Table 3. *Bond lengths* (Å) *and angles* (°)

	LuFeCoO$_4$	LuFe$_2$O$_4$
Lu—O(2^i) (6×)	2·230 (1)	2·237 (2)
Lu—O(1) (2×)	3·247 (3)	3·240 (8)
O(2^i)—O(2^{ii}) (6×)	3·418 (1)	3·441 (1)
O(2^i)—O(2^{iii}) (6×)	2·865 (3)	2·861 (4)
O(2^i)—Lu—O(2^{ii}) (6×)	100·1 (1)	100·5 (1)
O(2^i)—Lu—O(2^{iii}) (6×)	79·9 (1)	79·5 (1)
Fe/Co—O(1^i) (3×)	1·989 (1)	2·002 (1)
Fe/Co—O(2)	1·957 (2)	1·957 (4)
Fe/Co—O(1)	2·185 (3)	2·200 (8)
O(1^i)—O(1^{ii}) (3×)	3·418 (1)	3·441 (1)
O(2)—O(1^i) (3×)	2·962 (3)	2·972 (6)
O(1)—O(1^i) (3×)	2·763 (3)	2·782 (8)
O(1^i)—Fe/Co—O(1^{ii}) (3×)	118·4 (1)	118·4 (1)
O(2)—Fe/Co—O(1^i) (3×)	97·3 (1)	97·3 (2)
O(1)—Fe/Co—O(1^i) (3×)	82·7 (1)	82·8 (2)

Symmetry code: (i) $\frac{2}{3}, \frac{1}{3}, \frac{1}{3} - z$; (ii) $-\frac{1}{3}, \frac{1}{3}, \frac{1}{3} - z$; (iii) $\frac{1}{3}, -\frac{1}{3}, -\frac{1}{3} + z$.

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Structure of
[10-(2-Aminophenyl)-5-methyl-1,5,9-triaza-9-decene-*N*,*N'*,*N''*,*N'''*]iodocopper(II) Iodide

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Abstract. [CuI(C$_{14}$H$_{24}$N$_4$)]I, $M_r = 565·73$, monoclinic, $P2_1/c$, $a = 9·277$ (1), $b = 18·200$ (4), $c = 11·749$ (1) Å, $\beta = 92·925$ (8)°, $V = 1981·1$ (5) Å^3, $Z = 4$, $D_m = 1·91$ (1), $D_x = 1·897$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 4·19$ mm^{-1}, $F(000) = 1084$, room temperature, $R = 0·0349$ for 2625 reflections. The Cu^{2+} coordination sphere has a distorted square-pyramidal geometry with four equatorial Cu—N bonds varying from 2·016 (5) to 2·064 (5) Å and an axial Cu—I bond of 2·788 (1) Å. The N atom displacements from the N$_4$ best plane vary from −0·019 (5) to 0·019 (5) Å and the angle between the Cu—I bond and the N$_4$ plane is 85·1°. The second iodide which is 5·88 Å from Cu^{2+} acts as a counter-ion in the structure. The three chelate ring conformations can be described as half chair, distorted chair and distorted chair. Both amino groups form hydrogen bonds with the iodide ions.

Experimental. Crystals were from methanol–water solution, density by flotation. Data collected for 0·5 × 0·35 × 0·45 mm crystal on a Syntex $P2_1$ diffractometer, 15 reflections $17 < 2\theta < 25°$ were used to obtain lattice parameters, 3333 unique reflections were measured up to $2\theta = 50°$ (h: ±11, k: 0–21, l: 0–13) using graphite-monochromated Mo $K\alpha$ radiation, $\lambda = 0·71069$ Å, profile analysis according to Lehmann & Larsen (1974). Two standards (054 and

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Table 1. *Fractional coordinates and equivalent isotropic thermal parameters* ($Å^2$)

$$U_{eq} = \tfrac{1}{3}\Sigma_i\Sigma_j a_i^* a_j^* \mathbf{a}_i \mathbf{a}_j.$$

	x	y	z	U_{eq}
Cu(1)	0·16899 (8)	0·07148 (4)	0·30831 (6)	0·0347 (2)
N(1)	−0·0498 (5)	0·0552 (3)	0·2785 (4)	0·037 (2)
C(1)	−0·1122 (6)	0·1199 (3)	0·2277 (5)	0·037 (2)
C(2)	−0·1902 (7)	0·1169 (4)	0·1237 (5)	0·048 (2)
C(3)	−0·2530 (8)	0·1796 (4)	0·0772 (6)	0·062 (3)
C(4)	−0·2407 (8)	0·2451 (4)	0·1331 (7)	0·061 (3)
C(5)	−0·1620 (7)	0·2492 (4)	0·2365 (7)	0·057 (3)
C(6)	−0·0956 (6)	0·1870 (3)	0·2837 (5)	0·041 (2)
C(7)	−0·0061 (7)	0·1939 (4)	0·3892 (6)	0·045 (2)
N(2)	0·1029 (6)	0·1513 (3)	0·4135 (4)	0·043 (2)
C(8)	0·1837 (8)	0·1635 (4)	0·5233 (5)	0·056 (3)
C(9)	0·3346 (8)	0·1906 (4)	0·5009 (6)	0·063 (3)
C(10)	0·4245 (7)	0·1368 (4)	0·4359 (6)	0·056 (3)
N(3)	0·3720 (6)	0·1181 (3)	0·3162 (4)	0·045 (2)
C(11)	0·4885 (7)	0·0676 (4)	0·2769 (6)	0·050 (3)
C(12)	0·4609 (7)	0·0346 (4)	0·1582 (6)	0·059 (3)
C(13)	0·3440 (7)	−0·0201 (4)	0·1496 (6)	0·054 (3)
N(4)	0·1991 (5)	0·0153 (3)	0·1636 (4)	0·046 (2)
C(14)	0·3655 (8)	0·1845 (4)	0·2423 (6)	0·063 (3)
I(1)	0·21383 (5)	−0·04910 (3)	0·45209 (4)	0·049 (1)
I(2)	0·15178 (6)	0·39035 (3)	0·38803 (4)	0·063 (2)

Table 2. *Selected bond lengths* ($Å$) *and angles* (°), *with e.s.d.'s*

Cu(1)—N(1)	2·064 (5)	N(2)—C(8)	1·476 (7)
Cu(1)—N(2)	2·023 (5)	C(8)—C(9)	1·520 (10)
Cu(1)—N(3)	2·064 (5)	C(9)—C(10)	1·518 (9)
Cu(1)—N(4)	2·016 (5)	C(10)—N(3)	1·503 (8)
Cu(1)—I(1)	2.788 (1)	N(3)—C(11)	1·509 (8)
N(1)—C(1)	1·429 (7)	C(11)—C(12)	1·528 (9)
C(6)—C(7)	1·462 (8)	C(12)—C(13)	1·471 (9)
C(7)—N(2)	1·294 (7)	C(13)—N(4)	1·507 (8)
		N(4)—C(14)	1·488 (8)

N(2)—Cu(1)—N(1)	83·2 (2)	C(13)—N(4)—Cu(1)	118·1 (4)
N(3)—Cu(1)—N(1)	162·6 (2)	C(2)—C(1)—N(1)	121·0 (6)
N(3)—Cu(1)—N(2)	88·9 (2)	C(6)—C(1)—N(1)	119·5 (5)
N(4)—Cu(1)—N(1)	87·8 (2)	N(2)—C(7)—C(6)	122·6 (6)
N(4)—Cu(1)—N(2)	159·9 (2)	C(7)—C(6)—C(5)	119·3 (6)
N(4)—Cu(1)—N(3)	94·6 (2)	C(8)—N(2)—C(7)	117·3 (6)
I(1)—Cu(1)—N(1)	96·0 (1)	C(9)—C(8)—N(2)	109·2 (6)
I(1)—Cu(1)—N(2)	103·6 (1)	C(10)—C(9)—C(8)	114·4 (6)
I(1)—Cu(1)—N(3)	100·9 (1)	N(3)—C(10)—C(9)	117·2 (6)
I(1)—Cu(1)—N(4)	95·1 (2)	C(11)—N(3)—C(10)	102·8 (5)
C(1)—N(1)—Cu(1)	109·0 (3)	C(14)—N(3)—C(10)	111·3 (5)
C(7)—N(2)—Cu(1)	123·6 (4)	C(14)—N(3)—C(11)	108·9 (5)
C(8)—N(2)—Cu(1)	119·1 (4)	C(12)—C(11)—N(3)	115·5 (5)
C(10)—N(3)—Cu(1)	112·7 (4)	C(13)—C(12)—C(11)	114·6 (6)
C(11)—N(3)—Cu(1)	113·7 (4)	N(4)—C(13)—C(12)	111·2 (6)
C(14)—N(3)—Cu(1)	107·3 (4)		

214) measured every 100 reflections showed no significant intensity variation, no absorption correction. Structure solved by Patterson method (*SHELXS*86; Sheldrick, 1986). H-atom positions were calculated from geometry and not refined. Non-H-atom parameters and extinction refined in full-matrix least squares, $\Sigma w(\Delta F)^2$ minimized using *SHELX*76 (Sheldrick, 1976), 2625 observed reflections $I > 3\sigma(I)$, $w = \sigma^{-2}(F)$, extinction $x = 0.00077$ (3) in F_c' = $F_c(1 - 0.0001xF_c^2/\sin\theta)$, final $R = 0.0349$, $wR = 0.0345$, $S = 1.364$, $|\Delta/\sigma|_{max} = 0.155$ in final refinement, $\Delta\rho_{max} = 0.48$, $\Delta\rho_{min} = -0.47$ e $Å^{-3}$, scat-

tering factors from *International Tables for X-ray Crystallography* (1974). Other programs: *ORTEP*II (Johnson, 1976), *PLUTO* (Motherwell & Clegg, 1978) and local programs (Jaskólski, 1982), RIAD-32 computer. Atomic parameters and bond lengths and angles are given in Tables 1 and 2 respectively.* The atom-numbering scheme and packing diagram are shown in Figs. 1 and 2.

* Lists of structure factors, anisotropic thermal parameters, H-atom parameters, details of hydrogen bonds and best planes, and fuller lists of bond lengths and angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52781 (18 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.
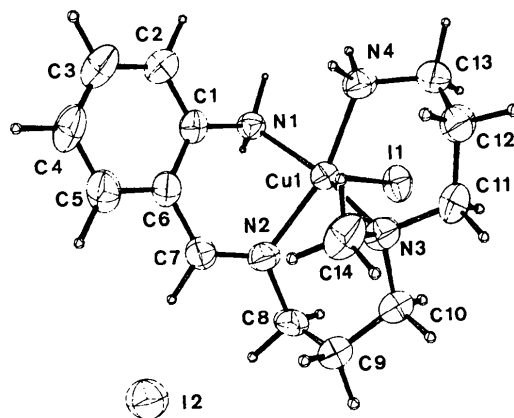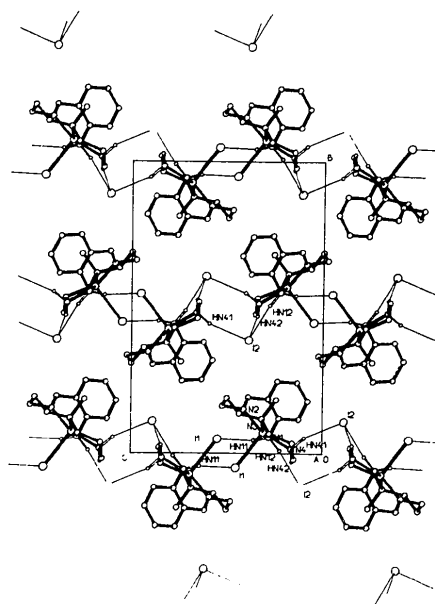

Fig. 1. A perspective view of the chemical unit with atomic numbering scheme.

Fig. 2. Projection of the structure down the *a* axis. Hydrogen bonds are shown as thin lines.

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A Redetermination of the Structures of Bis(salicylideneaminato)nickel(II) and Monoclinic and Orthorhombic Forms of Bis(*N*-methylsalicylideneaminato)nickel(II)

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Abstract. (I): Bis(salicylideneaminato)nickel(II), [Ni(C₇H₆NO)₂], $M_r = 298.97$, monoclinic, $P2_1/c$, $a = 12.959 (3)$, $b = 5.848 (1)$, $c = 8.147 (1)$ Å, $\beta = 95.98 (1)°$, $V = 614.10$ Å³, $Z = 2$, $D_x = 1.617$ Mg m⁻³, λ(Mo $K\alpha$) = 0.7107 Å, $\mu = 1.580$ mm⁻¹, $F(000) = 308$, room temperature, final $R = 0.028$ for 1083 reflections. (II): Bis(*N*-methylsalicylideneaminato)nickel(II), [Ni(C₈H₈NO)₂], $M_r = 327.03$, monoclinic, $P2_1/c$, $a = 12.119 (6)$, $b = 7.090 (2)$, $c = 8.348 (1)$ Å, $\beta = 92.75 (6)°$, $V = 716.47$ Å³, $Z = 2$, $D_x = 1.516$ Mg m⁻³, λ(Mo $K\alpha$) = 0.7107 Å, $\mu = 1.289$ mm⁻¹, $F(000) = 340$, room temperature, final $R = 0.029$ for 1195 reflections. (III): Bis(*N*-methylsalicylideneaminato)nickel(II), [Ni(C₈H₈NO)₂], $M_r = 327.03$, orthorhombic, *Ibam*, $a = 9.189 (2)$, $b = 24.331 (5)$, $c = 6.600 (2)$ Å, $V = 1475.61$ Å³, $Z = 4$, $D_x = 1.472$ Mg m⁻³, λ(Mo $K\alpha$) = 0.7107 Å, $\mu = 1.252$ mm⁻¹, $F(000) = 680$, room temperature, final $R = 0.030$ for 670 reflections. The redeterminations of the title structures based on diffractometer data have yielded more precise structural parameters than the previous photographic results [(I): Stewart & Lingafelter (1959). *Acta Cryst.* **12**, 842–845; (II): Frasson, Panattoni & Sacconi (1959). *J. Phys. Chem.* **63**, 1908–1911; (III): Fox & Lingafelter (1967). *Acta Cryst.* **22**, 943–944] thus extending the data to give a better understanding of the reasons for differences in the molecular conformations of these complexes. All three complexes have molecular centres of symmetry and Ni atoms in a square-planar coordination. Molecule (I) is almost completely planar with the molecular step between planes through the two benzene rings of 0.098 Å, molecule (II) is distinctively 'stepped' (step height of 0.782 Å),

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