

**substance: boron compounds, general properties**

**property: structure group of the orthorhombic MgAlB<sub>14</sub>-type borides**

The unit cell consists of four B<sub>12</sub> icosahedra, which are arranged in a distorted hexagonal packing, eight additional single B atoms and up to eight metal atoms, i.e. in total 64 atoms in the idealized unit cell (Fig. 1). The structure is characterized by a largely covalently bonded network formed by chains of icosahedra arranged parallel to the *c* axis and in the <110> direction. The external bonds of the icosahedra are part directly inter-icosahedral and part indirectly inter-icosahedral via the single boron or metal atoms. The metal atoms are accommodated outside the B<sub>12</sub> icosahedra in the large holes of the boron framework. In the most cases the metal sites are only partly occupied.

# Representatives of the orthorhombic MgAlB<sub>14</sub> type borides

Chemical formula (idealized)	Structural formula	
LiAlB <sub>14</sub>		93H, 80H, 81H
NaB <sub>0.8</sub> B <sub>14</sub>		70N
MgAlB <sub>14</sub>		93H, 83H, 93G, 81H, 81G
Mg <sub>2</sub> B <sub>14</sub>	Fe-doped	88K, 91D
TbAlB <sub>14</sub>		88K, 91D
DyAlB <sub>14</sub>		88K, 91D
HoAlB <sub>14</sub>		88K, 91D
ErAlB <sub>14</sub>		88K, 92K
TmAlB <sub>14</sub>		93K
YbAlB <sub>14</sub>		88K
LuAlB <sub>14</sub>		88K
YAlB <sub>14</sub>		92K, 92K

New rare earth aluminum borides with structure of MgAlB<sub>14</sub> type [88K].

Comparison of the interatomic distances in LiAlB<sub>14</sub>, MgAlB<sub>14</sub>, Mg<sub>2</sub>B<sub>14</sub> and NaB<sub>0.8</sub> B<sub>14</sub> in [81H].

Optical absorption spectra of LiAlB<sub>14</sub>, MgAlB<sub>14</sub>, ErAlB<sub>14</sub>, in particular in the range of the absorption edges in Fig. 2 [93W].

Optical reflectivity spectra of LiAlB<sub>14</sub> and MgAlB<sub>14</sub> in Fig. 3 [93W].

Optical absorption spectra of LiAlB<sub>14</sub> and ErAlB<sub>14</sub> in the range of single atom vibrations in Fig. 4 [93W].

Optical absorption spectra of LiAlB<sub>14</sub>, MgAlB<sub>14</sub>, ErAlB<sub>14</sub> in the range of the phonon frequencies in Fig. 5 [93W].

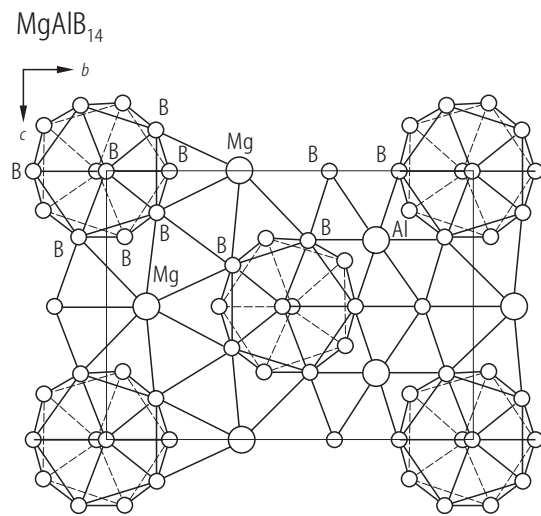
Optical and electronic properties of the orthorhombic MgAlB<sub>14</sub>-type borides in [93W].

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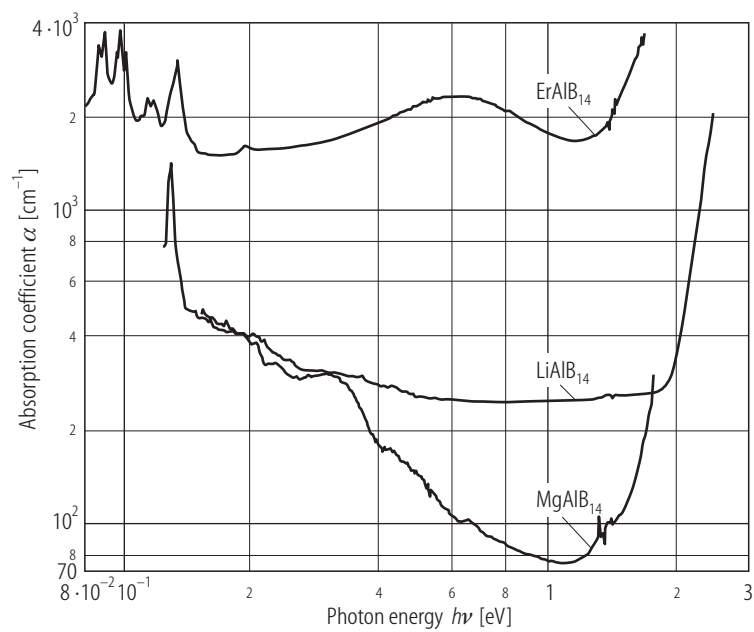
**Fig. 1.**

MgAlB<sub>14</sub> type orthorhombic structure group. Structure in a view parallel to [100]. Single atoms with  $-1/4 < x < +1/4$  are shown [77M].



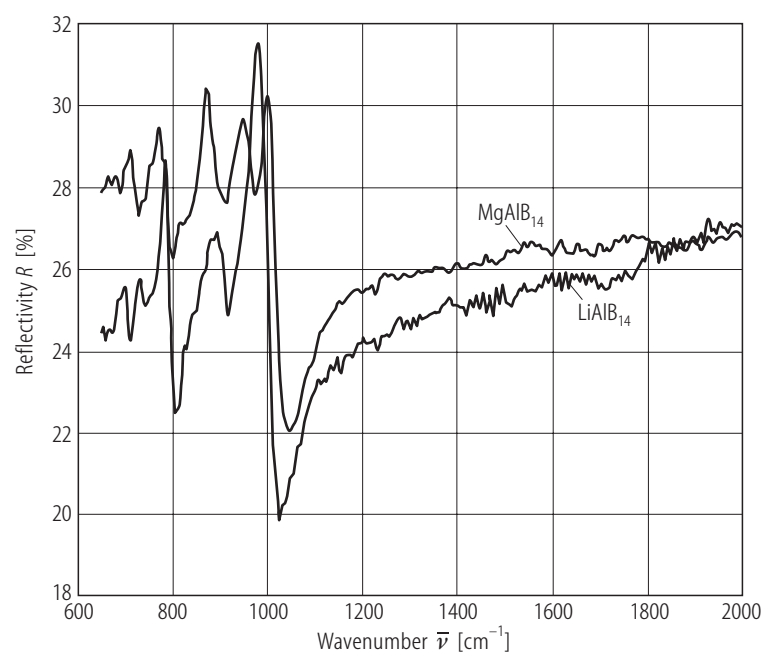
**Fig. 2.**

MgAlB<sub>14</sub> type orthorhombic structure group (LiAlB<sub>14</sub>, MgAlB<sub>14</sub>, ErAlB<sub>14</sub>). Optical absorption spectra, in particular in the range of the absorption edge [93W].



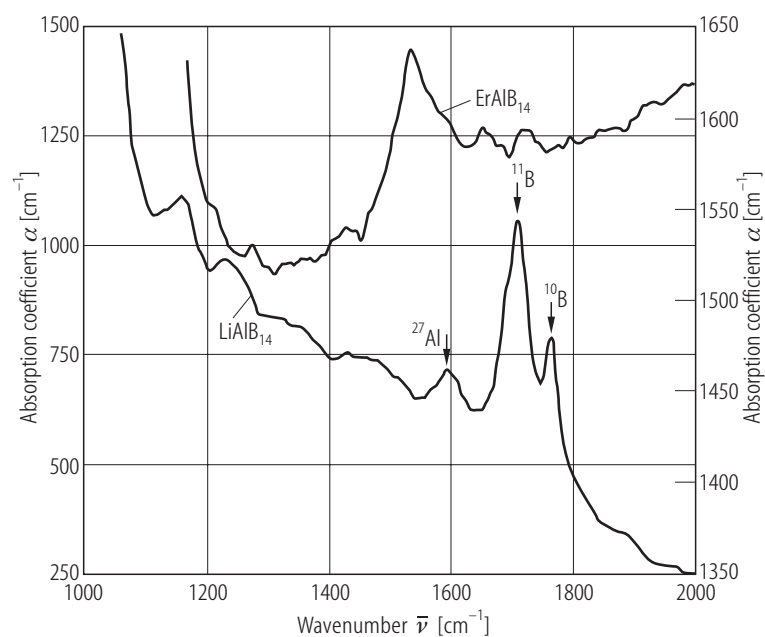
**Fig. 3.**

MgAlB<sub>14</sub> type orthorhombic structure group (LiAlB<sub>14</sub>, MgAlB<sub>14</sub>). Reflectivity spectra [93W].



**Fig. 4.**

MgAlB<sub>14</sub> type orthorhombic structure group (LiAlB<sub>14</sub> (left ordinate), ErAlB<sub>14</sub> (right ordinate)). Optical absorption spectra in the range of single atom vibrations [93W].



**Fig. 5.**

MgAlB<sub>14</sub> type orthorhombic structure group (LiAlB<sub>14</sub>, MgAlB<sub>14</sub>, ErAlB<sub>14</sub>). Optical absorption spectra in the range of phonon frequencies [93W].

