ALNO

ALNO

[Отпеск 12937] 1981

Энергии связи, кв. мех. расчет

Quinn Ch. M., Schwartz M. E.,

J. Chem. Phys., 1981, 74 (9), 5781–5785

оттиск 12816 1981

AlNO

(кв.-мех. расчет).

95: 86709j Studies of clusters using self-consistent field molecular orbital theory and a combination of all-electron real atoms and valence-electron model atoms. Schwartz, Maurice E.; Quinn, Charles M. (Dep. Chem., Univ. Notre Dame, Notre Dame, IN 46556 USA). *Surf. Sci.* 1981, 106(1-3), 258-64 (Eng). A valence-electron theory on model potentials for at. cores is developed to calc. for clusters such quantities as relative geometries and energies, valence orbital energies and ionization energies, charge distributions, and so on. To examine core-electron binding energies, the theor is extended by making a composite system consisting of an all-electron real atom for the atom whose core is to be examd. while describing the remainder of the system by the valence-electron model potential theory. Some illustrations of 2*p* core ionization in Al_2 and Al_4 show the accuracy of the techniques for both frozen-orbital ionization ("Koopmans theorem") and relaxed ionic state ionization (ΔE_{SCF}). The structures and both O and N 1*s* ionizations are discussed in AlNO and AlON, along with some chem. interesting results for NO + Al_2. Finally, some investigations of O atoms

(+2)

см. на обороте.

C.A 1981, 95, N10. (см. Al_2; III)

and the clusters Al, Al_2, Al_3, and Al_4 are analyzed. In OAl_2, OAl_3, and OAl_4, the most stable geometry occurs when the O "penetrates" the cluster to lie in the plane, sym. centered amongst the Al atoms, causing substantial lengthening of the Al–Al distance from bulk value in Al_2 and Al_3, but not in Al_4. Population analyses of the optimum planar OAl_3 and OAl_4 geometries show a transfer of about 1.4 electrons to the O $2p$ orbitals from Al $3s$ and $3p$, and indicate clearly the strong participation of the doubly degenerate O$2p\sigma$ in-surface orbitals in the clusters.

AlNO
AlON
NAlO
AlNO⁻

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Om 39432 "a"

1998

129: 114895h **Matrix Infrared Spectra and Density Functional Calculations of Three Al, N, O Isomers.** Andrews, Lester; Zhou, Mingfei; Bare, William D. (Department of Chemistry, University of Virginia, Charlottesville, VA 22901 USA). *J. Phys. Chem. A* 1998, 102(26), 5019–5026 (Eng), American Chemical Society. Laser–ablated Al atoms were reacted with NO, ^{15}NO, and $^{15}N^{18}O$ during condensation in excess Ar using a variety of concns. and laser energies/cm^2. Four of the five major product absorptions with higher laser energy were also obsd. with lower laser energy. The isotopic frequency ratios characterize different normal modes, and these are uniquely matched to the stretching modes of triplet AlON (1282.1, 566.7 cm^{-1}) and triplet AlNO (1644.3, 510.2 cm^{-1}) by d. functional theory (DFT) isotopic frequency calcns. The 5th band (1079.5 cm^{-1}) is due to a terminal Al–O stretching mode that is consistent with triplet NAlO based on DFT isotopic frequency calcns. The total product yield depended on laser energy; both AlON and AlNO addn. products were produced with lower energy, but the insertion product NAlO required higher energy. Anions were favored with lower laser energy, and a weak 1380.6 cm^{-1} band is assigned to AlNO$^-$ in accord with DFT isotopic frequency calcns.

CA 1998, 129, 114895h

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Zuning Zhang, Mingfei Zhou[+];

Chem. Phys., 2000, 236, N2, 185-194.