Related literature. This work was initiated because of an unexpected ligand decomposition during complex formation. The structure has provided further insight into extensively hydrogen-bonded systems and may be compared to ammonium perchlorate (Lundgren, 1979) and methylammonium perchlorate (Zanazzi, 1968).

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References

CSSR (1984). *Crystal Structure Search and Retrieval Instruction Manual.* SERC Daresbury Laboratory, Warrington, England.

Lundgren, J. O. (1979). *Acta Cryst.* B35, 1027–1033.

Motherwell, W. D. S. & Clegg, W. (1978). *PLUTO*. Program for plotting molecular and crystal structures. Univ. of Cambridge, England.

Sheldrick, G. M. (1976). *SHELX76*. Program for crystal structure determination. Univ. of Cambridge, England.

Sheldrick, G. M. (1985). *SHELXS86*. In *Crystallographic Computing* 3, edited by G. M. Sheldrick, C. Krüger & R. Goddard, pp. 175–189. Oxford Univ. Press.

Zanazzi, P. F. (1968). *Acta Cryst.* B24, 499–504.

Acta Cryst. (1992). C48, 193–194

Structure of *N*-(Indol-3-ylethyl)-4-hydroxyphenylacetamide

By Toshimasa Ishida, Akira Negi, Yasuko In and Masatoshi Inoue

Osaka University of Pharmaceutical Sciences, 2–10–65 *Kawai, Matsubara, Osaka* 580, *Japan*

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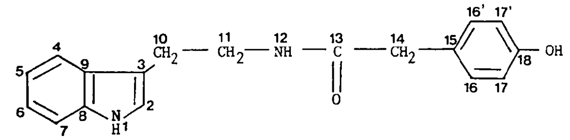
Abstract. $C_{18}H_{18}N_2O_2$, $M_r = 294.36$, monoclinic, $P2_1/a$, $a = 8.403\ (4)$, $b = 5.405\ (3)$, $c = 33.005\ (16)$ Å, $\beta = 91.07\ (4)°$, $V = 1499.0\ (13)$ Å^3, $Z = 4$, $D_m = 1.301\ (3)$, $D_x = 1.305$ g cm^{-3}, $\lambda(\text{Cu}\ K\alpha) = 1.5418$ Å, $\mu = 6.52$ cm^{-1}, $F(000) = 624$, $T = 293$ K, final $R = 0.046$ for 2088 independent reflections with $|F_o| > 0.0$. The molecule takes an extended conformation without specific interaction between the indole and phenol rings, where the torsion angles of C(2)—C(3)—C(10)—C(11), C(3)—C(10)—C(11)—N(12), C(10)—C(11)—N(12)—C(13), C(11)—N(12)—C(13)—C(14), N(12)—C(13)—C(14)—C(15) and C(13)—C(14)—C(15)—C(16) are 9.3 (2), 173.1 (2), 85.1 (2), −175.7 (2), −116.8 (2) and 95.7 (2)°, respectively, and the indole ring makes a dihedral angle of 70.2 (1)° with the phenol ring. In the crystal structure, two kinds of hydrogen bonds are formed between the phenol OH related by diad screw symmetry $[\text{O}(18)(x,\ y,\ z)\cdots\text{O}(18)(\tfrac{1}{2}-x,\ y-\tfrac{1}{2},\ -z) = 2.915\ (2)$ Å] and between the carbamoyl groups by glide symmetry $[\text{N}(12)(x,\ y,\ z)\cdots\text{O}(13)(x-\tfrac{1}{2},\ \tfrac{1}{2}-y,\ z) = 2.841\ (2)$ Å], forming infinite chains along the *b* and *a* axes, respectively.

Experimental. Platelet crystals of (1) from 70% aqueous ethanol; D_m by the flotation method in a C_6H_6/CCl_4 mixture; 0.15 × 0.20 × 0.40 mm; Rigaku AFC-5 diffractometer with graphite-monochromated Cu $K\alpha$ radiation; unit-cell dimensions by a least-squares fit of 2θ values of 25 reflections in the 2θ range 44–55°; intensities by θ–2θ-scan technique with a scan speed of 4° min^{-1} in 2θ; scan width of $\Delta(2\theta) = (2.5 + 0.15\tan\theta)°$; 5 s background measurements at both ends of a scan peak; four standard reflections remeasured at 100 reflection intervals; no significant intensity variation (< ±0.1%); a total of 2559 independent reflections within $\theta_{\max} = 65.01°$ ($\sin\theta/\lambda = 0.588$ Å^{-1}) collected (h 0 − 9, k 0 − 6, l − 38 − 38), 2088 for $|F_o| > 0.0$ and 1808 for $|F_o| \geq 3\sigma(F_o)$; intensity corrections for Lorentz and polarization effects; no absorption or extinction corrections.



(1)

The structure was solved by direct methods using *MULTAN*87 (Debaerdemaeker, Germain, Main, Tate & Woolfson, 1987); refinement by the block-diagonal least-squares procedure using 2088 reflections with $|F_o| > 0.0$; the function $\sum w(|F_o| - |F_c|)^2$ was minimized. The ideal positions of all H atoms were calculated on the basis of stereochemical considerations and, except for the phenol OH, were verified on a difference Fourier map. The electron density corresponding to H(18) was not clearly revealed on the map, although it suggested two possible locations around O(18). The non-H and H atoms refined anisotropically and isotropically respectively; in the last refinement, $w = 1.0/[\sigma(F_o)^2 - 0.84070|F_o| + 0.01195|F_o|^2]$; number of observations

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Table 1. *Fractional atomic coordinates and equivalent isotropic temperature factors* ($Å^2$) *for non*-H *atoms with their e.s.d.'s in parentheses*

$B_{eq} = \frac{4}{3}\sum_i\sum_j \mathbf{a}_i.\mathbf{a}_j B_{ij}.$

	x	y	z	B_{eq}
N(1)	0.3564 (2)	−0.2705 (4)	0.36652 (5)	4.47 (9)
C(2)	0.3229 (3)	−0.1717 (5)	0.32873 (7)	4.21 (9)
C(3)	0.2255 (2)	0.0266 (4)	0.33221 (6)	3.44 (8)
C(4)	0.1083 (2)	0.2282 (5)	0.39725 (6)	4.1 (1)
C(5)	0.1035 (3)	0.1943 (6)	0.43899 (7)	5.1 (1)
C(6)	0.1819 (3)	0.0019 (6)	0.45814 (7)	5.6 (1)
C(7)	0.2764 (3)	−0.1690 (5)	0.43691 (7)	4.7 (1)
C(8)	0.2797 (2)	−0.1310 (4)	0.39486 (6)	3.72 (9)
C(9)	0.1987 (2)	0.0601 (4)	0.37486 (6)	3.43 (8)
C(10)	0.1514 (2)	0.1814 (4)	0.29894 (6)	3.71 (9)
C(11)	0.1748 (2)	0.0692 (5)	0.25754 (6)	3.91 (9)
N(12)	0.0860 (2)	0.2045 (4)	0.22563 (5)	4.12 (8)
C(13)	0.1391 (2)	0.4015 (4)	0.20719 (6)	3.49 (8)
O(13)	0.2738 (2)	0.4865 (4)	0.21343 (5)	4.89 (8)
C(14)	0.0217 (2)	0.5228 (5)	0.17724 (6)	4.1 (1)
C(15)	0.0873 (2)	0.5114 (4)	0.13406 (6)	3.36 (8)
C(16)	0.0392 (2)	0.3189 (5)	0.10847 (6)	3.95 (9)
C(16′)	0.1860 (2)	0.6910 (4)	0.11962 (6)	3.89 (9)
C(17)	0.0966 (3)	0.3031 (5)	0.06954 (6)	4.3 (1)
C(17′)	0.2470 (3)	0.6760 (5)	0.08029 (6)	4.3 (1)
C(18)	0.1980 (2)	0.4851 (4)	0.05578 (6)	3.60 (9)
O(18)	0.2588 (2)	0.4800 (4)	0.01643 (4)	5.53 (8)

per refined parameters = 2088/276 = 7.57; $S = 0.822$, final $R = 0.046$, $wR = 0.066$, $(\Delta/\sigma)_{max} = 0.10$ and $|\Delta\rho|_{max} = 0.27$ e $Å^{-3}$. The atomic scattering factors were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV). For all crystallographic computations *The Universal Crystallographic Computing System* (1979) was used. All computations were performed on a MicroVAX II computer at the Computation Center, Osaka University of Pharmaceutical Sciences.

The final atomic coordinates and equivalent isotropic temperature factors are given in Table 1.* The molecular conformation and crystal packing in the unit cell are shown in Figs. 1 and 2.

Related literature. The electron transfer within a protein *via* the intramolecular charge transfer between the aromatic rings of tyrosine and tryptophan residues is of importance in biological oxidation–reduction systems (Ghiron, Bazin & Santus, 1986; Faraggi, DeFelippis & Klapper, 1989). As part of a structural study on the indole–phenol ring interactions at the atomic level (Ishida & Inoue, 1981), the crystal structure of the title compound was analysed.

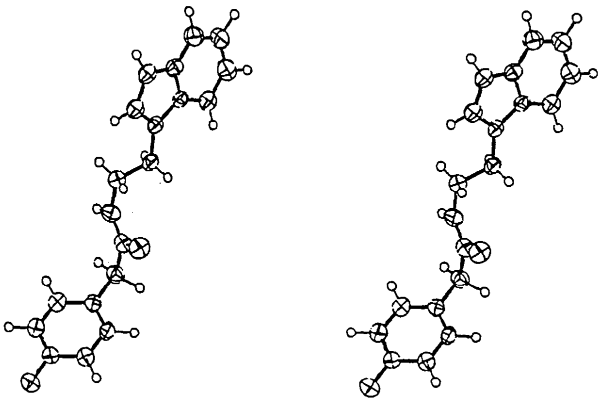

Fig. 1. A stereoscopic view of (1). The H atom of the phenol OH group is omitted.

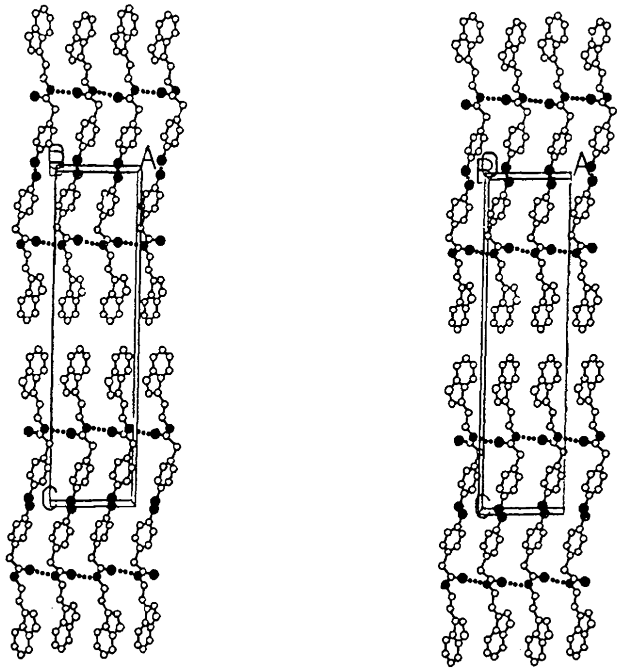

Fig. 2. A stereoscopic view of the crystal packing of (1), viewed along the *b* axis. Filled circles represent N or O atoms participating in hydrogen bonds.

References

Debaerdemaeker, T., Germain, G., Main, P., Tate, C. & Woolfson, M. M. (1987). *MULTAN87. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data.* Univs. of York, England, and Louvain, Belgium.

Faraggi, M., DeFelippis, M. R. & Klapper, M. H. (1989). *J. Am. Chem. Soc.* **111**, 5141–5145.

Ghiron, C. A., Bazin, M. & Santus, R. (1986). *Biochim. Biophys. Acta*, **873**, 102–107.

Ishida, T. & Inoue, M. (1981). *Acta Cryst.* B**37**, 2117-2120.

The Universal Crystallographic Computing System (1979). The Computation Center, Osaka Univ., Japan.

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* Lists of structure factors, anisotropic thermal parameters, H-atom coordinates with isotropic thermal parameters, bond lengths and angles, torsion angles, and possible hydrogen bonds and short contacts less than 3.4 Å have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54485 (12 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: AS0500]