**substance: boron compounds with group V elements**
**property: properties of boron-arsenic compounds**

**$B_6As$ ($B_{12}As_2$); $B_{13}As_2$**

**Structure**

For structure determination, see [61L, 61M, 66S, 70E, 73H, 77M1, 77M2].

Preparation of clear and black crystals from Pd and Ni flux and by chemical vapor deposition [87A].

α-rhombohedral boron structure group

Space group: $D_{3d}^5 - R\bar{3}m$ .

**lattice parameters**
(hexagonal presentation)

| | | |
|---|---|---|
| *a* | 6.169(4) Å | 86M, |
| *c* | 11.900(6) Å | 87M |
| *c*/*a* | 1.93 | 91L |
| *V* | 392.2 Å$^3$ | 94L |
| *a* | 6.142 Å | 61L, |
| *c* | 11.892 Å | 61M, |
| | | 77M1, |
| | | 77M2 |

(rhombohedral presentation)

| | | |
|---|---|---|
| *a* | 5.3 Å | 61L, |
| $\alpha$ | 70º30' | 61M, |
| | | 77M1, |
| | | 77M2 |

Other indication of the lattice structure:

**lattice:** orthorhombic [74G].

**lattice parameters**

| | | | |
|---|---|---|---|
| *a* | 9.709 Å | *T* = 300 K | 74G |
| *b* | 4.343 Å | | |
| *c* | 3.069 Å | | |

**interatomic distances**
(in Å)

| | | | | |
|---|---|---|---|---|
| *d* | 1.77 | | inter-icosahedral | 91L |
| | 1.81 | | intra-icosahedral | |
| | 1.65 | | origin to 6 B(1) | |
| | 1.80 | | origin to 6 B(2) | |
| | 2.39 | | X – X (chain) | |
| | 2.00 | | X – 3 B(1) | |

Ab initio calculated lattice constants in [92M].

Structure refinement of a crystal with $a$ = 6.149(2) Å and $c$ = 11.914(3) Å (2 specimens) [87M].

($U_{ij}$ in $10^{-4}$ Å$^2$)

| Atom | $x$ | $z$ | $U_{11}$ | $U_{33}$ | $U_{12}$ |
|---|---|---|---|---|---|
| B(1) | 0.1825(2) | 0.3618(2) | 35(4) | 37(5) | 19(5) |
| | 0.1823(2) | 0.3615(2) | 32(5) | 31(6) | 14(6) |
| B(2) | 0.1029(2) | 0.0(2) | 38(4) | 15(4) | 20(5) |
| | 0.1035(3) | 0.1191(2) | 38(6) | 27(6) | 11(6) |
| As | 0 | 0.39981(2) | 6(1) | 11(2) | 0 |
| | 0 | 0.39983(2) | 5(1) | 18(2) | 0 |

$y = -x$; $U_{22} = U_{11}$, $U_{13} = U_{23} = 0$

**Physical properties**

**Electronic properties**

For X-ray emission, see [76D].

Electronic band structure, calculated with the first-principles orthogonalized linear combination of atomic orbitals method in Fig. 1 [95L].

Ab initio pseudopotential calculation of the electronic band structure in [92M]. Erratum in [93M].

Further electronic band structure calculations in [84A] and [89H].

Calculated total and partial densities of states in Fig. 2 [95L].

Orbital-resolved partial density of states vs. energy. in Fig. 3 [95L].

Further density of states calculations in [90B2], [88W], [83A] and [84A].

**calculated Mulliken effective charge**

| | | | | |
|---|---|---|---|---|
| *q* | 3.01(6) *e* | B(1) | | 95L |
| | 3.19(6) *e* | B(2) | | |
| | 4.40(2) *e* | (As) | | |

**energy gap**
(in eV)

| | | | | |
|---|---|---|---|---|
| $E_g$ | 3.47 | $T$ = 300 K | optical (from plot $\alpha^{1/2}$ vs. $E$) | 83S |
| | 2.78 | | Z → A(calculated) | 95L |
| | 4.81 | | Γ (calculated) | |
| | 4.21 | | X (calculated) | |
| | 3.07 | | Z (calculated) | |
| | 2.97 | | A (calculated) | |
| | 4.21 | | D (calculated) | |

(The band gap of 1.45 eV, which has been ascribed to $B_{13}As_2$ in [79G], belongs in fact to BAs.)

**Impurities and defects**

Irradiation-induced damage rates in [95C].

**Lattice properties**

Calculated dispersion curves for nondegenerate lattice vibration modes in Fig. 4 [90B1].

**thermal conductivity**

| | | | | |
|---|---|---|---|---|
| $\kappa$ | 1.2 W cm$^{-1}$ K$^{-1}$ | $T$ = 300 K | crystal orientation not reported | 71S |

Temperature dependence of thermal conductivity in Figs. 5, 10 [86T].

**phonon mean free path**

| | | | | |
|---|---|---|---|---|
| $\Lambda$ | $\approx 10^{-1}$ cm | $T$ < 10 K | Temperature dependence: Fig. 6. | 71S |

**force field constants**
(in mdyn/Å)

| | | | | |
|---|---|---|---|---|
| $k_{BB}$ | 1.0 | | intra-icosahedral, calculated | 91B, |
| | 1.3 | | | 90B1 |
| | 1.6 | | | |
| $k_{(2-center)}$ | 1.8 | | inter-icosahedral, calculated | |
| $k_{icosahedron-chain}$ | 2.8 | | | |
| $k_{chain-chain}$ | 1.8 | | | |

**acoustic wave velocities**
(in $10^6$ cm s$^{-1}$)

| | | | | |
|---|---|---|---|---|
| $v_l$ | 0.64 | | c-direction ($C_3$ axis) | 91B |
| $v_t$ | 0.42 | | | 90B1 |
| $v_l$ | 0.88 | | c-direction ($C_3$ axis) | |
| $v_t$ | 0.45 | | | |
| | 0.39 | | | |

**acoustic phonon cutoff**

| | | | | |
|---|---|---|---|---|
| | 170 cm$^{-1}$ | | | 81S |

**elastic moduli and bulk modulus**
(in $10^{11}$ N m$^{-2}$)

| | | | | |
|---|---|---|---|---|
| $c_{11}$ | 4.3258 | | calculated | 93L |
| $c_{21}$ | 0.9221 | | | |
| $c_{31}$ | 0.6361 | | | |
| $c_{51}$ | 0.0447 | | | |
| $c_{33}$ | 3.5596 | | | |
| $B_0$ | 1.819 | | | |
| $B_0$ | 1.82 | $T$ = 300 K | calculated | 92L, |
| | | | | 97L |

**Optical properties**

Calculated optical properties (optical conductivity σ, real and imaginary part of the dielectric function, energy loss) in Fig. 7 [95L].

**refractive index**

| | | | | |
|---|---|---|---|---|
| *n* | 2.70 | *T* = 300 K | visible range | 83S |

Absorption edge in Fig. 8 [83S].

Raman spectrum in Fig. 9 [91T].

Raman spectrum in [86S].

**Further properties**

**Debye temperature**

| | | | | |
|---|---|---|---|---|
| $\Theta_D$ | 940 K | calculated from sound velocities | | 71S, 74G |

**density**

| | | | | |
|---|---|---|---|---|
| *d* | 3.583 g cm$^{-3}$ | *T* = 300 K | X-ray | 71S |
| | 3.59(5) g cm$^{-3}$ | *T* = 300 K | pycnometric | 71S |

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## Fig. 1.

$B_{12}As_2$. Electronic band structure, calculated with the first-principles orthogonalized linear combination of atomic orbitals method [95L].

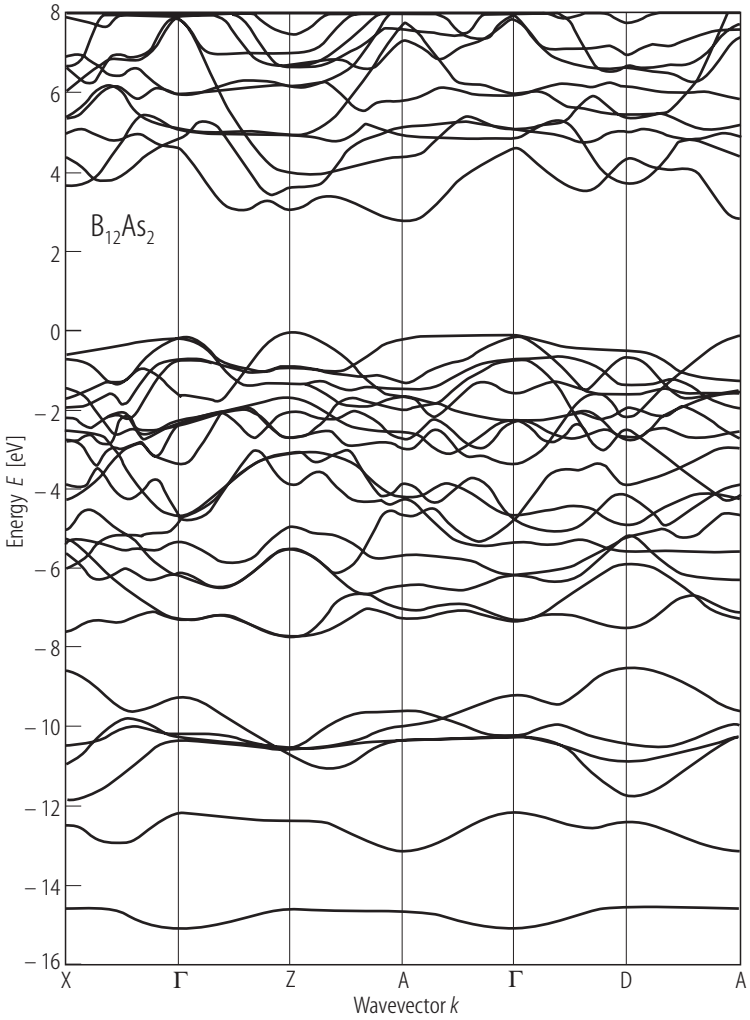


**Fig. 2.**

$B_{12}As_2$. **(a)** Total density of states,**(b)** partial density of states for B and **(c)** partial density of states for As vs. energy [95L].

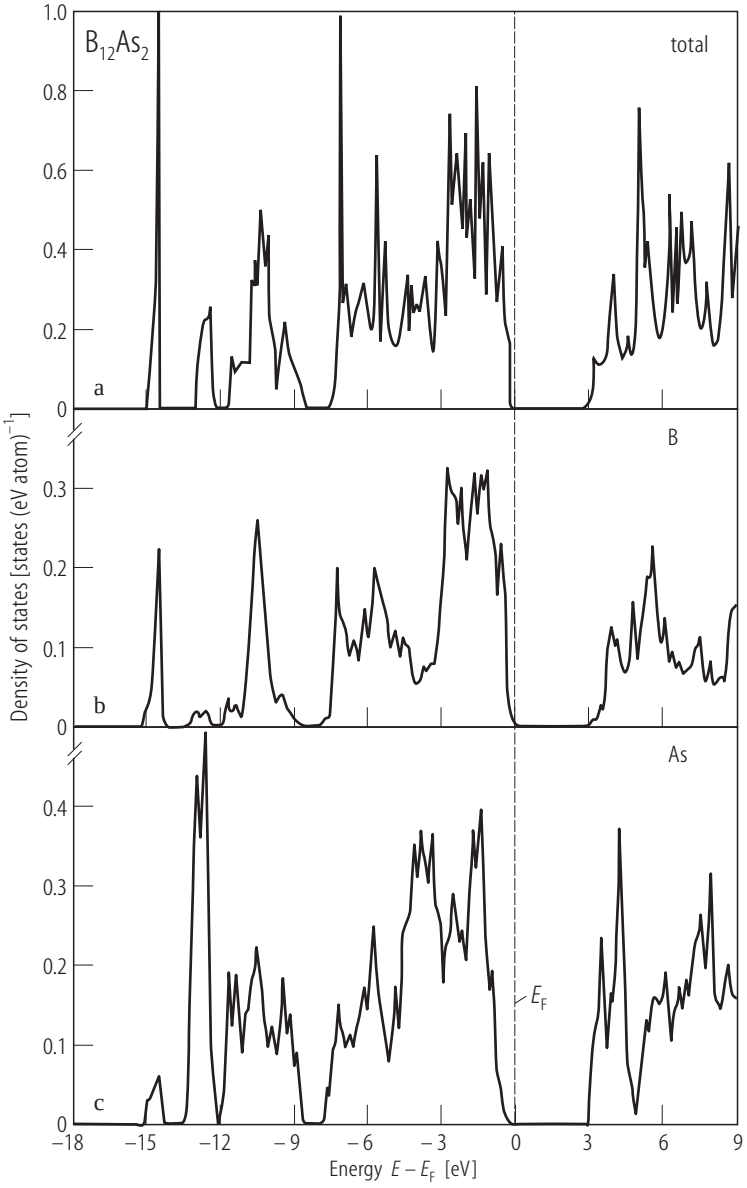
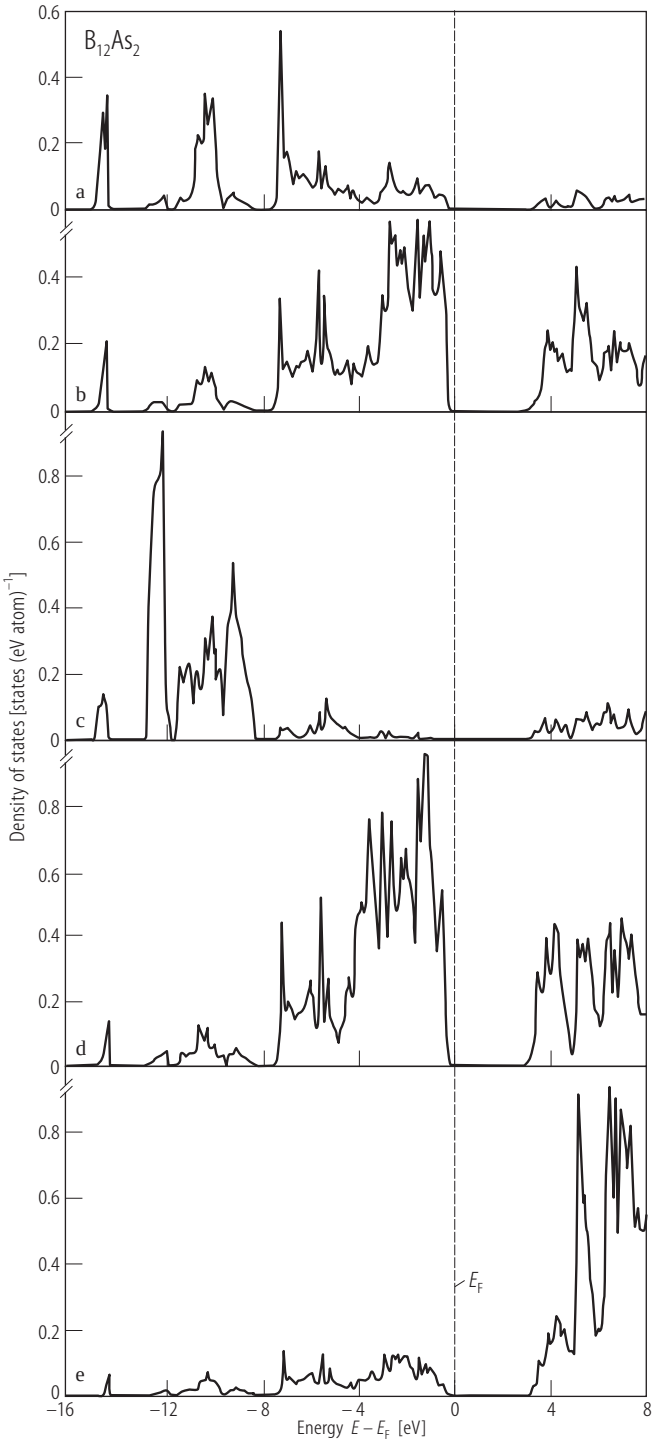


**Fig. 3.**

$B_{12}As_2$. Orbital-resolved partial density of states vs. energy. **(a)** B-s, **(b)** B-p, **(c)** As-s, **(d)** As-p, **(e)** As-d [95L].



## Fig. 4.

$B_{12}As_2$. Calculated dispersion curves for nondegenerate lattice vibration modes extending from $q$ = 0 to the zone edge in the *c*-direction [90B1].

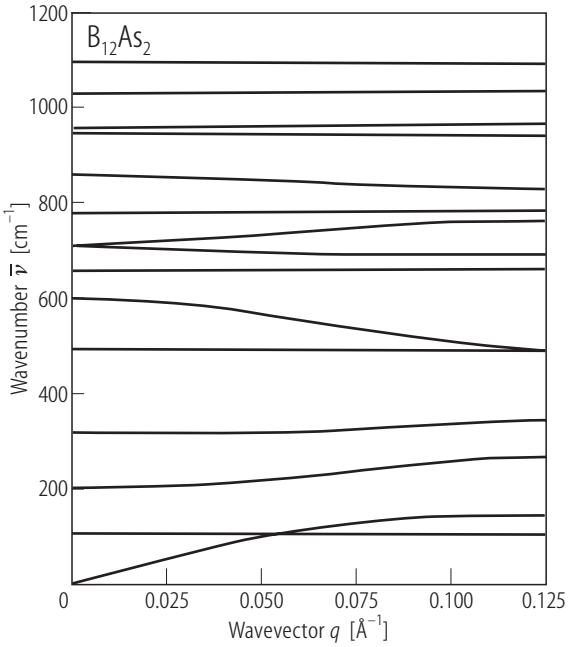
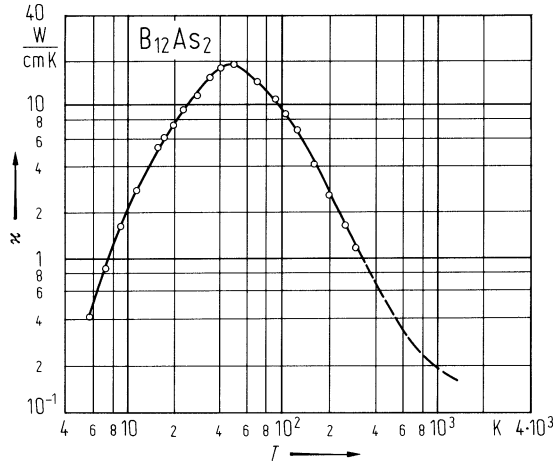


**Fig. 5.**

$B_{12}As_2$. Thermal conductivity vs. temperature [71S]. Crystal orientation not reported.



## Fig. 6.

$B_{12}As_2$. Phonon mean free path vs. temperature derived from the heat capacity. The dashed line represents the behavior of the acoustic phonons only and corresponds to the mean free path of the actual carriers with thermal energy [71S].

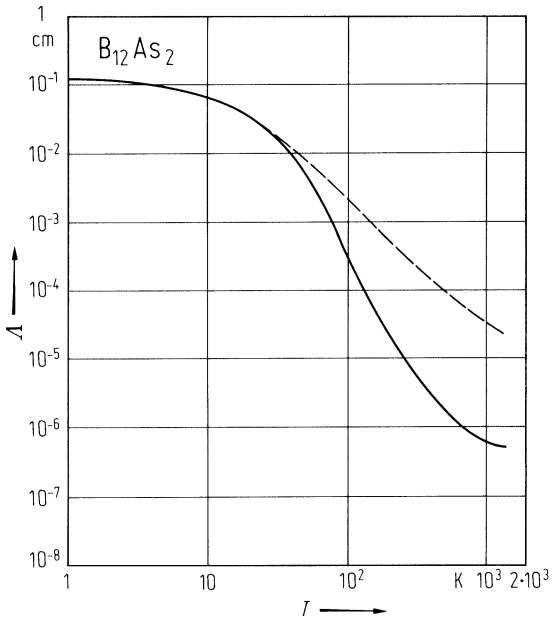


**Fig. 7.**

$B_{12}As_2$**.** Calculated optical properties. vs. photon energy. **(a)** Optical conductivity, **(b)** dielectric constants, **(c)** energy-loss function [95L].

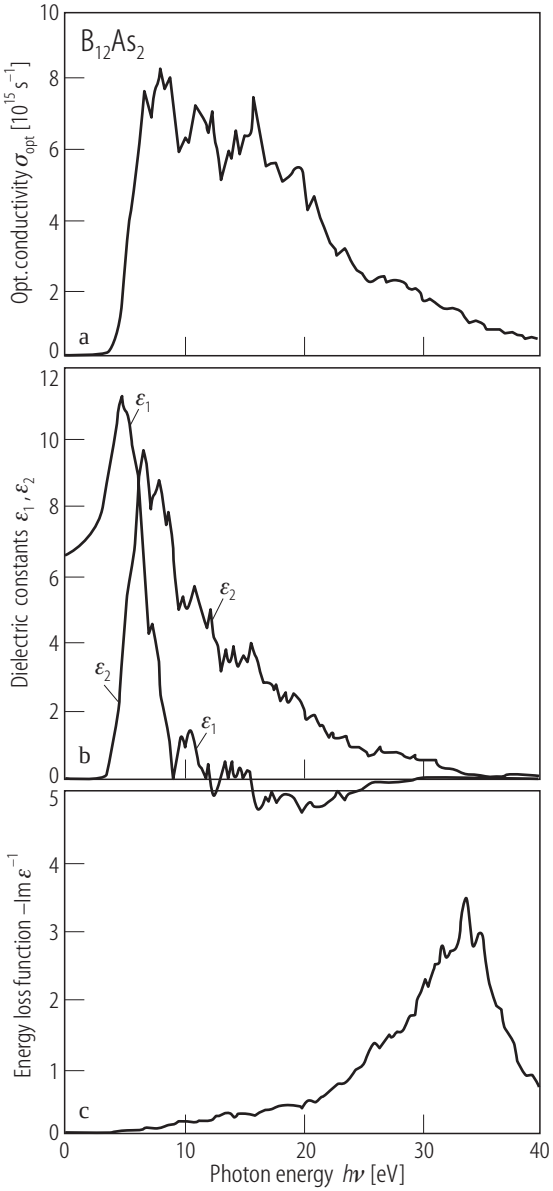


**Fig. 8.**

$B_{12}As_2$. Absorption edge. Absorption coefficient vs. photon energy [83S].

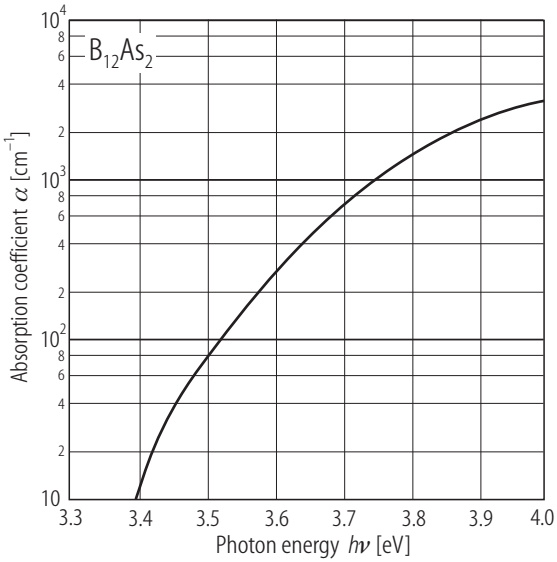
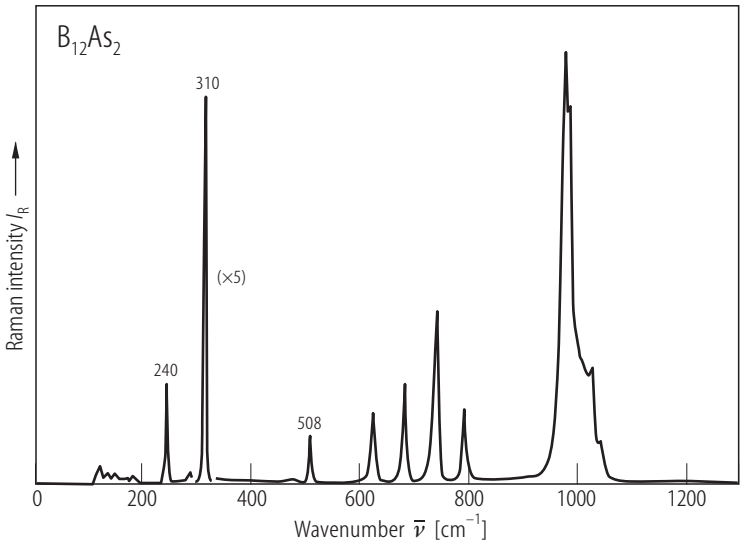


**Fig. 9.**

$B_{12}As_2$. Raman spectrum; intensity vs. Raman shift [91T].



## Fig. 10.

$B_{12}As_2$. Thermal conductivity vs. temperature.(Open circles ) [71S], (full circles) [87T], (------) fit by inclusion of a point scattering term into the Debye integral, (⋯⋯⋯) enhanced boundary scattering only [87T].