Knappe, 1965). It is, however, perfectly symmetrical, because of the molecular mirror plane which passes through the five atoms O(S), S, C(3), C(4), C(5) [only the three atoms C(1), C(2) and O are in general positions in the assymetric unit]. In the S heterocycle the bonds S—C(1) [1·809 (3)] and C(1)—C(2) [1·512 (4) Å] are significantly shorter than the corresponding bonds in the dimethyl derivative [1·822 (7), 1·842 (7) and 1·551 (9), 1·530 (10) Å]. The angles are nearly the same in both compounds. On the other hand, in the dioxolane ring the bonds C(2)—O [1·428 (3)] and O—C(3) [1·431 (3) Å] are significantly longer than the corresponding bonds of the dimethyl derivative [1·419 (9), 1·409 (8) and 1·413 (9), 1·407 (9) Å] but here also the angles remain nearly the same for both molecules. The angles between the different planes (Fig. 1*b*) of the two rings, *i.e.* C(1)—S—C(1$^{\rm i}$), C(1)—C(2)—C(2$^{\rm i}$)—C(1$^{\rm i}$), C(2)—O—O$^{\rm i}$—C(2$^{\rm i}$) and O—C(3)—O$^{\rm i}$ are sequentially 138, 117 and 146°.When these dihedral angles are compared to those of the dimethyl sulfoxide (132, 119, and 147° respectively) and of biotin (142, 118°, the third not cited), we note a close similarity, except for the first dihedral angle which differs significantly between the three compounds. Of particular interest is the value of 91° (Table 3) found for the dihedral angle between the atoms H2(C1) and H(C2) through the C(1)—C(2) bond, close to that which had been predicted (90°) from NMR measurements (Lett & Marquet, 1974). The packing is governed by hydrogen bonds [2·776 (5) Å] between the two centrosymmetric water molecules [O(*W*)H2 and O(*W*$^{\rm iv}$)H2] on the twofold axis and the O(S) and O(S$^{\rm iv}$) atoms of the two centrosymmetric sulfoxide molecules.

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Structure of the 1:1 Adduct of Orthoperiodic Acid and Urea

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Abstract. $H_5IO_6.CH_4N_2O$, monoclinic, $P2_1/c$, $a = 5{\cdot}175\,(1)$, $b = 6{\cdot}870\,(2)$, $c = 20{\cdot}480\,(5)$ Å, $\beta = 90{\cdot}96\,(2)°$ at 293 K, $Z = 4$, $D_{\rm pyc} = 2{\cdot}60\,(1)$ at 298 K, $D_c = 2{\cdot}627$ Mg m^{-3}, $R = 0{\cdot}054$, $R_w = 0{\cdot}081$ for 1254 reflexions. The structure consists of orthoperiodic acid and urea molecules, connected by relatively strong hydrogen bonds, forming a three-dimensional network.

Introduction. The title compound $IO(OH)_5.CO(NH_2)_2$ was studied as an analogue of the adduct of orthotelluric acid and urea, $Te(OH)_6.2CO(NH_2)_2$ (Loub, Haase & Mergehenn, 1979). The adduct was prepared by crystallization from a concentrated aqueous solution of orthoperiodic acid and urea with a molar ratio of 1:2 at 298 K. With increasing temperature and time of crystallization, ammonium periodate, NH_4IO_4, is gradually formed. Clear crystals were obtained as multiface prisms with well developed (001) faces. The cell dimensions were determined from the setting angles of 15 reflexions measured on an automatic Syntex $P2_1$ four-circle diffractometer with graphite-monochromated Mo $K\alpha$ radiation. 1290 independent inten-

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sities were collected with the same instrument from a sphere-shaped crystal with a volume of 0·05 mm^3 for $2\theta = 3$–50°. 72 reflexions (of 1290) did not meet the condition $I > 1\cdot96\ \sigma_1(I)$. Absorption was neglected ($\mu = 4\cdot46$ mm^{-1}). The iodine-atom position was obtained from a Patterson synthesis. The remaining non-H atoms were located by Fourier and ΔF syntheses and refined by the least-squares method to $R = \sum||F_o| - |F_c||/\sum|F_o| = 0\cdot068$ with isotropic temperature factors. In further cycles, with anisotropic temperature factors, the refinement converged to $R = 0\cdot054$, $R_w = [\sum w(|F_o| - |F_c|)^2/\sum w|F_o|^2]^{1/2} = 0\cdot081$ with weights $w = \sigma^{-2}(F_o)$ derived from $\sigma_2(I) = [\sigma_1^2(I) + (0\cdot06\ I)^2]^{1/2}$.[*] 36 reflexions (of 1290) which did not meet the condition $1/3 < |F_o/F_c| < 3$ were omitted. In the final cycle no parameter shift was >0·18 times its e.s.d. The localization of the H atoms using the difference syntheses was unsuccessful. The final difference map showed no residual electron density greater than 0·55 e Å^{-3}. The scattering factors for neutral atoms and the anomalous-dispersion correction for the I atom were taken from *International Tables for X-ray Crystallography* (1974). The calculations were performed with the *TLS* programs (Sklenář, 1973) on an ICL 4–72 computer. The final atomic parameters are given in Table 1. The projection of the structure in the *XZ* plane is depicted in Fig. 1.

Table 1. *Atomic coordinates* ($\times 10^4$) *and isotropic temperature factors with e.s.d.'s in parentheses.*

$$B_{\rm eq} = 4[V^2 \det(\beta_{ij})]^{1/3}.$$

	x	y	z	$B_{\rm eq}$ (Å^2)
I	3686·9 (7)	2414·6 (5)	811·9 (2)	0·69 (2)
O(1)	1073 (15)	2293 (7)	1401 (4)	1·5 (2)
O(2)	1360 (15)	2130 (8)	88 (4)	1·6 (2)
O(3)	6297 (17)	2576 (5)	223 (4)	1·1 (3)
O(4)	6038 (17)	2581 (6)	1535 (5)	1·6 (2)
O(5)	4110 (9)	−347 (10)	862 (2)	1·5 (1)
O(6)	3295 (9)	5158 (11)	819 (2)	1·8 (2)
O(7)	833 (8)	1143 (8)	2552 (2)	2·1 (2)
N(1)	1175 (15)	2025 (11)	3596 (3)	2·2 (2)
N(2)	4255 (13)	3004 (10)	2873 (3)	2·5 (2)
C	2125 (14)	2053 (10)	3003 (3)	1·5 (2)

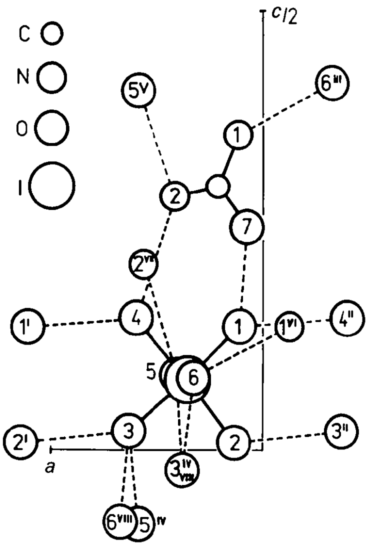

Fig. 1. Schematic projection of the structure in the *XZ* plane.

Discussion. The more important interatomic distances and bond angles, given in Table 2, are in agreement with expected values. The orthoperiodic acid group forms a distorted octahedron with an average I—O distance 1·88 (3) Å and O—I—O angle 90 (2)°. In contrast to free orthoperiodic acid, IO(OH)$_5$, no I—O distance in the adduct is so short that it could be unambiguously decided which oxygen carries no hydrogen atom. In orthoperiodic acid, the shortest I—O distance is 1·78 Å, the average value of the other I—O distances is 1·89 Å and the average value of the O—I—O angles is the same as in the adduct (Feikema, 1966). The urea group is practically planar ($\chi^2 = 2\cdot06$, $\nu = 1$).

Between the orthoperiodic acid and urea molecules there are eight different distances shorter than 3·11 Å, *i.e.* the distance corresponding to possible hydrogen

Table 2. *Interatomic distances* (Å) *and angles* (°) *and intermolecular distances* (Å) <3·11 Å *with e.s.d.'s in parentheses*

I—O(1)	1·830 (8)	O(1)—I—O(2)	92·5 (3)
I—O(2)	1·904 (8)	O(1)—I—O(3)	179·1 (2)
I—O(3)	1·829 (8)	O(1)—I—O(4)	87·7 (4)
I—O(4)	1·904 (10)	O(1)—I—O(5)	90·3 (2)
I—O(5)	1·912 (7)	O(1)—I—O(6)	87·7 (2)
I—O(6)	1·896 (8)	O(2)—I—O(3)	87·5 (4)
		O(2)—I—O(4)	177·5 (2)
C—O(7)	1·292 (8)	O(2)—I—O(5)	90·6 (2)
C—N(1)	1·318 (9)	O(2)—I—O(6)	92·4 (2)
C—N(2)	1·313 (10)	O(3)—I—O(4)	92·3 (4)
		O(3)—I—O(5)	90·6 (2)
O(1)—O(7)	2·491 (9)	O(3)—I—O(6)	91·4 (2)
O(1)—O(4$^{\rm ii}$)	2·632 (12)	O(4)—I—O(5)	86·9 (2)
O(2)—O(3$^{\rm ii}$)	2·657 (12)	O(4)—I—O(6)	90·1 (2)
O(3)—O(5$^{\rm iv}$)	2·704 (9)	O(5)—I—O(6)	176·5 (2)
O(3)—O(6$^{\rm viii}$)	2·653 (9)		
O(4)—N(2)	2·920 (12)	O(7)—C—N(1)	117·1 (6)
O(5)—N(2$^{\rm vii}$)	2·939 (8)	O(7)—C—N(2)	121·5 (5)
O(6)—N(1$^{\rm vi}$)	2·920 (9)	N(1)—C—N(2)	121·4 (6)

Symmetry code

(i)	$1 + x$,	y,	z	(v)	$1 - x$,	$\frac{1}{2} + y$,	$\frac{1}{2} - z$
(ii)	$x - 1$,	y,	z	(vi)	$\bar{x}$,	$\frac{1}{2} + y$,	$\frac{1}{2} - z$
(iii)	$\bar{x}$,	$y - \frac{1}{2}$,	$\frac{1}{2} - z$	(vii)	$1 - x$,	$y - \frac{1}{2}$,	$\frac{1}{2} - z$
(iv)	$1 - x$,	$\bar{y}$,	$\bar{z}$	(viii)	$1 - x$,	$1 - y$,	$\bar{z}$

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[*] Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 36550 (10 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

bonds. As the positions of the H atoms have not been determined, hydrogen bonds cannot be clearly identified. Bands in the Raman spectrum (at 2180 *vw*, 3000, 3250, 3335, 3450 and 3510, all *w*, cm^{-1}) and in the infrared spectrum (at 2380 *w* and 2760–3480 *s* cm^{-1}) indicate the presence of possible hydrogen bonds of the O(H)···(H)O, O(H)···O, O(H)···(H)N and O···(H)N types. The shortest distance, between O(1) and O(7), 2·491 (9) Å, indicates a strong hydrogen bond. This hydrogen bond causes a lengthening of the O(7)—C distance and shortening of the N—C distances, compared with the corresponding distances in urea (Mullen & Hellner, 1978). Analogous shortest intermolecular distances are O(N)···O(C) = 2·596 for urea nitrate (Worsham & Busing, 1969), O(P)···O(C) = 2·400 for urea phosphate (Nozik, Fykin, Bukin & Muradjan, 1976) and O(Te)···O(C) = 2·621 (5) and 2·696 (7) Å for urea tellurate (Loub, Haase & Mergehenn, 1979). Therefore, the adduct consists of hydrogen-bonded molecules of orthoperiodic acid and urea, forming a three-dimensional network.

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Commission on Journals

Deposition of Macromolecular Atomic Coordinates and Structure Factors with the Protein Data Bank – Modified Policy

Commission policy that *all* structural papers should be equally subject to the requirement of deposition of atomic coordinates and lists of structure factors, as recently reaffirmed in the announcement giving full deposition details [*Acta Cryst.* (1981), B**37**, 1161–1162], has been modified at the request of the Commission on Biological-Macromolecule Crystallography. It was pointed out that most biological-macromolecule structural investigations currently pass through several stages of improving resolution and that the required deposition and resulting public availability of the structure factors may deprive the investigator of a hard-earned advantage.

Under the modified policy, atomic coordinates and structure factors of biological macromolecules are still to be deposited in machine-readable form. However, it is possible for an author who expects to be disadvantaged by having his list of structure factors made generally available to request that this list be granted a privileged status for a period no longer than four years from the date of publication. Earlier release would require the specific consent of the authors.

Papers concerned with new techniques for solving or refining biological-macromolecule structures are exempt from the deposition requirement.