an improved scale factor and overall temperature factor were obtained by the Thewlis (1952) method.

The phased structure factors were then used in the computation of (100) and (010) electron density maps. From these maps all atomic positions except those of the hydrogen atoms were found and refined isotropically by the method of least squares until the residual index R had steadied at 0·147.

Table 1. *Atomic coordinates**

The fractional coordinates are multiplied by 10^4.

	x	y	z
Br	1283	5123	4251
O	8588	3563	6137
N	9392	6661	5538
C(1)	8812	6222	7205
C(2)	8510	4371	7029
C(3)	8045	2993	7791
C(4)	8026	3845	8716
C(5)	8103	6317	8966
C(6)	8686	6744	8194
C(7)	9240	7310	6446
C(8)	9683	7872	4841
C(9)	9282	9823	4646
C(10)	9558	0898	3960
C(11)	0422	0547	3267
C(12)	0808	8720	3350
C(13)	0517	7532	4110

* The mean standard deviation for the bromine atom was 0·008 Å and for the other atoms (excluding hydrogen) was 0·05 Å.

Discussion

Since only two-dimensional data were used the e.s.d.'s of the positional parameters were much higher than would be the case in a three-dimensional structure determination. In view of this it was felt that the inclusion of anisotropic temperature factors and hydrogen atoms in the refinement would be unjustified.

The main interest of this structure lay in the comparative intramolecular and intermolecular O····N distances. After computation of the interatomic spacings in the two cases it was found that the intramolecular distance (2·62±0·08 Å) was less than the shortest intermolecular O····N distance (4·99±08 Å), thus supporting the thesis that the movement of the hydroxylic hydrogen atom during the photochromic change is intramolecular rather than intermolecular.

The structure was also compared with the isomorphous chloro derivative (Bregman, Leiserowitz & Osaki, 1964) to examine any possible effect of the change of halogen atom. Apart from minor differences (such as the expected lengthening of the halogen–aryl contact) no significant change could be detected as far as the existing e.s.d.'s allowed.

No further work on this compound is envisaged.

This work was presented in a thesis by one of us (ADH) for the Master's degree of the University of Wales.

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Space groups of L-tyrosine and L-tryptophane – a corrigendum. By B. KHAWAS and G.S.R. KRISHNA MURTI,

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It has been kindly pointed out to us by Dr Gerald Strahs (New York Medical College, New York) that the centric space groups *Pnam* and *Pmmm* assigned to L-tyrosine and L-tryptophane (Khawas & Krishna Murti, 1969) demand the presence of DL-tyrosine and DL-tryptophane in the crystals and that the contradiction for L-tryptophane can be removed by assigning the acentric space group *P*222 instead of *Pmmm*. No acentric space group can be assigned to

L-tyrosine satisfying the apparent systematic extinctions of X-ray reflexion. Presumably the extinctions are accidental.

Reference

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