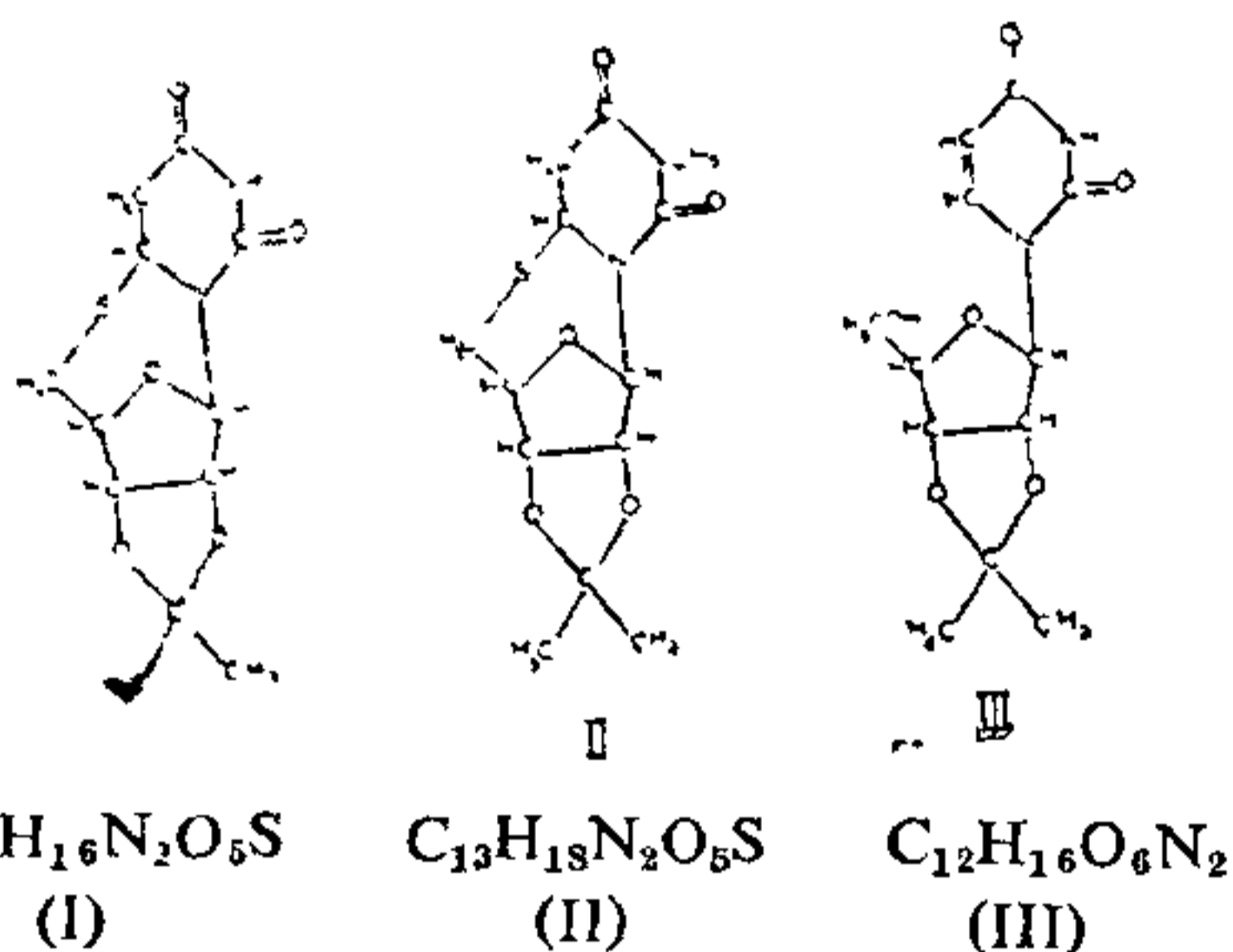


LETTERS TO THE EDITOR

CRYSTAL DATA ON THIONUCLEOSIDES

We wish to report here the crystal data of the following thionucleosides:

- (1) 5'-deoxy-5', 6-epithio-5, 6-dihydro-
2', 3'-O-isopropylidene uridine (I)
- (2) 5'-deoxy-5', 6-epithio-5, 6-dihydro-
N-methyl-2', 3'-O-isopropylidene uridine (II)



Compounds I and II are purely synthetic and are of interest in connection with the work being done to provide an explanation for how substituents like CH_3 are put on to C-5 position (Private communication from Dr. D. M. Brown, University of Cambridge, U.K.). There are many minor nucleo-

sides in tRNA as well as in DNA with C-5 substituents. It is important to know whether the sulphur atom is axial or equatorial on the dihydrouracil ring. We also report here the crystal data of 2', 3'-O-isopropylidene uridine (III), an important intermediate in the preparation of many 5'-substituted uridines.

In crystallizing compounds (I) and (II), about 3 mg of the substance was dissolved in 1 ml of acetone and the solution was layered on a column of distilled water (about 4 ml) in a suitable test tube and allowed to diffuse slowly. Crystals appeared either at the interface or on the top of the acetone column in about 10 to 15 days.

Compound (I) crystallized as needles (about 2 mm long, 0.5 mm cross-section). Compound (II) crystallized as thin plates (about $1.5 \times 1 \times 0.1$ mm). Compound (III) was crystallized by slow evaporation of its solution containing 50% acetone and 50% water. All the crystals are found to be stable in air.

The unit cell dimensions and the space groups of the crystals were determined from rotation, Weissenberg and precession photographs. They belong to orthorhombic system. The densities of (I) and (III) were determined by flotation method using chlorobenzene and bromobenzene. Crystal data are summarised in Table I.

TABLE I

	Crystal I	Crystal II	Crystal III
<i>a</i>	36.129 Å	39.526 Å	19.846 Å
<i>b</i>	14.664 Å	6.607 Å	12.774 Å
<i>c</i>	5.469 Å	5.661 Å	5.222 Å
Volume	2897.45 Å ³	1478.36 Å ³	1323.77 Å ³
Systematic absences	$h00: h = 2n + 1$	$h00: h = 2n + 1$	$h00: h = 2n + 1$
	$0k0: k = 2n + 1$	$0k0: k = 2n + 1$	$0k0: k = 2n + 1$
		$00l: l = 2n + 1$	$00l: l = 2n + 1$
Space group	$P2_12_12$	$P2_12_12_1$	$P2_12_12_1$
Z	8	4	4
ρ_{obs}	1.39 gm/cc	No suitable liquid for experimental determination	1.41 gm/cc.
ρ_{cal}	1.40 gm/cc.	1.44 (?) gm/cc	1.40 gm/cc

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RELATION BETWEEN FORCE FIELD
PARAMETER AND MASS RATIO

THE fundamental problem of intra-molecular mechanics is the determination of the normal coordinate transformation matrix L which may be written as $L = TA$, normalised to the inverse kinetic energy matrix G in the sense $T\tilde{T} = G$. A is an orthogonal matrix. For a two-dimensional vibrational species, the A matrix can be generated by a single parameter c . From studies conducted on isotopic species¹ it is clear that the parameter c is mass-dependent, but the true functional form of this dependence cannot be determined from the theory of molecular vibrations. Müller and collaborators² have investigated the variation of the ratio L_{12}/L_{21} with the mass coupling parameter defined as $T = G_{12}/|G|^{1/2}$ which turns out to be a function of masses and geometry of the molecule and have

noted certain regularities. In the present note we have, however, studied the variation of the parameter c with the mass-ratio m_y/m_x in a number of molecules of the XY_2 and XY_4 types.

TABLE I
Values of mass-ratio and parameter

Molecular Type	Molecule	Mass ratio m_y/m_x	Parameter c	Reference for exact force fields
XY ₂	SeO ₂	0.203	0.046	3
	ClO ₂	0.451	0.082	4
	SO ₂	0.499	0.084	5
	OF ₂	1.188	1.156	6
	OCl ₂	2.216	0.256	7
XY ₄	GeF ₄	0.262	-0.048	8
	GeCl ₄	0.469	-0.013	8
	VCl ₄	0.696	0.02	8
	TiCl ₄	0.740	0.022	8
	CF ₄	1.582	0.15	8

TABLE II
Force fields* and coriolis constants for XY₂ and XY₄ type molecules

Molecule	XY ₂			Molecule	XY ₄			Coriolis constants ζ_4		
	Force fields (A ₁)				Force fields (F ₂)			Coriolis constants ζ_4		
	Present Work	Previous Result	Reference		Present Work	Previous Result	Reference	Present Work	Previous Result	Reference
NO ₂	12.375 0.390 1.188	12.309 0.592 1.100	9	SiF ₄	6.592 0.345 0.435	6.406 ± 0.37 0.291 ± 0.15 0.438 ± 0.01	8	0.506	0.56	14
Cl ₂ S	2.586 -0.021 0.295	2.58 0 0.294	10	SiCl ₄	2.744 0.109 0.242	2.96 ± 0.09 0.14 ± 0.03 0.236 ± 0.005	8	-0.361	-0.23 ± 0.05	15
MgF ₂	2.236 -0.02 0.1465	2.321 0.03 0.141	11	SnCl ₄	2.530 0.121 0.122	2.688 ± 0.08 0.22 ± 0.1 0.118 ± 0.01	8	0.284	0.27 ± 0.05	16
SiF ₂	5.0398 -0.063 0.362	5.329 0.174 0.44	12	RuO ₄	6.699 0.369 0.390	6.49 ± 0.05 0.07 ± 0.05 0.381 ± 0.05	8	0.420	0.32	17
CaF ₂	2.364 0.014 0.085	2.48 0.05 0.08	13	CsO ₄	7.903 0.358 0.441	8.11 ± 0.08 0.1 ± 0.1 0.47 ± 0.01	8	0.507	0.407	17

* The three values of the force constants reported correspond to F_{11} , F_{12} , and F_{22} in the case of XY₂ type molecules and F_{33} , F_{31} and F_{32} in the case of XY₄ type molecules.