

substance: boron compounds with group VI elements
property: properties of boron-selenium compounds

B₁₃Se

Structure formula B₁₂Se_{2-x} B_x

α-rhombohedral boron structure group

Space group: R $\bar{3}$ m

lattice parameters

| | | | | |
|------------|-------------|------------------|-------------------|-----|
| <i>a</i> | 5.9041(4) Å | <i>T</i> = 300 K | X-ray diffraction | 93B |
| <i>c</i> | 11.947(1) Å | | | |
| <i>c/a</i> | 2.02 | | | |

hexagonal position parameters and occupancies

| Atom | Position | Coordinates | <i>x</i> | <i>z</i> | Occupancy | |
|------|----------|---------------------------------|-----------|-----------|-----------|-----|
| B(1) | 18(h) | <i>x</i> , \bar{x} , <i>z</i> | 0.1707(2) | 0.6370(3) | 1.0 | 93B |
| B(2) | 18(h) | <i>x</i> , <i>x</i> , <i>z</i> | 0.1059(3) | 0.8828(2) | 1.0 | |
| B(3) | 6(c) | 0,0, <i>z</i> | 0.382(1) | 0.531(2) | | |
| Se | 6(c) | 0,0, <i>z</i> | 0.4192(1) | 0.469(2) | | |

B₂Se₃

Structure

crystalline structure: monoclinic [72H2, 77G]

space group: P₂P_m (?) or C_{2h}¹ – P2/m [77G]

lattice parameters

| | | | | |
|----------|------------|------------------|-------------------|------|
| <i>a</i> | 4.06(1) Å | <i>T</i> = 300 K | X-ray diffraction | 72H2 |
| <i>b</i> | 38.6(1) Å | | | |
| <i>c</i> | 10.43(2) Å | | | |
| <i>β</i> | 90° | | | |

Physical properties

No detailed investigations on the electronic properties are available. But the obtained materials, either in crystalline or glassy form are reported to be colored in red, orange or yellow [62H, 67C, 70G, 71D, 72D, 72H1, 77G]. Therefore semiconducting behavior can be expected.

IR spectra absorption maxima wavenumbers

B₂Se₃ (polycrystal)

| | | | | |
|----------------|----------------------|------------------|---------------|-------|
| (<i>ν/c</i>) | 768 cm ⁻¹ | <i>T</i> = 300 K | IR absorption | 72H2, |
| | 789 cm ⁻¹ | | | 77G |
| | 804 cm ⁻¹ | | | |
| | 831 cm ⁻¹ | | | |
| | 868 cm ⁻¹ | | | |
| | 883 cm ⁻¹ | | | |

B₂Se₃ (glass)

| | | | | |
|----------------|----------------------|------------------|---------------|-------|
| (<i>ν/c</i>) | 775 cm ⁻¹ | <i>T</i> = 300 K | IR absorption | 72H2, |
| | 838 cm ⁻¹ | | | 77G |
| | 861 cm ⁻¹ | | | |

Deviating results on IR spectra are reported in [62H].

density

| | | | |
|----------|-------------------------|------------|-----|
| <i>d</i> | 2.10 g cm ⁻³ | calculated | 77G |
|----------|-------------------------|------------|-----|

melting point

| | | |
|----------------------|-------|------|
| <i>T_m</i> | 753 K | 69B, |
| | | 72H2 |

glass softening temperature

T_{gs} 325°C

beginning of glass softening

71D,
72D

References:

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