$0,9451X - 0,3263Y - 0,0197Z + 1,6324 = 0$ (III)
durch die Atome S(2), C(2), N(2), C(5).

(Orthogonales Achsensystem mit X parallel **a** und Z parallel **c***.) Der Winkel zwischen den Ebenen (II)–(III) beträgt 11,4°, während die Winkel zwischen den Ebenen (I)–(II) 73,4 ° und den Ebenen (I)–(III) 81,5 ° betragen (Fig. 2).

Aus der vorliegenden Konformation ist ersichtlich, dass in Lösung eine ungehinderte Rotation beider Thiocyanatgruppen um die C(3)–C(4)- bzw. C(4)–C(5)-Achse vonstatten gehen kann. Eine Wechselwirkung der freien Elektronenpaare an den Stickstoffatomen untereinander oder mit dem π-Elektronenpaar der C(4)–C(6)-Bindung ist auszuschliessen.

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DL-1-Amino-1,2-dicarboxyethane (Aspartic Acid) Hydrochloride

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Abstract. $C_4H_8NO_4Cl$, monoclinic, $P2_1/a$, $a = 11 \cdot 14_4$, $b = 6 \cdot 31_4$, $c = 11 \cdot 24_8$ Å, $\beta = 120 \cdot 20\,(2)°$, $Z = 4$, $D_c = 1 \cdot 65$ g cm^{-3}, μ(Cu $K\bar{\alpha}$) = 46·8 cm^{-1}. The bond lengths and angles are consistent with those in the closely-related structures of DL-aspartic acid and L-aspartic acid.

Introduction. The facility with which modern computers manipulate 3D data has relegated the role of generalized projections (Cochran & Dyer, 1952) to one of historical interest. Nevertheless, the structure analysis reported here is worthy of note as a striking illustration of the way in which atoms that overlap in projection could be resolved with less-demanding 2D Fourier summations. Furthermore, the clarity with which the H atoms are resolved carries its own commentary on the quality of the experimental intensities derived visually. It therefore has some relevance to the present resurgence of interest in photographic methods (IUCr Tenth International Congress, 1975).

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* B. Dawson died on February 20, 1974. The text presented here was prepared by his colleagues, being based on the records left by Dr Dawson. Unfortunately these records do not include a list of the structure factor data used for the structure determination. Publication of the paper has, however, been permitted in view of the circumstances. The paper is communicated by the Chief, Division of Chemical Physics, to whom any correspondence should be directed.

This work was undertaken originally as part of a programme of amino acid analyses (Dawson & Mathieson, 1951; Dawson, 1953; Mathieson, 1952, 1953) and reported briefly (Dawson, 1960), but full details were not given. The refinement of this structure is of

Table 1. *Atomic fractional coordinates with standard deviations for the non-hydrogen atoms*

The temperature factor is of the form
$$\exp[-(B_{11}h^2 + B_{22}k^2 + B_{33}l^2 + B_{13}hl + B_{23}kl)].$$
All values have been multiplied by 10^4 except the H thermal parameter.

	x	y	z	B_{11}	B_{22}	B_{33}	B_{13}	B_{23}
C(1)	3854 (7)	6840 (22)	897 (7)	29	85	20	17	0
C(2)	4185 (7)	7500 (22)	2345 (7)	25	66	20	9	0
C(3)	3135 (7)	6660 (22)	2690 (7)	30	66	20	16	0
C(4)	3552 (7)	7040 (22)	4175 (7)	29	78	20	17	0
O(1)	3005 (5)	5510 (22)	243 (5)	39	92	30	32	−0·2
O(2)	4592 (5)	7980 (22)	502 (5)	34	85	23	25	0
O(3)	2570 (5)	6480 (22)	4453 (5)	31	91	23	19	0
O(4)	4682 (5)	7740 (22)	5027 (5)	37	91	25	28	0
N	4300 (6)	9845 (16)	2491 (6)	25	79	20	9	−0·1
Cl	1424 (2)	1718 (3)	2469 (2)	35	80	22	26	0

	x	y	z	B_{iso}		x	y	z	B_{iso}
H(1)	5000	6800	2950	2·52	H(5)	4550	300	3300	2·52
H(2)	3000	5200	2550	2·52	H(6)	4900	400	2300	2·52
H(3)	2200	7200	2100	2·52	H(7)	4350	7600	9250	2·52
H(4)	3500	500	1900	2·52	H(8)	3000	6400	5250	2·52

historical importance as it constituted a valuable experimental basis for the early development of the generalized structure factor formalism (Dawson, 1975).

Unit-cell dimensions were determined from Weissenberg photographs calibrated against Ag and Pt (Fridrichsons, 1959). Following the standard practice of that era, intensities (Cu $K\bar{\alpha}$ radiation) were recorded on Weissenberg photographs of several layers about a and b, the intensities being estimated visually. Since a crystal of ca 0·1 mm maximum dimension was used, no absorption corrections were applied.

The atomic parameters, refined by normal and generalized Fourier projections, are listed in Table 1; owing to the restrictions of the recorded data, the cross terms B_{12} and B_{23} of the anisotropic temperature factors are set at zero. The resultant bond lengths and angles are given in Table 2, and Fig. 1.
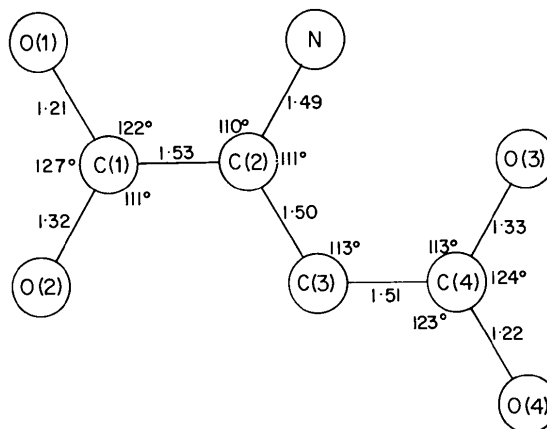

Fig. 1. Diagram of the molecular ion, with dimensions in Å and degrees.

Table 2. *Bond lengths and angles with standard deviations*

|					
C(1)—C(2)	1·531 (12) Å	O(2)—H(7)	0·79 Å	N—C(2)—H(1)	113°
C(2)—C(3)	1·503 (13)	O(3)—H(8)	0·78	C(2)—C(3)—H(2)	113
C(3)—C(4)	1·511 (12)	C(1)—C(2)—C(3)	112·4 (0·7)°	C(4)—C(3)—H(2)	106
C(1)—O(1)	1·214 (16)	C(2)—C(3)—C(4)	112·5 (0·7)	C(2)—C(3)—H(3)	114
C(1)—O(2)	1·316 (14)	C(2)—C(1)—O(1)	121·7 (1·0)	C(4)—C(3)—H(3)	109
C(4)—O(3)	1·328 (11)	C(2)—C(1)—O(2)	111·3 (0·9)	H(2)—C(3)—H(3)	102
C(4)—O(4)	1·219 (12)	O(1)—C(1)—O(2)	126·9 (1·4)	C(2)—N—H(4)	112
C(2)—N	1·488 (18)	C(3)—C(4)—O(3)	112·7 (0·7)	C(2)—N—H(5)	114
C(2)—H(1)	0·93	C(3)—C(4)—O(4)	123·2 (0·8)	C(2)—N—H(6)	114
C(3)—H(2)	0·93	O(3)—C(4)—O(4)	124·0 (0·8)	H(4)—N—H(5)	108
C(3)—H(3)	0·97	C(1)—C(2)—N	109·7 (1·0)	H(4)—N—H(6)	103
N—H(4)	0·90	C(3)—C(2)—N	111·0 (1·0)	H(5)—N—H(6)	104
N—H(5)	0·86	C(1)—C(2)—H(1)	106	C(1)—O(2)—H(7)	105
N—H(6)	0·87	C(3)—C(2)—H(1)	104	C(4)—O(3)—H(8)	101

(a) (b)
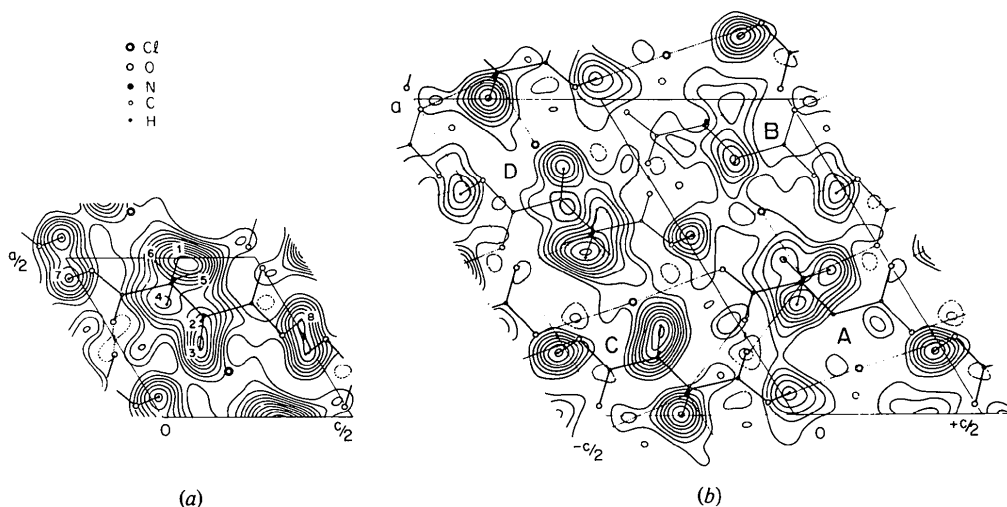
Fig. 2. (a) Zero-layer difference synthesis projected down b showing hydrogen atoms. (b) Combination of the zero-layer (O), cosine (C_1) and sine (S_1) components of the first-layer generalized projection. The combinations are as follows: in sector A, $O + C_1 + S_1$, sector B, $O - C_1 + S_1$, sector C, $O - C_1 - S_1$, and sector D, $O + C_1 - S_1$.

H atoms were located as follows. Fig. 2(*a*) shows the difference projection from only *h0l* data. This projection reveals the existence of H atoms but owing to considerable overlap only three of the eight, H(4), H(7) and H(8), are delineated with reasonable clarity. The other H atoms are distinguished individually, as shown in Fig. 2(*b*), by calculation of appropriate combinations of the first-layer (*h1l*) cosine (C_1) and sine (S_1) generalized difference projections with the zero-layer *h0l* (designated *O*) difference projection. Thus, in sector *A* ($O + C_1 + S_1$), H(4), H(5) and H(6) attached to N, and H(7), H(8) attached to O(2), O(3) respectively are clearly portrayed. In sector *B* ($O - C_1 + S_1$), H(2) attached to C(3) is shown while H(3), also attached to C(3), appears clearly in sector *D* ($O + C_1 - S_1$). H(1) attached to C(2) is clearly depicted in sector *C* ($O - C_1 - S_1$).

Discussion. This work complements that on the closely-related structures of DL-aspartic acid (Amirthalingam & Ramachandran, 1955; Rao, Srinivasan & Valambal, 1968; Rao, 1973) and L-aspartic acid (Derissen, Endeman & Peerdeman, 1968). The bond lengths found in the former are consistent with those presented here, to within the limits of experimental error. The results for the latter are also consistent with the present work except that the C(1)O(1)-O(2) carboxyl group is evidently ionized to form a zwitterion. In all three analyses, the C atom skeleton maintains a planar zigzag conformation.

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Structural Studies of Precursor and Partially Oxidized Conducting Complexes. III. A Neutron Diffraction Study of Barium Tetracyanoplatinate(II) Tetrahydrate*

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Abstract. Ba[Pt(CN)$_4$].4H$_2$O, monoclinic $C2/c$ (C_{2h}^6), $a = 12\cdot278$ (9), $b = 13\cdot882$ (10), $c = 6\cdot641$ (5) Å, $\beta = 107\cdot75$ (4)°, $Z = 4$, $D_m = 3\cdot09$ (1), $D_x = 3\cdot13$ g cm^{-3}. A room-temperature, single-crystal neutron diffraction study was performed. The structural solution was obtained by direct methods, and refinement by full-matrix least-squares techniques gave $R(F_o^2) = 0\cdot052$ for 1437 observed reflections $> \sigma(F_o^2)$. The Pt atoms, at the centers of the planar tetracyanoplatinate anions, are arranged in a linear chain, separated by $3\cdot321$ (3) Å.

Introduction. As a result of our ongoing study of par-

tially oxidized tetracyanoplatinate conducting salts, we are able to explain why some cations are more favorable for the formation of these salts, while other cations are unsuitable. Alkali metal ions such as K$^+$ (Williams, Keefer, Washecheck & Enright, 1976; Williams, Petersen, Gerdes & Peterson, 1974) as well as the organic guanidium cation [C(NH$_2$)$_3$]$^+$ (Williams, Cornish, Washecheck & Johnson, 1976), are all known to form partially oxidized tetracyanoplatinate compounds. To date, however, no such compounds with divalent cations have been prepared (Koch, Gebert & Williams, 1976). With this room-temperature, single-crystal neutron diffraction study of Ba[Pt(CN)$_4$].4H$_2$O, we are able to rationalize the non-existence of partially oxidized barium tetracyanoplatinates and, more generally, the entire series of tetracyanoplatinates which might contain divalent cations.