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Di-μ-iodo-1:2κ^4I:I-diiodo-2κ^2I-tris(1,10-phenanthroline)-1κ^2N,N';2κ^2N,N'-bismuth(III)sodium(I)

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The title compound, $[BiNaI_4(C_{12}H_8N_2)_3]$, contains a bimetallic neutral cluster, with the metal atoms bridged by two iodide ions. The NaN_4I_2 coordination is irregular and the BiN_2I_4 coordination is distorted octahedral. A number of π–π stacking interactions involving the phenanthroline rings help to establish the crystal packing.

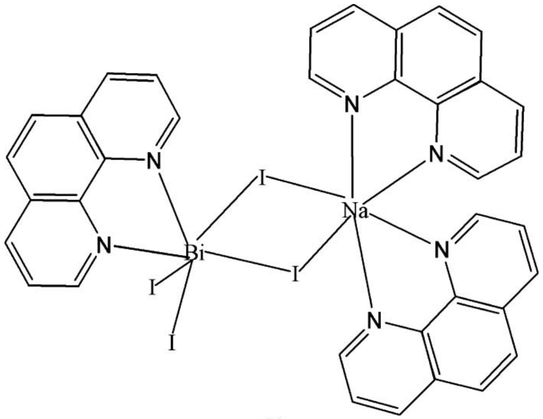
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.012 Å
R factor = 0.032
wR factor = 0.077
Data-to-parameter ratio = 15.4

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

Comment

There has recently been increasing interest in bismuth(III) coordination chemistry, particularly in the light of the role of bismuth compounds in ^{212}Bi isotope therapy in cancer research (Sun *et al.*, 1997) and the use of bismuth complexes in the treatment of peptic ulcers (Baxter *et al.*, 1992). In particular, the interaction of bismuth(III) salts with chelating nitrogen-base ligands has been actively studied (Hancock *et al.*, 1993). As a continuation of our interest in nitrogen-containing ligands, we report here the synthesis and structure of the title compound, (I), a novel bimetallic complex containing bismuth(III), Na$^+$, I$^-$ and 1,10-phenanthroline (phen).



(I)

The molecular structure of (I) and the packing are shown in Figs. 1 and 2, respectively. Selected bond lengths and angles are listed in Table 1. Compound (I) is monomeric, with the Bi and Na atoms both chelated by phen and also bonded to iodide anions. The metals are bridged by atoms I2 and I3.

Bi1 is surrounded equatorially by I1, I3, N1 and N2, and axially by I2 and I4. The sum of the equatorial-plane angles is 360.9°, which shows that these atoms are approximately coplanar. The axial I2—Bi1—I4 angle of 168.442 (19)° indicates a fair degree of distortion from a regular octahedron. The Bi—N distances for the coordinated phen are normal (Baraanyi *et al.*, 1977).

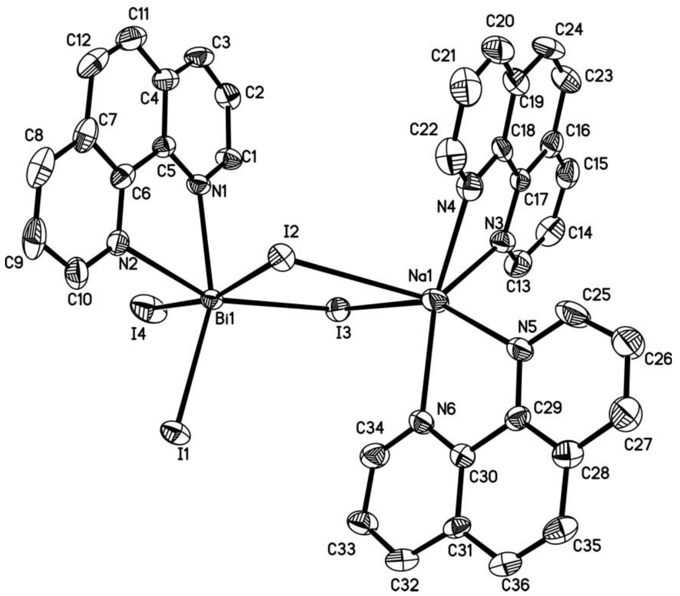


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids. H atoms have been omitted for clarity.

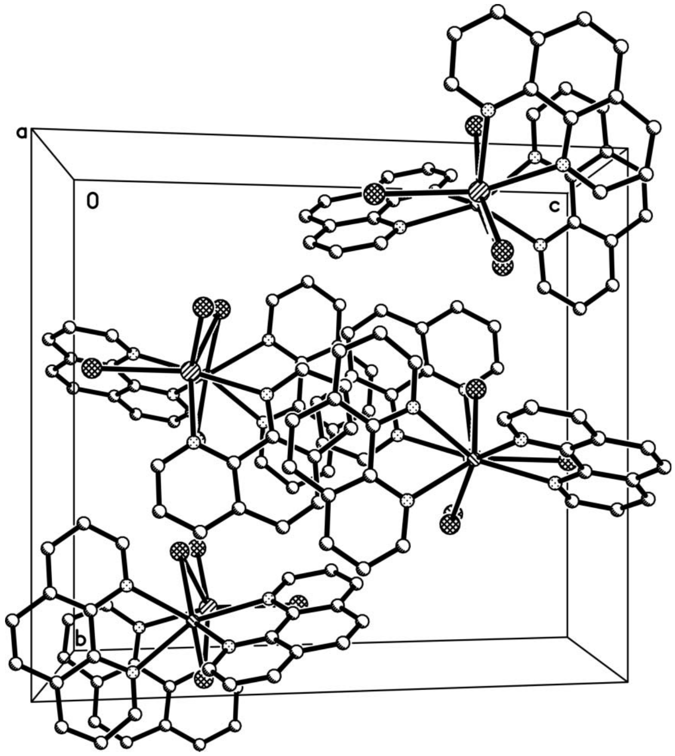


Figure 2
The packing of (I). H atoms have been omitted.

The coordination around the Na atom can not be described in terms of a regular polyhedron, but atoms N3, N4, N6 and Na1 are roughly coplanar (r.m.s. deviation = 0.1523 Å). Atom N5 deviates from this plane in one direction, and I2 and I3 in the other. The plane defined by atoms Bi1, I2 and I3 is approximately perpendicular to the above plane [dihedral angle = 91.6 (4)°].

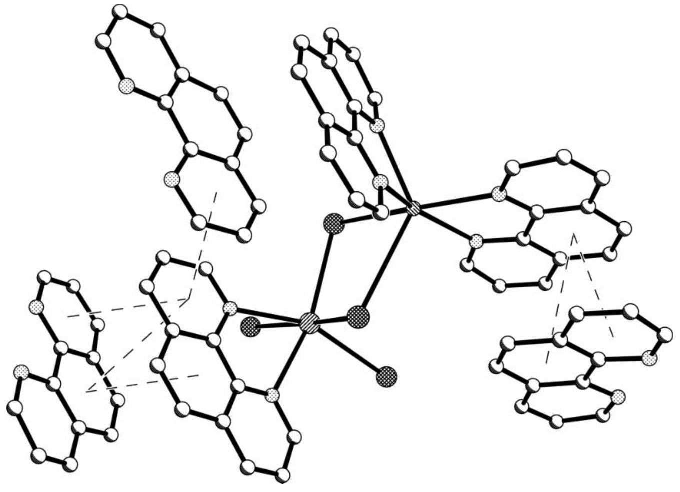


Figure 3
Detail of (I), showing π–π stacking interactions as dashed lines (H atoms have been omitted for clarity).

A number of π–π stacking interactions involving the phen rings help to consolidate the crystal packing (Fig. 3). The $Cg\cdots Cg$ (Cg = ring centroid) distances lie in the range 3.672–3.952 Å, which is normal for such interactions (Janiak, 2000).

Experimental

Phenanthroline (0.0297 g, 0.15 mmol) and NaI (0.0222 g, 0.15 mmol) were added to a stirred solution of BiI_3 (0.0884 g, 0.15 mmol) in acetonitrile (*ca* 20 ml) resulting in an orange solution. After concentration and cooling, small orange–red crystals of (I) (0.1212 g) were collected and dried *in vacuo* [yield 80%, m.p. 552 K (decomposition)]. Analysis calculated (%) for $C_{36}H_{24}BiI_4N_6Na$: C 33.77, H 1.89, N 6.56; found: C 33.53, H 1.98, N 6.78.

Crystal data

$[BiNaI_4(C_{12}H_8N_2)_3]$
M_r = 1280.18
Monoclinic, $P2_1/n$
a = 14.464 (2) Å
b = 15.579 (2) Å
c = 17.467 (3) Å
β = 104.906 (2)°
V = 3803.3 (10) Å^3
Z = 4
D_x = 2.236 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5357 reflections
θ = 2.5–26.7°
μ = 7.93 mm^{-1}
T = 298 (2) K
Block, orange–red
0.35 × 0.33 × 0.30 mm

Data collection

Siemens SMART CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min}$ = 0.078, $T_{\max}$ = 0.093
19705 measured reflections
6685 independent reflections
4689 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.043
$\theta_{\max}$ = 25.0°
$h = -17 \rightarrow 16$
$k = -17 \rightarrow 18$
$l = -11 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.077
S = 1.00
6685 reflections
433 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0325P)^2 + 0.5298P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max}$ = 1.17 e Å^{-3}
$\Delta\rho_{\min}$ = −1.14 e Å^{-3}

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Table 1
Selected geometric parameters (Å, °).

Bi1—N1	2.528 (6)	Na1—N5	2.453 (7)
Bi1—N2	2.563 (6)	Na1—N6	2.490 (6)
Bi1—I4	3.0056 (7)	Na1—N3	2.492 (7)
Bi1—I3	3.0159 (6)	Na1—N4	2.503 (7)
Bi1—I1	3.0171 (7)	Na1—I2	3.376 (3)
Bi1—I2	3.0869 (6)	Na1—I3	3.473 (3)
N5—Na1—N6	67.0 (2)	N4—Na1—I2	84.12 (16)
N5—Na1—N3	102.6 (2)	N5—Na1—I3	152.56 (19)
N6—Na1—N3	130.0 (2)	N6—Na1—I3	88.88 (16)
N5—Na1—N4	87.7 (2)	N3—Na1—I3	82.47 (16)
N6—Na1—N4	151.6 (2)	N4—Na1—I3	118.43 (17)
N3—Na1—N4	66.2 (2)	I2—Na1—I3	76.06 (6)
N5—Na1—I2	117.67 (19)	Bi1—I2—Na1	97.37 (5)
N6—Na1—I2	95.94 (17)	Bi1—I3—Na1	96.69 (5)
N3—Na1—I2	128.64 (17)		

All H atoms were positioned geometrically (C—H = 0.93 Å) and refined as riding, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(carrier). The highest peak and deepest hole in the final difference map were 1.08 and 0.90 Å, repsectively, from atom I4.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL* (Sheldrick, 1997*b*).

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