Electronic Supplementary Material for CrystEngComm

Supplementary materials

Ab-initio Prediction of Materials Properties with CRYSTAL: MOF-5 as a case study

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Table 1(ESI) Calculated vibrational frequencies (cm^{-1}) of MOF-5 and symmetry of the modes[a].

Symm	ω	*Symm*	ω	*Symm*	ω	*Symm*	ω
B_g	9.1	E_u	292.7	F_{1u}	830.0	E_u	1415.7
F_{2u}	19.5	B_u	295.1	B_u	838.2	F_{1u}	1421.3
F_{1g}	30.9	F_{2g}	368.6	B_g	868.0	F_{2u}	1444.4
F_{2u}	33.7	F_{1g}	371.0	F_{1g}	868.8	F_{1u}	1446.4
E_g	43.4	A_u	421.2	E_g	869.6	B_u	1463.1
F_{1u}	51.8	F_{2u}	421.5	E_g	872.8	E_g	1463.4
A_u	56.2	E_u	421.6	F_{2g}	874.7	F_{2g}	1465.2
F_{1g}	62.4	F_{2g}	467.4	A_g	877.8	A_g	1477.9
E_u	70.9	A_g	470.7	F_{2u}	901.2	E_u	1549.8
B_g	74.7	E_g	471.5	F_{1u}	901.8	F_{1u}	1549.8
F_{1g}	82.8	F_{2u}	476.7	A_u	995.0	B_u	1551.6
F_{2g}	86.8	F_{1u}	478.1	F_{2u}	995.3	F_{1g}	1567.7
F_{2u}	97.1	F_{1u}	511.7	E_u	995.5	F_{2u}	1587.6
F_{2g}	110.4	F_{2g}	522.5	F_{1g}	1004.1	F_{2g}	1604.8
F_{1u}	113.9	E_u	575.7	F_{2g}	1004.4	F_{1g}	1642.7
F_{1g}	125.2	F_{1u}	579.4	E_u	1039.6	F_{1u}	1648.6
E_g	125.4	B_u	586.2	F_{1u}	1040.0	F_{2g}	1669.5
F_{1u}	136.2	F_{2u}	597.9	B_u	1041.1	E_g	1669.8
F_{2u}	138.0	F_{1u}	606.1	F_{2u}	1140.1	A_g	1670.8
E_u	150.9	F_{1g}	623.5	F_{1u}	1140.5	F_{2g}	1670.8
F_{2g}	152.2	F_{2g}	631.0	E_g	1170.1	F_{1u}	3230.3
F_{1g}	160.1	F_{1g}	648.6	F_{2g}	1170.7	E_u	3230.3
F_{2u}	160.2	F_{2g}	649.0	A_g	1171.5	B_u	3230.4
F_{1u}	178.3	F_{1g}	691.5	E_u	1180.2	F_{2g}	3230.9
F_{2g}	184.2	F_{2g}	692.9	F_{1u}	1180.8	F_{1g}	3231.0
E_g	192.7	E_g	713.7	B_u	1182.1	F_{1u}	3242.8
B_u	198.2	F_{2g}	715.4	E_g	1212.4	F_{2u}	3243.0
A_g	252.7	A_g	722.3	F_{2g}	1212.8	A_g	3243.8
F_{1u}	262.8	F_{2u}	744.8	A_g	1215.3	E_g	3244.6
F_{1g}	267.9	F_{1u}	748.7	F_{1g}	1336.6	F_{2g}	3244.8
F_{2u}	269.0	F_{1g}	817.6	F_{2g}	1337.1		
F_{2g}	278.8	F_{2g}	819.4	F_{2u}	1371.8		
F_{1u}	286.7	E_u	827.2	F_{1u}	1372.3		

[a] The modes are ordered by increasing frequency.