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Structures of Bis(3-phenylsydnone) Sulfide (1), Bis[3-(*p*-methoxyphenyl)sydnone] Sulfide (2), and Bis[3-(*p*-ethoxyphenyl)sydnone] Sulfide (3)

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Abstract. (1) $C_{16}H_{10}N_4O_4S$, $M_r = 354$, monoclinic, $P2_1/n, a = 10.347(2), b = 7.777(1), c = 19.796(4)$ Å, $\beta = 100.33 (2)^{\circ}, \quad V = 1567.13 \text{ Å}^3, \quad Z = 4, \quad D_m = 100.33 (2)^{\circ}, \quad V = 1567.13 \text{ Å}^3, \quad Z = 4, \quad D_m = 100.33 (2)^{\circ}, \quad V = 1567.13 \text{ Å}^3, \quad Z = 4, \quad D_m = 100.33 (2)^{\circ}, \quad V = 1567.13 \text{ Å}^3, \quad Z = 4, \quad D_m = 100.33 (2)^{\circ}, \quad V = 1567.13 \text{ Å}^3, \quad Z = 4, \quad D_m = 100.33 (2)^{\circ}, \quad V = 1567.13 \text{ Å}^3, \quad Z = 4, \quad D_m = 100.33 (2)^{\circ}, \quad V = 100.33 (2)$ 1.52 (3), $D_x = 1.50 \text{ g cm}^{-3}$, $\lambda(\text{Mo } K\alpha) = 0.7093 \text{ Å}$, μ (Mo K α) = 2.26 cm⁻¹, F(000) = 728, T = 298 K, final R = 0.033 for 2922 observed reflections. (2) C₁₈- $H_{14}N_4O_6S$, $M_r = 414$, monoclinic, $P2_1/c$, a =14.255 (2), b = 9.344 (1), c = 15.250 (2) Å, $\beta =$ 116.61 (1)°, $V = 1816.12 \text{ Å}^3$, Z = 4, $D_m = 1.50$ (3), $D_r = 1.52 \text{ g cm}^{-3}$, $\lambda(\text{Mo } K\alpha) = 0.7093 \text{ Å}$, $\mu(\text{Mo } K\alpha)$ $= 2 \cdot 14 \text{ cm}^{-1}$, F(000) = 856, T = 298 K, final R =0.039 for 2066 observed reflections. (3) C₂₀H₁₈N₄O₆S, $M_r = 442$, monoclinic, C2/c, a = 20.724 (5), b =12.157 (3), c = 8.201 (3) Å, $\beta = 95.10$ (2)°, V =2057.88 Å³, Z = 4, $D_m = 1.45$ (3), $D_x = 1.43$ g cm⁻³, $\mu(\text{Mo } K\alpha) = 1.94 \text{ cm}^{-1},$ λ (Mo K α) = 0.7093 Å, F(000) = 920, T = 298 K, final R = 0.039 for 1088 observed reflections. The bond lengths of the sydnone ring are similar in all three compounds and comparable to those of other 3,4-disubstituted sydnone derivatives.

The N(1)–C(7) bonds of the title compounds are apparently longer than those of 3-substituted sydnone derivatives which may be attributed to steric effects. A survey of S–C bond lengths and angles between planes of different substituted diaryl sulfides does not show any correlation with the type of substituents. The shortening of the S–C bond lengths of the title compounds *versus* the average bond lengths in the cyclic 1,3,5-trithiane may be attributable to orbital electronegativity effects. In contrast to the 'morino' conformation found in most other diaryl sulfides, all three title compounds appear in the butterfly conformation.

Introduction. The crystal structures of a few 3,4disubstituted sydnone derivatives have recently been studied (Ueng, Wang & Yeh, 1987a,b) and the bond lengths of the sydnone rings were compared with those of 3-substituted sydnone derivatives. As part of a series of studies on 3,4-disubstituted sydnone compounds, the three bis-sydnone sulfide structures were investigated in order to confirm further the steric effect between the phenyl ring and the sydnone ring. In addition, the lone-pair electrons on the S atom may have some effect

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on the S-C bond for these compounds. The conformation of such compounds around the S atom is also of interest.

Table 1. Atomic positional parameters and equivalent isotropic temperature factors for (1), (2) and (3)

$$B_{eq} = (8/3)\pi^2 \sum_i \sum_i U_{ii} a_i^* a_i^* a_i \cdot a_i.$$

$\begin{array}{c c c c c c c c c c c c c c c c c c c $		x	v	z	$B_{\rm es}({\rm \AA}^2)$
	Compound (1)		,	_	- eq /
$\begin{array}{cccc} C14 & 0.6655 (1) & 0.3777 (2) & 0.2852 (1) & 3-1 (1) \\ C34 & 0.6579 (2) & 0.4576 (2) & 0.3461 (1) & 3-7 (1) \\ C34 & 0.4260 (2) & 0.4900 (3) & 0.3226 (1) & 4-6 (1) \\ C44 & 0.4260 (2) & 0.3302 (3) & 0.2618 (1) & 4-8 (1) \\ C54 & 0.9508 (2) & 0.3302 (3) & 0.2618 (1) & 4-8 (1) \\ C54 & 0.9908 (2) & 0.3242 (2) & 0.2535 (1) & 3-0 (1) \\ C34 & 0.9986 (2) & 0.3242 (2) & 0.2535 (1) & 3-0 (1) \\ N24 & 0.79964 (1) & 0.4266 (2) & 0.2023 (1) & 4-0 (1) \\ N24 & 0.7964 (1) & 0.4266 (2) & 0.2033 (1) & 4-0 (1) \\ O24 & 1.1142 (1) & 0.2957 (2) & 0.2580 (1) & 4-9 (1) \\ O24 & 1.1142 (1) & 0.2957 (2) & 0.2580 (1) & 4-9 (1) \\ C28 & 1.2302 (1) & 0.1406 (2) & 0.44757 (1) & 4-1 (1) \\ C28 & 1.3307 (2) & -0.0713 (3) & 0.3322 (1) & 4-1 (1) \\ C58 & 1.3307 (2) & -0.0977 (3) & 0.4109 (1) & 4+4 (1) \\ C58 & 1.3307 (2) & -0.0977 (3) & 0.4109 (1) & 4+4 (1) \\ C58 & 1.3307 (2) & -0.0977 (3) & 0.4109 (1) & 4+4 (1) \\ C58 & 1.3453 (2) & 0.524 (2) & 0.4475 (1) & 4+1 (1) \\ C58 & 1.3407 (2) & -0.3475 (2) & 0.4478 (1) & 3-1 (1) \\ C18 & 1.1564 (1) & 0.366 (2) & 0.4417 (1) & 4+4 (1) \\ C18 & 1.1564 (1) & 0.5751 (2) & 0.4649 (1) & 3-1 (1) \\ C14 & 0.0708 (2) & 0.2708 (3) & 0.1663 (2) & 2-9 (1) \\ N14 & 0.0708 (2) & 0.2708 (3) & 0.1663 (2) & 2-9 (1) \\ N14 & 0.0708 (2) & 0.2708 (3) & 0.1663 (2) & 2-9 (1) \\ N14 & 0.0708 (2) & 0.2708 (3) & 0.1663 (2) & 2-9 (1) \\ N24 & 0.0310 (2) & 0.2708 (3) & 0.1663 (2) & 2-9 (1) \\ N14 & 0.0708 (2) & 0.2708 (3) & 0.1663 (2) & 2-9 (1) \\ N14 & 0.0708 (2) & 0.2708 (3) & 0.1059 (2) & 5-5 (2) \\ C14 & 0.3980 (2) & 0.2708 (3) & 0.1059 (2) & 5-5 (2) \\ C14 & 0.3980 (2) & 0.2708 (3) & 0.1059 (2) & 5-7 (2) \\ C44 & 0.3980 (2) & 0.2024 (4) & 0.3866 (2) & 3-7 (2) \\ C54 & 0.3261 (2) & 0.3374 (3) & 0.3148 (2) & 3-7 (2) \\ C54 & 0.3261 (2) & 0.3374 (3) & 0.3148 (2) & 3-7 (2) \\ C18 & 0.4381 (2) & 0.2028 (4) & 0.1059 (2) & 5-5 (1) \\ N18 & 0.1053 (2) & 0.2034 (4) & 0.2302 (2) & 2-9 (1) \\ N18 & 0.1053 (2) & 0.2034 (4) & 0.2305 (2) & 5-6 (1) \\ N18 & 0.1053 (2) & 0.2303 (3) & 0.3337 (3) & 0.1985 (2) & 5-6 (1) \\ C28 & 0.5118 (3) & 0.3946 (3) & 0.0963$	S	0.9319(1)	0.2026(1)	0-37728 (2)	3.1(1)
$\begin{array}{cccc} C24 & 0.6579 (2) & 0.4576 (2) & 0.3461 (1) & 3.7 (1) \\ C34 & 0.5355 (2) & 0.4717 (3) & 0.36451 (1) & 4.6 (1) \\ C44 & 0.4260 (2) & 0.3003 (3) & 0.2618 (1) & 4.8 (1) \\ C54 & 0.4362 (2) & 0.303 (3) & 0.2618 (1) & 4.8 (1) \\ C74 & 0.9058 (1) & 0.2990 (2) & 0.2969 (1) & 2.9 (1) \\ N14 & 0.7920 (1) & 0.3656 (2) & 0.2635 (1) & 3.0 (1) \\ N14 & 0.7920 (1) & 0.3656 (2) & 0.2635 (1) & 3.0 (1) \\ N14 & 0.7920 (1) & 0.4027 (2) & 0.1948 (1) & 4.3 (1) \\ O14 & 0.9252 (1) & 0.4027 (2) & 0.1948 (1) & 4.3 (1) \\ O14 & 0.9252 (1) & 0.4027 (2) & 0.1948 (1) & 4.3 (1) \\ O14 & 0.9252 (1) & 0.4005 (2) & 0.5321 (1) & 3.6 (1) \\ C1B & 1.2362 (1) & 0.1406 (2) & 0.4572 (1) & 3.1 (1) \\ C4B & 1.3722 (2) & -0.0971 (3) & 0.4109 (1) & 4.4 (1) \\ C5B & 1.3037 (2) & -0.0971 (3) & 0.4109 (1) & 4.4 (1) \\ C6B & 1.2619 (2) & 0.0545 (2) & 0.4276 (1) & 3.8 (1) \\ C1B & 1.0438 (1) & 0.3466 (2) & 0.4181 (1) & 2.9 (1) \\ C8B & 1.0342 (2) & 0.5246 (2) & 0.4276 (1) & 3.6 (1) \\ N1B & 1.1719 (1) & 0.3061 (2) & 0.4490 (1) & 3.1 (1) \\ N2B & 1.2402 (1) & 0.4359 (2) & 0.4785 (1) & 4.2 (1) \\ O2B & 0.9470 (1) & 0.6275 (2) & 0.4117 (1) & 4.4 (1) \\ Compound (2) \\ S & 0.0283 (1) & 0.3751 (1) & 0.0874 (1) & 3.1 (1) \\ N14 & 0.0708 (2) & 0.2709 (3) & 0.1663 (2) & 2.9 (1) \\ N14 & 0.0708 (2) & 0.2708 (3) & 0.1693 (2) & 5.5 (2) \\ C34 & -0.183 (2) & 0.2578 (3) & 0.1591 (2) & 3.9 (2) \\ C14 & 0.183 (2) & 0.2578 (3) & 0.1591 (2) & 3.9 (2) \\ C14 & 0.183 (2) & 0.2578 (3) & 0.1591 (2) & 3.9 (2) \\ C14 & 0.183 (2) & 0.2578 (3) & 0.1591 (2) & 5.5 (2) \\ C34 & 0.3449 (2) & 0.3286 (3) & 0.3666 (2) & 3.7 (2) \\ C34 & 0.3449 (2) & 0.3286 (3) & 0.3666 (2) & 3.7 (2) \\ C34 & 0.3449 (2) & 0.2268 (3) & 0.1591 (2) & 5.5 (2) \\ C34 & 0.3449 (2) & 0.3286 (3) & 0.3666 (2) & 3.7 (2) \\ C34 & 0.5320 (1) & 0.192 (2) & 0.2466 (2) & 3.7 (2) \\ C34 & 0.5320 (1) & 0.1632 (2) & -0.0097 (3) & 3.5 (1) \\ N18 & 0.1033 (2) & 0.2395 (2) & 4.5 (2) \\ C18 & 0.2395 (2) & 0.0337 (3) & 0.0985 (2) & 4.5 (2) \\ C36 & 0.3414 (1) & 0.0332 (2) & 0.2306 (4) & 4.6 (2) \\ C3 & 0.5233 (2) & 0.1488 (2) & 0.2302 (4) & 4.8 (2) \\ C26$	CIA	0.6655 (1)	0.3777 (2)	0.2852(1)	3.1(1)
$\begin{array}{cccc} C34 & 0.4355 (2) & 0.4717 (3) & 0.3645 (1) & 4.6 (1) \\ C54 & 0.4362 (2) & 0.302 (3) & 0.2226 (1) & 4.9 (1) \\ C54 & 0.9986 (2) & 0.313 (3) & 0.2618 (1) & 4.8 (1) \\ C64 & 0.9986 (2) & 0.313 (3) & 0.2618 (1) & 4.9 (1) \\ C84 & 0.9986 (2) & 0.3242 (2) & 0.2533 (1) & 3.5 (1) \\ N14 & 0.7926 (1) & 0.4564 (2) & 0.2023 (1) & 4.0 (1) \\ O14 & 0.9252 (1) & 0.4027 (2) & 0.1948 (1) & 4.3 (1) \\ O24 & 1.1142 (1) & 0.2957 (2) & 0.2380 (1) & 4.9 (1) \\ C18 & 1.2362 (1) & 0.1406 (2) & 0.4572 (1) & 3.1 (1) \\ C28 & 1.2750 (2) & -0.0905 (2) & 0.5321 (1) & 3.6 (1) \\ C3B & 1.3435 (2) & -0.0721 (3) & 0.5322 (1) & 4.1 (1) \\ C5B & 1.3307 (2) & -0.0977 (3) & 0.4109 (1) & 4.4 (1) \\ C5B & 1.3017 (2) & -0.0977 (3) & 0.4109 (1) & 4.4 (1) \\ C5B & 1.3017 (2) & -0.0977 (3) & 0.4109 (1) & 4.4 (1) \\ C5B & 1.3017 (2) & -0.0977 (3) & 0.4109 (1) & 3.8 (1) \\ N18 & 1.1719 (1) & 0.3061 (2) & 0.4490 (1) & 3.1 (1) \\ N2B & 1.0483 (1) & 0.5751 (2) & 0.4785 (1) & 4.2 (1) \\ O1B & 1.402 (2) & 0.5246 (2) & 0.4181 (1) & 2.9 (1) \\ N2B & 1.0947 (1) & 0.6273 (2) & 0.4107 (1) & 4.4 (1) \\ Compound (2) \\ S & 0.9470 (1) & 0.6273 (2) & 0.4107 (1) & 4.1 (1) \\ C74 & 0.0003 (2) & 0.2709 (3) & 0.1663 (2) & 2.9 (1) \\ N14 & 0.0708 (2) & 0.217 (2) & 0.2466 (2) & 3.1 (1) \\ O14 & -0.0757 (2) & 0.1430 (2) & 0.2395 (2) & 4.8 (1) \\ O24 & -0.310 (2) & 0.2396 (3) & 0.3066 (2) & 3.7 (2) \\ C34 & 0.0310 (2) & 0.2362 (3) & 0.1591 (2) & 3.9 (2) \\ C44 & 0.3980 (2) & 0.0217 (2) & 0.2466 (2) & 3.8 (1) \\ O14 & -0.0757 (2) & 0.1430 (2) & 0.2392 (2) & 2.9 (1) \\ N14 & 0.0708 (2) & 0.217 (2) & 0.2466 (2) & 3.1 (1) \\ O14 & -0.0757 (2) & 0.133 (0) & 0.1659 (2) & 5.5 (2) \\ C34 & 0.0310 (2) & 0.2362 (3) & 0.1059 (2) & 5.5 (2) \\ C34 & 0.0349 (2) & 0.0217 (2) & 0.2466 (2) & 3.7 (1) \\ O14 & -0.0757 (2) & 0.1236 (3) & 0.3056 (2) & 3.7 (2) \\ C34 & 0.0349 (2) & 0.0208 (4) & 0.3656 (2) & 3.7 (2) \\ C34 & 0.0349 (2) & 0.0308 (2) & 0.0019 (2) & 2.8 (1) \\ N14 & 0.0708 (2) & 0.2022 (2) & 2.9 (1) \\ N14 & 0.0708 (2) & 0.0034 (1) & 0.2500 & 3.5 (1) \\ O25 & 0.248 (1) & 0.0336 (2) & 0.0038 (2) & 3.5 (1) \\ O3 $	C2A	0-6579 (2)	0.4576 (2)	0-3461 (1)	3.7(1)
$\begin{array}{cccc} C44 & 0-4260 (2) & 0-4090 (3) & 0-3226 (1) & 4-9 (1) \\ C54 & 0-4362 (2) & 0-3302 (3) & 0-2218 (1) & 4-8 (1) \\ C64 & 0-5569 (2) & 0-3135 (3) & 0-2417 (1) & 3-9 (1) \\ C74 & 0-9086 (2) & 0-3242 (2) & 0-2535 (1) & 3-5 (1) \\ N14 & 0-7920 (1) & 0-3656 (2) & 0-2335 (1) & 3-6 (1) \\ N14 & 0-7920 (1) & 0-3656 (2) & 0-2033 (1) & 4-0 (1) \\ O14 & 0-9252 (1) & 0-4027 (2) & 0-1948 (1) & 4-3 (1) \\ O24 & 1-1142 (1) & 0-2957 (2) & 0-2032 (1) & 4-1 (1) \\ C1B & 1-2362 (1) & 0-1406 (2) & 0-4572 (1) & 3-1 (1) \\ C2B & 1-3262 (2) & -0.0058 (2) & 0-5231 (1) & 3-6 (1) \\ C3B & 1-3435 (2) & -0-0771 (3) & 0-4109 (1) & 4+4 (1) \\ C5B & 1-3307 (2) & -0-0977 (3) & 0-4109 (1) & 4+4 (1) \\ C6B & 1-2619 (2) & 0-0545 (2) & 0-4003 (1) & 3-8 (1) \\ N1B & 1-1719 (1) & 0-366 (2) & 0-4767 (1) & 3-5 (1) \\ N1B & 1-1719 (1) & 0-366 (2) & 0-4767 (1) & 3-1 (1) \\ C2B & 1-0483 (1) & 0-3466 (2) & 0-4767 (1) & 3-1 (1) \\ C2B & 1-0483 (1) & 0-3455 (2) & 0-4787 (1) & 3-1 (1) \\ C7A & 0-0003 (2) & 0-2709 (3) & 0-1663 (2) & 2-9 (1) \\ N1A & 0-0708 (2) & 0-2709 (3) & 0-1663 (2) & 2-9 (1) \\ N1A & 0-0708 (2) & 0-2707 (3) & 0-1663 (2) & 2-9 (1) \\ N1A & 0-0708 (2) & 0-2707 (3) & 0-1663 (2) & 2-9 (1) \\ N1A & 0-0708 (2) & 0-2707 (3) & 0-1663 (2) & 2-9 (1) \\ N1A & 0-0708 (2) & 0-2707 (3) & 0-1663 (2) & 2-9 (1) \\ N1A & 0-0708 (2) & 0-2707 (3) & 0-1663 (2) & 2-9 (1) \\ N1A & 0-0708 (2) & 0-2707 (3) & 0-1663 (2) & 2-9 (1) \\ N1A & 0-0708 (2) & 0-2707 (3) & 0-1663 (2) & 2-9 (1) \\ N1A & 0-0708 (2) & 0-2707 (3) & 0-1663 (2) & 2-9 (1) \\ N1A & 0-0708 (2) & 0-2707 (3) & 0-156 (3) & 0-1597 (2) & 3-7 (2) \\ C44 & 0-3880 (2) & 0-2044 (3) & 0-3148 (2) & 3-7 (2) \\ C54 & 0-3449 (2) & 0-3256 (3) & 0-1059 (2) & 3-7 (2) \\ C54 & 0-3449 (2) & 0-3256 (3) & 0-3066 (2) & 3-7 (2) \\ C54 & 0-3449 (2) & 0-3286 (3) & 0-3066 (2) & 3-7 (2) \\ C34 & 0-3489 (2) & 0-0044 (2) & 0-1155 (3) & 4-64 (1) \\ O18 & -0-0258 (2) & 0-0312 (2) & -00494 (2) & 3-18 (1) \\ N1B & 0-1053 (2) & 0-0363 (3) & 0-0605 (2) & 3-7 (2) \\ C44 & 0-2344 (2) & 0-2360 (3) & 0-3354 (3) & 0-0963 (2) & 3-5 (4) \\ C5B & 0-3518 (3) & 0-3946 ($	C3A	0.5355 (2)	0.4717(3)	0.3645(1)	4.6(1)
$\begin{array}{cccc} C34 & 0-362 (2) & 0-302 (3) & 0-2018 (1) & 4-8 (1) \\ C54 & 0-556 (2) & 0-313 (3) & 0-2417 (1) & 3-9 (1) \\ C7A & 0-9058 (1) & 0-2990 (2) & 0-2969 (1) & 2-9 (1) \\ C84 & 0-996 (2) & 0-324 (2) & 0-2335 (1) & 3-5 (1) \\ N14 & 0-7920 (1) & 0-3656 (2) & 0-2635 (1) & 3-5 (1) \\ N24 & 0-7964 (1) & 0-4264 (2) & 0-2023 (1) & 4-0 (1) \\ N24 & 1-9252 (1) & 0-4027 (2) & 0-1948 (1) & 4-3 (1) \\ O24 & 1-1142 (1) & 0-2957 (2) & 0-2880 (1) & 4-9 (1) \\ C1B & 1-3262 (1) & 0-1406 (2) & 0-4572 (1) & 3-1 (1) \\ C2B & 1-23750 (2) & 0-0805 (2) & 0-5321 (1) & 3-6 (1) \\ C3B & 1-3372 (2) & -0-1593 (2) & 0-4767 (1) & 4-1 (1) \\ C5B & 1-3307 (2) & -0-0977 (3) & 0-4109 (1) & 4-4 (1) \\ C5B & 1-3307 (2) & -0-0977 (3) & 0-4109 (1) & 4-4 (1) \\ C5B & 1-3021 (2) & 0-545 (2) & 0-4003 (1) & 3-8 (1) \\ N1B & 1-1719 (1) & 0-3661 (2) & 0-4499 (1) & 3-1 (1) \\ N1B & 1-1719 (1) & 0-3661 (2) & 0-4499 (1) & 3-1 (1) \\ N1B & 1-1719 (1) & 0-3671 (2) & 0-4499 (1) & 3-1 (1) \\ O2B & 0-9470 (1) & 0-6275 (2) & 0-41177 (1) & 4-4 (1) \\ Compound (2) \\ S & 0-0283 (1) & 0-3751 (1) & 0.0874 (1) & 3-1 (1) \\ N1A & 0-0708 (2) & 0-2709 (3) & 0-1663 (2) & 2-9 (1) \\ N1A & 0-0707 (2) & 0-1430 (2) & 0-2295 (2) & 4-3 (1) \\ O1A & -00757 (2) & 0-1430 (2) & 0-2295 (2) & 4-3 (1) \\ O1A & -00757 (2) & 0-1430 (2) & 0-2295 (2) & 4-3 (1) \\ O1A & -00757 (2) & 0-1430 (2) & 0-2295 (2) & 4-3 (1) \\ O2A & 0-0380 (2) & 0-2014 (3) & 0-3292 (2) & 2-9 (1) \\ N1A & 0-0310 (2) & 0-22678 (3) & 0.1591 (2) & 5-5 (2) \\ C3A & 0-3499 (2) & 0-2364 (3) & 0.3117 (2) & 3-5 (1) \\ O2A & 0-2366 (2) & 0-0731 (3) & 0.3148 (2) & 3-7 (2) \\ C4A & 0-3380 (2) & 0-2014 (3) & 0-3050 (2) & 2-9 (2) \\ C5A & 0-3494 (2) & 0.3286 (3) & 0.3117 (2) & 3-5 (1) \\ O3A & 0-5044 (2) & 0.3294 (3) & 0.3117 (2) & 3-5 (1) \\ O3A & 0-5044 (2) & 0.3394 (3) & 0.3117 (2) & 3-5 (1) \\ O2B & -0.0611 (2) & 0-3034 (1) & 0-2302 (2) & 2-9 (1) \\ N2B & 0-0817 (2) & 0-2365 (2) & 0-1135 (1) & 4-4 (1) \\ O2B & -0.0611 (2) & 0-3034 (1) & 0-2307 (2) & 3-7 (2) \\ C5B & 0-32414 (1) & 0-00335 (2) & 0-2376 (4) & 4-6 (2) \\ C5B & 0-3414 (1) & 0-0335 (2) & 0-2307 ($	C4A	0-4260 (2)	0.4090 (3)	0.3226(1)	4.9(1)
Cbd 0-5369 (2) 0-3135 (3) 0-241 (1) 3-9 (1) C74 0-9058 (1) 0-2990 (2) 0-2266 (1) 3-9 (1) C84 0-9986 (2) 0-3242 (2) 0-2533 (1) 3-0 (1) N14 0-7926 (1) 0-4565 (2) 0-2033 (1) 4-0 (1) O14 0-9252 (1) 0-4027 (2) 0-1948 (1) 4-3 (1) C1B 1-2362 (1) 0-4027 (2) 0-1948 (1) 4-1 (1) C1B 1-2362 (1) 0-4005 (2) 0-4572 (1) 3-1 (1) C2B 1-2362 (2) 0-0050 (2) 0-5231 (1) 3-6 (1) C3B 1-3307 (2) -0-0977 (3) 0-4109 (1) 4-1 (1) C5B 1-3307 (2) -0-0977 (3) 0-4109 (1) 4-1 (1) C6B 1-2619 (2) 0-0545 (2) 0-4003 (1) 3-8 (1) C7B 1-0482 (1) 0-3466 (2) 0-4767 (1) 3-5 (1) N1B 1-1719 (1) 0-3061 (2) 0-4479 (1) 3-1 (1) C2B 1-2402 (1) 0-4359 (2) 0-4489 (1) 3-1 (1) C2B 0-9470 (1) 0-6275 (2) 0-4181 (1) 2-9 (1) N1B 1-1564 (1) 0-5751 (2) 0-4649 (1) 4-3 (1) O2B 0-9470 (1) 0-6275 (2) 0-4117 (1) 4-4 (1) Compound (2) S 0-0283 (1) 0-3751 (1) 0-0874 (1) 3-1 (1) N24 0-0708 (2) 0-2079 (3) 0-1663 (2) 2-9 (1) N14 0-0708 (2) 0-2017 (2) 0-2466 (2) 3-1 (1) N24 0-0310 (2) 0-2078 (3) 0-1659 (2) 2-9 (1) N14 0-0708 (2) 0-2017 (3) 0-2392 (2) 4-3 8 (1) O24 -0-1883 (2) 0-2678 (3) 0-1591 (2) 3-9 (2) C44 0-3980 (2) 0-2014 (3) 0-2926 (2) 4-3 (1) D1A 0-0308 (2) 0-2014 (3) 0-2926 (2) 4-3 (1) N24 0-0310 (2) 0-2046 (3) 0-3348 (2) 3-7 (2) C44 0-3980 (2) 0-2044 (4) 0-3866 (2) 3-7 (2) C44 0-2361 (2) 0-1207 (3) 0-0197 (2) 3-9 (3) C1B 0-20258 (2) 0-1332 (3) 0-04097 (3) 3-6 (1) N2B 0-0053 (2) 0-07072 (3) 0-3148 (2) 3-7 (1) D2B -0-0153 (2) 0-07072 (3) 3-0107 (2) 3-7 (1) D2B -0-0163 (2) 0-07072 (2) 3-206 (2) 3-7 (1) D2B -0-0163 (2) 0-0208 (2) -0-0079 (3) 3-7 (1) D2B 0-0258 (1) 0-1034 (1) 0-2500 (3) 3-5 (1) D3B 0-5250 (1) 0-1034 (1) 0-2500 (3) 3-5 (1) D4 0-4035 (1) 0-2354 (2) 0-0058 (3) 3-4 (1)	C5A	0.4362(2)	0.3302(3)	0.2618(1)	4.8(1)
$\begin{array}{c ccccc} CAA & 0-9986 (2) & 0-2990 (2) & 0-2990 (1) & 2-911 \\ 2-811 \\ N1A & 0-9986 (2) & 0-3242 (2) & 0-2335 (1) & 3-5 (1) \\ N1A & 0-9926 (1) & 0-4264 (2) & 0-2033 (1) & 3-5 (1) \\ OLA & 0-9252 (1) & 0-4027 (2) & 0-1948 (1) & 4-3 (1) \\ OLA & 1-1142 (1) & 0-2957 (2) & 0-2380 (1) & 4-9 (1) \\ C1B & 1-2362 (1) & 0-4065 (2) & 0-4572 (1) & 3-1 (1) \\ C2B & 1-2350 (2) & 0-0805 (2) & 0-5231 (1) & 3-6 (1) \\ C3B & 1-3435 (2) & -0-077 (3) & 0-4109 (1) & 4-4 (1) \\ C5B & 1-2619 (2) & -0-0593 (2) & 0-4767 (1) & 4-1 (1) \\ C6B & 1-2619 (2) & -0.0545 (2) & 0-4003 (1) & 3-8 (1) \\ C7B & 1-0483 (1) & 0-3466 (2) & 0-4181 (1) & 2-9 (1) \\ N2B & 1-0342 (2) & 0-5246 (2) & 0-4206 (1) & 3-5 (1) \\ N1B & 1-1719 (1) & 0-3061 (2) & 0-4499 (1) & 3-1 (1) \\ N2B & 1-1564 (1) & 0-5751 (2) & 0-4449 (1) & 4-3 (1) \\ O2B & 0-9470 (1) & 0-6275 (2) & 0-4417 (1) & 4-4 (1) \\ Compound (2) \\ S & 0-0283 (1) & 0-3751 (1) & 0.0874 (1) & 3-1 (1) \\ N2A & 0.0310 (2) & 0-2396 (3) & 0-1663 (2) & 2-9 (1) \\ N1A & 0-07057 (2) & 0-1430 (2) & 0-2295 (2) & 4-38 (1) \\ O2A & -0-1883 (2) & 0-2578 (3) & 0-1059 (2) & 5-5 (2) \\ C1A & 0-03980 (2) & 0-2074 (3) & 0-3364 (2) & 4-02 (2) \\ C2A & 0-2366 (2) & 0-731 (3) & 0-3148 (2) & 3-7 (2) \\ C4A & 0-3389 (2) & 0-025 (3) & 0-3168 (2) & 3-7 (2) \\ C4A & 0-3389 (2) & 0-2284 (3) & 0-3159 (2) & 5-5 (2) \\ C5A & 0-2361 (2) & 0-3304 (3) & 0-3117 (2) & 3-5 (1) \\ O3A & 0-5044 (2) & 0.189 (13) & 0-4350 (2) & -0.013 (2) & -0.0049 (2) & 3-1 (1) \\ N2B & 0-0817 (2) & 0-3294 (3) & 0-3162 (5) & 0-4667 (3) & 6-9 (3) \\ C7B & 0-0222 (2) & 0-2490 (3) & 0-3162 (5) & 0-4115 (1) & 4-4 (1) \\ D2B & -0-1611 (2) & 0-1903 (3) & -0.0049 (2) & 3-1 (1) \\ D2B & -0.0161 (2) & 0-2395 (2) & 0-2306 (2) & 3-7 (2) \\ C3B & 0-3081 (2) & 0-3034 (1) & 0-2300 (3) & -0.0049 (2) & 3-1 (1) \\ D2B & -0.0161 (2) & 0-2394 (3) & 0-3162 (5) & 0-4067 (3) & 6-9 (3) \\ C3B & 0-3081 (2) & 0-3034 (1) & 0-2300 (3) & -0.0075 (2) & 3-7 (1) \\ D3B & 0-0025 (2) & 0-2000 (4) & 0-335 (2) & 0-0004 (4) & 3-35 (1) \\ C4B & 0-4224 (2) & 0-2395 (3) & 0-0005 (2) & 3-7 (2) \\ C5B & 0-3091 (1) & 0-1352 (2$	COA	0.3369(2)	0.3135(3)	0.2417(1)	3.9(1)
Carl 0.9780 (2) 0.2242 (2) 0.2233 (1) 3.0 (1) N14 0.7920 (1) 0.3556 (2) 0.2233 (1) 4.0 (1) O14 0.9252 (1) 0.405 (2) 0.2233 (1) 4.3 (1) O24 1.1142 (1) 0.2957 (2) 0.2380 (1) 4.9 (1) C18 1.2362 (1) 0.1406 (2) 0.4572 (1) 3.1 (1) C28 1.2350 (2) 0.0805 (2) 0.4572 (1) 3.6 (1) C38 1.3307 (2) -0.0977 (3) 0.4109 (1) 4.4 (1) C58 1.0310 (2) 0.0545 (2) 0.4403 (1) 3.8 (1) N1B 1.1719 (1) 0.3061 (2) 0.4493 (1) 3.5 (1) N1B 1.1719 (1) 0.3061 (2) 0.4493 (1) 3.1 (1) N2B 1.2602 (1) 0.4559 (2) 0.4493 (1) 3.1 (1) N2B 1.2602 (1) 0.4559 (2) 0.4493 (1) 3.1 (1) O2B 0.9470 (1) 0.6275 (2) 0.4117 (1) 4.4 (1) Compound (2) S 0.0283 (1) 0.3751 (1) 0.0874 (1) 3.1 (1) C74 0.0003 (2) 0.2709 (3) 0.1663 (2) 2.9 (1) N14 0.0708 (2) 0.2709 (3) 0.1663 (2) 2.9 (1) N14 0.0708 (2) 0.2217 (2) 0.2466 (2) 3.1 (1) O24 -0.1883 (2) 0.2578 (3) 0.1059 (2) 5.5 (2) C84 -0.0996 (2) 0.2362 (3) 0.1391 (2) 3.9 (2) C14 0.1843 (2) 0.2017 (3) 0.3314 (2) 3.7 (2) C34 0.3399 (2) 0.0275 (3) 0.3314 (2) 3.7 (2) C34 0.3399 (2) 0.0204 (4) 0.2396 (2) 3.3 (1) (2) 3.9 (2) C34 0.3499 (2) 0.2204 (3) 0.3017 (2) 3.5 (1) O34 0.5044 (2) 0.1891 (3) 0.3418 (2) 3.7 (2) C34 0.3499 (2) 0.2204 (3) 0.30147 (2) 3.5 (1) O34 0.5044 (2) 0.1391 (3) 0.3117 (2) 3.5 (1) O34 0.5044 (2) 0.1391 (3) 0.3117 (2) 3.5 (1) O34 0.5042 (2) 0.0324 (3) 0.3017 (2) 3.5 (1) D34 0.5044 (2) 0.1391 (3) 0.3117 (2) 3.5 (1) D34 0.5044 (2) 0.1391 (3) 0.3117 (2) 3.5 (1) D34 0.5044 (2) 0.1391 (3) 0.3117 (2) 3.5 (1) D34 0.5042 (2) 0.2294 (3) 0.3017 (2) 3.7 (2) C64 0.2361 (2) 0.03294 (3) 0.3017 (2) 3.7 (2) C64 0.2361 (2) 0.03294 (3) 0.3017 (2) 3.7 (2) C64 0.2361 (2) 0.03294 (3) 0.3017 (2) 3.5 (1) D18 0.4053 (2) 0.0003 (2) -0.0073 (2) 3.7 (2) C64 0.2414 (1) 0.1933 (2) 0.0006 (2) 3.7 (2) C10 0.9885 (2) 0.132 (4) 0.148 (2) 0.2300 (3) 5.0 (1) C38 0.3388 (2) 0.1337 (3) 0.0963 (2) 4.5 (2) C39 0.3088 (2) 0.00034 (1) 0.2250 (3) 5.5 (1) D38 0.3088 (2) 0.0004 (2) 0.1207 (4) 4.1 (2) C5 0.2888 0.3004 (3)	CIA CIA	0.9038(1)	0.2990(2) 0.3242(2)	0.2909(1) 0.2535(1)	2.9(1) 3.5(1)
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	N14	0.7920(2)	0.3656(2)	0.2635(1)	3.0(1)
$\begin{array}{ccccc} \hline 0.14 & 0.9252 (1) & 0.4027 (2) & 0.1948 (1) & 4.3 (1) \\ 02.4 & 1.1142 (1) & 0.2957 (2) & 0.2580 (1) & 4.9 (1) \\ C1B & 1.2362 (1) & 0.1406 (2) & 0.4572 (1) & 3.1 (1) \\ C2B & 1.2750 (2) & 0.0805 (2) & 0.5231 (1) & 3.6 (1) \\ C3B & 1.3435 (2) & -0.0771 (3) & 0.4109 (1) & 4.4 (1) \\ C4B & 1.3722 (2) & -0.1593 (2) & 0.4767 (1) & 4.1 (1) \\ C5B & 1.307 (2) & -0.0977 (3) & 0.4109 (1) & 4.4 (1) \\ C5B & 1.307 (2) & -0.0977 (3) & 0.4109 (1) & 4.4 (1) \\ C7B & 1.0483 (1) & 0.3466 (2) & 0.44181 (1) & 2.9 (1) \\ C8B & 1.042 (2) & 0.524 (2) & 0.4276 (1) & 3.5 (1) \\ N1B & 1.1719 (1) & 0.3061 (2) & 0.4276 (1) & 3.5 (1) \\ N2B & 1.2402 (1) & 0.4359 (2) & 0.4489 (1) & 3.1 (1) \\ N2B & 1.2602 (1) & 0.4359 (2) & 0.4489 (1) & 4.3 (1) \\ O2B & 0.9470 (1) & 0.6275 (2) & 0.4117 (1) & 4.4 (1) \\ \hline Compound (2) \\ S & 0.0283 (1) & 0.3751 (1) & 0.0874 (1) & 3.1 (1) \\ N24 & 0.0310 (2) & 0.2017 (2) & 0.2466 (2) & 3.1 (1) \\ N24 & 0.0310 (2) & 0.2017 (2) & 0.2266 (2) & 4.3 (1) \\ N14 & 0.0708 (2) & 0.2017 (2) & 0.2395 (2) & 4.8 (1) \\ O24 & -0.1883 (2) & 0.2678 (3) & 0.1591 (2) & 3.9 (2) \\ C14 & 0.1843 (2) & 0.0214 (3) & 0.2902 (2) & 2.9 (1) \\ C34 & 0.3380 (2) & 0.0725 (3) & 0.3634 (2) & 4.0 (2) \\ C44 & 0.3980 (2) & 0.0725 (3) & 0.3634 (2) & 4.0 (2) \\ C44 & 0.3980 (2) & 0.0725 (3) & 0.3636 (2) & 3.7 (2) \\ C54 & 0.2361 (2) & 0.3128 (3) & 0.3117 (2) & 3.5 (1) \\ O34 & 0.5642 (3) & 0.3162 (5) & 0.4667 (3) & 6.9 (3) \\ C7B & 0.0222 (2) & 0.2490 (3) & -0.0192 (2) & 2.9 (1) \\ C2B & 0.2051 (2) & 0.1820 (3) & -0.0788 (2) & 3.0 (1) \\ C2B & 0.0617 (2) & 0.3294 (3) & 0.3117 (2) & 3.5 (1) \\ O1B & -0.0228 (2) & 0.0725 (3) & 0.3606 (2) & 3.7 (1) \\ D2B & -0.0611 (2) & 0.1903 (3) & -0.0049 (2) & 3.1 (1) \\ D2B & -0.0611 (2) & 0.1903 (3) & -0.0049 (2) & 3.1 (1) \\ D2B & -0.0611 (2) & 0.1903 (3) & -0.0048 (2) & 3.0 (1) \\ C2B & 0.2350 (1) & 0.1320 (3) & -0.0158 (2) & 4.0 (2) \\ C54 & 0.2341 (4) & 0.2352 (3) & 0.0258 (2) & 3.0 (1) \\ C3B & 0.3280 (2) & 0.0033 (1) & 0.2500 & 3.5 (1) \\ C3B & 0.5243 (2) & 0.1337 (3) & 0.1898 (2) & 5.6 (2) \\ C44 & 0.2414 (1) & 0.0335 (2$	N24	0.7964(1)	0.4264(2)	0.2023(1)	4.0(1)
$\begin{array}{ccccc} \hline 0.24 & 1-1142 (1) & 0-2957 (2) & 0-2580 (1) & 4-9 (1) \\ C1B & 1-2362 (1) & 0-1406 (2) & 0.4572 (1) & 3-1 (1) \\ C3B & 1-3435 (2) & -0.0805 (2) & 0.5231 (1) & 3-6 (1) \\ C3B & 1-3435 (2) & -0.0721 (3) & 0.5322 (1) & 4-1 (1) \\ C5B & 1-307 (2) & -0.0977 (3) & 0.4109 (1) & 4-4 (1) \\ C5B & 1-2619 (2) & 0.0545 (2) & 0.4003 (1) & 3-8 (1) \\ C7B & 1-0442 (2) & 0.5246 (2) & 0.4216 (1) & 3-1 (1) \\ C8B & 1-0342 (2) & 0.5246 (2) & 0.4216 (1) & 3-1 (1) \\ N1B & 1-1719 (1) & 0.3061 (2) & 0.4496 (1) & 4-3 (1) \\ 01B & 1-1546 (1) & 0.5751 (2) & 0.4649 (1) & 4-3 (1) \\ 02B & 0.9470 (1) & 0.6275 (2) & 0.4117 (1) & 4-4 (1) \\ \hline Compound (2) \\ S & 0.0283 (1) & 0.3751 (1) & 0.0874 (1) & 3-1 (1) \\ C7A & 0.0003 (2) & 0.2709 (3) & 0.1663 (2) & 2-9 (1) \\ N1A & 0.0708 (2) & 0.2117 (2) & 0.2466 (2) & 3-1 (1) \\ N2A & 0.0310 (2) & 0.1239 (3) & 0.2926 (2) & 4-38 (1) \\ 02A & -0.0986 (2) & 0.2617 (3) & 0.1059 (2) & 5-5 (2) \\ C8A & -0.0996 (2) & 0.2261 (3) & 0.1059 (2) & 5-5 (2) \\ C4A & 0.3980 (2) & 0.2014 (3) & 0.2902 (2) & 2-9 (1) \\ C2A & 0.2366 (2) & 0.0731 (3) & 0.3148 (2) & 3-7 (2) \\ C5A & 0.348 (2) & 0.2004 (4) & 0.3866 (2) & 3-7 (2) \\ C5A & 0.349 (2) & 0.3294 (3) & 0.3117 (2) & 3-5 (1) \\ 03A & 0.5044 (2) & 0.3294 (3) & 0.3117 (2) & 3-5 (1) \\ 03A & 0.5044 (2) & 0.3294 (3) & 0.3117 (2) & 3-5 (1) \\ 03A & 0.5044 (2) & 0.3294 (3) & 0.3117 (2) & 3-5 (1) \\ 03B & -0.0228 (2) & 0.0416 (3) & -0.0705 (2) & 3-7 (2) \\ C5B & 0.0517 (2) & 0.0432 (3) & -0.0705 (2) & 3-7 (2) \\ C5B & 0.0518 (2) & 0.193 (2) & -0.0193 (2) & -0.0193 (2) & -0.019 (2) & -2.8 (1) \\ N1B & 0.0103 (2) & 0.193 (2) & -0.0049 (2) & 3-1 (1) \\ 02B & -0.0679 (2) & 0.1820 (3) & -0.0705 (2) & 3-7 (2) \\ C3B & 0.328 (2) & 0.1312 (2) & -0.0135 (1) & -0.0705 (2) & 3-7 (1) \\ 02B & -0.0679 (2) & 0.1323 (3) & -0.0705 (2) & 3-7 (1) \\ 03B & 0.5243 (2) & 0.1337 (3) & 0.1985 (2) & 5-6 (2) \\ C5B & 0.3213 (2) & 0.148 (2) & 0.2306 (2) & 3-7 (1) \\ 03B & 0.5243 (2) & 0.0337 (3) & 0.1985 (2) & 5-6 (2) \\ C5B & 0.0513 (1) & 0.0334 (1) & 0.2500 & 3.55 (1) \\ C1 & 0.328 (2) & 0.0334 (1) & 0.2503 (3) & -$	014	0.9252(1)	0.4027 (2)	0.1948(1)	4.3(1)
	02 <i>A</i>	1.1142(1)	0.2957 (2)	0.2580(1)	4.9(1)
$\begin{array}{ccccc} 228 & 1.2750 (2) & 0.0805 (2) & 0.5221 (1) & 3.6 (1) \\ C3B & 1.3435 (2) & -0.0721 (3) & 0.5322 (1) & 4.1 (1) \\ C5B & 1.3307 (2) & -0.0977 (3) & 0.4109 (1) & 4.4 (1) \\ C5B & 1.3307 (2) & -0.0977 (3) & 0.4109 (1) & 4.4 (1) \\ C5B & 1.0342 (2) & 0.5246 (2) & 0.4205 (1) & 3.8 (1) \\ C7B & 1.0483 (1) & 0.3466 (2) & 0.44181 (1) & 2.9 (1) \\ C8B & 1.0342 (2) & 0.5246 (2) & 0.4276 (1) & 3.5 (1) \\ N1B & 1.1719 (1) & 0.3061 (2) & 0.4490 (1) & 3.1 (1) \\ N2B & 1.2402 (1) & 0.4359 (2) & 0.4785 (1) & 4.2 (1) \\ O2B & 0.9470 (1) & 0.5751 (2) & 0.4649 (1) & 4.3 (1) \\ O2B & 0.9470 (1) & 0.5751 (2) & 0.4619 (1) & 4.3 (1) \\ O2B & 0.9470 (1) & 0.6275 (2) & 0.4117 (1) & 4.4 (1) \\ \hline Compound (2) \\ S & 0.0283 (1) & 0.3751 (1) & 0.0874 (1) & 3.1 (1) \\ N2A & 0.0310 (2) & 0.2107 (2) & 0.2466 (2) & 3.1 (1) \\ N2A & 0.0310 (2) & 0.2139 (3) & 0.2926 (2) & 4.8 (1) \\ O2A & -0.1883 (2) & 0.2678 (3) & 0.1059 (2) & 5.5 (2) \\ C8A & -0.0996 (2) & 0.2362 (3) & 0.1591 (2) & 3.9 (2) \\ C1A & 0.3439 (2) & 0.0725 (3) & 0.6364 (2) & 4.0 (2) \\ C4A & 0.3800 (2) & 0.2004 (4) & 0.3866 (2) & 3.8 (2) \\ C5A & 0.3449 (2) & 0.3284 (3) & 0.3017 (2) & 5.6 (1) \\ C9A & 0.5642 (3) & 0.3191 (3) & 0.3148 (2) & 3.7 (2) \\ C5A & 0.3449 (2) & 0.3284 (3) & 0.3060 (2) & 3.7 (2) \\ C5A & 0.3449 (2) & 0.3284 (3) & 0.3016 (2) & 3.7 (2) \\ C5A & 0.3449 (2) & 0.3284 (3) & 0.3017 (2) & 5.6 (1) \\ C9A & 0.5642 (3) & 0.3162 (2) & -0.0135 (1) & 4.4 (1) \\ D2B & -0.053 (2) & 0.0913 (2) & -0.0949 (2) & 3.1 (1) \\ N1B & 0.1053 (2) & 0.0916 (3) & -0.07987 (2) & 5.6 (1) \\ C1B & -0.0258 (2) & 0.0812 (2) & -0.1135 (1) & 4.4 (1) \\ D2B & -0.0611 (2) & 0.1930 (2) & -0.0498 (2) & 3.7 (1) \\ C3B & 0.5642 (3) & 0.337 (3) & 0.1985 (2) & 5.6 (2) \\ C3B & 0.5885 (1) & -0.1933 (2) & -0.0498 (2) & 3.7 (1) \\ C3B & 0.5283 (2) & 0.1332 (4) & 0.1534 (4) & 0.455 (2) \\ C6B & 0.2470 (2) & 0.3337 (3) & 0.1985 (2) & 5.6 (2) \\ C5B & 0.5200 & 0.0334 (1) & 0.2500 & 3.5 (1) \\ C1 & 0.320 (1) & 0.1247 (2) & 0.1819 (4) & 4.5 (2) \\ C5B & 0.5200 & 0.0334 (1) & 0.2500 & 3.5 (1) \\ C1 & 0.4635 (1) & 0.2234 (2) & -0.0944 (2$	C1B	1.2362 (1)	0-1406 (2)	0.4572 (1)	3-1(1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C2B	1.2750 (2)	0.0805 (2)	0.5231(1)	3.6(1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C3 <i>B</i>	1.3435 (2)	-0.0721 (3)	0.5322(1)	4.1(1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C4B	1.3722 (2)	-0.1593 (2)	0.4767 (1)	4.1(1)
$\begin{array}{ccccc} C6B & 1-2619(2) & 0-0346(2) & 0-4003(1) & 3-8(1) \\ C7B & 1-0432(2) & 0-3466(2) & 0-4181(1) & 2-9(1) \\ C8B & 1-0342(2) & 0-5246(2) & 0-4276(1) & 3-5(1) \\ N1B & 1-1719(1) & 0-3061(2) & 0-4490(1) & 3-1(1) \\ N2B & 1-2402(1) & 0-4359(2) & 0-4785(1) & 4-2(1) \\ O1B & 1-1564(1) & 0-5751(2) & 0-4649(1) & 4-3(1) \\ O2B & 0-9470(1) & 0-6275(2) & 0-4117(1) & 4-4(1) \\ C7A & 0.0003(2) & 0-2709(3) & 0-1663(2) & 2-9(1) \\ N1A & 0-0708(2) & 0-217(2) & 0-2466(2) & 3-1(1) \\ N2A & 0-0310(2) & 0-2395(3) & 0-2926(2) & 4-3(1) \\ O2A & -0.0757(2) & 0-1430(2) & 0-2395(2) & 4-8(1) \\ O2A & -0.083(2) & 0-2678(3) & 0-1059(2) & 5-5(2) \\ C8A & -0.0996(2) & 0-2362(3) & 0-1591(2) & 3-9(2) \\ C1A & 0.1843(2) & 0-2014(3) & 0-3902(2) & 2-9(1) \\ C2A & 0-2366(2) & 0-0731(3) & 0-3148(2) & 3-7(2) \\ C3A & 0-3439(2) & 0-0725(3) & 0-3634(2) & 4-0(2) \\ C4A & 0-3980(2) & 0-2004(4) & 0-3866(2) & 3-8(2) \\ C5A & 0-3449(2) & 0-3286(3) & 0-3606(2) & 3-7(2) \\ C6A & 0-2361(2) & 0-3294(3) & 0-3117(2) & 3-5(1) \\ O3A & 0-5044(2) & 0-1891(3) & -0-0498(2) & 5-0(1) \\ C9A & 0-5042(3) & 0-3162(5) & 0-4667(3) & 6-9(3) \\ C7B & 0-0222(2) & 0-2490(3) & -0-0798(2) & 4-2(1) \\ O1B & -0-0238(2) & 0-0816(2) & -0-0798(2) & 4-2(1) \\ O1B & -0-0238(2) & 0-0816(3) & -0-0798(2) & 4-2(1) \\ O1B & -0-0238(2) & 0-0816(3) & -0-0798(2) & 4-2(1) \\ O1B & -0-0238(2) & 0-0816(3) & -0-0798(2) & 3-1(1) \\ N2B & 0.0817(2) & 0-916(3) & -0-0788(2) & 3-0(1) \\ C2B & 0-3816(2) & 0-1325(3) & -00705(2) & 3-7(2) \\ C4B & 0-2419(2) & 0-2256(3) & 0-1037(2) & 3-9(2) \\ C3B & 0-3885(2) & 0-1325(4) & 0-1534(2) & 4-1(2) \\ C5B & 0-3518(3) & 0-3946(3) & 0-0963(2) & 4-5(2) \\ C5B & 0-23518(3) & 0-3946(3) & 0-0963(2) & 4-5(2) \\ C5B & 0-2358(1) & -0-0044(2) & 0-1819(4) & 4-5(2) \\ C5B & 0-3518(3) & 0-3946(3) & 0-0963(2) & 4-5(2) \\ C5B & 0-3518(3) & 0-3946(3) & 0-0963(2) & 4-5(2) \\ C5B & 0-2358(1) & -0-0040(2) & 0-1819(4) & 4-5(2) \\ C5 & 0-2858(1) & -0-0040(2) & 0-1819(4) & 4-5(2) \\ C5 & 0-2858(1) & -0-0040(2) & 0-1819(4) & 4-5(2) \\ C5 & 0-2858(1) & -0-00404(2) & 0-1819(4) & 4-5(2) \\ C5 & 0-3518(3) & 0-2350(3) & -3$	C5B	1.3307 (2)	-0.0977 (3)	0.4109(1)	4.4(1)
$\begin{array}{cccccc} C/B & 1-0483 (1) & 0-3400 (2) & 0-4181 (1) & 2-9 (1) \\ C8B & 1-0483 (2) & 0-5246 (2) & 0-4276 (1) & 3-5 (1) \\ N1B & 1-1719 (1) & 0-3061 (2) & 0-4499 (1) & 3-1 (1) \\ N2B & 1-2402 (1) & 0-4359 (2) & 0-4785 (1) & 4-2 (1) \\ O1B & 1-1564 (1) & 0-5751 (2) & 0-4649 (1) & 4-3 (1) \\ O2B & 0-9470 (1) & 0-6275 (2) & 0-4117 (1) & 4-4 (1) \\ Compound (2) \\ S & 0-0283 (1) & 0-3751 (1) & 0-0874 (1) & 3-1 (1) \\ C7A & 0-0003 (2) & 0-2709 (3) & 0-1663 (2) & 2-9 (1) \\ N1A & 0-0708 (2) & 0-2017 (2) & 0-2466 (2) & 3-1 (1) \\ N2A & 0-0310 (2) & 0-1239 (3) & 0-2926 (2) & 4-3 (1) \\ O1A & -0-0757 (2) & 0-1430 (2) & 0-2395 (2) & 4-88 (1) \\ O2A & -0-1883 (2) & 0-2678 (3) & 0-1059 (2) & 5-5 (2) \\ C8A & -0-0996 (2) & 0-2362 (3) & 0-1591 (2) & 3-9 (2) \\ C1A & 0-1843 (2) & 0-2014 (3) & 0-2902 (2) & 2-9 (1) \\ C2A & 0-2366 (2) & 0-0731 (3) & 0-3448 (2) & 3-7 (2) \\ C3A & 0-3439 (2) & 0-0725 (3) & 0-3634 (2) & 4-0 (2) \\ C5A & 0-3449 (2) & 0-3286 (3) & 0-3606 (2) & 3-7 (2) \\ C6A & 0-2361 (2) & 0-3294 (3) & 0-3117 (2) & 3-5 (1) \\ O3A & 0-5044 (2) & 0-1891 (3) & 0-4350 (2) & 3-0 (1) \\ C9A & 0-5642 (3) & 0-3162 (5) & 0-4667 (3) & 6-9 (3) \\ C7B & 0-0232 (2) & 0-2490 (3) & -00798 (2) & 3-1 (1) \\ N2B & 0-0817 (2) & 0-0916 (3) & -0-0728 (2) & 4-2 (1) \\ O2B & -0-1611 (2) & 0-1903 (2) & -0-0049 (2) & 3-1 (1) \\ N2B & 0-0817 (2) & 0-0812 (3) & -00705 (2) & 3-7 (2) \\ C3B & 0-3885 (2) & 0-1532 (4) & 0-1534 (2) & 4-1 (2) \\ C5B & 0-3518 (3) & 0-3346 (3) & 0-0685 (2) & 3-7 (1) \\ C3B & 0-5243 (2) & 0-3337 (3) & 0-1985 (2) & 5-6 (2) \\ C9B & 0-6034 (3) & 0-2288 (5) & 0-2450 (3) & 6-9 (3) \\ Compound (3) \\ S \\ Compound (3) \\ S \\ Compound (3) \\ S \\ Compound (3) \\ C \\ C \\ C \\ C \\ C \\ O \\ 0 \\ C \\ C \\ C \\ O \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0$	C6B	1.2619 (2)	0.0545(2)	0.4003(1)	3.8(1)
$\begin{array}{cccc} Colored Colo$	C/B	1.0483 (1)	0.3400(2)	0.4181(1) 0.4276(1)	2.9(1) 3.5(1)
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	NIP	1.0342(2)	0.3240(2)	0.4490 (1)	3.1(1)
$\begin{array}{ccccc} 122 & 0.1264 (1) & 0.5751 (2) & 0.4649 (1) & 4.3 (1) \\ 02B & 0.9470 (1) & 0.6275 (2) & 0.4117 (1) & 4.4 (1) \\ \hline \\ Compound (2) \\ S & 0.0283 (1) & 0.3751 (1) & 0.0874 (1) & 3.1 (1) \\ C7A & 0.0003 (2) & 0.2709 (3) & 0.1663 (2) & 2.9 (1) \\ N1A & 0.0708 (2) & 0.2017 (2) & 0.2466 (2) & 3.1 (1) \\ N2A & 0.0310 (2) & 0.1239 (3) & 0.2926 (2) & 4.3 (1) \\ 01A & -0.0757 (2) & 0.1430 (2) & 0.2395 (2) & 4.8 (1) \\ 02A & -0.1883 (2) & 0.2678 (3) & 0.1059 (2) & 5.5 (2) \\ C8A & -0.0996 (2) & 0.2362 (3) & 0.1591 (2) & 3.9 (2) \\ C1A & 0.1843 (2) & 0.2014 (3) & 0.2902 (2) & 2.9 (1) \\ C2A & 0.2366 (2) & 0.0731 (3) & 0.3148 (2) & 3.7 (2) \\ C3A & 0.3439 (2) & 0.0725 (3) & 0.3634 (2) & 4.0 (2) \\ C4A & 0.3980 (2) & 0.2024 (3) & 0.3106 (2) & 3.7 (2) \\ C6A & 0.2361 (2) & 0.3286 (3) & 0.3606 (2) & 3.7 (2) \\ C6A & 0.2361 (2) & 0.3294 (3) & 0.3117 (2) & 3.5 (1) \\ 03A & 0.5044 (2) & 0.1891 (3) & -0.0987 (2) & 5.0 (1) \\ C9A & 0.5642 (3) & 0.3162 (5) & 0.4667 (3) & 6.9 (3) \\ C7B & 0.0222 (2) & 0.2490 (3) & -0.0078 (2) & 4.2 (1) \\ N1B & 0.1053 (2) & 0.1903 (2) & -0.00987 (2) & 3.1 (1) \\ N2B & 0.0817 (2) & 0.0916 (3) & -0.0728 (2) & 4.2 (1) \\ 01B & -0.0258 (2) & 0.0812 (2) & -0.1135 (1) & 4.4 (1) \\ 02B & -0.1611 (2) & 0.1900 (3) & -0.07987 (2) & 5.0 (1) \\ C3B & 0.0817 (2) & 0.1205 (3) & 0.0508 (2) & 3.0 (1) \\ C2B & 0.0817 (2) & 0.1205 (3) & -0.0705 (2) & 3.7 (2) \\ C1B & 0.2149 (2) & 0.2256 (3) & 0.0508 (2) & 3.0 (1) \\ 02B & 0.0815 (2) & 0.1352 (4) & 0.1504 (2) & 4.1 (2) \\ C4B & 0.4224 (2) & 0.2899 (4) & 0.1504 (2) & 4.1 (2) \\ C4B & 0.4224 (2) & 0.289 (3) & 0.0466 (2) & 3.7 (1) \\ 03B & 0.5233 (2) & 0.1337 (3) & 0.1985 (2) & 5.6 (2) \\ C3B & 0.3855 (2) & 0.1352 (4) & 0.1504 (2) & 4.1 (2) \\ C5B & 0.2450 (3) & 0.2288 (5) & 0.2450 (3) & 6.9 (3) \\ Compound (3) \\ S & 0.5000 & 0.0334 (1) & 0.2500 & 3.5 (1) \\ C1 & 0.3520 (1) & 0.1424 (2) & 0.1504 (2) & 4.1 (2) \\ C5B & 0.2450 (3) & 0.3373 (3) & 0.1985 (2) & 5.6 (2) \\ C10 & 0.0840 (2) & -0.0040 (2) & 0.1207 (4) & 4.6 (2) \\ C2 & 0.3091 (1) & 0.1224 (2) & 0.0970 (3) & 3.1 (1) \\ C9 & 0.1403 (2) & 0.0$	N7R	1.2402 (1)	0.4359(2)	0.4785(1)	4.2(1)
O2B 0.9470 (1) 0.6275 (2) 0.4117 (1) 4.4 (1)Compound (2)S 0.0283 (1) 0.3751 (1) 0.0874 (1) 3.1 (1)C7A 0.0003 (2) 0.2709 (3) 0.1663 (2) 2.9 (1)N1A 0.0708 (2) 0.2017 (2) 0.2466 (2) 3.1 (1)OLA -0.0757 (2) 0.1430 (2) 0.2395 (2) 4.8 (1)O2A -0.01833 (2) 0.2678 (3) 0.1059 (2) 5.5 (2)C8A -0.0996 (2) 0.2362 (3) 0.1591 (2) 3.9 (2)C1A 0.1843 (2) 0.2014 (3) 0.2902 (2) 2.9 (1)C2A 0.233980 (2) 0.2004 (4) 0.3866 (2) 3.9 (2)C4A 0.33980 (2) 0.2004 (4) 0.3866 (2) 3.8 (2)C5A 0.3439 (2) 0.2004 (4) 0.3866 (2) 3.7 (2)C6A 0.2361 (2) 0.3294 (3) 0.3117 (2) 3.5 (1)O3A 0.5044 (2) 0.1891 (3) 0.4350 (2) 5.0 (1)C7B 0.0222 (2) 0.2490 (3) 0.0019 (2) 2.8 (1)N1B 0.1053 (2) 0.916 (3) -0.0728 (2) 4.2 (1)O1B -0.0581 (2) 0.9116 (3) -0.0705 (2) 3.7 (2)C7B 0.02258 (2) 0.1903 (2) -0.0049 (2) 3.111 (1)N2B 0.0817 (2) 0.919 (3) -0.0705 (2) 3.7 (1)O2B -0.0679 (2) 0.820 (3) -0.0705 (2) 3.7 (1)D2B 0.0817 (2) 0.9193 (2) <td>O1B</td> <td>1.1564(1)</td> <td>0.5751(2)</td> <td>0.4649(1)</td> <td>$4 \cdot 3(1)$</td>	O1B	1.1564(1)	0.5751(2)	0.4649(1)	$4 \cdot 3(1)$
Compound (2) S 0-283 (1) 0-3751 (1) 0-0874 (1) 3-1 (1) N1A 0-0708 (2) 0-2709 (3) 0-1663 (2) 2-9 (1) N1A 0-0708 (2) 0-219 (3) 0-2926 (2) 4-3 (1) N2A 0-0310 (2) 0-1239 (3) 0-2926 (2) 4-3 (1) O1A -0-0757 (2) 0-1430 (2) 0-2395 (2) 4-8 (1) O2A -0-1883 (2) 0-2678 (3) 0-1059 (2) 5-5 (2) C8A -0-0996 (2) 0-2362 (3) 0-1591 (2) 3-9 (2) C1A 0-1843 (2) 0-2014 (3) 0-2902 (2) 2-9 (1) C2A 0-2366 (2) 0-0731 (3) 0-3148 (2) 3-7 (2) C3A 0-3439 (2) 0-0725 (3) 0-3634 (2) 4-0 (2) C4A 0-3380 (2) 0-0204 (4) 0-3866 (2) 3-7 (2) C4A 0-3489 (2) 0-3286 (3) 0-3606 (2) 3-7 (2) C6A 0-2361 (2) 0-3294 (3) 0-3117 (2) 3-5 (1) O3A 0-5044 (2) 0-1891 (3) 0-4350 (2) 3-7 (2) C6A 0-2361 (2) 0-3294 (3) 0-3117 (2) 3-5 (1) O3A 0-5044 (2) 0-1891 (3) 0-4350 (2) 2-0 (1) C7B 0-0222 (2) 0-2490 (3) 0-0019 (2) 2-8 (1) N1B 0-1053 (2) 0-1903 (2) -0-0049 (2) 3-1 (1) N2B 0-0817 (2) 0-0916 (3) -0-0728 (2) 4-2 (1) O1B -0-0258 (2) 0-0812 (2) -0-1135 (1) 4-4 (1) O2B -0-0611 (2) 0-1900 (3) -0-0977 (2) 3-7 (2) C1B 0-2149 (2) 0-2256 (3) 0-0508 (2) 3-0 (1) C2B 0-2836 (2) 0-1205 (3) 0-1027 (2) 3-9 (2) C3B 0-3885 (2) 0-1322 (4) 0-1544 (2) 4-1 (2) C4B 0-4224 (2) 0-2899 (4) 0-1504 (2) 4-1 (2) C4B 0-32520 (1) 0-1074 (2) 0-1353 (3) 3-4 (1) C2 0-3091 (1) 0-1824 (2) 0-2302 (4) 4-8 (2) C4 0-2318 (3) 0-3946 (3) 0-0963 (2) 4-5 (2) C6 0-3314 (1) -0-0040 (2) 0-1207 (4) 4-6 (2) C3 0-2353 (2) 0-1448 (2) 0-2302 (4) 4-8 (2) C4 0-2414 (1) 0-0335 (2) 0-2376 (4) 4-0 (2) C5 0-2858 (1) -0-0404 (2) 0-1819 (4) 4-5 (2) C6 0-3314 (1) 0-1933 (2) 0-0406 (4) 3-8 (2) C7 0-4727 (1) 0-1247 (2) 0-0970 (3) 3-1 (1) C9 0-1403 (2) 0-0605 (3) 0-3354 (4) 5-6 (2) C9 0-1403 (2) 0-0605 (3) 0-3354 (4) 5-6 (2) C10 0-0840 (2) -0-0080 (3) 0-3893 (5) 8-1 (3) N1 0-4098 (1) 0-1933 (2) -0-0042 (2) 4-8 (1) O2 0-5671 (1) 0-2096 (2) -0-0099 (3) 5-3 (1) O3 0-1879 (1) -0-0123 (2) 0-2945 (3) 5-2 (2)	O2B	0.9470(1)	0.6275(2)	0.4117(1)	4.4(1)
$\begin{array}{c} \mbox{Compound (2)} \\ \mbox{S} & 0.0283 (1) & 0.3751 (1) & 0.0874 (1) & 3.1 (1) \\ \mbox{C7A} & 0.0003 (2) & 0.2709 (3) & 0.1663 (2) & 2.9 (1) \\ \mbox{N1A} & 0.0708 (2) & 0.2017 (2) & 0.2466 (2) & 3.1 (1) \\ \mbox{N2A} & 0.0310 (2) & 0.1239 (3) & 0.2926 (2) & 4.3 (1) \\ \mbox{O1A} & -0.0757 (2) & 0.1430 (2) & 0.2395 (2) & 4.8 (1) \\ \mbox{O2A} & -0.1883 (2) & 0.2678 (3) & 0.1059 (2) & 5.5 (2) \\ \mbox{C8A} & -0.0996 (2) & 0.2362 (3) & 0.1591 (2) & 3.9 (2) \\ \mbox{C1A} & 0.1883 (2) & 0.2014 (3) & 0.2902 (2) & 2.9 (1) \\ \mbox{C2A} & 0.2366 (2) & 0.0731 (3) & 0.3148 (2) & 3.7 (2) \\ \mbox{C3A} & 0.3498 (2) & 0.2024 (4) & 0.3866 (2) & 3.7 (2) \\ \mbox{C4A} & 0.3380 (2) & 0.2004 (4) & 0.3866 (2) & 3.7 (2) \\ \mbox{C4A} & 0.3980 (2) & 0.2326 (3) & 0.3606 (2) & 3.7 (2) \\ \mbox{C4A} & 0.3980 (2) & 0.2004 (4) & 0.3866 (2) & 3.7 (2) \\ \mbox{C5A} & 0.3449 (2) & 0.3286 (3) & 0.3606 (2) & 3.7 (2) \\ \mbox{C6A} & 0.2361 (2) & 0.3294 (3) & 0.3117 (2) & 3.5 (1) \\ \mbox{O3A} & 0.5044 (2) & 0.1891 (3) & 0.4350 (2) & 5.0 (1) \\ \mbox{C9A} & 0.5642 (3) & 0.3162 (5) & 0.4667 (3) & 6.9 (3) \\ \mbox{C7B} & 0.0222 (2) & 0.2490 (3) & 0.0019 (2) & 2.8 (1) \\ \mbox{N1B} & 0.1053 (2) & 0.0916 (3) & -0.0728 (2) & 4.2 (1) \\ \mbox{O1B} & -0.0258 (2) & 0.0812 (2) & -0.1135 (1) & 4.4 (1) \\ \mbox{O2B} & -0.0611 (2) & 0.1903 (2) & -0.0498 (2) & 3.1 (1) \\ \mbox{C4B} & 0.4224 (2) & 0.289 (4) & 0.1504 (2) & 4.1 (2) \\ \mbox{C4B} & 0.4224 (2) & 0.289 (4) & 0.1504 (2) & 4.1 (2) \\ \mbox{C4B} & 0.4224 (2) & 0.289 (4) & 0.1504 (2) & 4.1 (2) \\ \mbox{C4B} & 0.4224 (2) & 0.289 (4) & 0.1504 (2) & 4.1 (2) \\ \mbox{C4B} & 0.4224 (2) & 0.289 (4) & 0.1504 (2) & 4.1 (2) \\ \mbox{C4B} & 0.4224 (2) & 0.3337 (3) & 0.1985 (2) & 5.6 (1) \\ \mbox{C3B} & 0.5000 & 0.0334 (1) & 0.2500 & 3.5 (1) \\ \mbox{C1} & 0.3520 (1) & 0.1027 (2) & 0.351 (4) & 4.6 (2) \\ \mbox{C3B} & 0.5233 (2) & 0.1448 (2) & 0.2302 (4) & 4.8 (2) \\ \mbox{C4B} & 0.4241 (1) & 0.0335 (2) & 0.2376 (4) & 4.0 (2) \\ \mbox{C5B} & 0.5000 & 0.0334 (1) & 0.2500 & 3.5 (1) \\ \mbox{C4B} & 0.4241 (1) & 0.0335 (2) & 0.2376 (4) $	010	0) 0 (1)	0 0210 (2)		(-,
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Compound (2)		/		
$\begin{array}{ccccc} C7A & 0.0003 (2) & 0.2709 (3) & 0.1663 (2) & 2.9 (1) \\ N1A & 0.0708 (2) & 0.2017 (2) & 0.2466 (2) & 3.1 (1) \\ 01A & -0.0757 (2) & 0.1430 (2) & 0.2395 (2) & 4.8 (1) \\ 02A & -0.1883 (2) & 0.2678 (3) & 0.1059 (2) & 5.5 (2) \\ C8A & -0.0996 (2) & 0.2362 (3) & 0.1591 (2) & 3.9 (2) \\ C1A & 0.1843 (2) & 0.2014 (3) & 0.2902 (2) & 2.9 (1) \\ C2A & 0.2366 (2) & 0.0731 (3) & 0.3148 (2) & 3.7 (2) \\ C3A & 0.3439 (2) & 0.0725 (3) & 0.3634 (2) & 4.0 (2) \\ C4A & 0.3980 (2) & 0.2024 (3) & 0.3666 (2) & 3.8 (2) \\ C5A & 0.3449 (2) & 0.3286 (3) & 0.3606 (2) & 3.7 (2) \\ C6A & 0.2361 (2) & 0.3286 (3) & 0.3606 (2) & 3.7 (2) \\ C6A & 0.2361 (2) & 0.3286 (3) & 0.3606 (2) & 3.7 (2) \\ C6A & 0.2361 (2) & 0.3284 (3) & 0.3117 (2) & 3.5 (1) \\ 03A & 0.5044 (2) & 0.1891 (3) & 0.4350 (2) & 5.0 (1) \\ C9A & 0.5642 (3) & 0.3162 (5) & 0.4667 (3) & 6.9 (3) \\ C7B & 0.0222 (2) & 0.2490 (3) & 0.0019 (2) & 2.8 (1) \\ N1B & 0.1053 (2) & 0.1903 (2) & -0.0049 (2) & 3.1 (1) \\ N2B & 0.0817 (2) & 0.0916 (3) & -0.0728 (2) & 4.2 (1) \\ 01B & -0.0258 (2) & 0.0812 (2) & -0.1135 (1) & 4.4 (1) \\ 02B & -0.6179 (2) & 0.1820 (3) & -0.07087 (2) & 5.0 (1) \\ C3B & 0.3855 (2) & 0.1532 (4) & 0.1504 (2) & 4.1 (2) \\ C4B & 0.4224 (2) & 0.2256 (3) & 0.0508 (2) & 3.7 (1) \\ C3B & 0.3855 (2) & 0.1532 (4) & 0.1504 (2) & 4.1 (2) \\ C4B & 0.4224 (2) & 0.2899 (4) & 0.1504 (2) & 4.1 (2) \\ C5B & 0.3518 (3) & 0.3946 (3) & 0.0963 (2) & 4.5 (2) \\ C6B & 0.2470 (2) & 0.3337 (3) & 0.1985 (2) & 5.6 (2) \\ C9B & 0.6034 (3) & 0.2288 (5) & 0.2450 (3) & 6.9 (3) \\ \hline Compound (3) \\ S & 0.5000 & 0.0334 (1) & 0.2500 & 3.5 (1) \\ C1 & 0.3520 (1) & 0.1824 (2) & 0.1700 (4) & 4.6 (2) \\ C5 & 0.2838 (1) & -0.0404 (2) & 0.1819 (4) & 4.5 (2) \\ C6 & 0.3314 (1) & -0.0040 (2) & 0.1207 (4) & 4.8 (2) \\ C4 & 0.2414 (1) & -0.0340 (2) & 0.2376 (4) & 4.0 (2) \\ C5 & 0.2858 (1) & -0.0404 (2) & 0.1819 (4) & 4.5 (2) \\ C7 & 0.4727 (1) & 0.1247 (2) & 0.0970 (3) & 3.1 (1) \\ C9 & 0.1403 (2) & 0.0605 (3) & 0.3534 (4) & 5.6 (2) \\ C10 & 0.0840 (2) & -0.0080 (3) & 0.3893 (5) & 8.1 (3) \\ N1 & 0.4098 (1) & 0.1491 (2) & 0.0508 (3$	S	0.0283 (1)	0-3751(1)	0.0874 (1)	3.1(1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C7A	0.0003(2)	0.2709 (3)	0.1663(2)	2.9(1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	NIA	0.0708 (2)	0.2017(2)	0.2466(2)	$3 \cdot 1(1)$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	NZA OLA	0.0310(2)	0.1239(3)	0.2920(2) 0.2305(2)	4.8(1)
$\begin{array}{ccccc} 0.103 (2) & 0.236 (3) & 0.1591 (2) & 3.9 (2) \\ 0.236 (3) & 0.1591 (2) & 3.9 (2) \\ 0.24 & 0.236 (2) & 0.0731 (3) & 0.3148 (2) & 3.7 (2) \\ 0.34 & 0.3439 (2) & 0.0725 (3) & 0.3634 (2) & 4.0 (2) \\ 0.386 (2) & 3.86 (2) & 0.3634 (2) & 4.0 (2) \\ 0.34 & 0.3439 (2) & 0.3286 (3) & 0.3606 (2) & 3.7 (2) \\ 0.34 & 0.5044 (2) & 0.3286 (3) & 0.3606 (2) & 3.7 (2) \\ 0.34 & 0.5044 (2) & 0.3286 (3) & 0.4667 (3) & 6.9 (3) \\ 0.34 & 0.5044 (2) & 0.1891 (3) & 0.4350 (2) & 5.0 (1) \\ 0.34 & 0.5044 (2) & 0.1891 (3) & 0.4350 (2) & 5.0 (1) \\ 0.94 & 0.5642 (3) & 0.3162 (5) & 0.4667 (3) & 6.9 (3) \\ 0.7B & 0.0222 (2) & 0.2490 (3) & 0.0019 (2) & 2.8 (1) \\ 0.1B & 0.1053 (2) & 0.1903 (2) & -0.0049 (2) & 3.1 (1) \\ 0.2B & -0.6817 (2) & 0.0916 (3) & -0.0728 (2) & 4.2 (1) \\ 0.2B & -0.1611 (2) & 0.1900 (3) & -0.0987 (2) & 5.0 (1) \\ 0.2B & -0.0679 (2) & 0.1820 (3) & -0.0708 (2) & 3.7 (2) \\ 0.1B & 0.2124 (2) & 0.2256 (3) & 0.0508 (2) & 3.7 (1) \\ 0.2B & 0.2836 (2) & 0.1205 (3) & 0.1027 (2) & 3.9 (2) \\ 0.3B & 0.3885 (2) & 0.1532 (4) & 0.1504 (2) & 4.1 (2) \\ 0.5B & 0.43518 (3) & 0.3946 (3) & 0.0963 (2) & 4.5 (2) \\ 0.3B & 0.32518 (3) & 0.3946 (3) & 0.0963 (2) & 4.5 (2) \\ 0.3B & 0.5233 (2) & 0.1334 (1) & 0.2500 & 3.5 (1) \\ 0.3B & 0.5233 (2) & 0.1344 (2) & 0.2150 (3) & 6.9 (3) \\ \hline Compound (3) \\ S & 0.5000 & 0.0334 (1) & 0.2302 (4) & 4.8 (2) \\ 0.46 & 0.2414 (1) & 0.0335 (2) & 0.2376 (4) & 4.0 (2) \\ 0.5 & 0.2838 (1) & -0.0404 (2) & 0.1819 (4) & 4.5 (2) \\ 0.5 & 0.2838 (1) & -0.0404 (2) & 0.1819 (4) & 4.5 (2) \\ 0.5 & 0.2838 (1) & -0.0404 (2) & 0.1819 (4) & 4.5 (2) \\ 0.5 & 0.2838 (1) & -0.0404 (2) & 0.1819 (4) & 4.5 (2) \\ 0.5 & 0.2838 (1) & -0.0404 (2) & 0.1819 (4) & 4.5 (2) \\ 0.5 & 0.2838 (1) & -0.0404 (2) & 0.1819 (4) & 4.5 (2) \\ 0.5 & 0.2838 (1) & -0.0404 (2) & 0.1819 (4) & 4.5 (2) \\ 0.5 & 0.2838 (1) & -0.0404 (2) & 0.1819 (4) & 4.5 (2) \\ 0.5 & 0.2838 (1) & -0.0404 (2) & 0.1819 (4) & 4.5 (2) \\ 0.5 & 0.2838 (1) & -0.0404 (2) & 0.1819 (4) & 4.5 (2) \\ 0.5 & 0.2838 (1) & -0.0404 (2) & 0.1819 (4) & 4.5 (2) \\ 0.5 & 0.2838 (1) & -0.0404 (2) & 0.1819 (4) &$	024	-0.1883(2)	0.2678(3)	0.1059(2)	5.5(2)
$\begin{array}{cccccc} C1A & 0.1843 (2) & 0.2014 (3) & 0.2902 (2) & 2.9 (1) \\ C2A & 0.2366 (2) & 0.0731 (3) & 0.3148 (2) & 3.7 (2) \\ C3A & 0.3439 (2) & 0.0725 (3) & 0.3634 (2) & 4.0 (2) \\ C4A & 0.3980 (2) & 0.2004 (4) & 0.3866 (2) & 3.8 (2) \\ C5A & 0.3449 (2) & 0.3286 (3) & 0.3606 (2) & 3.7 (2) \\ C6A & 0.2361 (2) & 0.3294 (3) & 0.3117 (2) & 3.5 (1) \\ C3A & 0.5044 (2) & 0.1891 (3) & 0.4350 (2) & 5.0 (1) \\ C9A & 0.5642 (3) & 0.3162 (5) & 0.4667 (3) & 6.9 (3) \\ C7B & 0.022 (2) & 0.2490 (3) & 0.0019 (2) & 2.8 (1) \\ N1B & 0.1053 (2) & 0.1903 (2) & -0.0049 (2) & 3.1 (1) \\ N2B & 0.0817 (2) & 0.0916 (3) & -0.0728 (2) & 4.2 (1) \\ O1B & -0.0258 (2) & 0.0812 (2) & -0.1135 (1) & 4.4 (1) \\ O2B & -0.1611 (2) & 0.1900 (3) & -0.0977 (2) & 3.7 (2) \\ C1B & 0.2149 (2) & 0.2256 (3) & 0.0508 (2) & 3.0 (1) \\ C2B & 0.2836 (2) & 0.1205 (3) & 0.1027 (2) & 3.9 (2) \\ C3B & 0.3885 (2) & 0.1322 (4) & 0.1544 (2) & 4.1 (2) \\ C4B & 0.4224 (2) & 0.2899 (4) & 0.1504 (2) & 4.1 (2) \\ C4B & 0.4224 (2) & 0.2899 (3) & 0.0466 (2) & 3.7 (1) \\ O3B & 0.5243 (2) & 0.3337 (3) & 0.1985 (2) & 5.6 (2) \\ C6B & 0.2470 (2) & 0.3337 (3) & 0.1985 (2) & 5.6 (2) \\ C3B & 0.5000 & 0.0334 (1) & 0.2500 & 3.5 (1) \\ C1 & 0.3520 (1) & 0.1074 (2) & 0.1155 (3) & 3.4 (1) \\ C2 & 0.3091 (1) & 0.1284 (2) & 0.2302 (4) & 4.8 (2) \\ C4 & 0.22414 (1) & 0.0335 (2) & 0.2376 (4) & 4.0 (2) \\ C5 & 0.2838 (1) & -0.0404 (2) & 0.1819 (4) & 4.5 (2) \\ C6 & 0.3414 (1) & -0.0040 (2) & 0.1207 (4) & 4.6 (2) \\ C7 & 0.4727 (1) & 0.1247 (2) & 0.0970 (3) & 3.1 (1) \\ C9 & 0.103 (2) & 0.0605 (3) & 0.3384 (4) & 5.6 (2) \\ C10 & 0.0840 (2) & -0.0080 (3) & 0.3893 (5) & 8.1 (3) \\ N1 & 0.4098 (1) & 0.1931 (2) & -0.0970 (3) & 3.4 (1) \\ C9 & 0.5671 (1) & 0.2096 (2) & -0.0094 (2) & 4.8 (1) \\ O2 & 0.5671 (1) & 0.2096 (2) & -0.0094 (2) & 4.8 (1) \\ O2 & 0.5671 (1) & 0.2096 (2) & -0.0094 (2) & 4.8 (1) \\ O3 & 0.1879 (1) & -0.0123 (2) & -0.2945 (3) & 5.3 (1) \\ O3 & 0.1879 (1) & -0.0123 (2) & -0.2945 (3) & 5.3 (1) \\ O3 & 0.1879 (1) & -0.0123 (2) & -0.2945 (3) & 5.3 (1) \\ O3 & 0.1879 (1) & -0.0123 (2) & -0.2945 (3) & 5.3 (1) \\ O3$	C84	-0.0996(2)	0.2362(3)	0.1591(2)	3.9(2)
$\begin{array}{ccccc} C2A & 0.2366(2) & 0.0731(3) & 0.3148(2) & 3.7(2) \\ C3A & 0.3439(2) & 0.0725(3) & 0.3634(2) & 4.0(2) \\ C4A & 0.3980(2) & 0.2004(4) & 0.3866(2) & 3.8(2) \\ C5A & 0.3449(2) & 0.3286(3) & 0.3606(2) & 3.7(2) \\ C6A & 0.2361(2) & 0.3294(3) & 0.3117(2) & 3.5(1) \\ O3A & 0.5042(2) & 0.1891(3) & 0.4350(2) & 5.0(1) \\ C9A & 0.5642(3) & 0.3162(5) & 0.4667(3) & 6.9(3) \\ C7B & 0.0222(2) & 0.2490(3) & 0.0019(2) & 2.8(1) \\ N1B & 0.1053(2) & 0.1903(2) & -0.0049(2) & 3.1(1) \\ N2B & 0.0817(2) & 0.0916(3) & -0.0728(2) & 4.2(1) \\ O1B & -0.0258(2) & 0.0812(2) & -0.0149(2) & 3.1(1) \\ C2B & -0.0679(2) & 0.1820(3) & -0.0705(2) & 3.7(2) \\ C1B & 0.2149(2) & 0.2256(3) & 0.00987(2) & 5.0(1) \\ C2B & 0.3855(2) & 0.1532(4) & 0.1027(2) & 3.9(2) \\ C3B & 0.3885(2) & 0.1532(4) & 0.1524(2) & 4.1(2) \\ C4B & 0.4224(2) & 0.2899(4) & 0.1504(2) & 4.1(2) \\ C4B & 0.4224(2) & 0.289(4) & 0.1504(2) & 4.1(2) \\ C5B & 0.3318(3) & 0.3946(3) & 0.0963(2) & 3.7(1) \\ O3B & 0.5243(2) & 0.3337(3) & 0.1985(2) & 5.6(2) \\ C9B & 0.6034(3) & 0.2288(5) & 0.2450(3) & 6.9(3) \\ Compound (3) \\ Compound (3) \\ Compound (3) \\ C1 & 0.3520(1) & 0.1074(2) & 0.1155(3) & 3.4(1) \\ C2 & 0.3091(1) & 0.1824(2) & 0.2302(4) & 4.8(2) \\ C4 & 0.2414(1) & 0.0335(2) & 0.2376(4) & 4.0(2) \\ C5 & 0.2858(1) & -0.0404(2) & 0.1207(4) & 4.8(2) \\ C4 & 0.2414(1) & 0.0335(2) & 0.2376(4) & 4.0(2) \\ C5 & 0.2858(1) & -0.0404(2) & 0.1819(4) & 4.5(2) \\ C6 & 0.3414(1) & -0.0404(2) & 0.1819(4) & 4.5(2) \\ C6 & 0.3414(1) & -0.0404(2) & 0.1819(4) & 4.5(2) \\ C7 & 0.4727(1) & 0.1247(2) & 0.0970(3) & 3.1(1) \\ C9 & 0.1403(2) & -0.0080(3) & 0.3893(5) & 8.1(3) \\ N1 & 0.4098(1) & 0.1931(2) & -0.0924(3) & 3.4(1) \\ N2 & 0.4018(1) & 0.2231(2) & -0.0652(3) & 4.6(2) \\ O1 & 0.4635(1) & 0.2331(2) & -0.0692(3) & 3.4(1) \\ N2 & 0.4018(1) & 0.2231(2) & -0.0692(3) & 3.4(1) \\ N2 & 0.4018(1) & 0.2231(2) & -0.0692(3) & 3.4(1) \\ N2 & 0.4018(1) & 0.2231(2) & -0.0692(3) & 3.4(1) \\ N2 & 0.4018(1) & 0.2231(2) & -0.0692(3) & 3.4(1) \\ N2 & 0.4018(1) & 0.2231(2) & -0.0692(3) & 3.4(1) \\ N2 & 0.4018(1) & 0.2031(2) & -0.2945(3) & 5.2(1) \\ $	CIA	0.1843 (2)	0.2014 (3)	0.2902 (2)	2.9(1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C2A	0.2366 (2)	0.0731 (3)	0.3148 (2)	3.7 (2)
$\begin{array}{ccccc} C44 & 0.3980(2) & 0.2004(4) & 0.3866(2) & 3.8(2) \\ C5A & 0.3449(2) & 0.3286(3) & 0.3606(2) & 3.7(2) \\ C6A & 0.2361(2) & 0.3294(3) & 0.3117(2) & 3.5(1) \\ O3A & 0.5044(2) & 0.1891(3) & 0.4350(2) & 5.0(1) \\ C9A & 0.5642(3) & 0.3162(5) & 0.4667(3) & 6.9(3) \\ C7B & 0.022(2) & 0.2490(3) & 0.0019(2) & 2.8(1) \\ N1B & 0.1053(2) & 0.1903(2) & -0.0049(2) & 3.1(1) \\ N2B & 0.0817(2) & 0.0916(3) & -0.0728(2) & 4.2(1) \\ O1B & -0.0258(2) & 0.0812(2) & -0.1135(1) & 4.4(1) \\ O2B & -0.1611(2) & 0.1900(3) & -0.0987(2) & 5.0(1) \\ C8B & -0.0679(2) & 0.1820(3) & -0.0705(2) & 3.7(2) \\ C1B & 0.2184(2) & 0.2256(3) & 0.0508(2) & 3.0(1) \\ C2B & 0.2836(2) & 0.1205(3) & 0.1027(2) & 3.9(2) \\ C3B & 0.3885(2) & 0.1532(4) & 0.1544(2) & 4.1(2) \\ C5B & 0.3518(3) & 0.3946(3) & 0.0963(2) & 4.5(2) \\ C6B & 0.2470(2) & 0.3337(3) & 0.1985(2) & 5.6(2) \\ C9B & 0.6034(3) & 0.2288(5) & 0.2450(3) & 6.9(3) \\ \hline Compound (3) \\ S & 0.5000 & 0.0334(1) & 0.2500 & 3.5(1) \\ C1 & 0.3520(1) & 0.1074(2) & 0.1155(3) & 3.4(1) \\ C2 & 0.3091(1) & 0.1824(2) & 0.1700(4) & 4.6(2) \\ C5 & 0.2838(1) & -0.0404(2) & 0.189(4) & 4.5(2) \\ C44 & 0.2414(1) & 0.0335(2) & 0.2376(4) & 4.0(2) \\ C5 & 0.2858(1) & -0.0404(2) & 0.1819(4) & 4.5(2) \\ C7 & 0.4727(1) & 0.1247(2) & 0.3737(4) & 4.8(2) \\ C7 & 0.4727(1) & 0.1247(2) & 0.0970(3) & 3.1(1) \\ C9 & 0.1403(2) & -0.0080(3) & 0.3893(5) & 8.1(3) \\ N1 & 0.4098(1) & 0.1941(2) & 0.0508(3) & 3.4(1) \\ C9 & 0.1403(2) & -0.0080(3) & 0.3893(5) & 8.1(3) \\ N1 & 0.4098(1) & 0.1941(2) & -0.052(3) & 4.6(2) \\ C1 & 0.4635(1) & 0.2331(2) & -0.0094(2) & 4.8(1) \\ O2 & 0.5671(1) & 0.2096(2) & -0.0094(2) & 4.8(1) \\ O2 & 0.5671(1) & 0.2096(2) & -0.0094(3) & 5.3(1) \\ O3 & 0.1879(1) & -0.0123(2) & -22945(3) & 5.2(2) \\ \end{array} \right$	C3A	0.3439 (2)	0.0725 (3)	0.3634 (2)	4.0 (2)
$\begin{array}{ccccc} C5A & 0.3449 (2) & 0.3286 (3) & 0.3606 (2) & 3.7 (2) \\ C6A & 0.2361 (2) & 0.3294 (3) & 0.3117 (2) & 3.5 (1) \\ O3A & 0.5044 (2) & 0.1891 (3) & 0.4350 (2) & 5.0 (1) \\ C9A & 0.5642 (3) & 0.3162 (5) & 0.4667 (3) & 6.9 (3) \\ C7B & 0.0222 (2) & 0.2490 (3) & 0.0019 (2) & 2.8 (1) \\ N1B & 0.1053 (2) & 0.1903 (2) & -0.0049 (2) & 3.1 (1) \\ N2B & 0.0817 (2) & 0.0916 (3) & -0.0728 (2) & 4.2 (1) \\ O1B & -0.0258 (2) & 0.0812 (2) & -0.1135 (1) & 4.4 (1) \\ O2B & -0.1611 (2) & 0.1900 (3) & -0.0987 (2) & 5.0 (1) \\ C8B & -0.0679 (2) & 0.1820 (3) & -0.0705 (2) & 3.7 (2) \\ C1B & 0.2186 (2) & 0.1205 (3) & 0.1027 (2) & 3.9 (2) \\ C3B & 0.3885 (2) & 0.1252 (4) & 0.1544 (2) & 4.1 (2) \\ C4B & 0.4224 (2) & 0.2899 (4) & 0.1504 (2) & 4.1 (2) \\ C4B & 0.4224 (2) & 0.3393 (3) & 0.0466 (2) & 3.7 (1) \\ O3B & 0.5243 (2) & 0.3337 (3) & 0.1985 (2) & 5.6 (2) \\ C9B & 0.6034 (3) & 0.2288 (5) & 0.2450 (3) & 6.9 (3) \\ Compound (3) \\ C6 & 0.3414 (1) & -0.0040 (2) & 0.1207 (4) & 4.6 (2) \\ C4 & 0.2414 (1) & 0.1335 (2) & 0.2376 (4) & 4.0 (2) \\ C5 & 0.2838 (1) & -0.00404 (2) & 0.1819 (4) & 4.5 (2) \\ C6 & 0.3414 (1) & -0.0040 (2) & 0.1207 (4) & 4.8 (2) \\ C7 & 0.4727 (1) & 0.1247 (2) & 0.0970 (3) & 3.1 (1) \\ C9 & 0.1033 (2) & -0.0040 (4) & 3.88 (2) \\ C7 & 0.4727 (1) & 0.1247 (2) & 0.0970 (3) & 3.1 (1) \\ C9 & 0.103 (2) & -0.0080 (3) & -33893 (5) & 8.1 (3) \\ N1 & 0.4098 (1) & 0.1931 (2) & -0.0924 (2) & 4.8 (1) \\ O1 & 0.4635 (1) & 0.2331 (2) & -0.0652 (3) & 3.4 (1) \\ N2 & 0.4018 (1) & 0.2331 (2) & -0.0632 (3) & 3.4 (1) \\ N2 & 0.4018 (1) & 0.2331 (2) & -0.0638 (3) & 3.4 (1) \\ N2 & 0.4018 (1) & 0.2331 (2) & -0.0692 (3) & 3.3 (1) \\ O3 & 0.1879 (1) & -0.0123 (2) & -2945 (3) & 5.2 (1) \\ O3 & 0.1879 (1) & -0.0123 (2) & -2945 (3) & 5.3 (1) \\ O3 & 0.1879 (1) & -0.0123 (2) & -2945 (3) & 5.3 (1) \\ O3 & 0.1879 (1) & -0.0123 (2) & -2945 (3) & 5.3 (1) \\ O3 & 0.1879 (1) & -0.0123 (2) & -2945 (3) & 5.3 (1) \\ O3 & 0.1879 (1) & -0.0123 (2) & -2945 (3) & 5.2 (2) \\ \end{array}$	C4A	0.3980 (2)	0-2004 (4)	0.3866 (2)	3.8 (2)
$\begin{array}{ccccc} C6A & 0.2361 (2) & 0.3294 (3) & 0.3117 (2) & 3.5 (1) \\ O3A & 0.5044 (2) & 0.1891 (3) & 0.4350 (2) & 5.0 (1) \\ C9A & 0.5642 (3) & 0.3162 (5) & 0.4667 (3) & 6.9 (3) \\ C7B & 0.0222 (2) & 0.2490 (3) & 0.0019 (2) & 2.8 (1) \\ N1B & 0.1053 (2) & 0.1903 (2) & -0.0049 (2) & 3.1 (1) \\ N2B & 0.0817 (2) & 0.0916 (3) & -0.0728 (2) & 4.2 (1) \\ O1B & -0.0258 (2) & 0.0812 (2) & -0.1135 (1) & 4.4 (1) \\ O2B & -0.1611 (2) & 0.1900 (3) & -0.0987 (2) & 5.0 (1) \\ C2B & 0.2149 (2) & 0.2256 (3) & 0.0508 (2) & 3.0 (1) \\ C2B & 0.2836 (2) & 0.1532 (4) & 0.1544 (2) & 4.1 (2) \\ C4B & 0.4224 (2) & 0.2899 (4) & 0.1504 (2) & 4.1 (2) \\ C4B & 0.4224 (2) & 0.2899 (4) & 0.1504 (2) & 4.1 (2) \\ C5B & 0.3518 (3) & 0.3946 (3) & 0.0963 (2) & 4.5 (2) \\ C6B & 0.2470 (2) & 0.3539 (3) & 0.0466 (2) & 3.7 (1) \\ O3B & 0.5243 (2) & 0.3337 (3) & 0.1985 (2) & 5.6 (2) \\ C9B & 0.6034 (3) & 0.2288 (5) & 0.2450 (3) & 6.9 (3) \\ Compound (3) \\ Compound (3) \\ C5 & 0.2858 (1) & -0.0404 (2) & 0.1155 (3) & 3.4 (1) \\ C2 & 0.3091 (1) & 0.1824 (2) & 0.1270 (4) & 4.6 (2) \\ C5 & 0.2858 (1) & -0.0404 (2) & 0.1819 (4) & 4.6 (2) \\ C5 & 0.2858 (1) & -0.0404 (2) & 0.1819 (4) & 4.6 (2) \\ C5 & 0.2858 (1) & -0.0404 (2) & 0.1819 (4) & 4.6 (2) \\ C6 & 0.3414 (1) & -0.0335 (2) & 0.2376 (4) & 4.0 (2) \\ C5 & 0.2858 (1) & -0.0404 (2) & 0.1819 (4) & 4.5 (2) \\ C7 & 0.4727 (1) & 0.1247 (2) & 0.0970 (3) & 3.1 (1) \\ C9 & 0.1403 (2) & -0.0080 (3) & 0.3833 (5) & 8.1 (3) \\ N1 & 0.4098 (1) & 0.1491 (2) & 0.0508 (3) & 3.4 (1) \\ D2 & 0.5671 (1) & 0.2096 (2) & -0.0094 (2) & 4.8 (1) \\ O2 & 0.5671 (1) & 0.2096 (2) & -0.0094 (2) & 4.8 (1) \\ O2 & 0.5671 (1) & 0.2096 (2) & -0.0094 (2) & 4.8 (1) \\ O3 & 0.1879 (1) & -0.0123 (2) & 0.2945 (3) & 5.2 (1) \\ \end{array}$	C5A	0-3449 (2)	0.3286 (3)	0.3606 (2)	3.7 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C6A	0.2361 (2)	0-3294 (3)	0.3117(2)	3.5(1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	03A	0.5044(2)	0.1891(3)	0.4350 (2)	5.0(1)
$\begin{array}{ccccc} CIB & 0.70222 (2) & 0.7290 (3) & 0.0019 (2) & 2.6 (1) \\ N1B & 0.1053 (2) & 0.1903 (2) & -0.0049 (2) & 3.1 (1) \\ N2B & 0.0817 (2) & 0.0916 (3) & -0.0728 (2) & 4.2 (1) \\ 01B & -0.0258 (2) & 0.0812 (2) & -0.1135 (1) & 4.4 (1) \\ 02B & -0.1611 (2) & 0.1900 (3) & -0.0987 (2) & 5.0 (1) \\ CBB & -0.0679 (2) & 0.1820 (3) & -0.0705 (2) & 3.7 (2) \\ C1B & 0.2149 (2) & 0.2256 (3) & 0.0508 (2) & 3.0 (1) \\ C2B & 0.2836 (2) & 0.1205 (3) & 0.1027 (2) & 3.9 (2) \\ C3B & 0.3885 (2) & 0.1322 (4) & 0.1544 (2) & 4.1 (2) \\ C4B & 0.4224 (2) & 0.2899 (4) & 0.1504 (2) & 4.1 (2) \\ C5B & 0.3518 (3) & 0.3946 (3) & 0.0963 (2) & 4.5 (2) \\ C6B & 0.2470 (2) & 0.3639 (3) & 0.0466 (2) & 3.7 (1) \\ O3B & 0.5243 (2) & 0.3337 (3) & 0.1985 (2) & 5.6 (2) \\ C9B & 0.6034 (3) & 0.2288 (5) & 0.2450 (3) & 6.9 (3) \\ Compound (3) \\ S & 0.5000 & 0.0334 (1) & 0.2500 & 3.5 (1) \\ C1 & 0.3520 (1) & 0.1074 (2) & 0.1155 (3) & 3.4 (1) \\ C2 & 0.3091 (1) & 0.1824 (2) & 0.2030 (4) & 4.8 (2) \\ C4 & 0.2414 (1) & 0.0335 (2) & 0.2376 (4) & 4.0 (2) \\ C5 & 0.2858 (1) & -0.0404 (2) & 0.1819 (4) & 4.5 (2) \\ C6 & 0.3414 (1) & -0.0040 (2) & 0.1207 (4) & 4.6 (2) \\ C7 & 0.4727 (1) & 0.1247 (2) & 0.0970 (3) & 3.1 (1) \\ C9 & 0.1403 (2) & 0.00605 (3) & 0.3534 (4) & 5.6 (2) \\ C10 & 0.0840 (2) & -0.0080 (3) & 0.3893 (5) & 8.1 (3) \\ N1 & 0.4098 (1) & 0.1491 (2) & 0.0508 (3) & 3.4 (1) \\ N2 & 0.4018 (1) & 0.2231 (2) & -0.0652 (3) & 4.6 (2) \\ C1 & 0.4635 (1) & 0.2331 (2) & -0.0970 (3) & 3.1 (1) \\ C9 & 0.5671 (1) & 0.2096 (2) & -0.0094 (2) & 4.8 (1) \\ O2 & 0.5671 (1) & 0.2096 (2) & -0.0094 (2) & 4.8 (1) \\ O3 & 0.1879 (1) & -0.0123 (2) & 0.2245 (3) & 5.2 (2) \\ \end{array}$	C9A C7P	0.3642(3)	0.3102(3)	0.4007(3)	3 9 (3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		0.0222(2)	0.2490 (3)	-0.0019(2)	3.1(1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N2R	0.0817(2)	0.0916(3)	-0.0728(2)	4.2 (1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	OIR .	-0.0258(2)	0.0812(2)	-0.1135(1)	$4 \cdot 4(1)$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O2B	-0.1611(2)	0.1900 (3)	-0.0987 (2)	5.0(1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C8 <i>B</i>	-0.0679 (2)	0.1820 (3)	-0.0705 (2)	3.7 (2)
$\begin{array}{ccccc} C2B & 0.2836 (2) & 0.1205 (3) & 0.1027 (2) & 3.9 (2) \\ C3B & 0.3885 (2) & 0.1532 (4) & 0.1544 (2) & 4.1 (2) \\ C4B & 0.4224 (2) & 0.2899 (4) & 0.1504 (2) & 4.1 (2) \\ C5B & 0.3518 (3) & 0.3946 (3) & 0.0963 (2) & 4.5 (2) \\ C6B & 0.2470 (2) & 0.3639 (3) & 0.0466 (2) & 3.7 (1) \\ 03B & 0.5243 (2) & 0.3337 (3) & 0.1985 (2) & 5.6 (2) \\ C9B & 0.6034 (3) & 0.2288 (5) & 0.2450 (3) & 6.9 (3) \\ \hline \\ Compound (3) \\ \hline \\ S & 0.5000 & 0.0334 (1) & 0.2500 & 3.5 (1) \\ C1 & 0.3520 (1) & 0.1074 (2) & 0.1155 (3) & 3.4 (1) \\ C2 & 0.3091 (1) & 0.1824 (2) & 0.1700 (4) & 4.6 (2) \\ C3 & 0.2533 (2) & 0.1448 (2) & 0.2302 (4) & 4.8 (2) \\ C4 & 0.2414 (1) & 0.0335 (2) & 0.2376 (4) & 4.0 (2) \\ C5 & 0.2858 (1) & -0.0040 (2) & 0.1207 (4) & 4.5 (2) \\ C6 & 0.3414 (1) & -0.0340 (2) & 0.1207 (4) & 4.5 (2) \\ C7 & 0.4727 (1) & 0.1247 (2) & 0.0970 (3) & 3.1 (1) \\ C9 & 0.1403 (2) & 0.0605 (3) & 0.3534 (4) & 5.6 (2) \\ C10 & 0.0840 (2) & -0.0080 (3) & 0.3893 (5) & 8.1 (3) \\ N1 & 0.4098 (1) & 0.1491 (2) & 0.0508 (3) & 3.4 (1) \\ O2 & 0.5671 (1) & 0.2096 (2) & -0.0094 (2) & 4.8 (1) \\ O2 & 0.5671 (1) & 0.2096 (2) & -0.0094 (3) & 5.3 (1) \\ O3 & 0.1879 (1) & -0.0123 (2) & 0.2945 (3) & 5.2 (2) \\ \end{array}$	C1 <i>B</i>	0.2149 (2)	0-2256 (3)	0.0508 (2)	3.0(1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C2 <i>B</i>	0-2836 (2)	0-1205 (3)	0.1027 (2)	3.9 (2)
$\begin{array}{ccccc} C4B & 0.4224 (2) & 0.2899 (4) & 0.1504 (2) & 4.1 (2) \\ C5B & 0.3518 (3) & 0.3946 (3) & 0.0963 (2) & 4.5 (2) \\ C6B & 0.2470 (2) & 0.3639 (3) & 0.0466 (2) & 3.7 (1) \\ 03B & 0.5243 (2) & 0.3337 (3) & 0.1985 (2) & 5.6 (2) \\ C9B & 0.6034 (3) & 0.2288 (5) & 0.2450 (3) & 6.9 (3) \\ \hline \\ Compound (3) \\ S & 0.5000 & 0.0334 (1) & 0.2500 & 3.5 (1) \\ C1 & 0.3520 (1) & 0.1074 (2) & 0.1155 (3) & 3.4 (1) \\ C2 & 0.3091 (1) & 0.1824 (2) & 0.1700 (4) & 4.6 (2) \\ C3 & 0.2533 (2) & 0.1448 (2) & 0.2302 (4) & 4.8 (2) \\ C4 & 0.2414 (1) & 0.0335 (2) & 0.2376 (4) & 4.0 (2) \\ C5 & 0.2858 (1) & -0.0404 (2) & 0.1819 (4) & 4.5 (2) \\ C6 & 0.3414 (1) & -0.0303 (2) & 0.0040 (4) & 3.8 (2) \\ C7 & 0.4727 (1) & 0.1247 (2) & 0.0970 (3) & 3.1 (1) \\ C9 & 0.1403 (2) & 0.0605 (3) & 0.3534 (4) & 5.6 (2) \\ C10 & 0.0840 (2) & -0.0080 (3) & 0.3893 (5) & 8.1 (3) \\ N1 & 0.4098 (1) & 0.1491 (2) & 0.0508 (3) & 3.4 (1) \\ N2 & 0.4018 (1) & 0.2331 (2) & -0.0652 (3) & 4.6 (2) \\ O1 & 0.4635 (1) & 0.2331 (2) & -0.00944 (2) & 4.8 (1) \\ O2 & 0.5671 (1) & 0.2096 (2) & -0.0099 (3) & 5.3 (1) \\ O3 & 0.1879 (1) & -0.0123 (2) & 0.2945 (3) & 5.2 (2) \\ \end{array}$	C3B	0.3885 (2)	0.1532 (4)	0.1544 (2)	4.1(2)
$\begin{array}{ccccc} C3B & 0.3518 (3) & 0.3946 (3) & 0.0965 (2) & 4.5 (2) \\ C6B & 0.2470 (2) & 0.3639 (3) & 0.0466 (2) & 3.7 (1) \\ O3B & 0.5243 (2) & 0.3337 (3) & 0.1985 (2) & 5.6 (2) \\ C9B & 0.6034 (3) & 0.2288 (5) & 0.2450 (3) & 6.9 (3) \\ \hline \\ Compound (3) \\ S & 0.5000 & 0.0334 (1) & 0.2500 & 3.5 (1) \\ C1 & 0.3520 (1) & 0.1074 (2) & 0.1155 (3) & 3.4 (1) \\ C2 & 0.3091 (1) & 0.1824 (2) & 0.1700 (4) & 4.6 (2) \\ C3 & 0.2533 (2) & 0.1448 (2) & 0.2302 (4) & 4.8 (2) \\ C4 & 0.2414 (1) & 0.0335 (2) & 0.2376 (4) & 4.0 (2) \\ C5 & 0.2858 (1) & -0.0404 (2) & 0.1819 (4) & 4.5 (2) \\ C6 & 0.3414 (1) & -0.0040 (2) & 0.1207 (4) & 4.1 (2) \\ C8 & 0.5104 (1) & 0.1237 (2) & 0.0970 (3) & 3.1 (1) \\ C9 & 0.1403 (2) & 0.0605 (3) & 0.3534 (4) & 5.6 (2) \\ C10 & 0.0840 (2) & -0.0080 (3) & 0.3893 (5) & 8.1 (3) \\ N1 & 0.4098 (1) & 0.1491 (2) & 0.0508 (3) & 3.4 (1) \\ N2 & 0.4018 (1) & 0.2231 (2) & -0.0652 (3) & 4.6 (2) \\ O1 & 0.4635 (1) & 0.2231 (2) & -0.0924 (2) & 4.8 (1) \\ O2 & 0.5671 (1) & 0.2096 (2) & -0.0099 (3) & 5.3 (1) \\ O3 & 0.1879 (1) & -0.0123 (2) & 0.2945 (3) & 5.2 (2) \\ \end{array}$	C4B	0-4224 (2)	0.2899 (4)	0.1504(2)	4.1(2)
$\begin{array}{ccccc} Cobs & 0.2470(2) & 0.5359(3) & 0.0466(2) & 3.7(1) \\ 03B & 0.5243(2) & 0.3337(3) & 0.1985(2) & 5.6(2) \\ C9B & 0.6034(3) & 0.2288(5) & 0.2450(3) & 6.9(3) \\ \hline \\ Compound (3) \\ S & 0.5000 & 0.0334(1) & 0.2500 & 3.5(1) \\ C1 & 0.3520(1) & 0.1074(2) & 0.1155(3) & 3.4(1) \\ C2 & 0.3091(1) & 0.1824(2) & 0.1700(4) & 4.6(2) \\ C3 & 0.2533(2) & 0.1448(2) & 0.2302(4) & 4.8(2) \\ C4 & 0.2414(1) & 0.0335(2) & 0.2376(4) & 4.0(2) \\ C5 & 0.2858(1) & -0.0404(2) & 0.1819(4) & 4.5(2) \\ C6 & 0.3414(1) & -0.0040(2) & 0.1207(4) & 4.1(2) \\ C8 & 0.5104(1) & 0.1933(2) & 0.0040(4) & 3.8(2) \\ C7 & 0.4727(1) & 0.1247(2) & 0.0970(3) & 3.1(1) \\ C9 & 0.1403(2) & 0.0605(3) & 0.3534(4) & 5.6(2) \\ C10 & 0.0840(2) & -0.0080(3) & 0.3893(5) & 8.1(3) \\ N1 & 0.4098(1) & 0.1491(2) & 0.0508(3) & 3.4(1) \\ N2 & 0.4018(1) & 0.2231(2) & -0.0622(3) & 4.6(2) \\ O1 & 0.4635(1) & 0.2331(2) & -0.0924(2) & 4.8(1) \\ O2 & 0.5671(1) & 0.2096(2) & -0.0099(3) & 5.3(1) \\ O3 & 0.1879(1) & -0.0123(2) & 0.2945(3) & 5.2(2) \\ \end{array}$	CSB	0.3518(3)	0.3940(3)	0.0903(2)	4.5(2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	018	0.2470(2) 0.5243(2)	0.3337(3)	0.1985(2)	5.6 (2)
$\begin{array}{c} \text{Compound (3)} \\ \text{S} & 0.5000 & 0.0334 (1) & 0.2500 & 3.5 (1) \\ \text{C1} & 0.3520 (1) & 0.1074 (2) & 0.1155 (3) & 3.4 (1) \\ \text{C2} & 0.3091 (1) & 0.1824 (2) & 0.1700 (4) & 4.6 (2) \\ \text{C3} & 0.2533 (2) & 0.1448 (2) & 0.2302 (4) & 4.8 (2) \\ \text{C4} & 0.2414 (1) & -0.035 (2) & 0.2376 (4) & 4.0 (2) \\ \text{C5} & 0.2858 (1) & -0.0404 (2) & 0.1819 (4) & 4.5 (2) \\ \text{C6} & 0.3414 (1) & -0.0040 (2) & 0.1207 (4) & 4.1 (2) \\ \text{C8} & 0.5104 (1) & 0.1237 (2) & 0.0970 (3) & 3.1 (1) \\ \text{C9} & 0.1403 (2) & 0.0605 (3) & 0.3534 (4) & 5.6 (2) \\ \text{C10} & 0.0840 (2) & -0.0080 (3) & 0.3893 (5) & 8.1 (3) \\ \text{N1} & 0.4098 (1) & 0.1491 (2) & 0.0508 (3) & 3.4 (1) \\ \text{N2} & 0.4018 (1) & 0.2231 (2) & -0.0924 (2) & 4.8 (1) \\ \text{O2} & 0.5671 (1) & 0.2096 (2) & -0.0090 (3) & 5.3 (1) \\ \text{O3} & 0.1879 (1) & -0.0123 (2) & 0.2945 (3) & 5.2 (2) \\ \end{array}$	C9B	0.5243(2) 0.6034(3)	0.2288(5)	0.2450 (3)	6.9(2)
$\begin{array}{c} \mbox{Compound (3)} \\ S & 0.5000 & 0.0334 (1) & 0.2500 & 3.5 (1) \\ C1 & 0.3520 (1) & 0.1074 (2) & 0.1155 (3) & 3.4 (1) \\ C2 & 0.3091 (1) & 0.1824 (2) & 0.1700 (4) & 4.6 (2) \\ C3 & 0.2533 (2) & 0.1448 (2) & 0.2302 (4) & 4.8 (2) \\ C4 & 0.2414 (1) & 0.0335 (2) & 0.2376 (4) & 4.0 (2) \\ C5 & 0.2858 (1) & -0.0404 (2) & 0.1819 (4) & 4.5 (2) \\ C6 & 0.3414 (1) & -0.0040 (2) & 0.1207 (4) & 4.1 (2) \\ C8 & 0.5104 (1) & 0.1933 (2) & 0.0040 (4) & 3.8 (2) \\ C7 & 0.4727 (1) & 0.1247 (2) & 0.0970 (3) & 3.1 (1) \\ C9 & 0.1403 (2) & 0.0605 (3) & 0.3893 (5) & 8.1 (3) \\ N1 & 0.4098 (1) & 0.1491 (2) & 0.0508 (3) & 3.4 (1) \\ N2 & 0.4018 (1) & 0.2231 (2) & -0.0652 (3) & 4.6 (2) \\ O1 & 0.4635 (1) & 0.2231 (2) & -0.0924 (2) & 4.8 (1) \\ O2 & 0.5671 (1) & 0.2096 (2) & -0.0009 (3) & 5.3 (1) \\ O3 & 0.1879 (1) & -0.0123 (2) & 0.2945 (3) & 5.2 (2) \\ \end{array}$	-			/	/
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Compound (3))			
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	S	0.5000	0.0334(1)	0.2500	3.5(1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C1	0.3520(1)	0.1074(2)	0.1155(3)	3.4(1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C2	0.3091(1) 0.2533(2)	0.1024 (2)	0.1700(4) 0.2302(4)	4.0(2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C4	0.2414(1)	0.0335(2)	0.2376 (4)	4.0(2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C5	0.2858 (1)	-0.0404 (2)	0.1819 (4)	4.5 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C6	0.3414 (1)	-0.0040 (2)	0.1207 (4)	4·1 (2)
$\begin{array}{ccccccc} C7 & 0.4727(1) & 0.1247(2) & 0.0970(3) & 3.1(1) \\ C9 & 0.1403(2) & 0.0605(3) & 0.3534(4) & 5.6(2) \\ C10 & 0.0840(2) & -0.0080(3) & 0.3893(5) & 8.1(3) \\ N1 & 0.4098(1) & 0.1491(2) & 0.0508(3) & 3.4(1) \\ N2 & 0.4018(1) & 0.2231(2) & -0.0652(3) & 4.6(2) \\ O1 & 0.4635(1) & 0.2334(2) & -0.0944(2) & 4.8(1) \\ O2 & 0.5671(1) & 0.2096(2) & -0.0009(3) & 5.3(1) \\ O3 & 0.1879(1) & -0.0123(2) & 0.2945(3) & 5.2(2) \\ \end{array}$	C8	0-5104 (1)	0-1933 (2)	0.0040 (4)	3.8(2)
$\begin{array}{cccc} C9 & 0.1403 \left(2\right) & 0.0605 \left(3\right) & 0.3534 \left(4\right) & 5.6 \left(2\right) \\ C10 & 0.0840 \left(2\right) & -0.0080 \left(3\right) & 0.3893 \left(5\right) & 8.1 \left(3\right) \\ N1 & 0.4098 \left(1\right) & 0.1491 \left(2\right) & 0.0508 \left(3\right) & 3.4 \left(1\right) \\ N2 & 0.4018 \left(1\right) & 0.2231 \left(2\right) & -0.0652 \left(3\right) & 4.6 \left(2\right) \\ O1 & 0.4635 \left(1\right) & 0.2334 \left(2\right) & -0.0944 \left(2\right) & 4.8 \left(1\right) \\ O2 & 0.5671 \left(1\right) & 0.2096 \left(2\right) & -0.0009 \left(3\right) & 5.3 \left(1\right) \\ O3 & 0.1879 \left(1\right) & -0.0123 \left(2\right) & 0.2945 \left(3\right) & 5.2 \left(2\right) \end{array}$	C7	0-4727 (1)	0-1247 (2)	0.0970 (3)	3.1(1)
$ \begin{array}{cccccc} C10 & 0.0840 \left(2\right) & -0.0080 \left(3\right) & 0.3893 \left(5\right) & 8\cdot1 \left(3\right) \\ N1 & 0.4098 \left(1\right) & 0.1491 \left(2\right) & 0.0508 \left(3\right) & 3\cdot4 \left(1\right) \\ N2 & 0.4018 \left(1\right) & 0.2231 \left(2\right) & -0.0652 \left(3\right) & 4\cdot6 \left(2\right) \\ O1 & 0.4635 \left(1\right) & 0.2354 \left(2\right) & -0.0944 \left(2\right) & 4\cdot8 \left(1\right) \\ O2 & 0.5671 \left(1\right) & 0.2096 \left(2\right) & -0.0009 \left(3\right) & 5\cdot3 \left(1\right) \\ O3 & 0.1879 \left(1\right) & -0.0123 \left(2\right) & 0.2945 \left(3\right) & 5\cdot2 \left(2\right) \\ \end{array} $	C9	0.1403 (2)	0.0605 (3)	0.3534 (4)	5.6(2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C10	0.0840 (2)	-0.0080 (3)	0.3893 (5)	8.1 (3)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	NI	0.4098 (1)	0-1491 (2)	0.0508 (3)	3.4(1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N2 01	0.4018(1)	0.2231(2) 0.2534(2)	-0.0032(3) -0.0044(2)	4.8(1)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	02	0.5671(1)	0.2096 (2)	-0.0009 (3)	5.3(1)
	03 03	0.1879(1)	-0.0123 (2)	0.2945 (3)	5.2 (2)

Experimental. (1) $C_{16}H_{10}N_4O_4S$, crystal $0.4 \times 0.4 \times 0.6$ mm. CAD-4 diffractometer. Unit-cell dimensions: 25 reflections, 2θ range 17 to 31° . D_m by flotation (CCl₄/CHCl₃). Absorption corrections were made according to experimental ψ rotation; normalized transmission coefficients 0.97-1.00. $2\theta_{max} = 60^\circ$. Ranges of *h*, *k*, *l*; -14 to 14, 0 to 10, 0 to 27, respectively. Three standard reflections monitored every 2 h: variation < 3%. 4538 unique reflections, 2922 observed with $I > 3\sigma(I)$. R = 0.033, wR = 0.028, S = 2.30. Weighting scheme from counting statistics. Structure solved by heay-atom method. H atoms found in difference Fourier map after isotropic refinement and then refined. $(\Delta/\sigma)_{max} = 0.37$. Peaks in final $\Delta\rho$ map



(3) Fig. 1. The crystal structures of (1), (2) and (3).

0.24 to -0.21 e Å⁻³. Extinction coefficient 1.96 (length in µm). Atomic scattering factors from International Tables for X-ray Crystallography (1974). Computing programs: NRCC SDP PDP-11 package (Gabe & Lee, 1981), MULTAN and ORTEP from Enraf-Nonius (1979) Structure Determination Package. (2) C_{18} - $H_{14}N_4O_6S$, crystal $0.2 \times 0.4 \times 0.4$ mm. Unit cell: 25 reflections, 2θ range 15 to 23°. Normalized transmission coefficients 0.97-1.00. Ranges of h, k, l: -20 to 20, 0 to 13, 0 to 21, respectively. 5267 unique reflections, 2066 observed with $I > 2\sigma(I)$. R = 0.039, wR = 0.037, S = 1.63. Structure solved by direct method using the MULTAN program. $(\Delta/\sigma)_{max} = 0.37$. Peaks in final $\Delta \rho$ map 0.17 to -0.18 e Å⁻³. Extinction coefficient 0.302 (length in μ m). Other details as for (1). (3) $C_{20}H_{18}N_4O_6S$, crystal $0.2 \times 0.2 \times 0.3$ mm. Unit cell: 25 reflections, 2θ range 10 to 24° . D_m by flotation (CCl₄/CH₂Cl₂). Normalized transmission coefficients 0.94-1.00. Ranges of h, k, l: -29 to 29, 0 to 17, 0 to 11, respectively. 3004 unique reflections, 1088 observed with $I > 2\sigma(I)$. R = 0.039, wR = 0.033, S = 1.67. Structure solved by direct method using the MULTAN program, $(\Delta/\sigma)_{max} = 0.31$. Peaks in final $\Delta\rho$ map 0.15 to -0.16 e Å⁻³. Extinction coefficient 0.078 (length in μ m). Other details as for (1).

Discussion. Atomic positional parameters and equivalent isotropic temperature factors are listed in Table 1.* The molecular structures and the crystal packing

*Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51476 (95 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. diagrams are shown in Figs. 1 and 2. The bond lengths and angles are shown in Tables 2 and 3.

The bond lengths of the sydnone ring are listed in Table 4 and compared with those from other 3,4disubstituted sydnone derivatives. The bond lengths of the sydnone ring are similar in these three title structures and comparable to those of other 3,4disubstituted sydnone derivatives. The N(1)-C(7) bond lengths of the title compounds are 1.350(1), 1.352(3) and 1.358(3) Å, respectively. As found before, the lengthening of the N(1)-C(7) bond compared with the

Table 2. Bond lengths (Å) for (1), (2) and (3)

Comp	ound (1)									
S	C7A	1.736 (2)	S	C7B	1.735 (2)	CIA	C2A	1.373 (2)			
C1A	C6A	1.381 (2)	CIA	N1A	1.452 (2)	C2A	C3A	1.382 (2)			
C3A	C4A	1.369 (3)	C4A	C5A	1.370 (3)	C5A	C6A	1.383 (3)			
C7A	C8A	1-412 (2)	C7A	N1A	1.347 (2)	C8A	01A	1.409 (2)			
C8A	O2 <i>A</i>	1.204 (2)	N1A	N2A	1.308 (2)	N2A	01 <i>A</i>	1.380 (2)			
C1B	C2B	1-376 (2)	C1B	C6B	1.377 (2)	C1 <i>B</i>	N1 <i>B</i>	1.445 (2)			
C2B	C3B	1-377 (3)	C3B	C4B	1.369 (3)	C4B	C5B	1.383 (3)			
C5B	C6B	1-378 (3)	C7B	C8 <i>B</i>	1.408 (2)	C7B	N1 <i>B</i>	1.352 (2)			
C8B	O1B	1.402 (2)	C8B	O2B	1.205 (2)	N1 <i>B</i>	N2B	1.307 (2)			
N2 <i>B</i>	O1 <i>B</i>	1.383 (2)									
Compound (2)											
S	C7A	1.729 (3)	S	C7B	1.730 (3)	C7A	N1 <i>A</i>	1.351 (4)			
C7A	C8A	1.415 (4)	N1A	N2A	1.303 (3)	NIA	C1A	1.448 (3)			
N2A	01A	1.377 (3)	01A	C8A	1.416 (3)	O2A	C8A	1.194 (3)			
C1A	C2A	1.373 (4)	CIA	C6A	1.366 (4)	C2A	C3A	1.369 (4)			
C3A	C4A	1.380 (5)	C4A	C5A	1.378 (4)	C4A	O3A	1.361 (4)			
C5A	C6A	1.388 (4)	O3A	C9A	1.414 (5)	C7B	N1 <i>B</i>	1.352 (4)			
C7B	C8B	1.411 (4)	N1 <i>B</i>	N2 <i>B</i>	1.312 (3)	N1 <i>B</i>	C1 <i>B</i>	1.443 (3)			
N2 <i>B</i>	O1B	1.375 (3)	01 <i>B</i>	C8B	1.425 (4)	O2 <i>B</i>	C8 <i>B</i>	1.201 (4)			
C1 <i>B</i>	C2B	1.362 (4)	C1B	C6B	1.382 (4)	C2B	C3B	1.376 (4)			
C3B	C4 <i>B</i>	1.377 (5)	C4 <i>B</i>	C5B	1.381 (5)	C4B	O3B	1.364 (4)			
C5B	C6 <i>B</i>	1.369 (4)	O3 <i>B</i>	C9 <i>B</i>	1-421 (5)						
Compound (3)											
S	C7	1.732 (3)				CI	C2	1.376 (4)			
čı	Č6	1.373 (4)	CL	NI	1.445 (4)	Č2	Č3	1.375 (4)			
~	23	1.373(4)	č.		1 202 (4)	<u> </u>	õ	1 250 (4)			

C8 C7 N1

1.370 (4)

1-196 (4)

1.442 (4)

C7 N1

N2





01 C10

1.410(4)

1.483 (5)

1.373 (3)

C8 C9

1.411 (4)

1.358(3)

1.309 (3)

Fig. 2. Packing diagrams for (1), (2) and (3).

C5 C8 C9 C6 O2 O3

	Table 3. Bond angles $(^{\circ})$ for (1) , (2) and (3)							Table 3 (cont.)							
								C2A	C1A	C6A	122.0 (3)	C1A	C2A	C3A	119-4 (3)
Comp	ound (1)							C2A	C3A	C4A	119-8 (3)	C3A	C4A	C5A	120-5 (3)
C7A	S	C7B	97.38 (7)	C2A	C1A	C6A	122.9 (2)	C3A	C4A	O3A	115-5 (3)	C5A	C4A	03 <i>A</i>	124.0 (3)
C2A	C1A	N1A	119.1 (1)	C6A	C1A	N1A	117.9(1)	C4A	C5A	C6A	119-8 (3)	C1A	C6A	C5A	118-6 (3)
C1A	C2A	C3A	117.9 (2)	C2A	C3A	C4A	120-6 (2)	C4A	O3A	C9A	118-4 (3)	S	C7B	N1 <i>B</i>	125.7 (2)
C3A	C4A	C5A	120.4 (2)	C4A	C5A	C6A	120.7 (2)	S	C7B	C8B	127.8 (2)	N1 <i>B</i>	C7B	C8 <i>B</i>	106-4 (2)
C1A	C6A	C5A	117.5 (2)	S	C7A	C8A	127-4 (1)	C7B	N1 <i>B</i>	N2 <i>B</i>	115.0 (2)	C7B	N1 <i>B</i>	C1B	128-1 (2)
S	C7A	N1A	126-5(1)	C8A	C7A	N1 <i>A</i>	106-1 (2)	N2 <i>B</i>	N1 <i>B</i>	C1B	116-9 (2)	N1 <i>B</i>	N2 <i>B</i>	01 <i>B</i>	104.3 (2)
C7A	C8A	014	103.7(1)	C7A	C8A	O2A	134-8 (2)	N2 <i>B</i>	01 <i>B</i>	C8B	111.1 (2)	C7B	C8 <i>B</i>	01 <i>B</i>	103.3 (2)
01 <i>A</i>	C8A	O2A	121.5 (1)	C1A	NIA	C7A	129-4 (1)	C7B	C8 <i>B</i>	O2 <i>B</i>	136-5 (3)	01 <i>B</i>	C8 <i>B</i>	O2 <i>B</i>	120.2(3)
C1A	N1A	N2A	115-7 (1)	C7A	N 1 <i>A</i>	N2A	115-0(1)	N1 <i>B</i>	C1 <i>B</i>	C2B	119.0 (3)	N 1 <i>B</i>	C1 <i>B</i>	C6B	118.7 (3)
N1A	N24	01 <i>A</i>	104-2 (1)	C8A	01 <i>A</i>	N2A	110-9(1)	C2B	C1 <i>B</i>	C6B	122.3 (3)	CIB	C2B	C3B	119-1 (3)
C2 <i>B</i>	C 1 <i>B</i>	C6 <i>B</i>	123.0 (2)	C2 <i>B</i>	C 1 <i>B</i>	N1 <i>B</i>	117-4 (1)	C2B	C3B	C4B	119.6 (3)	C3B	C4B	CSB	120.5 (3)
C6 <i>B</i>	C1 <i>B</i>	N1 <i>B</i>	119-5 (1)	C1 <i>B</i>	C2B	C3B	118-2 (2)	C3B	C4B	O3B	124.4 (3)	CSB	C4B	038	115.1 (3)
C2B	C 3 <i>B</i>	C4 <i>B</i>	120-2 (2)	C3 <i>B</i>	C4B	C5B	120.7 (2)	C4 <i>B</i>	C5B	C6B	120.3 (3)	C1B	C6B	C 5B	118-2 (3)
C4 <i>B</i>	C5B	C6 <i>B</i>	120-3 (2)	C1 <i>B</i>	C6 <i>B</i>	C5B	117-6 (2)	C4 <i>B</i>	O3B	C9 <i>B</i>	118-5 (3)				
S	C7B	C8B	128-1(1)	S	C7B	N1B	125-6(1)	<u> </u>	1/7	、					
C8 <i>B</i>	C7B	N1 <i>B</i>	106-3 (1)	C7B	C8B	01B	103.9(1)	Comp	ouna (3)		~ ~	.	~ ~	
C7B	C8 <i>B</i>	02 <i>B</i>	135-2 (2)	O1B	C8B	028	120.9 (2)	C7	S	C7	100-3(1)	C2	CI	C6	122-3 (3)
C1 <i>B</i>	N1 <i>B</i>	C7B	129-6 (1)	C1 <i>B</i>	N1B	N2B	115-9(1)	C2	Cl	N1	117-8 (3)	C6	Cl	NI	119.9 (3)
C7B	N1 <i>B</i>	N2 <i>B</i>	114-4 (1)	N1 <i>B</i>	N2B	OIB	104-4 (1)	C1	C2	C3	118-9 (3)	C2	C3	C4	120.2(3)
~		、 、						C3	C4	C5	119.5 (3)	C3	C4	03	124.9 (3)
Comp	ound (2)		_	-			C5	C4	03	115.5 (3)	C4	CS	C6	120.9 (3)
C7A	S	C7B	101.0(1)	S	C7A	NIA	126.2(2)	C1	C6	CS	118-2(3)	01	C8	01	$103 \cdot 3(2)$
S	C7A	C8A	127.8 (2)	N1A	C7A	C8A	106.0 (2)	C7	C8	02	135-0 (3)	01	C8	02	121.6 (3)
C7A	N1A	N2A	115-4 (2)	C7A	N1A	CIA	129.9 (2)	S	C7	C8	127-6 (2)	S	07	NI	125.8 (2)
N2A	NIA	C 1A	114.7 (2)	N1A	N24	01A	104-1 (2)	C8	C7	NI	106-4 (2)	010	09	03	107.2 (3)
N2A	01 <i>A</i>	C8A	111.3 (2)	C7A	C8A	01A	$103 \cdot 3(2)$	C1	NI	C7	128.9(2)	CI	NI	N2	110.9(2)
C7A	C8A	02 <i>A</i>	136-0 (3)	01 <i>A</i>	C8A	O2A	120.7 (3)	C7	N1	N2	114.2(2)	NI	N2	01	104.5 (2)
N1A	C1A	C2A	119-1 (3)	N1A	C1A	C6A	118.7(3)	C8	01	N2	111-5 (2)	C4	03	C9	117.9 (2)

Table 4. Comparison of selected bond lengths (Å) and some conformational parameters of the sydnone ring in 3,4-disubstituted compounds

O(1)–C(8)	(1) ^a 1·409 (2) 1·402 (2)	(2) ^a 1·416 (3) 1·425 (4)	(3) ^a 1·410 (4)	(4) ^b 1-419 (4)	(5) ⁶ 1·399 (2)	(6) ^c 1·406 (3)	(7) ^d 1·400 (4)	(8) ^e § 1-416 (6)
O(1)N(2)	1·380 (2) 1·383 (2)	1·377 (3) 1·375 (3)	1.373 (3)	1-379 (3)	1.382 (2)	1.379 (2)	1.380 (4)	1.368 (5)
N(2)—N(1)	1·308 (2) 1·307 (2)	1·303 (3) 1·312 (3)	1.309 (3)	1.295 (3)	1.309 (2)	1.318 (2)	1.325 (4)	1-318 (5)
N(1)-C(7)	1·347 (2) 1·352 (2)	1·351 (4) 1·352 (4)	1.358 (3)	1.350(3)	1.352 (2)	1.351 (2)	1.350 (4)	1.358 (6)
C(7)–C(8)	1-412 (2) 1-408 (2)	1·415 (4) 1·411 (4)	1.411 (4)	1-413 (4)	1.420 (3)	1.416 (2)	1-418 (4)	1.417 (7)
C(8)—O(2)	1·204 (2) 1·205 (2)	1 · 194 (3) 1 · 201 (4)	1.196 (4)	1 · 196 (3)	1-212 (2)	1.217 (2)	1.205 (4)	1-196 (6)
C(7)–C(9)				1-444 (2)	1.453 (4)	1-465 (3)	1.464 (4)	1-429 (6)
S-C(7)	1·736 (2) 1·735 (2)	1·729 (3) 1·730 (3)	1.732 (3)					
⊿[O(2)]*	0·047 (3) 0·015 (3)	0-037 (5) 0-029 (5)	0.044 (4)	0.011 (6)	0.001 (3)	0.041 (2)	0.013 (2)	0.019 (4)
⊿[S]†	0·053 (3) 0·045 (3)	0·078 (5) 0·100 (5)	0.055 (4)					
ω(°)	53·7 (1) 62·8 (1)	51·0 (1) 59·2 (1)	53-5 (1)	68-4 (2)	78-6 (1)	54-9	63-8	63.0 (2)
x ²‡	84·5 43·4	7·1 41·4	37-0	5-4	16-4	195-6	21.1	0.7
Color	Light brown	Transparent	Transparent	Brown	Light brown	Transparent	Bright yellow	Light brown

References: (a) this work; (b) Ueng, Wang & Yeh (1987a); (c) Hašek, Obrda, Kuml, Nešpurek, Chojnacki & Šorm (1978); (d) Hašek, Obrda, Kuml. Nešpurek & Šorm (1979); (e) Ueng, Wang & Yeh (1987b).

* Deviation (Å) of O(2) the mean plane of the sydnone ring.

† Deviation (Å) of S from the mean plane of the sydnone ring.

 $\ddagger \chi^2 \text{ is defined as } \sum_{i=1}^n \Delta d_i^2 / (\sigma_x^2 + \sigma_y^2 + \sigma_z^2 \text{ as in } (b).$

§ (4) 4-acetyl-3-(p-tolyl)sydnone; (5) 4-acetyl-3-phenylsydnone oxime; (6) 4-(3-methyl-1-buten-2-yl)-3-phenylsydnone; (7) 4-(cyclohexen-1-yl)-3-phenylsydnone; (8) 3-phenyl-4-(N-carbamoyl-1,4,2-oxathiazolimin-3-yl)sydnone.

corresponding bond in 3,4-disubstituted sydnone derivatives may also be attributed to the steric effect (Ueng, Wang & Yeh, 1987a,b).

The bond lengths (S-C), bond angles (CSC') and the angles between the CSC' plane and the sydnone ring of the title compounds and other diaryl sulfides are comparable (Von Deuten & Klar, 1981). There is no apparent trend in such bond lengths. A π interaction between the S atom and the sydnone ring would be expected if the CSC plane and the aryl ring were coplanar. However, this is not obvious; as an example 4-(dimethylamino)phenyl 4-nitrophenyl sulfide (Von Deuten & Klar, 1981) does have one of the aryl rings which is coplanar with the CSC plane, but both S-C lengths are about the same. The shortening of the S-C bonds of the title compounds relative to those of other diaryl sulfides and the average bond lengths of 1,3,5-trithiane [1.818 (5) Å (Fleming & Lynton, 1967)] may be attributable to orbital eletronegativity effects.

The C(7)–S(1)–C(7') bond angles of the title compounds $[97.4(1), 101.0(1) \text{ and } 100.3(1)^{\circ}]$ are comparable with corresponding angles in the cyclic 1,3,5-trithane $[99.2(6) \text{ and } 100.7(5)^{\circ}]$. The dihedral angles (ω) between the sydnone ring and the phenyl ring are listed in Table 4 for 3,4-disubstituted compounds. It is certainly clear that all such compounds have angles greater than 50°.

Compound (3) has exact C_2 molecular symmetry bisecting the C-S-C' angle which coincides with the crystallographic twofold axis along the *b* axis. Compound (1) has a pseudo twofold axis; the two sydnone-aryl parts of the compound are essentially the same. However, compound (2) adopts a quite different conformation from those of the other two compounds. The difference can be seen clearly in Fig. 1. The packing in the crystal is also quite different (Fig. 2).

Instead of the 'morino' conformation (Von Deuten & Klar, 1981) with one ring in the C–S–C' plane and the other perpendicular, as found in most other diaryl sulfides, the three title compounds have the butterfly conformation $[61.7 (1), 59.3 (1); 88.1 (1), 73.6 (1); 72.9 (1), 72.9 (1)^{\circ}$, respectively].

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Structures of two Psychoactive 1,4-Benzodiazepines

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Abstract. (I) 8-Chloro-6-(2-chlorophenyl)-2-methyl-4H-imidazo[1,2-a][1,4]benzodiazepine, $C_{18}H_{13}Cl_2N_3$, $M_r = 342 \cdot 2$, monoclinic, $P2_1/c$, $a = 13 \cdot 168$ (3), b =14·852 (3), $c = 8 \cdot 286$ (2) Å, $\beta = 94 \cdot 45$ (2)°, V =1615·6 Å³, Z = 4, $D_x = 1 \cdot 407$ g cm⁻³, λ (Mo K α) = 0·71069 Å, $\mu = 3 \cdot 95$ cm⁻¹, F(000) = 704, T = 293 K, R = 0.042 for 796 observed reflections. (II) 8-Chloro-6-(2-chlorophenyl)-1-(4-pyridyl)-1,2,4-triazolo[4,3-a]-[1,4]benzodiazepine, $C_{21}H_{13}Cl_2N_5$, $M_r = 406 \cdot 3$, orthorhombic, *Pbca*, $a = 21 \cdot 560$ (3), $b = 8 \cdot 790$ (1), c =19·866 (5) Å, $V = 3764 \cdot 9$ Å³, Z = 8, $D_x =$ 1.434 g cm⁻³, λ (Mo K α) = 0.71069 Å, μ = 3.5 cm⁻¹, F(000) = 1664, T = 293 K, R = 0.042 for 2196 observed reflections. The angle between the mean planes of the chlorophenyl ring and the fused benzo moiety is 77 (1)° in (I) and 78 (1)° in (II). The seven-membered heterocyclic ring adopts a cycloheptatriene-like boat conformation with bow and stern angles of 55 (1) and 33 (1)° in (I), and 53.4 (7) and 34.3 (7)° in (II). In both compounds the five-membered heterocyclic ring and the two aromatic rings are each planar to within +0.02 Å. Bond lengths and angles are normal.

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