08.1-20 A COMPUTER DETERMINATION OF 2V OF ANTH-
RACENE FROM EXTINCTION DATA. By Maureen M. Julian,
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In biaxial crystals, measurement of the angle between
the two optic axes, 2V, is constant for a given crystal,
at a given temperature, and for a given wavelength. A
study of the optical properties of anthracene was done
because of conflicting results in the literature and
because recently developed techniques (Bloss, 1981) in-
troduce computer and statistical methods into the prac-
tice of optical crystallography permitting greater
accuracy. The work was complicated by the fact that
the anthracene crystal rapidly dissolves in immersion
media. Data were completed on four separate crystals,
three at 540 nm and one at 900 nm. The data were
analyzed by the Bloss-Riess-Roher program "excalibr"
using Joel's equation to find the optic axes and refine-
ment was done by least squares to calculate an accurate
2V.

Bloss, F.D. "The Spindle Stage: Principles and Prac-
tice". CUP, 1981.

actions. S-S bond lengths are 2.067(2) $\overset{o}{A}$. The
geometry of the B_8S_{16} molecule (transannular
S..S distances ca. 4.6 $\overset{o}{A}$) allows the preparation
of transition metal complexes with tetragonal
planar coordination by the tetradentate B_8S_{16}
ligand.
Two different isotypic compounds BS_2 and BSe_2
with the same 1:2 boron-to-chalcogen ratio as
in B_8S_{16} are obtained, if the conditions of pre-
paration are varied slightly. They are monocli-
nic, space group $P2_1/c$, with a = 6.800(2), b =
10.545(3), c = 7.828(2) $\overset{o}{A}$, ß = 117.27(3)$^{\circ}$, Z =
8 BS_2, d_x = 1.995 g.cm^{-3} for BS_2, and a = 7.205
(2), b = 11.202(3), c = 8.123(2)$\overset{o}{A}$, ß =117.62(3)$^{\circ}$,
d_x = 3.858 g.cm^{-3} for BSe_2. The crystal struc-
tures (R = 6.2% and 5.2%) of both show endless
chains along the b axis, consisting of five-
membered B_2S_3 (B_2Se_3) rings as in the porphin-
like isomer, the rings being linked through
B-S-B (B-Se-B) bridges. Rather short interannu-
lar S..S and Se..Se contacts of 3.167(3) and
3.295(3) $\overset{o}{A}$ appear to be essential for the stabi-
lization of the strictly planar chains as a
whole. As in B_8S_{16}, the boron-chalcogen bond
lengths are quite uniform with B-S and B-Se
values of 1.783(9) ...1.824(8) $\overset{o}{A}$ (mean 1.803) and
of 1.90(3) ...1.98(3) $\overset{o}{A}$ (mean 1.93) respectively.
The structural results indicate that, in con-
trast to some ternary phases such as $Pb_4B_4S_{10}$
and $Ag_6B_{10}S_{18}$ and in accordance to investigat-
ions on BS_2, BSe_2 and B_2S_3 glasses, trigonal
planar coordination of boron is prevalent in
binary sulfides and selenides.

08.2-01 STRUCTURES, CRYSTAL CHEMISTRY AND PRO-
PERTIES OF NOVEL BORON SULFIDES AND SELENIDES:
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Only very limited knowledge is available on the
compositions and structural properties of bin-
ary boron sulfides and selenides. B_2S_3, which
was prepared as twinned single crystals from
thermal decomposition of $Ag_6B_{10}S_{18}$, was shown
to form a layer structure containing planar
B_2S_2 and B_3S_3 rings (Krebs, Diercks, Acta Cryst.
A31, S66 (1975); Diercks, Krebs, Angew. Chem.
Int. Ed. Engl. 16, 313 (1977)).
We could now prepare three novel compounds in
this class and determine their crystal struc-
tures from single crystal diffractometer data.
A molecular boron sulfide B_8S_{16} is obtained from
stoichiometric B_2S_3-S_8 mixtures in graphitized
reaction tubes at 300/100°C or from thiolysis
of halogen-substituted trithiadiborolanes
$B_2S_3Hal_2$. It crystallizes in space group $P2_1/c$
with a = 12.091(2), b = 4.063(1), c = 21.870(4)
$\overset{o}{A}$, ß = 107.64(3)$^{\circ}$, Z = 2, d_x = 1.944, d_m = 1.92
(2) g.cm^{-3} (at 20°C) and contains centrosymmetric
exactly planar B_8S_{16} molecules with a porphin-
like structure of four five-membered 1.2.4.3.5-
trithiadiborolane rings linked through S bridges
(R = 5.4% for 20°C data, 4.7% for -130°C data).
The average B-S bond length of 1.807 $\overset{o}{A}$ (indivi-
dual values 1.795(6) ...1.820(6) $\overset{o}{A}$) corresponds
to the 1.808 $\overset{o}{A}$ value in B_2S_3 and indicates, in
accordance to the planarity of the molecule
and to CNDO calculations, strong pπ-pπ inter-

08.2-02 THE CRYSTAL AND MOLECULAR STRUCTURE
OF TETRABORATE OF CALCIUM AND POTASSIUM, DODE-
CAHYDRATE. By X. Solans and M. Font-Altaba.
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$(B_4O_5(OH)_4)_2$ Ca K_2. 12H_2O. Orthorhombic,
$P2_12_12_1$, a = 16.597(3), b = 12.469(3), c =
11.569(2)$\overset{o}{A}$.

Intensity data were recorded on a Philips
PW-1100 four circle diffractometer using MoK
radiation, monochromatized by reflexion from
a graphite crystal. 3175 reflections in the
range 2θ ⩽ 30° were considered as observed
applying the condition I ⩾ 2.5 σ (I).

The structure was solved with the MULTAN 80
system of computer programs and refined by full
matrix least-squares method with the SHELX 76
program.

The Ca^{2+} and K^+ ions have a distorted eight-
coordination. No great differences are obser-
ved in the $B_4O_5(OH)_4$ ions.