Crystal structure of dirubidium barium bis(tetracyanoplatinate(II)), $Rb_2Ba[Pt(CN)_4]_2$

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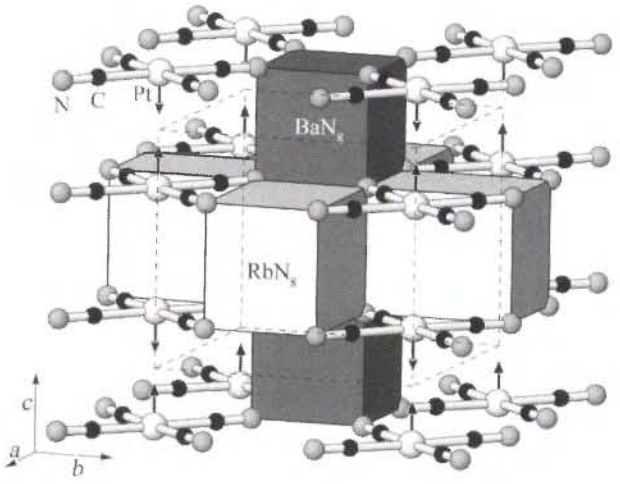

Abstract

$BaN_8C_8Pt_2Rb_2$, tetragonal, *P4/mmm* (no. 123), $a = 7.788(1)$ Å, $c = 6.971(1)$ Å, $V = 422.8$ Å^3, $Z = 1$, $R_{gt}(F) = 0.046$, $wR_{ref}(F^2) = 0.134$, $T = 298$ K.

Source of material

A concentrated aqueous solution of $Ba[Pt(CN)_4] \cdot 4H_2O$ (Chempur, 99.9 %) was added to a stoichiometric amount of an aqueous solution of Rb_2SO_4 (Sigma-Aldrich, 99.8 %) as described in [1]. After removing $BaSO_4$ by filtration, the clear residual solution was slowly evaporated at room temperature. Transparent green crystals of $Rb_2Ba[Pt(CN)_4]_2$ were obtained together with the main product of $Rb_2[Pt(CN)_4] \cdot 1.5H_2O$.

Discussion

In $Rb_2Ba[Pt(CN)_4]_2$ platinum is square-planar coordinated by the cyanide ligands. The Pt—C distances of 1.99(2) Å are in good agreement with literature data [2,3]. The nitrogen atoms form a cubic primitive packing, with ¼ of the cubes centered by Rb and ⅛ by Ba. RbN_8 and BaN_8 cubes alternate in the *c* direction. The Pt atoms are located on the faces of ⅖ of the remaining empty cubes (⅝), forming one-dimensional $[Pt(CN)_4]$ stacks along [001] with alternating Pt—Pt distances of 3.389(3) Å and 3.582(3) Å. This alternation is depending on the distances of d(Ba—N) = 2.90(2) Å and d(Rb—N) = 3.33(1) Å, which are known from compounds like $Ba[Pt(CN)_4] \cdot 4H_2O$ [4] and $Rb_2[Pt(CN)_4] \cdot 1.5H_2O$ [1], and is not caused by direct Pt—Pt interactions.

Table 1. Data collection and handling.

Crystal:	green block, size 0.15 × 0.20 × 0.25 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	245.30 cm^{-1}
Diffractometer, scan mode:	Bruker AXS SMART APEX CCD, ω
$2\theta_{max}$:	57.82°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	4579, 379
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 298
$N(param)_{refined}$:	21
Programs:	SHELXTL [5], ATOMS [6]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pt	2*g*	0	0	0.2431(2)	0.0207(4)	U_{11}	0.0270(7)	0	0	0
Ba	1*c*	½	½	0	0.0182(7)	U_{11}	0.028(1)	0	0	0
Rb	2*e*	0	½	½	0.043(2)	0.029(2)	0.044(2)	0	0	0
C	8*r*	0.181(1)	x	0.240(2)	0.025(4)	U_{11}	0.023(7)	0.007(6)	0.003(4)	U_{13}
N	8*r*	0.283(2)	x	0.237(2)	0.041(5)	U_{11}	0.044(9)	−0.008(7)	0.004(5)	U_{13}

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