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*Acta Cryst.* (1991). C**47**, 2127–2131

# Structure of 4-Cyano-4′-iodobiphenyl at 297 and 183 K

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(*Received* 6 *June* 1990; *accepted* 2 *April* 1991)

**Abstract.** 4′-Iodobiphenyl-4-carbonitrile, $C_{13}H_8IN$, $M_r = 305{\cdot}12$, monoclinic, $P2_1/c$, $Z = 8$, Mo $K\alpha$, $\lambda = 0{\cdot}71069$ Å, $F(000) = 1168$. At 297 (2) K, $a = 9{\cdot}854\,(2)$, $b = 14{\cdot}869\,(3)$, $c = 17{\cdot}103\,(5)$ Å, $\beta = 115{\cdot}44\,(2)°$, $V = 2262{\cdot}9$ Å$^3$, $D_x = 1{\cdot}791\,(2)$ g cm$^{-3}$, $\mu = 27{\cdot}64$ cm$^{-1}$, $R = 0{\cdot}043$ for 3950 reflections. At 183 (4) K, $a = 9{\cdot}766\,(3)$, $b = 14{\cdot}850\,(8)$, $c = 16{\cdot}806\,(6)$ Å, $\beta = 115{\cdot}24\,(3)°$, $V = 2204{\cdot}6$ Å$^3$, $D_x = 1{\cdot}838\,(4)$ g cm$^{-3}$, $\mu = 28{\cdot}37$ cm$^{-1}$, $R = 0{\cdot}054$ for 6128 reflections. The two crystallographically independent molecules (*A* and *B*) are similar and both have the expected geometry and dimensions. Each molecule is part of a chain of crystallographically equivalent molecules with short intermolecular N···I distances [3·243 (8) and 3·180 (8) Å at 297 K] and approximately linear C—N···I—C in each chain. There is disorder such that between 1 and 2% of the molecules appear to have I and CN interchanged; presumably any particular chain is ordered but 1 to 2% of the chains are in the opposite direction to the majority.

**Introduction.** As part of a study of intermolecular donor–acceptor interactions in crystals we have looked for examples of interactions between nitrile N atoms and I atoms in *p*-iodobenzonitrile (Schlemper & Britton, 1965), *o*-iodobenzonitrile (Lam & Britton, 1974) and 2,6-dibromo-4-iodobenzonitrile (Gleason & Britton, 1978). The expected interaction was found in the two compounds with I *para* to the CN but not in the *ortho* compound, where iodine–iodine and nitrile–nitrile interactions occurred. We report here the crystal structure of another member of this series. The structure has been determined at two temperatures, 297 and 183 K. This was carried out in response to a referee's comment on the disorder reported in the 297 K determination (see below).

**Experimental.** The compound was prepared as described by McNamara & Gleason (1976) and recrystallized from ethanol. Experimental data are given in Table 1. Data were collected on an Enraf–Nonius CAD-4 diffractometer equipped with a graphite monochromator. Systematic extinctions (0*k*0, *k* odd; *h*0*l*, *l* odd) uniquely determined the space group. Data were collected using *ω* scans. Absorption corrections were made using *DIFABS* (Walker & Stuart, 1983). The unit cell was very similar to that of the analogous bromine compound (Kronebusch, Gleason & Britton, 1976*a*) and the positional parameters from that structure were successfully used to provide a trial structure. The structure was refined with full-matrix least-squares refinement on *F*'s. All non-H atoms were given anisotropic thermal parameters; H atoms were included at idealized positions with isotropic *B* values 20% larger than the equivalent isotropic *B* value of the attached atom. Refinement of the initial data set (297 K) converged with $R = 0{\cdot}044$, $wR = 0{\cdot}048$ and $S = 1{\cdot}58$; $w = 1/\sigma^2(F)$ was calculated from $\sigma^2(I) = \sigma^2(I)_c + (0{\cdot}04I)^2$, where $\sigma(I)_c$ is the standard deviation in *I* based solely on counting statistics. However, the C1—N1 and C2—C1 distances were abnormal [for example, the C1—N1 distances were 1·027 (8) and 1·074 (8) Å, respectively, shorter than usual and in poor agreement with each other]. The possibility of disorder was considered, and tested by including an I atom 2·10 Å from each C2 atom with fixed positional parameters and fixed isotropic $B = 4{\cdot}60$ Å$^2$, the average of the equivalent isotropic *B*'s of

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Table 1. *Experimental data*

| | 297 K | 183 K |
|---|---|---|
| Crystal size (mm) | 0·20 × 0·25 × 0·35 | 0·35 × 0·35 × 0·40 |
| Reflections used for lattice parameters | | |
| Number | 24 | 24 |
| $\theta$ range (°) | 13–19 | 13–22 |
| Data collection | | |
| $\theta$ range (°) | 0–26 | 0–32 |
| $h, k, l$ | 0–12, 0–18, −21–21 | −14–14, 0–22, −25–25 |
| Number of reflections collected | 4550 | 15220 |
| Number of unique reflections | 4429 | 7633 |
| $R_{\rm int}$ | 0·014 | 0·028 |
| Number of reflections used | 3950 | 6128 |
| Criterion for reflections used | $I > \sigma(I)$ | $I > 2\sigma(I)$ |
| Check reflections | 3 | 3 |
| Time between checks (s) | 10000 | 3000 |
| Crystal decay | None | None |
| Absorption corrections | 0·68–1·56 | 0·71–1·25 |
| Secondary-extinction coefficient | $4·47 \times 10^{-8}$ | $2·58 \times 10^{-7}$ |
| $R$ | 0·043 | 0·053 |
| $wR$ | 0·047 | 0·066 |
| $S$ | 1·56 | 1·53 |
| $(\Delta/\sigma)_{\rm max}$ | 0·02 | 0·04 |
| $(\Delta\rho)_{\rm max,min}$ (e Å$^{-3}$) | 0·58, −0·91 | 2·11, −1·81 |

the I atoms attached to C11; only the occupancies of these disordered I atoms were allowed to vary, with the constraint that the total $I$ population was 1·000 per molecule. This refinement converged with $R$ = 0·043, $wR$ = 0·047 and $S$ = 1·56, with occupancies for I2*A* and I2*B* of 0·016 (2) and 0·011 (2), respectively. This was accepted as the final refinement. Atomic scattering factors and anomalous-dispersion corrections for all atoms were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV). The computer programs used were from *TEXSAN* (Molecular Structure Corporation, 1985).

At this point the determination seemed complete. However, two referees for the original manuscript questioned the reality of an apparent disorder as small as this. We felt that it was real because other nitrile structures do not show such short C—N distances. If we use the $\mathcal{R}$ factor (Hamilton, 1965) to assess the significance of the improvement, the experimental $\mathcal{R}$ is approximately 1·02, while $\mathcal{R}_{2,3676,0·005}$ = 1·0015. Therefore we would say that the hypothesis that there is no disorder can be rejected at the 99·5% confidence level or higher. Nevertheless, as a further test of the reality of the disorder, we decided to collect another data set, at low temperature, using a different crystal from the same synthetic batch.

The data-collection parameters are given in Table 1. The same procedures were used and refinement converged, assuming no disorder, with $R$ = 0·054, $wR$ = 0·067 and $S$ = 1·562. Again the C1—N1 distances, 1·055 (8) and 1·095 (7) Å, respectively, were abnormal. Again disordered I atoms were put in both molecules at the distance and with the isotropic thermal parameters found for the primary positions, and with only the two occupancies as variables. This refinement converged with $R$ = 0·053, $wR$ = 0·066 and $S$ = 1·533, with occupancies for I2*A* and I2*B* of 0·019 (1) and 0·013 (1), respectively. These values agree well with the values from the 297 K refinement. Since the low-temperature data contain a larger fraction of high-angle data, which are less affected by the outer shell electrons, we regard this as good confirmation of the reality of the proposed disorder.

As a further check on the reality of the disorder Fig. 1 shows difference Fourier maps in the region of the CN group, for both the ordered and disordered model. In the map for the disordered model, the C and N atoms have been kept at their final positions, but the minor component of the I atoms has been omitted in $F_C$. In the map from the ordered model there is a small peak beween C1*A* and N1*A*, but it is not among the higher peaks on the map, which are all near the major I-atom positions. In the map from the disordered model the minor component of the I shows up as the highest peak on the map, although the other peaks change very little. Maps for molecule *B* are not shown but they are quite similar.

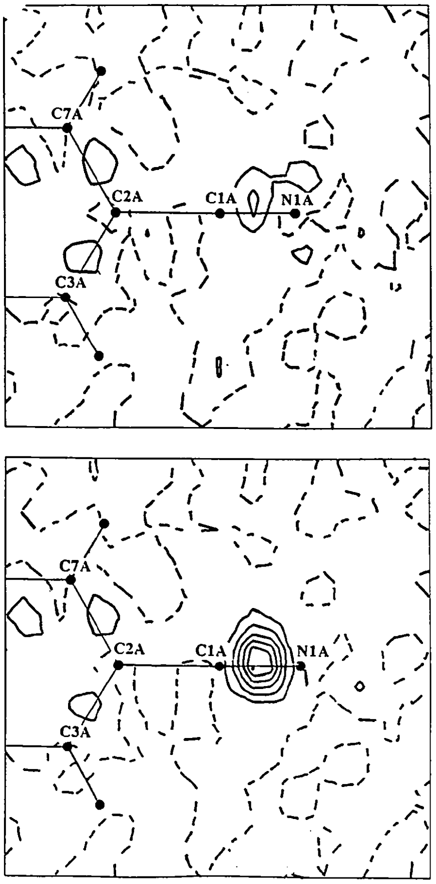

Fig. 1. Difference Fourier maps in the region of the CN group from molecule *A*. Solid lines – positive contours at 0·50 e Å$^{-3}$ intervals; dashed lines – zero contour. Above: map based on the final refinement assuming complete order. Below: map based on the final parameters from the disordered structure, but with the minor component of the disordered I removed.

Table 2. *Atomic coordinates and equivalent isotropic thermal parameters*

$$B_{eq} = (8\pi^2/3)\textstyle\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

| | $x$ | $y$ | $z$ | $B_{eq}$(Å$^2$) |
|---|---|---|---|---|
| 297 K | | | | |
| N1*A* | 0·0167 (8) | −0·2076 (4) | 0·1127 (4) | 8·7 (4) |
| C1*A* | 0·0211 (9) | −0·1323 (6) | 0·1130 (4) | 7·1 (4) |
| C2*A* | 0·0188 (7) | −0·0354 (3) | 0·1159 (3) | 4·7 (2) |
| C3*A* | 0·1526 (6) | 0·0114 (3) | 0·1599 (3) | 4·7 (2) |
| C4*A* | 0·1492 (5) | 0·1036 (3) | 0·1650 (3) | 4·3 (2) |
| C5*A* | 0·0147 (5) | 0·1494 (3) | 0·1255 (3) | 3·7 (2) |
| C6*A* | −0·1175 (6) | 0·1029 (3) | 0·0806 (4) | 4·8 (2) |
| C7*A* | −0·1156 (7) | 0·0104 (4) | 0·0762 (4) | 5·4 (2) |
| C8*A* | 0·0104 (4) | 0·2508 (3) | 0·1309 (3) | 3·6 (2) |
| C9*A* | 0·0979 (5) | 0·2951 (3) | 0·2073 (3) | 4·1 (2) |
| C10*A* | 0·0953 (5) | 0·3881 (3) | 0·2128 (3) | 4·2 (2) |
| C11*A* | 0·0043 (5) | 0·4373 (3) | 0·1410 (3) | 3·7 (2) |
| C12*A* | −0·0839 (6) | 0·3952 (3) | 0·0647 (3) | 4·3 (2) |
| C13*A* | −0·0814 (6) | 0·3018 (3) | 0·0590 (3) | 4·4 (2) |
| I1*A* | 0·00447 (4) | 0·57836 (2) | 0·14558 (3) | 4·55 (2) |
| N1*B* | 0·4929 (6) | 0·0478 (4) | 0·1106 (4) | 7·4 (3) |
| C1*B* | 0·4922 (8) | 0·1239 (6) | 0·1116 (4) | 6·3 (3) |
| C2*B* | 0·4945 (5) | 0·2201 (3) | 0·1170 (3) | 4·1 (2) |
| C3*B* | 0·6291 (6) | 0·2666 (3) | 0·1455 (4) | 4·7 (2) |
| C4*B* | 0·6278 (5) | 0·3591 (3) | 0·1489 (3) | 4·1 (2) |
| C5*B* | 0·4949 (5) | 0·4067 (3) | 0·1266 (3) | 3·4 (2) |
| C6*B* | 0·3624 (5) | 0·3597 (3) | 0·0998 (3) | 3·9 (2) |
| C7*B* | 0·3599 (6) | 0·2661 (3) | 0·0938 (3) | 4·5 (2) |
| C8*B* | 0·4960 (5) | 0·5069 (3) | 0·1288 (3) | 3·3 (2) |
| C9*B* | 0·5852 (5) | 0·5557 (3) | 0·1001 (3) | 3·8 (2) |
| C10*B* | 0·5841 (5) | 0·6487 (3) | 0·1004 (3) | 3·8 (2) |
| C11*B* | 0·4917 (5) | 0·6940 (3) | 0·1294 (3) | 3·6 (2) |
| C12*B* | 0·4020 (5) | 0·6460 (3) | 0·1599 (3) | 4·2 (2) |
| C13*B* | 0·4063 (5) | 0·5541 (3) | 0·1594 (3) | 3·9 (2) |
| I1*B* | 0·48721 (4) | 0·83494 (2) | 0·12689 (2) | 4·66 (2) |
| 183 K | | | | |
| N1*A* | 0·0227 (7) | −0·2110 (4) | 0·1161 (4) | 4·7 (2) |
| C1*A* | 0·0240 (7) | −0·1343 (4) | 0·1145 (4) | 3·6 (2) |
| C2*A* | 0·0216 (6) | −0·0376 (3) | 0·1163 (3) | 2·4 (1) |
| C3*A* | 0·1560 (5) | 0·0100 (3) | 0·1604 (3) | 2·5 (1) |
| C4*A* | 0·1524 (5) | 0·1031 (3) | 0·1653 (3) | 2·4 (1) |
| C5*A* | 0·0159 (5) | 0·1487 (3) | 0·1256 (3) | 2·0 (1) |
| C6*A* | −0·1161 (5) | 0·1005 (3) | 0·0812 (3) | 2·4 (1) |
| C7*A* | −0·1161 (5) | 0·0088 (3) | 0·0766 (4) | 2·8 (2) |
| C8*A* | 0·0114 (4) | 0·2499 (3) | 0·1311 (3) | 2·1 (1) |
| C9*A* | 0·1010 (5) | 0·2950 (3) | 0·2083 (3) | 2·4 (1) |
| C10*A* | 0·0983 (5) | 0·3879 (3) | 0·2140 (3) | 2·3 (1) |
| C11*A* | 0·0041 (4) | 0·4369 (3) | 0·1418 (3) | 2·1 (1) |
| C12*A* | −0·0882 (5) | 0·3938 (3) | 0·0634 (3) | 2·4 (1) |
| C13*A* | −0·0845 (5) | 0·3003 (3) | 0·0588 (3) | 2·4 (1) |
| I1*A* | 0·00351 (3) | 0·57797 (2) | 0·14552 (2) | 2·38 (1) |
| N1*B* | 0·4928 (6) | 0·0448 (3) | 0·1091 (4) | 4·1 (2) |
| C1*B* | 0·4889 (7) | 0·1219 (3) | 0·1098 (4) | 3·4 (2) |
| C2*B* | 0·4917 (5) | 0·2185 (3) | 0·1162 (3) | 2·4 (1) |
| C3*B* | 0·6290 (5) | 0·2645 (3) | 0·1453 (3) | 2·6 (2) |
| C4*B* | 0·6281 (5) | 0·3578 (3) | 0·1493 (3) | 2·3 (1) |
| C5*B* | 0·4950 (4) | 0·4052 (3) | 0·1270 (3) | 1·9 (1) |
| C6*B* | 0·3597 (5) | 0·3587 (3) | 0·0989 (3) | 2·2 (1) |
| C7*B* | 0·3571 (5) | 0·2645 (3) | 0·0922 (3) | 2·5 (1) |
| C8*B* | 0·4950 (4) | 0·5056 (3) | 0·1297 (3) | 2·0 (1) |
| C9*B* | 0·5851 (5) | 0·5546 (3) | 0·1002 (3) | 2·1 (1) |
| C10*B* | 0·5830 (5) | 0·6472 (3) | 0·0999 (3) | 2·2 (1) |
| C11*B* | 0·4920 (4) | 0·6935 (3) | 0·1305 (3) | 2·0 (1) |
| C12*B* | 0·3987 (5) | 0·6452 (3) | 0·1603 (3) | 2·2 (1) |
| C13*B* | 0·4035 (5) | 0·5522 (3) | 0·1599 (3) | 2·2 (1) |
| I1*B* | 0·48567 (3) | 0·83435 (2) | 0·12652 (2) | 2·42 (1) |

**Discussion.** The final positional parameters are given in Table 2.* The thermal ellipsoids and labelling of the atoms are shown in Figs. 2 and 3, for 297 and 183 K, respectively. Bond lengths and angles are

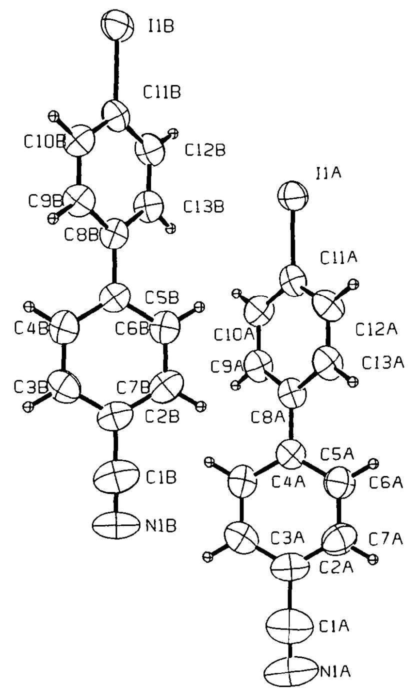

Fig. 2. View along the *c* axis of the two molecules in the asymmetric unit. Thermal ellipsoids are shown at the 50% probability level for the structure at 297 K. H atoms are shown with arbitrary size.

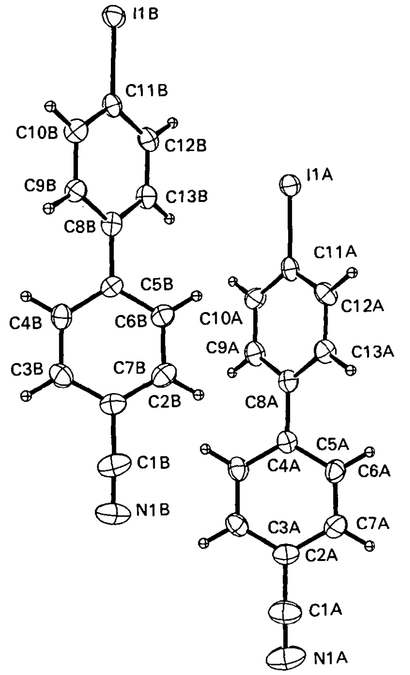

Fig. 3. View along the *c* axis of the two molecules in the asymmetric unit. Thermal ellipsoids are shown at the 50% probability level for the structure at 183 K. H atoms are shown with arbitrary size.

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* Lists of structure factors, anisotropic thermal parameters, H-atom positional parameters and deviations from the mean planes of the benzene rings have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54123 (80 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 3. *Bond lengths* (Å) *and angles* (°)

| | 297 K | | 183 K | |
|---|---|---|---|---|
| | Molecule *A* | Molecule *B* | Molecule *A* | Molecule *B* |
| N1—C1 | 1·121 (12) | 1·132 (12) | 1·140 (8) | 1·147 (7) |
| C1—C2 | 1·442 (10) | 1·432 (10) | 1·437 (7) | 1·438 (7) |
| C2—C3 | 1·391 (7) | 1·386 (7) | 1·394 (7) | 1·395 (6) |
| C3—C4 | 1·375 (7) | 1·377 (7) | 1·386 (6) | 1·386 (6) |
| C4—C5 | 1·382 (6) | 1·391 (6) | 1·387 (6) | 1·383 (6) |
| C5—C6 | 1·380 (7) | 1·374 (6) | 1·382 (6) | 1·383 (6) |
| C6—C7 | 1·378 (7) | 1·396 (6) | 1·364 (6) | 1·402 (6) |
| C7—C2 | 1·381 (8) | 1·390 (7) | 1·401 (7) | 1·380 (6) |
| C5—C8 | 1·513 (6) | 1·491 (6) | 1·508 (6) | 1·492 (6) |
| C8—C9 | 1·385 (6) | 1·382 (6) | 1·389 (6) | 1·387 (6) |
| C9—C10 | 1·386 (6) | 1·382 (6) | 1·384 (6) | 1·375 (6) |
| C10—C11 | 1·378 (7) | 1·384 (6) | 1·377 (6) | 1·384 (6) |
| C11—C12 | 1·369 (7) | 1·401 (6) | 1·395 (6) | 1·409 (6) |
| C12—C13 | 1·394 (7) | 1·367 (6) | 1·393 (6) | 1·382 (6) |
| C13—C8 | 1·396 (6) | 1·395 (6) | 1·394 (6) | 1·386 (6) |
| C11—I1 | 2·099 (5) | 2·096 (5) | 2·096 (5) | 2·093 (5) |
| N1—C1—C2 | 175·8 (8) | 177·5 (7) | 176·4 (7) | 176·4 (6) |
| C1—C2—C3 | 119·5 (6) | 120·5 (5) | 119·8 (5) | 120·0 (4) |
| C1—C2—C7 | 120·2 (6) | 119·1 (5) | 120·2 (5) | 119·1 (4) |
| C7—C2—C3 | 120·4 (5) | 120·4 (4) | 119·9 (4) | 120·9 (4) |
| C2—C3—C4 | 119·3 (5) | 119·3 (5) | 119·7 (4) | 118·8 (4) |
| C3—C4—C5 | 120·4 (5) | 121·4 (4) | 120·1 (4) | 121·3 (4) |
| C4—C5—C6 | 120·2 (5) | 118·7 (4) | 119·4 (4) | 119·3 (4) |
| C4—C5—C8 | 120·5 (4) | 120·4 (4) | 120·3 (4) | 120·9 (4) |
| C6—C5—C8 | 119·3 (4) | 120·8 (4) | 120·3 (4) | 119·8 (4) |
| C5—C6—C7 | 119·9 (5) | 121·1 (4) | 121·7 (4) | 120·5 (4) |
| C6—C7—C2 | 119·9 (5) | 119·0 (4) | 119·1 (4) | 119·2 (4) |
| C5—C8—C9 | 120·6 (4) | 121·0 (4) | 121·0 (4) | 120·3 (4) |
| C5—C8—C13 | 120·8 (4) | 120·8 (4) | 120·5 (4) | 121·3 (4) |
| C9—C8—C13 | 118·6 (5) | 118·1 (4) | 118·5 (4) | 118·4 (4) |
| C8—C9—C10 | 121·0 (4) | 121·1 (4) | 121·5 (4) | 121·0 (4) |
| C9—C10—C11 | 119·5 (5) | 119·7 (4) | 119·4 (4) | 120·4 (4) |
| C10—C11—C12 | 120·7 (5) | 120·2 (4) | 120·7 (4) | 119·7 (4) |
| C10—C11—I1 | 120·5 (4) | 119·5 (3) | 120·7 (3) | 119·9 (3) |
| C12—C11—I1 | 118·8 (3) | 120·4 (3) | 118·5 (3) | 120·3 (3) |
| C11—C12—C13 | 119·9 (4) | 118·8 (4) | 119·2 (4) | 118·6 (4) |
| C12—C13—C8 | 120·2 (5) | 122·1 (4) | 120·7 (4) | 122·0 (4) |

Table 4. *Geometry* (Å, °) *of the* C1—N1···I1—C11 *contacts*

| | Molecule *A* | | Molecule *B* | |
|---|---|---|---|---|
| | 297 K | 183 K | 297 K | 183 K |
| N1···I1 | 3·243 (8) | 3·190 (6) | 3·180 (8) | 3·142 (5) |
| C1—N1···I1 | 169·8 (8) | 170·9 (6) | 173·4 (8) | 172·2 (6) |
| N1···I1—C11 | 166·8 (3) | 167·4 (3) | 174·8 (3) | 174·5 (3) |

Table 5. *Packing* (Å, °) *in isomorphous compounds* $X—C_6H_4—C_6H_4—Y$

Degree to which the *X*–*Y* vector in the molecule is not parallel to the *b* axis.

| | | Molecule *A* | | Molecule *B* | | |
|---|---|---|---|---|---|---|
| *X* | *Y* | Distance* | Angle† | Distance* | Angle† | Ref. |
| $CH_3$ | $CH_3$ | 0·933 | 5·3 | 0·804 | 4·6 | (*a*) |
| Br | Br | 0·878 | 4·7 | 1·015 | 5·4 | (*b*) |
| Cl | Cl | 0·844 | 4·6 | 0·859 | 4·7 | (*c*) |
| Br | CN | 0·713 | 3·6 | 0·435 | 2·2 | (*d*) |
| I | CN | 0·623 | 3·1 | 0·307 | 1·5 | (*e*) |

References: (*a*) Casalone, Mariani, Mugnoli & Simonetta (1969); (*b*) Kronebusch, Gleason & Britton (1976*b*); (*c*) Brock, Kuo & Levy (1978); (*d*) Kronebusch, Gleason & Britton (1976*a*); (*e*) this work, only the room temperature values are used since the other structures were all determined at room temperature.

* Length of the component perpendicular to the *b* axis of the *X*—*Y* distance.

† Angle between the intramolecular *X*–*Y* vector and the *b* axis.

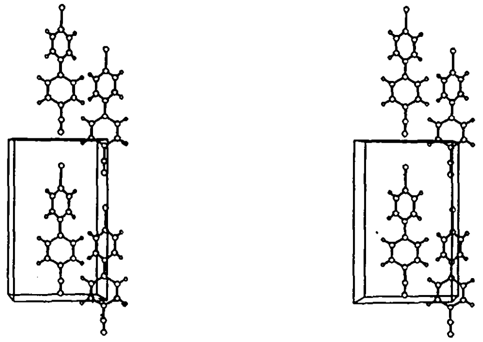

Fig. 4. The packing. Molecules approximately parallel to the *b* axis form chains exactly parallel to **b**.

given in Table 3. Half-normal probability plots (Abrahams & Keve, 1971) comparing the bond lengths between the independent molecules in Table 3 suggest that the e.s.d.'s should be about 50% larger at both temperatures but that, if this is allowed for, there are no significant differences between the two molecules. The four $C_6$ rings are planar within experimental error. The dihedral angles between the rings are: *A* 40·8 (4) and 40·0 (3); *B* 41·6 (4) and 41·6 (3)°, for 297 and 183 K, respectively, similar to values found in a number of other *para*-substituted biphenyls (Brock & Minton, 1989).

The only intermolecular distances shorter than the usual van der Waals distances are the N···I distances in each chain. [If we use the van der Waals radii of Nyburg & Faerman (1985), which allow for variation of the radii with orientation, we expect an N···I contact distance of 3·36 Å for a linear C—N···I—C contact.] The parameters for these contacts, which vary slightly from linear, are given in Table 4. For comparison, Cody & Murray-Rust (1984) in a survey using the Cambridge Structural Database (1988) found 14 I···N contacts with an average I···N distance of 3·14 Å and an average N···I—C angle of 174°. In a more specific comparison, in *p*-iodobenzonitrile (Schlemper & Britton, 1965; Desiraju & Harlow, 1989) the molecules lie on a twofold axis, and the C—N···I—C contact, which is exactly linear, was interpreted as a significant intermolecular interaction between the lone pair on the N atom and an empty orbital on the I atom, an interaction that would be maximized for the linear arrangement. The question then arises: why are the interactions not closer to linear in the present compound? This compound is isomorphous with four other 4,4′-*XY* disubstituted biphenyls and in all of them the molecules are only approximately parallel to the *b* axis. In Table 5 these structures are compared with respect to how far they are from parallel to the *b* axis. This comparison is made in two ways, first, by the distance the *X* atom would have to be moved perpendicular to the *b* axis in order to make the *X*–*Y* vector exactly parallel to **b**, and second by the angle between the *X*–*Y* vector and the *b* axis. It can be seen from the first three entries in Table 5 that the packing forces tend to incline both molecules about 5° away from parallel to the $b$ axis, but in the two cases where we propose a linear interaction the angles are less than 5°. Furthermore in the iodo compound (Fig. 4) where we would expect a stronger interaction, iodine being a stronger Lewis acid than bromine, the effect is greater. When the iodine is replaced with fluorine, which does not show Lewis acidic behavior at all, the crystals are not isomorphous and there is no short F···N contact (Gleason, Brostrom, Etter & Johnson, 1991).

The small amount of disorder, described earlier, does not affect the preceding argument. Since we regard the CN···I interaction as a specific one, we feel that the disorder probably occurs for entire chains rather than for isolated molecules, but the crystallographic data can be interpreted equally well with either model. In further support of the suggested disorder, in their recent reexamination of the structures of the 4-halobenzonitriles, Desiraju & Harlow (1989) suggest that disorder occurs in 4-bromobenzonitrile and in one of the forms of 4-chlorobenzonitrile although they do not report any measure of the amount of disorder.

All of the compounds in Table 5 have two molecules in the asymmetric unit related by pseudosymmetry. This has been described in detail by Brock, Kuo & Levy (1978) in their determination of the isomorphous 4,4′-dichlorobiphenyl.

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# Structure of 4-Cyano-4′-fluorobiphenyl

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(*Received* 14 *December* 1990; *accepted* 15 *March* 1991)

**Abstract.** 4′-Fluorobiphenyl-4-carbonitrile, $C_{13}H_8FN$, $M_r = 197{\cdot}2$, orthorhombic, $Pbca$, $a = 22{\cdot}525\ (2)$, $b = 11{\cdot}730\ (2)$, $c = 7{\cdot}568\ (2)$ Å, $V = 1999{\cdot}7$ Å$^3$, $Z = 8$, $D_x = 1{\cdot}31$ g cm$^{-3}$, $\lambda(\text{Mo}\ K\alpha) = 0{\cdot}71073$ Å, $\mu = 0{\cdot}8$ cm$^{-1}$, $F(000) = 816$, $T = 298\ (1)$ K, $R = 0{\cdot}033$ for 840 observed reflections. A number of isomorphous 4,4′-disubstituted biphenyl derivatives have been reported with the prototype being 4,4′-dimethyl-

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0108-2701/91/102131-04$03.00