

Compound [ICSD, S.G.]	Raman Table	Compound [ICSD, S.G.]	Raman Table
Al ₂ SiO ₅ [84613, 58]	Al2SiO5_58_icsd84613	P ₂ S ₃ [423037, 11]	P2S3_11_icsd423037
BaTi(SiO ₃) ₃ [18100, 188]	BaTi(SiO3)3_188_icsd18100	Ca ₂ ZnSi ₂ O ₇ [186944, 113]	Ca2ZnSi2O7_113_icsd186944
Sb ₂ O ₃ [240206, 227]	Sb2O3_227_icsd240206	P ₄ S ₃ [406048, 62]	P4S3_62_icsd406048
Li ₃ PO ₄ [257440, 62]	Li3PO4_62_icsd257440	P ₂ S ₅ [409061, 2]	P2S5_2_icsd409061
Sb ₂ O ₃ [414463, 19]	Sb2O3_19_icsd414463	CoS ₂ [86351, 205]	CoS2_205_icsd86351
NaS [73173, 194]	NaS_194_icsd73173	HgS [81923, 152]	HgS_152_icsd81923
Na ₂ O ₂ [134060, 189]	Na2O2_189_icsd134060	MgTiO ₃ [55285, 148]	MgTiO3_148_icsd55285
BeAl ₂ O ₄ [72416, 62]	BeAl2O4_62_icsd72416	NaP ₅ [99177, 62]	NaP5_62_icsd99177
Mg ₃ (BO ₃) ₂ [31385, 58]	Mg3(BO3)2_58_icsd31385	NaP ₁₅ [239084, 2]	NaP15_2_icsd239084
P ₂ O ₃ [24407, 11]	P2O3_11_icsd24407	CoAsS [69129, 29]	CoAsS_29_icsd69129
Na ₂ Mg(CO ₃) ₂ [100482, 148]	Na2Mg(CO3)2_148_icsd100482	As ₄ S ₅ [16107, 11]	As4S5_11_icsd16107
FeAsS [185809, 14]	FeAsS_14_icsd185809	P ₂ S ₇ [423062, 2]	P2S7_2_icsd423062
P ₂ Se ₅ [74546, 14]	P2Se5_14_icsd74546	Si ₃ (BiO ₃) ₄ [69430, 220]	Si3(BiO3)4_220_icsd69430
BeO [15620, 186]	BeO_186_icsd15620	ZnO ₂ [38979, 205]	ZnO2_205_icsd38979
Li ₄ P ₂ O ₇ [130427, 153]	Li4P2O7_153_icsd130427	Na ₃ PS ₄ [121567, 114]	Na3PS4_114_icsd121567
TeO ₂ [26844, 61]	TeO2_61_icsd26844	LiP [100465, 14]	LiP_14_icsd100465
As ₂ S ₃ [15239, 14]	As2S3_14_icsd15239	CuSbS ₂ [171051, 62]	CuSbS2_62_icsd171051
PS [1703, 15]	PS_15_icsd1703	BaBe ₂ Si ₂ O ₇ [100030, 62]	BaBe2Si2O7_62_icsd100030
Sb ₂ Te [69557, 164]	Sb2Te_164_icsd69557	P ₂ S ₇ [423061, 14]	P2S7_14_icsd423061
Te ₃ As ₂ [18208, 12]	Te3As2_12_icsd18208	AsSe [2056, 14]	AsSe_14_icsd2056
FeSbS [24161, 14]	FeSbS_14_icsd24161	TiO ₂ [9161, 136]	TiO2_136_icsd9161
AsS [86228, 15]	AsS_15_icsd86228	Li ₃ P [240861, 194]	Li3P_194_icsd240861
ZnS [67453, 186]	ZnS_186_icsd67453	ZrO ₂ [86692, 14]	ZrO2_14_icsd86692
As ₂ O ₃ [238641, 14]	As2O3_14_icsd238641	Li ₅ Ge ₂ [121533, 166]	Li5Ge2_166_icsd121533
TiO ₂ [9852, 141]	TiO2_141_icsd9852	HgO [14124, 62]	HgO_62_icsd14124
FeS ₂ [42415, 58]	FeS2_58_icsd42415	Li ₄ GeS ₄ [95649, 62]	Li4GeS4_62_icsd95649
As ₂ S ₃ [185819, 2]	As2S3_2_icsd185819	PbO [15466, 129]	PbO_129_icsd15466
GeS ₂ [44, 7]	GeS2_7_icsd44	Zn(AsO ₂) ₂ [202249, 14]	Zn(AsO2)2_14_icsd202249
LiI [414242, 186]	LiI_186_icsd414242	PbSeO ₃ [98376, 11]	PbSeO3_11_icsd98376
Na ₃ PO ₄ [97205, 114]	Na3PO4_114_icsd97205	SbCl ₃ [8258, 62]	SbCl3_62_icsd8258
CdS [154186, 186]	CdS_186_icsd154186	ZnSe [77091, 216]	ZnSe_216_icsd77091
ZnO [44477, 186]	ZnO_186_icsd44477	As ₄ S ₃ [16105, 62]	As4S3_62_icsd16105
CuAgS [66580, 36]	CuAgS_36_icsd66580	Na ₃ PS ₄ [121566, 114]	Na3PS4_114_icsd121566
NaS ₂ [2586, 122]	NaS2_122_icsd2586	As ₈ S ₉ [98792, 13]	As8S9_13_icsd98792
Al ₂ ZnO ₄ [185709, 227]	Al2ZnO4_227_icsd185709	HgS [38471, 154]	HgS_154_icsd38471
AsS ₂ [424590, 4]	AsS2_4_icsd424590	Ba(NO ₃) ₂ [35495, 205]	Ba(NO3)2_205_icsd35495
PbCO ₃ [166089, 62]	PbCO3_62_icsd166089	ZnTe [77072, 216]	ZnTe_216_icsd77072
Sb ₂ O ₃ [2033, 56]	Sb2O3_56_icsd2033	P ₄ S ₅ [1995, 11]	P4S5_11_icsd1995
PO ₂ [42777, 15]	PO2_15_icsd42777	Li ₃ PO ₄ [77095, 62]	Li3PO4_62_icsd77095
SbO ₂ [153156, 15]	SbO2_15_icsd153156	BaCO ₃ [158378, 62]	BaCO3_62_icsd158378
CaTa ₂ O ₆ [24091, 62]	CaTa2O6_62_icsd24091	Li ₂ O [257372, 225]	Li2O_225_icsd257372
Ca ₃ Si ₂ O ₇ [2282, 14]	Ca3Si2O7_14_icsd2282	Sb ₂ Se ₃ [30973, 62]	Sb2Se3_62_icsd30973
Al ₂ Si(O ₂ F) ₂ [59410, 62]	Al2Si(O2F)2_62_icsd59410	TiO ₂ [36408, 61]	TiO2_61_icsd36408
ZnS [136503, 216]	ZnS_216_icsd136503	Ag ₂ HgS ₂ [201713, 14]	Ag2HgS2_14_icsd201713
PbClF [39165, 129]	PbClF_129_icsd39165	GeP ₃ [16294, 166]	GeP3_166_icsd16294
ZnF ₂ [280605, 136]	ZnF2_136_icsd280605	AsS [360, 14]	AsS_14_icsd360
SiO ₂ [90145, 152]	SiO2_152_icsd90145	LiP ₅ [88710, 33]	LiP5_33_icsd88710
Li ₃ P ₇ [60774, 19]	Li3P7_19_icsd60774	CaMgCO ₃₂ [52149, 148]	CaMgCO32_148_icsd52149
Bi ₂ Se ₃ [60205, 62]	Bi2Se3_62_icsd60205	K ₃ Na(SO ₄) ₂ [26014, 164]	K3Na(SO4)2_164_icsd26014
ZnP ₄ [40428, 92]	ZnP4_92_icsd40428	KNbO ₃ [190923, 160]	KNbO3_160_icsd190923
NaHCO ₃ [18183, 14]	NaHCO3_14_icsd18183	NaMgF ₃ [72318, 62]	NaMgF3_62_icsd72318
ZnAs [427612, 61]	ZnAs_61_icsd427612	Mg ₃ (PO ₄) ₂ [31005, 14]	Mg3(PO4)2_14_icsd31005

Table 1. List of computed compounds in the database and their Raman information, such as Raman-active frequencies and Raman intensities. The database currently contains 145 compounds and constantly grows. ICSD codes and space group (S.G.) numbers, of compounds are provided.

Compound [ICSD, S.G.]	Raman Table	Compound [ICSD, S.G.]	Raman Table
As ₂ Se ₃ [29535, 14]	As2Se3_14_icsd29535	SiC [156190, 186]	SiC_186_icsd156190
CaTiO ₃ [62149, 62]	CaTiO3_62_icsd62149	Ag ₃ AsS ₃ [36352, 15]	Ag3AsS3_15_icsd36352
CaCO ₃ [15194, 62]	CaCO3_62_icsd15194	As ₂ O ₃ [238665, 14]	As2O3_14_icsd238665
Li ₃ N [156894, 191]	Li3N_191_icsd156894	BaSO ₄ [33730, 62]	BaSO4_62_icsd33730
NaP [14009, 19]	NaP_19_icsd14009	Li ₂ O ₂ [50658, 194]	Li2O2_194_icsd50658
SbI ₃ [30906, 14]	SbI3_14_icsd30906	CoAsS [610107, 198]	CoAsS_198_icsd610107
AsO ₂ [10436, 62]	AsO2_62_icsd10436	FeS ₂ [316, 205]	FeS2_205_icsd316
CuBiS ₂ [34936, 62]	CuBiS2_62_icsd34936	Sb ₂ O ₅ [1422, 15]	Sb2O5_15_icsd1422
P ₂ O ₅ [79698, 62]	P2O5_62_icsd79698	CaMg ₃ (CO ₃) ₄ [201729, 155]	CaMg3(CO3)4_155_icsd201729
AsBr ₃ [26774, 19]	AsBr3_19_icsd26774	LiCaAlF ₆ [150332, 163]	LiCaAlF6_163_icsd150332
Sb ₂ PbO ₆ [81387, 162]	Sb2PbO6_162_icsd81387	As ₂ Se ₃ [291473, 12]	As2Se3_12_icsd291473
Ca ₂ CO ₃ F ₂ [100607, 60]	Ca2CO3F2_60_icsd100607	SiO ₂ [403365, 92]	SiO2_92_icsd403365
PbSO ₄ [16916, 62]	PbSO4_62_icsd16916	NaBe ₄ SbO ₇ [27599, 186]	NaBe4SbO7_186_icsd27599
KAlSiO ₄ [83449, 159]	KAlSiO4_159_icsd83449	RuS ₂ [68472, 205]	RuS2_205_icsd68472
BaBe ₂ Si ₂ O ₇ [20409, 31]	BaBe2Si2O7_31_icsd20409	BaSi ₂ O ₅ [100313, 62]	BaSi2O5_62_icsd100313
Ag ₂ S [262636, 14]	Ag2S_14_icsd262636	Na ₂ Si ₂ O ₅ [34688, 14]	Na2Si2O5_14_icsd34688
SbO ₂ [153154, 33]	SbO2_33_icsd153154	PSe [74878, 14]	PSe_14_icsd74878
TlAsS ₂ [81094, 14]	TlAsS2_14_icsd81094	CaCO ₃ [18166, 167]	CaCO3_167_icsd18166
Al ₂ SiO ₅ [24275, 58]	Al2SiO5_58_icsd24275	ZnN ₆ [430428, 14]	ZnN6_14_icsd430428
SbCl ₅ [250363, 194]	SbCl5_194_icsd250363	AsI ₃ [23003, 148]	AsI3_148_icsd23003
As ₂ O ₃ [238612, 227]	As2O3_227_icsd238612	ZnCl ₂ [2459, 33]	ZnCl2_33_icsd2459
Li ₂ S [657596, 225]	Li2S_225_icsd657596	P ₄ O ₉ [300205, 167]	P4O9_167_icsd300205
KBF ₄ [9875, 62]	KBF4_62_icsd9875	MgCO ₃ [80870, 167]	MgCO3_167_icsd80870
SbI ₃ [26082, 148]	SbI3_148_icsd26082	Na ₂ S ₅ [430333, 32]	Na2S5_32_icsd430333
Na ₂ S ₅ [38349, 62]	Na2S5_62_icsd38349	Na ₃ P [433838, 185]	Na3P_185_icsd433838
P ₄ O ₇ [16452, 14]	P4O7_14_icsd16452	SbBr ₃ [14217, 19]	SbBr3_19_icsd14217
Cu ₂ O [172174, 224]	Cu2O_224_icsd172174	Sb ₂ Te ₃ [2084, 166]	Sb2Te3_166_icsd2084
WS ₂ [202366, 194]	WS2_194_icsd202366	Na ₂ Ca(SO ₄) ₂ [16901, 15]	Na2Ca(SO4)2_15_icsd16901
Li ₃ PO ₄ [257439, 31]	Li3PO4_31_icsd257439		

Table 1. Continued. List of computed compounds in the database and their Raman information, such as Raman-active frequencies and Raman intensities. The database currently contains 145 compounds and constantly grows. ICSD codes and space group (S.G.) numbers, of compounds are provided.