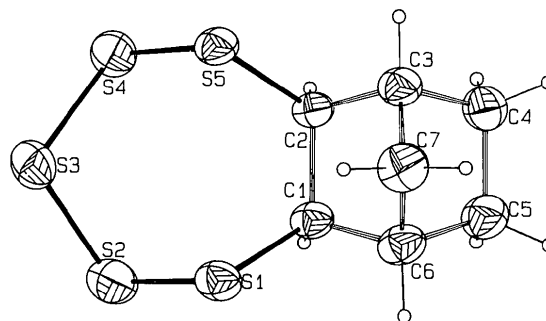


Table 1. Atomic coordinates and equivalent isotropic thermal parameters (\AA^2)
$$B_{\text{eq}} = (8\pi^2/3) \sum_i \sum_j U_{ij} a_i^* a_j^* a_i a_j$$

	x	y	z	B_{eq}
S(1)	0.3325 (1)	0.0813 (1)	1.1465 (1)	2.91
S(2)	0.2228 (1)	0.0747 (1)	1.2719 (1)	3.61
S(3)	0.1812 (1)	0.2523 (1)	1.3020 (1)	3.43
S(4)	0.0233 (1)	0.3039 (1)	1.1042 (1)	3.31
S(5)	0.1318 (1)	0.3212 (1)	0.9784 (1)	2.72
C(1)	0.1911 (3)	0.0639 (2)	0.9633 (3)	2.37
C(2)	0.1015 (3)	0.1778 (2)	0.8829 (3)	2.20
C(3)	0.1482 (3)	0.1959 (3)	0.7598 (3)	2.76
C(4)	0.0743 (4)	0.0967 (3)	0.6477 (3)	3.25
C(5)	0.1577 (4)	-0.0187 (3)	0.7245 (3)	3.41
C(6)	0.2699 (3)	0.0285 (3)	0.8697 (3)	2.96
C(7)	0.3066 (3)	0.1526 (3)	0.8280 (4)	3.47

Fig. 1. Perspective view of the $\text{C}_7\text{H}_{10}\text{S}_5$ molecule with atom-numbering schemeTable 2. Bond distances (\AA) and angles ($^\circ$)

S(1)—S(2)	2.034 (1)	S(1)—C(1)	1.829 (3)
S(3)—S(4)	2.063 (1)	S(4)—S(5)	2.034 (1)
C(1)—C(2)	1.570 (4)	C(1)—C(6)	1.541 (4)
C(2)—C(3)	1.543 (4)	C(3)—C(4)	1.538 (4)
C(4)—C(5)	1.546 (5)	C(5)—C(6)	1.540 (4)
S(2)—S(3)	2.066 (1)	C(3)—C(7)	1.534 (5)
S(5)—C(2)	1.825 (2)	C(6)—C(7)	1.535 (5)
S(2)—S(1)—C(1)	104.3 (1)	S(1)—S(2)—S(3)	105.2 (1)
S(2)—S(3)—S(4)	103.9 (1)	S(3)—S(4)—S(5)	104.3 (1)
S(4)—S(5)—C(2)	104.3 (1)	S(1)—C(1)—C(2)	118.8 (2)
S(1)—C(1)—C(6)	106.3 (2)	C(2)—C(1)—C(6)	102.5 (2)
S(5)—C(2)—C(1)	119.4 (2)	S(5)—C(2)—C(3)	106.7 (2)
C(1)—C(2)—C(3)	102.9 (2)	C(2)—C(3)—C(4)	107.4 (2)
C(2)—C(3)—C(7)	102.4 (2)	C(4)—C(3)—C(7)	101.6 (3)
C(3)—C(4)—C(5)	103.0 (2)	C(4)—C(5)—C(6)	103.4 (3)
C(1)—C(6)—C(5)	108.3 (3)	C(1)—C(6)—C(7)	101.4 (2)
C(5)—C(6)—C(7)	101.9 (2)	C(3)—C(7)—C(6)	94.3 (3)

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1,3-Propanediammonium Diperchlorate

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Abstract. $\text{C}_3\text{H}_{12}\text{N}_2^{2+} \cdot 2\text{ClO}_4^-$, $M_r = 275.04$, monoclinic, $P2_1/c$, $a = 7.298$ (4), $b = 14.388$ (9), $c = 9.708$ (6) \AA , $\beta = 96.79$ (4) $^\circ$, $V = 1012.2$ \AA^3 , $Z = 4$, $D_x = 1.80$ Mg m^{-3} , $\lambda(\text{Mo } K\alpha) = 0.71073$ \AA , $\mu = 0.596$ mm^{-1} , $F(000) = 568$, $T = 293$ K, $R = 0.053$ for 1053 unique reflexions [$F \geq 3\sigma(F)$]. The crystal

structure is composed of doubly charged 1,3-propanediammonium cations and tetrahedral perchlorate anions. One N atom is surrounded by eight perchlorate O atoms and the other by seven in the weakly hydrogen-bonding range 2.95 (1)–3.23 (1) \AA . The ammonium groups have a conformation with

five of the six hydrogen atoms utilized in seven hydrogen bonds, with O...H distances ranging from 2.3 (1) to 2.5 (1) Å. One perchlorate O atom is involved in two hydrogen bonds and is further distinguished by an extended Cl—O bond of 1.445 (4) Å [*cf.* 1.406 (4)—1.425 (4) Å].

Experimental. Colourless crystals of the title compound were formed as a by-product when the sodium salt of *N,N*-disalicyloyl-1,3-propanediamine (0.0142 mol) in 60 ml ethanol/methanol (1/1) was mixed with 30 ml of an ethanolic solution of iron(III) perchlorate (0.0284 mol), stirred for 45 min at room temperature and cooled to induce crystallization.

Crystal dimensions 0.30 × 0.10 × 0.10 mm, Enraf-Nonius CAD-4 diffractometer, graphite-monochromated Mo $K\alpha$ radiation, unit-cell dimensions from setting angles of 25 accurately centred reflexions ($5.6 \leq \theta \leq 6.4^\circ$), ω - 2θ scan mode, ω scan width ($0.70 + 0.35 \tan \theta$)° and scan speed ranging from 1.0 to 5.0° min⁻¹ according to the intensity gathered in a pre-scan, $-8 \leq h \leq 8$, $0 \leq k \leq 17$, $0 \leq l \leq 11$, $0 \leq \theta \leq 25^\circ$, 2838 reflexions measured, 1371 unique ($R_{\text{int}} = 0.016$), 1053 observed [$F \geq 3\sigma(F)$], intensity standards (200, 041, 122) measured every 2.5 h, no systematic drift, Lp corrections applied, absorption ignored, *SHELXS* Patterson interpretation technique (Sheldrick, 1985) used to solve the phase problem, all non-H atoms found in Fourier map, H atoms from ΔF synthesis, full-matrix least squares based on F using *SHELX76* (Sheldrick, 1976), final $R = 0.053$, $wR = 0.047$ [$w = 1.74260/[\sigma^2(F) + 0.00030F^2]$], $S = 2.8$, anisotropic thermal parameters for heavier atoms, isotropic for H atoms. Empirical extinction correction applied (0.00259). N atoms given a slightly reduced site occupancy (0.93) and O slightly increased (1.03) in an attempt to allow for charges. Max. fluctuation in final ΔF map in range -0.4 to 0.4 e \AA^{-3} , max. Δ/σ 0.08. Scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV), computation carried out on the Amdahl 5890 system of the University of Manchester Computing Centre. Literature surveyed via the Cambridge Structural Database using the Crystal Structure Search and Retrieval interactive system (CSSR, 1984). Fractional atomic coordinates and vibrational parameters for non-H atoms are presented in Table 1* and selected bond lengths and angles in Table 2. Molecular packing, including atomic labelling, is displayed in Fig. 1.

* Lists of structure factors, H-atom coordinates, all bond lengths and angles and anisotropic vibrational parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54166 (8 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. Fractional atomic coordinates and vibrational parameters (\AA^2) for non-H atoms

$$U_{\text{eq}} = (1/3) \sum_i \sum_j U_{ij} a_i^* a_j^* a_i \cdot a_j$$

	<i>x</i>	<i>y</i>	<i>z</i>	U_{eq}
Cl(1)	0.2233 (2)	0.2584 (1)	0.6102 (1)	0.0301 (4)
O(1)	0.0704 (6)	0.3069 (3)	0.5412 (4)	0.046 (1)
O(2)	0.3921 (6)	0.3025 (3)	0.5803 (4)	0.048 (1)
O(3)	0.2226 (7)	0.1645 (3)	0.5651 (5)	0.053 (1)
O(4)	0.2174 (6)	0.2612 (3)	0.7563 (4)	0.058 (1)
Cl(2)	0.3020 (2)	0.5702 (1)	0.7382 (2)	0.0309 (3)
O(5)	0.4167 (6)	0.6232 (3)	0.6597 (5)	0.059 (1)
O(6)	0.1687 (7)	0.6286 (3)	0.7883 (5)	0.066 (1)
O(7)	0.2087 (7)	0.5018 (4)	0.6533 (5)	0.071 (1)
O(8)	0.4107 (7)	0.5279 (3)	0.8513 (5)	0.067 (1)
N(1)	0.7950 (11)	0.5541 (5)	0.6505 (9)	0.032 (2)
C(1)	0.7633 (11)	0.4560 (5)	0.6805 (7)	0.036 (2)
C(2)	0.8249 (10)	0.4328 (5)	0.8309 (7)	0.036 (2)
C(3)	0.7666 (12)	0.3374 (5)	0.8703 (8)	0.043 (2)
N(2)	0.5709 (11)	0.3346 (6)	0.8942 (9)	0.040 (2)

Table 2. Selected bond lengths (\AA), angles ($^\circ$) and H bonds (\AA , $^\circ$)

Cl(1)—O(1)	1.415 (4)	Cl(1)—O(2)	1.445 (4)	
Cl(1)—O(3)	1.420 (4)	Cl(1)—O(4)	1.425 (4)	
Cl(2)—O(5)	1.420 (4)	Cl(2)—O(6)	1.415 (4)	
Cl(2)—O(7)	1.406 (4)	Cl(2)—O(8)	1.414 (4)	
N(1)—C(1)	1.465 (9)	C(1)—C(2)	1.514 (9)	
C(2)—C(3)	1.500 (9)	C(3)—N(2)	1.48 (1)	
C(2)—C(1)—N(1)	111.6 (6)	C(3)—C(2)—C(1)	112.8 (6)	
N(2)—C(3)—C(2)	112.0 (7)			
H bonds				
N	O	N...O	H...O	N—H...O
N(1) ⁱ	O(1)	2.98 (1)	2.46 (8)	127 (1)
N(1)	O(5)	2.95 (1)	2.31 (6)	136 (1)
N(1) ⁱⁱ	O(6)	3.08 (1)	2.36 (6)	168 (1)
N(1) ^j	O(7)	3.05 (1)	2.42 (8)	143 (1)
N(2)	O(2)	3.20 (1)	2.38 (11)	144 (1)
N(2) ⁱⁱⁱ	O(2)	3.07 (1)	2.44 (6)	149 (1)
N(2)	O(4)	2.96 (1)	2.30 (11)	126 (1)

Symmetry code: (i) $1 - x, 1 - y, 1 - z$; (ii) $1 + x, y, z$; (iii) $x, \frac{1}{2} - y, z - \frac{1}{2}$.

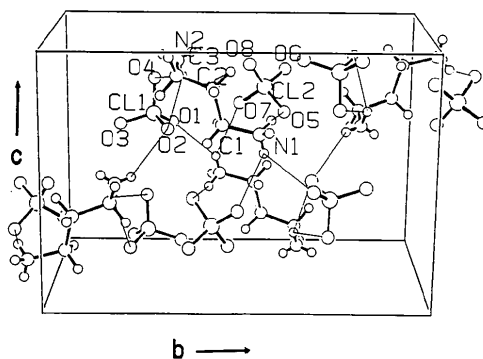


Fig. 1. Molecular packing, including labelling scheme and H bonding, drawn using *PLUTO* (Motherwell & Clegg, 1978).

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

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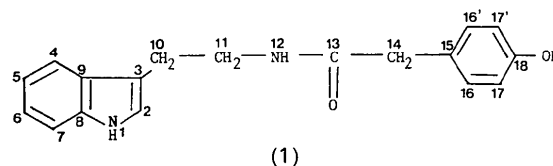
Abstract. $C_{18}H_{18}N_2O_2$, $M_r = 294.36$, monoclinic, $P2_1/a$, $a = 8.403$ (4), $b = 5.405$ (3), $c = 33.005$ (16) Å, $\beta = 91.07$ (4)°, $V = 1499.0$ (13) Å³, $Z = 4$, $D_m = 1.301$ (3), $D_x = 1.305$ g cm⁻³, $\lambda(\text{Cu } K\alpha) = 1.5418$ Å, $\mu = 6.52$ cm⁻¹, $F(000) = 624$, $T = 293$ 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 $[O(18)(x, y, z) \cdots O(18)(\frac{1}{2} - x, y - \frac{1}{2}, -z) = 2.915$ (2) Å] and between the carbamoyl groups by glide symmetry $[N(12)(x, y, z) \cdots O(13)(x - \frac{1}{2}, \frac{1}{2} - y, z) = 2.841$ (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; $0.15 \times 0.20 \times 0.40$ 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 $\Delta(2\theta) = (2.5 +$

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$0.15 \tan \theta$)°; 5 s background measurements at both ends of a scan peak; four standard reflections remeasured at 100 reflection intervals; no significant intensity variation ($< \pm 0.1\%$); a total of 2559 independent reflections within $\theta_{\max} = 65.01^\circ$ ($\sin \theta / \lambda = 0.588 \text{ \AA}^{-1}$) 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.



The structure was solved by direct methods using *MULTAN87* (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