Electronic Supplementary Information for Dalton Transactions

Structure determination of β-Pb_2ZnF_6 by coupling multinuclear solid state NMR, powder XRD and ab initio calculations

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Electronic Supplementary Information

Table 1 Conditions of X-ray data collection and refinement parameters of β-Pb_2ZnF_6

Diffractometer	PANalytical X'pert PRO equipped with an Anton Paar HTK 1200 high-temperature heating chamber
Radiation	CuKα, 40kV, 35mA
Divergence, antiscattering slits/°	0.50
Receiving slit/°	1.00
Angular range/°2θ	5-140
Step scan increment/°2θ	0.017
Count time/sec.step^{-1}	500
Temperature/°C	90 (under argon atmosphere)
Space group	$P4_2/ncm$ (No.138)
Cell parameters/Å	a = 5.632 (1), c = 16.247 (1)
Volume/Å^3; Z	515.35 (1); Z = 4
Number of reflections	286
Number of refined parameters	17
Half-width parameters	U = 0.042 (2), V = -0.014 (2), W = 0.0071 (3)
Peak shape	Pseudo-Voigt 0.63 (2)
Zero point/°2θ	0.0456 (3)
Reliability factors	R_p = 0.159, R_{wp} = 0.133, R_{exp} = 0.0549, χ^2 = 5.83, R_{Bragg} = 0.095