compared with those of the triselenylimide ion in $K_3(NSeO_2)_3$ (Kocman & Rucklidge, 1974) in Table 5.

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# The Crystal Structure of Methyl Sulphimide, (CH3NSO2)3

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The structure of $(CH_3NSO_2)_3$ has been determined by X-ray diffraction. Least-squares refinement with 1177 reflexions gave a final $R$ of 0·037 for 96 parameters. The intensities were collected on a semi-automatic diffractometer with monochromatized Mo $K\alpha$ radiation. The sulphimide molecule is in the chair form and has symmetry $3m$ ($C_{3v}$) within experimental error, the mean S–N distance is 1·669 (1) Å, S–O$_{ax}$ 1·407 (1) Å, S–O$_{eq}$ 1·409 (1) Å, C–N 1·492 (2) Å. The geometry of the molecule is compared with that of sulphanuric chloride, $(NSOCl)_3$, and with the trisulphimide ion, $(NSO_2)_3^{3-}$.

## Introduction

The sulphur–nitrogen bonds in $\alpha$-sulphanuric chloride, $(NSOCl)_3$, are short and equal in length (Hazell, Wiegers & Vos, 1966). The shortness of the bonds is explained, *e.g.* Salem (1966), by two kinds of $\pi$-bonding: between $d$-orbitals on the sulphur atom and the $p_z$ orbital on the nitrogen atom, and to exocyclic $\pi'$-bonding in the plane of the nitrogen atom and its adjacent sulphur atoms from the overlap of the lone pair on the $sp^2$ hybridized nitrogen atom with $d$-orbitals from the sulphur atoms.

The structures of the trisulphimide ion, $(NSO_2^-)_3$, in the silver salt (Dalgaard, Hazell & Hazell, 1974) and of methyl sulphimide, $(CH_3NSO_2)_3$, have been studied. In the methyl compound the lone pairs on the nitrogen atoms are replaced by methyl groups which would if the nitrogen atom retained its $sp^2$ hybridization remove the possibility of $\pi'$-bonding. Alternatively, the nitrogen atom could become $sp^3$ hybridized with the lone pair in the axial or the equatorial position.

The S–N bonds are found to be significantly longer than those in sulphanuric chloride or in the sulphimide ion (Table 1) but the geometry about the nitrogen atom is intermediate between planar trigonal and tetrahedral.

## Crystal data

Methyl sulphimide, $(CH_3NSO_2)_3$; $M = 279\cdot3$. Orthorhombic, $a = 8\cdot021$ (10), $b = 10\cdot648$ (10), $c = 11\cdot537$ (10) Å, $U = 985\cdot4$ Å$^3$; $D_c = 1\cdot88$, $Z = 4$. The systematic absences are: $0kl$ for $k + l$ odd, and $hk0$ for $h + k$ odd; the space group is $Pnma$ (No. 62) or $Pn2_1a$ (No. 33). The structure determination confirms $Pnma$. The compound crystallizes from toluene as colourless needles elongated in the [010] direction. $\mu$ for Mo $K\alpha$ radiation is 7·48 cm$^{-1}$.

## Experimental

The crystals were provided by Dr A. J. Banister.

Intensities were collected on a linear diffractometer of the Arndt & Phillips (1961) design. Mo $K\alpha$ radiation

monochromatized by means of a graphite crystal (Rasmussen & Henriksen, 1970) was used in conjunction with a scintillation counter and a pulse-height analyser. The background-peak-background method was used.

1393 independent reflexions with sin $\theta/\lambda < 0.7$ were measured. In most cases four symmetry-related reflexions were recorded. Of these 1393 reflexions 1198 had $I > 2\sigma_c(I)$ where $\sigma_c(I)$ is the square-root of the total number of counts per reflexion.

The crystal, which was mounted with its needle axis parallel to the rotation axis, was 1·4 mm long and approximately 0·25 × 0·38 mm in cross-section. Corrections were made for absorption and the mean path lengths for the different reflexions were calculated.

## Structure determination and refinement

The structure was determined by Patterson and Fourier methods. Least-squares refinement of atomic coor-

dinates, thermal parameters, an overall scale factor, and an isotropic extinction parameter reduced $R$ to 0·037 for 1177 reflexions and 96 parameters; the weighted $R$ was 0·048. Only reflexions for which $I > 2\sigma_c(I)$ were used, and those reflexions close to the rotation axis of the crystal ($h^2 + l^2 < 3$) were also omitted. The value of the extinction parameter, $g$, was 2·6 (5) × $10^{-5}$; the largest correction was to $F(002)$ for which $F_{obs}/F_{corr}$ was 0·80.

The atomic coordinates and thermal parameters are listed in Table 2, and observed and calculated structure factors in Table 3.

## Correction of parameters for thermal motion

The thermal motion of the non-hydrogen atoms was analysed, assuming rigid-body motion, by the method of Schomaker & Trueblood (1968). The contributions of each atom were weighted inversely as the atomic number. The r.m.s. value of $\Delta u_{ij}$, where $\Delta u_{ij}$ is the

Table 1. *Molecular geometry for six-membered sulphur–nitrogen compounds,* $(NSOX)_3$, *and some related compounds*

| | | | | S–O | S–N | $\angle$X–S–O | $\angle$N–S–N | $\angle$S–N–S | Reference |
|---|---|---|---|---|---|---|---|---|---|
| I | $\alpha(NSOCl)_3$ | chair | eq | 1·407 (7) | 1·571 (4) | 107·9 (4) | 112·8 (4) | 122·0 (4) | Hazell, Wiegers & Vos (1966) |
| II | $(NSO_2^-)_3$ (silver salt) | chair | ax eq | 1·456 (6) 1·436 (6) | 1·636 (4) | 117·4 (4) | 106·1 (4) | 115·0 (3) | Dalgaard, Hazell & Hazell (1974) |
| III | $(CH_3NSO_2)_3$ | chair | ax eq | 1·407 (1) 1·409 (1) | 1·669 (1) | 121·9 (1) | 104·5 (1) | 117·1 (1) | This work |
| IV | $(NSCl)_3$ | chair | – | | 1·605 (5) | – | 113·4 (3) | 123·9 (3) | Wiegers & Vos (1966) |
| V | $(NSF)_3$ | chair | – | | 1·593 (2) | – | 112·6 (2) | 123·2 (1) | Krebs & Pohl (1973) |
| VI | $(NSOF)_2NSOC_6H_5$ | deformed-chair | eq | 1·410 (20) | 1·52–1·63 | 108·2 (4) | 113·9 (4) | 119·5 (2) | Arrington, Moeller & Paul (1970) |
| VII | $(NSOCl)_2NPCl_2$ | deformed-chair | eq | 1·421 (13) | 1·540 (10) 1·578 (10) | 106·0 (4) 104·4 (3)* | 115·0 (7) | 120·3 (8) | van de Grampel & Vos (1969) |
| VIII | $(NS)_3P(C_6H_5)_3$ | half-chair | – | | 1·56–1·68 | – | – | – | Holt & Holt (1970) |
| IX | $\gamma(SO_3)_3$ | chair | ax eq | 1·371 (13) 1·430 (13) | – | 126·1 (7) | – | – | McDonald & Cruickshank (1967) |
| X | $(PNF_2)_3$ | planar | – | | – | 99·2 (5)* | | | Dougill (1963) |
| XI | $(PNCl_2)_3$ | planar | – | | – | 102·0 (3)* | | | Wilson & Carroll (1960) |

\* $\angle$X–P–X

Table 2(*a*). *Atomic coordinates, as fractions* $\times 10^5$, *and thermal parameters in* $Å^2 \times 10^{-4}$ *and their estimated standard deviations*

| | $x$ | $y$ | $z$ | $u_{11}$ | $u_{22}$ | $u_{33}$ | $u_{12}$ | $u_{13}$ | $u_{23}$ |
|---|---|---|---|---|---|---|---|---|---|
| S(1) | 22126 (8) | 11652 (5) | 9378 (5) | 375 (3) | 290 (3) | 281 (3) | –3 (2) | 12 (2) | 48 (2) |
| S(2) | 264 (11) | 25000 | –5589 (8) | 286 (4) | 433 (5) | 408 (5) | 0 | –92 (4) | 0 |
| O(1) | 9874 (23) | 11653 (16) | 18063 (14) | 570 (12) | 505 (10) | 335 (9) | –84 (8) | 131 (8) | 94 (7) |
| O(2) | 33925 (24) | 1941 (15) | 8516 (16) | 581 (11) | 390 (9) | 522 (11) | 131 (8) | –52 (9) | 62 (7) |
| O(3) | –3874 (37) | 25000 | –17471 (24) | 683 (20) | 618 (16) | 522 (17) | 0 | –361 (15) | 0 |
| O(4) | –11947 (29) | 25000 | 3169 (26) | 230 (12) | 719 (18) | 755 (21) | 0 | 91 (13) | 0 |
| N(1) | 12577 (23) | 12589 (16) | –3485 (15) | 355 (10) | 319 (9) | 277 (10) | –10 (7) | 3 (8) | –36 (6) |
| N(2) | 32776 (33) | 25000 | 10339 (22) | 298 (14) | 315 (12) | 332 (14) | 0 | –40 (11) | 0 |
| C(1) | 21869 (43) | 7582 (32) | –13615 (25) | 569 (18) | 575 (17) | 332 (14) | 8 (14) | 78 (13) | –93 (12) |
| C(2) | 50389 (46) | 25000 | 6079 (43) | 255 (18) | 559 (22) | 555 (25) | 0 | 7 (17) | 0 |

Table 2(*b*). *Atomic coordinates of hydrogen atoms, as fractions* $\times 10^3$, *and isotropic temperature factor coefficients, and their estimated standard deviations*

| | $x$ | $y$ | $z$ | $B$ | | $x$ | $y$ | $z$ | $B$ |
|---|---|---|---|---|---|---|---|---|---|
| H(11) | 139 (4) | 85 (3) | –201 (3) | 7·7 (0·9) | H(21) | 506 (5) | 250 | –26 (4) | 5·4 (1·0) |
| H(12) | 244 (4) | 1 (3) | –122 (3) | 5·4 (0·8) | H(22) | 557 (4) | 194 (4) | 85 (3) | 9·9 (0·9) |
| H(13) | 318 (4) | 133 (3) | –147 (3) | 6·7 (0·8) | | | | | |

Table 3. *Observed and calculated structure factors* ( × 10)

| K | L | FOBS | FCALC |
|---|---|---|---|
| * | H= | 0 | * |
| 0 | 2 | 1847 | 1836 |
| 0 | 4 | 1407 | -1429 |
| 0 | 6 | 791 | -844 |
| 0 | 8 | 648 | -668 |
| 0 | 10 | 294 | 291 |
| 0 | 12 | 200 | 213 |
| 0 | 14 | 253 | -247 |
| 1 | 3 | 670 | -666 |
| 1 | 5 | 180 | 186 |
| 1 | 7 | 802 | 799 |
| 1 | 9 | 598 | 626 |
| 1 | 11 | 195 | -195 |
| 1 | 13 | 426 | -431 |
| 2 | 2 | 611 | -671 |
| 2 | 4 | 607 | -616 |
| 2 | 6 | 184 | -179 |
| 2 | 8 | 355 | 363 |
| 2 | 10 | 268 | 276 |
| 2 | 12 | 151 | 153 |
| 2 | 14 | 63 | 70 |
| 3 | 3 | 515 | -548 |
| 3 | 5 | 94 | -85 |
| 3 | 7 | 120 | 123 |
| 3 | 9 | 809 | 849 |
| 3 | 11 | 184 | 205 |
| 3 | 13 | 285 | -281 |
| 4 | 2 | 459 | 477 |
| 4 | 4 | 330 | 360 |
| 4 | 6 | 93 | -90 |
| 4 | 8 | 201 | -206 |
| 4 | 10 | 431 | -496 |
| 4 | 12 | 188 | -197 |
| 4 | 14 | 205 | 213 |
| 5 | 3 | 76 | 68 |
| 5 | 5 | 241 | -267 |
| 5 | 9 | 250 | -250 |
| 5 | 11 | 81 | -96 |
| 6 | 2 | 323 | -322 |
| 6 | 4 | 222 | 201 |
| 6 | 6 | 59 | 41 |
| 6 | 8 | 196 | 202 |
| 6 | 10 | 118 | 106 |
| 7 | 3 | 241 | 253 |
| 7 | 5 | 219 | -231 |
| 7 | 7 | 478 | -499 |
| 7 | 9 | 405 | -411 |
| 7 | 11 | 129 | 130 |
| 7 | 13 | 314 | 322 |
| 8 | 2 | 598 | 640 |
| 8 | 4 | 278 | -283 |
| 8 | 6 | 490 | -494 |
| 8 | 8 | 374 | -369 |
| 8 | 10 | 220 | 222 |
| 8 | 12 | 136 | 140 |
| 9 | 3 | 212 | -197 |
| 9 | 5 | 197 | 209 |
| 9 | 7 | 387 | 395 |
| 9 | 9 | 152 | 160 |
| 9 | 11 | 104 | -107 |
| 10 | 2 | 39 | -105 |
| 10 | 4 | 156 | -170 |
| 10 | 6 | 89 | -84 |
| 10 | 8 | 46 | 50 |
| 10 | 10 | 157 | 175 |
| 11 | 3 | 471 | -484 |
| 11 | 5 | 50 | -54 |
| 11 | 7 | 205 | 194 |
| 11 | 9 | 305 | 308 |
| 12 | 4 | 99 | 103 |
| 12 | 6 | 95 | 99 |
| 12 | 8 | 52 | -45 |
| * | H= | 1 | * |
| 0 | 2 | 1493 | -1485 |
| 0 | 3 | 243 | -211 |
| 0 | 4 | 684 | -671 |
| 0 | 5 | 846 | 813 |
| 0 | 6 | 448 | 443 |
| 0 | 7 | 89 | -87 |
| 0 | 8 | 1184 | 1184 |
| 0 | 9 | 479 | -473 |
| 0 | 10 | 584 | 605 |
| 0 | 11 | 70 | -53 |
| 0 | 12 | 441 | -428 |
| 0 | 13 | 158 | -146 |
| 0 | 14 | 352 | -343 |
| 1 | 2 | 759 | 758 |
| 1 | 3 | 641 | 631 |
| 1 | 4 | 835 | 825 |
| 1 | 5 | 766 | 768 |
| 1 | 6 | 426 | 405 |
| 1 | 7 | 299 | 290 |
| 1 | 8 | 186 | 181 |
| 1 | 9 | 252 | -252 |
| 1 | 11 | 310 | -317 |
| 1 | 12 | 203 | -199 |
| 1 | 13 | 51 | 34 |
| 1 | 14 | 135 | -128 |
| 2 | 2 | 133 | -120 |
| 2 | 3 | 236 | -232 |
| 2 | 4 | 586 | -565 |
| 2 | 5 | 83 | -68 |
| 2 | 6 | 315 | -300 |
| 2 | 7 | 286 | 291 |
| 2 | 8 | 151 | 155 |
| 2 | 9 | 310 | 311 |
| 2 | 10 | 171 | 176 |
| 2 | 11 | 87 | 76 |
| 2 | 12 | 44 | -26 |
| 2 | 14 | 87 | -79 |
| 3 | 2 | 960 | -950 |
| 3 | 3 | 420 | 420 |
| 3 | 4 | 58 | 56 |
| 3 | 5 | 402 | 414 |
| 3 | 6 | 227 | -247 |
| 3 | 7 | 174 | 178 |
| 3 | 8 | 53 | 56 |
| 3 | 9 | 94 | -92 |
| 3 | 10 | 357 | 371 |
| 3 | 11 | 267 | -268 |
| 3 | 12 | 37 | 45 |
| 3 | 14 | 74 | 69 |
| 4 | 2 | 416 | 447 |
| 4 | 3 | 339 | 298 |
| 4 | 4 | 48 | 63 |
| 4 | 5 | 145 | 139 |
| 4 | 6 | 183 | -171 |
| 4 | 7 | 27 | 23 |
| 4 | 8 | 508 | -519 |
| 4 | 9 | 194 | -193 |
| 4 | 10 | 244 | -254 |
| 4 | 11 | 237 | -240 |
| 4 | 12 | 257 | 258 |
| 4 | 14 | 183 | 163 |
| 5 | 2 | 831 | 810 |
| 5 | 3 | 171 | 157 |
| 5 | 4 | 142 | 148 |
| 5 | 5 | 123 | 120 |
| 5 | 6 | 136 | 142 |
| 5 | 7 | 133 | -124 |
| 5 | 8 | 112 | -116 |
| 5 | 10 | 267 | -269 |
| 5 | 11 | 153 | 151 |
| 5 | 12 | 56 | -63 |
| 5 | 13 | 51 | -58 |
| 5 | 14 | 70 | -67 |
| 6 | 2 | 77 | 54 |
| 6 | 3 | 23 | 19 |
| 6 | 4 | 38 | 5 |
| 6 | 5 | 58 | -40 |
| 6 | 6 | 33 | -38 |
| 6 | 7 | 170 | 152 |
| 6 | 8 | 177 | -181 |
| 6 | 9 | 243 | 247 |
| 6 | 10 | 117 | -120 |
| 6 | 12 | 125 | 128 |
| 6 | 14 | 91 | 85 |
| 7 | 2 | 50 | -53 |
| 7 | 3 | 232 | -235 |
| 7 | 4 | 286 | -292 |
| 7 | 5 | 404 | -414 |
| 7 | 6 | 247 | -255 |
| 7 | 7 | 210 | -215 |
| 7 | 8 | 186 | -186 |
| 7 | 9 | 170 | 172 |
| 7 | 10 | 58 | -56 |
| 7 | 11 | 291 | 292 |
| 7 | 12 | 140 | 135 |
| 7 | 14 | 107 | 105 |
| 8 | 2 | 775 | -771 |
| 8 | 3 | 54 | 46 |
| 8 | 4 | 238 | -234 |
| 8 | 5 | 160 | 165 |
| 8 | 6 | 358 | 365 |
| 8 | 7 | 129 | -124 |
| 8 | 8 | 519 | 518 |
| 8 | 9 | 200 | -202 |
| 8 | 10 | 185 | 185 |
| 8 | 12 | 191 | -187 |
| 8 | 13 | 86 | -83 |
| 9 | 2 | 256 | 273 |
| 9 | 4 | 325 | 324 |
| 9 | 5 | 233 | 241 |
| 9 | 6 | 201 | 197 |
| 9 | 7 | 180 | 181 |
| 9 | 8 | 62 | 58 |
| 9 | 9 | 120 | -116 |
| 9 | 10 | 59 | -56 |
| 9 | 11 | 143 | -140 |
| 9 | 12 | 68 | -66 |
| 10 | 2 | 212 | -224 |
| 10 | 3 | 113 | -116 |
| 10 | 4 | 190 | -189 |
| 10 | 5 | 27 | -37 |
| 10 | 7 | 71 | 74 |
| 10 | 8 | 143 | 141 |
| 10 | 9 | 103 | 105 |
| 10 | 10 | 115 | 114 |
| 10 | 11 | 88 | 91 |
| 11 | 2 | 197 | -212 |
| 11 | 4 | 51 | -44 |
| 11 | 5 | 267 | 268 |
| 11 | 6 | 56 | -57 |
| 11 | 7 | 241 | 229 |
| 11 | 9 | 67 | -71 |
| 11 | 10 | 96 | 100 |
| 12 | 2 | 226 | 236 |
| 12 | 3 | 37 | 37 |
| 12 | 4 | 71 | 71 |
| 12 | 6 | 131 | -137 |
| 12 | 8 | 187 | -189 |
| 12 | 9 | 59 | -63 |
| * | H= | 2 | * |
| 0 | 0 | 759 | -774 |
| 0 | 1 | 201 | -187 |
| 0 | 2 | 137 | -133 |
| 0 | 3 | 957 | 922 |
| 0 | 4 | 1272 | 1255 |
| 0 | 5 | 855 | 832 |
| 0 | 6 | 835 | 814 |
| 0 | 8 | 636 | -646 |
| 0 | 9 | 379 | 398 |
| 0 | 10 | 692 | -689 |
| 0 | 11 | 77 | 99 |
| 0 | 12 | 258 | -260 |
| 0 | 13 | 145 | -137 |
| 0 | 14 | 74 | 56 |
| 1 | 0 | 511 | -502 |
| 1 | 1 | 642 | 655 |
| 1 | 2 | 118 | 109 |
| 1 | 3 | 1036 | 1031 |
| 1 | 5 | 478 | 463 |
| 1 | 6 | 53 | -32 |
| 1 | 7 | 226 | -218 |
| 1 | 8 | 187 | 187 |
| 1 | 9 | 378 | -388 |
| 1 | 10 | 49 | -49 |
| 1 | 13 | 156 | 161 |
| 1 | 14 | 59 | 61 |
| 2 | 0 | 1635 | -1682 |
| 2 | 1 | 234 | 233 |
| 2 | 2 | 610 | -614 |
| 2 | 3 | 134 | 135 |
| 2 | 4 | 228 | 193 |
| 2 | 5 | 123 | -98 |
| 2 | 6 | 263 | 265 |
| 2 | 7 | 83 | -93 |
| 2 | 8 | 394 | 404 |
| 2 | 9 | 89 | -91 |
| 2 | 10 | 214 | 213 |
| 2 | 11 | 84 | -91 |
| 2 | 14 | 72 | -53 |
| 3 | 0 | 1606 | -1579 |
| 3 | 1 | 310 | -278 |
| 3 | 2 | 245 | -224 |
| 3 | 3 | 334 | 340 |
| 3 | 4 | 91 | 89 |
| 3 | 5 | 239 | 215 |
| 3 | 6 | 249 | -244 |
| 3 | 7 | 673 | -679 |
| 3 | 8 | 113 | 102 |
| 3 | 9 | 409 | -421 |
| 3 | 10 | 90 | -79 |
| 3 | 11 | 137 | 138 |
| 3 | 13 | 333 | 332 |
| 3 | 14 | 161 | 163 |
| 4 | 0 | 1392 | 1396 |
| 4 | 1 | 753 | 724 |
| 4 | 2 | 642 | 655 |
| 4 | 3 | 582 | 570 |
| 4 | 4 | 367 | -365 |
| 4 | 5 | 63 | -58 |
| 4 | 6 | 614 | -617 |
| 4 | 7 | 308 | -316 |
| 4 | 8 | 266 | -269 |
| 4 | 9 | 495 | -507 |
| 4 | 10 | 109 | 106 |
| 4 | 12 | 114 | 117 |
| 4 | 13 | 179 | 176 |
| 5 | 0 | 1165 | 1095 |
| 5 | 1 | 88 | 67 |
| 5 | 2 | 438 | 402 |
| 5 | 3 | 104 | -94 |
| 5 | 4 | 60 | -57 |
| 5 | 5 | 195 | 194 |
| 5 | 6 | 96 | -92 |
| 5 | 7 | 461 | 455 |
| 5 | 8 | 121 | -123 |
| 5 | 9 | 49 | 40 |
| 5 | 10 | 124 | 128 |
| 5 | 11 | 135 | -137 |
| 5 | 13 | 128 | -125 |
| 5 | 14 | 149 | -147 |
| 6 | 0 | 294 | -287 |
| 6 | 1 | 123 | 121 |
| 6 | 2 | 233 | -227 |
| 6 | 3 | 86 | 69 |
| 6 | 4 | 271 | -270 |
| 6 | 5 | 49 | -7 |
| 6 | 6 | 42 | -11 |
| 6 | 7 | 29 | 14 |
| 6 | 8 | 358 | 353 |
| 6 | 9 | 155 | -159 |
| 6 | 10 | 231 | 231 |
| 6 | 11 | 87 | -89 |
| 6 | 12 | 70 | 66 |
| 6 | 13 | 58 | 60 |
| 7 | 0 | 544 | 542 |
| 7 | 1 | 388 | -410 |
| 7 | 2 | 83 | 84 |
| 7 | 3 | 696 | -712 |
| 7 | 4 | 151 | -142 |
| 7 | 5 | 293 | -295 |
| 7 | 6 | 138 | -132 |
| 7 | 7 | 243 | 249 |
| 7 | 8 | 159 | -163 |
| 7 | 9 | 300 | 305 |
| 7 | 10 | 109 | 102 |
| 7 | 12 | 98 | 94 |
| 7 | 13 | 147 | -142 |
| 8 | 0 | 128 | -119 |
| 8 | 1 | 158 | -160 |
| 8 | 2 | 77 | -73 |
| 8 | 3 | 140 | 141 |
| 8 | 4 | 350 | 361 |
| 8 | 5 | 284 | 288 |
| 8 | 6 | 406 | 411 |
| 8 | 7 | 96 | 95 |
| 8 | 8 | 199 | -206 |
| 8 | 9 | 164 | 183 |
| 8 | 10 | 438 | -432 |
| 8 | 12 | 200 | -196 |
| 8 | 13 | 60 | -51 |
| 9 | 0 | 95 | 100 |
| 9 | 1 | 274 | 279 |
| 9 | 3 | 397 | 391 |
| 9 | 4 | 131 | -134 |
| 9 | 5 | 85 | 78 |
| 9 | 6 | 61 | -58 |
| 9 | 7 | 80 | -79 |
| 9 | 8 | 38 | 37 |
| 9 | 9 | 40 | -41 |
| 9 | 12 | 50 | 62 |
| 10 | 0 | 457 | -470 |
| 10 | 1 | 91 | -98 |
| 10 | 2 | 237 | -240 |
| 10 | 3 | 110 | -117 |
| 10 | 4 | 83 | 86 |
| 10 | 6 | 243 | 239 |
| 10 | 7 | 33 | 33 |
| 10 | 8 | 193 | 189 |
| 10 | 9 | 56 | 54 |
| 11 | 0 | 231 | -246 |
| 11 | 1 | 147 | 146 |
| 11 | 2 | 51 | -52 |
| 11 | 3 | 284 | 281 |
| 11 | 7 | 313 | -320 |
| 11 | 8 | 39 | 29 |
| 11 | 9 | 171 | -166 |
| 11 | 10 | 72 | -65 |
| 12 | 0 | 286 | 321 |
| 12 | 1 | 104 | 104 |
| 12 | 2 | 181 | 181 |
| 12 | 3 | 83 | 76 |
| 12 | 4 | 98 | -101 |
| 12 | 5 | 57 | -56 |
| 12 | 6 | 234 | -224 |
| 12 | 7 | 117 | -113 |
| 12 | 8 | 82 | -75 |
| 12 | 9 | 128 | -122 |
| * | H= | 3 | * |
| 0 | 1 | 125 | -116 |
| 0 | 2 | 280 | 285 |
| 0 | 3 | 104 | -93 |
| 0 | 4 | 1450 | 1432 |
| 0 | 5 | 233 | -204 |
| 0 | 6 | 50 | 42 |
| 0 | 7 | 245 | -250 |
| 0 | 8 | 539 | -541 |
| 0 | 9 | 240 | -241 |
| 0 | 10 | 38 | 43 |
| 0 | 11 | 106 | -96 |
| 0 | 12 | 219 | 221 |
| 0 | 14 | 233 | 232 |
| 1 | 1 | 580 | 581 |
| 1 | 2 | 649 | 654 |
| 1 | 3 | 85 | -68 |
| 1 | 4 | 422 | 409 |
| 1 | 5 | 625 | -633 |
| 1 | 6 | 435 | 435 |
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| 1 | 8 | 57 | -63 |
| 1 | 9 | 251 | 248 |
| 1 | 10 | 274 | -276 |
| 1 | 11 | 165 | 161 |
| 1 | 12 | 64 | -60 |
| 1 | 13 | 78 | 78 |
| 1 | 14 | 54 | -46 |
| 2 | 1 | 101 | -122 |
| 2 | 2 | 183 | -178 |
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| 2 | 5 | 84 | -80 |
| 2 | 7 | 30 | 29 |
| 2 | 8 | 71 | -62 |
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| 2 | 10 | 88 | -84 |
| 2 | 11 | 110 | 101 |
| 2 | 12 | 53 | 44 |
| 2 | 13 | 75 | 73 |
| 2 | 14 | 64 | 54 |
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| 3 | 9 | 358 | 369 |
| 3 | 10 | 54 | -51 |
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| 3 | 12 | 276 | 269 |
| 3 | 13 | 125 | 128 |
| 3 | 14 | 197 | 186 |
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| 4 | 6 | 210 | 213 |
| 4 | 7 | 502 | -497 |
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| 4 | 9 | 54 | -49 |
| 4 | 11 | 171 | 175 |
| 4 | 12 | 186 | -181 |
| 4 | 13 | 59 | -51 |
| 4 | 14 | 215 | -210 |
| 5 | 1 | 116 | 115 |
| 5 | 2 | 108 | -102 |
| 5 | 3 | 28 | -28 |
| 5 | 4 | 203 | 208 |
| 5 | 5 | 478 | 481 |
| 5 | 6 | 603 | 617 |
| 5 | 7 | 220 | 216 |
| 5 | 8 | 427 | 430 |
| 5 | 9 | 201 | -202 |
| 5 | 11 | 190 | -182 |
| 5 | 12 | 188 | -176 |
| 5 | 13 | 87 | -91 |
| 5 | 14 | 144 | -141 |
| 6 | 1 | 42 | 49 |
| 6 | 3 | 71 | -69 |
| 6 | 4 | 326 | -337 |
| 6 | 5 | 101 | -99 |
| 6 | 6 | 78 | -74 |
| 6 | 7 | 55 | 60 |
| 6 | 8 | 201 | 210 |
| 6 | 9 | 121 | 123 |
| 6 | 10 | 55 | 54 |
| 6 | 11 | 112 | 109 |
| 6 | 12 | 44 | -54 |
| 6 | 13 | 94 | 88 |
| 6 | 14 | 76 | -60 |
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| 7 | 4 | 437 | -428 |
| 7 | 5 | 503 | 518 |
| 7 | 6 | 187 | -180 |
| 7 | 7 | 185 | 182 |
| 7 | 8 | 186 | 193 |
| 7 | 9 | 197 | -206 |
| 7 | 10 | 241 | 240 |
| 7 | 11 | 189 | -193 |
| 7 | 13 | 92 | -88 |
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| 8 | 3 | 41 | -51 |
| 8 | 4 | 529 | 535 |
| 8 | 6 | 139 | -140 |
| 8 | 8 | 246 | -254 |
| 8 | 9 | 146 | -147 |
| 8 | 10 | 73 | 66 |
| 8 | 11 | 122 | -118 |
| 8 | 12 | 104 | 106 |
| 9 | 2 | 119 | 103 |
| 9 | 4 | 76 | 59 |
| 9 | 5 | 98 | -101 |
| 9 | 6 | 116 | 116 |
| 9 | 8 | 65 | 68 |
| 9 | 9 | 76 | 81 |
| 9 | 11 | 85 | 84 |
| 9 | 12 | 76 | -80 |
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| 10 | 2 | 126 | 129 |
| 10 | 3 | 24 | 36 |
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| 10 | 6 | 69 | -63 |
| 10 | 7 | 107 | 112 |
| 10 | 8 | 153 | -156 |
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| 10 | 10 | 46 | -46 |
| 10 | 11 | 52 | -47 |
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| 11 | 4 | 114 | -106 |
| 11 | 5 | 315 | -313 |
| 11 | 6 | 230 | -227 |
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| 11 | 9 | 138 | 140 |
| 12 | 1 | 272 | 271 |
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| 12 | 3 | 43 | 36 |
| 12 | 4 | 160 | -160 |
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| 12 | 7 | 145 | -129 |
| 12 | 8 | 88 | 85 |
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| 0 | 2 | 201 | 198 |
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| 0 | 9 | 182 | -196 |
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| 0 | 12 | 103 | 102 |
| 0 | 13 | 97 | 90 |
| 0 | 14 | 85 | 81 |
| 1 | 0 | 208 | 211 |
| 1 | 1 | 250 | 232 |
| 1 | 2 | 96 | 98 |
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| 1 | 4 | 133 | -144 |
| 1 | 5 | 38 | 31 |
| 1 | 6 | 123 | -119 |
| 1 | 7 | 459 | 462 |
| 1 | 8 | 40 | 41 |
| 1 | 9 | 82 | 75 |
| 1 | 10 | 67 | 69 |
| 1 | 11 | 121 | -121 |
| 1 | 12 | 72 | 67 |
| 1 | 13 | 211 | -201 |
| 2 | 0 | 515 | -493 |
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| 2 | 2 | 211 | -210 |
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| 2 | 4 | 57 | -49 |
| 2 | 5 | 127 | -111 |
| 2 | 6 | 219 | 224 |
| 2 | 8 | 422 | 430 |
| 2 | 10 | 162 | 165 |
| 2 | 11 | 53 | 51 |
| 2 | 13 | 72 | 71 |
| 3 | 0 | 386 | 377 |
| 3 | 1 | 233 | -244 |
| 3 | 2 | 293 | 304 |
| 3 | 3 | 608 | -600 |
| 3 | 4 | 365 | -357 |
| 3 | 5 | 666 | -676 |
| 3 | 6 | 489 | -493 |
| 3 | 8 | 144 | 153 |
| 3 | 9 | 114 | 105 |
| 3 | 10 | 147 | 204 |
| 3 | 11 | 53 | -51 |
| 3 | 12 | 46 | 51 |
| 3 | 13 | 122 | -119 |
| 4 | 0 | 120 | 122 |
| 4 | 1 | 304 | -358 |
| 4 | 2 | 31 | -32 |
| 4 | 3 | 723 | -714 |
| 4 | 4 | 560 | 565 |
| 4 | 5 | 149 | -145 |
| 4 | 6 | 462 | 475 |
| 4 | 7 | 448 | 461 |
| 4 | 8 | 406 | -412 |
| 4 | 9 | 274 | 287 |
| 4 | 10 | 443 | -446 |
| 4 | 11 | 67 | -78 |
| 4 | 12 | 259 | -206 |
| 4 | 13 | 199 | -199 |
| 5 | 0 | 203 | -190 |
| 5 | 1 | 397 | 400 |
| 5 | 2 | 257 | -262 |
| 5 | 3 | 787 | 775 |
| 5 | 4 | 188 | 183 |
| 5 | 5 | 436 | 409 |
| 5 | 6 | 423 | 429 |
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| 5 | 10 | 137 | -202 |
| 5 | 11 | 40 | 37 |
| 5 | 12 | 78 | -72 |
| 5 | 13 | 50 | 37 |
| 6 | 0 | 510 | -527 |
| 6 | 1 | 54 | 54 |
| 6 | 2 | 274 | -280 |
| 6 | 3 | 154 | -153 |
| 6 | 4 | 135 | 139 |
| 6 | 5 | 236 | -236 |
| 6 | 6 | 299 | 304 |
| 6 | 7 | 103 | 97 |
| 6 | 8 | 211 | 213 |
| 6 | 9 | 170 | 170 |
| 6 | 10 | 106 | 95 |
| 6 | 11 | 38 | 25 |
| 6 | 13 | 53 | -25 |
| 7 | 0 | 361 | -330 |
| 7 | 1 | 28 | 32 |
| 7 | 2 | 183 | -164 |
| 7 | 3 | 333 | 320 |
| 7 | 4 | 238 | 187 |
| 7 | 5 | 49 | 45 |
| 7 | 6 | 275 | 257 |
| 7 | 7 | 408 | -402 |
| 7 | 9 | 141 | -142 |
| 7 | 10 | 136 | -135 |
| 7 | 11 | 84 | 89 |
| 7 | 12 | 107 | -104 |
| 7 | 13 | 131 | 176 |
| 8 | 0 | 246 | 258 |
| 8 | 1 | 44 | 29 |
| 8 | 2 | 160 | 162 |
| 8 | 3 | 215 | 210 |
| 8 | 4 | 223 | -231 |
| 8 | 5 | 62 | 67 |
| 8 | 6 | 390 | -393 |
| 8 | 7 | 213 | -213 |
| 8 | 8 | 103 | -105 |
| 8 | 9 | 75 | -64 |
| 8 | 10 | 92 | 94 |
| 8 | 11 | 40 | 31 |
| 8 | 12 | 137 | 115 |
| 9 | 0 | 84 | -92 |
| 9 | 1 | 38 | 38 |
| 9 | 3 | 48 | 47 |
| 9 | 4 | 54 | 48 |
| 9 | 5 | 145 | 138 |
| 9 | 6 | 32 | 26 |
| 9 | 7 | 105 | 95 |
| 9 | 9 | 82 | -86 |
| 9 | 11 | 74 | -77 |
| 10 | 0 | 54 | -38 |
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| 10 | 3 | 105 | 110 |
| 10 | 4 | 98 | -103 |
| 10 | 6 | 77 | -82 |
| 10 | 7 | 93 | -92 |
| 10 | 8 | 128 | 123 |
| 10 | 9 | 66 | -65 |
| 10 | 10 | 133 | 134 |
| 11 | 0 | 131 | 127 |
| 11 | 1 | 150 | -152 |
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| 11 | 3 | 344 | -338 |
| 11 | 4 | 90 | -100 |
| 11 | 5 | 162 | -160 |
| 11 | 6 | 202 | -203 |
| 11 | 7 | 76 | 78 |
| 12 | 0 | 51 | 59 |
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| 12 | 3 | 195 | -186 |
| 12 | 4 | 159 | 149 |
| 12 | 6 | 174 | 112 |
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| 0 | 7 | 279 | -277 |
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| 0 | 12 | 186 | -179 |
| 0 | 13 | 103 | 112 |
| 0 | 14 | 137 | -145 |
| 1 | 1 | 81 | -91 |
| 1 | 2 | 265 | 256 |
| 1 | 5 | 259 | 255 |
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| 1 | 8 | 283 | 302 |
| 1 | 9 | 100 | -112 |
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| 1 | 12 | 174 | -167 |
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| 2 | 3 | 63 | -63 |
| 2 | 5 | 66 | -57 |
| 2 | 6 | 54 | 54 |
| 2 | 7 | 210 | 208 |
| 2 | 8 | 93 | 97 |
| 2 | 9 | 193 | 195 |
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| 3 | 6 | 286 | -296 |
| 3 | 8 | 216 | 227 |
| 3 | 9 | 134 | -128 |
| 3 | 10 | 93 | 82 |
| 3 | 11 | 164 | -167 |
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| 3 | 14 | 63 | -48 |
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| 4 | 3 | 88 | 83 |
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| 4 | 5 | 645 | 658 |
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| 4 | 11 | 264 | -265 |
| 4 | 12 | 137 | 132 |
| 4 | 13 | 134 | -134 |
| 5 | 1 | 157 | 148 |
| 5 | 2 | 598 | 598 |
| 5 | 3 | 230 | -232 |
| 5 | 4 | 622 | 622 |
| 5 | 5 | 246 | -250 |
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| 5 | 8 | 43 | -36 |
| 5 | 9 | 85 | 82 |
| 5 | 11 | 196 | 193 |
| 5 | 13 | 49 | 27 |
| 6 | 1 | 288 | -271 |
| 6 | 2 | 101 | 109 |
| 6 | 3 | 33 | -18 |
| 6 | 4 | 93 | 90 |
| 6 | 5 | 182 | 172 |
| 6 | 6 | 78 | 58 |
| 6 | 7 | 174 | 175 |
| 6 | 8 | 35 | -33 |
| 6 | 9 | 67 | 80 |
| 6 | 10 | 68 | -71 |
| 6 | 11 | 47 | 34 |
| 7 | 1 | 236 | 237 |
| 7 | 3 | 40 | -29 |
| 7 | 4 | 117 | 108 |
| 7 | 5 | 327 | -322 |
| 7 | 6 | 293 | -287 |
| 7 | 7 | 152 | -158 |
| 7 | 8 | 287 | -281 |
| 7 | 9 | 92 | 90 |
| 7 | 11 | 140 | 145 |
| 7 | 12 | 138 | 133 |
| 8 | 1 | 160 | 150 |
| 8 | 2 | 218 | -226 |
| 8 | 3 | 43 | 45 |
| 8 | 4 | 114 | -100 |
| 8 | 5 | 304 | -294 |
| 8 | 7 | 218 | -213 |
| 8 | 9 | 40 | 48 |
| 8 | 11 | 92 | 98 |
| 9 | 1 | 96 | 96 |
| 9 | 2 | 46 | 59 |
| 9 | 4 | 117 | 109 |
| 9 | 6 | 194 | 179 |
| 9 | 10 | 72 | -72 |
| 10 | 2 | 93 | -92 |
| 10 | 4 | 104 | -108 |
| 10 | 5 | 114 | -115 |
| 10 | 6 | 64 | 65 |
| 10 | 8 | 103 | 118 |
| 10 | 9 | 112 | 113 |
| 11 | 1 | 56 | -61 |
| 11 | 2 | 298 | -298 |
| 11 | 3 | 80 | 80 |
| 11 | 4 | 324 | -323 |
| 11 | 5 | 126 | 129 |
| 11 | 7 | 36 | 38 |
| 11 | 8 | 98 | 106 |
| 12 | 1 | 46 | -35 |
| 12 | 2 | 170 | 163 |
| 12 | 3 | 40 | 54 |
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| 12 | 5 | 201 | 192 |
| 12 | 6 | 41 | -33 |
| * | H= | 6 | * |
| 0 | 0 | 207 | 202 |
| 0 | 1 | 244 | -254 |
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| 0 | 3 | 612 | -627 |
| 0 | 4 | 183 | 162 |
| 0 | 5 | 365 | -376 |
| 0 | 6 | 210 | -221 |
| 0 | 7 | 100 | 95 |
| 0 | 8 | 210 | -208 |
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| 0 | 11 | 91 | -94 |
| 0 | 12 | 108 | -113 |
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| 1 | 0 | 289 | -285 |
| 1 | 1 | 220 | 223 |
| 1 | 2 | 247 | -244 |
| 1 | 3 | 242 | 233 |
| 1 | 4 | 248 | 252 |
| 1 | 5 | 225 | 226 |
| 1 | 6 | 364 | 368 |
| 1 | 7 | 155 | 174 |
| 1 | 8 | 67 | -66 |
| 1 | 9 | 112 | -108 |
| 1 | 10 | 143 | -149 |
| 1 | 11 | 53 | -55 |
| 1 | 12 | 122 | -126 |
| 2 | 0 | 363 | -379 |
| 2 | 1 | 88 | 86 |
| 2 | 2 | 205 | -210 |
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| 2 | 5 | 74 | -71 |
| 2 | 6 | 107 | 105 |
| 2 | 7 | 159 | 163 |
| 2 | 8 | 156 | 159 |
| 2 | 9 | 126 | 126 |
| 2 | 10 | 106 | 106 |
| 2 | 11 | 46 | 31 |
| 2 | 12 | 79 | 81 |
| 3 | 0 | 251 | -251 |
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| 3 | 2 | 49 | 52 |
| 3 | 4 | 473 | 485 |
| 3 | 5 | 232 | -237 |
| 3 | 6 | 281 | 284 |
| 3 | 7 | 210 | -209 |
| 3 | 8 | 106 | -100 |
| 3 | 9 | 150 | -140 |
| 3 | 10 | 187 | -185 |
| 3 | 11 | 76 | 63 |
| 3 | 12 | 156 | -149 |
| 3 | 13 | 196 | 201 |
| 4 | 0 | 892 | 903 |
| 4 | 1 | 129 | 137 |
| 4 | 2 | 311 | 318 |
| 4 | 3 | 498 | 506 |
| 4 | 4 | 249 | -251 |
| 4 | 5 | 206 | 206 |
| 4 | 6 | 348 | -350 |
| 4 | 7 | 315 | -327 |
| 4 | 8 | 251 | -252 |
| 4 | 9 | 159 | -160 |
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| 4 | 11 | 72 | 68 |
| 4 | 12 | 66 | 68 |
| 5 | 0 | 56 | -53 |
| 5 | 1 | 128 | -141 |
| 5 | 2 | 111 | -124 |
| 5 | 3 | 69 | -77 |
| 5 | 4 | 190 | -204 |
| 5 | 5 | 208 | 203 |
| 5 | 6 | 126 | -120 |
| 5 | 7 | 234 | 232 |
| 5 | 9 | 103 | 101 |
| 5 | 10 | 156 | 156 |
| 5 | 11 | 87 | -83 |
| 5 | 12 | 115 | 113 |
| 6 | 0 | 151 | -137 |
| 6 | 2 | 150 | -143 |
| 6 | 3 | 65 | 61 |
| 6 | 4 | 101 | -109 |
| 6 | 5 | 100 | 98 |
| 6 | 6 | 62 | 53 |
| 6 | 8 | 124 | 127 |
| 6 | 9 | 76 | -63 |
| 6 | 10 | 103 | 94 |
| 6 | 12 | 92 | 88 |
| 7 | 0 | 209 | 208 |
| 7 | 1 | 217 | -216 |
| 7 | 2 | 150 | 152 |
| 7 | 3 | 289 | -286 |
| 7 | 4 | 298 | -286 |
| 7 | 5 | 167 | -164 |
| 7 | 6 | 301 | -301 |
| 7 | 7 | 41 | -40 |
| 7 | 9 | 129 | 124 |
| 7 | 10 | 136 | 139 |
| 7 | 11 | 53 | 44 |
| 8 | 0 | 119 | 104 |
| 8 | 1 | 220 | -194 |
| 8 | 2 | 170 | 165 |
| 8 | 3 | 367 | -348 |
| 8 | 4 | 85 | 78 |
| 8 | 5 | 102 | -99 |
| 8 | 6 | 77 | -77 |
| 8 | 7 | 82 | 79 |
| 8 | 8 | 93 | -86 |
| 8 | 10 | 137 | -123 |
| 9 | 0 | 45 | -31 |
| 9 | 1 | 43 | 41 |
| 9 | 2 | 54 | -40 |
| 9 | 3 | 44 | 34 |
| 9 | 4 | 69 | 60 |
| 9 | 5 | 81 | 70 |
| 9 | 6 | 128 | 123 |
| 9 | 7 | 89 | 98 |
| 10 | 0 | 229 | -239 |
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| 10 | 3 | 108 | -114 |
| 10 | 4 | 52 | 52 |
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| 10 | 6 | 94 | 98 |
| 10 | 7 | 126 | 122 |
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| 11 | 2 | 50 | -42 |
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| 11 | 4 | 146 | 157 |
| 11 | 5 | 95 | -94 |
| 11 | 6 | 191 | 183 |
| 12 | 0 | 233 | 218 |
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| 12 | 3 | 208 | 203 |
| 12 | 4 | 61 | -58 |
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| 0 | 8 | 150 | -139 |
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| 1 | 3 | 113 | -118 |
| 1 | 4 | 500 | 510 |
| 1 | 5 | 89 | 93 |
| 1 | 6 | 180 | 185 |
| 1 | 8 | 157 | -157 |
| 1 | 10 | 145 | -138 |
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| 1 | 12 | 61 | 42 |
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| 2 | 3 | 105 | -110 |
| 2 | 4 | 60 | -59 |
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| 2 | 7 | 140 | 137 |
| 2 | 8 | 74 | 77 |
| 2 | 9 | 91 | 94 |
| 2 | 11 | 73 | 57 |
| 2 | 12 | 90 | 71 |
| 3 | 1 | 301 | 303 |
| 3 | 2 | 128 | 137 |
| 3 | 4 | 38 | 37 |
| 3 | 5 | 103 | -95 |
| 3 | 6 | 176 | -184 |
| 3 | 7 | 81 | -70 |
| 3 | 8 | 215 | -218 |
| 3 | 9 | 47 | 42 |
| 3 | 10 | 50 | -42 |
| 3 | 11 | 54 | 53 |
| 3 | 12 | 208 | 212 |
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| 4 | 2 | 290 | -293 |
| 4 | 3 | 67 | -66 |
| 4 | 5 | 288 | -290 |
| 4 | 6 | 56 | 60 |
| 4 | 7 | 201 | -197 |
| 4 | 8 | 141 | 128 |
| 4 | 10 | 87 | 82 |
| 4 | 11 | 132 | 142 |
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| 5 | 2 | 60 | -55 |
| 5 | 3 | 33 | -43 |
| 5 | 4 | 138 | 130 |
| 5 | 5 | 93 | 98 |
| 5 | 6 | 204 | 203 |
| 5 | 7 | 50 | 75 |
| 5 | 8 | 47 | 47 |
| 5 | 9 | 38 | -38 |
| 5 | 10 | 62 | -70 |
| 6 | 1 | 50 | -51 |
| 6 | 3 | 165 | -157 |
| 6 | 5 | 110 | -112 |
| 6 | 7 | 86 | 83 |
| 6 | 8 | 58 | 57 |
| 6 | 9 | 117 | 101 |
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| 7 | 1 | 86 | -92 |
| 7 | 2 | 377 | -373 |
| 7 | 3 | 54 | 77 |
| 7 | 4 | 356 | -350 |
| 7 | 6 | 75 | -78 |
| 7 | 7 | 35 | 21 |
| 7 | 8 | 129 | 126 |
| 7 | 10 | 91 | 85 |
| 8 | 1 | 63 | -50 |
| 8 | 3 | 170 | 167 |
| 8 | 4 | 44 | -57 |
| 8 | 5 | 238 | 237 |
| 8 | 6 | 53 | -51 |
| 8 | 7 | 63 | 68 |
| 8 | 8 | 60 | -84 |
| 8 | 9 | 133 | -147 |
| 9 | 2 | 270 | 256 |
| 9 | 4 | 215 | 203 |
| 9 | 5 | 73 | 80 |
| 9 | 6 | 65 | 67 |
| 10 | 1 | 189 | -170 |
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| 10 | 3 | 34 | -47 |
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| 11 | 1 | 102 | 95 |
| 11 | 2 | 166 | 161 |
| 11 | 4 | 73 | 63 |
| * | H= | 8 | * |
| 0 | 0 | 472 | 462 |
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| 0 | 7 | 255 | -264 |
| 0 | 8 | 195 | -195 |
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| 0 | 10 | 107 | -114 |
| 1 | 0 | 340 | 349 |
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| 1 | 4 | 218 | -223 |
| 1 | 5 | 158 | 162 |
| 1 | 6 | 102 | -98 |
| 1 | 7 | 92 | 75 |
| 1 | 10 | 173 | 167 |
| 2 | 0 | 278 | -293 |
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| 2 | 4 | 125 | -123 |
| 2 | 5 | 56 | 52 |
| 2 | 6 | 63 | 67 |
| 2 | 7 | 55 | 50 |
| 2 | 8 | 163 | 167 |
| 2 | 9 | 45 | -43 |
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| 3 | 0 | 411 | 412 |
| 3 | 1 | 107 | -81 |
| 3 | 2 | 113 | 117 |
| 3 | 3 | 114 | -100 |
| 3 | 4 | 228 | -237 |
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| 3 | 6 | 207 | -213 |
| 3 | 7 | 48 | 47 |
| 3 | 8 | 44 | -39 |
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| 3 | 10 | 96 | 96 |
| 4 | 0 | 81 | 82 |
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| 4 | 3 | 173 | -179 |
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| 4 | 6 | 48 | -48 |
| 4 | 7 | 64 | 62 |
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| 5 | 0 | 109 | -106 |
| 5 | 1 | 44 | 44 |
| 5 | 2 | 64 | -50 |
| 5 | 3 | 81 | 76 |
| 5 | 5 | 60 | 43 |
| 5 | 6 | 109 | 104 |
| 5 | 7 | 59 | -59 |
| 5 | 8 | 54 | 48 |
| 5 | 9 | 76 | -73 |
| 6 | 0 | 244 | -243 |
| 6 | 2 | 176 | -178 |
| 6 | 3 | 77 | -71 |
| 6 | 4 | 75 | -67 |
| 6 | 5 | 46 | -35 |
| 6 | 6 | 76 | 74 |
| 6 | 7 | 76 | 74 |
| 6 | 8 | 131 | 130 |
| 6 | 9 | 76 | 84 |
| 7 | 0 | 247 | -250 |
| 7 | 2 | 45 | -21 |
| 7 | 3 | 100 | -98 |
| 7 | 4 | 163 | 162 |
| 7 | 5 | 123 | -113 |
| 7 | 6 | 90 | 91 |
| 7 | 7 | 56 | -59 |
| 8 | 0 | 232 | 220 |
| 8 | 1 | 195 | 187 |
| 8 | 2 | 173 | 177 |
| 8 | 3 | 269 | 256 |
| 8 | 4 | 93 | 100 |
| 8 | 6 | 50 | -30 |
| 8 | 7 | 164 | -160 |
| 9 | 0 | 104 | 98 |
| 9 | 1 | 40 | 45 |
| 9 | 3 | 63 | 69 |
| 9 | 4 | 51 | -56 |
| 9 | 5 | 78 | 81 |
| 10 | 0 | 101 | -91 |
| 10 | 1 | 54 | 54 |
| 10 | 2 | 110 | -98 |
| 10 | 3 | 79 | 71 |
| * | H= | 9 | * |
| 0 | 1 | 563 | 588 |
| 0 | 4 | 64 | 88 |
| 0 | 5 | 271 | -272 |
| 0 | 7 | 217 | -210 |
| 1 | 2 | 95 | -99 |
| 1 | 4 | 62 | 67 |
| 1 | 5 | 54 | 42 |
| 1 | 6 | 198 | 200 |
| 1 | 8 | 218 | 195 |
| 2 | 1 | 119 | -115 |
| 2 | 2 | 63 | -55 |
| 2 | 3 | 120 | -131 |
| 2 | 4 | 80 | -77 |
| 2 | 7 | 65 | 61 |
| 3 | 1 | 55 | -53 |
| 3 | 2 | 237 | -240 |
| 3 | 3 | 64 | -67 |
| 3 | 4 | 233 | -235 |
| 3 | 5 | 46 | -46 |
| 3 | 6 | 90 | -80 |
| 3 | 8 | 149 | 165 |
| 4 | 1 | 64 | -64 |
| 4 | 3 | 129 | 136 |
| 4 | 5 | 115 | 109 |
| 4 | 6 | 57 | -54 |
| 5 | 2 | 164 | 154 |
| 5 | 4 | 142 | 134 |
| 5 | 5 | 52 | 54 |
| 5 | 6 | 46 | 39 |
| 6 | 1 | 205 | -196 |
| 6 | 4 | 59 | -54 |
| 6 | 5 | 76 | 63 |
| 6 | 7 | 58 | 59 |
| 7 | 2 | 121 | 110 |
| 8 | 1 | 298 | 292 |
| 8 | 3 | 56 | 39 |
| * | H= | 10 | |
| 0 | 0 | 215 | 245 |
| 0 | 1 | 96 | -104 |
| 0 | 2 | 94 | 124 |
| 0 | 3 | 129 | -143 |
| 0 | 4 | 56 | 9 |
| 1 | 0 | 207 | -206 |
| 1 | 2 | 83 | -74 |
| 1 | 3 | 69 | 52 |
| 1 | 4 | 133 | 147 |
| 2 | 0 | 179 | -183 |
| 2 | 2 | 156 | -154 |
| 2 | 3 | 44 | -45 |
| 2 | 4 | 50 | -40 |
| 3 | 0 | 217 | -214 |
| 3 | 1 | 49 | -52 |
| 3 | 2 | 91 | -99 |
| 3 | 3 | 72 | -83 |
| 4 | 0 | 70 | 57 |
| 4 | 1 | 80 | 59 |
| 4 | 2 | 118 | 118 |
| 4 | 3 | 134 | 121 |
| 4 | 4 | 78 | 77 |
| 5 | 0 | 86 | 83 |
| 5 | 1 | 42 | 58 |
| 5 | 2 | 64 | 70 |
| 5 | 3 | 75 | 93 |
| 6 | 0 | 159 | -160 |
| 6 | 2 | 101 | -104 |
| * | H= | 11 | * |
| 1 | 2 | 161 | 160 |
| 2 | 1 | 49 | -54 |

difference between $u_{ij}$ observed and $u_{ij}$ calculated, was 0·0009 Å$^2$. **T**, **L**, and **S**, their standard deviations and **T**′, **L**′, and **S**′, the values transposed to an inertial axial system, are given in Table 6. **S**′ is almost zero. The value of **L** was used to correct the bond lengths and angles for thermal motion. The corrected and uncorrected values of the bond lengths are given in Table 4; for the angles the maximum difference between corrected and uncorrected values was 0·02° and only the corrected values are given (Table 5).

Table 4. *Bond lengths, l, and their estimated standard deviations, and the values, $l_{corr}$, corrected for thermal vibration* (Å)

| | $l$ | $l_{corr}$ |
|---|---|---|
| S(1)—O(1)$_{axial}$ | 1·403 (2) | 1·405 |
| S(1)—O(2)$_{eq}$ | 1·405 (2) | 1·407 |
| S(2)—O(3)$_{eq}$ | 1·410 (3) | 1·412 |
| S(2)—O(4)$_{axial}$ | 1·407 (3) | 1·409 |
| S(1)—N(1) | 1·673 (2) | 1·675 |
| S(1)—N(2) | 1·662 (1) | 1·664 |
| S(2)—N(1) | 1·668 (2) | 1·669 |
| N(1)—C(1) | 1·485 (3) | 1·487 |
| N(2)—C(2) | 1·496 (4) | 1·498 |
| C(1)—H(11) | 0·84 (3) | |
| C(1)—H(12) | 0·99 (5) | |
| C(1)—H(13) | 1·01 (3) | |
| C(2)—H(21) | 0·99 (4) | |
| C(2)—H(22) | 0·79 (4) | |

## Computational details

Least-squares refinement was carried out with the full-matrix program *LINUS* (Coppens & Hamilton, 1970); the quantity minimized was $r=\sum w||F_o|-|F_c||^2/\sum w|F_o|^2$ where $w=1/\sigma^2$ and $\sigma=\sqrt{[\sigma_c(F_o^2)+1{\cdot}02F_o^2]}-|F_o|$.

The scattering factors were those of Doyle & Turner (1968) for sulphur, Cromer & Mann (1968) for oxygen, nitrogen, and carbon, and for hydrogen that of Stewart, Davidson & Simpson (1965) for a spherically symmetric atom. No corrections were made for anomalous dispersion.

Calculations of **T**, **L**, and **S** and the correction of bond lengths and angles for thermal vibration were

made with a modified version of the Schomaker & Trueblood (1968) program. Standard deviations were calculated with *ORFFE* (Busing, Martin & Levy, 1964); the drawing was made with *ORTEP* (Johnson, 1965).

## Discussion

The molecule, which is chair formed and has approximate symmetry $3m$ $(C_{3v})$, lies on a crystallographic mirror plane with atoms S(2), N(2), O(3), O(4), and H(22) in the plane. The packing is shown in Fig. 1. The carbon atoms do not lie in the SNS planes, the carbon-nitrogen bond being bent 28·1° out of the plane. For a trigonally hybridized carbon atom the bond would lie in the plane and for a tetrahedrally hybridized nitrogen atom the angle would be 54·7°. The mean carbon–nitrogen distance is 1·492 (2) Å.

In $(NSOCl)_3$ the $\pi$-electrons are shared between six sulphur–nitrogen bonds and three sulphur–oxygen bonds giving short S–N bonds, 1·571 (4) Å, and short S–O bonds, 1·407 (7) Å. In $(NSO_2)_3^-$ the $\pi$-electrons are shared between six S–N bonds and six S–O bonds resulting in longer S–N bonds, 1·636 (4) Å, and also longer S–O bonds, 1·456 (6) and 1·436 (6) Å. The attachment of methyl groups to the nitrogen atoms in

$(CH_3NSO_2)_3$ reduces the $\pi$-bonding in the ring still further, S–N being 1·669 (1) Å, leaving more electrons available for the S–O bonds which are 1·407 (1) Å. In methyl sulphimide the axial and equatorial S–O bonds are equal within experimental error. The $(SN)_3$ ring in $(NSOCl)_3$ is more nearly planar than those in the other two compounds, the mean deviations of the nitrogen atoms from the plane through the sulphur atoms being $(NSOCl)_3$ 0·253, $(NSO_2)_3^-$ 0·514, and $(CH_3NSO_2)_3$ 0·521 Å.

In the series $(NSOCl)_3$, $(NSO_2)_3^-$, $(CH_3NSO_2)_3$ the angles N–S–N and X–S–Y vary systematically with the S–N $\pi$-bond order (Fig. 2) demonstrating the importance of repulsion between bonding electrons in determining molecular geometry. In Fig. 3 the exocyclic angle X–S–Y for a group of $(NS)_3$ and related compounds is plotted against the mean bond order for S–X and S–Y, showing that the greater the double-bond character the greater the repulsion between the bonds and the greater the angle X–S–Y. The S–N–S angle for $(NSO_2)_3^-$ is smaller than that in $(NSOCl)_3$ or $(CH_3NSO_2)_3$ as there are weak bonds from the nitrogen atom to two silver atoms. The $\pi$-bond orders were obtained from the bond-order bond-length curves of Cruickshank (1961) for sulphur–oxygen and of

Table 5. *Angles and their estimated standard deviations*

Atoms marked with primes are related to atoms at $x,y,z$ by $x,\frac{1}{2}-y,z$. Angles involving hydrogen atoms are not corrected for thermal vibration.

| | | | |
|---|---|---|---|
| O(1)—S(1)—O(2) | 121·50 (11) | O(3)—S(2)—N(1) | 106·31 (10) |
| O(3)—S(2)—O(4) | 122·28 (18) | O(4)—S(2)—N(1) | 107·93 (9) |
| N(1)—S(1)—N(2) | 104·09 (10) | S(1)—N(1)—S(2) | 116·59 (10) |
| N(1)—S(2)—N(1') | 104·81 (13) | S(1)—N(2)—S(1') | 117·55 (16) |
| O(1)—S(1)—N(1) | 108·22 (10) | S(1)—N(1)—C(1) | 116·54 (18) |
| O(1)—S(1)—N(2) | 108·20 (12) | S(2)—N(1)—C(1) | 117·85 (18) |
| O(2)—S(1)—N(1) | 106·82 (10) | S(1)—N(2)—C(2) | 117·63 (10) |
| O(2)—S(1)—N(2) | 106·71 (11) | | |
| | | | |
| N(1)—C(1)—H(11) | 103·4 (2·1) | H(12)-C(1)–H(13) | 111·0 (2·7) |
| N(1)—C(1)–H(12) | 107·9 (2·2) | N(2)—C(2)–H(21) | 110·0 (2·3) |
| N(1)—C(1)–H(13) | 105·8 (1·9) | N(2)—C(2)–H(22) | 113·3 (2·6) |
| H(11)-C(1)–H(12) | 113·4 (3·0) | H(21)-C(2)–H(22) | 110·6 (2·9) |
| H(11)-C(1)–H(13) | 114·4 (2·7) | H(22)-C(2)–H(22') | 98·4 (5·9) |

Table 6. **T, L,** *and* **S** *and their estimated standard deviations*

**T'**, **L'**, and **S'** are referred to molecular axes, the transformation from axes parallel to **a**, **b**, and **c** to the molecular axes is given by **A**; for comparison transformation, **B**, to the principal axes of **L** is also given. T is in $\text{Å} \times 10^4$, L in $(°)^2$, and S in $(°)$ $\text{Å} \times 10^{-4}$.

$$\mathbf{T} = \begin{pmatrix} 89 & 0 & 12 \\ & 53 & 0 \\ & & 20 \end{pmatrix} \quad \sigma(\mathbf{T}) = \begin{pmatrix} 10 & 0 & 9 \\ & 10 & 0 \\ & & 11 \end{pmatrix} \quad \mathbf{T'} = \begin{pmatrix} 53 & 0 & 0 \\ & 67 & 34 \\ & & 42 \end{pmatrix}$$

$$\mathbf{L} = \begin{pmatrix} 2·48 & 0 & 0·70 \\ & 5·15 & 0 \\ & & 3·57 \end{pmatrix} \quad \sigma(\mathbf{L}) = \begin{pmatrix} 0·82 & 0 & 0·64 \\ & 0·86 & 0 \\ & & 0·80 \end{pmatrix} \quad \mathbf{L'} = \begin{pmatrix} 5·15 & 0 & 0 \\ & 3·71 & -0·55 \\ & & 2·34 \end{pmatrix}$$

$$\mathbf{S} = \begin{pmatrix} 0 & 8 & 0 \\ 48 & 0 & 313 \\ 0 & -196 & 0 \end{pmatrix} \quad \sigma(\mathbf{S}) = \begin{pmatrix} 0 & 151 & 0 \\ 153 & 0 & 151 \\ 0 & 153 & 0 \end{pmatrix} \quad \mathbf{S'} = \begin{pmatrix} 0 & 254 & -190 \\ -132 & 0 & 0 \\ 146 & 0 & 0 \end{pmatrix}$$

R.m.s. delta for $U_{ij}$obs. $- U_{ij}$calc. $= 0·0009$ Å².

$$\mathbf{A} = \begin{pmatrix} 0 & 1 & 0 \\ 0·7126 & 0 & 0·7016 \\ 0·7016 & 0 & -0·7126 \end{pmatrix} \quad \mathbf{B} = \begin{pmatrix} 0 & 1 & 0 \\ 0·4381 & 0 & 0·8989 \\ 0·8989 & 0 & -0·4381 \end{pmatrix}$$
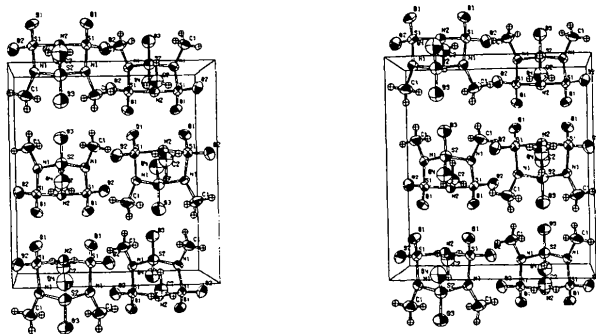
Fig. 1. Stereoscopic view of the unit cell contents; the *b* axis is across and the *c* axis down the page.
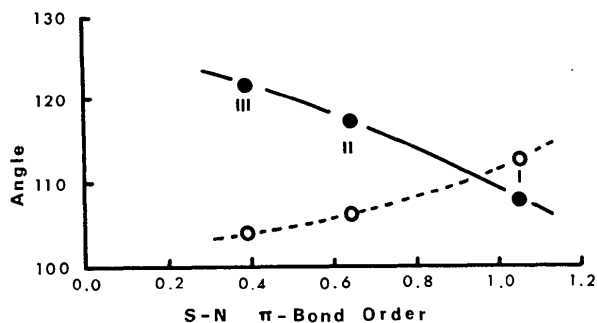


Fig. 2. Angles at sulphur *vs.* the bond order of the sulphur nitrogen bond for $(CH_3NSO_2)_3$, $(NSO_2)_3^{3-}$, and for $(NSOCl)_3$. The open circles denote $\angle$ N–S–N, the full ones $\angle$ X–S–Y. The Roman numerals relate to Table 5.



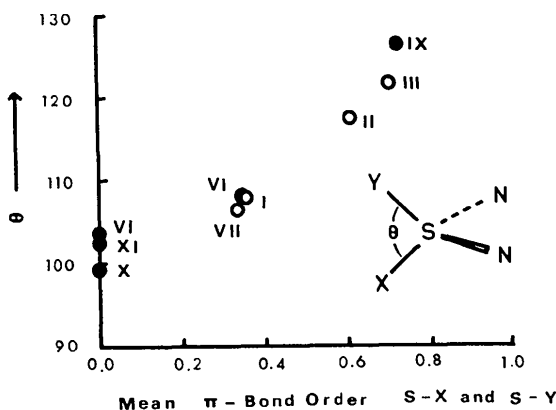Fig. 3. The exocyclic angles $\angle$ X–S–Y plotted against the mean bond orders for S–X and S–Y. The open circles denote $(NS)_3$ compounds, the full circles to related compounds. The Roman numerals relate to Table 5.

Chapman & Waddington (1962) for sulphur–nitrogen.

Although methyl sulphimide and sulphanuric chloride have the same space group and similar cell dimensions $[(CH_3NSO_2)_3: 8·02, 10·65, 11·54$ Å and $(NSOCl)_3: 7·56, 11·54, 10·08$ Å] they are not isostructural.

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