Electronic Supplementary Material (ESI) for CrystEngComm

Supporting Information

Synthesis, Crystal Growth and Characterization of a New Noncentrosymmetric Borophosphate: $RbPbBP_2O_8$

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Table S1. Atomic Coordinates and Equivalent Isotropic Displacement Parameters for $RbPbBP_2O_8$.

atom	Wyck.	S.O.F.	*x/a*	*y/b*	*z/c*	U_{eq} [a]
Rb(1) | Pb(1)	8d	0.5	0.6360(1)	0.7500	0.1250	0.026(1)
B(1)	4a	1.0	1.0000	0.0000	0.0000	0.045(3)
P(1)	8d	1.0	0.8432(6)	0.2500	0. 1250	0.033(1)
O(1)	16e	1.0	0.7274(17)	0.3925(13)	0.0768(8)	0.055(2)
O(2)	16e	1.0	0.9914(16)	0.1613(14)	0.0570(7)	0.049(2)

[a] U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Table S2. Bond-valence sums for $RbPbBP_2O_8$, calculated with the bond-length/bond-strength concept ($\sum V$) and the CHARDI concept ($\sum Q$).

	Rb(1) | Pb(1)	B(1)	P(1)	O(1)	O(2)
$\sum V$	1.35	3.58	4.96	-1.92	-2.14
$\sum Q$	1.52	2.91	5.03	-1.94	-2.06

Table S3. Dipole Moments of MO_8 (M = K, Rb, Sr, Ba, and Pb) Polyhedra in $KSrBP_2O_8$, $KBaBP_2O_8$, and $RbPbBP_2O_8$.

Species	*x (a)*	*y (b)*	*z (c)*	Polyhedral dipole moment (Debye)
KO_8 [a]	-2.287	-0.3808	0	2.32
KO_8 [b]	-2.519	0.2688	0	2.53
RbO_8	2.355	0.0153	0	2.36
SrO_8	-1.696	-0.1557	0	1.70
BaO_8	-2.834	0.1783	0	2.84
PbO_8 [c]	-4.056	-5.987	-1.936	7.48

[a] In $KSrBP_2O_8$ and [b] in $KBaBP_2O_8$, the cif files are obtained from Ref. 14.

[c] For Pb^{2+} cations, the lone pair is given a charge of -2 and localized 0.86 Å from the Pb^{2+} cation. (J. Galy, G. Meunier, S. Andersson and A. Astrom, *J. Solid State Chem.*, 1975, **13**, 142)

Fig. S1 Coordinated environment of mixed occupied Rb/Pb atoms.

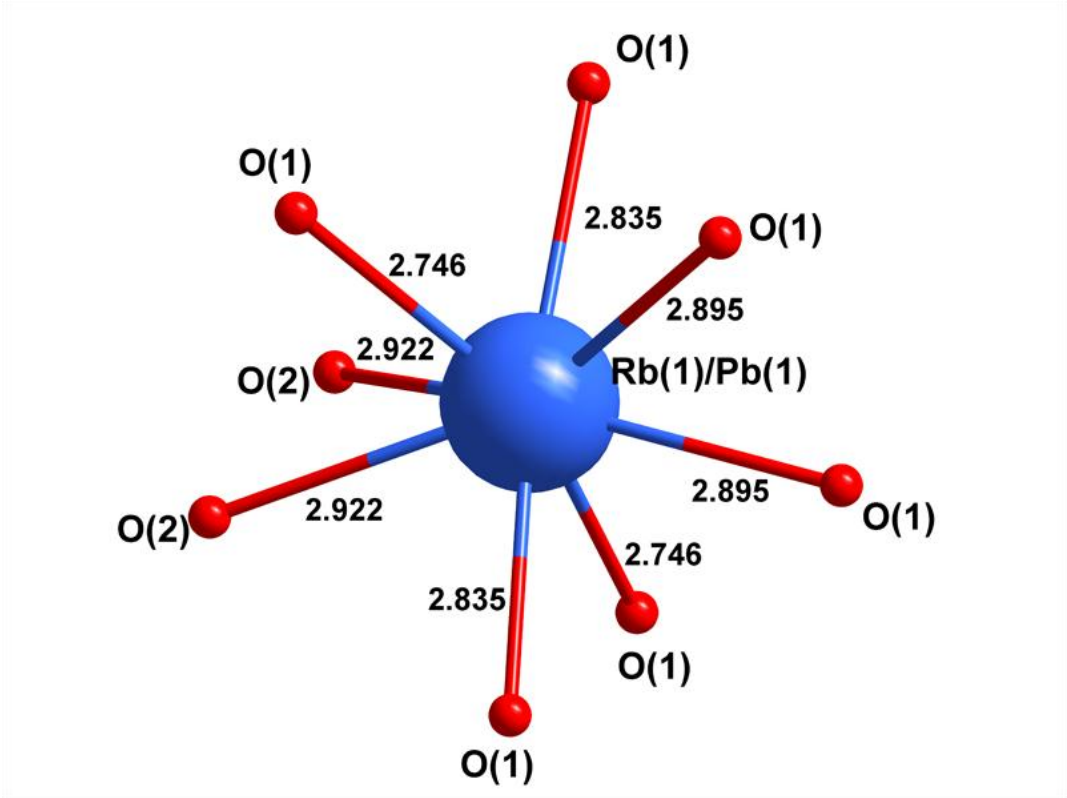

Fig. S2 Phase matching curve, *i.e.*, particle size *vs* SHG intensity, data for $RbPbBP_2O_8$. The curve is drawn to guide the eye and is not a fit to the data.