and the type of the acceptor ligand. The C=C bond distance of the coordinated alkenes also provides no explanation for the difference. The average C=C bond distance of the coordinated butene ligand in the two independent molecules is 1·45 (4) Å and this is not significantly different from that of the coordinated ethylene [1·449 (6) Å] or that of the coordinated styrene [1·46 (2) Å]. The C=C bond distance in the *trans*-stilbene complex is, however, 1·38 (2) Å, and since this complex has the longest Zr—P distance of the series this suggests an inverse relationship between the C=C and Zr—P bond distances in these compounds. Although the trend can be observed in the other complexes the differences are not significant. In all cases the C—C bond of the coordinated alkyne or alkene is coplanar with the Zr and the P atoms. The preference for the single-faced π-acceptor ligands to adopt this conformation has been discussed by Lauher & Hoffmann (1976).

There are no important short intermolecular contacts between non-H atoms. Intermolecular distances less than 3·7 Å are given in Table 2(*d*).

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Structure of Cobalt Diquinoline Diisothiocyanate

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Abstract. Diisothiocyanatobis(quinoline)cobalt, $[\mathrm{Co(NCS)_2(C_9H_7N)_2}]$, $M_r = 433{\cdot}42$, monoclinic, $P2_1/c$, $a = 14{\cdot}834\ (2)$, $b = 8{\cdot}435\ (1)$, $c = 15{\cdot}392\ (2)$ Å, $\beta = 92{\cdot}03\ (1)^\circ$, $V = 1924\ (1)$ Å^3, $Z = 4$, $F(000) = 884$, $D_m = 1{\cdot}49\ (1)$ Mg m^{-3}, $D_x = 1{\cdot}496$ Mg m^{-3}, $\lambda(\mathrm{Mo}\ K\alpha) = 0{\cdot}71069$ Å, $\mu = 1{\cdot}109$ mm^{-1}, $T = 293\ (1)$ K. Patterson and Fourier methods were used for solving the structure. The final values for R and wR were 0·047 and 0·035 respectively for 2356 observed reflections. The Co atom is four-coordinated by two N atoms from the isothiocyanate groups and two N atoms from the quinoline ligands.

Introduction. The determination of the unit-cell dimensions and crystal structure of the title compound is part of our research project concerning the X-ray diffraction and spectroscopic studies of the halogen and pseudohalogen quinoline complexes of divalent metals from the transition series (Mirčeva & Golič, 1987; Golič & Mirčeva, 1988). The structures of many pyridine complexes of that type are known but only a few structures of quinoline analogues have been determined.

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Table 1. *Final fractional coordinates* (× 10^4) *and equivalent isotropic temperature factors* U_{eq} ($Å^2 \times 10^3$)

	x	y	z	U_{eq}
Co	2518·3 (2)	4778 (1)	5862·0 (2)	49·1 (2)
N(10)	2599 (2)	7065 (4)	5812 (2)	65 (2)
C(10)	2671 (2)	8403 (4)	5976 (2)	51 (2)
S(1)	2790 (1)	10242 (1)	6212 (1)	76 (1)
N(20)	2333 (2)	4311 (4)	7077 (2)	70 (2)
C(20)	2137 (2)	4514 (3)	7796 (2)	51 (2)
S(2)	1888 (1)	4799 (1)	8787 (1)	66 (1)
N(1)	1397 (1)	3846 (3)	5244 (2)	47 (1)
C(1)	926 (2)	2812 (4)	5685 (2)	55 (2)
C(2)	134 (2)	2108 (4)	5367 (3)	61 (2)
C(3)	−184 (2)	2495 (4)	4558 (3)	64 (2)
C(4)	297 (2)	3592 (3)	4047 (2)	51 (2)
C(5)	14 (2)	4039 (4)	3198 (2)	66 (2)
C(6)	501 (3)	5085 (4)	2742 (2)	71 (2)
C(7)	1298 (2)	5739 (4)	3109 (2)	63 (2)
C(8)	1589 (2)	5353 (4)	3928 (2)	53 (2)
C(9)	1093 (2)	4243 (3)	4419 (2)	45 (2)
N(2)	3622 (1)	3727 (3)	5375 (2)	46 (1)
C(11)	3536 (2)	3017 (4)	4610 (2)	57 (2)
C(12)	4223 (2)	2130 (4)	4249 (2)	66 (2)
C(13)	5009 (2)	1949 (4)	4699 (3)	68 (2)
C(14)	5137 (2)	2667 (4)	5520 (2)	58 (2)
C(15)	5936 (2)	2501 (5)	6035 (3)	77 (2)
C(16)	6030 (2)	3249 (6)	6815 (3)	88 (3)
C(17)	5337 (2)	4218 (6)	7119 (2)	82 (2)
C(18)	4541 (2)	4380 (4)	6642 (2)	65 (2)
C(19)	4426 (2)	3589 (3)	5841 (2)	49 (2)

Experimental. Well shaped crystals obtained by recrystallization, from ethanol, of compound prepared by reaction between cobalt nitrate, quinoline and potassium thiocyanate in appropriate molar ratio. D_m by flotation. Crystal dimensions 0·22 × 0·33 × 0·53 mm. Cell dimensions determined by least-squares refinement of θ angles of 79 strong reflections in the range $8 < \theta < 14$°; Enraf–Nonius CAD-4 diffractometer, graphite-monochromatized Mo $K\alpha$ radiation; ω–2θ scan mode, 2θ scan width $(0·7 + 0·3\tan\theta)$°, aperture $(2·4 + 0·9\tan\theta)$ mm, maximum scan time 40 s; $2\theta_{max}$50°; $(\sin\theta)/\lambda \leq 0·595$ Å^{-1}; sphere with index range $-17 \leq h \leq 17$, $-10 \leq k \leq 10$ and $-18 \leq l \leq 18$ measured; three standard reflections 240, 4$\bar{1}$3, 150 checked every 168 reflections measured, orientation controlled every 336 reflections using three reflections; intensity decreased 0·5% during the data collection, 13702 reflections collected, 3386 independent reflections after merging of data produced with $R_{int} = 0·06$ from measuring of equivalent reflections, 2356 observed $[I > 2·5\sigma(I)]$, $\sigma(I)$ based on counting statistics. Data corrected for Lorentz and polarization effects, no absorption correction. Position of the Co atom determined from Patterson map, other non-H atoms found from Fourier synthesis, H atoms located at calculated positions, not refined; anisotropic full-matrix least squares for all non-H atoms, H atoms included in the last cycle of the refinement with isotropic thermal parameters of attached atoms; the empirical

Table 2. *Bond distances* (Å) *and angles* (°)

Co—N(10)	1·934 (3)	C(3)—C(4)	1·423 (5)
Co—N(20)	1·940 (3)	C(4)—C(5)	1·410 (5)
Co—N(1)	2·043 (2)	C(4)—C(9)	1·405 (4)
Co—N(2)	2·028 (2)	C(5)—C(6)	1·353 (5)
N(10)—C(10)	1·161 (5)	N(2)—C(11)	1·324 (4)
N(20)—C(20)	1·167 (5)	C(11)—C(12)	1·396 (5)
C(10)—S(1)	1·601 (4)	C(12)—C(13)	1·344 (5)
C(20)—S(2)	1·601 (4)	C(13)—C(14)	1·408 (5)
C(6)—C(7)	1·405 (5)	C(14)—C(15)	1·409 (5)
C(7)—C(8)	1·358 (4)	C(14)—C(19)	1·414 (4)
C(8)—C(9)	1·425 (5)	C(15)—C(16)	1·358 (6)
C(9)—N(1)	1·375 (4)	C(16)—C(17)	1·407 (6)
N(1)—C(1)	1·320 (4)	C(17)—C(18)	1·374 (5)
C(1)—C(2)	1·390 (5)	C(18)—C(19)	1·408 (4)
C(2)—C(3)	1·356 (6)	C(19)—N(2)	1·375 (3)
N(10)—Co—N(20)	104·6 (1)	C(6)—C(7)—C(8)	121·0 (3)
N(10)—Co—N(1)	114·6 (1)	C(7)—C(8)—C(9)	119·7 (3)
N(10)—Co—N(2)	111·7 (1)	C(8)—C(9)—N(1)	119·4 (2)
N(20)—Co—N(1)	103·3 (1)	C(8)—C(9)—C(4)	118·9 (3)
N(1)—Co—N(2)	108·3 (1)	C(4)—C(9)—N(1)	121·7 (2)
N(20)—Co—N(2)	114·3 (1)	C(11)—N(2)—C(19)	118·7 (2)
N(10)—C(10)—S(1)	178·8 (3)	N(2)—C(11)—C(12)	123·2 (3)
N(20)—C(20)—S(2)	178·8 (3)	C(11)—C(12)—C(13)	119·2 (3)
Co—N(10)—C(10)	165·2 (3)	C(12)—C(13)—C(14)	120·1 (3)
Co—N(20)—C(20)	158·9 (3)	C(13)—C(14)—C(15)	123·1 (3)
C(1)—N(1)—C(9)	118·2 (2)	C(13)—C(14)—C(19)	118·1 (3)
N(1)—C(1)—C(2)	123·9 (3)	C(15)—C(14)—C(19)	118·7 (3)
C(1)—C(2)—C(3)	118·8 (3)	C(14)—C(15)—C(16)	120·6 (3)
C(2)—C(3)—C(4)	120·0 (3)	C(15)—C(16)—C(17)	120·8 (3)
C(3)—C(4)—C(5)	123·2 (3)	C(16)—C(17)—C(18)	120·2 (3)
C(3)—C(4)—C(9)	117·3 (3)	C(17)—C(18)—C(19)	119·7 (3)
C(5)—C(4)—C(9)	119·4 (3)	C(18)—C(19)—N(2)	119·5 (3)
C(4)—C(5)—C(6)	120·6 (3)	C(18)—C(19)—C(14)	119·9 (3)
C(5)—C(6)—C(7)	120·3 (3)	C(14)—C(19)—N(2)	120·6 (3)

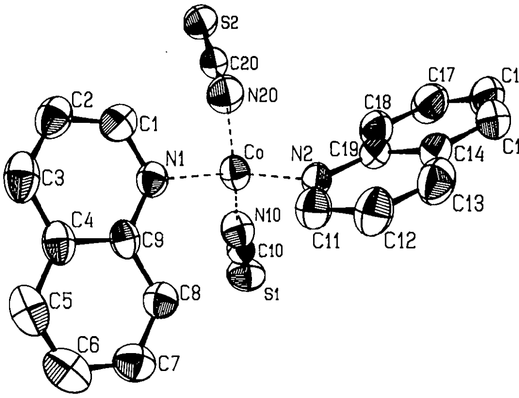

Fig. 1. *ORTEP* (Johnson, 1965) view of the molecule. The atoms are represented by thermal ellipsoids at the 50% probability level.

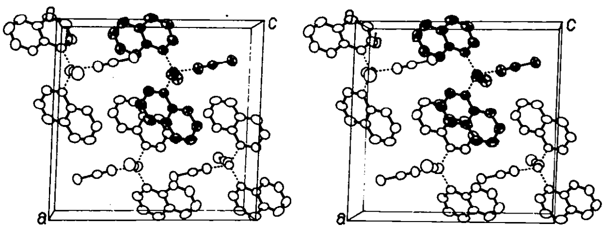

Fig. 2. Stereoview of the molecular packing.

weighting function $w = 6 \times (W_f \times W_s)$ where $W_f(|F_o| < 12{\cdot}0) = (|F_o|/12{\cdot}0)^{6{\cdot}0}$, $W_f(|F_o| > 24{\cdot}0) = (24{\cdot}0/|F_o|^{2{\cdot}0}$, $W_f(12{\cdot}0 < |F_o| < 24{\cdot}0) = 1{\cdot}0$ and $W_s(\sin\theta < 0{\cdot}26) = (\sin\theta/0{\cdot}26)^{3{\cdot}0}$, $W_s(\sin\theta > 0{\cdot}32) = (0{\cdot}32/\sin\theta)^{7{\cdot}0}$, $W_s(0{\cdot}26 < \sin\theta < 0{\cdot}32) = 1{\cdot}0$ was applied to keep $\sum w(\Delta F)^2$ uniform over the ranges of $|F_o|$ and $(\sin\theta)/\lambda$; in the final refinement cycle there were 2522 contributing reflections including observed reflections and those less-thans for which F_c was greater than F_o, 244 variables, $S = 1{\cdot}13$, average shift/e.s.d. 0·01, max. shift/e.s.d. 0·14 at U_{11} of C(12) atom, max. and min. heights in final difference Fourier map were 0·4 and $-1{\cdot}2$ e Å^{-3}; $R = 0{\cdot}047$, $wR = 0{\cdot}035$; atomic scattering and dispersion factors for the neutral atoms Co, S, N and C from Cromer & Mann (1968) and Cromer & Liberman (1970), and for H atoms from Stewart, Davidson & Simpson (1965); DEC-10 computer at RCU Ljubljana; *XRAY76* system of crystallographic programs (Stewart, Machin, Dickinson, Ammon, Heck & Flack, 1976).

Discussion. The final positional parameters with U_{eq} (Hamilton, 1959) for non-H atoms are listed in Table 1.* A view of the molecule of the cobalt complex is given in Fig. 1 (the atomic labelling scheme is also shown). Fig. 2 illustrates the packing of the molecules in the unit cell. Interatomic distances and angles are given in Table 2.

The structure consists of $\mathrm{Co(C_9H_7N)_2(NCS)_2}$ molecules between which are only van der Waals interactions (no intermolecular contacts of less than 3·4 Å for non-H atoms). The Co atom is tetrahedrally coordinated by N atoms (two denoted $\mathrm{N_Q}$ – from the quinoline ligands and two labelled $\mathrm{N_{CS}}$ – from the isothiocyanate groups). The Co—$\mathrm{N_Q}$ distances 2·043 (2) and 2·028 (2) Å compare well with the corresponding values found in the previously determined tetrahedral structure of $\mathrm{Co(C_9H_7N)_2Cl_2}$ (Golič & Mirčeva, 1988). The Co—$\mathrm{N_{CS}}$ distances 1·934 (3) and 1·940 (3) Å are close to those found in the tetrahedrally coordinated complex $\mathrm{K_2Co(NCS)_4.3H_2O}$ (Drew & Othman, 1975), and are, as expected, slightly shorter than those observed in octahedrally coordinated compounds (Cano & Garcia-Blanco, 1976; Hartl & Steidl, 1980; Hartl & Brüdgam, 1980). The angles in the coordination tetrahedron range from 103·3 (1) to 114·6 (1)°.

On the basis of a literature survey of structures of compounds containing isothiocyanate ligands, Knox & Eriks (1968) pointed out that the *M*—N—C(S) angles [*M* metal, C(S) carbon atom bonded to sulfur] vary in the range of 150 to 180°. Values for the Co—N—C(S) angles in $\mathrm{Co(C_9H_7N)_2(NCS)_2}$ are within that range [165·2 (3) and 158·9 (3)°].

The NCS groups are almost linear [both N—C—S angles being 178·8 (3)°] and consistent with values found in a great number of complexes (Ferrari, Braibanti, Bigliardi & Lanfredi, 1965; Mokuolu & Speakman, 1975).

The interatomic distances in NCS groups of our cobalt complex also agree with those in the above mentioned sources.

The bond lengths and angles in the quinoline ligands are close to the corresponding values found in the two previously determined structures of $\mathrm{Co(C_9H_7N)_2Cl_2}$ (Golič & Mirčeva, 1988) and $\mathrm{Zn(C_9H_7N)_2Cl_2}$ (Mirčeva & Golič, 1987), as well as to the values in many other complexes containing quinoline ligands (Horrocks, Templeton & Zalkin, 1968; Hursthouse & Malik, 1978).

The maximum deviations of the atoms from the corresponding mean planes of the ligands of 0·008 and 0·033 Å indicate that quinoline can be considered as being planar. The interplanar angle of the quinoline ligands is 76·7 (5)°.

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* Lists of structure factors, anisotropic thermal parameters, calculated H-atom coordinates and least-squares-planes equations have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52503 (17 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.