80.1-20 A COMPUTER DETERMINATION OF 2V OF ANTHE- 
RACENE FROM EXTINCTION DATA. By Maureen M. Julian, 
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In bidimensional crystals, measurement of the angle between 
the two optic axes, 2V, is constant for a given crystal, at 
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) introduce computer and statistical methods into the practice of optical crystallography permitting greater accuracy. The work was complicated by the fact that the anthracene crystal rapidly dissolves in immersion 
media. Data were collected on four separate crystals, three at 540 m and one at 900 m. The data were 
analyzed by the Bloss-Rüsen-Roher program "excellibr" 
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 Spinide Stage: Principles and Prac-
tice". OGF, 1981.

80.2-01 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 binary 
boron sulfides and selenides. B₂S₃, which 
was prepared as twinned single crystals from 
thermal decomposition of Ag⁺B⁺₁₂O⁺₁₈, was shown 
to form a layer structure containing planar 

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, BS₂₅₁₈, is obtained from 
stoichiometric B₂S₅-S₈ mixtures in graphitized 
reaction tubes at 300/100°C or from thiolysis of 
halogen-substituted trithiaborolanes 
B₂S₅Hal₂. It crystallizes in space group P2₁/c with 
a = 12.091(2), b = 4.063(1), c = 21.87:0(4) 
Å, β = 107.64(3)°, Z = 2, dₓ = 1.995 g.cm⁻³, dᵧ = 1.92 
(2) g.cm⁻³ (at 20°C) and contains centroymmetrically 
exactly planar BS₂₅₁₈ molecules with a porphin-
like structure of four five-membered 1.2.4.3.5-
trithiaborolane 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 Å (individ-
ual values 1.795(6) ... 1.820(6) Å) corresponds to 
the 1.808 Å value in B₂S₃ and indicates, in 
accordance to the planarity of the molecule 
and to CNDO calculations, strong pπ-pπ inter-
actions. S-S bond lengths are 2.067(2) Å. The 
geometry of the B₂S₅ molecule (transannular 
S-S distances ca. 4.6 Å) allows the preparation 
of transition metal complexes with tetragonal 
planar coordination by the tetradequate BS₂₅ ligand.

Two different isotypic compounds BS₂ and BSe₂ 
with the same 1:2 boron-to-chalcogen ratio as 
in B₂S₅ are obtained, if the conditions of pre-
paration are varied slightly. They are monoco-
nial, space group P2₁/c, with a = 6.800(2), b = 
10.545(3), c = 7.828(2) Å, β = 117.27(3)°, Z = 
8 B₂S₂, dₓ = 1.995 g.cm⁻³ for BS₂, and a = 7.205 
(2), b = 11.202(3), c = 8.123(2) Å, β = 117.62(3)°, 
 dryer = 3.858 g.cm⁻³ for BSe₂. The crystal struct-
ures (R = 6.2% and 5.2%) of both show less 
chains along the b axis, consisting of five-
membered B₂S₃ (B₂Se₃) 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) Å appear to be essential for the stabi-
ization of the strictly planar chains as a whole. As in B₂S₅, the boron-chalcogen bond 
lengths are quite uniform with 
B-S (mean 1.803) Å and 
B-Se (mean 1.93) Å respectively. 
The structural results indicate that, in con-
trast to some ternary phases such as Pb₂B₂Se₃ 
and Ag₂B₂S₅ and in accordance to investiga-
tions on BS₂, BSe₂ and B₂S₃ glasses, trigonal 
planar coordination of boron is prevalent in 
binary sulfides and selenides.

80.2-02 THE CRYSTAL AND MOLECULAR STRUCTURE 
OF TETRABORATE OF CALCIUM AND POTASSIUM, DOB-
CAHYDRATE. By X. Solans and M. Font-Altaba. 
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Spain, and J. Solans, Dept. Crystallography 
and Mineralogy, University of Oviedo, Afias 
de Velasco s/n, Oviedo, Spain.

[B₂O₅(OH)]₄⁻ Ca K₂. 12H₂O. Orthorhombic, 
P₂₁₂₁₂₁; a = 16.597(3), b = 12.469(3), c = 
11.569(2) Å. 

Intensity data were recorded on a Philips 
PW-1100 four circle diffractometer using MoKα 
radiation, monochromatized by reflection 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 SHELXL 76 
program.

The Ca²⁺ and K⁺ ions have a distorted eight-
coordination. No great differences are observed 
in the B₂O₅(OH)₄ ions.