

Fig. 1. ORTEP plot (Johnson, 1965) of [Cr(C₅Me₅)₂]⁺.1⁻. Thermal ellipsoids are drawn at the 50% probability level.

1.863 (5) Å]. The average metal—ring-centroid distance for this formally Cr^{3+} complex is slightly shorter than the distance found for $(C_5Me_5)_2Cr_2O_4$ [1.931 (6) Å] (Heberhold, Kremnitz, Razavi, Schollhorn & Thewalt, 1985) but slightly longer than that found for $(C_5Ph_4H)_2Cr$ [1.832 (5) Å] (Castellani, Geib, Rheingold & Trogler, 1987) which have formal oxidation states of +5 and +2 respectively. Metal—ring-C-atom averages are more consistent with values of 2.200 (4), 2.200 (6) and 2.197 (5) Å for

complexes with oxidation states of +5, +3 and +2 respectively.

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Structural Chirality of [Bis(desferrithiocin)]copper(II)

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Abstract. [2-(3-Hydroxy-2-pyridyl)-4-methyl-4,5-dihydro-4-thiazolecarboxylato(2-)][2-(3-hydroxy-2-pyridyl)-4-methyl-4,5-dihydro-4-thiazolecarboxylic acid]copper(II), [Cu(C₁₀H₈N₂O₃S)(C₁₀H₁₀N₂O₃S)], M_r = 538.06, monoclinic, $P2_1$, a = 10.412 (1), b = 6.656 (4), c = 16.788 (1) Å, $\beta = 98.59$ (3)°, V = 1150.5 Å³, Z =2, $D_x = 1.553$ Mg m⁻³, Cu K α , $\lambda = 1.54184$ Å, $\mu =$ 3.3739 mm⁻¹, F(000) = 550, T = 293 K. The final Rvalue is 0.039 for 3465 significant [$I > 3.\sigma(I)$] reflections. The Cu atom has a square-pyramidal coordination sphere and is bound to two O and two N atoms, each in a *trans* position, and to one N atom in an axial position. The last bond exhibits a pronounced elongation [2.340 (4) Å] due to Jahn-Teller distortion.

Introduction. Desferrithiocin $(dftH_2)$ is known to be a naturally occurring chelator and was isolated as the

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Table	1.	Data-collection	and	structure-refinement			
parameters							

 Table 2. Atomic positional and equivalent isotropic displacement parameters (Å²)

Diffractometer used CAD-4, Enraf-Nonius <i>Method of intensity measurement wθ scan</i> x <i>y z U_q</i> <i>No.; θ range</i> (°) of reflections for 25; 18–28 Cu 0-2895 (1) 0-8500 0-7547 (1) 0-034 (1) <i>lattice parameters</i> <i>Method used for absorption correction DIFABS</i> (Walker & Stuart, 1983) <i>Minimum absorption correction</i> 1-5790 Of 0-1445 (3) 0-9761 (5) 0-6859 (2) 0-041 (2) <i>Maximum absorption correction</i> 1-5790 O51 0-6510 (4) 0-6224 (7) 0-7957 (2) 0-068 (3) <i>Maximum value of</i> (sin θ)/λ (Å ⁻¹) 0-588 N1 0-3966 (4) 0-8816 (7) 0-6715 (2) 0-040 (2) <i>Maximum value of</i> (sin θ)/λ (Å ⁻¹) 0-588 N1 0-3966 (4) 0-8816 (7) 0-6715 (2) 0-040 (2) <i>Maximum value of</i> (sin θ)/λ (Å ⁻¹) 0-588 N1 0-3966 (4) 0-8816 (7) 0-6715 (2) 0-040 (3) <i>reached</i> in intensity measurement <i>Range of</i> h, k and <i>I</i> 0 → 12, 0 → 7, −19 → 19 C1 0-3558 (5) 0.8777 (9) 0-9594 (3) 0-0646 (3) <i>Standard reflections</i> 206, 125, 026 C2 0-5725 (7) 0-705 (1) 0-6239 (4) 0-080 (5) <i>Interval, standar dreflections</i> 2, no intensity variation C4 0-6143 (6) 1-021 (1) 0-7089 (5) 0-082 (5) <i>θ range</i> (°) (219 unobserved reflections) C7 0-1268 (5) 0-9329 (8) 0-5667 (3) 0-043 (3) <i>θ range</i> (°) (219 unobserved reflections) C7 0-1268 (5) 0-9329 (8) 0-5667 (3) 0-043 (3) <i>θ range</i> (°) (219 unobserved reflections) C9 -0-0157 (7) 1-0072 (9) 0-4480 (4) 0-063 (3) <i>θ range</i> (°) (219 unobserved reflection density <i>map,</i> positions included in 027 0-2597 (3) 0-9930 (6) 1-0648 (2) 0-063 (3) <i>θ range</i> (°) (1) <i>G reflecting F</i> <i>map,</i> positions included in 027 0-2597 (3) 0-9930 (6) 1-0648 (2) 0-063 (3) <i>Parameters refined</i> 298 N21 0-1160 (3) 0-776 (5) 0-7356 (5) 0-7356 (2) 0-0435	Crystal shape	Needles		U_{ec}	$= (1/3)\sum_i\sum_j U_{ij}$	a;*a;*a;.a;.	
Method of intensity measurement ωθ scan x y 2 U_{a} No: θ range (*) of reflections for 25; 18–28 Cu 0.2895 (1) 0.8500 0.7547 (1) 0.034 (1) lattice parameters DIFABS (Walker & Stuart, 1983) dft ²⁻ 51 0.4650 (2) 0.7902 (3) 0.5349 (1) 0.078 (1) Maximum absorption correction 1.5790 0.51 0.6510 (4) 0.6224 (7) 0.7977 (2) 0.068 (3) Maximum value of (sin θ)λ (Å ⁻¹) 0.588 N1 0.3966 (4) 0.888 (7) 0.6413 (3) 0.7080 (5) 0.8088 (2) 0.040 (2) Maximum value of (sin θ)λ (Å ⁻¹) 0.512 (0.26 C3 0.5339 (4) 0.8264 (9) 0.6373 (3) 0.064 (3) Range of h, k and l 0.512, 0.26 C3 0.5339 (4) 0.8264 (9) 0.6337 (3) 0.047 (3) measured (h) C5 0.5457 (5) 0.7069 (8) 0.7728 (3) 0.042 (3) 0.042 (3) 0.042 (3) 0.042 (3) 0.042 (3) 0.042 (3) 0.043 (1) 0.633 (3) 0.043 (1) 0.633 (3) 0.043 (1)	Diffractometer used	CAD-4, Enraf–Nonius					
No.; θ range (°) of reflections for 25; 18–28 Cu 0-2895 (1) 0-8500 0-7547 (1) 0-034 (1) lattice parameters Method used for absorption correction DIFABS (Walker & Stuart, 1983) Minimum absorption correction 0-5842 Si 0-041 (2) Maximum absorption correction 1-5790 Of 0-1445 (3) 0-9761 (5) 0-6859 (2) 0-041 (2) Maximum value of (sin θ)/ λ (Λ^{-1}) 0-588 Ni 0-052 0-4493 (3) 0-7080 (5) 0-8098 (2) 0-040 (3) masurement not not not not not not not not not n	Method of intensity measurement	ω/θ scan		<i>x</i>	у	<i>Z</i>	U_{eq}
lattice parametersdft²-Method used for absorption correctionDIFABS (Walker & Stuart, 1983)S10-4650 (2)0-7902 (3)0-5349 (1)0-078 (1)Minimum absorption correction1-5790O70-1445 (3)0-9761 (5)0-6859 (2)0-041 (2)Maximum value of (sinθ)/λ (Å ⁻¹)0-588N10-3966 (4)0-6821 (7)0-7957 (2)0-068 (3)Maximum value of (sinθ)/λ (Å ⁻¹)0-588N10-3966 (4)0-6815 (7)0-6715 (2)0-040 (2)Marinum value of (sinθ)/λ (Å ⁻¹)0-512 (0 → 7, -19 → 19C10-3558 (5)0-8777 (9)0-9543 (3)0-046 (3)Range of h, k and l0 → 12, 0 → 7, -19 → 19C10-3558 (5)0-8777 (9)0-9543 (3)0-046 (3)Standard reflections206, 125, 026C20-5725 (7)0-706 (1)0-6239 (4)0-080 (2)Interval, standard reflections measured;4443; 65C60-5249 (5)0-7089 (8)0-7728 (3)0-042 (3)Otal No. of reflections measured;4443; 65C60-2249 (5)0-9723 (7)0-6055 (3)0-043 (3)Ør ange (°)(219 unobserved reflections)C70-1268 (5)0-9723 (7)0-6055 (3)0-044 (3)No. of observed reflections3465 with <i>I</i> > 3σ(<i>I</i>) (FridelC80-0027 (1)0-9765 (9)0-4407 (3)0-065 (5)Use of <i>F</i> or <i>F</i> ² in LS refinement <i>F</i> fftH ₂ -Method locating H atomsFrom difference electron density210-1161 (1)0-6862 (2)0-9750 (1)0-04	No.; θ range (°) of reflections for	25; 18–28	Cu	0.2895 (1)	0.8200	0.7547 (1)	0.034 (1)
	lattice parameters		dft2-				
$\begin{array}{l l l l l l l l l l l l l l l l l l l $	Method used for absorption correction	DIFABS (Walker & Stuart, 1983)		0.4(50.(2))	0 7002 (2)	0.5240 (1)	0.070 (1)
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Average absorption correction1-0177OS20-040 (3)0-024 (7)0-7597 (2)0-040 (3)Maximum value of (sin θ/λ (Å ⁻¹)0-588N10-3966 (4)0-8816 (7)0-6715 (2)0-040 (3)reached in intensity measurementN20-2077 (5)0-9348 (7)0-6718 (2)0-040 (3)Range of h, k and I0 $\rightarrow 12, 0 \rightarrow 7, -19 \rightarrow 19$ C10-3558 (5)0-8777 (9)0-5954 (3)0-046 (3)Standard reflections206, 125, 026C20-5725 (7)0-706 (1)0-6229 (4)0-080 (5)Interval, standard reflections2, no intensity variationC40-6143 (6)1-021 (1)0-7089 (5)0-042 (3)Total No. of reflections measured;4443; 65C60-2249 (5)0-7069 (8)0-7728 (3)0-042 (3) θ range (°)(219 unobserved reflections)C70-128 (5)0-9723 (7)0-6055 (3)0-041 (3)No. of observed reflections3465 with $I > 3\sigma(I)$ (FriedelC80-0024 (6)0-0723 (9)0-6503 (3)0-044 (3)Use of F or F ² in LS refinementF0-0157 (7)1-0072 (9)0-4802 (4)0-063 (4)Weighting scheme1/ σ_f^2 0298N210-1161 (1)0-6862 (2)0-9750 (1)0-048 (1)Weighting scheme1/ σ_f^2 0298N210-1161 (1)0-6862 (2)0-9713 (2)0-048 (2)Weighting scheme1/ σ_f^2 02510-137 (3)0-2684 (5)0-7615 (2)0-048 (2)Value of R 0-039 (i	Maximum absorption correction	1.5790	051	0.1445(3)	0.9701 (3)	0.7057 (2)	0.041 (2)
Maximum value of $(\sin \theta)/\lambda$ (Å ⁻¹) 0.588 N1 0.3966 (4) 0.806 (7) 0.6715 (2) 0.040 (3) reached in intensity measurement N2 0.2077 (5) 0.9348 (7) 0.4778 (3) 0.0616 (4) Range of h, k and l 0 \rightarrow 12, 0 \rightarrow 7, $-19 \rightarrow$ 19 C1 0.3558 (5) 0.8777 (9) 0.9394 (7) 0.4477 (3) 0.064 (4) Standard reflections 206, 125, 026 C2 0.5725 (7) 0.705 (1) 0.6239 (4) 0.080 (5) Interval, standard reflections 2, no intensity variation C3 0.5339 (4) 0.8264 (9) 0.6937 (3) 0.042 (3) Total No. of reflections measured; 4443; 65 C6 0.2249 (5) 0.9329 (8) 0.5607 (3) 0.043 (3) No. of observed reflections 3465 with $I > 3\sigma(I)$ (Friedel C8 0.0024 (6) 1.0090 (9) 0.5630 (3) 0.043 (3) Methods used to solve structure Patterson C10 0.0871 (7) 0.9903 (6) 1.0648 (2) 0.061 (2) 0.0440 (3) Weighting scheme $1/\sigma_T^2$ O210 0.0877 (3) 0.9268 (5) 0.7615 (2) 0.0448 (2) Weighting scheme $1/\sigma_T^2$ <td< td=""><td>Average absorption correction</td><td>1.0177</td><td>052</td><td>0.4493 (3)</td><td>0.7080 (5)</td><td>0.8098 (2)</td><td>0.040 (3)</td></td<>	Average absorption correction	1.0177	052	0.4493 (3)	0.7080 (5)	0.8098 (2)	0.040 (3)
reached in intensity measurementN20-2077 (5)0-9348 (7)0-4778 (3)0-066 (4)Range of h, k and l0→12, 0→7, -19→19C10-3538 (5)0-8777 (9)0-95954 (3)0-046 (3)Standard reflections206, 125, 026C20-5725 (7)0-705 (1)0-6239 (4)0-080 (5)Interval, standard reflections2, no intensity variationC30-5339 (4)0-8264 (9)0-6937 (3)0-047 (3)measured (h)C50-5457 (5)0-7069 (8)0-7728 (3)0-042 (3)Total No. of reflections measured;4443; 65C60-2249 (5)0-9329 (8)0-6607 (3)0-042 (3)0o observed reflections3465 with <i>I</i> > 3σ(<i>I</i>) (FriedelC80-0024 (6)1-0000 (9)0-5630 (3)0-054 (3)0opposites)C9-0-0157 (7)1-0072 (9)0-4802 (4)0-063 (4)Method of locating H atomsFftftH2Weighting scheme1/ σ_F^2 02510-0177 (3)0-2684 (5)0-7132 (2)0-048 (2)Value of R0-039 (inverse model: 0-047)N220-318 (4)1-0799 (6)0-835 (2)0-033 (2)0-028 (2)Value of wR0-045 (inverse model: 0-047)N220-318 (4)0-999 (6)0-861 (2)0-037 (2)Value of wR0-045 (inverse model: 0-051)C20-1971 (4)0-812 (6)0-933 (2)0-031 (3)Ratio of max. LS shift to e.s.d. (Δ/σ)0-0007C230-0800 (4)0-5903 (7)0-818 (3)0-044 (3)Max. height	Maximum value of $(\sin\theta)/\lambda$ (Å ⁻¹)	0.588	NI	0.3966 (4)	0.8816(7)	0.6715(2)	0.040 (2)
Range of h, k and l $0 \rightarrow 12, 0 \rightarrow 7, -19 \rightarrow 19$ C1 $0 \rightarrow 3558$ (5) $0 + 8777$ (9) $0 \cdot 5934$ (3) 0.046 (3)Standard reflections206, 125, 026C2 $0 \cdot 5725$ (7) $0 \cdot 7051$ (1) $0 \cdot 6229$ (4) 0.080 (5)Interval, standard reflections2, no intensity variationC3 $0 \cdot 5339$ (4) $0 \cdot 8254$ (9) $0 \cdot 6937$ (3) $0 \cdot 047$ (3)Interval, standard reflections2, no intensity variationC4 $0 \cdot 6143$ (6) $1 \cdot 021$ (1) $0 \cdot 7089$ (5) $0 \cdot 042$ (3)Interval, standard reflections measured;4443; 65C5 $0 \cdot 52457$ (5) $0 \cdot 7089$ (8) $0 \cdot 7728$ (3) $0 \cdot 0442$ (3)Interval, standard reflections(219 unobserved reflections)C7 $0 \cdot 1268$ (5) $0 \cdot 9723$ (7) $0 \cdot 6655$ (3) $0 \cdot 0443$ (3)No. of observed reflections3465 with $I > 3\sigma(I)$ (FriedelC8 $0 \cdot 0024$ (6) $1 \cdot 0009$ (9) $0 \cdot 5630$ (3) $0 \cdot 0454$ (3)Methods used to solve structurePattersonC10 $0 \cdot 08717$ (7) $0 \cdot 9755$ (9) $0 \cdot 4407$ (3) $0 \cdot 0655$ (5)Use of F or F ² in LS refinementFfrom difference electron density map, positions included in structure-factor calculation 0251 $0 \cdot 0773$ (3) $0 \cdot 9750$ (1) $0 \cdot 0484$ (2)Weighting scheme $1/\sigma_F^2$ O252 $0 \cdot 1949$ (3) $0 \cdot 7766$ (6) $0 \cdot 7132$ (2) $0 \cdot 048$ (2)Parameters refined298N21 $0 \cdot 1051$ $0 \cdot 229 \cdot 0318$ (8) $0 \cdot 7766$ (6) $0 \cdot 7132$ (2) $0 \cdot 048$ (2)Value of R0 \cdot	reached in intensity measurement		N2	0.2077(5)	0.9348(7)	0.4778(3)	0.061 (4)
Standard reflections 206, 125, 026 C2 0-5725 (7) 0-705 (1) 0-6239 (4) 0-080 (5) Interval, standard reflections 2, no intensity variation C3 0-5339 (4) 0-8264 (9) 0-6937 (3) 0-047 (3) measured (h) C4 0-6143 (6) 1-021 (1) 0-7089 (5) 0-682 (5) Total No. of reflections measured; 4443; 65 C5 0-5457 (5) 0-7069 (8) 0-7728 (3) 0-042 (3) No. of observed reflections 3465 with $I > 3\sigma(I)$ (Friedel C8 0-0024 (6) 1-0090 (9) 0-5630 (3) 0-043 (3) No. of observed reflections 3465 with $I > 3\sigma(I)$ (Friedel C8 0-0024 (6) 1-0090 (9) 0-5630 (3) 0-043 (3) Wethod s used to solve structure Patterson C10 0-0871 (7) 0-9755 (9) 0-4407 (3) 0-065 (5) Use of F or F^2 in LS refinement F dftH2 Parameters refined 298 N21 0-1161 (1) 0-6862 (2) 0-9750 (1) 0-048 (2) 0-051 (2) 0-046 (2) Value of R 0-039 (inverse model: 0-047) N22 0-118 (4) <td< td=""><td>Range of h, k and l</td><td>$0 \rightarrow 12 0 \rightarrow 7 -19 \rightarrow 19$</td><td>C1</td><td>0.3558 (5)</td><td>0.8777 (9)</td><td>0.5954 (3)</td><td>0.046 (3)</td></td<>	Range of h, k and l	$0 \rightarrow 12 0 \rightarrow 7 -19 \rightarrow 19$	C1	0.3558 (5)	0.8777 (9)	0.5954 (3)	0.046 (3)
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Standard reflections	206 125 026	C2	0.5725 (7)	0·705 (Ì)	0.6239 (4)	0.080 (5)
Interview of the form	Interval standard reflections	2 no intensity variation	C3	0.5339 (4)	0.8264 (9)	0.6937 (3)	0.047 (3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	measured (h)	2, no intensity variation	C4	0.6143 (6)	1.021 (1)	0.7089 (5)	0.082 (5)
Average (*) (219 unobserved reflections) C6 -2249 (5) -03239 (8) -5607 (3) -045 (3) More of Parage (*) (219 unobserved reflections) C7 -1268 (5) -9723 (7) -6655 (3) -0443 (3) No. of observed reflections 3465 with $I > 3\sigma(I)$ (Friedel C8 -0024 (6) 1.0090 (9) -5630 (3) -0453 (3) Wethods used to solve structure Patterson C10 -00871 (7) -09755 (9) -44407 (3) -00655 (3) Use of F or F^2 in LS refinement F dftH2 Weighting scheme $1/\sigma_F^2$ C251 -01161 (1) -06862 (2) -07150 (2) -048 (2) Weighting scheme $1/\sigma_F^2$ C252 -1949 (3) -04766 (6) -7132 (2) -0448 (2) Value of R 0-039 (inverse model: 0-047) N22 -3188 (4) -10799 (6) 08614 (2) -0037 (2) Value of wR 0-045 (inverse model: 0-051) C21 $0-1971$ (4) 0.8121 (6) 0.9908 (2) 0.031 (3) Ratio of max. LS shift to e.s.d. (Δ/σ) $0-0007$ C22	Total No. of reflections measured:	1112 65	C5	0.5457 (5)	0.7069 (8)	0.7728 (3)	0.042 (3)
Weighting scheme $1/\sigma_r^2$ 021 (inverse model: 0-047) 022 (inverse model: 0-051) 021 (inverse model: 0-051) 022 (inverse model: 0-051	A range (°)	(210 uncheaned inflactions)	C6	0.2249 (5)	0.9329 (8)	0.5607 (3)	0.045 (3)
No. of observed reflections 3465 with $I > 3\sigma(I)$ (Friedel C8 00024 (b) 10000 (9) 0.5630 (3) 0034 (3) opposites opposites $C10$ 00871 (7) 1.0072 (9) 04802 (4) 0.063 (4) Methods used to solve structure Patterson C10 0.0871 (7) 0.9765 (9) 0.4407 (3) 0.063 (4) Method of locating H atoms F dftH2 0.077 (2) 0.9903 (6) 1.0648 (2) 0.051 (2) Weighting scheme I/σ_F^2 O251 0.0577 (3) 0.2884 (5) 0.7615 (2) 0.044 (2) Parameters refined 298 N21 0.1806 (3) 0.7466 (6) 0.7132 (2) 0.048 (2) Value of R 0.039 (inverse model: 0.047) N22 0.3188 (4) 1.0799 (6) 0.8614 (2) 0.037 (2) Value of wR 0.045 (inverse model: 0.051) C21 0.1971 (4) 0.8121 (6) 0.9068 (2) 0.031 (3) Ratio of max. LS shift to e.s.d. (Δ/σ) 0.0007 C23 0.0800 (4) 0.5903 (7) 0.8186 (3) 0.032 (2) 0.048 (3) 0.032 (2) <	Ve of observed reflections	(219 unobserved reflections)	C7	0.1268 (5)	0.9723 (7)	0.6055 (3)	0.041 (3)
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	No. of observed reflections	3465 with $I > 3\sigma(I)$ (Friedel		0.0024(6)	1.0090 (9)	0.5630 (3)	0.054 (3)
Methods used to solve structure Patterson C10 0.001 (1) 0.9703 (3) 0.4407 (3) 0.003 (3) Use of F or F^2 in LS refinement F dftH2 0.003 (3) 0.04407 (3) 0.003 (3) 0.003 (3) Use of F or F^2 in LS refinement F dftH2 0.001 (1) 0.66862 (2) 0.9750 (1) 0.0448 (1) 0.0488 (1) 0.0488 (1) 0.0488 (1) 0.0488 (1) 0.0488 (1) 0.0488 (1) 0.015 (2) 0.0468 (2) 0.051 (2) 0.0468 (2) 0.051 (2) 0.0468 (2) 0.051 (2) 0.0468 (2) 0.001 (2) 0.0488 (2) 0.025 (2) 0.0456 (6) 0.7132 (2) 0.048 (2) 0.023 (2) 0.048 (2) 0.023 (2) 0.048 (2) 0.023 (2) 0.028 (2) 0.028 (2) 0.023 (2) 0.0		opposites)	C10	-0.0137 (7)	0.0765 (0)	0.4802 (4)	0.065 (4)
Use of F or F' in LS refinement F dftH2 Method of locating H atoms From difference electron density S21 0.1161 (1) 0.6862 (2) 0.9750 (1) 0.048 (1) map, positions included in 027 0.2597 (3) 0.9903 (6) 1.0648 (2) 0.051 (2) Weighting scheme $1/\sigma_F^2$ 0251 0.0577 (3) 0.2684 (5) 0.7615 (2) 0.048 (2) Parameters refined 298 N21 0.186 (3) 0.7466 (5) 0.8336 (2) 0.028 (2) Value of R 0.039 (inverse model: 0.047) N22 0.3188 (4) 1.0799 (6) 0.8614 (2) 0.031 (3) Ratio of max. LS shift to e.s.d. (Δ/σ) 0.0007 C22 0.0659 (5) 0.4950 (8) 0.8995 (3) 0.041 (3) Max. height in final ΔF map (e Å ⁻³) 0.572 C24 -0.0465 (5) 0.6934 (9) 0.7806 (3) 0.048 (3) Error in an observation of unit weight 0.985 C25 0.1194 (4) 0.4022 (7) 0.7583 (3) 0.034 (2) Secondary-extinction coefficient 3.62 (1) × 10^{-6} (Zachariasen, 1963) C26 0.279 (4) 0.4902 (7) 0.7583 (3) 0.034 (2) 0.034 (2)	Methods used to solve structure	Patterson	CIU	0.0071 (7)	0.9703 (9)	0.4407 (3)	0.002 (2)
Method of locating H atomsFrom difference electron density map, positions included in structure-factor calculation $S21$ $O27$ $O2597$ $O-6862$ (2) $O-9750$ (1) $O-048$ (1) $O-048$ (2) $O-051$ (2) $O-046$ (2) $O-039$ (2) $O-046$ (2) $O-039$ (2) $O-046$ (2) $O-039$ (2) $O-046$ (2) $O-037$ (2) $O-047$ (2) $O-0318$ (4) $O-0799$ (6) $O-0456$ (3) $O-037$ (2) $O-0465$ (3) $O-0450$ (3) $O-037$ (3) $O-04650$ (3) $O-0450$ (3) $O-0470$ (3) <b< td=""><td>Use of F or F^2 in LS refinement</td><td>F</td><td>dftHa</td><td></td><td></td><td></td><td></td></b<>	Use of F or F^2 in LS refinement	F	dftHa				
map, positions included in structure-factor calculation 027 0251 0.101 0.9903 (6) 0.903 (7) 0.9903 (6) 0.9048 (1) 0.9903 (6)Weighting scheme $1/\sigma_F^2$ 0251 0.7615 0.0577 (3) 0.252 0.9903 (6) 0.9766 (6) 0.7132 (2) 0.9484 (2)Parameters refined298N21 0.939 (inverse model: 0.047)N22 N22 0.1886 (3) 0.7466 (6) 0.7322 (2) 0.9038 (2) 0.9037 (2)Value of R 0.039 (inverse model: 0.047)N22 0.22 0.3188 (4) 0.1971 (4) 0.8121 (6) 0.9068 (2) 0.9008 (2) 0.9037 (2)Value of wR 0.045 (inverse model: 0.051)C21 C22 0.0595 (5) 0.4950 (8) 0.4950 (8) 0.8995 (3) 0.0007 0.9007 C23 C23 0.0800 (4) 0.9908 (2) 0.9903 (7) 0.8186 (3) 0.925 (3) 0.948	Method of locating H atoms	From difference electron density	S21	0-1161 (1)	0.6862 (2)	0.9750 (1)	0.048 (1)
structure-factor calculation 0251 0.0777 (3) 0.2884 (5) 0.7615 (2) 0.046 (2) Weighting scheme $1/\sigma_F^2$ 0252 0.1949 (3) 0.4766 (6) 0.7132 (2) 0.048 (2) Parameters refined 298 N21 0.1806 (3) 0.7766 (5) 0.8336 (2) 0.028 (2) Value of R 0.039 (inverse model: 0.047) N22 0.3188 (4) 1.0799 (6) 0.8614 (2) 0.037 (2) Value of wR 0.045 (inverse model: 0.051) C21 0.1971 (4) 0.8121 (6) 0.9068 (2) 0.031 (3) Ratio of max. LS shift to e.s.d. (Δ/σ) 0.0007 C22 0.0659 (5) 0.4950 (8) 0.8995 (3) 0.041 (3) Max. height in final ΔF map (e Å $^{-3}$) 0.572 C24 -0.0465 (5) 0.6934 (9) 0.7806 (3) 0.048 (3) Error in an observation of unit weight 0.985 C25 0.1194 (4) 0.4402 (7) 0.7583 (3) 0.034 (2) Secondary-extinction coefficient 3.62 (1) $\times 10^{-6}$ (Zachariasen, 1963) C25 0.194 (4) 0.4925 (map, positions included in	027	0.2597 (3)	0.9903 (6)	1.0648 (2)	0.051 (2)
Weighting scheme $1/\sigma_F^2$ O252 0.149 (3) 0.4766 (6) 0.7132 (2) 0.048 (2) Parameters refined 298 N21 0.1806 (3) 0.7466 (5) 0.8336 (2) 0.028 (2) Value of R 0.039 (inverse model: 0.047) N22 0.3188 (4) 1.0799 (6) 0.8614 (2) 0.037 (2) Value of wR 0.045 (inverse model: 0.051) C21 0.1911 (4) 0.8121 (6) 0.9068 (2) 0.031 (3) Ratio of max. LS shift to e.s.d. (Δ/σ) 0.0007 C23 0.0600 (4) 0.5903 (7) 0.8186 (3) 0.032 (2) Max. height in final ΔF map (e \mathbb{A}^{-3}) 0.572 C24 -0.0465 (5) 0.6334 (9) 0.7806 (3) 0.048 (3) Error in an observation of unit weight 0.985 C25 0.1194 (4) 0.4402 (7) 0.7583 (3) 0.031 (3) Secondary-extinction coefficient 3.62 (1) × 10^{-6} (Zachariasen, 1963) C26 0.2759 (4) 0.9958 (7) 0.9258 (3) 0.031 (2)		structure-factor calculation	0251	0.0577(3)	0.2684(5)	0.7615(2)	0.046(2)
Parameters refined 298 N21 0-1806 (3) 0-7466 (5) 0.8336 (2) 0.028 (2) Value of R 0-039 (inverse model: 0-047) N22 0-3188 (4) 1-0799 (6) 0-8614 (2) 0.037 (2) Value of wR 0-045 (inverse model: 0-051) C21 0-1971 (4) 0-8121 (6) 0-9068 (2) 0.031 (3) Ratio of max. LS shift to e.s.d. (Δ/σ) 0-0007 C23 0-0659 (5) 0-4950 (8) 0-8995 (3) 0-041 (3) Max. height in final ΔF map (e \mathbb{A}^{-3}) 0-572 C23 0-0800 (4) 0-5903 (7) 0-8186 (3) 0-032 (2) Error in an observation of unit weight 0-985 C25 0-1194 (4) 0-4402 (7) 0-7583 (3) 0-044 (3) Secondary-extinction coefficient 3-62 (1) × 10^{-6} (Zachariasen, 1963) C26 0-2759 (4) 0-9958 (7) 0-9258 (3) 0-031 (3)	Weighting scheme	$1/\sigma_F^2$	O252	0.1949 (3)	0.4766 (6)	0.7132(2)	0.048(2)
Value of R 0.039 (inverse model: 0.047) N22 0.318 (4) 1.0799 (6) 0.8614 (2) 0.037 (2) Value of wR 0.045 (inverse model: 0.051) C21 0.1971 (4) 0.8121 (6) 0.9068 (2) 0.031 (3) Ratio of max. LS shift to e.s.d. (Δ/σ) 0.0007 C23 0.0600 (4) 0.5903 (7) 0.8186 (3) 0.042 (3) Max. height in final ΔF map (e A^{-3}) 0.572 C24 -0.0455 (5) 0.6934 (9) 0.7806 (3) 0.048 (3) Error in an observation of unit weight 0.985 C25 0.1194 (4) 0.4402 (7) 0.7583 (3) 0.034 (3) Secondary-extinction coefficient 3.62 (1) × 10^{-6} (Zachariasen, 1963) C26 0.2759 (4) 0.9958 (7) 0.9258 (3) 0.033 (2)	Parameters refined	298	N21	0·1806 (3)	0.7466 (5)	0.8336 (2)	0.028 (2)
Value of wR 0.045 (inverse model: 0.051) C21 0.1971 (4) 0.8121 (6) 0.9068 (2) 0.031 (3) Ratio of max. LS shift to e.s.d. (Δ/σ) 0.0007 C22 0.0659 (5) 0.4950 (8) 0.8995 (3) 0.041 (3) Max. height in final ΔF map (e Å ⁻³) 0.572 C24 -0.0465 (5) 0.6934 (9) 0.7806 (3) 0.048 (3) Error in an observation of unit weight 0.985 C25 0.1194 (4) 0.4402 (7) 0.7583 (3) 0.034 (2) Secondary-extinction coefficient 3.62 (1) × 10 ⁻⁶ (Zachariasen, 1963) C26 0.279 (4) 0.4902 (7) 0.9258 (3) 0.034 (2)	Value of R	0.039 (inverse model: 0.047)	N22	0.3188 (4)	1.0799 (6)	0.8614 (2)	0.037 (2)
C22 0.0659 (5) 0.4950 (8) 0.8995 (3) 0.041 (3) Max. height in final ΔF map (e Å ⁻³) 0.572 C23 0.0800 (4) 0.5903 (7) 0.8186 (3) 0.032 (2) Error in an observation of unit weight 0.985 C24 -0.0465 (5) 0.6934 (9) 0.7806 (3) 0.048 (3) Secondary-extinction coefficient 3.62 (1) × 10 ⁻⁶ (Zachariasen, 1963) C26 0.2759 (4) 0.9958 (7) 0.9258 (3) 0.034 (2)	Value of wR	0.045 (inverse model: 0.051)	C21	0.1971 (4)	0.8121 (6)	0.9068 (2)	0.031 (3)
Max. height in final ΔF map (e Å ⁻³) 0.572 C23 0.0800 (4) 0.5903 (7) 0.8186 (3) 0.032 (2) Error in an observation of unit weight 0.985 C24 -0.0465 (5) 0.6934 (9) 0.7806 (3) 0.048 (3) Secondary-extinction coefficient 3.62 (1) × 10 ⁻⁶ (Zachariasen, 1963) C25 0.1194 (4) 0.4402 (7) 0.7583 (3) 0.034 (2)	Ratio of max. LS shift to e.s.d. (Δ/σ)	0.0007	C22	0.0659 (5)	0·4950 (8)	0.8995 (3)	0.041 (3)
Error in an observation of unit weight 0.985 Secondary-extinction coefficient $3.62 (1) \times 10^{-6}$ (Zachariasen, 1963) C25 $0.194 (4)$ $0.4402 (7)$ $0.7583 (3)$ $0.034 (2)$ C25 $0.194 (4)$ $0.4402 (7)$ $0.7583 (3)$ $0.034 (2)$ C25 $0.2579 (4)$ $0.9958 (7)$ $0.9258 (3)$ $0.033 (2)$	Max. height in final ΔF map (e Å ⁻³)	0.572	C23	0.0800 (4)	0.5903 (7)	0.8186 (3)	0.032 (2)
Secondary-extinction coefficient $3.62 (1) \times 10^{-6}$ (Zachariasen, 1963) C26 $0.2759 (4)$ $0.9958 (7)$ $0.9258 (3)$ $0.034 (2)$	Error in an observation of unit weight	0.985	C24 C25	-0.0465 (5)	0.6934 (9)	0.7806 (3)	0.048 (3)
(2) (2)	Secondary-extinction coefficient	$3.62(1) \times 10^{-6}$ (Zacharizsen 1063)	C25	0.1194(4)	0.4402 (7)	0.7283(3)	0.034 (2)
Sources of atomic scattering factors International Tables for V_{ray} C27 0.3000 (4) 1.0242 (9) 1.0028 (2) 0.020 (2)	Sources of atomic scattering factors	International Tables for V rev	C20	0.2739 (4)	1.0942 (9)	0.9258 (3)	0.033 (2)
C_{11} C_{12} C	sources of atomic scattering factors	Crustalle anarby (1074)	C28	0.3645 (5)	1.2680 (8)	1.0002 (3)	0.039 (3)
Computer used DEC Micro 2500 C29 0-4446 (4) 1-357 (1) 0-9433 (3) 0-147 (5)	Computer used	DEC MianoVAX 2500	C29	0.4046 (4)	1.352 (1)	0.9433 (3)	0.044 (3)
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Drograma yead		C210	0.3825 (5)	1.2546 (8)	0.8695 (3)	0.045 (3)
Accepted Inc. Inc. Inc. Inc. Inc. Inc. Inc. Inc.	riograms used	Accordance Inc. 1086)		. ,	(-/	(-)	00.00(0)

iron complex from *Streptomyces antibioticus* (Peter, 1985). Likewise its copper complexes are of remarkable thermodynamical stability and are able to compete successfully with biological chelators including serum albumin. An interesting phenomenon of the Cu complexes is their Cu_2Zn_2 superoxide dismutase mimetic activity (Schechinge-, 1988).

Experimental. A green single crystal of approximate dimensions $0.10 \times 0.15 \times 0.15$ mm was mounted on a glass fiber. The systematic absences indicated space group $P2_1/m$ or $P2_1$, of which the non-centrosymmetric space group was confirmed by further calculations. In the final full-matrix least-squares refinement, all non-H atoms were assigned anisotropic atomic displacement parameters. The structure was successfully distinguished from its inverse by least-squares refinement of both alternative models. The R value of the incorrect model converged to 0.047, whereas the correct model led to R= 0.039 in the final refinement. Furthermore, all starting values of the parameter η refine to +1 also indicating the correct choice (Rogers, 1981; Jones, 1984). A summary of data-collection and structurerefinement parameters is given in Table 1. Final atomic coordinates are listed in Table 2, distances and angles in Table 3 and intermolecular hydrogen bonds in Table 4.* A graphic representation (Keller, 1988) of the molecule is shown in Fig. 1, a stereoview of the unit cell in Fig. 2.

Discussion. The Cu atom in the title compound $Cu(dft^{2-})(dftH_2)$ has a similar coordination sphere to that of the previously reported compound $Cu(dft^{2-})(H_2O)_2$ (Schechinger, Hiller, Maichle, Strähle & Weser, 1988). In both compounds one dft²⁻ group is bound to the Cu atom via the nitrogen (N1) of the dihydrothiazole, and, in trans positions, one oxygen (O52) of the carboxyl group and the oxygen (O7) of the phenolic hydroxyl group. Instead of the two water molecules in Cu(dft²⁻)- $(H_2O)_2$ these positions are now occupied by a dftH₂ molecule coordinating via the two N atoms N21 and N22. The Cu atom is situated 0.154 (1) Å above the plane O7,O52,N1,N21. Owing to Jahn-Teller distortion the bond distance to the axially bound N atom

^{*} Lists of structure factors, H-atom positions, least-squaresplanes details, and anisotropic atomic displacement parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52515 (17 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table	3.	Distances	(Å)	and	angle	es (°)	with	e.s.d.	's
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Cu Cu Cu	07 052 NI	1·948 (. 2·015 (4 1·925 (4	3) 4) 4)	Cu Cu Cu	N21 N22 O252	1·990 (4 2·340 (4 2·727 (4)))
S1 S1 O7 O51 O52 N1 N1 N2 C1 C2 C3 C3 C6 C7 C8 C9	C1 C2 C7 C5 C3 C1 C3 C6 C10 C6 C3 C4 C5 C7 C8 C9 C10	1-735 (: 1-819 (' 1-334 (t) 1-240 (t) 1-240 (t) 1-246 (' 1-470 (t) 1-376 (t) 1-376 (t) 1-376 (t) 1-545 (t) 1-537 (t) 1-376 (t) 1-376 (t) 1-376 (t) 1-36 (t) 1-376 (t) 1-36 (t) 1	5) 7) 5) 5) 5) 5) 5) 5) 5) 5) 5) 7) 8) 8) 8) 8) 8) 8) 8)	S21 S21 O27 O251 O252 N21 N22 C21 C22 C23 C23 C23 C26 C27 C28 C29	C21 C22 C27 C25 C25 C21 C23 C26 C21 C26 C23 C24 C23 C24 C25 C27 C28 C29 C210	1-736 (5 1-817 (6 1-335 (6 1-195 (7 1-291 (5 1-471 (6 1-350 (6 1-336 (7 1-537 (7 1-521 (7 1-537 (7 1-521 (7 1-537 (7 1-391 (7 1-368 (8 1-388 (8)))))))))))))))))))
07 07 07 07 07 052	Cu Cu Cu Cu	O52 N1 N21 N22 N1	171 1 (1) 90 2 (1) 94 3 (1) 100 0 (1) 81 8 (1)	O52 O52 N1 N1 N21	Cu Cu Cu Cu Cu	N21 N22 N21 N22 N22	92·6 (1) 87·3 (1) 165·9 (2) 117·5 (2) 75·0 (1)
Cl	SI	C2	90-0 (3)	C21	S21	C22	89·8 (2)
Cu Cu	O7 O52	C7 C5	124·7 (3) 116·3 (3)	Cu	O252	C25	105.6 (3)
Cu Cu C1 C6	NI NI NI N2	C1 C3 C3 C10	125·3 (3) 115·9 (3) 114·4 (5) 116·2 (5)	Cu Cu C21 C26 Cu Cu	N21 N21 N22 N22 N22 N22	C21 C23 C23 C210 C26 C210	120·5 (3) 126·4 (3) 113·1 (4) 119·9 (4) 108·7 (3) 130·8 (3)
S1 S1 N1 S1 N1 N1 C2 C2 C2 C4 O51 O51 O51 O51 O71 C1 O7 C6 C7 C8 N2	C1 C1 C2 C3 C3 C3 C3 C5 C5 C5 C6 C7 C7 C7 C8 C9 C1 C1 C1 C1 C1 C1 C1 C1 C2 C3 C3 C3 C3 C3 C3 C3 C3 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5	N1 C6 C3 C2 C4 C5 C5 C5 C3 C3 C1 C7 C7 C7 C6 C8 C8 C9 C19	$\begin{array}{c} 1161 \ (4) \\ 1206 \ (3) \\ 123\cdot3 \ (5) \\ 105\cdot5 \ (4) \\ 107\cdot2 \ (4) \\ 107\cdot2 \ (4) \\ 111\cdot9 \ (6) \\ 113\cdot2 \ (5) \\ 125\cdot7 \ (5) \\ 117\cdot1 \ (4) \\ 117\cdot2 \ (5) \\ 123\cdot6 \ (4) \\ 117\cdot3 \ (5) \\ 117\cdot1 \ (5) \$	S21 S21 S21 N21 S21 N21 N21 C22 C24 O251 O252 C25 N22 N22 C21 O27 C26 C27 C26 C27 C28 S22 S22 S22 S22 S22 S22 S22 S22 S22 S	C21 C21 C21 C22 C23 C23 C23 C23 C23 C23 C23 C23 C23	N21 C26 C23 C22 C24 C25 C25 C25 C25 C25 C23 C23 C21 C27 C27 C27 C27 C27 C27 C27 C27 C27 C27	$\begin{array}{c} 117.1 (3) \\ 124.4 (3) \\ 118.5 (4) \\ 105.9 (3) \\ 107.6 (3) \\ 107.6 (3) \\ 107.6 (3) \\ 107.6 (3) \\ 107.6 (3) \\ 107.6 (3) \\ 108.8 (4) \\ 111.4 (5) \\ 112.9 (4) \\ 108.5 (4) \\ 108.5 (4) \\ 108.5 (4) \\ 108.5 (4) \\ 111.4 (5) \\ 108.6 (3) \\ 108.6 (4) \\$

Table 4. Intermolecular hydrogen bonds O-H-O

Symmetry operators:	(i) $1 - x$, 0.5 + y, 2 -	-z; (ii) $x, y - 1, z$.
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H27—O27 H27…O51'	1·11 (1) Å 1·44 (1)	O27—H27…O51'	171 (1)°
H251	0·92 (1) Å 1·64 (1)	O251—H251…O7"	172 (1)°

[2.340 (4) Å] is significantly longer than the sum of the covalent radii. A weak electrostatic interaction is observed between Cu and O252. The distance Cu...O252 [2.727 (4) Å] is 0.65 Å shorter compared with the sum of the van der Waals radii but significantly longer than the sum of the covalent radii (Pauling, 1968).



Fig. 1. Plot of the molecule and numbering scheme.



Fig. 2. Stereoview of the unit cell; projection parallel to b.

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Structures of Polymeric Zinc 3,3-Dimethylacrylate and Zinc 2-Chlorobenzoate

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Abstract. (1): catena-Poly[zinc-tris- μ -(3,3-dimethylacrylato-O,O')-zinc- μ -(3,3-dimethylacrylato-O,O')] $[Zn_2{\mu-O_2CCH:C(CH_3)_2}_3{O_2CCH:C(CH_3)_2}], M_r =$ 527.2, orthorhombic, *Pbcn*, a = 19.881 (2), b =14.488 (2), c = 17.049 (2) Å, V = 4910.7 Å³, Z = 8, $D_x = 1.426$ Mg m⁻³, λ (Mo K α) = 0.71073 Å, $\mu =$ $2\cdot 04 \text{ mm}^{-1}$, $\breve{F}(000) = 2176$, T = 295 K, R = 0.0554for 2272 unique observed reflections. (2): catena-Poly[zinc-tris- μ -(2-chlorobenzoato-O,O')-zinc- μ -(2-chlorobenzoato-O,O')] [Zn₂(μ -O₂CC₆H₄Cl)₃(O₂C- C_6H_4Cl), $M_r = 753.0$, monoclinic, $P2_1/n$, a =11.219 (1), b = 13.536 (1), c = 19.790 (2) Å, $\beta =$ $V = 2918 \cdot 2 \text{ Å}^3$, 103·827 (9)°, 1·714 Mg m⁻³, Z = 4, $D_x =$ $\lambda(\mathrm{Cu}\;K\alpha) = 1.54184\;\mathrm{\AA},$ $\mu =$ 5.94 mm^{-1} , F(000) = 1504, T = 295 K, R = 0.0447for 3996 unique observed reflections. Both structures contain polymeric chains in which binuclear Zn₂(carboxylate) $_{3}^{+}$ units with three syn-syn bridging ligands are connected by single syn-anti carboxylate links.

Introduction. Anhydrous zinc carboxylates adopt a variety of structures. Features common to all so far reported are a tetrahedral coordination of Zn atoms and a bridging function for the carboxylate ligands. The acetate and propionate are both known in two different forms, with exclusively syn-anti carboxylate bridges which link the Zn atoms into either twodimensional sheets or a three-dimensional crosslinked network (Capilla & Aranda, 1979; Clegg, Little & Straughan, 1986b; Goldschmied, Rae & Stephenson, 1977; Clegg, Little & Straughan, 1987). The benzoate (Guseinov, Musaev, Usubaliev, Amiraslanov & Mamedov, 1984) and crotonate (Clegg, Little & Straughan, 1986a) form polymeric chains in which $Zn_2(carboxylate)_3^+$ binuclear units with three syn-syn bridges are connected by single syn-anti carboxylates. Only syn-syn bridges occur in the structure of the 2-chlorobenzoate reported by Nakacho, Misawa, Fujiwara, Wakahara & Tomita

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(1976), pairs of carboxylates linking the Zn atoms into chains.

As part of a continuing study of zinc carboxylate structures, in an attempt to understand the factors influencing the choice of structure adopted for a particular carboxylate, and to investigate polymorphism in these compounds, we have determined the structure of zinc 3,3-dimethylacrylate and a second form of zinc 2-chlorobenzoate, which are reported here.

Experimental. The compounds were synthesized by refluxing freshly prepared zinc hydroxide with the corresponding carboxylic acids in water and recrystallized from ethanol (1) or acetone (2). Information for (2) is given in square brackets where it differs from that for (1). Crystal size $0.37 \times 0.37 \times 0.42$ mm $[0.08 \times 0.20 \times 0.40 \text{ mm}]$, Stoe-Siemens diffractometer, unit-cell parameters from 2θ values of 32 reflections (20–25°) [(20–40°)] measured at $\pm \omega$. Data collection in $\omega - \theta$ scan mode, scan width 0.765° $[0.68^{\circ}]$ below α_1 to 0.765° $[0.68^{\circ}]$ above α_2 , scan time 14-56s, $2\theta_{\text{max}}$ 50° [130°], index ranges $h0 \rightarrow 23$, $k0 \rightarrow$ $17, l0 \rightarrow 20 \ [h - 13 \rightarrow 13, k0 \rightarrow 15, l - 23 \rightarrow 23]$, correction for small decay in intensities of three standard reflections, semi-empirical absorption corrections, transmission 0.303-0.352 [0.168-0.327], 4320 [9807] reflections measured, 4320 [4943] unique, 2272 [3996] with $F > 4\sigma(F)$, $[R_{int} = 0.0428]$.

Structure solution by Patterson and difference syntheses, blocked-cascade least-squares refinement on F, weighting $w^{-1} = \sigma^2(F)$, anisotropic thermal parameters for all non-H atoms, H atoms constrained (C—H 0.96 Å, H—C—H 109.5°), aromatic and olefinic H atoms on angle external bisectors, $U(H) = 1.2U_{eq}(C)$, extinction parameter x = 1.0 (2) $\times 10^{-7}$ [1.7 (1) $\times 10^{-6}$], whereby $F'_c = F_c/(1 + xF_c^2/$ $\sin 2\theta)^{1/4}$. [Twofold disorder of orientation for one 2-chlorobenzoate ligand; occupancy factors refined © 1990 International Union of Crystallography