Соединения

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YBO_3

1981

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Vandenborre M. T.,
Husson E., et al.

Vi, cem. J. Raman Spectrose.
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1989

111: 45509z The electronic structure of yttrium disilicide. Martinage, L. (CNRS, Univ. Joseph Fourier, 38042 Grenoble, Fr.). *J. Phys.: Condens. Matter* 1989, 1(15), 2593-6 (Eng). The electronic structure was studied of YSi_2. The d. of states is calcd. within a tight-binding scheme and charge transfer is treated in a self-consistent way. The results show that hybridization between Si and Y is mainly due to Si p_z and Y d coupling and that YSi_2 is a metal. The densities of states compare well with those from the UV photoemission and ion photoemission spectra.

Электрон. структура

C.A. 1989, 111, N 6

YNH
NYH

1990

114: 30436m Geometries and energy separations of low-lying states of yttrium imide and yttrium hydride nitride (YNH and NYH). Das, Kalyan K.; Balasubramanian, K. (Dep. Chem., Arizona State Univ., Tempe, AZ 85287-1604 USA). *J. Chem. Phys.* 1990, 93(9), 6671-5 (Eng). Complete active-space multiconfiguration SCF followed by multireference configuration-interaction calcns. are carried out on low-lying electronic states of YNH and NYH. We find the $X^2\Sigma^+$ linear state of Y-N-H to be 55 kcal/mol more stable than the bent NYH and 59 kcal/mol more stable than the linear N-Y-H. Our calcns. confirm the recent assignment of the first obsd. spectra generated by laser vaporization of Y metal + He/NH_3. The theor. dipole moment of the Y-N-H mol. (3.06 D) is in excellent agreement with an exptl. value of 3.06 K obtained by Simard et al. The theor. Y-N and N-H bond lengths are also in good agreement with the exptl. results.

геометрия, низколеж. электр. сост, расчет

C.A. 1991, 114, NY

X-N-H | OM 35367 | 1990

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Jet-cooled spectroscopy
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taining polyatomic molecules: The visible spectrum of ~~[illegible]~~ yttrium imide

1994

F: YHBr
P: 3

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РЖХ 1997

1994

F: YHI
P: 3
6Б146. Смешанные трехатомные молекулы гидрид-галогенидов переходных металлов второго переходного ряда. 2nd Row transition metal mixed hydride halide triatomic molecules / Siegbahn P. E. M. // Theor. chim. acta. - 1994. - 88, N 6. - С. 413-424. - Англ.

Рнх 1997

1996

F: YPO4
P: 3

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Исследованы спектры ЛМ матриц переменного состава Sc[x]Y[1-y]PO[4] (x=0,25; 0,5 и 0,75), а также ScVO[4]. Положение полос обусловлено взаимодействием катионных и анионных орбиталей. Обсуждены точечная симметрия активных центров, неприводимые представления уровней, природа наблюдаемой ЛМ и ее тушения при следовании по ряду соединений от слабой голубой в YPO[4] до красной ЛМ в ScPO[4].

РЖХ 1997

$(ScY_3)_2$

1997

Ezhov Yu. S., et al.,

J. Struct. Chem. (Transl. of Zh. Strukt. Khim.) 1997, 38 (3), 403-407

структура, Di, электронография

(см. ScY_3; III)

YPS_4

1998

130: 87532z **Raman spectroscopy of rare earth thiophosphate-($LnPS_4$, Ln = Y, La ~ Lu) series compounds.** Huang, Zhongle (Department of Chemistry, Xiamen University, Xiamen, Peop. Rep. China 361005). *Zhongguo Xitu Xuebao* **1998**, 16(3), 208–212 (Ch), Yejin Gongye Chubanshe. The Raman spectroscopy study of $LnPS_4$ series compds. with tetragonal xenotime structure shows that the sym. stretching vibration frequency ν_1 increases linearly with the lanthanide contraction, i.e., the decrease of the effective ionic radius r_{Ln}^{3+}. Also, the ν_1 frequency for the nontetragonal $LuPS_4$ falls off the line running through the corresponding values for the tetragonal phases. This tendency is consistent with their structural modifications.

(CKP, D_1)

$LnPS_4$ (Ln = La – Lu)

(4)

C. A. 1999, 130, N 7

F: AunYm+

P: 3

1999

132:140459 Stability effects of AunXm+ (X=Cu, Al, Y, In) clusters. Bouwen W.; Vanhoutte, F.; Despa, F.; Bouckaert, S.; Neukermans, S.; Theil Kuhn, Weidele, H.; Lievens, P.; Silverans, R. E. Laboratorium voor Vaste-Stoffysica en Magnetisme, K.U. Leuven Louvain B-3001, Belg. Chem. Phys. Lett., 314(3,4), 227-233 (English) 1999 Bimetallic AunXm clusters (X=Cu, Al, Y, In, n=1-65, m=1 and 2) were produced by a dual-target dual-laser vaporization source. Following mult absorption, the stability patterns resulting from fragmentation were investigated by time-of-flight mass abundance

C.A. 2000, 132

spectrometry. AunCum+ clus exhibit the same electronic shell effects as Aun+. Different abundance p are obsd. for AunAl1+ compared to AunY1+ or AunIn1+. The patterns are re to the magic nos. of the electronic shell model for clusters. The differ between the bimetallic clusters are interpreted in terms of different clu geometries dependent on the dopant atoms nature.

HeY^{3+}

re, Do, we
wexe, Be
Геор.расчет

опыск № 40049

1999

Wesendrup R., Pernpointner M.,
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Phys. Rev. A, 1999, 60, N5,
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Coulomb-stable triply charged
diatomic ●: HeY^{3+}

УВг3 | Оп. 40661 | 2000

Jonathan C Wasse et al.,

спр-ра J. Phys.: Condens. Matter
2000, 12, N 46, 9539-9550

YB_{56}

2001

134: 152890p **Atomic structure of YB_{56} studied by digital high-resolution electron microscopy and electron diffraction.** Oku, Takeo; Bovin, Jan-Olov; Higashi, Iwami; Tanaka, Takaho; Ishizawa, Yoshio (Institute of Scientific and Industrial Research, Osaka University, Ibaraki, Japan 567-0047). *J. Mater. Res.* 2001, 16(1), 101-107 (Eng), Materials Research Society. At. positions for Y atoms were detd. by using high-resoln. electron microscopy and electron diffraction. A slow-scan charge-coupled device camera which had high linearity and electron sensitivity was used to record high-resoln. images and electron diffraction patterns digitally. Crystallog. image processing was applied for image anal., which provided more accurate, averaged Y atom positions. In addn., at. disordering positions in YB_{56} were detected from the differential images between obsd. and simulated images based on x-ray data, which were B_{24} clusters around the Y-holes. The present work indicates that the structure anal. combined with digital high-resoln. electron microscopy, electron diffraction, and differential images is useful for the evaluation of at. positions and disordering in the boron-based crystals.

электронная дифракция. спр-ра.

C.A. 2001, 134, N11

YB_2	Vajeeston P. et al.,	2001
теорет. расчет электрон. стр-ры и св-в в осн. эл. сост.; $\Delta_f H$, Сеllg.	Phys. Rev. B: Condens. Matter Mater. Phys. 2001, 63 (4), 045115/1 — 045115/12	
	(см. ● ScB_2; III)	