Crystal Chemisty of $M^{2+}Be_2P_2O_8$ Beryllophosphates: a Comparison With Aluminosilicates

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Introduction

- New synthetic beryllophosphates
- Hydrothermal synthesis in the M^{2+}-Be-PO_4-H_2O system at 200, 400 and 600°C
- M^{2+} = Ca, Sr, Pb and Ba
- Structural analogies with aluminosilicates, borosilicates and gallogermanates

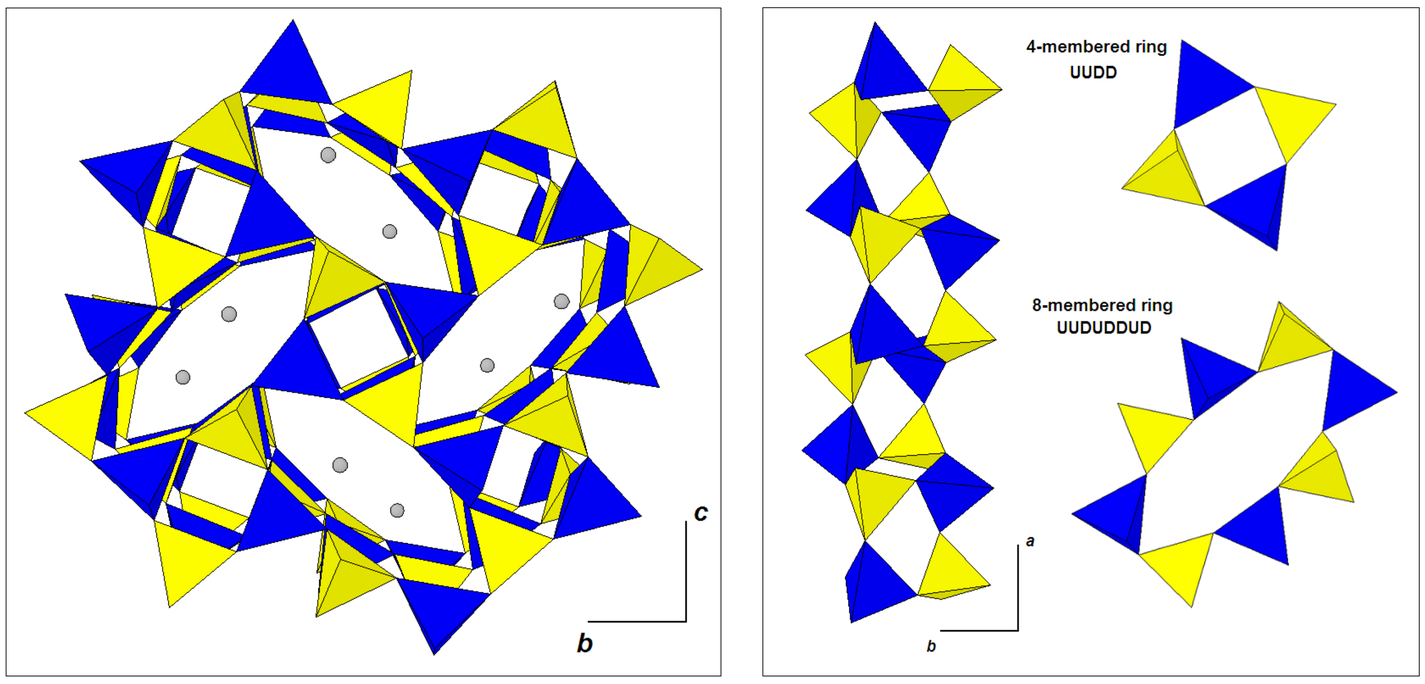
Comparison with natural analogues

	$CaBe_2P_2O_8$	$SrBe_2P_2O_8$	$PbBe_2P_2O_8$	$CaAl_2Si_2O_8$	$BaBe_2P_2O_8$	$CaAl_2Si_2O_8$
a (Å)	7.809(1)	8.000(1)	8.088(1)	8.580	5.028(1)	5.100
b	8.799(1)	8.986(1)	9.019(1)	9.583	5.028(1)	5.100
c	8.309(1)	8.418(1)	8.391(1)	9.090	7.466(1)	14.720
β (°)	90.51(1)	90.22(1)	90.12(1)	90.21	-	-
V (Å³)	570.98(2)	605.10(6)	612.22(1)	746.58	163.51(1)	
S.G.	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P6/mmm$	$P6_3/mcm$
Natural Analogues	Hurlbutite	Strontio-hurlbutite	-	Paracelsian	-	Dmisteinbergite

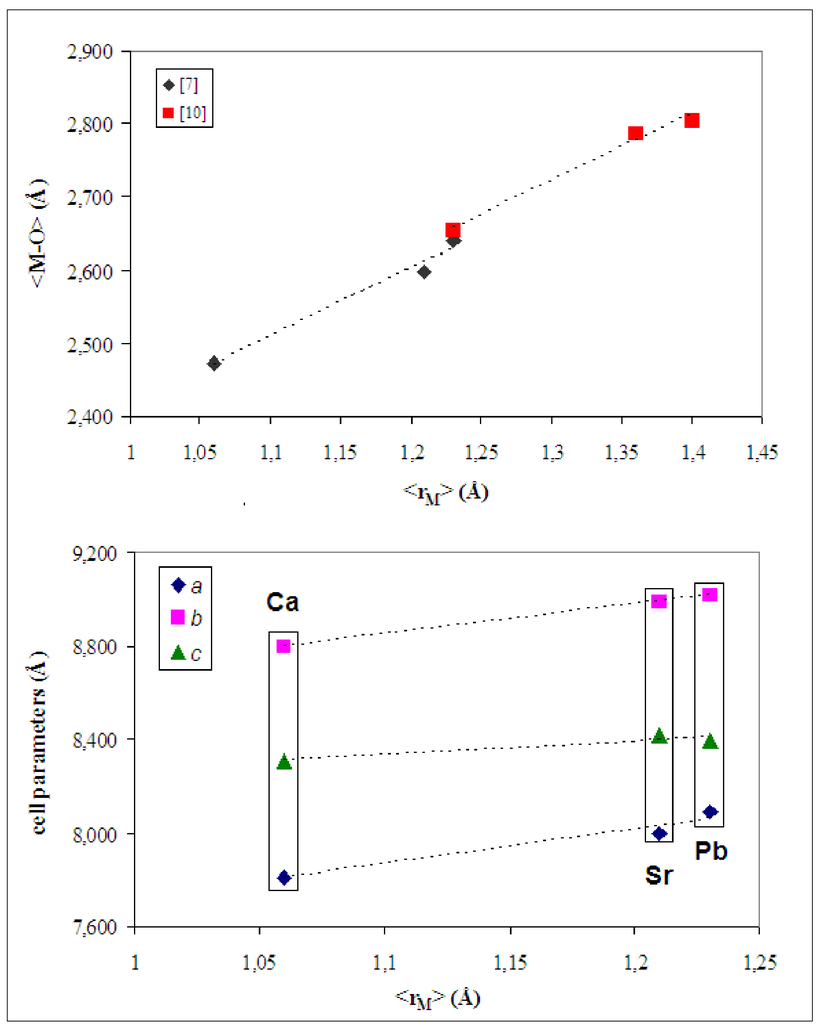
$CaBe_2P_2O_8$, $SrBe_2P_2O_8$ and $PbBe_2P_2O_8$

- Paracelsian-type structure
- Distinctive features: 4- and 8-membered rings with typical pattern and double-crankshaft chains
- Perfect alternation between the BeO_4 and PO_4 tetrahedra

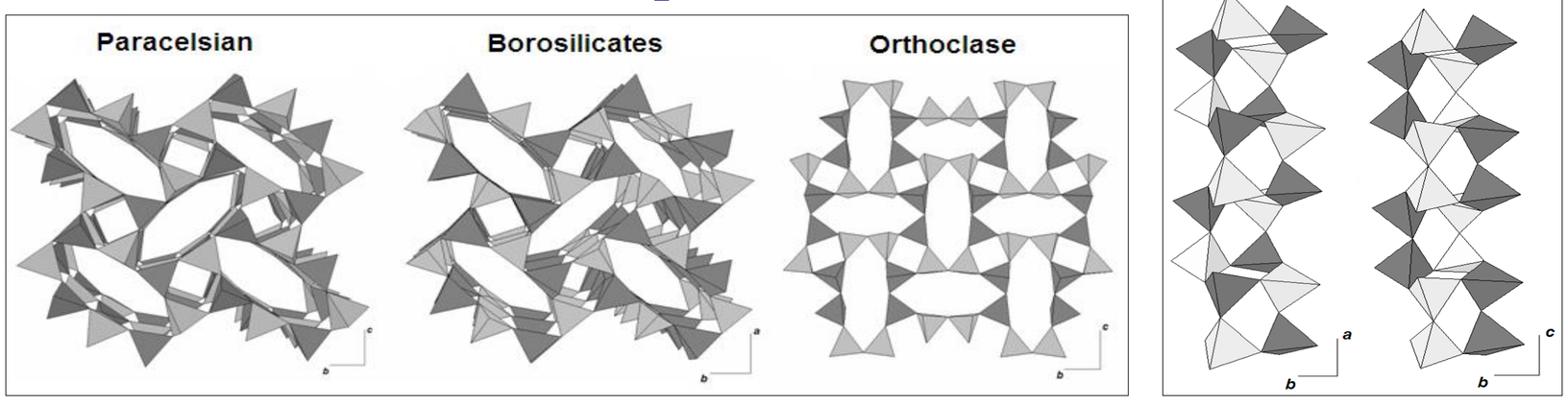
Paracelsian-type structure



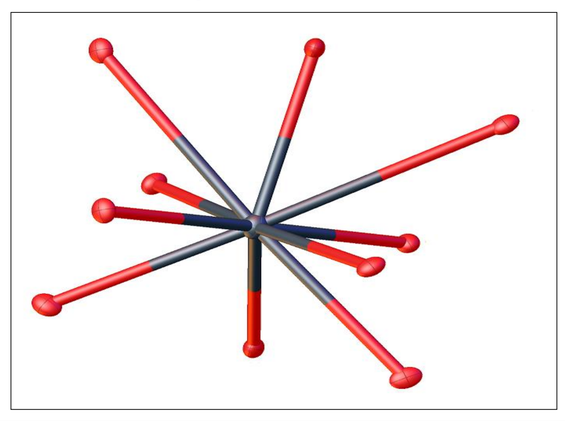
Variation of the crystallographic parameters



Structural comparison



$M^{2+}O_{10}$ polyhedron



$BaBe_2P_2O_8$

- Same structure than dmisteinbergite
- 6-membered rings assembled in double layers
- Be and P located in the same tetrahedra

Structure of $BaBe_2P_2O_8$