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A rotational search procedure for detecting a known molecule in a crystal. Errata.

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A recently published paper with the above title (Lattman & Love, 1970) contains three errors which require correction:

On page 1855, column 2, fourth line below equation (2), replace **C** by $\tilde{\mathbf{C}}$.

On page 1855, column 2, equation (4), replace $\tilde{\mathbf{C}}$ by **C**.

On page 1856, column 1, equation (6) and following, read:

$$\Delta^2 = (1/V) \cdot \int_V [R(\theta) - \bar{R}]^2 \mathrm{d}V. \qquad (6)$$

Here V is the volume explored in θ space, $\bar{R}$ is $\cdots$.

Reference

LATTMAN, E. E. & LOVE, W. E. (1970). *Acta Cryst.* B**26**, 1854.

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Further refinement of the structure of *p*-nitrobenzoic acid.*

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The structure of *p*-nitrobenzoic acid has been refined further after including hydrogen atoms and using anisotropic temperature factors; final R for 744 observed reflexions is 0·074 and the average estimated standard deviation in bond lengths is 0·006 Å. The central aromatic bonds are shortened from the normal value in crystalline benzene, although the shortening is more in *p*-nitroaniline and *p*-aminobenzoic acid; these results probably indicate that cooperative electronic interaction between the *para* substituents in the latter compounds must be only partly responsible for the shortening of the central aromatic bonds.

In the structure of *p*-nitrobenzoic acid reported earlier (Sakore & Pant, 1966; hereinafter referred to as paper I), the central aromatic bonds are of normal length. This result is expected because both the *para* substituents are electron-withdrawing groups and no resonance interaction is expected. However, in view of the shortening of the central aromatic bonds in terephthalic acid (Bailey & Brown, 1967), a molecule which has electron-withdrawing carboxylic groups in *para* positions, it was felt that the structure of *p*-nitrobenzoic acid should be refined thoroughly to decide whether there is in fact central-bond shortening in this molecule. In paper I, hydrogen atoms of the aromatic ring were not included in the structure refinement, and only individual isotropic temperature factors were used.

The refinement was started with the parameters given in paper I. Hydrogen atoms were included in the structure refinement and anisotropic temperature factors were introduced; five cycles of refinement decreased R by about

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Table 1. *Final atomic and thermal parameters*

Thermal parameters ($\times 10^4$) are of the form $T = \exp[-(b_{11}h^2 + b_{22}k^2 + b_{33}l^2 + 2b_{12}hk + 2b_{23}kl + 2b_{13}hl)]$.

	x	y	z	b_{11}	b_{22}	b_{33}	b_{12}	b_{23}	b_{13}
C(1)	0·4163±0·0003	0·4987±0·0009	0·0896±0·0002	49±2	308±18	16±1	−1±6	6±4	3±1
C(2)	0·4898±0·0003	0·6421±0·0009	0·1293±0·0002	42±2	346±20	20±1	−5±6	−7±4	1±1
C(3)	0·4590±0·0003	0·8345±0·0009	0·1689±0·0002	49±2	368±21	18±1	−11±6	−1±4	1±1
C(4)	0·3536±0·0003	0·8881±0·0009	0·1666±0·0002	54±2	275±17	15±1	−3±6	−2±3	4±1
C(5)	0·2790±0·0003	0·7492±0·0010	0·1281±0·0002	46±2	368±19	19±1	−1±6	−1±4	4±1
C(6)	0·3105±0·0003	0·5525±0·0009	0·0896±0·0002	40±2	338±20	20±1	−9±6	−9±4	4±1
C(7)	0·4525±0·0003	0·2878±0·0009	0·0490±0·0002	47±2	305±18	17±1	−1±6	8±4	2±1
O(1)	0·5464±0·0002	0·2407±0·0007	0·0487±0·0001	49±2	405±14	23±1	9±5	−21±3	3±1
O(2)	0·3798±0·0002	0·1585±0·0006	0·0147±0·0001	48±2	412±15	23±1	2±5	−35±3	2±1
O(3)	0·3821±0·0002	0·1783±0·0007	0·2504±0·0002	66±2	515±18	27±1	−15±6	−46±4	3±1
O(4)	0·2295±0·0002	0·1722±0·0007	0·1983±0·0001	60±2	440±16	28±1	32±5	−4±3	8±1
N	0·3184±0·0003	0·0933±0·0008	0·2085±0·0002	57±2	329±16	22±1	−12±6	−8±4	13±1
H(1)	0·408±0·004	0·034±0·012	−0·007±0·002						
H(2)	0·560±0·004	0·602±0·011	0·131±0·002						
H(3)	0·512±0·004	0·931±0·011	0·200±0·002						
H(5)	0·210±0·004	0·813±0·012	0·130±0·002						
H(6)	0·261±0·004	0·470±0·012	0·064±0·002						