B4 C

B_4C

1986

12 Д81. Мезонные атомы и молекулярная структура. 9. B_4C. Mesomic Atoms and Molecular Structure. 9. B_4C. Imanishi Nobutsugu, Ohashi Shigeyuki, Miyamoto Shinichi, Takeuchi Yuka, Iwasaki Matae. «Кёто дайгаку гэнси энэруги. кэнкюдзё ихо, Bull. Inst. Atom. Energy Kyoto Univ.», 1986, 69, March, 47 (яп.)

(м-л.)

сф. 1986, 18, N 12

2000

F: B4C
P: 3
133:257122 Atomic structure and vibrational properties of icosahedral .alpha.-boron and B4C boron carbide. Vast, N.; Besson, J. M.; Baroni, S.; Dal Corso, A.; Dal Corso, A. B.P. 12, CEA, Centre d'Etudes de Bruyeres Bruyeres Le Chatel 91680, Fr. Comput. Mater. Sci., 17(2-4), 127-132 (English) 2000. The Raman and IR spectra of .alpha.-rhombohedral boron B12 and of B4C boron carbide have been detd. by accurate first-principles calcns. based on d.-functional perturbation theory. Our results account for all the features obsd. exptl., including the

characteristic Raman-active mode around 530 cm-1, which is attributed to the libration of the icosahedra. A comparison of the calcd. vibrational spectra with exptl. data allows the first unambiguous detn. of the at. structure of B4C. Anal. of our data shows that the high bulk moduli of .alpha.-rhombohedral boron and of B4C boron carbide - 220 and 240 GPa, resp. - are mainly detd. by the stiff intramol. bonding within each icosahedron. This finding is at variance with the current interpretation of recent neutron diffraction data on B4C in terms of a postulated larger stiffness of the intermol. bonds in icosahedral solids (inverted mol. compressibility). Our results show that icosahedral boron-rich solids should be considered as members of a new class of covalently bonded materials.

B_4C

2000

135: 322947c **Atomic structure and vibrational properties of icosahedral B_4C boron carbide. [Erratum to document cited in CA131:342252].** Lazzari, R.; Vast, N.; Besson, J. M.; Baroni, S.; Dal Corso, A. (Centre d'Etudes de Bruyeres, CEA, 91680 Bruyeres Le Chatel, Fr.). *Phys. Rev. Lett.* 2000, 85(19), 4194 (Eng), American Physical Society. The energy difference between the polar and equatorial configurations of B_4C as predicted was underestd. by an order of magnitude. Recalcn. of the energy difference found it to amt. to 35 meV/atom, thus confirming that the polar configuration is the at. structure for B_4C boron carbide, as was deduced by the comparison of exptl. Raman and IR spectra with the theor. obtained with functional perturbation theory.

(структура)

C.A. 2001, 135, N22