nu_4 + 2\nu_5 + \nu_6$, A_{2g} (-0.75)	2008.052	$\nu_1 + \nu_2 + \nu_4 + \nu_5$, F_{1u} (0.70)	2550.478
$\nu_4 + 4\nu_6$, F_{2u} (0.76)	2008.081	$\nu_1 + \nu_2 + \nu_4 + \nu_5$, F_{2u} (0.76)	2550.479
$\nu_4 + 2\nu_5 + \nu_6$, A_{1g} (0.78)	2008.269	$\nu_2 + \nu_3 + \nu_4 + \nu_6$, F_{1u} (0.63)	2550.589
$\nu_4 + 2\nu_5 + \nu_6$, F_{1g} (0.59)	2008.383	$\nu_2 + 3\nu_5 + \nu_6$, E_u (0.59)	2550.639
$\nu_4 + 2\nu_5 + \nu_6$, E_g (0.65)	2008.420	$\nu_2 + 3\nu_5 + \nu_6$, F_{2u} (-0.65)	2551.166
$\nu_4 + 2\nu_5 + \nu_6$, F_{2g} (-0.76)	2008.503	$\nu_2 + 3\nu_5 + \nu_6$, F_{1u} (-0.73)	2551.328
$\nu_4 + 2\nu_5 + \nu_6$, A_{2g} (0.64)	2008.672	$\nu_2 + 3\nu_5 + \nu_6$, E_u (0.80)	2552.348
$\nu_4 + 2\nu_5 + \nu_6$, F_{2g} (-0.79)	2008.700	$\nu_2 + 3\nu_5 + \nu_6$, F_{1u} (-0.60)	2552.369
$\nu_4 + 2\nu_5 + \nu_6$, F_{1g} (0.65)	2008.747	$\nu_2 + 3\nu_5 + \nu_6$, F_{2u} (0.62)	2552.489
$\nu_4 + 4\nu_6$, A_{2u} (0.86)	2008.934	$\nu_2 + 3\nu_5 + \nu_6$, A_{1u} (-0.99)	2552.570
$\nu_4 + 2\nu_5 + \nu_6$, E_g (0.75)	2009.029	$\nu_2 + 3\nu_5 + \nu_6$, F_{1u} (-0.71)	2552.933
$\nu_4 + 4\nu_6$, F_{1u} (0.80)	2010.218	$\nu_2 + 3\nu_5 + \nu_6$, F_{2u} (0.51)	2553.453
$\nu_4 + 4\nu_6$, F_{2u} (0.86)	2010.348	$\nu_2 + 3\nu_5 + \nu_6$, E_u (-0.66)	2554.421
$\nu_4 + 4\nu_6$, E_u (0.98)	2010.610	$\nu_2 + 3\nu_5 + \nu_6$, A_{2u} (-0.93)	2554.612
$\nu_4 + 4\nu_6$, A_{1u} (-0.98)	2010.630	$\nu_2 + 3\nu_5 + \nu_6$, F_{1u} (0.64)	2554.711
$\nu_4 + 4\nu_6$, F_{2u} (-0.65)	2011.650	$\nu_2 + 3\nu_5 + \nu_6$, A_{1u} (0.91)	2554.956
$\nu_4 + 4\nu_6$, F_{1u} (0.65)	2011.763	$\nu_2 + 3\nu_5 + \nu_6$, F_{1u} (-0.61)	2555.355
$\nu_4 + 4\nu_6$, F_{1u} (-0.75)	2013.119	$\nu_2 + 3\nu_5 + \nu_6$, E_u (-0.69)	2555.448
$\nu_2 + 4\nu_6$, E_g (0.73)	2025.079	$\nu_2 + 3\nu_5 + \nu_6$, F_{2u} (-0.66)	2556.136
$\nu_2 + 4\nu_6$, F_{1g} (-0.87)	2026.000	$\nu_2 + 3\nu_5 + \nu_6$, F_{1u} (0.62)	2556.771
$\nu_2 + 4\nu_6$, F_{2g} (-0.69)	2027.711	$\nu_2 + 3\nu_5 + \nu_6$, E_u (-0.59)	2556.874
$\nu_1 + \nu_2 + \nu_4$, F_{1u} (-0.89)	2027.946	$\nu_2 + 3\nu_5 + \nu_6$, A_{2u} (-0.74)	2557.712
$\nu_1 + \nu_2 + \nu_4$, F_{2u} (0.89)	2028.280	$\nu_2 + 3\nu_5 + \nu_6$, F_{2u} (-0.70)	2557.860
$\nu_2 + 4\nu_6$, A_{1g} (-0.82)	2029.730	$\nu_2 + 3\nu_5 + \nu_6$, A_{1u} (0.91)	2558.573
$\nu_2 + 2\nu_5 + \nu_6$, A_{1u} (0.97)	2029.912	$\nu_2 + 3\nu_5 + \nu_6$, E_u (-0.61)	2558.965

Table 1 – continued

Band, Sym, Eig	Band center	Band, Sym, Eig	Band center
$\nu_2 + 2\nu_5 + \nu_6, F_{1u}$ (-0.85)	2029.920	$\nu_2 + 3\nu_5 + \nu_6, F_{1u}$ (-0.77)	2560.526
$\nu_2 + 4\nu_6, A_{2g}$ (-0.90)	2030.344	$\nu_2 + 3\nu_5 + \nu_6, F_{2u}$ (0.78)	2560.633
$\nu_2 + 2\nu_5 + \nu_6, F_{2u}$ (-0.59)	2030.626	$4\nu_2, E_g$ (0.58)	2565.138
$\nu_2 + 2\nu_5 + \nu_6, E_u$ (0.82)	2030.691	$4\nu_2, E_g$ (-0.64)	2568.017
$\nu_2 + 2\nu_5 + \nu_6, F_{1u}$ (-0.86)	2031.028	$4\nu_2, A_{1g}$ (-0.81)	2568.482
$\nu_2 + 4\nu_6, E_g$ (0.66)	2031.781	$2\nu_2 + \nu_3 + \nu_6, A_{2g}$ (0.69)	2569.227
$\nu_2 + 2\nu_5 + \nu_6, F_{2u}$ (0.87)	2031.841	$2\nu_2 + \nu_3 + \nu_6, F_{2g}$ (-0.66)	2571.962
$\nu_2 + 2\nu_5 + \nu_6, F_{2u}$ (-0.62)	2032.484	$2\nu_2 + \nu_3 + \nu_6, E_g$ (-0.69)	2572.645
$\nu_2 + 4\nu_6, F_{2g}$ (0.61)	2032.886	$2\nu_2 + \nu_3 + \nu_6, F_{1g}$ (-0.68)	2572.801
$\nu_2 + 2\nu_5 + \nu_6, F_{1u}$ (0.64)	2033.106	$2\nu_2 + \nu_3 + \nu_6, A_{1g}$ (0.60)	2574.137
$\nu_2 + 4\nu_6, F_{1g}$ (0.87)	2033.401	$\nu_1 + 2\nu_2 + \nu_5, F_{2g}$ (0.66)	2574.186
$\nu_2 + 2\nu_5 + \nu_6, A_{2u}$ (0.97)	2034.104	$2\nu_2 + \nu_3 + \nu_6, F_{1g}$ (0.77)	2574.414
$\nu_2 + 2\nu_5 + \nu_6, F_{1u}$ (-0.92)	2034.317	$2\nu_2 + \nu_3 + \nu_6, F_{2g}$ (-0.84)	2575.023
$\nu_2 + 4\nu_6, E_g$ (0.57)	2034.725	$4\nu_2, E_g$ (-0.56)	2575.750
$\nu_2 + 2\nu_5 + \nu_6, F_{2u}$ (-0.72)	2035.118	$\nu_1 + 2\nu_2 + \nu_5, F_{1g}$ (-0.80)	2576.015
$\nu_2 + 4\nu_6, F_{2g}$ (0.78)	2035.219	$2\nu_2 + \nu_3 + \nu_6, F_{2g}$ (0.54)	2577.030
$\nu_2 + 2\nu_5 + \nu_6, E_u$ (-0.83)	2035.243	$2\nu_2 + \nu_3 + \nu_6, F_{1g}$ (-0.74)	2578.187
$\nu_2 + 4\nu_6, A_{1g}$ (0.83)	2036.398	$\nu_1 + 2\nu_2 + \nu_5, F_{2g}$ (-0.57)	2578.360
$\nu_2 + 2\nu_5 + \nu_6, F_{1u}$ (0.67)	2036.643	$2\nu_3 + 2\nu_6, A_{1g}$ (-0.84)	2579.632
$\nu_2 + 2\nu_5 + \nu_6, F_{2u}$ (0.89)	2036.780	$2\nu_2 + \nu_3 + \nu_6, A_{2g}$ (-0.70)	2580.123
$\nu_2 + 4\nu_6, F_{1g}$ (-0.94)	2038.168	$2\nu_2 + \nu_3 + \nu_6, E_g$ (0.61)	2580.538
$\nu_2 + 4\nu_6, A_{2g}$ (0.90)	2039.267	$2\nu_3 + 2\nu_6, F_{2g}$ (0.85)	2581.152
$\nu_2 + 4\nu_6, E_g$ (0.65)	2040.787	$2\nu_3 + 2\nu_6, E_g$ (-0.77)	2581.860
$\nu_1 + 2\nu_2, E_g$ (0.85)	2055.481	$2\nu_3 + 2\nu_6, F_{1g}$ (-0.82)	2582.808
$\nu_1 + 2\nu_2, A_{1g}$ (-0.87)	2056.070	$2\nu_3 + 2\nu_6, E_g$ (0.85)	2582.872
$\nu_1 + \nu_3 + \nu_6, A_{2g}$ (-0.89)	2065.651	$2\nu_3 + 2\nu_6, F_{2g}$ (0.81)	2583.307
$\nu_1 + \nu_3 + \nu_6, F_{2g}$ (0.83)	2065.722	$\nu_1 + \nu_3 + \nu_5 + \nu_6, A_{1g}$ (-0.72)	2583.523
$\nu_1 + \nu_3 + \nu_6, E_g$ (-0.86)	2065.773	$2\nu_3 + 2\nu_6, E_g$ (-0.52)	2584.073
$\nu_1 + \nu_3 + \nu_6, F_{1g}$ (-0.89)	2066.683	$\nu_1 + \nu_3 + \nu_5 + \nu_6, F_{1g}$ (-0.86)	2584.147
$2\nu_1 + \nu_5, F_{2g}$ (0.79)	2068.983	$\nu_1 + \nu_3 + \nu_5 + \nu_6, F_{2g}$ (0.63)	2584.635
$6\nu_6, A_{1g}$ (-0.80)	2077.095	$\nu_1 + \nu_3 + \nu_5 + \nu_6, F_{1g}$ (-0.68)	2584.804
$6\nu_6, F_{2g}$ (0.66)	2077.936	$2\nu_3 + 2\nu_6, A_{2g}$ (-0.72)	2585.208
$2\nu_5 + 3\nu_6, F_{2u}$ (-0.68)	2080.396	$2\nu_3 + 2\nu_6, A_{1g}$ (-0.74)	2585.214
$\nu_1 + \nu_4 + 2\nu_6, F_{1u}$ (0.94)	2081.108	$\nu_1 + \nu_3 + \nu_5 + \nu_6, E_g$ (0.73)	2585.581
$\nu_3 + \nu_4 + \nu_5, F_{1g}$ (-0.68)	2081.161	$\nu_1 + \nu_3 + \nu_5 + \nu_6, F_{2g}$ (0.78)	2585.680
$\nu_3 + \nu_4 + \nu_5, F_{2g}$ (-0.81)	2081.224	$2\nu_3 + 2\nu_6, F_{2g}$ (0.82)	2586.276
$2\nu_5 + 3\nu_6, F_{2u}$ (-0.51)	2081.301	$2\nu_1 + 3\nu_6, F_{2u}$ (-0.78)	2586.317
$2\nu_5 + 3\nu_6, E_u$ (0.76)	2081.384	$\nu_1 + \nu_3 + \nu_5 + \nu_6, E_g$ (0.68)	2586.422
$\nu_3 + \nu_4 + \nu_5, A_{2g}$ (0.95)	2081.430	$2\nu_3 + 2\nu_6, F_{1g}$ (-0.76)	2586.903
$\nu_3 + \nu_4 + \nu_5, E_g$ (0.70)	2081.464	$\nu_1 + \nu_3 + \nu_5 + \nu_6, A_{2g}$ (-0.70)	2587.137
$\nu_3 + \nu_4 + \nu_5, F_{1g}$ (0.94)	2081.519	$2\nu_3 + 2\nu_6, A_{1g}$ (0.93)	2587.407
$\nu_3 + \nu_4 + \nu_5, F_{2g}$ (0.68)	2081.791	$2\nu_3 + 2\nu_6, E_g$ (-0.87)	2587.676
$\nu_3 + \nu_4 + \nu_5, E_g$ (0.70)	2081.815	$2\nu_3 + 2\nu_6, F_{2g}$ (-0.57)	2587.800
$2\nu_5 + 3\nu_6, F_{1u}$ (-0.83)	2081.826	$\nu_1 + \nu_3 + \nu_5 + \nu_6, F_{1g}$ (-0.60)	2588.311
$\nu_3 + \nu_4 + \nu_5, A_{1g}$ (0.95)	2081.853	$2\nu_1 + 3\nu_6, A_{1u}$ (-0.93)	2588.536
$\nu_1 + \nu_4 + 2\nu_6, F_{2u}$ (0.96)	2082.443	$2\nu_3 + 2\nu_6, F_{2g}$ (0.71)	2588.603
$2\nu_5 + 3\nu_6, A_{1u}$ (0.90)	2082.574	$2\nu_3 + 2\nu_6, F_{1g}$ (-0.55)	2589.216
$2\nu_5 + 3\nu_6, E_u$ (-0.60)	2082.645	$2\nu_3 + 2\nu_6, F_{1g}$ (-0.76)	2589.393
$\nu_1 + \nu_4 + 2\nu_6, E_u$ (0.96)	2082.827	$2\nu_1 + 2\nu_5, F_{2g}$ (-0.66)	2590.065
$\nu_1 + \nu_4 + 2\nu_6, A_{2u}$ (0.97)	2082.846	$2\nu_1 + 3\nu_6, F_{1u}$ (0.91)	2590.422
$2\nu_5 + 3\nu_6, F_{2u}$ (0.77)	2082.856	$2\nu_1 + 2\nu_5, A_{1g}$ (0.90)	2590.741
$2\nu_5 + 3\nu_6, F_{1u}$ (-0.76)	2082.867	$2\nu_3 + 2\nu_6, F_{2g}$ (0.70)	2591.036
$\nu_1 + \nu_4 + 2\nu_6, F_{1u}$ (-0.88)	2083.104	$2\nu_1 + 2\nu_5, E_g$ (0.90)	2591.069
$6\nu_6, E_g$ (0.68)	2083.401	$2\nu_1 + 3\nu_6, F_{2u}$ (-0.73)	2592.537
$2\nu_5 + 3\nu_6, F_{2u}$ (0.59)	2083.643	$\nu_3 + \nu_4 + 3\nu_6, F_{2u}$ (0.47)	2592.728

Table 1 – continued

Band, Sym, Eig	Band center	Band, Sym, Eig	Band center
$\nu_1 + \nu_4 + 2\nu_6, F_{2u}$ (-0.96)	2084.771	$\nu_3 + \nu_4 + 3\nu_6, F_{2u}$ (0.77)	2597.800
$\nu_3 + \nu_4 + \nu_5, F_{2g}$ (-0.70)	2084.870	$\nu_3 + \nu_4 + 3\nu_6, F_{1u}$ (0.59)	2597.903
$6\nu_6, F_{2g}$ (-0.56)	2084.933	$\nu_3 + \nu_4 + 3\nu_6, A_{2u}$ (-0.81)	2597.932
$2\nu_5 + 3\nu_6, F_{1u}$ (0.60)	2084.994	$\nu_3 + \nu_4 + 3\nu_6, F_{1u}$ (-0.69)	2598.033
$\nu_1 + \nu_4 + 2\nu_6, F_{1u}$ (0.88)	2085.062	$\nu_3 + \nu_4 + 3\nu_6, F_{2u}$ (0.61)	2598.239
$\nu_3 + \nu_4 + \nu_5, F_{2g}$ (0.63)	2085.127	$\nu_3 + \nu_4 + 3\nu_6, E_u$ (0.66)	2598.402
$\nu_3 + \nu_4 + \nu_5, F_{1g}$ (-0.68)	2085.225	$\nu_3 + \nu_4 + 3\nu_6, F_{2u}$ (0.50)	2598.691
$2\nu_5 + 3\nu_6, F_{1u}$ (0.63)	2085.300	$\nu_3 + \nu_4 + 3\nu_6, F_{1u}$ (-0.65)	2598.721
$2\nu_5 + 3\nu_6, A_{1u}$ (-0.95)	2085.325	$\nu_3 + \nu_4 + 3\nu_6, E_u$ (0.73)	2598.839
$2\nu_5 + 3\nu_6, F_{2u}$ (-0.60)	2085.392	$\nu_3 + \nu_4 + 3\nu_6, A_{1u}$ (-0.83)	2599.213
$2\nu_5 + 3\nu_6, A_{2u}$ (0.96)	2086.783	$\nu_3 + \nu_4 + 3\nu_6, F_{2u}$ (0.65)	2599.719
$2\nu_5 + 3\nu_6, F_{1u}$ (0.95)	2087.249	$\nu_3 + \nu_4 + 3\nu_6, F_{1u}$ (0.88)	2600.315
$2\nu_5 + 3\nu_6, A_{1u}$ (-0.91)	2087.293	$\nu_3 + \nu_4 + 3\nu_6, E_u$ (0.91)	2600.338
$2\nu_5 + 3\nu_6, F_{2u}$ (-0.67)	2087.651	$\nu_3 + \nu_4 + 3\nu_6, F_{2u}$ (-0.83)	2600.890
$2\nu_5 + 3\nu_6, E_u$ (0.65)	2087.688	$\nu_3 + \nu_4 + 3\nu_6, A_{1u}$ (0.79)	2600.910
$6\nu_6, F_{1g}$ (0.70)	2088.782	$\nu_3 + \nu_4 + 2\nu_5, F_{2g}$ (-0.70)	2601.198
$2\nu_5 + 3\nu_6, F_{2u}$ (-0.78)	2089.284	$\nu_3 + \nu_4 + 2\nu_5, F_{1g}$ (0.73)	2601.252
$2\nu_5 + 3\nu_6, F_{1u}$ (0.58)	2089.464	$\nu_1 + \nu_4 + \nu_5 + 2\nu_6, E_u$ (-0.70)	2601.260
$2\nu_5 + 3\nu_6, F_{2u}$ (-0.49)	2090.595	$\nu_3 + \nu_4 + 2\nu_5, F_{2g}$ (-0.80)	2601.322
$2\nu_5 + 3\nu_6, E_u$ (0.61)	2090.773	$\nu_1 + \nu_4 + \nu_5 + 2\nu_6, A_{2u}$ (0.90)	2601.326
$6\nu_6, A_{1g}$ (-0.79)	2090.872	$\nu_1 + \nu_4 + \nu_5 + 2\nu_6, F_{1u}$ (-0.75)	2601.532
$4\nu_5, F_{2g}$ (0.98)	2091.624	$\nu_1 + \nu_4 + \nu_5 + 2\nu_6, F_{2u}$ (-0.69)	2601.562
$2\nu_5 + 3\nu_6, F_{1u}$ (0.51)	2091.631	$\nu_1 + \nu_4 + \nu_5 + 2\nu_6, F_{2u}$ (-0.47)	2601.631
$2\nu_5 + 3\nu_6, F_{2u}$ (0.57)	2091.895	$\nu_1 + \nu_4 + \nu_5 + 2\nu_6, F_{1u}$ (-0.80)	2601.848
$6\nu_6, E_g$ (-0.64)	2091.996	$\nu_1 + \nu_4 + \nu_5 + 2\nu_6, E_u$ (0.59)	2601.969
$4\nu_5, A_{1g}$ (0.98)	2092.588	$\nu_3 + \nu_4 + 3\nu_6, F_{2u}$ (-0.62)	2601.971
$4\nu_5, E_g$ (-0.98)	2092.925	$\nu_3 + \nu_4 + 3\nu_6, F_{1u}$ (0.69)	2602.028
$4\nu_5, F_{2g}$ (-0.98)	2093.724	$\nu_1 + 3\nu_5 + \nu_6, F_{2u}$ (-0.40)	2602.063
$4\nu_5, F_{1g}$ (0.98)	2094.302	$\nu_3 + \nu_4 + 2\nu_5, E_g$ (0.76)	2602.144
$6\nu_6, F_{2g}$ (0.73)	2095.173	$\nu_3 + \nu_4 + 2\nu_5, F_{1g}$ (0.74)	2602.214
$6\nu_6, F_{1g}$ (-0.70)	2095.760	$\nu_3 + \nu_4 + 3\nu_6, F_{1u}$ (0.54)	2602.219
$2\nu_4 + \nu_5 + \nu_6, E_u$ (-0.82)	2097.197	$\nu_3 + \nu_4 + 3\nu_6, A_{2u}$ (-0.88)	2602.232
$2\nu_4 + \nu_5 + \nu_6, F_{2u}$ (-0.85)	2097.372	$\nu_3 + \nu_4 + 2\nu_5, F_{2g}$ (0.71)	2602.233
$2\nu_4 + \nu_5 + \nu_6, A_{1u}$ (0.97)	2097.404	$\nu_3 + \nu_4 + 3\nu_6, E_u$ (-0.68)	2602.275
$4\nu_5, E_g$ (0.98)	2097.493	$\nu_3 + \nu_4 + 2\nu_5, A_{2g}$ (-0.99)	2602.314
$4\nu_5, A_{1g}$ (0.98)	2097.529	$\nu_3 + \nu_4 + 3\nu_6, F_{1u}$ (-0.63)	2602.474
$2\nu_4 + \nu_5 + \nu_6, F_{1u}$ (-0.82)	2098.087	$\nu_3 + \nu_4 + 2\nu_5, F_{1g}$ (0.66)	2602.610
$2\nu_4 + \nu_5 + \nu_6, A_{2u}$ (0.98)	2098.312	$\nu_3 + \nu_4 + 3\nu_6, F_{2u}$ (0.52)	2602.719
$2\nu_4 + \nu_5 + \nu_6, F_{2u}$ (-0.72)	2098.358	$\nu_3 + \nu_4 + 2\nu_5, A_{1g}$ (0.77)	2602.802
$6\nu_6, A_{2g}$ (-0.95)	2098.361	$\nu_3 + \nu_4 + 3\nu_6, F_{1u}$ (0.49)	2602.818
$2\nu_4 + \nu_5 + \nu_6, F_{1u}$ (-0.88)	2098.379	$\nu_3 + \nu_4 + 3\nu_6, A_{1u}$ (0.50)	2602.907
$2\nu_4 + \nu_5 + \nu_6, E_u$ (0.67)	2098.513	$\nu_3 + \nu_4 + 2\nu_5, F_{2g}$ (0.67)	2602.925
$2\nu_4 + \nu_5 + \nu_6, F_{1u}$ (0.82)	2098.610	$\nu_3 + \nu_4 + 2\nu_5, E_g$ (0.91)	2602.942
$2\nu_4 + \nu_5 + \nu_6, F_{2u}$ (0.67)	2098.666	$\nu_3 + \nu_4 + 3\nu_6, F_{2u}$ (-0.65)	2603.025
$6\nu_6, A_{1g}$ (0.82)	2098.735	$\nu_3 + \nu_4 + 3\nu_6, E_u$ (-0.81)	2603.056
$2\nu_4 + \nu_5 + \nu_6, A_{1u}$ (-0.93)	2099.344	$\nu_1 + \nu_4 + \nu_5 + 2\nu_6, A_{2u}$ (-0.79)	2603.072
$2\nu_4 + \nu_5 + \nu_6, E_u$ (0.75)	2099.365	$\nu_1 + \nu_4 + \nu_5 + 2\nu_6, F_{1u}$ (0.51)	2603.413
$2\nu_4 + \nu_5 + \nu_6, F_{1u}$ (0.71)	2099.526	$\nu_3 + \nu_4 + 3\nu_6, F_{2u}$ (-0.51)	2603.430
$2\nu_4 + \nu_5 + \nu_6, F_{2u}$ (0.72)	2099.534	$\nu_1 + \nu_4 + \nu_5 + 2\nu_6, A_{1u}$ (-0.74)	2603.722
$2\nu_4 + \nu_5 + \nu_6, E_u$ (0.83)	2099.669	$\nu_1 + \nu_4 + \nu_5 + 2\nu_6, F_{1u}$ (-0.60)	2603.814
$2\nu_4 + \nu_5 + \nu_6, A_{2u}$ (0.99)	2099.700	$\nu_3 + \nu_4 + 3\nu_6, F_{2u}$ (0.59)	2603.840
$2\nu_4 + \nu_5 + \nu_6, F_{1u}$ (0.77)	2099.725	$\nu_1 + \nu_4 + \nu_5 + 2\nu_6, E_u$ (0.67)	2603.990
$2\nu_4 + \nu_5 + \nu_6, F_{2u}$ (0.72)	2099.777	$\nu_3 + \nu_4 + 3\nu_6, F_{2u}$ (-0.62)	2604.272
$2\nu_4 + \nu_5 + \nu_6, F_{2u}$ (-0.83)	2099.953	$\nu_3 + \nu_4 + 3\nu_6, F_{1u}$ (0.46)	2604.340
$6\nu_6, F_{2g}$ (-0.73)	2099.990	$\nu_3 + \nu_4 + 2\nu_5, F_{1g}$ (0.72)	2604.368

Table 1 – continued

Band, Sym, Eig	Band center	Band, Sym, Eig	Band center
$2\nu_4 + \nu_5 + \nu_6, E_u$ (0.68)	2100.229	$\nu_1 + \nu_4 + \nu_5 + 2\nu_6, F_{2u}$ (0.45)	2604.468
$2\nu_4 + \nu_5 + \nu_6, A_{1u}$ (-0.93)	2100.232	$\nu_3 + \nu_4 + 2\nu_5, E_g$ (0.90)	2604.511
$2\nu_4 + \nu_5 + \nu_6, F_{1u}$ (0.58)	2100.432	$\nu_3 + \nu_4 + 3\nu_6, E_u$ (-0.58)	2604.567
$2\nu_4 + \nu_5 + \nu_6, F_{2u}$ (-0.65)	2100.435	$\nu_3 + \nu_4 + 3\nu_6, F_{2u}$ (-0.45)	2604.630
$6\nu_6, E_g$ (-0.65)	2101.541	$\nu_3 + \nu_4 + 2\nu_5, A_{1g}$ (-0.98)	2604.698
$\nu_1 + \nu_2 + 2\nu_6, E_g$ (0.86)	2106.042	$\nu_3 + \nu_4 + 3\nu_6, F_{1u}$ (-0.53)	2604.706
$\nu_2 + \nu_3 + \nu_5, F_{1u}$ (0.69)	2106.699	$\nu_3 + \nu_4 + 2\nu_5, A_{2g}$ (0.99)	2604.857
$\nu_2 + \nu_3 + \nu_5, F_{2u}$ (-0.70)	2106.702	$\nu_3 + \nu_4 + 3\nu_6, A_{2u}$ (0.69)	2604.948
$\nu_1 + \nu_2 + 2\nu_6, F_{1g}$ (0.95)	2107.563	$\nu_3 + \nu_4 + 2\nu_5, F_{1g}$ (0.98)	2604.989
$\nu_1 + \nu_2 + 2\nu_6, A_{1g}$ (-0.94)	2108.569	$\nu_1 + \nu_4 + \nu_5 + 2\nu_6, F_{1u}$ (-0.82)	2604.990
$\nu_1 + \nu_2 + 2\nu_6, F_{2g}$ (0.95)	2109.569	$\nu_3 + \nu_4 + 2\nu_5, E_g$ (0.91)	2605.059
$\nu_2 + \nu_3 + \nu_5, F_{2u}$ (-0.71)	2111.259	$\nu_3 + \nu_4 + 2\nu_5, F_{2g}$ (0.62)	2605.067
$\nu_2 + \nu_3 + \nu_5, F_{1u}$ (-0.70)	2111.263	$\nu_1 + \nu_4 + \nu_5 + 2\nu_6, A_{1u}$ (0.61)	2605.183
$\nu_1 + \nu_2 + 2\nu_6, E_g$ (-0.86)	2111.395	$\nu_3 + \nu_4 + 2\nu_5, F_{2g}$ (0.55)	2605.206
$\nu_2 + \nu_3 + \nu_5, E_u$ (-0.72)	2111.903	$\nu_3 + \nu_4 + 3\nu_6, E_u$ (0.63)	2605.331
$\nu_2 + \nu_3 + \nu_5, A_{2u}$ (-0.93)	2112.105	$\nu_3 + \nu_4 + 3\nu_6, F_{1u}$ (0.55)	2605.629
$\nu_1 + \nu_2 + 2\nu_6, A_{2g}$ (0.96)	2112.541	$\nu_1 + \nu_4 + \nu_5 + 2\nu_6, F_{2u}$ (0.77)	2605.723
$\nu_2 + \nu_3 + \nu_5, E_u$ (-0.73)	2113.008	$\nu_1 + \nu_4 + \nu_5 + 2\nu_6, A_{2u}$ (-0.71)	2606.088
$\nu_2 + \nu_3 + \nu_5, A_{1u}$ (0.94)	2113.110	$\nu_1 + \nu_4 + \nu_5 + 2\nu_6, F_{2u}$ (0.69)	2606.343
$\nu_2 + \nu_4 + \nu_5 + \nu_6, F_{1g}$ (0.59)	2122.788	$\nu_1 + \nu_4 + \nu_5 + 2\nu_6, E_u$ (0.68)	2606.415
$\nu_2 + \nu_4 + \nu_5 + \nu_6, F_{1g}$ (0.56)	2122.934	$\nu_1 + \nu_4 + \nu_5 + 2\nu_6, F_{1u}$ (-0.59)	2606.462
$\nu_2 + \nu_4 + \nu_5 + \nu_6, F_{2g}$ (-0.65)	2123.128	$\nu_1 + 2\nu_2 + \nu_4, F_{2u}$ (-0.50)	2606.567
$\nu_2 + \nu_4 + \nu_5 + \nu_6, A_{1g}$ (0.81)	2123.167	$\nu_1 + \nu_4 + \nu_5 + 2\nu_6, A_{1u}$ (-0.65)	2606.709
$\nu_2 + \nu_4 + \nu_5 + \nu_6, E_g$ (-0.80)	2123.204	$\nu_1 + \nu_4 + \nu_5 + 2\nu_6, E_u$ (-0.63)	2606.736
$\nu_2 + \nu_4 + \nu_5 + \nu_6, E_g$ (-0.80)	2123.292	$\nu_1 + \nu_4 + \nu_5 + 2\nu_6, F_{1u}$ (-0.53)	2607.135
$\nu_2 + \nu_4 + \nu_5 + \nu_6, F_{2g}$ (0.78)	2123.301	$\nu_3 + \nu_4 + 2\nu_5, A_{1g}$ (0.78)	2609.249
$\nu_2 + \nu_4 + \nu_5 + \nu_6, A_{2g}$ (0.78)	2123.356	$\nu_3 + \nu_4 + 2\nu_5, E_g$ (0.84)	2609.250
$\nu_2 + \nu_4 + \nu_5 + \nu_6, F_{1g}$ (0.89)	2123.510	$\nu_3 + \nu_4 + 2\nu_5, F_{2g}$ (0.71)	2609.695
$\nu_2 + \nu_4 + \nu_5 + \nu_6, F_{2g}$ (-0.80)	2123.979	$\nu_3 + \nu_4 + 2\nu_5, F_{1g}$ (0.71)	2609.713
$\nu_2 + \nu_4 + \nu_5 + \nu_6, F_{1g}$ (0.97)	2125.285	$\nu_2 + \nu_3 + 3\nu_6, A_{2g}$ (0.77)	2613.106
$\nu_2 + \nu_4 + \nu_5 + \nu_6, F_{2g}$ (0.97)	2125.466	$5\nu_5, F_{2g}$ (-0.99)	2614.105
$\nu_2 + \nu_4 + \nu_5 + \nu_6, F_{2g}$ (-0.95)	2125.673	$\nu_2 + \nu_3 + 3\nu_6, F_{1g}$ (0.71)	2614.424
$\nu_2 + \nu_4 + \nu_5 + \nu_6, F_{1g}$ (0.98)	2125.697	$5\nu_5, A_{1g}$ (-1.00)	2614.728
$\nu_2 + \nu_4 + \nu_5 + \nu_6, F_{2g}$ (-0.76)	2126.610	$\nu_1 + 3\nu_4, F_{1u}$ (-0.93)	2614.842
$\nu_2 + \nu_4 + \nu_5 + \nu_6, F_{1g}$ (0.78)	2126.847	$\nu_1 + 3\nu_4, F_{1u}$ (-0.93)	2615.212
$\nu_2 + \nu_4 + \nu_5 + \nu_6, F_{2g}$ (-0.73)	2126.900	$\nu_1 + 3\nu_4, F_{2u}$ (0.97)	2615.268
$\nu_2 + \nu_4 + \nu_5 + \nu_6, A_{2g}$ (0.79)	2126.925	$\nu_1 + 3\nu_4, A_{2u}$ (0.97)	2615.395
$\nu_2 + \nu_4 + \nu_5 + \nu_6, E_g$ (0.75)	2127.006	$5\nu_5, E_g$ (1.00)	2615.621
$\nu_2 + \nu_4 + \nu_5 + \nu_6, E_g$ (-0.77)	2127.125	$\nu_2 + \nu_3 + 3\nu_6, E_g$ (0.67)	2616.052
$\nu_2 + \nu_4 + \nu_5 + \nu_6, A_{1g}$ (0.81)	2127.162	$5\nu_5, F_{2g}$ (-0.97)	2616.349
$\nu_2 + \nu_4 + \nu_5 + \nu_6, F_{1g}$ (-0.75)	2127.577	$5\nu_5, F_{1g}$ (-0.98)	2616.527
$2\nu_2 + \nu_5 + \nu_6, F_{2u}$ (-0.75)	2148.574	$5\nu_5, F_{1g}$ (-0.98)	2618.883
$2\nu_2 + \nu_5 + \nu_6, F_{1u}$ (0.72)	2148.680	$5\nu_5, F_{2g}$ (-0.98)	2618.894
$2\nu_2 + \nu_5 + \nu_6, E_u$ (0.92)	2150.315	$\nu_2 + \nu_3 + 3\nu_6, F_{2g}$ (0.66)	2620.227
$2\nu_2 + \nu_5 + \nu_6, A_{1u}$ (0.95)	2150.978	$\nu_2 + \nu_3 + 3\nu_6, E_g$ (0.64)	2621.960
$2\nu_2 + \nu_5 + \nu_6, F_{1u}$ (0.91)	2151.027	$\nu_2 + \nu_3 + 3\nu_6, F_{1g}$ (0.55)	2623.232
$2\nu_2 + \nu_5 + \nu_6, A_{2u}$ (-0.93)	2152.213	$\nu_2 + \nu_3 + 3\nu_6, A_{2g}$ (0.65)	2623.262
$2\nu_2 + \nu_5 + \nu_6, E_u$ (-0.92)	2152.293	$5\nu_5, F_{2g}$ (0.99)	2623.425
$2\nu_2 + \nu_5 + \nu_6, F_{2u}$ (0.91)	2152.358	$\nu_2 + \nu_3 + 3\nu_6, F_{2g}$ (-0.64)	2623.609
$2\nu_2 + \nu_5 + \nu_6, A_{1u}$ (0.92)	2152.401	$\nu_2 + \nu_3 + 3\nu_6, E_g$ (-0.68)	2624.353
$2\nu_2 + \nu_5 + \nu_6, E_u$ (0.96)	2152.998	$\nu_1 + \nu_2 + \nu_5 + 2\nu_6, A_{2g}$ (0.63)	2624.971
$2\nu_2 + \nu_5 + \nu_6, F_{1u}$ (-0.64)	2155.545	$\nu_2 + \nu_3 + 3\nu_6, F_{2g}$ (0.57)	2625.306
$2\nu_2 + \nu_5 + \nu_6, F_{2u}$ (-0.74)	2155.614	$\nu_1 + \nu_2 + \nu_5 + 2\nu_6, F_{1g}$ (0.66)	2625.354
$\nu_3 + \nu_5 + 2\nu_6, F_{1u}$ (0.89)	2158.735	$\nu_2 + \nu_3 + 2\nu_5, E_u$ (-0.70)	2625.378
$\nu_3 + \nu_5 + 2\nu_6, F_{2u}$ (-0.87)	2158.798	$\nu_2 + \nu_3 + 3\nu_6, E_g$ (-0.59)	2625.380

Table 1 – continued

Band, Sym, Eig	Band center	Band, Sym, Eig	Band center
$\nu_3 + \nu_5 + 2\nu_6$, A_{2u} (-0.88)	2158.889	$\nu_2 + \nu_3 + 2\nu_5$, A_{2u} (-0.98)	2625.414
$\nu_1 + 4\nu_6$, A_{1g} (-0.80)	2159.129	$\nu_2 + \nu_3 + 3\nu_6$, F_{1g} (-0.48)	2625.782
$\nu_3 + \nu_5 + 2\nu_6$, E_u (-0.86)	2159.269	$\nu_2 + \nu_3 + 3\nu_6$, F_{1g} (-0.41)	2625.789
$\nu_3 + \nu_5 + 2\nu_6$, F_{2u} (-0.70)	2159.506	$\nu_1 + 3\nu_2$, A_{2g} (0.81)	2625.884
$\nu_3 + \nu_5 + 2\nu_6$, F_{2u} (-0.85)	2159.798	$\nu_1 + \nu_2 + \nu_5 + 2\nu_6$, F_{2g} (0.76)	2625.929
$2\nu_1 + \nu_4$, F_{1u} (0.85)	2159.926	$\nu_2 + \nu_3 + 2\nu_5$, F_{1u} (-0.78)	2626.010
$\nu_3 + \nu_5 + 2\nu_6$, F_{1u} (-0.67)	2160.049	$\nu_2 + \nu_3 + 2\nu_5$, F_{2u} (-0.94)	2626.171
$\nu_1 + 4\nu_6$, F_{2g} (-0.78)	2160.327	$\nu_2 + \nu_3 + 3\nu_6$, F_{1g} (0.45)	2626.283
$\nu_3 + \nu_5 + 2\nu_6$, E_u (0.87)	2160.371	$\nu_2 + \nu_3 + 3\nu_6$, A_{1g} (0.70)	2626.291
$\nu_3 + \nu_5 + 2\nu_6$, F_{1u} (-0.57)	2160.822	$\nu_1 + \nu_2 + \nu_5 + 2\nu_6$, F_{2g} (-0.48)	2626.779
$\nu_3 + \nu_5 + 2\nu_6$, A_{1u} (-0.90)	2160.833	$\nu_1 + \nu_2 + \nu_5 + 2\nu_6$, E_g (0.70)	2627.111
$\nu_3 + \nu_5 + 2\nu_6$, F_{2u} (0.51)	2161.277	$\nu_1 + \nu_2 + \nu_5 + 2\nu_6$, F_{2g} (-0.53)	2627.421
$\nu_3 + \nu_5 + 2\nu_6$, F_{1u} (0.63)	2161.877	$\nu_2 + \nu_3 + 3\nu_6$, A_{2g} (-0.91)	2627.735
$\nu_3 + \nu_5 + 2\nu_6$, A_{2u} (0.90)	2161.894	$\nu_1 + \nu_2 + \nu_5 + 2\nu_6$, F_{1g} (0.80)	2627.868
$\nu_3 + \nu_5 + 2\nu_6$, E_u (-0.86)	2161.991	$\nu_2 + \nu_3 + 3\nu_6$, E_g (0.50)	2628.085
$\nu_1 + 2\nu_5 + \nu_6$, F_{2u} (0.66)	2162.886	$\nu_1 + \nu_2 + \nu_5 + 2\nu_6$, F_{1g} (-0.58)	2628.179
$\nu_3 + \nu_5 + 2\nu_6$, F_{1u} (-0.63)	2163.002	$\nu_2 + \nu_3 + 3\nu_6$, F_{2g} (-0.79)	2628.496
$\nu_3 + \nu_5 + 2\nu_6$, F_{2u} (-0.52)	2163.175	$\nu_1 + \nu_2 + \nu_5 + 2\nu_6$, A_{1g} (-0.56)	2628.566
$\nu_3 + \nu_5 + 2\nu_6$, F_{1u} (-0.72)	2163.802	$\nu_2 + \nu_3 + 3\nu_6$, F_{1g} (-0.47)	2628.566
$\nu_1 + 2\nu_5 + \nu_6$, E_u (-0.83)	2163.962	$\nu_1 + \nu_2 + \nu_5 + 2\nu_6$, F_{2g} (-0.53)	2628.969
$\nu_1 + 4\nu_6$, E_g (0.76)	2164.084	$\nu_1 + \nu_2 + \nu_5 + 2\nu_6$, E_g (0.61)	2629.990
$\nu_3 + \nu_5 + 2\nu_6$, F_{1u} (-0.54)	2164.387	$\nu_2 + \nu_3 + 3\nu_6$, F_{1g} (-0.68)	2630.066
$\nu_3 + \nu_5 + 2\nu_6$, F_{2u} (0.57)	2164.615	$\nu_2 + \nu_3 + 2\nu_5$, F_{2u} (-0.97)	2630.073
$\nu_1 + 2\nu_5 + \nu_6$, A_{1u} (0.75)	2165.072	$\nu_1 + \nu_2 + \nu_5 + 2\nu_6$, F_{2g} (-0.64)	2630.164
$\nu_1 + 2\nu_5 + \nu_6$, F_{1u} (-0.50)	2165.251	$\nu_2 + \nu_3 + 2\nu_5$, F_{1u} (0.97)	2630.270
$\nu_1 + 2\nu_5 + \nu_6$, F_{2u} (-0.91)	2165.570	$\nu_1 + 3\nu_2$, E_g (-0.67)	2630.385
$\nu_3 + \nu_5 + 2\nu_6$, E_u (-0.79)	2165.817	$\nu_1 + \nu_2 + \nu_5 + 2\nu_6$, A_{1g} (-0.77)	2630.438
$\nu_3 + \nu_5 + 2\nu_6$, A_{2u} (-0.87)	2166.012	$\nu_2 + \nu_3 + 2\nu_5$, E_u (0.71)	2630.608
$\nu_1 + 4\nu_6$, F_{2g} (-0.78)	2166.295	$\nu_2 + \nu_3 + 2\nu_5$, A_{1u} (-0.99)	2630.638
$\nu_1 + 2\nu_5 + \nu_6$, F_{2u} (0.78)	2166.779	$\nu_1 + \nu_2 + \nu_5 + 2\nu_6$, F_{2g} (-0.56)	2630.657
$\nu_3 + \nu_5 + 2\nu_6$, E_u (-0.87)	2166.783	$\nu_2 + \nu_3 + 3\nu_6$, F_{1g} (-0.55)	2630.872
$\nu_1 + 2\nu_5 + \nu_6$, F_{1u} (0.73)	2166.798	$\nu_1 + \nu_2 + \nu_5 + 2\nu_6$, F_{2g} (-0.47)	2631.371
$\nu_3 + \nu_5 + 2\nu_6$, A_{1u} (-0.74)	2167.390	$\nu_1 + \nu_2 + \nu_5 + 2\nu_6$, F_{1g} (-0.56)	2631.755
$\nu_1 + 4\nu_6$, F_{1g} (-0.95)	2169.182	$\nu_1 + \nu_2 + \nu_3 + \nu_6$, A_{2g} (-0.77)	2631.951
$\nu_1 + 4\nu_6$, E_g (-0.76)	2169.950	$\nu_2 + \nu_3 + 3\nu_6$, E_g (-0.49)	2632.151
$\nu_1 + 4\nu_6$, A_{1g} (-0.80)	2171.475	$\nu_2 + \nu_3 + 2\nu_5$, F_{2u} (0.79)	2632.248
$\nu_3 + 2\nu_4$, F_{1u} (0.66)	2173.342	$\nu_2 + \nu_3 + 2\nu_5$, F_{1u} (-0.94)	2632.415
$\nu_3 + 2\nu_4$, F_{2u} (0.83)	2173.630	$\nu_1 + \nu_2 + \nu_5 + 2\nu_6$, F_{1g} (-0.75)	2632.457
$\nu_3 + 2\nu_4$, F_{1u} (0.78)	2173.990	$\nu_2 + \nu_3 + 3\nu_6$, F_{2g} (-0.60)	2632.542
$\nu_3 + 2\nu_4$, E_u (0.95)	2174.036	$\nu_2 + \nu_3 + 2\nu_5$, F_{1u} (0.97)	2632.798
$\nu_3 + 2\nu_4$, F_{2u} (0.84)	2174.186	$\nu_2 + \nu_3 + 2\nu_5$, F_{2u} (-0.97)	2632.948
$\nu_4 + \nu_5 + 3\nu_6$, F_{1g} (-0.67)	2174.406	$\nu_2 + \nu_3 + 3\nu_6$, A_{1g} (-0.90)	2633.989
$\nu_3 + 2\nu_4$, A_{2u} (0.95)	2174.536	$\nu_3 + 5\nu_6$, F_{2g} (0.61)	2634.337
$\nu_3 + 2\nu_4$, F_{1u} (-0.79)	2174.920	$\nu_1 + \nu_2 + \nu_3 + \nu_6$, F_{1g} (0.75)	2634.384
$\nu_4 + \nu_5 + 3\nu_6$, F_{1g} (0.59)	2175.147	$\nu_3 + 5\nu_6$, E_g (0.52)	2634.951
$\nu_4 + \nu_5 + 3\nu_6$, F_{2g} (0.76)	2175.229	$\nu_2 + \nu_3 + 2\nu_5$, F_{2u} (0.83)	2635.679
$\nu_4 + \nu_5 + 3\nu_6$, A_{1g} (0.80)	2175.307	$\nu_2 + \nu_3 + 2\nu_5$, F_{1u} (0.81)	2636.753
$\nu_4 + \nu_5 + 3\nu_6$, E_g (0.77)	2175.636	$\nu_1 + \nu_2 + 2\nu_4$, E_g (-0.74)	2640.114
$\nu_4 + \nu_5 + 3\nu_6$, F_{2g} (-0.71)	2175.681	$\nu_1 + \nu_2 + 2\nu_4$, A_{1g} (0.97)	2640.173
$\nu_4 + \nu_5 + 3\nu_6$, E_g (0.83)	2176.022	$\nu_1 + \nu_2 + 2\nu_4$, F_{1g} (0.97)	2640.472
$\nu_4 + \nu_5 + 3\nu_6$, F_{1g} (0.63)	2176.175	$\nu_1 + \nu_2 + 2\nu_4$, E_g (0.74)	2640.780
$\nu_4 + \nu_5 + 3\nu_6$, F_{2g} (0.79)	2176.186	$\nu_1 + \nu_2 + 2\nu_4$, F_{2g} (0.97)	2640.811
$\nu_4 + \nu_5 + 3\nu_6$, A_{2g} (0.60)	2176.270	$\nu_1 + \nu_2 + 2\nu_4$, A_{2g} (-0.97)	2640.832
$\nu_4 + \nu_5 + 3\nu_6$, F_{1g} (0.56)	2176.623	$\nu_1 + 2\nu_3$, A_{1g} (-0.85)	2658.574
$\nu_4 + \nu_5 + 3\nu_6$, A_{2g} (0.69)	2176.677	$\nu_1 + 2\nu_3$, E_g (-0.85)	2661.173

Table 1 – continued

Band, Sym, Eig	Band center	Band, Sym, Eig	Band center
$\nu_4 + \nu_5 + 3\nu_6, F_{2g}$ (-0.62)	2177.107	$\nu_1 + 2\nu_3, F_{2g}$ (-0.86)	2665.412
$\nu_4 + \nu_5 + 3\nu_6, E_g$ (-0.72)	2177.465	$3\nu_1 + \nu_6, F_{2u}$ (0.89)	2665.431
$\nu_4 + \nu_5 + 3\nu_6, F_{1g}$ (-0.70)	2177.609	$\nu_1 + 2\nu_2 + \nu_4, F_{1u}$ (0.86)	2666.946
$\nu_4 + \nu_5 + 3\nu_6, F_{2g}$ (-0.62)	2178.786	$\nu_1 + 2\nu_2 + \nu_4, F_{2u}$ (0.74)	2667.134
$\nu_4 + \nu_5 + 3\nu_6, F_{1g}$ (-0.59)	2179.087	$\nu_1 + 2\nu_2 + \nu_4, F_{1u}$ (-0.88)	2667.819
$\nu_4 + \nu_5 + 3\nu_6, F_{2g}$ (0.80)	2179.210	$\nu_3 + 2\nu_5 + 2\nu_6, A_{2u}$ (0.64)	2670.741
$\nu_4 + \nu_5 + 3\nu_6, A_{1g}$ (-0.90)	2179.752	$\nu_3 + 5\nu_6, E_g$ (0.65)	2675.801
$\nu_4 + \nu_5 + 3\nu_6, F_{1g}$ (0.82)	2179.929	$\nu_3 + 5\nu_6, F_{2g}$ (0.72)	2676.328
$\nu_4 + \nu_5 + 3\nu_6, F_{2g}$ (-0.77)	2179.972	$\nu_3 + 5\nu_6, E_g$ (0.59)	2676.460
$\nu_4 + \nu_5 + 3\nu_6, E_g$ (0.67)	2180.188	$\nu_3 + 5\nu_6, A_{2g}$ (-0.65)	2676.730
$\nu_4 + \nu_5 + 3\nu_6, F_{1g}$ (0.58)	2180.392	$\nu_3 + 5\nu_6, F_{1g}$ (0.56)	2676.818
$\nu_4 + \nu_5 + 3\nu_6, A_{2g}$ (0.67)	2180.526	$\nu_3 + 2\nu_5 + 2\nu_6, F_{1u}$ (-0.68)	2677.332
$\nu_4 + \nu_5 + 3\nu_6, E_g$ (0.89)	2180.560	$\nu_1 + \nu_3 + \nu_4 + \nu_6, F_{2u}$ (0.82)	2677.364
$\nu_4 + \nu_5 + 3\nu_6, F_{2g}$ (0.48)	2180.792	$\nu_1 + \nu_3 + \nu_4 + \nu_6, F_{1u}$ (0.64)	2677.384
$\nu_4 + \nu_5 + 3\nu_6, F_{1g}$ (0.63)	2182.056	$\nu_3 + 2\nu_5 + 2\nu_6, A_{2u}$ (0.74)	2677.388
$\nu_4 + \nu_5 + 3\nu_6, E_g$ (0.72)	2182.308	$\nu_3 + 2\nu_5 + 2\nu_6, F_{1u}$ (0.53)	2677.496
$\nu_4 + 3\nu_5, F_{1u}$ (-0.91)	2182.418	$\nu_3 + 2\nu_5 + 2\nu_6, F_{2u}$ (0.60)	2677.522
$\nu_4 + \nu_5 + 3\nu_6, F_{2g}$ (0.52)	2182.598	$\nu_1 + \nu_3 + \nu_4 + \nu_6, A_{2u}$ (0.89)	2677.523
$\nu_4 + \nu_5 + 3\nu_6, F_{1g}$ (0.53)	2182.733	$\nu_3 + 2\nu_5 + 2\nu_6, E_u$ (0.98)	2677.541
$\nu_4 + \nu_5 + 3\nu_6, F_{2g}$ (0.42)	2182.860	$\nu_1 + \nu_3 + \nu_4 + \nu_6, F_{2u}$ (0.74)	2677.659
$\nu_4 + \nu_5 + 3\nu_6, A_{2g}$ (0.60)	2183.220	$\nu_1 + \nu_3 + \nu_4 + \nu_6, F_{1u}$ (0.86)	2677.744
$\nu_4 + 3\nu_5, F_{1u}$ (-0.78)	2183.299	$\nu_3 + 2\nu_5 + 2\nu_6, A_{1u}$ (-0.73)	2677.794
$\nu_4 + \nu_5 + 3\nu_6, F_{1g}$ (-0.52)	2183.393	$\nu_1 + \nu_3 + \nu_4 + \nu_6, E_u$ (-0.86)	2677.809
$\nu_4 + 3\nu_5, A_{2u}$ (-0.95)	2183.416	$\nu_3 + 2\nu_5 + 2\nu_6, F_{1u}$ (-0.48)	2677.821
$\nu_4 + 3\nu_5, E_u$ (0.79)	2183.423	$\nu_3 + 5\nu_6, F_{1g}$ (-0.91)	2677.987
$\nu_4 + \nu_5 + 3\nu_6, A_{1g}$ (-0.74)	2183.599	$\nu_3 + 2\nu_5 + 2\nu_6, E_u$ (-0.68)	2678.013
$\nu_4 + \nu_5 + 3\nu_6, E_g$ (0.75)	2183.689	$\nu_3 + 2\nu_5 + 2\nu_6, F_{2u}$ (-0.58)	2678.143
$\nu_4 + 3\nu_5, F_{2u}$ (0.97)	2183.716	$\nu_1 + \nu_3 + \nu_4 + \nu_6, F_{2u}$ (-0.55)	2678.278
$\nu_4 + 3\nu_5, A_{1u}$ (0.99)	2183.844	$\nu_1 + \nu_3 + \nu_4 + \nu_6, F_{1u}$ (0.67)	2678.295
$\nu_4 + \nu_5 + 3\nu_6, F_{2g}$ (-0.65)	2183.951	$\nu_1 + \nu_3 + \nu_4 + \nu_6, E_u$ (-0.90)	2678.584
$\nu_4 + 3\nu_5, E_u$ (-0.77)	2183.962	$\nu_1 + \nu_3 + \nu_4 + \nu_6, A_{1u}$ (-0.96)	2678.829
$\nu_4 + 3\nu_5, F_{2u}$ (-0.98)	2183.964	$\nu_3 + 2\nu_5 + 2\nu_6, F_{1u}$ (0.48)	2679.045
$\nu_4 + \nu_5 + 3\nu_6, F_{1g}$ (0.51)	2184.014	$\nu_3 + 2\nu_5 + 2\nu_6, F_{2u}$ (-0.57)	2679.056
$\nu_4 + 3\nu_5, F_{1u}$ (-0.80)	2184.050	$\nu_1 + \nu_3 + \nu_4 + \nu_6, F_{2u}$ (-0.69)	2679.523
$\nu_4 + 3\nu_5, E_u$ (-0.97)	2185.717	$\nu_3 + 2\nu_5 + 2\nu_6, F_{2u}$ (0.47)	2679.712
$\nu_4 + 3\nu_5, A_{2u}$ (-0.95)	2185.839	$\nu_3 + 2\nu_5 + 2\nu_6, E_u$ (-0.68)	2679.714
$2\nu_1 + \nu_2, E_g$ (-0.82)	2186.021	$\nu_3 + 2\nu_5 + 2\nu_6, F_{1u}$ (0.42)	2679.728
$\nu_4 + 3\nu_5, F_{1u}$ (0.98)	2186.265	$\nu_3 + 2\nu_5 + 2\nu_6, A_{2u}$ (0.72)	2680.062
$\nu_4 + 3\nu_5, F_{2u}$ (0.97)	2186.300	$\nu_3 + 2\nu_5 + 2\nu_6, F_{1u}$ (-0.53)	2680.094
$3\nu_4 + \nu_6, E_g$ (-0.80)	2190.629	$\nu_3 + 2\nu_5 + 2\nu_6, E_u$ (0.70)	2680.177
$3\nu_4 + \nu_6, A_{2g}$ (0.82)	2190.793	$\nu_3 + 2\nu_5 + 2\nu_6, F_{2u}$ (0.48)	2680.507
$3\nu_4 + \nu_6, F_{2g}$ (0.75)	2190.895	$2\nu_2 + \nu_3 + \nu_5, A_{2u}$ (0.58)	2680.635
$3\nu_4 + \nu_6, F_{1g}$ (0.78)	2191.243	$\nu_3 + 2\nu_5 + 2\nu_6, F_{1u}$ (0.96)	2680.682
$3\nu_4 + \nu_6, E_g$ (-0.79)	2191.272	$\nu_3 + 2\nu_5 + 2\nu_6, F_{2u}$ (0.72)	2680.711
$3\nu_4 + \nu_6, F_{2g}$ (-0.95)	2191.311	$2\nu_1 + \nu_4 + \nu_5, A_{2u}$ (-0.85)	2680.820
$3\nu_4 + \nu_6, A_{1g}$ (-0.99)	2191.355	$\nu_3 + 5\nu_6, A_{1g}$ (0.69)	2680.970
$3\nu_4 + \nu_6, F_{1g}$ (-0.68)	2191.368	$\nu_3 + 2\nu_5 + 2\nu_6, F_{2u}$ (0.50)	2680.981
$3\nu_4 + \nu_6, F_{1g}$ (-0.69)	2191.680	$\nu_3 + 5\nu_6, F_{2g}$ (0.70)	2681.029
$3\nu_4 + \nu_6, F_{2g}$ (-0.72)	2191.695	$\nu_3 + 2\nu_5 + 2\nu_6, F_{1u}$ (-0.58)	2681.242
$3\nu_4 + \nu_6, A_{2g}$ (0.82)	2192.602	$2\nu_1 + \nu_4 + \nu_5, F_{2u}$ (0.88)	2681.298
$3\nu_4 + \nu_6, E_g$ (0.69)	2192.836	$2\nu_1 + \nu_4 + \nu_5, E_u$ (-0.89)	2681.318
$3\nu_4 + \nu_6, F_{1g}$ (0.61)	2193.035	$2\nu_1 + \nu_4 + \nu_5, F_{1u}$ (0.89)	2681.377
$\nu_2 + \nu_5 + 3\nu_6, F_{1u}$ (0.62)	2199.299	$\nu_3 + 5\nu_6, E_g$ (0.57)	2681.390
$\nu_2 + \nu_5 + 3\nu_6, F_{2u}$ (-0.54)	2199.329	$\nu_3 + 5\nu_6, F_{1g}$ (-0.66)	2681.460
$\nu_2 + \nu_5 + 3\nu_6, E_u$ (0.67)	2199.331	$2\nu_1 + \nu_5 + 2\nu_6, F_{2g}$ (-0.82)	2681.798

Table 1 – continued

Band, Sym, Eig	Band center	Band, Sym, Eig	Band center
$\nu_2 + \nu_3 + \nu_4, A_{1g}$ (0.93)	2199.375	$\nu_3 + 2\nu_5 + 2\nu_6, E_u$ (0.91)	2681.997
$\nu_2 + \nu_3 + \nu_4, E_g$ (-0.74)	2199.796	$\nu_3 + 5\nu_6, E_g$ (0.55)	2682.157
$\nu_2 + \nu_3 + \nu_4, F_{2g}$ (0.84)	2199.846	$\nu_3 + 2\nu_5 + 2\nu_6, F_{2u}$ (-0.52)	2682.177
$\nu_2 + \nu_3 + \nu_4, F_{1g}$ (-0.80)	2200.051	$\nu_3 + 2\nu_5 + 2\nu_6, A_{1u}$ (-0.84)	2682.179
$\nu_2 + \nu_5 + 3\nu_6, A_{1u}$ (-0.75)	2200.806	$\nu_3 + 2\nu_5 + 2\nu_6, F_{1u}$ (0.56)	2682.442
$\nu_2 + \nu_5 + 3\nu_6, E_u$ (-0.78)	2200.894	$2\nu_1 + \nu_5 + 2\nu_6, F_{1g}$ (0.79)	2682.579
$\nu_2 + \nu_5 + 3\nu_6, F_{1u}$ (0.52)	2200.969	$\nu_3 + 2\nu_5 + 2\nu_6, F_{2u}$ (-0.57)	2682.792
$\nu_2 + \nu_5 + 3\nu_6, A_{2u}$ (0.90)	2201.135	$\nu_3 + 2\nu_5 + 2\nu_6, F_{1u}$ (-0.48)	2683.070
$\nu_2 + \nu_5 + 3\nu_6, F_{2u}$ (-0.75)	2201.949	$\nu_3 + 2\nu_5 + 2\nu_6, F_{2u}$ (-0.70)	2683.184
$\nu_2 + \nu_5 + 3\nu_6, F_{1u}$ (-0.73)	2202.750	$\nu_3 + 2\nu_5 + 2\nu_6, E_u$ (0.65)	2683.265
$\nu_2 + \nu_5 + 3\nu_6, A_{1u}$ (-0.77)	2202.768	$\nu_3 + 2\nu_5 + 2\nu_6, A_{2u}$ (-0.60)	2683.334
$\nu_2 + \nu_3 + \nu_4, A_{2g}$ (-0.94)	2202.780	$\nu_3 + 2\nu_5 + 2\nu_6, A_{1u}$ (0.71)	2683.372
$\nu_2 + \nu_3 + \nu_4, F_{1g}$ (-0.81)	2202.884	$\nu_3 + 2\nu_5 + 2\nu_6, F_{1u}$ (-0.44)	2683.701
$\nu_2 + \nu_5 + 3\nu_6, F_{2u}$ (-0.65)	2202.962	$\nu_3 + 2\nu_5 + 2\nu_6, F_{2u}$ (0.39)	2683.853
$\nu_2 + \nu_3 + \nu_4, F_{2g}$ (-0.85)	2203.090	$\nu_3 + 2\nu_5 + 2\nu_6, E_u$ (0.70)	2683.877
$\nu_2 + \nu_3 + \nu_4, E_g$ (0.74)	2203.381	$2\nu_1 + \nu_5 + 2\nu_6, E_g$ (0.69)	2683.920
$\nu_2 + \nu_5 + 3\nu_6, F_{1u}$ (0.54)	2203.727	$\nu_3 + 2\nu_5 + 2\nu_6, F_{1u}$ (0.53)	2684.102
$\nu_2 + \nu_5 + 3\nu_6, E_u$ (-0.72)	2204.456	$\nu_3 + 2\nu_5 + 2\nu_6, F_{2u}$ (-0.64)	2684.167
$\nu_2 + \nu_5 + 3\nu_6, E_u$ (-0.66)	2205.164	$\nu_3 + 5\nu_6, F_{1g}$ (-0.64)	2684.259
$\nu_2 + \nu_5 + 3\nu_6, F_{1u}$ (0.57)	2205.621	$\nu_3 + 5\nu_6, A_{2g}$ (0.55)	2684.319
$\nu_2 + \nu_5 + 3\nu_6, F_{2u}$ (-0.60)	2205.810	$\nu_1 + 3\nu_5 + \nu_6, E_u$ (0.61)	2684.397
$\nu_2 + \nu_5 + 3\nu_6, F_{2u}$ (-0.56)	2205.960	$\nu_3 + 5\nu_6, F_{2g}$ (0.67)	2684.753
$\nu_2 + \nu_5 + 3\nu_6, A_{2u}$ (-0.79)	2206.099	$\nu_3 + 2\nu_5 + 2\nu_6, F_{1u}$ (-0.69)	2684.927
$\nu_2 + \nu_5 + 3\nu_6, F_{2u}$ (-0.71)	2207.298	$\nu_3 + 2\nu_5 + 2\nu_6, F_{2u}$ (0.49)	2685.253
$\nu_2 + 3\nu_5, F_{1g}$ (0.71)	2207.896	$\nu_3 + 2\nu_5 + 2\nu_6, F_{1u}$ (0.47)	2685.763
$\nu_2 + 3\nu_5, F_{2g}$ (-0.71)	2207.922	$\nu_1 + 3\nu_5 + \nu_6, A_{1u}$ (0.75)	2685.794
$\nu_2 + \nu_5 + 3\nu_6, E_u$ (0.46)	2208.007	$\nu_1 + 3\nu_5 + \nu_6, A_{2u}$ (0.84)	2685.947
$\nu_2 + 3\nu_5, E_g$ (0.98)	2208.507	$\nu_1 + 3\nu_5 + \nu_6, F_{2u}$ (-0.52)	2685.986
$\nu_2 + \nu_5 + 3\nu_6, F_{1u}$ (0.62)	2208.534	$\nu_1 + 3\nu_5 + \nu_6, F_{1u}$ (0.74)	2686.434
$\nu_2 + \nu_5 + 3\nu_6, A_{1u}$ (-0.65)	2208.713	$\nu_1 + 3\nu_5 + \nu_6, F_{1u}$ (0.72)	2686.765
$\nu_2 + \nu_5 + 3\nu_6, A_{2u}$ (-0.77)	2208.748	$\nu_3 + 5\nu_6, F_{1g}$ (0.82)	2687.297
$\nu_2 + 3\nu_5, F_{1g}$ (0.97)	2209.032	$\nu_1 + 3\nu_5 + \nu_6, E_u$ (-0.53)	2687.309
$\nu_2 + \nu_5 + 3\nu_6, E_u$ (0.59)	2210.181	$\nu_3 + 5\nu_6, F_{2g}$ (0.90)	2687.643
$\nu_2 + \nu_5 + 3\nu_6, F_{2u}$ (0.63)	2210.785	$\nu_3 + 2\nu_5 + 2\nu_6, F_{2u}$ (0.42)	2687.694
$\nu_2 + \nu_5 + 3\nu_6, F_{1u}$ (-0.68)	2211.312	$\nu_3 + 2\nu_5 + 2\nu_6, F_{1u}$ (-0.43)	2687.918
$\nu_2 + 3\nu_5, F_{2g}$ (-0.71)	2211.455	$\nu_3 + 5\nu_6, E_g$ (0.54)	2688.000
$\nu_2 + 3\nu_5, F_{1g}$ (-0.71)	2211.475	$\nu_1 + \nu_3 + 2\nu_5, F_{2u}$ (0.56)	2688.282
$\nu_2 + 3\nu_5, F_{2g}$ (-0.98)	2215.084	$\nu_3 + 2\nu_5 + 2\nu_6, A_{2u}$ (0.76)	2688.368
$\nu_2 + 2\nu_4 + \nu_6, F_{2u}$ (-0.63)	2215.714	$\nu_3 + 5\nu_6, F_{1g}$ (0.56)	2688.545
$\nu_2 + 2\nu_4 + \nu_6, F_{2u}$ (-0.82)	2216.319	$\nu_1 + 3\nu_5 + \nu_6, E_u$ (0.64)	2688.548
$\nu_2 + 2\nu_4 + \nu_6, F_{1u}$ (-0.71)	2216.346	$\nu_3 + 5\nu_6, E_g$ (-0.62)	2689.162
$\nu_2 + 2\nu_4 + \nu_6, F_{1u}$ (-0.95)	2216.428	$\nu_3 + 5\nu_6, F_{2g}$ (-0.76)	2689.169
$\nu_2 + 2\nu_4 + \nu_6, F_{2u}$ (0.73)	2216.431	$\nu_3 + 2\nu_5 + 2\nu_6, F_{1u}$ (-0.54)	2689.379
$\nu_2 + 2\nu_4 + \nu_6, E_u$ (-0.71)	2216.586	$\nu_1 + 3\nu_5 + \nu_6, F_{2u}$ (-0.75)	2689.382
$\nu_2 + 2\nu_4 + \nu_6, A_{1u}$ (0.99)	2216.618	$\nu_1 + 3\nu_5 + \nu_6, E_u$ (-0.57)	2689.397
$\nu_2 + 2\nu_4 + \nu_6, F_{1u}$ (0.83)	2218.195	$\nu_3 + 5\nu_6, A_{2g}$ (-0.69)	2689.401
$\nu_2 + 2\nu_4 + \nu_6, F_{1u}$ (0.69)	2218.257	$\nu_1 + 3\nu_5 + \nu_6, A_{1u}$ (0.77)	2689.558
$\nu_2 + 2\nu_4 + \nu_6, F_{2u}$ (-0.98)	2218.311	$\nu_3 + 5\nu_6, F_{2g}$ (0.59)	2689.704
$\nu_2 + 2\nu_4 + \nu_6, E_u$ (-0.71)	2218.406	$\nu_1 + 3\nu_5 + \nu_6, F_{1u}$ (0.74)	2689.868
$\nu_2 + 2\nu_4 + \nu_6, A_{2u}$ (0.99)	2218.422	$\nu_3 + 5\nu_6, F_{1g}$ (-0.57)	2690.030
$\nu_2 + 2\nu_4 + \nu_6, F_{2u}$ (0.88)	2219.019	$\nu_3 + 5\nu_6, A_{2g}$ (0.67)	2690.316
$\nu_2 + 2\nu_4 + \nu_6, F_{1u}$ (0.66)	2219.226	$\nu_1 + \nu_3 + 3\nu_6, E_g$ (0.75)	2690.362
$2\nu_2 + \nu_3, F_{1u}$ (0.65)	2226.973	$\nu_3 + 2\nu_5 + 2\nu_6, F_{2u}$ (-0.54)	2690.383
$2\nu_2 + \nu_3, F_{2u}$ (0.82)	2229.033	$2\nu_1 + \nu_5 + 2\nu_6, F_{2g}$ (0.49)	2690.454
$2\nu_2 + \nu_3, F_{1u}$ (0.67)	2233.246	$\nu_3 + 5\nu_6, A_{1g}$ (-0.69)	2691.510

Table 1 – continued

Band, Sym, Eig	Band center	Band, Sym, Eig	Band center
$2\nu_3 + \nu_6, F_{2u}$ (0.87)	2235.276	$2\nu_1 + \nu_5 + 2\nu_6, F_{1g}$ (-0.65)	2691.650
$2\nu_3 + \nu_6, F_{2u}$ (0.86)	2237.368	$\nu_1 + \nu_3 + 3\nu_6, A_{2g}$ (-0.77)	2692.304
$2\nu_3 + \nu_6, F_{1u}$ (-0.84)	2237.718	$\nu_1 + \nu_3 + 3\nu_6, E_g$ (0.74)	2692.337
$\nu_1 + \nu_3 + \nu_5, F_{2u}$ (0.83)	2239.525	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, E_g$ (-0.48)	2692.922
$\nu_1 + \nu_3 + \nu_5, F_{1u}$ (0.78)	2239.624	$\nu_1 + \nu_2 + \nu_3 + \nu_6, F_{2g}$ (-0.63)	2692.937
$2\nu_1 + 2\nu_6, A_{1g}$ (-0.93)	2239.783	$\nu_3 + 2\nu_4 + \nu_5, E_u$ (-0.93)	2693.499
$2\nu_1 + 2\nu_6, F_{2g}$ (0.93)	2241.381	$\nu_3 + 2\nu_4 + \nu_5, F_{2u}$ (-0.77)	2693.514
$2\nu_3 + \nu_6, E_u$ (0.76)	2241.676	$\nu_3 + 2\nu_4 + \nu_5, F_{1u}$ (-0.82)	2693.524
$2\nu_3 + \nu_6, F_{2u}$ (-0.91)	2241.992	$\nu_3 + 2\nu_4 + \nu_5, F_{2u}$ (0.81)	2693.553
$2\nu_3 + \nu_6, F_{1u}$ (-0.90)	2242.059	$\nu_3 + 2\nu_4 + \nu_5, F_{1u}$ (0.87)	2693.674
$2\nu_2 + \nu_4 + \nu_6, E_g$ (-0.67)	2242.071	$\nu_3 + 2\nu_4 + \nu_5, A_{1u}$ (-1.00)	2693.850
$2\nu_2 + \nu_4 + \nu_6, A_{2g}$ (-0.78)	2242.260	$2\nu_2 + \nu_3 + \nu_4, A_{2g}$ (0.55)	2694.009
$2\nu_2 + \nu_4 + \nu_6, F_{1g}$ (-0.65)	2242.532	$\nu_3 + 2\nu_4 + \nu_5, F_{2u}$ (-0.56)	2694.023
$2\nu_2 + \nu_4 + \nu_6, F_{2g}$ (-0.64)	2242.563	$\nu_3 + 2\nu_4 + \nu_5, A_{2u}$ (0.98)	2694.110
$\nu_1 + \nu_3 + \nu_5, A_{2u}$ (-0.88)	2242.704	$\nu_3 + 2\nu_4 + \nu_5, F_{1u}$ (0.88)	2694.127
$2\nu_3 + \nu_6, A_{1u}$ (-0.95)	2243.239	$\nu_3 + 2\nu_4 + \nu_5, E_u$ (-0.92)	2694.217
$2\nu_1 + 2\nu_6, E_g$ (-0.91)	2243.345	$\nu_3 + 2\nu_4 + \nu_5, F_{2u}$ (-0.85)	2694.272
$\nu_1 + \nu_3 + \nu_5, E_u$ (-0.71)	2243.635	$\nu_3 + 2\nu_4 + \nu_5, F_{1u}$ (-0.69)	2694.392
$2\nu_2 + \nu_4 + \nu_6, A_{1g}$ (-0.93)	2243.645	$\nu_3 + 5\nu_6, F_{1g}$ (0.51)	2694.595
$2\nu_2 + \nu_4 + \nu_6, F_{1g}$ (0.73)	2243.976	$\nu_3 + 2\nu_4 + \nu_5, F_{2u}$ (0.71)	2694.604
$2\nu_2 + \nu_4 + \nu_6, F_{2g}$ (0.74)	2244.002	$\nu_3 + 2\nu_4 + \nu_5, F_{1u}$ (-0.59)	2694.643
$2\nu_2 + \nu_4 + \nu_6, E_g$ (0.65)	2244.319	$\nu_1 + 3\nu_2, A_{1g}$ (-0.90)	2694.917
$2\nu_2 + \nu_4 + \nu_6, F_{1g}$ (0.73)	2246.499	$2\nu_1 + \nu_5 + 2\nu_6, F_{2g}$ (0.76)	2694.959
$2\nu_2 + \nu_4 + \nu_6, F_{2g}$ (-0.73)	2246.537	$2\nu_1 + 2\nu_2, E_g$ (-0.40)	2695.714
$2\nu_2 + \nu_4 + \nu_6, E_g$ (0.66)	2246.898	$\nu_3 + 2\nu_4 + \nu_5, A_{2u}$ (0.75)	2697.079
$2\nu_2 + \nu_4 + \nu_6, A_{2g}$ (0.80)	2247.193	$\nu_3 + 2\nu_4 + \nu_5, E_u$ (-0.83)	2697.306
$\nu_5 + 5\nu_6, A_{1u}$ (-0.68)	2251.103	$\nu_3 + 2\nu_4 + \nu_5, F_{1u}$ (-0.66)	2697.583
$\nu_5 + 5\nu_6, F_{1u}$ (-0.64)	2251.826	$\nu_3 + 2\nu_4 + \nu_5, A_{2u}$ (-0.77)	2697.622
$\nu_5 + 5\nu_6, E_u$ (-0.62)	2252.070	$\nu_3 + 2\nu_4 + \nu_5, E_u$ (-0.78)	2697.628
$\nu_5 + 5\nu_6, F_{2u}$ (-0.51)	2252.157	$\nu_3 + 2\nu_4 + \nu_5, F_{2u}$ (0.72)	2697.751
$\nu_3 + \nu_4 + 2\nu_6, E_g$ (-0.93)	2252.195	$\nu_3 + 2\nu_4 + \nu_5, E_u$ (0.80)	2697.777
$\nu_3 + \nu_4 + 2\nu_6, F_{1g}$ (-0.93)	2252.412	$\nu_3 + 2\nu_4 + \nu_5, A_{1u}$ (-1.00)	2697.803
$\nu_3 + \nu_4 + 2\nu_6, F_{2g}$ (-0.89)	2252.645	$\nu_3 + 2\nu_4 + \nu_5, F_{1u}$ (-0.77)	2697.906
$\nu_3 + \nu_4 + 2\nu_6, A_{1g}$ (-0.84)	2252.927	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, A_{2g}$ (-0.85)	2698.246
$\nu_5 + 5\nu_6, F_{2u}$ (-0.86)	2253.070	$\nu_1 + \nu_2 + \nu_3 + \nu_6, E_g$ (0.65)	2701.712
$\nu_3 + \nu_4 + 2\nu_6, F_{1g}$ (0.88)	2253.520	$2\nu_1 + \nu_2 + \nu_5, F_{1g}$ (0.83)	2702.779
$\nu_3 + \nu_4 + 2\nu_6, E_g$ (-0.82)	2253.578	$2\nu_2 + \nu_3 + \nu_4, A_{2g}$ (-0.58)	2703.490
$\nu_3 + \nu_4 + 2\nu_6, A_{2g}$ (-0.92)	2253.616	$\nu_1 + \nu_2 + \nu_3 + \nu_6, F_{2g}$ (-0.95)	2703.734
$\nu_3 + \nu_4 + 2\nu_6, F_{2g}$ (-0.52)	2253.876	$2\nu_1 + \nu_2 + \nu_5, F_{2g}$ (-0.81)	2705.392
$\nu_3 + \nu_4 + 2\nu_6, F_{2g}$ (0.81)	2253.975	$\nu_1 + \nu_3 + 3\nu_6, F_{1g}$ (-0.53)	2705.716
$\nu_3 + \nu_4 + 2\nu_6, F_{1g}$ (0.86)	2254.051	$\nu_1 + \nu_2 + \nu_3 + \nu_6, F_{1g}$ (-0.89)	2706.408
$\nu_3 + \nu_4 + 2\nu_6, E_g$ (-0.75)	2254.372	$2\nu_2 + \nu_3 + \nu_4, E_g$ (-0.65)	2706.672
$\nu_3 + \nu_4 + 2\nu_6, F_{1g}$ (0.86)	2254.440	$\nu_1 + \nu_2 + \nu_3 + \nu_6, A_{1g}$ (0.89)	2707.533
$\nu_3 + \nu_4 + 2\nu_6, F_{2g}$ (0.67)	2254.447	$2\nu_2 + \nu_3 + \nu_4, F_{2g}$ (0.45)	2707.843
$\nu_3 + \nu_4 + 2\nu_6, A_{1g}$ (-0.88)	2254.894	$\nu_2 + \nu_3 + \nu_4 + \nu_5, F_{2g}$ (0.68)	2718.068
$\nu_1 + \nu_4 + \nu_5 + \nu_6, F_{1g}$ (-0.88)	2255.193	$\nu_2 + \nu_3 + \nu_4 + \nu_5, F_{2g}$ (0.82)	2718.232
$\nu_3 + \nu_4 + 2\nu_6, F_{2g}$ (0.44)	2255.200	$\nu_2 + \nu_3 + \nu_4 + \nu_5, E_g$ (0.70)	2718.353
$\nu_3 + \nu_4 + 2\nu_6, A_{1g}$ (-0.84)	2255.396	$\nu_2 + \nu_3 + \nu_4 + \nu_5, A_{1g}$ (0.95)	2718.467
$3\nu_5 + 2\nu_6, F_{2g}$ (0.52)	2255.678	$\nu_2 + \nu_3 + \nu_4 + \nu_5, F_{1g}$ (0.92)	2718.523
$\nu_3 + \nu_4 + 2\nu_6, F_{1g}$ (0.72)	2255.810	$\nu_2 + \nu_3 + \nu_4 + \nu_5, F_{1g}$ (-0.61)	2718.552
$\nu_3 + \nu_4 + 2\nu_6, E_g$ (0.66)	2255.819	$\nu_2 + \nu_3 + \nu_4 + \nu_5, A_{2g}$ (0.93)	2718.621
$\nu_1 + \nu_4 + \nu_5 + \nu_6, F_{2g}$ (0.57)	2255.955	$\nu_2 + \nu_3 + \nu_4 + \nu_5, E_g$ (-0.69)	2718.748
$\nu_3 + \nu_4 + 2\nu_6, A_{2g}$ (-0.90)	2256.124	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, A_{2u}$ (0.72)	2722.192
$\nu_3 + \nu_4 + 2\nu_6, F_{1g}$ (-0.84)	2256.474	$\nu_2 + \nu_3 + \nu_4 + \nu_5, F_{1g}$ (-0.85)	2722.507
$\nu_5 + 5\nu_6, A_{2u}$ (0.71)	2256.492	$\nu_2 + \nu_3 + \nu_4 + \nu_5, F_{2g}$ (-0.97)	2722.783

Table 1 – continued

Band, Sym, Eig	Band center	Band, Sym, Eig	Band center
$\nu_3 + \nu_4 + 2\nu_6, F_{2g}$ (0.63)	2256.523	$\nu_2 + \nu_3 + \nu_4 + \nu_5, F_{1g}$ (-0.67)	2722.797
$\nu_1 + \nu_4 + \nu_5 + \nu_6, E_g$ (-0.82)	2256.562	$\nu_2 + \nu_3 + \nu_4 + \nu_5, E_g$ (0.69)	2722.842
$\nu_5 + 5\nu_6, E_u$ (-0.65)	2256.574	$\nu_2 + \nu_3 + \nu_4 + \nu_5, F_{2g}$ (0.58)	2722.930
$\nu_1 + \nu_4 + \nu_5 + \nu_6, F_{1g}$ (0.67)	2256.653	$\nu_2 + \nu_3 + \nu_4 + \nu_5, A_{2g}$ (-0.97)	2722.959
$\nu_1 + \nu_4 + \nu_5 + \nu_6, A_{1g}$ (0.81)	2256.660	$\nu_2 + \nu_3 + \nu_4 + \nu_5, A_{1g}$ (0.96)	2723.125
$3\nu_5 + 2\nu_6, E_g$ (0.71)	2256.812	$\nu_2 + \nu_3 + \nu_4 + \nu_5, E_g$ (-0.70)	2723.233
$\nu_3 + \nu_4 + 2\nu_6, F_{2g}$ (-0.65)	2256.821	$\nu_2 + \nu_3 + \nu_4 + \nu_5, F_{2g}$ (0.65)	2723.764
$\nu_3 + \nu_4 + 2\nu_6, E_g$ (-0.59)	2257.100	$\nu_2 + \nu_3 + \nu_4 + \nu_5, F_{1g}$ (-0.60)	2723.778
$3\nu_5 + 2\nu_6, A_{1g}$ (0.97)	2257.256	$\nu_2 + \nu_3 + \nu_4 + \nu_5, F_{2g}$ (-0.57)	2723.912
$\nu_5 + 5\nu_6, F_{1u}$ (0.68)	2257.367	$\nu_2 + \nu_3 + \nu_4 + \nu_5, F_{1g}$ (-0.65)	2724.681
$\nu_1 + \nu_4 + \nu_5 + \nu_6, F_{1g}$ (-0.79)	2257.484	$\nu_2 + \nu_3 + \nu_4 + \nu_5, F_{2g}$ (-0.54)	2724.719
$\nu_1 + \nu_4 + \nu_5 + \nu_6, F_{2g}$ (-0.92)	2257.567	$\nu_2 + \nu_3 + \nu_4 + \nu_5, F_{1g}$ (-0.56)	2724.798
$3\nu_5 + 2\nu_6, F_{1g}$ (-0.71)	2257.637	$2\nu_2 + \nu_3 + \nu_5, F_{2u}$ (-0.75)	2744.076
$\nu_5 + 5\nu_6, F_{2u}$ (0.60)	2257.647	$2\nu_2 + \nu_3 + \nu_5, F_{1u}$ (0.75)	2744.088
$\nu_1 + \nu_4 + \nu_5 + \nu_6, F_{2g}$ (-0.76)	2257.928	$2\nu_2 + \nu_3 + \nu_5, F_{1u}$ (-0.74)	2747.354
$\nu_1 + \nu_4 + \nu_5 + \nu_6, E_g$ (-0.82)	2257.970	$\nu_1 + \nu_3 + 3\nu_6, F_{1g}$ (-0.86)	2747.396
$\nu_1 + \nu_4 + \nu_5 + \nu_6, A_{2g}$ (0.89)	2258.005	$2\nu_2 + \nu_3 + \nu_5, F_{2u}$ (-0.75)	2747.465
$\nu_1 + \nu_4 + \nu_5 + \nu_6, F_{1g}$ (-0.72)	2258.302	$2\nu_1 + \nu_3 + \nu_6, A_{2g}$ (-0.59)	2748.953
$3\nu_5 + 2\nu_6, F_{2g}$ (-0.94)	2258.310	$2\nu_2 + \nu_3 + \nu_5, A_{1u}$ (0.75)	2750.877
$3\nu_5 + 2\nu_6, F_{1g}$ (-0.91)	2258.444	$2\nu_2 + \nu_3 + \nu_5, A_{2u}$ (0.81)	2750.908
$3\nu_5 + 2\nu_6, F_{2g}$ (-0.65)	2258.845	$2\nu_2 + \nu_3 + \nu_5, E_u$ (0.82)	2750.945
$\nu_5 + 5\nu_6, F_{2u}$ (-0.62)	2259.072	$2\nu_2 + \nu_3 + \nu_5, E_u$ (0.82)	2751.269
$3\nu_5 + 2\nu_6, A_{1g}$ (0.90)	2259.125	$2\nu_3 + \nu_5 + \nu_6, F_{1u}$ (0.66)	2752.303
$3\nu_5 + 2\nu_6, F_{1g}$ (-0.84)	2259.129	$2\nu_2 + \nu_3 + \nu_5, F_{2u}$ (0.47)	2752.496
$3\nu_5 + 2\nu_6, F_{2g}$ (-0.54)	2259.719	$2\nu_3 + \nu_5 + \nu_6, A_{1u}$ (-0.69)	2752.602
$\nu_5 + 5\nu_6, E_u$ (-0.64)	2259.877	$2\nu_2 + \nu_3 + \nu_5, A_{2u}$ (-0.57)	2753.022
$3\nu_5 + 2\nu_6, E_g$ (0.87)	2260.150	$2\nu_2 + \nu_3 + \nu_5, E_u$ (-0.74)	2753.129
$3\nu_5 + 2\nu_6, F_{2g}$ (0.94)	2260.759	$2\nu_3 + \nu_5 + \nu_6, E_u$ (0.73)	2753.339
$3\nu_5 + 2\nu_6, A_{2g}$ (-0.98)	2260.946	$2\nu_3 + \nu_5 + \nu_6, F_{1u}$ (0.46)	2753.406
$\nu_5 + 5\nu_6, F_{1u}$ (-0.63)	2261.021	$2\nu_3 + \nu_5 + \nu_6, F_{2u}$ (0.53)	2753.958
$3\nu_5 + 2\nu_6, F_{1g}$ (0.65)	2261.310	$2\nu_3 + \nu_5 + \nu_6, F_{1u}$ (0.72)	2754.603
$\nu_5 + 5\nu_6, A_{1u}$ (-0.55)	2261.539	$2\nu_3 + \nu_5 + \nu_6, E_u$ (-0.69)	2754.726
$3\nu_5 + 2\nu_6, F_{2g}$ (-0.56)	2261.844	$2\nu_3 + \nu_5 + \nu_6, F_{2u}$ (-0.80)	2755.256
$\nu_5 + 5\nu_6, F_{2u}$ (-0.62)	2262.353	$2\nu_3 + \nu_5 + \nu_6, A_{2u}$ (-0.94)	2755.409
$\nu_5 + 5\nu_6, F_{1u}$ (0.67)	2262.356	$\nu_1 + \nu_3 + 3\nu_6, E_g$ (-0.53)	2756.058
$3\nu_5 + 2\nu_6, E_g$ (0.69)	2262.618	$\nu_1 + \nu_3 + 3\nu_6, F_{2g}$ (-0.75)	2756.111
$3\nu_5 + 2\nu_6, F_{1g}$ (0.69)	2262.886	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, A_{2g}$ (-0.57)	2756.540
$\nu_5 + 5\nu_6, E_u$ (-0.63)	2263.431	$\nu_1 + \nu_3 + 3\nu_6, F_{1g}$ (-0.55)	2757.007
$3\nu_5 + 2\nu_6, A_{1g}$ (-0.89)	2263.506	$2\nu_2 + \nu_3 + \nu_4, F_{1g}$ (-0.63)	2758.567
$3\nu_5 + 2\nu_6, F_{2g}$ (-0.61)	2263.838	$\nu_1 + \nu_3 + 2\nu_5, E_u$ (0.91)	2758.616
$3\nu_5 + 2\nu_6, F_{1g}$ (0.60)	2264.600	$\nu_1 + \nu_3 + 2\nu_5, A_{2u}$ (-0.88)	2758.703
$\nu_5 + 5\nu_6, A_{1u}$ (0.62)	2264.862	$2\nu_3 + \nu_5 + \nu_6, F_{2u}$ (-0.61)	2758.816
$3\nu_5 + 2\nu_6, E_g$ (0.56)	2264.878	$2\nu_3 + \nu_5 + \nu_6, F_{1u}$ (-0.63)	2758.818
$3\nu_5 + 2\nu_6, F_{2g}$ (0.60)	2264.976	$2\nu_3 + \nu_5 + \nu_6, F_{2u}$ (0.74)	2759.138
$\nu_5 + 5\nu_6, E_u$ (-0.60)	2265.046	$\nu_1 + \nu_3 + 3\nu_6, A_{1g}$ (-0.86)	2759.822
$\nu_5 + 5\nu_6, F_{2u}$ (-0.52)	2265.467	$\nu_1 + \nu_3 + 3\nu_6, F_{2g}$ (0.78)	2759.895
$\nu_5 + 5\nu_6, F_{1u}$ (0.51)	2265.533	$\nu_1 + \nu_3 + 3\nu_6, F_{2g}$ (-0.43)	2760.089
$3\nu_5 + 2\nu_6, F_{1g}$ (0.70)	2266.019	$\nu_1 + \nu_3 + 2\nu_5, F_{1u}$ (0.65)	2760.209
$3\nu_5 + 2\nu_6, F_{2g}$ (-0.68)	2266.058	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, E_g$ (0.59)	2760.262
$\nu_5 + 5\nu_6, F_{1u}$ (0.56)	2266.262	$\nu_1 + \nu_3 + 2\nu_5, F_{2u}$ (0.72)	2760.345
$\nu_5 + 5\nu_6, A_{1u}$ (0.63)	2267.995	$\nu_1 + \nu_3 + 3\nu_6, F_{1g}$ (0.52)	2760.428
$\nu_5 + 5\nu_6, F_{2u}$ (0.55)	2268.698	$2\nu_3 + \nu_5 + \nu_6, E_u$ (-0.67)	2760.434
$2\nu_4 + 3\nu_6, F_{2u}$ (0.54)	2268.911	$2\nu_3 + \nu_5 + \nu_6, A_{1u}$ (-0.86)	2760.672
$2\nu_4 + 3\nu_6, F_{1u}$ (0.60)	2269.153	$2\nu_3 + \nu_5 + \nu_6, F_{2u}$ (0.47)	2760.769
$\nu_5 + 5\nu_6, F_{1u}$ (0.53)	2269.274	$\nu_1 + \nu_3 + 3\nu_6, F_{2g}$ (0.36)	2760.863

Table 1 – continued

Band, Sym, Eig	Band center	Band, Sym, Eig	Band center
$2\nu_4 + 3\nu_6, E_u$ (0.84)	2269.603	$\nu_1 + \nu_3 + 2\nu_5, F_{1u}$ (0.62)	2760.896
$2\nu_4 + 3\nu_6, F_{2u}$ (0.66)	2269.606	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, E_g$ (-0.57)	2761.663
$\nu_5 + 5\nu_6, A_{2u}$ (-0.70)	2269.659	$2\nu_3 + \nu_5 + \nu_6, F_{2u}$ (0.58)	2761.997
$3\nu_2 + \nu_6, F_{2u}$ (0.76)	2269.688	$2\nu_3 + \nu_5 + \nu_6, E_u$ (0.95)	2762.034
$2\nu_4 + 3\nu_6, F_{1u}$ (-0.71)	2269.912	$\nu_1 + \nu_3 + 2\nu_5, F_{1u}$ (-0.54)	2762.318
$3\nu_2 + \nu_6, F_{1u}$ (-0.71)	2269.965	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{1g}$ (-0.44)	2762.339
$2\nu_4 + 3\nu_6, A_{1u}$ (-0.76)	2270.036	$2\nu_2 + 2\nu_3, A_{2g}$ (-0.48)	2762.351
$\nu_5 + 5\nu_6, E_u$ (0.56)	2271.018	$2\nu_3 + \nu_5 + \nu_6, A_{2u}$ (0.86)	2762.351
$2\nu_4 + 3\nu_6, F_{2u}$ (0.66)	2271.083	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, E_g$ (0.59)	2762.519
$\nu_5 + 5\nu_6, F_{2u}$ (-0.56)	2271.135	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{1g}$ (0.45)	2762.594
$2\nu_4 + 3\nu_6, E_u$ (-0.92)	2271.805	$2\nu_3 + \nu_5 + \nu_6, F_{2u}$ (0.48)	2762.897
$2\nu_4 + 3\nu_6, F_{2u}$ (0.85)	2272.026	$2\nu_3 + \nu_5 + \nu_6, F_{1u}$ (0.70)	2763.003
$2\nu_4 + 3\nu_6, A_{1u}$ (0.90)	2272.219	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{2g}$ (0.38)	2763.154
$3\nu_2 + \nu_6, F_{2u}$ (0.71)	2273.133	$2\nu_3 + \nu_5 + \nu_6, A_{1u}$ (-0.96)	2763.230
$2\nu_4 + 3\nu_6, F_{1u}$ (-0.70)	2273.236	$2\nu_3 + \nu_5 + \nu_6, F_{1u}$ (-0.59)	2763.351
$2\nu_4 + 3\nu_6, A_{2u}$ (-0.99)	2273.340	$2\nu_3 + \nu_5 + \nu_6, E_u$ (0.94)	2763.425
$2\nu_4 + 3\nu_6, F_{2u}$ (-0.74)	2273.478	$2\nu_1 + \nu_5 + 2\nu_6, A_{1g}$ (0.84)	2763.586
$2\nu_4 + 3\nu_6, F_{1u}$ (-0.90)	2273.611	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, A_{1g}$ (-0.56)	2763.629
$2\nu_4 + 2\nu_5, A_{1g}$ (0.88)	2273.816	$2\nu_3 + \nu_5 + \nu_6, F_{2u}$ (0.60)	2763.962
$2\nu_4 + 2\nu_5, F_{1g}$ (0.82)	2274.070	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{2g}$ (-0.37)	2764.852
$2\nu_4 + 2\nu_5, F_{2g}$ (0.73)	2274.140	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, A_{2g}$ (0.82)	2764.923
$2\nu_4 + 2\nu_5, E_g$ (-0.87)	2274.464	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{1g}$ (0.43)	2765.155
$2\nu_4 + 3\nu_6, F_{1u}$ (-0.66)	2274.490	$\nu_1 + \nu_3 + 2\nu_5, F_{1u}$ (-0.77)	2766.957
$2\nu_4 + 2\nu_5, F_{2g}$ (-0.65)	2274.625	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{2g}$ (-0.72)	2771.127
$2\nu_4 + 3\nu_6, F_{2u}$ (0.68)	2274.636	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{1g}$ (-0.62)	2771.165
$2\nu_4 + 3\nu_6, E_u$ (0.87)	2274.762	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, A_{2g}$ (-0.63)	2771.380
$2\nu_4 + 2\nu_5, F_{1g}$ (-0.86)	2274.763	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{1g}$ (0.75)	2771.397
$2\nu_4 + 2\nu_5, F_{2g}$ (-0.70)	2274.972	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, E_g$ (0.70)	2771.416
$2\nu_4 + 2\nu_5, E_g$ (0.66)	2275.198	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{2g}$ (-0.64)	2771.453
$2\nu_4 + 2\nu_5, A_{1g}$ (-0.85)	2275.248	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{2g}$ (-0.51)	2771.726
$2\nu_4 + 3\nu_6, F_{2u}$ (-0.65)	2275.276	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, E_g$ (-0.58)	2771.733
$3\nu_2 + \nu_6, F_{1u}$ (-0.70)	2275.314	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{1g}$ (0.52)	2771.802
$2\nu_4 + 2\nu_5, F_{2g}$ (-0.94)	2275.566	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, A_{1g}$ (0.78)	2771.803
$2\nu_4 + 2\nu_5, E_g$ (0.69)	2275.817	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{2g}$ (-0.41)	2771.833
$2\nu_4 + 2\nu_5, A_{1g}$ (0.84)	2275.912	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, E_g$ (0.56)	2771.882
$2\nu_4 + 2\nu_5, F_{1g}$ (-0.94)	2275.935	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, A_{2g}$ (0.69)	2771.966
$2\nu_4 + 3\nu_6, F_{2u}$ (-0.77)	2275.976	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{1g}$ (0.57)	2772.161
$2\nu_4 + 2\nu_5, E_g$ (0.85)	2276.062	$2\nu_1 + 2\nu_4, A_{1g}$ (0.93)	2772.218
$2\nu_4 + 2\nu_5, A_{2g}$ (0.99)	2276.075	$2\nu_1 + 2\nu_4, E_g$ (0.93)	2772.306
$2\nu_4 + 3\nu_6, F_{1u}$ (0.80)	2276.090	$2\nu_1 + 2\nu_4, F_{2g}$ (0.74)	2772.451
$2\nu_4 + 2\nu_5, F_{2g}$ (-0.93)	2276.133	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, E_g$ (0.43)	2772.474
$2\nu_4 + 3\nu_6, E_u$ (-0.77)	2276.207	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{1g}$ (-0.41)	2772.507
$2\nu_4 + 3\nu_6, A_{1u}$ (0.78)	2276.529	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, A_{1g}$ (0.70)	2772.524
$2\nu_4 + 3\nu_6, F_{1u}$ (-0.76)	2277.036	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{1g}$ (-0.51)	2772.539
$2\nu_4 + 3\nu_6, F_{2u}$ (0.54)	2277.304	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{2g}$ (-0.63)	2772.584
$\nu_2 + \nu_3 + 2\nu_6, F_{1u}$ (-0.76)	2277.766	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{2g}$ (-0.42)	2772.667
$\nu_2 + \nu_3 + 2\nu_6, F_{2u}$ (-0.63)	2278.497	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, A_{2g}$ (0.54)	2772.916
$\nu_2 + \nu_3 + 2\nu_6, F_{1u}$ (0.45)	2279.398	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{2g}$ (-0.55)	2773.123
$\nu_2 + \nu_3 + 2\nu_6, F_{2u}$ (0.62)	2279.864	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{1g}$ (-0.40)	2773.130
$\nu_2 + \nu_3 + 2\nu_6, A_{2u}$ (-0.92)	2280.517	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, E_g$ (0.57)	2773.196
$\nu_2 + \nu_3 + 2\nu_6, E_u$ (0.80)	2280.850	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{1g}$ (-0.59)	2773.339
$\nu_1 + \nu_2 + \nu_5 + \nu_6, E_u$ (-0.93)	2281.003	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{2g}$ (0.55)	2773.391
$\nu_1 + \nu_2 + \nu_5 + \nu_6, F_{1u}$ (-0.57)	2281.105	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, A_{1g}$ (-0.77)	2773.393
$\nu_1 + \nu_2 + \nu_5 + \nu_6, F_{2u}$ (0.65)	2281.117	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{1g}$ (0.48)	2773.511
$\nu_2 + \nu_3 + 2\nu_6, A_{1u}$ (0.82)	2281.432	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, E_g$ (-0.76)	2773.611

Table 1 – continued

Band, Sym, Eig	Band center	Band, Sym, Eig	Band center
$\nu_2 + \nu_3 + 2\nu_6, F_{1u}$ (0.68)	2281.530	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{2g}$ (-0.49)	2773.783
$\nu_2 + \nu_3 + 2\nu_6, E_u$ (0.91)	2282.338	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{2g}$ (0.43)	2774.053
$\nu_2 + \nu_3 + 2\nu_6, F_{1u}$ (0.56)	2283.107	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, E_g$ (-0.61)	2774.167
$\nu_2 + \nu_3 + 2\nu_6, F_{2u}$ (0.44)	2283.133	$\nu_3 + 3\nu_4, A_{2g}$ (0.79)	2774.187
$\nu_1 + \nu_2 + \nu_5 + \nu_6, A_{2u}$ (0.90)	2283.308	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{2g}$ (-0.45)	2774.315
$\nu_1 + \nu_2 + \nu_5 + \nu_6, E_u$ (0.83)	2283.373	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{1g}$ (0.44)	2774.337
$\nu_1 + \nu_2 + \nu_5 + \nu_6, A_{1u}$ (0.82)	2283.400	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{2g}$ (0.70)	2774.644
$\nu_2 + \nu_3 + 2\nu_6, F_{2u}$ (-0.59)	2283.669	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, A_{1g}$ (-0.55)	2774.717
$\nu_1 + \nu_2 + \nu_5 + \nu_6, F_{1u}$ (0.50)	2284.297	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{1g}$ (0.56)	2774.752
$\nu_1 + \nu_2 + \nu_5 + \nu_6, F_{2u}$ (0.64)	2284.967	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, E_g$ (0.46)	2774.765
$\nu_2 + \nu_3 + 2\nu_6, F_{1u}$ (0.70)	2285.450	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{2g}$ (-0.54)	2774.808
$\nu_2 + \nu_3 + 2\nu_6, F_{2u}$ (0.84)	2286.259	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{1g}$ (0.53)	2775.023
$\nu_2 + \nu_4 + 3\nu_6, A_{2g}$ (-0.68)	2293.143	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{2g}$ (0.51)	2775.563
$\nu_2 + \nu_4 + 3\nu_6, F_{1g}$ (-0.68)	2293.639	$2\nu_3 + \nu_5 + 2\nu_6, A_{2g}$ (0.73)	2775.750
$\nu_2 + \nu_4 + 3\nu_6, E_g$ (0.68)	2293.692	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, E_g$ (-0.55)	2775.785
$\nu_2 + \nu_4 + 3\nu_6, F_{2g}$ (-0.58)	2293.970	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{1g}$ (-0.52)	2775.844
$\nu_2 + \nu_4 + 3\nu_6, A_{1g}$ (-0.85)	2294.978	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{2g}$ (0.46)	2775.849
$\nu_2 + \nu_4 + 3\nu_6, F_{1g}$ (0.75)	2295.098	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{1g}$ (-0.49)	2775.919
$\nu_2 + \nu_4 + 3\nu_6, F_{2g}$ (0.74)	2295.183	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{2g}$ (-0.48)	2775.974
$\nu_2 + \nu_4 + 3\nu_6, E_g$ (0.77)	2295.788	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, E_g$ (0.56)	2776.085
$\nu_2 + \nu_4 + 3\nu_6, F_{1g}$ (-0.94)	2297.236	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, A_{1g}$ (0.55)	2776.201
$\nu_2 + \nu_4 + 3\nu_6, F_{2g}$ (-0.91)	2297.502	$2\nu_3 + \nu_5 + 2\nu_6, E_g$ (0.52)	2776.362
$\nu_2 + \nu_4 + 3\nu_6, E_g$ (-0.46)	2298.059	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{2g}$ (0.52)	2776.504
$\nu_2 + \nu_4 + 3\nu_6, F_{1g}$ (-0.56)	2298.382	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{1g}$ (-0.37)	2776.508
$\nu_2 + \nu_4 + 3\nu_6, F_{2g}$ (-0.75)	2298.712	$2\nu_2 + \nu_3 + \nu_4, A_{1g}$ (0.80)	2776.667
$\nu_2 + \nu_4 + 2\nu_5, F_{2u}$ (0.72)	2299.017	$\nu_1 + \nu_3 + \nu_4 + \nu_5, E_g$ (-0.42)	2776.787
$\nu_2 + \nu_4 + 2\nu_5, A_{2u}$ (0.99)	2299.340	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{1g}$ (0.47)	2776.904
$\nu_2 + \nu_4 + 2\nu_5, F_{1u}$ (0.73)	2299.406	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{2g}$ (0.40)	2776.985
$\nu_2 + \nu_4 + 3\nu_6, A_{1g}$ (-0.86)	2299.417	$2\nu_3 + \nu_5 + 2\nu_6, E_g$ (-0.48)	2777.073
$\nu_2 + \nu_4 + 2\nu_5, E_u$ (0.73)	2299.446	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{1g}$ (-0.44)	2777.212
$\nu_2 + \nu_4 + 2\nu_5, F_{2u}$ (0.62)	2299.573	$3\nu_1 + \nu_5, F_{2g}$ (0.59)	2777.364
$\nu_2 + \nu_4 + 3\nu_6, E_g$ (0.76)	2299.581	$\nu_1 + \nu_3 + \nu_4 + \nu_5, A_{2g}$ (-0.74)	2777.414
$\nu_2 + \nu_4 + 2\nu_5, F_{1u}$ (0.66)	2299.614	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{2g}$ (0.46)	2777.416
$\nu_2 + \nu_4 + 3\nu_6, A_{2g}$ (-0.70)	2299.731	$2\nu_3 + \nu_5 + 2\nu_6, E_g$ (0.57)	2777.462
$\nu_2 + \nu_4 + 2\nu_5, F_{2u}$ (-0.62)	2299.798	$\nu_1 + \nu_3 + \nu_4 + \nu_5, F_{1g}$ (0.41)	2777.498
$\nu_2 + \nu_4 + 3\nu_6, F_{1g}$ (0.70)	2299.866	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, A_{1g}$ (-0.77)	2777.512
$\nu_2 + \nu_4 + 3\nu_6, F_{2g}$ (0.86)	2300.019	$\nu_1 + \nu_3 + \nu_4 + \nu_5, F_{2g}$ (0.39)	2778.157
$\nu_2 + \nu_4 + 3\nu_6, A_{2g}$ (0.62)	2300.292	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{1g}$ (-0.39)	2778.253
$\nu_2 + \nu_4 + 3\nu_6, F_{2g}$ (-0.57)	2300.560	$\nu_1 + \nu_3 + \nu_4 + \nu_5, A_{1g}$ (0.85)	2778.319
$\nu_2 + \nu_4 + 3\nu_6, E_g$ (-0.66)	2301.051	$\nu_1 + \nu_3 + \nu_4 + \nu_5, F_{1g}$ (-0.53)	2778.375
$\nu_2 + \nu_4 + 2\nu_5, F_{1u}$ (0.83)	2301.185	$\nu_3 + \nu_4 + \nu_5 + 2\nu_6, F_{2g}$ (-0.36)	2778.687
$\nu_2 + \nu_4 + 3\nu_6, F_{1g}$ (0.66)	2301.198	$2\nu_3 + \nu_4 + \nu_6, F_{1g}$ (0.45)	2778.696
$\nu_2 + \nu_4 + 2\nu_5, F_{2u}$ (0.90)	2301.448	$\nu_1 + \nu_3 + \nu_4 + \nu_5, F_{1g}$ (-0.54)	2778.819
$\nu_2 + \nu_4 + 2\nu_5, A_{1u}$ (0.99)	2301.647	$\nu_3 + 3\nu_5 + \nu_6, F_{2g}$ (0.56)	2778.832
$\nu_2 + \nu_4 + 2\nu_5, E_u$ (0.73)	2301.775	$\nu_1 + \nu_3 + \nu_4 + \nu_5, F_{2g}$ (-0.36)	2778.939
$\nu_2 + \nu_4 + 2\nu_5, F_{1u}$ (0.78)	2303.255	$\nu_1 + \nu_3 + \nu_4 + \nu_5, F_{1g}$ (-0.57)	2779.453
$\nu_2 + \nu_4 + 3\nu_6, F_{2g}$ (-0.77)	2303.560	$\nu_1 + \nu_3 + \nu_4 + \nu_5, F_{2g}$ (0.59)	2779.667
$\nu_2 + \nu_4 + 3\nu_6, F_{1g}$ (0.75)	2303.782	$\nu_3 + 3\nu_5 + \nu_6, F_{1g}$ (0.59)	2780.421
$\nu_2 + \nu_4 + 2\nu_5, F_{2u}$ (-0.68)	2303.793	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, E_u$ (-0.49)	2784.746
$\nu_2 + \nu_4 + 3\nu_6, E_g$ (0.68)	2303.825	$\nu_3 + 3\nu_4, E_g$ (-0.77)	2785.562
$\nu_2 + \nu_4 + 2\nu_5, F_{1u}$ (0.87)	2303.916	$\nu_3 + 3\nu_4, F_{1g}$ (-0.66)	2785.778
$\nu_2 + \nu_4 + 3\nu_6, A_{1g}$ (-0.82)	2304.558	$\nu_3 + 3\nu_4, A_{1g}$ (-0.89)	2785.895
$3\nu_1, A_{1g}$ (0.78)	2318.552	$2\nu_3 + \nu_4 + \nu_6, A_{2g}$ (-0.69)	2786.118
$2\nu_2 + 3\nu_6, F_{2u}$ (0.51)	2318.620	$\nu_3 + 3\nu_4, F_{2g}$ (-0.71)	2786.268
$2\nu_2 + 3\nu_6, F_{1u}$ (-0.73)	2319.864	$\nu_3 + 3\nu_4, F_{2g}$ (-0.88)	2786.464

Table 1 – continued

Band, Sym, Eig	Band center	Band, Sym, Eig	Band center
$2\nu_2 + 3\nu_6, F_{2u}$ (-0.59)	2321.415	$\nu_3 + 3\nu_4, E_g$ (0.82)	2786.575
$2\nu_2 + 3\nu_6, E_u$ (0.90)	2323.449	$\nu_3 + 3\nu_4, F_{1g}$ (0.69)	2786.636
$2\nu_2 + 3\nu_6, F_{2u}$ (0.61)	2323.982	$\nu_3 + 3\nu_4, F_{1g}$ (-0.72)	2786.742
$2\nu_2 + 3\nu_6, A_{1u}$ (-0.95)	2324.289	$\nu_3 + 3\nu_4, F_{2g}$ (0.83)	2787.161
$2\nu_2 + 2\nu_5, A_{1g}$ (0.69)	2324.712	$\nu_3 + 3\nu_4, E_g$ (0.81)	2787.600
$2\nu_2 + 2\nu_5, E_g$ (-0.65)	2324.764	$\nu_3 + 3\nu_4, A_{1g}$ (-0.89)	2787.719
$2\nu_2 + 3\nu_6, F_{1u}$ (-0.89)	2325.418	$\nu_3 + 3\nu_4, F_{2g}$ (-0.61)	2787.898
$2\nu_2 + 2\nu_5, F_{2g}$ (0.72)	2325.552	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, A_{2u}$ (0.62)	2788.895
$2\nu_2 + 3\nu_6, F_{1u}$ (-0.62)	2325.591	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, E_u$ (0.48)	2790.999
$2\nu_2 + 2\nu_5, F_{1g}$ (-0.92)	2327.104	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, E_u$ (0.48)	2791.938
$2\nu_2 + 3\nu_6, F_{2u}$ (-0.63)	2327.832	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, E_u$ (-0.67)	2792.754
$2\nu_2 + 2\nu_5, E_g$ (0.67)	2328.397	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, A_{2u}$ (0.55)	2792.934
$2\nu_2 + 2\nu_5, A_{2g}$ (0.94)	2328.518	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, F_{2u}$ (0.65)	2794.848
$2\nu_2 + 3\nu_6, F_{1u}$ (0.51)	2328.697	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, F_{1u}$ (-0.48)	2795.192
$2\nu_2 + 2\nu_5, F_{2g}$ (0.74)	2329.515	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, E_u$ (0.48)	2795.925
$\nu_3 + 4\nu_6, F_{1u}$ (-0.63)	2329.951	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, F_{2u}$ (-0.58)	2795.970
$\nu_3 + 4\nu_6, F_{2u}$ (-0.73)	2330.702	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, F_{1u}$ (-0.67)	2796.244
$\nu_3 + 4\nu_6, E_u$ (-0.71)	2330.904	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, A_{1u}$ (-0.96)	2797.079
$\nu_3 + 4\nu_6, F_{1u}$ (-0.76)	2331.097	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, A_{1u}$ (-0.81)	2797.105
$\nu_1 + \nu_3 + \nu_4, E_g$ (-0.88)	2331.409	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, F_{1u}$ (-0.68)	2797.112
$\nu_1 + \nu_3 + \nu_4, F_{1g}$ (0.88)	2331.606	$2\nu_1 + \nu_2 + \nu_4, F_{1u}$ (-0.93)	2797.427
$\nu_1 + \nu_3 + \nu_4, F_{2g}$ (0.88)	2331.954	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, F_{2u}$ (0.54)	2797.544
$2\nu_2 + 2\nu_5, A_{1g}$ (0.65)	2331.971	$\nu_1 + \nu_3 + \nu_5 + 2\nu_6, A_{2u}$ (-0.74)	2797.611
$2\nu_2 + 2\nu_5, E_g$ (0.66)	2332.019	$2\nu_1 + \nu_2 + \nu_4, F_{2u}$ (-0.80)	2797.786
$\nu_3 + 4\nu_6, A_{2u}$ (0.73)	2332.233	$2\nu_1 + \nu_2 + \nu_4, F_{2u}$ (-0.47)	2797.817
$\nu_1 + \nu_3 + \nu_4, A_{1g}$ (-0.87)	2332.745	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, E_u$ (0.53)	2797.942
$2\nu_2 + 3\nu_6, F_{2u}$ (0.64)	2332.752	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, F_{1u}$ (0.72)	2798.005
$\nu_1 + \nu_5 + 3\nu_6, A_{1u}$ (-0.71)	2332.839	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, F_{1u}$ (0.58)	2798.227
$\nu_3 + 2\nu_5 + \nu_6, F_{1g}$ (-0.72)	2332.932	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, F_{2u}$ (0.49)	2798.712
$\nu_3 + 2\nu_5 + \nu_6, F_{2g}$ (0.68)	2332.990	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, F_{1u}$ (-0.50)	2798.730
$\nu_1 + \nu_5 + 3\nu_6, F_{1u}$ (-0.67)	2333.746	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, F_{2u}$ (0.45)	2799.082
$\nu_3 + 2\nu_5 + \nu_6, F_{1g}$ (-0.83)	2333.772	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, A_{1u}$ (0.85)	2799.751
$\nu_1 + \nu_5 + 3\nu_6, F_{2u}$ (0.70)	2334.130	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, F_{2u}$ (0.65)	2799.823
$\nu_1 + \nu_5 + 3\nu_6, E_u$ (-0.79)	2334.559	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, A_{2u}$ (0.59)	2799.840
$\nu_3 + 2\nu_5 + \nu_6, A_{2g}$ (0.73)	2334.565	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, E_u$ (0.64)	2799.849
$\nu_3 + 2\nu_5 + \nu_6, E_g$ (-0.69)	2334.588	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, F_{1u}$ (0.55)	2800.218
$\nu_3 + 2\nu_5 + \nu_6, F_{2g}$ (-0.78)	2334.795	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, E_u$ (-0.68)	2800.376
$\nu_3 + 4\nu_6, F_{2u}$ (-0.57)	2334.884	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, E_u$ (0.56)	2800.833
$\nu_3 + 2\nu_5 + \nu_6, F_{1g}$ (-0.67)	2334.975	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, A_{1u}$ (0.66)	2801.236
$\nu_3 + 4\nu_6, F_{1u}$ (-0.63)	2334.981	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, F_{2u}$ (-0.56)	2801.350
$\nu_3 + 2\nu_5 + \nu_6, E_g$ (-0.56)	2335.511	$\nu_1 + \nu_2 + \nu_3 + \nu_5, A_{2u}$ (0.86)	2801.590
$\nu_1 + \nu_5 + 3\nu_6, F_{2u}$ (0.62)	2335.550	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, F_{2u}$ (-0.56)	2801.601
$\nu_3 + 2\nu_5 + \nu_6, A_{1g}$ (-0.74)	2335.602	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, E_u$ (0.77)	2801.632
$\nu_3 + 2\nu_5 + \nu_6, F_{2g}$ (-0.63)	2335.880	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, F_{1u}$ (-0.44)	2801.659
$\nu_3 + 4\nu_6, A_{2u}$ (0.61)	2335.903	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, F_{2u}$ (0.37)	2801.874
$\nu_3 + 2\nu_5 + \nu_6, F_{1g}$ (-0.58)	2336.308	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, A_{1u}$ (-0.63)	2801.938
$\nu_3 + 4\nu_6, F_{2u}$ (0.66)	2336.663	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, F_{1u}$ (-0.66)	2801.952
$\nu_3 + 2\nu_5 + \nu_6, E_g$ (-0.82)	2336.903	$\nu_1 + \nu_2 + \nu_3 + \nu_5, E_u$ (0.59)	2802.348
$\nu_3 + 2\nu_5 + \nu_6, A_{2g}$ (0.88)	2336.928	$\nu_2 + 2\nu_3 + \nu_6, F_{2u}$ (-0.36)	2802.732
$\nu_1 + \nu_5 + 3\nu_6, E_u$ (-0.60)	2336.988	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, F_{1u}$ (0.39)	2802.896
$\nu_3 + 2\nu_5 + \nu_6, F_{2g}$ (0.70)	2337.044	$\nu_1 + \nu_3 + \nu_5 + 2\nu_6, A_{2u}$ (0.62)	2802.901
$\nu_3 + 2\nu_5 + \nu_6, F_{1g}$ (0.69)	2337.210	$\nu_1 + \nu_3 + \nu_5 + 2\nu_6, F_{2u}$ (0.38)	2802.940
$\nu_3 + 2\nu_5 + \nu_6, F_{2g}$ (0.62)	2337.264	$\nu_1 + \nu_3 + \nu_5 + 2\nu_6, F_{2u}$ (0.50)	2803.305
$\nu_3 + 4\nu_6, F_{1u}$ (-0.76)	2337.309	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, F_{1u}$ (-0.60)	2803.631
$\nu_3 + 4\nu_6, E_u$ (-0.54)	2337.389	$\nu_1 + \nu_2 + \nu_3 + \nu_5, F_{2u}$ (-0.52)	2803.760

Table 1 – continued

Band, Sym, Eig	Band center	Band, Sym, Eig	Band center
$\nu_3 + 2\nu_5 + \nu_6, A_{1g}$ (0.80)	2337.643	$\nu_2 + 2\nu_3 + \nu_6, E_u$ (-0.63)	2803.780
$\nu_1 + \nu_5 + 3\nu_6, F_{1u}$ (0.69)	2338.115	$\nu_2 + \nu_3 + \nu_5 + 2\nu_6, F_{1u}$ (0.66)	2803.939
$\nu_1 + \nu_5 + 3\nu_6, A_{2u}$ (0.80)	2338.318	$\nu_1 + \nu_2 + \nu_3 + \nu_5, F_{1u}$ (-0.56)	2804.227
$\nu_3 + 2\nu_5 + \nu_6, F_{1g}$ (0.86)	2338.530	$\nu_1 + \nu_3 + \nu_5 + 2\nu_6, A_{2u}$ (0.56)	2804.415
$\nu_3 + 2\nu_5 + \nu_6, E_g$ (-0.95)	2338.558	$\nu_2 + 2\nu_3 + \nu_6, F_{2u}$ (-0.44)	2804.566
$\nu_1 + \nu_5 + 3\nu_6, F_{2u}$ (0.59)	2338.803	$\nu_1 + \nu_2 + \nu_3 + \nu_5, E_u$ (0.61)	2804.808
$\nu_3 + 4\nu_6, F_{2u}$ (-0.71)	2339.089	$3\nu_2 + \nu_3, F_{1u}$ (0.77)	2805.062
$\nu_3 + 4\nu_6, F_{1u}$ (0.80)	2339.806	$\nu_1 + \nu_2 + \nu_3 + \nu_5, F_{1u}$ (0.51)	2805.594
$\nu_3 + 4\nu_6, A_{1u}$ (0.83)	2339.905	$\nu_1 + \nu_2 + \nu_3 + \nu_5, A_{1u}$ (-0.81)	2805.752
$\nu_3 + 4\nu_6, F_{1u}$ (0.63)	2340.207	$\nu_1 + \nu_2 + \nu_3 + \nu_5, E_u$ (0.77)	2805.783
$\nu_3 + 4\nu_6, E_u$ (0.65)	2340.323	$3\nu_2 + \nu_3, F_{2u}$ (-0.61)	2806.119
$\nu_1 + 3\nu_5, A_{1g}$ (-0.84)	2340.581	$\nu_2 + 2\nu_3 + \nu_6, A_{2u}$ (-0.70)	2806.744
$\nu_3 + 4\nu_6, F_{2u}$ (-0.58)	2340.746	$\nu_1 + \nu_3 + \nu_5 + 2\nu_6, E_u$ (-0.76)	2806.768
$\nu_1 + 3\nu_5, F_{2g}$ (-0.89)	2341.059	$\nu_2 + \nu_3 + 2\nu_4, A_{1u}$ (0.65)	2806.899
$\nu_1 + 3\nu_5, F_{1g}$ (-0.86)	2341.264	$\nu_1 + \nu_3 + \nu_5 + 2\nu_6, E_u$ (0.61)	2807.552
$\nu_1 + \nu_5 + 3\nu_6, F_{1u}$ (0.57)	2341.381	$\nu_2 + \nu_3 + 2\nu_4, F_{1u}$ (0.62)	2810.976
$\nu_3 + 2\nu_5 + \nu_6, E_g$ (0.79)	2341.573	$\nu_2 + \nu_3 + 2\nu_4, F_{2u}$ (-0.62)	2811.558
$\nu_3 + 2\nu_5 + \nu_6, A_{2g}$ (0.78)	2341.712	$\nu_2 + \nu_3 + 2\nu_4, F_{1u}$ (-0.76)	2811.615
$\nu_3 + 4\nu_6, F_{2u}$ (-0.66)	2341.841	$\nu_2 + \nu_3 + 2\nu_4, F_{1u}$ (0.73)	2811.762
$\nu_3 + 4\nu_6, E_u$ (0.70)	2341.928	$\nu_2 + \nu_3 + 2\nu_4, A_{2u}$ (-0.87)	2811.769
$\nu_1 + \nu_5 + 3\nu_6, A_{1u}$ (0.62)	2342.424	$\nu_2 + \nu_3 + 2\nu_4, F_{2u}$ (-0.74)	2811.901
$\nu_3 + 2\nu_5 + \nu_6, F_{1g}$ (0.64)	2342.828	$\nu_2 + \nu_3 + 2\nu_4, E_u$ (0.73)	2812.023
$\nu_3 + 2\nu_5 + \nu_6, F_{2g}$ (0.64)	2342.865	$\nu_2 + \nu_3 + 2\nu_4, F_{2u}$ (0.80)	2814.352
$\nu_3 + 4\nu_6, F_{1u}$ (-0.62)	2343.307	$\nu_2 + \nu_3 + 2\nu_4, A_{1u}$ (0.74)	2814.579
$\nu_1 + 3\nu_5, F_{2g}$ (-0.94)	2343.656	$\nu_2 + \nu_3 + 2\nu_4, F_{1u}$ (0.97)	2814.624
$\nu_4 + 5\nu_6, E_g$ (0.65)	2346.640	$\nu_2 + \nu_3 + 2\nu_4, F_{2u}$ (-0.76)	2814.669
$\nu_4 + 5\nu_6, F_{2g}$ (-0.63)	2346.833	$\nu_2 + \nu_3 + 2\nu_4, E_u$ (-0.75)	2814.884
$\nu_4 + 5\nu_6, F_{1g}$ (-0.59)	2347.347	$\nu_2 + \nu_3 + 2\nu_4, F_{1u}$ (0.85)	2815.223
$\nu_4 + 5\nu_6, A_{2g}$ (0.61)	2348.415	$\nu_1 + 2\nu_2 + \nu_3, F_{2u}$ (-0.47)	2815.332
$\nu_1 + 2\nu_4 + \nu_6, F_{2u}$ (-0.58)	2348.445	$2\nu_2 + 2\nu_3, E_g$ (-0.52)	2824.073
$\nu_1 + 2\nu_4 + \nu_6, F_{1u}$ (-0.97)	2348.777	$2\nu_1 + 2\nu_2, A_{1g}$ (-0.92)	2824.737
$\nu_4 + 5\nu_6, F_{1g}$ (0.88)	2348.818	$3\nu_3, F_{1u}$ (-0.88)	2828.780
$\nu_1 + 2\nu_4 + \nu_6, F_{2u}$ (-0.74)	2348.956	$2\nu_3 + \nu_5 + 2\nu_6, F_{2g}$ (0.47)	2835.543
$\nu_1 + 2\nu_4 + \nu_6, F_{1u}$ (0.96)	2349.031	$\nu_1 + \nu_2 + \nu_3 + \nu_4, A_{2g}$ (0.57)	2835.590
$\nu_4 + 2\nu_5 + 2\nu_6, F_{1u}$ (-0.76)	2349.091	$2\nu_3 + \nu_5 + 2\nu_6, E_g$ (0.58)	2835.619
$\nu_1 + 2\nu_4 + \nu_6, E_u$ (-0.97)	2349.157	$2\nu_3 + \nu_5 + 2\nu_6, F_{1g}$ (-0.43)	2836.620
$\nu_1 + 2\nu_4 + \nu_6, A_{1u}$ (-0.97)	2349.185	$2\nu_2 + \nu_3 + \nu_4, E_g$ (0.64)	2837.644
$\nu_4 + 2\nu_5 + 2\nu_6, F_{2u}$ (-0.53)	2350.024	$2\nu_2 + \nu_3 + \nu_4, A_{1g}$ (0.97)	2837.835
$\nu_1 + 2\nu_4 + \nu_6, F_{2u}$ (0.79)	2350.195	$2\nu_2 + \nu_3 + \nu_4, F_{1g}$ (0.77)	2838.073
$\nu_4 + 2\nu_5 + 2\nu_6, F_{1u}$ (-0.73)	2350.213	$2\nu_2 + \nu_3 + \nu_4, F_{2g}$ (0.71)	2838.184
$\nu_4 + 2\nu_5 + 2\nu_6, E_u$ (-0.63)	2350.219	$2\nu_3 + \nu_5 + 2\nu_6, F_{2g}$ (0.49)	2839.466
$\nu_4 + 2\nu_5 + 2\nu_6, A_{1u}$ (0.67)	2350.255	$3\nu_3, F_{1u}$ (-0.90)	2839.485
$\nu_4 + 2\nu_5 + 2\nu_6, F_{1u}$ (0.58)	2350.549	$2\nu_3 + \nu_4 + \nu_6, A_{2g}$ (0.55)	2839.832
$\nu_4 + 2\nu_5 + 2\nu_6, E_u$ (0.91)	2350.694	$2\nu_3 + \nu_4 + \nu_6, F_{1g}$ (-0.52)	2840.012
$\nu_4 + 2\nu_5 + 2\nu_6, F_{2u}$ (-0.87)	2350.727	$2\nu_2 + \nu_3 + \nu_4, F_{2g}$ (-0.53)	2840.131
$\nu_4 + 2\nu_5 + 2\nu_6, A_{2u}$ (0.89)	2350.894	$2\nu_3 + \nu_4 + \nu_6, E_g$ (0.59)	2840.205
$\nu_4 + 2\nu_5 + 2\nu_6, F_{2u}$ (-0.70)	2351.362	$3\nu_3, F_{2u}$ (-0.90)	2840.786
$\nu_4 + 2\nu_5 + 2\nu_6, A_{2u}$ (-0.67)	2351.388	$2\nu_3 + \nu_4 + \nu_6, F_{1g}$ (-0.49)	2843.972
$\nu_4 + 2\nu_5 + 2\nu_6, F_{1u}$ (-0.49)	2351.401	$2\nu_3 + \nu_4 + \nu_6, F_{2g}$ (0.48)	2844.108
$\nu_4 + 2\nu_5 + 2\nu_6, E_u$ (0.60)	2351.550	$2\nu_2 + 2\nu_3, E_g$ (0.67)	2844.330
$\nu_4 + 2\nu_5 + 2\nu_6, F_{2u}$ (-0.58)	2351.577	$2\nu_3 + \nu_4 + \nu_6, A_{1g}$ (0.96)	2844.659
$\nu_4 + 2\nu_5 + 2\nu_6, F_{1u}$ (-0.82)	2351.623	$3\nu_3, A_{2u}$ (-0.94)	2845.310
$\nu_4 + 5\nu_6, A_{1g}$ (-0.72)	2351.823	$2\nu_3 + \nu_4 + \nu_6, E_g$ (-0.74)	2846.178
$\nu_4 + 2\nu_5 + 2\nu_6, F_{1u}$ (0.46)	2351.982	$2\nu_3 + \nu_4 + \nu_6, F_{1g}$ (-0.76)	2846.479
$\nu_4 + 5\nu_6, F_{2g}$ (-0.69)	2352.014	$2\nu_3 + \nu_4 + \nu_6, F_{2g}$ (0.79)	2846.534

Table 1 – continued

Band, Sym, Eig	Band center	Band, Sym, Eig	Band center
$\nu_4 + 2\nu_5 + 2\nu_6, F_{2u}$ (0.92)	2352.085	$2\nu_3 + \nu_4 + \nu_6, A_{2g}$ (0.74)	2847.091
$\nu_4 + 2\nu_5 + 2\nu_6, F_{1u}$ (-0.63)	2352.097	$\nu_1 + \nu_2 + \nu_3 + \nu_4, A_{2g}$ (-0.48)	2848.398
$\nu_4 + 5\nu_6, E_g$ (0.66)	2352.449	$\nu_3 + 3\nu_5 + \nu_6, F_{2g}$ (-0.57)	2848.418
$\nu_4 + 2\nu_5 + 2\nu_6, F_{1u}$ (0.74)	2352.873	$2\nu_3 + \nu_4 + \nu_6, E_g$ (-0.79)	2848.470
$\nu_4 + 2\nu_5 + 2\nu_6, A_{1u}$ (-0.72)	2352.880	$\nu_3 + 3\nu_5 + \nu_6, F_{1g}$ (0.60)	2848.569
$\nu_4 + 2\nu_5 + 2\nu_6, F_{2u}$ (-0.87)	2352.987	$2\nu_3 + \nu_4 + \nu_6, F_{2g}$ (0.62)	2848.654
$\nu_4 + 5\nu_6, F_{1g}$ (-0.69)	2353.006	$2\nu_3 + \nu_4 + \nu_6, F_{1g}$ (0.84)	2848.663
$\nu_4 + 2\nu_5 + 2\nu_6, E_u$ (0.72)	2353.075	$2\nu_3 + \nu_4 + \nu_6, A_{1g}$ (-0.99)	2848.893
$\nu_4 + 2\nu_5 + 2\nu_6, F_{2u}$ (-0.62)	2353.178	$2\nu_3 + \nu_4 + \nu_6, F_{1g}$ (-0.79)	2849.007
$\nu_4 + 2\nu_5 + 2\nu_6, A_{2u}$ (-0.99)	2353.454	$2\nu_3 + \nu_4 + \nu_6, F_{2g}$ (-0.85)	2849.094
$\nu_4 + 2\nu_5 + 2\nu_6, E_u$ (-0.97)	2353.490	$2\nu_3 + \nu_4 + \nu_6, E_g$ (-0.79)	2849.571
$\nu_4 + 2\nu_5 + 2\nu_6, F_{1u}$ (0.80)	2353.556	$\nu_3 + 3\nu_5 + \nu_6, F_{1g}$ (0.44)	2850.944
$\nu_4 + 2\nu_5 + 2\nu_6, A_{2u}$ (0.88)	2353.914	$\nu_3 + 3\nu_5 + \nu_6, F_{2g}$ (-0.56)	2850.966
$\nu_4 + 2\nu_5 + 2\nu_6, F_{1u}$ (0.61)	2354.234	$\nu_3 + 3\nu_5 + \nu_6, F_{1g}$ (0.55)	2850.989
$\nu_4 + 2\nu_5 + 2\nu_6, F_{2u}$ (-0.74)	2354.325	$\nu_3 + 3\nu_5 + \nu_6, A_{2g}$ (0.54)	2851.121
$\nu_4 + 2\nu_5 + 2\nu_6, E_u$ (-0.66)	2354.332	$\nu_3 + 3\nu_5 + \nu_6, F_{1g}$ (0.49)	2851.218
$\nu_4 + 5\nu_6, A_{2g}$ (0.61)	2354.827	$\nu_1 + \nu_3 + \nu_4 + \nu_5, E_g$ (0.64)	2851.265
$\nu_4 + 5\nu_6, F_{2g}$ (-0.68)	2355.057	$\nu_1 + \nu_3 + \nu_4 + \nu_5, F_{2g}$ (0.45)	2851.486
$\nu_4 + 2\nu_5 + 2\nu_6, F_{2u}$ (-0.89)	2355.339	$\nu_3 + 3\nu_5 + \nu_6, A_{1g}$ (0.61)	2851.488
$\nu_4 + 5\nu_6, F_{1g}$ (0.63)	2355.470	$\nu_1 + \nu_3 + \nu_4 + \nu_5, E_g$ (-0.42)	2851.516
$\nu_4 + 2\nu_5 + 2\nu_6, F_{1u}$ (-0.87)	2355.533	$\nu_3 + 3\nu_5 + \nu_6, F_{2g}$ (-0.53)	2851.953
$\nu_4 + 2\nu_5 + 2\nu_6, F_{2u}$ (0.69)	2355.792	$\nu_3 + 3\nu_5 + \nu_6, A_{2g}$ (-0.64)	2851.995
$\nu_4 + 2\nu_5 + 2\nu_6, E_u$ (0.67)	2355.834	$\nu_3 + 3\nu_5 + \nu_6, E_g$ (-0.56)	2852.170
$\nu_4 + 2\nu_5 + 2\nu_6, F_{1u}$ (-0.62)	2355.942	$\nu_3 + 3\nu_5 + \nu_6, F_{2g}$ (-0.46)	2852.569
$\nu_4 + 5\nu_6, E_g$ (0.66)	2355.945	$2\nu_3 + \nu_4 + \nu_6, F_{2g}$ (0.53)	2852.873
$\nu_4 + 2\nu_5 + 2\nu_6, F_{2u}$ (-0.46)	2356.176	$2\nu_3 + \nu_4 + \nu_6, E_g$ (-0.73)	2852.963
$\nu_4 + 2\nu_5 + 2\nu_6, F_{1u}$ (-0.64)	2356.422	$2\nu_3 + \nu_4 + \nu_6, F_{1g}$ (-0.79)	2852.979
$\nu_4 + 2\nu_5 + 2\nu_6, F_{2u}$ (0.59)	2356.468	$2\nu_3 + \nu_5 + 2\nu_6, A_{1g}$ (0.60)	2853.028
$\nu_4 + 2\nu_5 + 2\nu_6, A_{2u}$ (-0.73)	2356.502	$2\nu_3 + \nu_4 + \nu_6, F_{2g}$ (0.67)	2853.096
$\nu_4 + 2\nu_5 + 2\nu_6, A_{1u}$ (-0.74)	2356.589	$2\nu_3 + \nu_4 + \nu_6, F_{2g}$ (-0.61)	2853.291
$\nu_4 + 2\nu_5 + 2\nu_6, E_u$ (0.75)	2356.654	$2\nu_3 + \nu_4 + \nu_6, F_{1g}$ (0.69)	2853.463
$\nu_4 + 2\nu_5 + 2\nu_6, F_{2u}$ (0.76)	2357.071	$2\nu_2 + 2\nu_3, F_{1g}$ (0.66)	2853.505
$\nu_4 + 2\nu_5 + 2\nu_6, F_{1u}$ (-0.73)	2357.093	$2\nu_3 + 2\nu_4, A_{2g}$ (0.71)	2853.526
$\nu_4 + 2\nu_5 + 2\nu_6, F_{1u}$ (-0.75)	2357.146	$2\nu_3 + \nu_4 + \nu_6, E_g$ (-0.71)	2853.666
$\nu_1 + \nu_2 + \nu_3, F_{1u}$ (0.86)	2357.353	$\nu_3 + 3\nu_5 + \nu_6, F_{2g}$ (0.58)	2853.897
$\nu_4 + 5\nu_6, F_{1g}$ (0.85)	2358.400	$\nu_3 + 3\nu_5 + \nu_6, F_{1g}$ (0.68)	2853.923
$\nu_4 + 5\nu_6, F_{2g}$ (-0.93)	2358.480	$\nu_3 + 3\nu_5 + \nu_6, F_{1g}$ (-0.61)	2854.295
$\nu_4 + 5\nu_6, A_{2g}$ (-0.63)	2359.442	$\nu_3 + 3\nu_5 + \nu_6, A_{1g}$ (0.89)	2854.389
$\nu_4 + 5\nu_6, F_{2g}$ (0.67)	2359.811	$\nu_1 + \nu_3 + \nu_4 + \nu_5, F_{2g}$ (0.52)	2854.506
$\nu_4 + 5\nu_6, E_g$ (0.71)	2360.022	$\nu_3 + 3\nu_5 + \nu_6, E_g$ (-0.85)	2854.518
$\nu_1 + \nu_2 + \nu_3, F_{2u}$ (0.86)	2360.411	$\nu_3 + 3\nu_5 + \nu_6, F_{2g}$ (0.47)	2854.727
$\nu_4 + 5\nu_6, F_{1g}$ (0.61)	2360.686	$2\nu_3 + \nu_5 + 2\nu_6, F_{1g}$ (-0.41)	2854.793
$\nu_4 + 5\nu_6, A_{1g}$ (-0.71)	2361.156	$\nu_3 + 3\nu_5 + \nu_6, F_{2g}$ (0.52)	2855.248
$\nu_4 + 5\nu_6, F_{1g}$ (0.65)	2361.404	$\nu_3 + 3\nu_5 + \nu_6, F_{1g}$ (0.41)	2855.304
$\nu_4 + 5\nu_6, E_g$ (-0.57)	2362.019	$\nu_3 + 3\nu_5 + \nu_6, F_{1g}$ (0.56)	2855.306
$\nu_4 + 5\nu_6, F_{2g}$ (-0.66)	2362.484	$\nu_3 + 3\nu_5 + \nu_6, F_{2g}$ (0.46)	2855.611
$\nu_4 + 5\nu_6, F_{1g}$ (0.69)	2363.848	$2\nu_3 + 2\nu_5, F_{2g}$ (-0.51)	2855.932
$\nu_4 + 5\nu_6, E_g$ (-0.64)	2364.060	$\nu_3 + 3\nu_5 + \nu_6, A_{2g}$ (0.48)	2856.056
$\nu_4 + 5\nu_6, F_{2g}$ (0.61)	2364.509	$\nu_3 + 3\nu_5 + \nu_6, E_g$ (-0.85)	2856.147
$\nu_4 + 5\nu_6, A_{2g}$ (-0.61)	2365.279	$\nu_3 + 3\nu_5 + \nu_6, F_{1g}$ (0.49)	2856.218
$3\nu_4 + \nu_5, A_{2u}$ (0.89)	2365.485	$\nu_3 + 3\nu_5 + \nu_6, F_{1g}$ (0.52)	2856.742
$3\nu_4 + \nu_5, E_u$ (0.91)	2365.602	$\nu_3 + 3\nu_5 + \nu_6, E_g$ (-0.78)	2856.948
$3\nu_4 + \nu_5, F_{1u}$ (-0.67)	2365.869	$\nu_3 + 3\nu_5 + \nu_6, A_{1g}$ (0.72)	2857.342
$3\nu_4 + \nu_5, F_{2u}$ (0.83)	2366.256	$2\nu_3 + 2\nu_5, F_{2g}$ (-0.69)	2857.391
$3\nu_4 + \nu_5, E_u$ (0.81)	2366.380	$\nu_3 + 3\nu_5 + \nu_6, A_{2g}$ (-0.57)	2857.455

Table 1 – continued

Band, Sym, Eig	Band center	Band, Sym, Eig	Band center
$3\nu_4 + \nu_5, F_{1u}$ (0.97)	2366.399	$\nu_3 + 3\nu_5 + \nu_6, F_{1g}$ (0.65)	2857.483
$3\nu_4 + \nu_5, A_{1u}$ (1.00)	2366.608	$2\nu_3 + 2\nu_5, F_{2g}$ (0.64)	2857.715
$3\nu_4 + \nu_5, F_{1u}$ (-0.66)	2366.672	$\nu_3 + 3\nu_5 + \nu_6, E_g$ (0.83)	2857.766
$3\nu_4 + \nu_5, F_{2u}$ (-0.77)	2366.687	$2\nu_3 + 2\nu_5, F_{1g}$ (0.51)	2857.825
$3\nu_4 + \nu_5, A_{2u}$ (-0.88)	2366.765	$\nu_3 + 3\nu_5 + \nu_6, F_{2g}$ (0.56)	2858.647
$3\nu_4 + \nu_5, F_{2u}$ (-0.61)	2366.795	$2\nu_3 + 2\nu_5, F_{2g}$ (0.47)	2858.981
$3\nu_4 + \nu_5, E_u$ (0.81)	2366.884	$2\nu_3 + 2\nu_5, F_{1g}$ (-0.80)	2858.995
$3\nu_4 + \nu_5, F_{1u}$ (-0.67)	2367.007	$2\nu_3 + 2\nu_5, F_{1g}$ (0.48)	2860.543
$\nu_2 + 5\nu_6, F_{2u}$ (-0.66)	2371.238	$2\nu_3 + 2\nu_5, A_{1g}$ (0.83)	2860.651
$\nu_2 + 5\nu_6, F_{1u}$ (-0.51)	2372.209	$2\nu_3 + \nu_5 + 2\nu_6, F_{2g}$ (-0.46)	2860.652
$\nu_1 + \nu_2 + \nu_4 + \nu_6, A_{2g}$ (-0.96)	2373.082	$2\nu_3 + 2\nu_5, E_g$ (0.56)	2860.730
$\nu_1 + \nu_2 + \nu_4 + \nu_6, E_g$ (-0.82)	2373.528	$\nu_1 + 2\nu_3 + \nu_5, F_{1g}$ (-0.39)	2860.848
$\nu_2 + 5\nu_6, E_u$ (-0.94)	2373.589	$2\nu_3 + 2\nu_5, F_{2g}$ (0.47)	2861.701
$\nu_1 + \nu_2 + \nu_4 + \nu_6, F_{2g}$ (0.86)	2373.657	$\nu_3 + 3\nu_5 + \nu_6, E_g$ (0.54)	2862.089
$\nu_1 + \nu_2 + \nu_4 + \nu_6, F_{1g}$ (-0.86)	2373.663	$\nu_3 + 3\nu_5 + \nu_6, A_{2g}$ (0.57)	2862.280
$\nu_2 + 2\nu_5 + 2\nu_6, F_{2g}$ (0.81)	2374.240	$2\nu_3 + \nu_5 + 2\nu_6, F_{2g}$ (0.46)	2862.993
$\nu_2 + 2\nu_5 + 2\nu_6, F_{1g}$ (0.47)	2374.348	$2\nu_3 + 2\nu_5, A_{1g}$ (-0.83)	2863.514
$\nu_2 + 2\nu_5 + 2\nu_6, E_g$ (0.63)	2374.348	$2\nu_3 + 2\nu_5, E_g$ (-0.87)	2864.018
$\nu_2 + 2\nu_5 + 2\nu_6, F_{2g}$ (-0.48)	2374.625	$2\nu_3 + 2\nu_5, F_{1g}$ (0.41)	2864.814
$\nu_2 + 2\nu_5 + 2\nu_6, A_{2g}$ (-0.89)	2374.790	$\nu_2 + 2\nu_3 + \nu_6, F_{2u}$ (0.63)	2865.383
$\nu_2 + 2\nu_5 + 2\nu_6, E_g$ (0.61)	2375.167	$3\nu_2 + \nu_3, F_{1u}$ (0.87)	2865.680
$\nu_1 + \nu_2 + \nu_4 + \nu_6, A_{1g}$ (0.96)	2375.532	$\nu_2 + 2\nu_3 + \nu_5, F_{1g}$ (0.64)	2866.191
$\nu_1 + \nu_2 + \nu_4 + \nu_6, F_{2g}$ (0.86)	2375.629	$2\nu_3 + \nu_5 + 2\nu_6, F_{2g}$ (-0.44)	2867.599
$\nu_1 + \nu_2 + \nu_4 + \nu_6, F_{1g}$ (0.86)	2375.631	$\nu_1 + 2\nu_3 + \nu_5, F_{1g}$ (0.55)	2867.632
$\nu_2 + 2\nu_5 + 2\nu_6, F_{1g}$ (-0.56)	2375.757	$\nu_2 + 2\nu_3 + \nu_6, F_{1u}$ (-0.68)	2870.255
$\nu_2 + 2\nu_5 + 2\nu_6, A_{1g}$ (0.61)	2376.126	$\nu_2 + 2\nu_3 + \nu_6, F_{2u}$ (0.57)	2872.600
$\nu_1 + \nu_2 + \nu_4 + \nu_6, E_g$ (-0.81)	2376.224	$\nu_2 + 2\nu_3 + \nu_6, F_{1u}$ (-0.66)	2872.881
$\nu_2 + 2\nu_5 + 2\nu_6, E_g$ (-0.66)	2376.414	$\nu_2 + 2\nu_3 + \nu_6, F_{2u}$ (0.66)	2873.204
$\nu_2 + 2\nu_5 + 2\nu_6, F_{1g}$ (0.68)	2376.440	$\nu_2 + 2\nu_3 + \nu_6, F_{2u}$ (0.56)	2874.658
$\nu_2 + 2\nu_5 + 2\nu_6, A_{2g}$ (0.80)	2377.051	$\nu_1 + \nu_2 + \nu_3 + \nu_5, F_{1u}$ (0.52)	2875.434
$\nu_2 + 2\nu_5 + 2\nu_6, F_{2g}$ (-0.59)	2377.062	$\nu_1 + \nu_2 + \nu_3 + \nu_5, F_{2u}$ (-0.64)	2875.556
$\nu_2 + 5\nu_6, F_{1u}$ (0.69)	2377.329	$\nu_2 + 2\nu_3 + \nu_6, F_{1u}$ (0.62)	2878.387
$\nu_2 + 2\nu_5 + 2\nu_6, F_{1g}$ (0.54)	2377.422	$2\nu_3 + 3\nu_6, F_{2u}$ (0.45)	2878.435
$\nu_2 + 2\nu_5 + 2\nu_6, E_g$ (-0.57)	2377.588	$\nu_2 + 2\nu_3 + \nu_6, F_{1u}$ (0.61)	2878.624
$\nu_2 + 2\nu_5 + 2\nu_6, F_{2g}$ (0.66)	2377.725	$\nu_1 + \nu_2 + \nu_3 + \nu_5, F_{1u}$ (0.47)	2879.725
$\nu_2 + 5\nu_6, F_{2u}$ (0.67)	2377.826	$\nu_2 + 2\nu_3 + \nu_6, F_{2u}$ (-0.61)	2879.760
$\nu_2 + 2\nu_5 + 2\nu_6, F_{2g}$ (0.52)	2378.383	$\nu_1 + \nu_3 + \nu_5 + 2\nu_6, A_{2u}$ (0.59)	2879.845
$\nu_2 + 2\nu_5 + 2\nu_6, F_{1g}$ (-0.64)	2378.504	$\nu_2 + 2\nu_3 + \nu_6, E_u$ (-0.72)	2879.977
$\nu_2 + 2\nu_5 + 2\nu_6, A_{1g}$ (-0.81)	2378.629	$\nu_1 + \nu_3 + \nu_5 + 2\nu_6, F_{2u}$ (0.51)	2880.039
$\nu_2 + 2\nu_5 + 2\nu_6, A_{1g}$ (-0.71)	2378.841	$\nu_2 + 2\nu_3 + \nu_6, F_{1u}$ (0.56)	2880.529
$\nu_2 + 5\nu_6, F_{2u}$ (-0.63)	2379.549	$\nu_2 + 2\nu_3 + \nu_6, A_{1u}$ (-0.92)	2880.558
$\nu_2 + 2\nu_5 + 2\nu_6, E_g$ (0.50)	2379.891	$\nu_1 + \nu_3 + \nu_5 + 2\nu_6, E_u$ (0.61)	2880.807
$\nu_2 + 2\nu_5 + 2\nu_6, F_{1g}$ (0.46)	2380.154	$\nu_1 + \nu_3 + 2\nu_4, A_{2u}$ (0.88)	2881.698
$\nu_2 + 2\nu_5 + 2\nu_6, F_{2g}$ (0.57)	2380.664	$2\nu_3 + 3\nu_6, E_u$ (-0.52)	2881.818
$\nu_2 + 2\nu_5 + 2\nu_6, A_{2g}$ (-0.65)	2380.706	$2\nu_3 + 3\nu_6, E_u$ (-0.45)	2882.300
$\nu_2 + 2\nu_5 + 2\nu_6, E_g$ (0.59)	2380.800	$\nu_1 + \nu_3 + \nu_5 + 2\nu_6, A_{1u}$ (0.79)	2882.435
$\nu_2 + 5\nu_6, F_{1u}$ (0.59)	2381.546	$\nu_1 + \nu_3 + \nu_5 + 2\nu_6, F_{2u}$ (-0.51)	2883.286
$\nu_2 + 2\nu_5 + 2\nu_6, F_{1g}$ (0.62)	2382.278	$\nu_1 + \nu_3 + \nu_5 + 2\nu_6, F_{1u}$ (0.55)	2883.531
$\nu_2 + 5\nu_6, A_{1u}$ (-0.92)	2382.350	$2\nu_3 + 3\nu_6, E_u$ (0.70)	2919.585
$\nu_2 + 2\nu_5 + 2\nu_6, F_{2g}$ (0.67)	2382.497	$2\nu_3 + 3\nu_6, F_{2u}$ (0.66)	2923.806
$\nu_2 + 2\nu_5 + 2\nu_6, F_{2g}$ (0.78)	2382.797	$2\nu_3 + 3\nu_6, F_{2u}$ (0.49)	2924.917
$\nu_2 + 2\nu_5 + 2\nu_6, F_{1g}$ (-0.83)	2383.120	$\nu_1 + \nu_2 + \nu_3 + \nu_4, F_{2g}$ (0.44)	2926.278
$\nu_2 + 2\nu_5 + 2\nu_6, A_{1g}$ (0.77)	2383.667	$2\nu_3 + 2\nu_5, A_{1g}$ (-0.81)	2926.662
$\nu_2 + 2\nu_5 + 2\nu_6, E_g$ (0.67)	2383.676	$2\nu_3 + 2\nu_5, E_g$ (-0.61)	2926.840
$\nu_2 + 5\nu_6, F_{1u}$ (-0.60)	2384.019	$2\nu_3 + 3\nu_6, A_{1u}$ (0.80)	2926.893

Table 1 – continued

Band, Sym, Eig	Band center	Band, Sym, Eig	Band center
$\nu_2 + 5\nu_6, E_u$ (-0.91)	2384.112	$2\nu_3 + 3\nu_6, F_{2u}$ (0.73)	2926.964
$\nu_2 + 2\nu_5 + 2\nu_6, A_{2g}$ (-0.72)	2384.736	$2\nu_3 + 3\nu_6, F_{1u}$ (0.85)	2927.083
$\nu_2 + 2\nu_5 + 2\nu_6, E_g$ (0.64)	2384.825	$2\nu_3 + 2\nu_5, E_g$ (-0.50)	2928.546
$\nu_2 + 5\nu_6, F_{2u}$ (0.57)	2384.979	$2\nu_3 + 3\nu_6, E_u$ (-0.61)	2928.633
$\nu_2 + 5\nu_6, A_{2u}$ (-0.96)	2385.460	$2\nu_3 + 2\nu_5, A_{2g}$ (0.96)	2928.689
$\nu_2 + 5\nu_6, F_{2u}$ (0.56)	2386.030	$2\nu_3 + 3\nu_6, F_{1u}$ (-0.64)	2928.786
$\nu_2 + 5\nu_6, F_{1u}$ (-0.64)	2388.221	$2\nu_3 + 3\nu_6, F_{1u}$ (0.73)	2928.871
$\nu_2 + 5\nu_6, F_{2u}$ (0.54)	2389.687	$\nu_1 + \nu_3 + \nu_5 + 2\nu_6, F_{2u}$ (-0.70)	2929.068
$\nu_2 + 2\nu_4 + \nu_5, F_{1g}$ (0.80)	2390.995	$\nu_1 + \nu_3 + \nu_5 + 2\nu_6, F_{1u}$ (0.70)	2929.177
$\nu_2 + 2\nu_4 + \nu_5, F_{1g}$ (-0.75)	2391.066	$\nu_2 + 2\nu_3 + \nu_4, A_{2u}$ (-0.70)	2929.428
$\nu_2 + 2\nu_4 + \nu_5, F_{2g}$ (0.76)	2391.100	$2\nu_3 + 3\nu_6, E_u$ (0.56)	2929.557
$\nu_2 + 2\nu_4 + \nu_5, F_{2g}$ (-0.84)	2391.176	$2\nu_3 + 3\nu_6, F_{2u}$ (0.63)	2929.594
$\nu_2 + 2\nu_4 + \nu_5, A_{2g}$ (0.99)	2391.217	$2\nu_3 + 3\nu_6, F_{2u}$ (-0.56)	2929.906
$\nu_2 + 2\nu_4 + \nu_5, E_g$ (-0.74)	2391.335	$2\nu_3 + 3\nu_6, F_{1u}$ (0.65)	2929.946
$\nu_2 + 2\nu_4 + \nu_5, F_{1g}$ (-0.80)	2391.507	$3\nu_1 + \nu_4, F_{1u}$ (0.89)	2930.131
$\nu_2 + 5\nu_6, F_{1u}$ (-0.76)	2392.370	$2\nu_3 + 3\nu_6, F_{2u}$ (0.59)	2930.471
$\nu_2 + 2\nu_4 + \nu_5, F_{2g}$ (0.72)	2392.648	$2\nu_3 + 3\nu_6, E_u$ (-0.57)	2930.544
$\nu_2 + 2\nu_4 + \nu_5, F_{1g}$ (-0.85)	2393.183	$2\nu_3 + 3\nu_6, F_{2u}$ (-0.66)	2930.874
$\nu_2 + 2\nu_4 + \nu_5, F_{2g}$ (0.86)	2393.336	$\nu_1 + \nu_3 + \nu_5 + 2\nu_6, F_{1u}$ (0.63)	2930.917
$\nu_2 + 2\nu_4 + \nu_5, F_{2g}$ (-0.69)	2393.474	$2\nu_3 + 3\nu_6, A_{1u}$ (0.85)	2930.999
$\nu_2 + 2\nu_4 + \nu_5, F_{1g}$ (-0.98)	2393.551	$2\nu_3 + 3\nu_6, F_{1u}$ (0.64)	2931.152
$\nu_2 + 2\nu_4 + \nu_5, A_{1g}$ (-0.99)	2393.566	$\nu_1 + \nu_3 + 2\nu_4, E_u$ (-0.72)	2931.218
$\nu_2 + 2\nu_4 + \nu_5, E_g$ (0.74)	2393.684	$\nu_1 + \nu_3 + 2\nu_4, F_{2u}$ (-0.60)	2931.285
$\nu_1 + 2\nu_2 + \nu_6, F_{2u}$ (0.70)	2399.473	$\nu_1 + \nu_3 + \nu_5 + 2\nu_6, F_{1u}$ (0.58)	2931.980
$\nu_1 + 2\nu_2 + \nu_6, F_{1u}$ (-0.90)	2401.061	$2\nu_3 + 3\nu_6, F_{2u}$ (0.52)	2932.196
$\nu_1 + 2\nu_2 + \nu_6, F_{2u}$ (0.71)	2403.720	$2\nu_1 + \nu_3 + \nu_5, A_{2u}$ (-0.75)	2932.239
$2\nu_3 + \nu_5, F_{2g}$ (-0.83)	2407.980	$2\nu_3 + 3\nu_6, F_{2u}$ (0.42)	2932.351
$2\nu_3 + \nu_5, F_{1g}$ (-0.93)	2409.907	$\nu_1 + \nu_3 + \nu_5 + 2\nu_6, F_{1u}$ (-0.61)	2932.408
$\nu_1 + \nu_3 + 2\nu_6, F_{1u}$ (-0.88)	2410.546	$2\nu_3 + 3\nu_6, A_{1u}$ (-0.61)	2932.447
$\nu_1 + \nu_3 + 2\nu_6, F_{2u}$ (0.88)	2412.014	$2\nu_3 + 3\nu_6, F_{1u}$ (-0.40)	2932.611
$\nu_1 + \nu_3 + 2\nu_6, F_{1u}$ (-0.85)	2412.020	$\nu_1 + 2\nu_3 + \nu_5, F_{2g}$ (0.44)	2932.909
$\nu_1 + \nu_3 + 2\nu_6, E_u$ (0.88)	2412.128	$2\nu_1 + \nu_3 + \nu_5, E_u$ (-0.84)	2932.934
$2\nu_1 + \nu_5 + \nu_6, A_{1u}$ (-0.93)	2413.482	$\nu_1 + \nu_2 + \nu_3 + \nu_4, F_{2g}$ (-0.50)	2933.016
$\nu_1 + \nu_3 + 2\nu_6, A_{2u}$ (-0.96)	2413.543	$\nu_1 + 2\nu_3 + \nu_6, F_{2u}$ (-0.51)	2933.215
$\nu_1 + \nu_3 + 2\nu_6, F_{1u}$ (-0.74)	2413.771	$2\nu_3 + 3\nu_6, F_{1u}$ (0.42)	2933.793
$2\nu_3 + \nu_5, A_{1g}$ (0.94)	2414.318	$\nu_1 + 2\nu_3 + \nu_6, F_{2u}$ (0.85)	2934.054
$\nu_1 + \nu_3 + 2\nu_6, F_{2u}$ (0.77)	2414.388	$\nu_1 + 2\nu_3 + \nu_5, F_{1g}$ (0.43)	2934.424
$2\nu_3 + \nu_5, E_g$ (-0.94)	2414.445	$2\nu_3 + \nu_4 + \nu_5, A_{2u}$ (0.89)	2934.496
$2\nu_1 + \nu_5 + \nu_6, F_{1u}$ (0.74)	2415.122	$\nu_2 + 2\nu_3 + \nu_4, E_u$ (-0.54)	2934.607
$2\nu_1 + \nu_5 + \nu_6, E_u$ (0.87)	2415.858	$\nu_1 + 2\nu_2 + \nu_3, F_{1u}$ (-0.46)	2934.683
$2\nu_3 + \nu_5, F_{2g}$ (-0.83)	2416.274	$\nu_1 + 2\nu_2 + \nu_3, F_{1u}$ (-0.52)	2934.887
$2\nu_1 + \nu_5 + \nu_6, F_{2u}$ (-0.77)	2416.409	$2\nu_3 + \nu_4 + \nu_5, A_{1u}$ (0.90)	2935.084
$2\nu_2 + \nu_4 + \nu_5, F_{2u}$ (-0.65)	2417.221	$\nu_2 + 2\nu_3 + \nu_4, F_{2u}$ (-0.38)	2935.118
$2\nu_2 + \nu_4 + \nu_5, F_{1u}$ (-0.68)	2417.228	$2\nu_3 + \nu_5 + 2\nu_6, F_{2g}$ (0.50)	2935.306
$2\nu_2 + \nu_4 + \nu_5, A_{2u}$ (-0.69)	2417.341	$2\nu_3 + \nu_4 + \nu_5, E_u$ (-0.65)	2935.340
$2\nu_2 + \nu_4 + \nu_5, E_u$ (0.64)	2417.407	$2\nu_1 + \nu_3 + \nu_4, F_{1g}$ (-0.44)	2935.383
$2\nu_3 + \nu_5, F_{2g}$ (0.93)	2417.883	$\nu_1 + \nu_3 + 2\nu_4, F_{1u}$ (-0.65)	2935.625
$2\nu_3 + \nu_5, F_{1g}$ (0.94)	2418.012	$\nu_1 + 2\nu_3 + \nu_6, F_{2u}$ (0.54)	2935.804
$2\nu_2 + \nu_4 + \nu_5, E_u$ (0.72)	2418.855	$\nu_1 + 2\nu_2 + \nu_3, F_{1u}$ (-0.69)	2936.353
$2\nu_2 + \nu_4 + \nu_5, F_{2u}$ (-0.87)	2419.066	$2\nu_3 + \nu_4 + \nu_5, E_u$ (0.57)	2936.466
$2\nu_2 + \nu_4 + \nu_5, A_{1u}$ (0.96)	2419.093	$2\nu_3 + \nu_4 + \nu_5, A_{2u}$ (-0.94)	2936.942
$2\nu_2 + \nu_4 + \nu_5, F_{1u}$ (-0.88)	2419.172	$2\nu_3 + \nu_4 + \nu_5, E_u$ (-0.58)	2937.205
$2\nu_2 + \nu_4 + \nu_5, A_{2u}$ (-0.71)	2420.708	$2\nu_1 + \nu_3 + \nu_5, F_{1u}$ (-0.69)	2937.344
$2\nu_2 + \nu_4 + \nu_5, E_u$ (0.78)	2420.878	$\nu_2 + 2\nu_3 + \nu_4, F_{2u}$ (0.71)	2937.497
$2\nu_2 + \nu_4 + \nu_5, F_{2u}$ (0.73)	2421.408	$\nu_1 + 2\nu_3 + \nu_6, A_{1u}$ (0.78)	2937.519

Table 1 – continued

Band, Sym, Eig	Band center	Band, Sym, Eig	Band center
$2\nu_2 + \nu_4 + \nu_5, F_{1u}$ (0.75)	2421.449	$\nu_1 + \nu_2 + \nu_3 + \nu_4, A_{1g}$ (-0.53)	2938.699
$2\nu_5 + 4\nu_6, A_{1g}$ (-0.80)	2425.656	$2\nu_3 + 2\nu_5, E_g$ (-0.45)	2938.942
$\nu_3 + \nu_4 + \nu_5 + \nu_6, F_{1u}$ (0.75)	2426.064	$2\nu_3 + \nu_4 + \nu_5, E_u$ (0.66)	2939.236
$\nu_3 + \nu_4 + \nu_5 + \nu_6, E_u$ (-0.90)	2426.166	$2\nu_3 + \nu_4 + \nu_5, A_{1u}$ (-0.97)	2939.345
$\nu_3 + \nu_4 + \nu_5 + \nu_6, F_{2u}$ (0.76)	2426.388	$3\nu_3 + \nu_5, A_{1u}$ (-0.84)	2939.511
$\nu_3 + \nu_4 + \nu_5 + \nu_6, A_{1u}$ (0.76)	2426.468	$\nu_1 + 2\nu_3 + \nu_5, F_{2g}$ (-0.44)	2939.963
$2\nu_5 + 4\nu_6, F_{2g}$ (-0.79)	2426.493	$\nu_1 + 2\nu_3 + \nu_5, F_{1g}$ (0.41)	2940.154
$\nu_3 + \nu_4 + \nu_5 + \nu_6, F_{1u}$ (0.78)	2426.540	$3\nu_1 + \nu_2, E_g$ (-0.83)	2941.863
$2\nu_5 + 4\nu_6, F_{1g}$ (-0.59)	2426.614	$4\nu_1, A_{1g}$ (-0.63)	2941.916
$\nu_3 + \nu_4 + \nu_5 + \nu_6, F_{2u}$ (-0.76)	2426.640	$\nu_1 + \nu_3 + 2\nu_4, F_{1u}$ (0.54)	2942.937
$7\nu_6, F_{2u}$ (-0.51)	2426.687	$\nu_1 + \nu_3 + 2\nu_4, F_{2u}$ (-0.83)	2943.149
$\nu_3 + \nu_4 + \nu_5 + \nu_6, F_{1u}$ (0.66)	2426.754	$2\nu_3 + \nu_4 + \nu_5, E_u$ (-0.70)	2943.511
$\nu_3 + \nu_4 + \nu_5 + \nu_6, E_u$ (-0.62)	2426.793	$\nu_1 + 2\nu_3 + \nu_6, F_{1u}$ (0.57)	2943.518
$\nu_3 + \nu_4 + \nu_5 + \nu_6, E_u$ (0.65)	2427.005	$2\nu_3 + \nu_4 + \nu_5, F_{2u}$ (-0.50)	2943.706
$\nu_3 + \nu_4 + \nu_5 + \nu_6, A_{1u}$ (-0.79)	2427.046	$2\nu_3 + \nu_4 + \nu_5, A_{2u}$ (-0.81)	2944.052
$\nu_3 + \nu_4 + \nu_5 + \nu_6, F_{1u}$ (-0.51)	2427.123	$\nu_1 + \nu_3 + 2\nu_4, F_{1u}$ (-0.71)	2944.859
$2\nu_5 + 4\nu_6, E_g$ (0.48)	2427.138	$2\nu_3 + \nu_5 + 2\nu_6, E_g$ (-0.53)	2955.353
$\nu_3 + \nu_4 + \nu_5 + \nu_6, A_{2u}$ (-0.73)	2427.220	$\nu_1 + \nu_2 + \nu_3 + \nu_4, E_g$ (0.48)	2955.363
$\nu_3 + \nu_4 + \nu_5 + \nu_6, F_{2u}$ (-0.63)	2427.276	$\nu_1 + \nu_2 + \nu_3 + \nu_4, A_{1g}$ (0.67)	2967.952
$\nu_3 + \nu_4 + \nu_5 + \nu_6, F_{1u}$ (0.52)	2427.293	$\nu_1 + \nu_2 + \nu_3 + \nu_4, F_{2g}$ (0.70)	2968.338
$\nu_1 + \nu_4 + 3\nu_6, E_g$ (-0.70)	2427.314	$\nu_1 + \nu_2 + \nu_3 + \nu_4, E_g$ (0.65)	2968.487
$\nu_3 + \nu_4 + \nu_5 + \nu_6, F_{2u}$ (0.63)	2427.331	$2\nu_3 + \nu_5 + 2\nu_6, F_{1g}$ (-0.41)	2968.562
$2\nu_5 + 4\nu_6, F_{2g}$ (0.57)	2427.332	$\nu_1 + \nu_2 + 2\nu_3, A_{2g}$ (0.69)	2971.162
$7\nu_6, A_{1u}$ (0.78)	2427.449	$\nu_1 + \nu_2 + 2\nu_3, F_{1g}$ (0.44)	2971.169
$\nu_1 + \nu_4 + 3\nu_6, F_{2g}$ (0.82)	2427.538	$\nu_1 + \nu_2 + \nu_3 + \nu_4, F_{2g}$ (-0.44)	2971.402
$\nu_3 + \nu_4 + \nu_5 + \nu_6, A_{2u}$ (-0.96)	2427.561	$\nu_1 + 2\nu_3 + \nu_5, E_g$ (0.52)	2971.934
$2\nu_5 + 4\nu_6, A_{1g}$ (-0.79)	2427.785	$2\nu_1 + \nu_2 + \nu_3, F_{1u}$ (-0.53)	2994.712
$\nu_3 + \nu_4 + \nu_5 + \nu_6, F_{1u}$ (0.70)	2427.820	$\nu_1 + 2\nu_3 + \nu_6, F_{2u}$ (-0.49)	2996.661