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Key indicators

Single-crystal X-ray study
 T = 295 K
 Mean $\sigma(C-C)$ = 0.005 Å
 R factor = 0.031
 wR factor = 0.074
 Data-to-parameter ratio = 22.7

For details of how these key indicators were
 automatically derived from the article, see
<http://journals.iucr.org/e>.

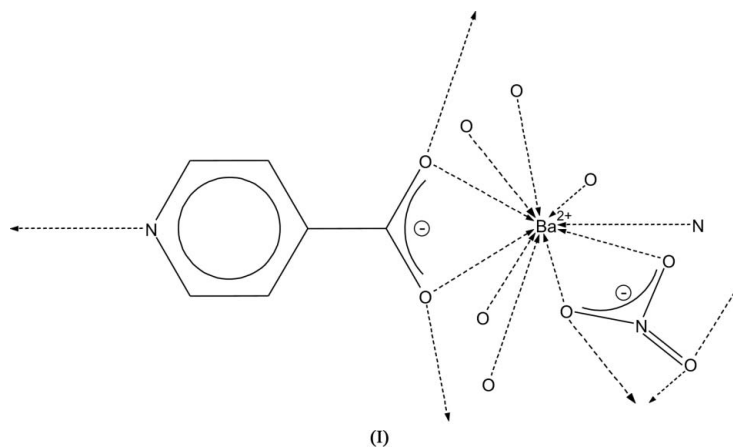
Poly[μ_4 -isonicotinato- μ_3 -nitrate-barium(II)]

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The title compound, $[Ba(C_6H_4NO_2)(NO_3)]_n$, was formed by the hydrothermal reaction of $Ba(NO_3)_2$, isonicotinamide and KOH with release of ammonia. The Ba ion is ten-coordinated by nine O atoms and one N atom. Five of these O atoms derive from one monodentate and two bidentate nitrate anions. The other O atoms derive from one bidentate and two monodentate carboxylate groups of the isonicotinate anions. The coordination is completed by an N atom of the isonicotinate anion. These units are connected to form a three-dimensional framework structure.

Comment

Recently, we have found that coordination polymers composed of linear and trigonal-planar anions show a high tendency to crystallize in non-centrosymmetric space groups (Schuy *et al.*, 2005). During our systematic search to find more examples of this, colourless crystals of the title compound, (I), were synthesized by hydrothermal methods.



The crystal structure of (I) contains barium ions coordinated by nine O atoms from three nitrate anions [Ba–O = 2.881 (3)–2.985 (4) Å] and three isonicotinate anions [Ba–O = 2.682 (3)–2.964 (3) Å] and by one N atom from a fourth isonicotinate anion [Ba–N = 2.964 (4) Å; Fig. 1]. Each nitrate anion connects three barium ions, two in a bidentate chelating mode and one in a monodentate mode. Each isonicotinate anion connects four barium ions, three in a bridging-chelating tetradentate mode and the fourth barium ion *via* the N atom. This leads to a complex three-dimensional structure of the anhydrous title compound. BaO_9 polyhedra are connected in layers parallel to the (110) plane. Adjacent layers are connected by the isonicotinate anions, forming a three-dimensional network (Fig. 2). The Ba–O and Ba–N

distances are within the ranges of literature values (e.g. Schuy *et al.*, 2005), as are the intramolecular bonds of the anions (Cai *et al.*, 2003).

Experimental

Isonicotinamide (0.25 g, 2 mmol), Ba(NO₃)₂ (0.66 g, 2.5 mmol), KOH (0.11 g, 2 mmol) and deionized water (5 ml) were placed in a Teflon-lined autoclave and heated at 423 K for 50 h. The autoclave was then cooled to room temperature at a rate of 5 K h⁻¹. A clear solution was obtained, from which barium nitrate crystallized. These crystals were filtered off. Colourless column-shaped crystals of (I) crystallized from the filtrate after 2 d. Elemental analysis calculated for C₆H₄BaN₂O₅: C 22.42, H 1.25, N 8.71%; found: C 22.01, H 0.88, N 8.69%. No yield was determined.

Crystal data

[Ba(C₆H₄NO₂)(NO₃)]
M_r = 321.45
 Triclinic, *P* $\bar{1}$
a = 5.6416 (10) Å
b = 8.0487 (15) Å
c = 9.7998 (18) Å
 α = 93.525 (15)°
 β = 106.058 (14)°
 γ = 96.254 (15)°

V = 423.12 (13) Å³
Z = 2
D_x = 2.523 Mg m⁻³
 Mo *K*α radiation
 μ = 4.69 mm⁻¹
T = 295 (2) K
 Column, colourless
 0.7 × 0.3 × 0.2 mm

Data collection

Stoe IPDS-II diffractometer
 ω and φ scans
 Absorption correction: numerical
 [X-RED32 (Stoe & Cie, 2001)
 after optimizing the crystal shape
 (X-SHAPE; Stoe & Cie, 1999)]
T_{min} = 0.367, *T_{max}* = 0.670

6949 measured reflections
 2928 independent reflections
 2604 reflections with *I* > 2σ(*I*)
R_{int} = 0.040
 θ_{max} = 32.2°

Refinement

Refinement on *F*²
R[*F*² > 2σ(*F*²)] = 0.031
wR(*F*²) = 0.074
S = 1.12
 2928 reflections
 129 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0237P)^2 + 1.55P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 (Δ/σ)_{max} = 0.001
 $\Delta\rho_{\text{max}} = 1.81 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\text{min}} = -1.34 \text{ e } \text{Å}^{-3}$
 Extinction correction: SHELXL97
 Extinction coefficient: 0.080 (3)

Table 1

Selected bond lengths (Å).

Ba1—O11 ⁱ	2.682 (3)	Ba1—O22	2.954 (4)
Ba1—O12	2.724 (3)	Ba1—O11 ⁱⁱ	2.964 (3)
Ba1—O12 ⁱⁱ	2.838 (3)	Ba1—N1 ^{iv}	2.964 (4)
Ba1—O21 ⁱⁱⁱ	2.881 (3)	Ba1—O23 ⁱ	2.978 (3)
Ba1—O23	2.938 (3)	Ba1—O21 ⁱ	2.985 (4)

Symmetry codes: (i) *x* + 1, *y*, *z*; (ii) $-x$, $-y$, $-z$; (iii) $-x$, $-y$ + 1, $-z$; (iv) *x* + 1, *y*, *z* + 1.

H atoms were placed in idealized positions and constrained to ride on their parent atoms, with a C—H distance of 0.93 Å. A common *U*_{iso}(H) value was refined for all four H atoms. The highest peak is located 1.07 Å from atom Ba1 and the deepest hole 0.74 Å from atom Ba1.

Data collection: X-Area (Stoe & Cie, 2001); cell refinement: X-Area; data reduction: X-Area; program(s) used to solve structure: SIR92 (Altomare *et al.*, 1993); program(s) used to refine

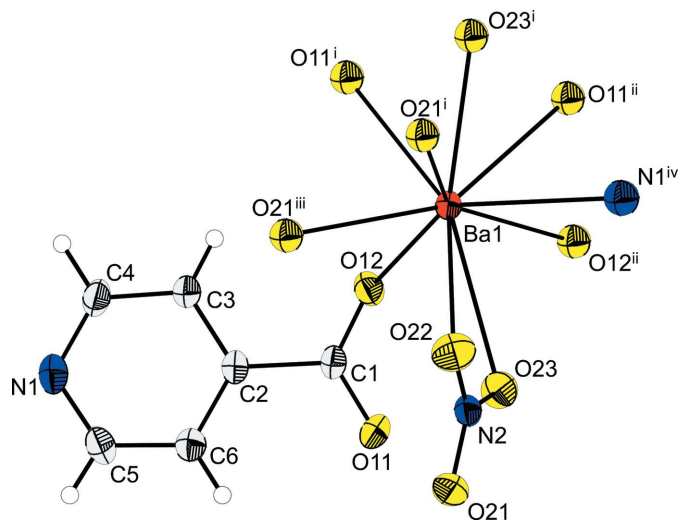


Figure 1

A view of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H-atom radii are arbitrary. [Symmetry codes: (i) *x* + 1, *y*, *z*; (ii) $-x$, $-y$, $-z$; (iii) $-x$, $-y$ + 1, $-z$; (iv) *x* + 1, *y*, *z* + 1.]

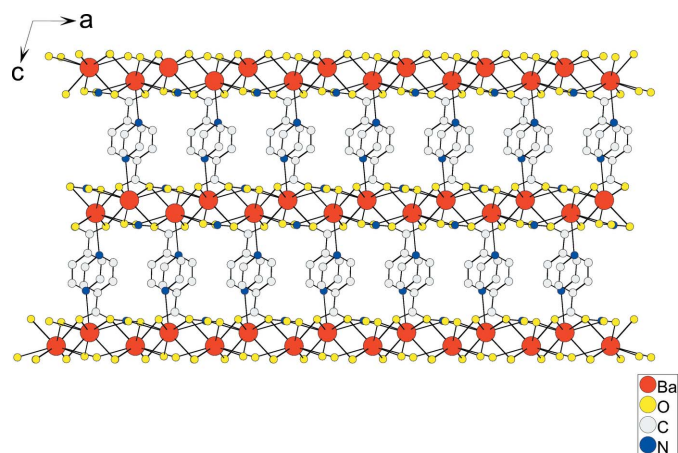


Figure 2

View of the crystal structure of (I), projected along [010]. H atoms have been omitted for clarity.

structure: SHELXL97 (Sheldrick, 1997); molecular graphics: DIAMOND (Brandenburg, 2004); software used to prepare material for publication: SHELXL97.

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