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## Database S2.2.2

## Non-perovskites found from internet mining

| Compound | Structure type | Reference |
|---|---|---|
| AgIO3 | edge sharing | ICSD |
| Ba2RhSbO6 | hexagonal | J. Inorg Nucl Chem 27, 994-1003 (1965) |
| Ba2ScMoO6 | hexagonal | Inorg Chem 10(5),922 (1971) |
| BaTeO3 | edge sharing | ICSD |
| Bi2TiFeO6 | edge sharing | ICSD |
| Bi2TiMoO6 | sheelite | Applied Catalysis A: General 110, 207-216 (1994) |
| Bi3YO6 | fluorite | Solid State Ionics 264, 49-53 (2014) |
| BiEuO3 | Bi2O3 type | ICSD |
| BiGdO3 | Bi2O3 type | ICSD |
| BiInS3 | edge sharing | ICSD |
| BiTbO3 | fluorite | J. Magnetism. and Magnetic Materials 398, 289-297 (2016) |
| BiYbO3 | | ICSD |
| Ca3NpO6 | | Handbook of Inorganic Substances, Walter de Gruyter GmbH & Co (2015), P. Villars, K. Cenzual, R. Gladyshevskii |
| CaPtO3 | pyroxene | ICSD |
| CaTeO3 | isolated octahedra | ICSD |
| Cd2GaTaO6 | pyrochlore | Int. J. of Hydrogen En. 35 (13) 7029-7035 (2010) |
| Cd2InSbO6 | amorphous | Vacuum 80, 1038-1041 (2006) |
| CdFeO3 | hexagonal | J Phys Chem Solids 36, 783-789 (1975) |
| CdTeO3 | isolated TeO3 pyramids | Acta Cryst. C41, 1152-1154 (1985) |
| Ce3LuSe6 | edge sharing | ICSD |
| CeBiO3 | layered | Phys. Stat. Solidi B 252 (12), 2680-2684 (2015) |
| CeBiS3 | | Springer Materials |

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|---|---|---|
| CeBiSe3 | | Springer Materials |
| CeDyS3 | edge sharing | ICSD |
| CeErS3 | edge sharing | ICSD |
| CeEuO3 | Sm2O3 type | Springer Materials |
| CeHoS3 | edge sharing | ICSD |
| CeInO3 | layered | ICSD |
| CeLaO3 | La2O3-type | Springer Materials |
| CeLuS3 | layered | ICSD |
| CePrO3 | | Springer Materials |
| CeSbO3 | pyrochlore | ICSD |
| CeTbO3 | | Springer Materials |
| CeTmS3 | layered | ICSD |
| CeYbS3 | layered | ICSD |
| CeYbSe3 | layered (ScUS3 type) | ICSD |
| CrFeO3 | Al2O3 type | Springer Materials |
| CrMoO3 | no octahedra | ICSD |
| CrRhO3 | Al2O3 type | Springer Materials |
| CrVO3 | corundum | J. Solid State Chem. 144, 392-397 (1999) |
| CrWO3 | no octahedra | ICSD |
| Cs2LiInCl6 | edge sharing | ICSD |
| Cs2NaTiF6 | hexagonal | Z. Anorg Chem. 403(2), 127-136 (1974) |
| Cs2TlBiCl6 | | Springer Materials |
| Cs3ErCl6 | isolated octahedra | Springer Materials |
| Cs3EuF6 | | Springer Materials |
| Cs3GdBr6 | isolated octahedra | J Luminesc. 153, 64-72 (2014) |

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|---|---|---|
| Cs3GdCl6 | isolated octahedra | J Luminesc. 153, 64-72 (2014) |
| Cs3InCl6 | isolated octahedra | PhD thesis Stephan Bremm, Uni Koln 2002 |
| Cs3LuF6 | isolated octahedra | Springer Materials |
| Cs3LaI6 | | J. Luminesc. 149, 374-384 (2014) |
| Cs3SmCl6 | isolated octahedra | Springer Materials |
| Cs3TlF6 | isolated octahedra | ICSD |
| Cs3UF6 | isolated octahedra | Springer Materials |
| CsCrCl3 | hexagonal | ICSD |
| CsFeCl3 | hexagonal | ICSD |
| CsMnBr3 | hexagonal | ICSD |
| CsPdCl3 | edge sharing | Z. Anorg. Chem. 625 (11), 1944-1950 (1999) |
| CsSrI3 | PuBr3-type structure | Phys. Chem. Chem. Phys. 18, 13196-13208 (2016) |
| CsTiBr3 | hexagonal | ICSD |
| CsTiCl3 | hexagonal | ICSD |
| CsVCl3 | BaNiO3 type | ICSD |
| Dy2TiCuO6 | layered | Solid State Sci 4, 1495-1498 (2002) |
| Dy3GaO6 | Er3GaS6 type | ICSD |
| DyBiO3 | | Springer Materials |
| Er2TiCuO6 | | Prog. Solid State Chem. 22, 197-233 (1993) |
| Er3GaO6 | Er3GaS6 type | ICSD |
| ErInO3 | hexagonal | J Inorg Nucl Chem 38, 1471-1475 (1976) |
| Eu3AuO6 | Au - planar coordinated | ICSD |
| Eu3GaO6 | Er3GaS6 type | ICSD |
| EuLuO3 | | Springer Materials |
| Fe3TiO6 | ilmenite | ICSD |

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|---|---|---|
| FeHfO3 | ilmenite | J. Magnetism and Magnetic Materials 394, 463-469 (2015) |
| FeRhO3 | ilmenite | Electro Ceramics Web course Indian Institute of Technology Kanpur (Ashish Garg, Department of Materials Science and Engineering) |
| Gd3AuO6 | Au - planar coordinated | Z. Anorg. Allg. Chem. 627, 439-444 (2001) |
| Gd3FeO6 | BiCa2VO6 type | ICSD |
| Gd3GaO6 | Er3GaS6 type | ICSD |
| GdErO3 | (Mn_0.5Fe_0.5)2O3 type | Springer Materials |
| GdInS3 | | Springer Materials |
| GdLaO3 | CeYbYb2S6-type | J Solid State Chemistry 177, 4142-4148 (2004) |
| GdLuO3 | bixbyite | ICSD |
| Hg3AsF6 | no octahedra | PRB 31(5) (2881-2885) (1985) |
| Hg3NbF6 | isolated octahedra | J. Solid State Chem. 57 (1) 34-42 (1985) |
| Hg3SbF6 | isolated octahedra | J. Solid State Chem. 57 (1) 34-42 (1985) |
| Hg3TaF6 | layered | Inorg Chem 23, 4506-4508 (1984) |
| HgVO3 | no octahedra | ICSD |
| Ho3ScO6 | edge sharing | ICSD |
| HoInO3 | hexagonal | J. Inorg. Nucl. Chem. 38 (8) 1471-1475 (1976) |
| In2FeRuO6 | bixbyite | Solid State Commun 152(2), 95-99 (2012) |
| InGaO3 | layered | ICSD |
| InMnO3 | layered | ICSD |
| K3CeF6 | | Springer Materials |
| K3ErCl6 | isolated octahedra | Z. Anorg. Allg. Chem. 627, 2317-2322 (2001) |
| K3InCl6 | isolated octahedra | Acta Cryst E62, i143-i144 (2006) |
| K3UF6 | isolated octahedra | Springer Materials |
| KCdBr3 | NH4CdCl3 - type | Phys. Stat. Solidi B 147 K195 (1988) |
| KDyI3 | | Springer Materials |

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|---|---|---|
| KMnBr3 | hexagonal | Mat Res Bul 17, 1421-1427 (1982) |
| KPbF3 | | Rep. Prog. Phys. 67, 1233-1314 (2004) |
| KPbI3 | NH4CdCl3-type | Springer Materials |
| KTiBr3 | hexagonal face sharing | Acta Cryst A 66(5) 558-590 (2010) |
| KTiCl3 | hexagonal face sharing | Acta Cryst A 66(5) 558-590 (2010) |
| KTmI3 | corner and edge sharing | Chemical Journal of Chinese Universities 19(3):335-339 (1998) |
| KVCl3 | hexagonal | Z. Anorg. Allg. Chem. doi: 10.1002/zaac.19603020506 (1960) |
| KYbI3 | layered | Z. Anorg. Allg. Chem. 618, 7-12 (1992) |
| La2KNbO6 | | Chem Mater 20 (10), 3327-3335 (2008) |
| La3FeO6 | BiCa2VO6 type | ICSD |
| La3InS6 | isolated octahedra | ICSD |
| La3LuSe6 | layered | http://escholarship.org/uc/item/697389n and (icsd) |
| LaAsO3 | KClO3 - type | ICSD |
| LaBiS3 | | Springer Materials |
| LaBiSe3 | | Springer Materials |
| LaDyO3 | | J. Alloys and Compounds 494 (1-2), 336 (2010) |
| LaErS3 | edge sharing | ICSD |
| LaEuO3 | hexagonal | PRB 40(1), 102 (1989) |
| LaHoS3 | edge sharing | ICSD |
| LaInS3 | | Springer Materials |
| LaSbO3 | | Springer Materials |
| LaSmO3 | | J. of Research of the National Bureau of Standards A Physics & Chem. 64A(4), 317 (1960) |
| LaTmS3 | face sharing | ICSD |
| LaYbSe3 | layered | J. Solid State Chem. 177, 709-713 (2004) |
| LaYS3 | LaErS3 type | Springer Materials |

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|---|---|---|
| Li3NiF6 | edge sharing | J. Fluorine Chem. 6(3) 267-274(1975) |
| Li3ScF6 | edge sharing | ICSD |
| Li3TiF6 | edge sharing | ICSD |
| LiSbO3 | edge sharing | ICSD |
| Lu2FeMoO6 | edge sharing | Sci Rep 6, 20133 (2016) |
| Lu2TiCuO6 | layered | Solid State Sci. 4, 1495-1498 (2002) |
| MgFeO3 | bixbyite | Springer Materials |
| Mn2FeMoO6 | edge sharing | Angew. Chem. 40(53), 10774-10778 (2014) |
| Mn2FeWO6 | edge sharing | ICSD |
| Mn2InSbO6 | edge sharing | ICSD |
| Mn3WO6 | edge sharing | Springer Materials |
| MnTbO3 | TbMnO3 perovskite | ICSD |
| Na3EuCl6 | edge sharing | Springer Materials |
| Na3GdI6 | edge sharing | Z. Anorg. Chem. 623 (1-6): 837-843 (1997) |
| Na3InCl6 | edge sharing | ICSD |
| Na3PdF6 | | Springer Materials |
| Na3SmBr6 | edge sharing chains | ICSD |
| Na3SmI6 | | Springer Materials |
| Na3TbCl6 | edge sharing | Springer Materials |
| Na3TlF6 | | Springer Materials |
| NaBiO3 | ilmenite | Inorg Chem. 55, 5747-5749 (2016) |
| NaCdCl3 | edge sharing | Eur. J. Inorg. Che. 1675-1680 (2003), doi:  10.1002/ejic.200200612 |
| NaHgCl3 | no octahedra | ICSD |
| NaMnCl3 | ilmenite | ICSD |
| NaTiCl3 | | Springer Materials |

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|---|---|---|
| Nd2CuZrO6 | layered | Chem Mater 10(10), 3124-3130 (1998) |
| Nd2KNbO6 | no octahedra | Chem Mater 20 (10), 3327-3335 (2008) |
| Nd3FeO6 | BiCa2VO6 type | ICSD |
| Nd3GaO6 | Er3GaS6 type | ICSD |
| NdBiS3 | | Springer Materials |
| NdEuO3 | monoclinic | PRB 40(1), 102 (1989) |
| NdLuS3 | layered | Springer Materials |
| NdLuSe3 | UFeS3 type | Inorg. Chem. doi: 10.1021/ic701012j (2007) |
| NdTmS3 | layered | Springer Materials |
| NdYbS3 | | J Solid State Chem. 7, 321-336 (1973) |
| NdYbSe3 | layered | J. Solid State Chem. 177 (3) 709-713 (2004) |
| Pb2NiTaO6 | pyrochlore | Springer Materials |
| Pb2VBiO6 | edge sharing | Solid State Sci. 6(8), 783-790 (2004) |
| Pb3UO6 | isolated octahedra | Acta Cryst. 23 264 (1967) |
| Pb3WO6 | edge sharing | J. Alloys and Compounds 545, 135-138 (2012) |
| PbReO3 | defect pyrochlore | Mater. Sci. Eng. 36, 231-239 (1978) |
| PbTcO3 | pyrochlore | Springer Materials |
| PbTeO3 | isolated octahedra | ICSD |
| Pr3InS6 | | Springer Materials |
| PrEuO3 | monoclinic | J. of the Less Common Metals, 149, 101-107 (1989) |
| PrInS3 | | Springer Materials |
| PrLuS3 | layered | ICSD |
| PrLuSe3 | layered | ICSD |
| PrSbO3 | | Springer Materials |
| PrTmS3 | layered | ICSD |

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|---|---|---|
| PrYbS3 | layered | ICSD |
| PrYbSe3 | layered | J. Solid State Chem. 177(3, 709-713 (2004) |
| Rb3BiBr6 | isolated octahedra | ICSD |
| Rb3DyCl6 | isolated octahedra | Springer Materials |
| Rb3ErCl6 | | Springer Materials |
| Rb3HoCl6 | | |
| Rb3InCl6 | isolated octahedra | Doctoral Thesis Stephan Bremm (Uni Koln 2002) |
| Rb3TlCl6 | K3InCl6 type | ICSD |
| Rb3YbCl6 | | Springer Materials |
| Rb3YbF6 | isolated octahedra | Springer Materials |
| RbMnBr3 | BaNiO3 type | ICSD |
| RbPbI3 | NH4CdCl3 type | ICSD |
| RbTiBr3 | BaNiO3-type | Springer Materials |
| RbTiCl3 | BaNiO3 type | Z. Anorg. Alg. Chem 524, 90-94 (1985) |
| RbVCl3 | BaNiO3 type | J. Solid State Chem. 56(3) 343-354 |
| SbAsO3 | As2O3 type | ICSD |
| Sc3CrO6 | Mg3TeO3 type | ICSD |
| Sm3AuO6 | Perovskite-Ba2LaRuO6(I1-) | ICSD |
| Sm3GaO6 | Er3GaS6-type | Springer Materials |
| Sm3InS6 | | Springer Materials |
| SmEuO3 | Sm2O3 type | PRB 40 (1), 102 (1989) |
| SmGdO3 | amorphous | Appl. Phys. Lett. 104, 073501 (2014) |
| SmLuO3 | | Arabian Journal of Chemistry (2016) http://dx.doi.org/10.1016/j.arabjc.2016.03.010 |
| SmYbSe3 | layered | J. Solid. State Chem. 177(3) 709-713 (2004) |
| Sr2TaBiO6 | layered | Abstract Nanocon 2011, http://nanocon2012.tanger.cz/files/proceedings/nanocon_11/lists/papers/1356.pdf |

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|---|---|---|
| SrTeO3 | edge sharing | ICSD |
| Tb2TiCuO6 | layered | Solid State Sciences 4, 1495-1498 (2002) |
| Tb3GaO6 | Er3GaS6-type | Springer Materials |
| TbNiO3 | oxidation state not stabilized | Chem Mater 11(9), (1999) |
| TiSbO3 | layered | Master Thesis Patrick Woodward Oregon State University (1996) |
| TiTaO3 | pyrochlore | Mat Res Bull 17, 917-933 (1982) |
| Tl3BiCl6 | isolated octahedra | ICSD |
| Tl3BiI6 | isolated octahedra | ICSD |
| TlCaBr3 | PuBr3 type | Z. anorg. allg. chem. 622 (1996) 759-765 |
| TlCdBr3 | NH4CdBr3 type | ICSD |
| TlCdI3 | NH4CdCl3 type | J. Luminesc. 79(2), 135-141 (1998) |
| TlFeCl3 | hexagonal | J. Magn. and Magn. Mater. 116(1-2), 80-82 (1992) |
| TlHgBr3 | face sharing octahedra | Opt. Mater. 49, 94-99 (2015) |
| TlHgCl3 | NH4CdCl3 type | ICSD |
| TlMnBr3 | (NH4)CdI3 type | J. Thermal Analysis 6(1), 175-182 (1974) |
| TlNbO3 | pyrochlore | Mat Res Bul 10, 933-940 (1975) |
| TlPbCl3 | Ga2Gd3 type | ICSD |
| TlSbO3 | layered | ICSD |
| TlTaO3 | pyrochlore | Solid State Commun. 17, 545-547 (1975) |
| TlVO3 | KVO3 type | Springer Materials |
| TlZnF3 | BaTiO3-hexagonal | J. Phys. Condens. Matter 17(29) 4653-4663 (2005) |
| Tm2TiCuO6 | layered | ICSD |
| VFeO3 | Al2O3 | Springer Materials |
| VTiO3 | Al2O3 | Springer Materials |
| Y2EuErO6 | Mn2O3 type | http://www.icdd.com/resources/axa/VOL55/V55_05.pdf |

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|---|---|---|
| Y2EuHoO6 | Mn2O3 type | http://www.icdd.com/resources/axa/VOL55/V55_05.pdf |
| Y2TiCuO6 | layered | ICSD |
| Y3GaO6 | er3gas6-type | ICSD |
| Yb2TiCuO6 | layered | PRB 82.134203(2010) |
| Yb2TiMnO6 | layered | Mat Res Bulletin 36 57-58 (2001) |
| YbInO3 | bixbyite | Dphil Thesis Daniel Giaquinta (Northwestern Uni, 1989) |
| YbLaO3 | LaYbO3 perovskite, no structure for YbLaO3 | |
| YGdO3 | bixbyite | ICSD |
| YLaO3 | LaYO3 perovskite, no structure for YLaO3 | |
| YPrO3 | bixbyite | ICSD |
| YTmO3 | bixbyite | ICSD |
| YYbO3 | bixbyite | ICSD |