scattering factors for neutral atoms and real and imaginary dispersion terms from *International Tables for X-ray Crystallography* (1974). Programs: *PARST* (Nardelli, 1983), *SHELXTL-Plus* (Sheldrick, 1987), *PCK*83 (Williams, 1984), *PLATON* (Spek, 1982), *MISSYM* (Le Page, 1987), *SCHAKAL* (Keller, 1986). The molecule, which is on a center of symmetry, and the numbering are shown in Fig. 1 and a stereoscopic view is in Fig. 2. Positional parameters and U_{eq} values for the non-H atoms are given in Table 1.* Bond lengths, bond angles, torsion angles, least-squares planes, dihedral angles and hydrogen-bond geometry are given in Table 2.

Related literature. The coordination chemistry of amino acids and Pt electrophiles has been the subject of numerous studies (Volshtein, 1975; Beck, 1988). The simplest amino acid, glycine (glyH), has been used particularly often. Of the various binding modes of deprotonated glycine (gly), both chelate formation (N,O) (Freeman & Golomb, 1969; Iakovidis, Hadjiliadis, Schöllhorn, Thewalt & Trötscher, 1989) and binding *via* the terminal amino group (Baidina, Podberezskaya, Borisov, Shestakova, Kuklina & Mal'chikov, 1979; Pesch, Preut & Lippert, 1990) have been established by X-ray analysis. In acidic medium, neutral glycine can bind both through oxygen and through nitrogen (Appleton, Hall & Ralph, 1985; Schwarz, Lippert, Iakovidis & Hadjiliadis, 1990).

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* Lists of structure factors, anisotropic thermal parameters, H-atom parameters, least-squares-planes data and complete hydrogen-bond geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52576 (10 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of Potassium Isocyanato[*N*-salicylidene-DL-alaninato(2 −)]cuprate(II)

BY VIKTOR KETTMANN

Department of Analytical Chemistry, Faculty of Pharmacy, University of Komensky, Odbojárov 10, 83232 *Bratislava, Czechoslovakia*

AND JURAJ KRÄTSMÁR-ŠMOGROVIČ AND OL'GA ŠVAJLENOVÁ

Department of Organic and Inorganic Chemistry, Faculty of Pharmacy, University of Komensky, Odbojárov 10, 83232 *Bratislava, Czechoslovakia*

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Abstract. K[Cu(NCO)($C_{10}H_9NO_3$)], $M_r = 335{\cdot}84$, monoclinic, $P2_1/c$, $a = 7{\cdot}925$ (3), $b = 17{\cdot}144$ (8), $c = 9{\cdot}231$ (5) Å, $\beta = 104{\cdot}53$ (5)°, $V = 1214{\cdot}0$ (8) Å^3, $Z = 4$, $D_m = 1{\cdot}84$ (1), $D_x = 1{\cdot}837$ Mg m^{-3}, λ(Cu $K\alpha$) = 1·54178 Å, $\mu = 4{\cdot}76$ mm^{-1}, $F(000) = 676$, $T = 293$ K, final $R = 0{\cdot}045$ for 1397 observed reflections. The Cu coordination can be described as square planar (with Cu bonded to the heteroatoms of the

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Table 1. *Final atomic coordinates* ($\times 10^4$) *with e.s.d.'s in parentheses and equivalent isotropic thermal parameters* ($Å^2$)

$B_{eq} = (4/3)\sum_i\sum_j \beta_{ij}\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	B_{eq}
Cu(1)	1862 (0)	4639 (0)	4430 (0)	2·96
K(1)	4099 (1)	4563 (0)	1644 (1)	2·61
O(1)	878 (2)	4430 (1)	2371 (2)	2·74
O(2)	2837 (3)	4802 (1)	6561 (2)	2·61
O(3)	3049 (3)	4294 (1)	8790 (2)	3·31
O(4)	5360 (3)	6285 (1)	5523 (2)	3·26
N(1)	602 (3)	3813 (1)	5105 (2)	2·13
N(2)	3128 (3)	5545 (1)	3930 (3)	2·54
C(1)	−502 (3)	4001 (2)	1820 (3)	2·07
C(2)	−1319 (3)	3521 (2)	2692 (3)	2·03
C(3)	−2813 (4)	3091 (2)	1999 (3)	2·43
C(4)	−3501 (4)	3129 (2)	475 (3)	2·72
C(5)	−2684 (4)	3583 (2)	−370 (3)	2·86
C(6)	−1215 (4)	3998 (2)	263 (3)	2·63
C(7)	−678 (3)	3438 (2)	4289 (3)	2·30
C(8)	1205 (4)	3648 (2)	6707 (3)	2·90
C(9)	2096 (5)	2867 (2)	7012 (4)	4·61
C(10)	2443 (4)	4295 (2)	7435 (3)	2·54
C(11)	4217 (3)	5909 (2)	4734 (3)	2·21

Table 2. *Bond lengths* (Å) *and angles* (°) *with e.s.d.'s in parentheses*

Cu—O(1)	1·899 (2)	C(6)—C(1)	1·406 (4)
Cu—O(2)	1·945 (2)	C(2)—C(7)	1·441 (4)
Cu—N(1)	1·925 (2)	C(7)—N(1)	1·275 (3)
Cu—N(2)	1·965 (2)	N(1)—C(8)	1·463 (3)
O(1)—C(1)	1·310 (3)	C(8)—C(9)	1·506 (5)
C(1)—C(2)	1·416 (4)	C(8)—C(10)	1·521 (4)
C(2)—C(3)	1·405 (4)	C(10)—O(2)	1·277 (3)
C(3)—C(4)	1·377 (4)	C(10)—O(3)	1·222 (3)
C(4)—C(5)	1·374 (4)	N(2)—C(11)	1·167 (4)
C(5)—C(6)	1·365 (4)	C(11)—O(4)	1·199 (4)

O(1)—Cu—N(1)	93·9 (1)	C(4)—C(5)—C(6)	121·7 (3)
O(1)—Cu—N(2)	91·2 (1)	C(5)—C(6)—C(1)	121·3 (3)
O(1)—Cu—O(2)	177·1 (1)	C(2)—C(7)—N(1)	125·3 (3)
N(1)—Cu—O(2)	83·4 (1)	Cu—N(1)—C(7)	125·5 (2)
N(1)—Cu—N(2)	173·9 (1)	Cu—N(1)—C(8)	113·9 (2)
O(2)—Cu—N(2)	91·6 (1)	C(7)—N(1)—C(8)	120·6 (2)
Cu—O(1)—C(1)	126·1 (2)	N(1)—C(8)—C(10)	108·4 (2)
O(1)—C(1)—C(2)	124·1 (2)	N(1)—C(8)—C(9)	112·4 (3)
O(1)—C(1)—C(6)	118·8 (2)	C(9)—C(8)—C(10)	110·2 (3)
C(2)—C(1)—C(6)	117·1 (2)	C(8)—C(10)—O(2)	116·7 (3)
C(1)—C(2)—C(7)	123·0 (2)	C(8)—C(10)—O(3)	119·7 (3)
C(1)—C(2)—C(3)	119·9 (2)	O(2)—C(10)—O(3)	123·5 (3)
C(3)—C(2)—C(7)	117·0 (2)	Cu—O(2)—C(10)	116·3 (2)
C(2)—C(3)—C(4)	120·9 (3)	Cu—N(2)—C(11)	127·8 (2)
C(3)—C(4)—C(5)	119·0 (3)	N(21)—C(11)—O(4)	178·0 (3)

tridentate Schiff-base ligand and to the N atom of the NCO group) but with the O4 atom of the adjacent complex anion involved in an additional semi-coordinate bond at a long distance [2·703 (2) Å] in the axial direction. The complex anions are held together *via* six-coordinate K^+ ions.

Experimental. Crystal size 0·2 × 0·2 × 0·4 mm; D_m by flotation in bromoform/cyclohexane; systematic absences $0k0$ for k odd and $h0l$ for l odd; Syntex $P2_1$ diffractometer, graphite-monochromatized Cu $K\alpha$ radiation; cell dimensions from 15 reflections, $15 < \theta < 35°$; intensity data ($h = 0$ to 8, $k = 0$ to 18, $l = -9$ to 9) by $\theta/2\theta$ scan, $2\theta \leq 110°$; two standards measured every 96 reflections, no significant systematic variations; 1740 reflections measured, 1527 unique, 1397 with $I \geq 2\sigma(I)$ considered observed and included in the refinement; Lp correction but none for absorption or extinction; structure solved by the heavy-atom method and refined by block-diagonal least squares. $\Delta\rho$ map showed positions of all H atoms, refinement continued on all positional parameters and anisotropic thermal parameters for non-H atoms (isotropic thermal parameters for H atoms were set at 0·5 higher than B_{eq} of the bonded atom and not refined); in final cycle $R = 0·045$, $wR = 0·074$ for observed reflections only, $S = 1·7$; max. shift/e.s.d. 0·02; function minimized $\sum w(\Delta F)^2$, where $w = 1$ if $|F_o| < 20$ and $w = 20/|F_o|$ if $|F_o| \geq 20$; max. and min. heights in final synthesis 0·37 and 0·53 e $Å^{-3}$; scattering factors for uncharged atoms from *International Tables for X-ray Crystallography* (1974); all calculations performed with local version of the *NRC* system (Ahmed, Hall, Pippy & Huber, 1973). Final atomic coordinates of non-H atoms and equivalent isotropic B's are listed in Table 1,* bond distances and angles in Table 2. A perspective drawing of the complex anion and numbering of the atoms is shown in Fig. 1.

Related literature. Ueki, Ashida, Sasada & Kakudo (1969); Pavelčík, Krätsmár-Šmogrović, Švajlenová &

* Lists of structure factors, anisotropic thermal parameters, H-atom parameters and least-squares planes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52561 (11 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

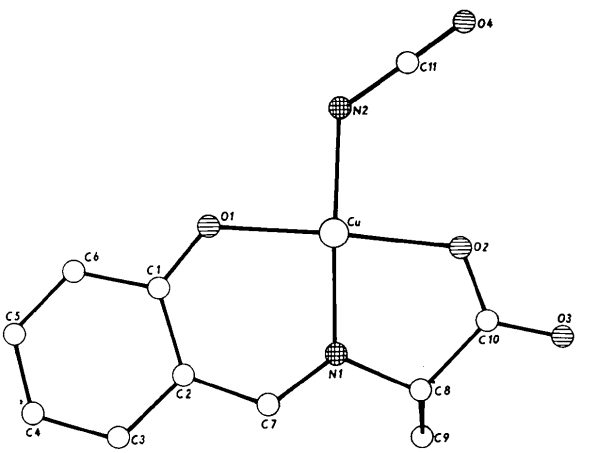

Fig. 1. A perspective view of the complex anion, showing the atomic numbering. H atoms are not drawn for clarity.

Majer (1981); Werner, Valent, Adelsköld & Švajlenová (1983).

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Methyl (*E*)-3-Benzamido-2-bromoacrylate

BY CHRISTOPHER J. EASTON AND GIOVANNA ROSITANO

Department of Organic Chemistry, University of Adelaide, South Australia 5001, *Australia*

AND EDWARD R. T. TIEKINK

Department of Physical and Inorganic Chemistry, University of Adelaide, South Australia 5001, *Australia*

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Abstract. $C_{11}H_{10}BrNO_3$, $M_r = 284{\cdot}1$, orthorhombic, $Pna2_1$, $a = 9{\cdot}915$ (1), $b = 17{\cdot}834$ (1), $c = 6{\cdot}442$ (1) Å, $V = 1139$ (1) Å^3, $Z = 4$, $D_x = 1{\cdot}657$ Mg m^{-3}, Mo $K\bar{\alpha}$ radiation, $\lambda = 0{\cdot}7107$ Å, $\mu = 3{\cdot}501$ mm^{-1}, $F(000) = 568$, $T = 295$ (2) K, $R = 0{\cdot}033$ for 1151 observed reflections. The structure investigation determines the stereochemistry of the title compound as *E*. Bond distances and angles are as expected. The non-phenyl portion of the molecule is planar [maximum deviation: 0·106 (5) Å] and forms a dihedral angle of 15·4° with the phenyl ring. There are no significant intermolecular contacts in the crystal lattice.

Experimental. A mixture of *N*-benzoyl-β-alanine methyl ester (0·3 g, 1·4 mmol), *N*-bromosuccinimide (0·26 g, 1·4 mmol) and 2,2′-azobisisobutyronitrile (*ca* 5 mg) in CCl_4 (15 ml) was heated for 2 h at reflux under N_2 whilst being irradiated with a 250 W Hg lamp. The filtrate was concentrated *in vacuo* and chromatographed on silica to give methyl (*E*)-3-benzamido-2-bromoacrylate (132 mg, 32%), isomer *A*, m.p. 371–372 K, found: C, 46·48; H, 3·53%; $C_{11}H_{10}BrNO_3$ requires C, 46·50; H, 3·54% and methyl (*Z*)-3-benzamido-2-bromoacrylate (62 mg, 15%), isomer *B*, m.p. 395·5–396·5 K, found: C, 46·51; H, 3·67%; $C_{11}H_{10}BrNO_3$ requires C, 46·50; H, 3·54%. Crystals of isomer *A* grown by slow evaporation of hexane into an ethyl acetate solution of the compound. Enraf–Nonius CAD-4F diffractometer controlled by a PDP8/A computer, graphite-monochromated Mo $K\bar{\alpha}$ radiation; ω:2θ-scan technique. Cell parameters on crystal 0·18 × 0·12 × 0·75 mm by least squares on 25 reflections ($8 \le \theta \le 12°$) (de Boer & Duisenberg, 1984). Analytical absorption correction applied; max. and min. transmission factors 0·710 and 0·520 (Sheldrick, 1976). Total of 2588 reflections ($1{\cdot}5 \le \theta \le 27{\cdot}5°$) measured in the range $0 \le h \le 12$, $-23 \le k \le 12$, $0 \le l \le 8$. No significant variation in the net intensities of three reference reflections ($2\bar{2}5$, $2\bar{3}4$, $1\bar{4}2$) measured every 7200 s. 1486 unique reflections (R_{int} 0·024) and 1151 satisfied $I \ge 2{\cdot}5\sigma(I)$. Structure solved by Patterson method, full-matrix least-squares refinement of 173 parameters based on *F* (Sheldrick, 1976). Anisotropic

Table 1. *Fractional atomic coordinates and* B_{eq} *values* (Å^2)

$B_{eq} = 8\pi^2(U_{11} + U_{22} + U_{33})/3$.

	x	*y*	*z*	B_{eq}
Br(2)	−0·06102 (4)	−0·05594 (3)	0	4·77
O(1)	−0·2244 (4)	0·0015 (3)	−0·3736 (8)	6·49
O(1′)	−0·3878 (5)	−0·0834 (3)	−0·3656 (7)	4·87
O(4)	−0·4316 (3)	−0·2594 (2)	0·1777 (6)	4·54
N(3)	−0·2455 (4)	−0·1872 (3)	0·1491 (7)	3·54
C(1)	−0·2761 (5)	−0·0516 (3)	−0·2937 (9)	3·54
C(1′)	−0·4478 (6)	−0·0519 (4)	−0·5501 (9)	5·41
C(2)	−0·2261 (5)	−0·0903 (3)	−0·1082 (8)	3·14
C(3)	−0·2894 (5)	−0·1479 (3)	−0·0213 (10)	3·15
C(4)	−0·3211 (5)	−0·2422 (3)	0·2438 (8)	3·27
C(41)	−0·2616 (5)	−0·2767 (3)	0·4353 (7)	3·11
C(42)	−0·1609 (5)	−0·2417 (3)	0·5468 (8)	3·55
C(43)	−0·1157 (6)	−0·2729 (4)	0·7321 (10)	4·62
C(44)	−0·1690 (6)	−0·3382 (4)	0·7993 (10)	5·01
C(45)	−0·2665 (7)	−0·3750 (4)	0·6880 (11)	5·21
C(46)	−0·3127 (5)	−0·3445 (3)	0·5021 (15)	4·44

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