

substance: boron compounds with lanthanides

property: properties of MgAlB₁₄ type orthorhombic borides with lanthanides

Structure: orthorhombic MgAlB₁₄ type

Space group: Imma or Ima2

Lattice parameters vs. metallic radii of metal atoms in Fig. 1 [91K].

TbAlB₁₄

On preparation and crystal habit see [94D].

lattice parameters

(in Å)

| | | | | |
|----------|-----------|------------------|-------------------|------|
| <i>a</i> | 5.836(7) | <i>T</i> = 300 K | X-ray diffraction | 91D2 |
| <i>b</i> | 10.419(9) | | | |
| <i>c</i> | 8.189(8) | | | |

magnetic moments

| | | | |
|---------------------------|---------------------|------------------------|-----|
| <i>p</i> _{eff} | 11.0 μ _B | <i>T</i> = 150...250 K | 88B |
| <i>p</i> _{theor} | 9.72 μ _B | | |

Temperature dependence of $1/\sigma_m$ ($\sigma_m \sim p_{\text{eff}}^2/(T - \Theta)$) in Fig. 2 [88B].

paramagnetic Curie temperature

| | | |
|----------|------|-----|
| Θ | 10 K | 88B |
|----------|------|-----|

microhardness

(for load *p* = 100 g, in kg mm⁻²)

| | | | | |
|-----------------------|----------------|------------------|----------------------------|-----|
| <i>H</i> _K | 2700/3400/2400 | <i>T</i> = 300 K | (001) for azimuth 0/45/90° | 94D |
| | 2600 | | (011) for azimuth 45° | |

DyAlB₁₄

On preparation and crystal habit see [94D].

lattice parameters

(in Å)

| | | | | |
|----------|-----------|------------------|-------------------|------|
| <i>a</i> | 5.846(5) | <i>T</i> = 300 K | X-ray diffraction | 91D2 |
| <i>b</i> | 10.420(6) | | | |
| <i>c</i> | 8.198(5) | | | |

magnetic moments

| | | | |
|---------------------------|----------------------|------------------------|-----|
| <i>p</i> _{eff} | 12.1 μ _B | <i>T</i> = 150...250 K | 88B |
| <i>p</i> _{theor} | 10.63 μ _B | | |

Temperature dependence of $1/\sigma_m$ ($\sigma_m \sim p_{\text{eff}}^2/(T - \Theta)$) in Fig. 2 [88B].

paramagnetic Curie temperature

| | | |
|----------|--------|-----|
| Θ | − 13 K | 88B |
|----------|--------|-----|

microhardness(for load $p = 100$ g, in kg mm^{-2})

| | | | | |
|-------|------|-------------|------------------------------|-----|
| H_K | 3700 | $T = 300$ K | (001) for azimuth 90° | 94D |
|-------|------|-------------|------------------------------|-----|

HoAlB₁₄

On preparation and crystal habit see [94D].

lattice parameters

(in Å)

| | | | | |
|-----|---------------|-------------|-------------------|-----|
| a | 5.81...5.84 | $T = 300$ K | X-ray diffraction | 93W |
| b | 8.18...8.27 | | | |
| c | 10.40...10.43 | | | 91K |

needles

| | | | | |
|-----|-----------|-------------|-------------------|------|
| a | 5.816(1) | $T = 300$ K | X-ray diffraction | 91D2 |
| b | 10.399(2) | | | |
| c | 8.182(2) | | | |

plates

| | | | | |
|-----|-----------|-------------|-------------------|------|
| a | 5.841(5) | $T = 300$ K | X-ray diffraction | 91D2 |
| b | 10.410(6) | | | |
| c | 8.188(5) | | | |

magnetic moments

| | | | | |
|------------------|--------------|-------------------|--|-----|
| p_{eff} | 11.8 μ_B | $T = 150...250$ K | | 88B |
|------------------|--------------|-------------------|--|-----|

| | | | | |
|--------------------|---------------|--|--|--|
| p_{theor} | 10.60 μ_B | | | |
|--------------------|---------------|--|--|--|

paramagnetic Curie temperature

| | | | | |
|----------|-------|--|--|-----|
| Θ | -16 K | | | 88B |
|----------|-------|--|--|-----|

microhardness(for load $p = 100$ g, in kg mm^{-2})

| | | | | |
|-------|--------------------|-------------|---------------------------------------|-----|
| H_K | 3800 / 3300 / 3000 | $T = 300$ K | (001) for azimuth $0 / 45 / 90^\circ$ | 94D |
| | 3400 / 2600 | | (011) for azimuth $0 / 45^\circ$ | |

ErAlB₁₄

On preparation and crystal habit see [94D].

lattice parameters

(in Å)

| | | | | |
|----------|---------------|------------------|---|------|
| <i>a</i> | 5.78...5.86 | <i>T</i> = 300 K | X-ray diffraction | 93W |
| <i>b</i> | 8.17...8.22 | | | |
| <i>c</i> | 10.30...10.47 | | | |
| <i>a</i> | 5.8200(1) | <i>T</i> = 300 K | Er _{0.62} Al _{0.73} B ₁₄ , X-ray diffraction | 92K2 |
| <i>b</i> | 8.1825(3) | | | |
| <i>c</i> | 10.3950(4) | | | |
| <i>a</i> | 5.8157(2) | | | 93W |
| <i>b</i> | 8.1816(3) | | | |
| <i>c</i> | 10.3936(4) | | | |
| needles | | | | |
| <i>a</i> | 5.839(7) | <i>T</i> = 300 K | X-ray diffraction | 91D2 |
| <i>b</i> | 10.390(9) | | | |
| <i>c</i> | 8.171(8) | | | |
| plates | | | | |
| <i>a</i> | 5.842(5) | | | |
| <i>b</i> | 10.406(6) | | | |
| <i>c</i> | 8.186(5) | | | |

atomic distances

(in Å)

| | | | |
|----------|----------------|----------|-----|
| <i>d</i> | 2.27 | Al – 12B | 93W |
| | 2.71 | Er – 16B | |
| | 2.91 | Al – Al | |
| | 3.17/3.40/3.64 | Er – Er | |

site occupancies

| | | | | |
|-------------|----------|------------------|---|------|
| Er | 0.310(1) | <i>T</i> = 300 K | Er _{0.62} Al _{0.73} B ₁₄ | 92K2 |
| Al | 0.732(4) | | | |
| B(1) – B(5) | 1 | | | |

Electronic properties

Relationship of electronic properties to those of quasicrystals in [97W].

energy gaps

(in eV)

| | | | | |
|----------------------|---------|------------------|---|-----|
| <i>E_g</i> | 0.33(3) | <i>T</i> = 300 K | deep level to band (probably due to Er) | 93W |
| | 0.97(1) | | indirect allowed interband | |
| | 1.30(1) | | indirect allowed interband | |

Lattice properties

phonon wavenumbers

(in cm^{-1})

| | | | |
|---------|------|---------------------|-----|
| ν/c | 1536 | $T = 300 \text{ K}$ | 93W |
| | 1065 | | |
| | 1027 | | |
| | 930 | | |
| | 902 | | |
| | 873 | | |
| | 801 | | |
| | 778 | | |
| | 761 | | |
| | 711 | | |
| | 691 | | |

Phonon spectrum in Fig. 3 [93W, 94W].

Optical properties

Optical absorption spectra of ErAlB_{14} (compared with LiAlB_{14} and MgAlB_{14}) in particular in the range of the absorption edge in Fig. 4 [93W].

Optical absorption spectra of ErAlB_{14} (compared with LiAlB_{14}) in the range of single atom vibrations in Fig. 5 [93W].

Optical absorption spectra of ErAlB_{14} (compared with LiAlB_{14} and MgAlB_{14} ,) in the range of the phonon frequencies in Fig. 6 [93W].

IR reflectivity spectrum and Drude fit in [94W].

Transport and further properties

electrical conductivity

| | | | |
|----------|--|---------------------|-----|
| σ | $3 \cdot 10^{-1} \Omega^{-1} \text{cm}^{-1}$ | $T = 300 \text{ K}$ | 94W |
|----------|--|---------------------|-----|

thermoelectric power

| | | | |
|-----|-------------------------------|---------------------|-----|
| S | $-140(10) \mu\text{V K}^{-1}$ | $T = 300 \text{ K}$ | 94W |
|-----|-------------------------------|---------------------|-----|

magnetic moments

| | | | |
|------------------|-----------------------|-------------------------------|-----|
| p_{eff} | $11.2 \mu_{\text{B}}$ | $T = 150 \dots 250 \text{ K}$ | 88B |
|------------------|-----------------------|-------------------------------|-----|

| | | | |
|--------------------|-----------------------|--|--|
| p_{theor} | $9.59 \mu_{\text{B}}$ | | |
|--------------------|-----------------------|--|--|

Temperature dependence of $1/\sigma_{\text{m}}$ ($\sigma_{\text{m}} \sim p_{\text{eff}}^2/(T - \Theta)$) in Fig. 2 [88B].

paramagnetic Curie temperature

| | | |
|----------|-----------------|-----|
| Θ | -19 K | 88B |
|----------|-----------------|-----|

decomposition temperature

| | | |
|---------------------|--------------------|-----|
| T_{decomp} | $> 2000 \text{ K}$ | 93W |
|---------------------|--------------------|-----|

microhardness

(for load $p = 100 \text{ g}$, in kg mm^{-2})

| | | | | |
|----------------|--------------------|---------------------|--------------------------------|-----|
| H_{K} | 4100 / 3800 / 3400 | $T = 300 \text{ K}$ | (001) for azimuth 0 / 45 / 90° | 94D |
| | 3300 / 3100 | | (011) for azimuth 0 / 45° | |

TmAlB₁₄

On preparation and crystal habit see [94D].

lattice parameters

(in Å)

| | | | | |
|----------|------------|------------------|-------------------|------|
| <i>a</i> | 5.8212(3) | <i>T</i> = 300 K | X-ray diffraction | 93W |
| <i>b</i> | 8.1762(3) | | | |
| <i>c</i> | 10.3837(2) | | | 92K1 |

microhardness

(for load *p* = 100 g, in kg mm⁻²)

| | | | | |
|----------------------|------------------|------------------|--------------------------------|-----|
| <i>H_K</i> | 3150 / 3400/3300 | <i>T</i> = 300 K | (001) for azimuth 0 / 45 / 90° | 94D |
|----------------------|------------------|------------------|--------------------------------|-----|

YbAlB₁₄

lattice parameters

(in Å)

| | | | | |
|----------|-----------|------------------|-------------------|------|
| <i>a</i> | 5.860(3) | <i>T</i> = 300 K | X-ray diffraction | 91D1 |
| <i>b</i> | 10.439(3) | | | |
| <i>c</i> | 8.222(2) | | | |

LuAlB₁₄

Preparation in [91D2].

lattice parameters

(in Å)

| | | | | |
|----------|-----------|------------------|-------------------|------|
| <i>a</i> | 5.867(7) | <i>T</i> = 300 K | X-ray diffraction | 91D2 |
| <i>b</i> | 10.364(8) | | | |
| <i>c</i> | 8.157(7) | | | |

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Fig. 1.

LnAlB_{14} (MgAlB_{14} -type lanthanide compounds). Lattice parameters vs. metallic radii of the metal atoms; data of LiAlB_{14} , MgAlB_{14} (full circles), MgMgB_{14} (crosses) and $\text{Na}_{1-x}\text{B}_{1-y}\text{B}_{14}$ (crossed oval circles) for comparison [91K].

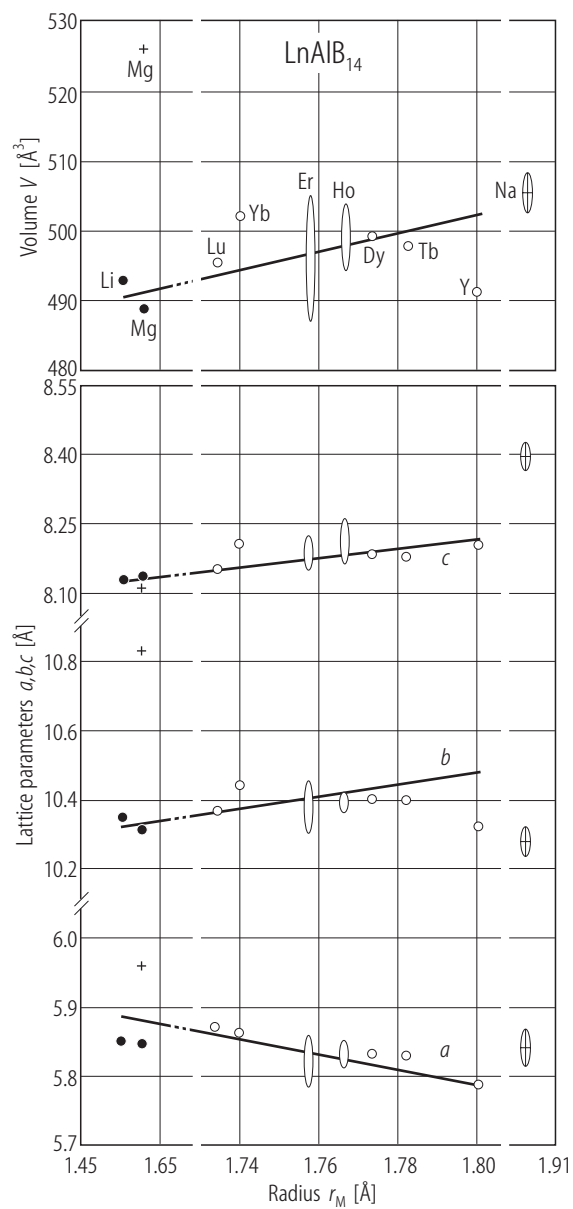


Fig. 2.

LnAlB_{14} (MgAlB_{14} -type lanthanide compounds). Temperature dependence of the reciprocal molar magnetization $1/\sigma_m$ ($\sigma_m \sim p_{\text{eff}}^2 / (T - \Theta)$) of single-crystal TbAlB_{14} , DyAlB_{14} , ErAlB_{14} [88B].

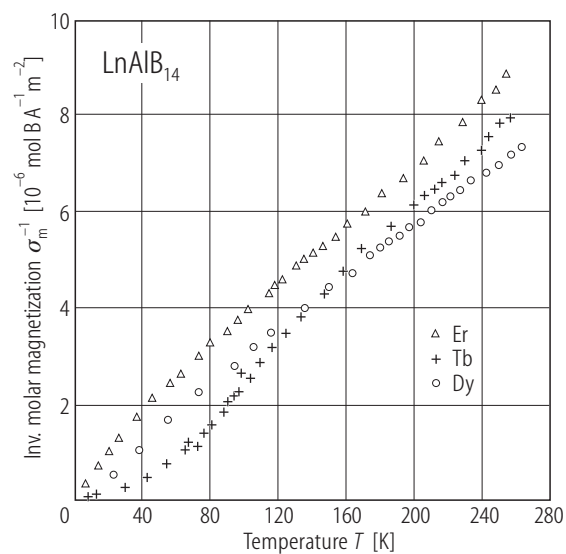


Fig. 3.

ErAlB₁₄. Absorption index vs. wavenumber. Spectra obtained by different experimental methods; (1) from reflectivity spectrum by KKR, (2) from transmission spectrum [93W, 94W].

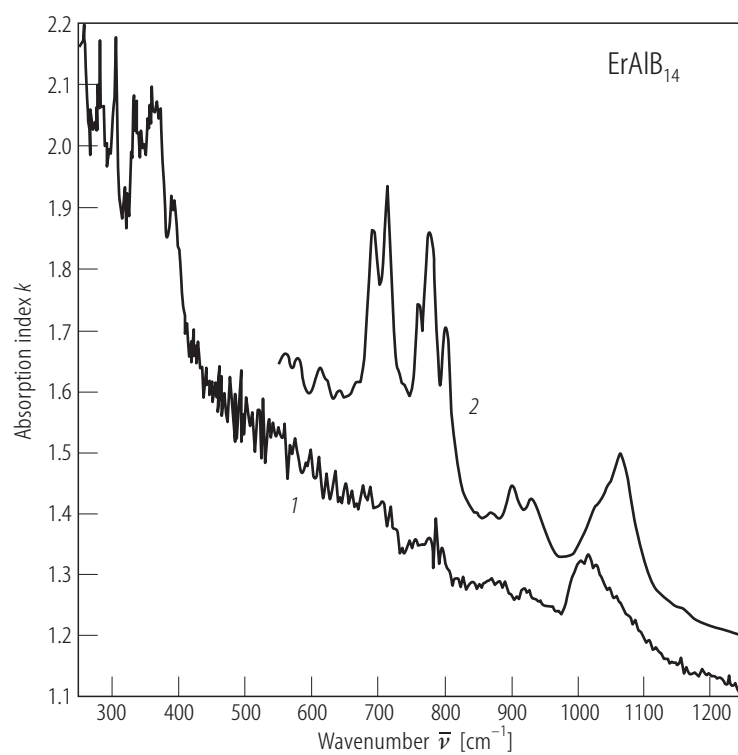


Fig. 4.

MgAlB₁₄ type orthorhombic structure group (LiAlB₁₄, MgAlB₁₄, ErAlB₁₄). Optical absorption spectra, in particular in the range of the absorption edge [93W].

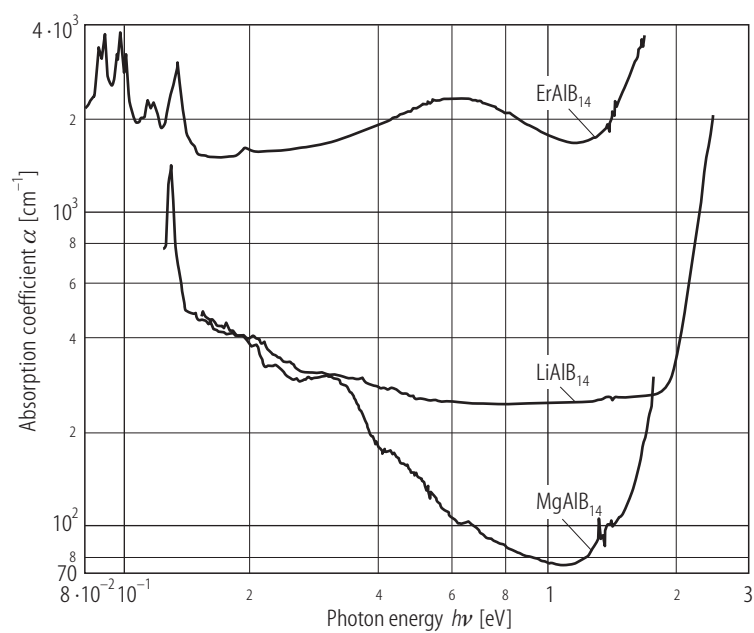


Fig. 5.

MgAlB₁₄ type orthorhombic structure group (LiAlB₁₄ (left ordinate), ErAlB₁₄ (right ordinate)). Optical absorption spectra in the range of single atom vibrations [93W].

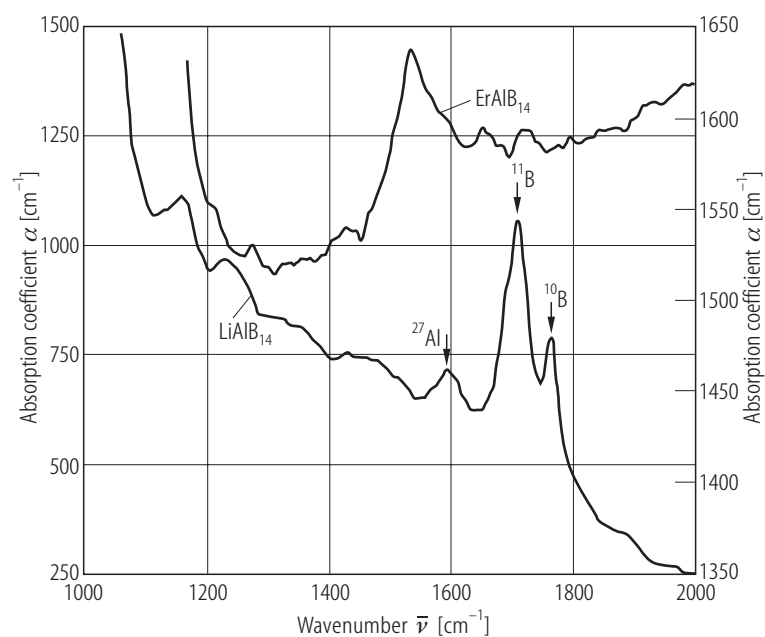


Fig. 6.

MgAlB₁₄ type orthorhombic structure group (LiAlB₁₄, MgAlB₁₄, ErAlB₁₄). Optical absorption spectra in the range of phonon frequencies [93W].

