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D_0

(Conf. VC) III

III

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VC4

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C.A. 1970. 72. 26

+2 I

+1 II

X

VC2

VC4

D0

C.A. 1970. 73.

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(+2) I

(+1) III IV

(V-C$_2$)($^3\Delta_u$)
(CuV$_2$)($^3\Delta_u$)
(CuC$_2$)($^3\Delta_u$)

7- VII 4875 1970

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(См. VCx) 1

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Ti_2C
Zr_2C

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4 Б27. Химическая связь в субкарбидах (Me_2C) переходных металлов IVa — Va подгрупп. Иванов-ский А. Л., Губанов В. А., Алямовский С. И., Швейкин Г. П. «Ж. неорган. химии», 1979, 24, № 11, 2897—2900

Расширенным методом Хюккеля рассчитаны кластеры в структурах V_2C и гипотетич. субкарбидах Ti_2C и Zr_2C. Установлено, что электронный спектр энергий V_2C состоит из трех отдельных зон, сформированных преимущественно вкладами C2*s*, C2*p* и *M*-*spd*-функциями. Хим. связь осуществляется в основном M—M-взаимодействиями. Уменьшение конц-ии валентных *d*-электронов в $M_2^{IV}C$ приводит к неустойчивости субкарбидов переходных металлов подгруппы IVa.

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$n \leq 10$

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η^6-$(C_6H_6)V$

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расчет электронного строения

(+1) IX

X. 1986, 19, N 15.

η^6-$(C_6F_6)V$

кольце зарядовая плотность выше, чем в обычном комплексе дибензолванадия. Главные нормальные колебания в существенной степени остаются невозмущенными в I. В II атом V подвергается внутр. окислению при контакте с кольцом гексафторбензола. И. А. Тополь

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Ом. 38515

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Robert G. A. R.; Scuseria, Gustavo E. (Department [illegible] polis, MN 55455–
Rice Quantum Institute, Rice University, Houston [illegible] (Eng), America
Chem. Phys. Lett. 1996, 262(1,2), 87–90 (Eng). [illegible] provides a rapi
is made of various ab initio methods, including [illegible] shape effects on
the $^2\Delta$ and $^2\Sigma$ states of VC. The calcns. confirm [illegible] this article the au
of VC is the $^2\Delta$ state. A $^2\Pi$ state is not well [illegible] rithms are useful fo
configuration. The bond length in the $^2\Delta$ state is [illegible] range of solute fu
energy 2.9 eV, and the harmonic vibrational [illegible] of aq. free energies
cm^{-1}. The B3LYP predictions are good, but not [illegible] The first new model
for TiC and CrC. [illegible] model for the solut

CA 1997, 126, N5

V-C60

1997

(фуллерены)

128: 196883u **Multiple dumbbell structures of vanadium–C_{60} clusters.** Nakajima, Atsushi; Nagao, Satoshi; Takeda, Hiroaki; Kurikawa, Tsuyoshi; Kaya, Koji (Faculty of Science and Technology, Department of Chemistry, Keio University, 3–14–1 Hiyoshi, Kohoku–ku, Yokohama, Japan 223). *J. Chem. Phys.* 1997, 107(16), 6491–6494 (Eng), American Institute of Physics. Vanadium (V)–C_{60} mixed clusters were produced by two laser vaporization methods. In the mass spectra of cationic $V_n(C_{60})_m^+$, the abundant clusters were produced at the compn. of (n,m)=(1,1), (1,2), (2,3), (3–4,4), and (5,5). This pattern is explicable in terms of a multiple dumbbell structure; V atom and C_{60} are alternatively piled up. The ionization energy and the reactivity of the dumbbell clusters toward O_2 and CO show $V_1(C_{60})_2$ takes a structure of $V_1(\eta^6–C_{60})_2$.

C.A. 1998, 128, N16

05.39917

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F: VC2-
P: 3
132:70925 Electronic structure and chemical bonding between the first row transition metals and C2: A photoelectron spectroscopy study of MC2- (M=Sc, V, Cr, Mn, Fe, and Co). Li, Xi; Wang, Lai-Sheng Department of Physics, Washington State University Richland, WA 99352, USA J. Chem. Phys., 111(18), 8389-8395 (English) 1999 Vibrationally resolved photoelectron spectra of MC2- (M = Sc, V, Cr, Mn, Fe, and Co) are reported at 2 detachment photon energies, 532 and 355 nm. All the spectra showed a well resolved vibrational progression in the ground state

C-A. 2000, 132

detachment features. Electron affinities, vibrational frequencies, and information about the low- lying electronic states were obtained for the 1st row transition metal dicarbide mols. The measured electron affinities for the MC2 species show strong metal-dependence with a min. at VC2 and a max. at MnC2. The ground state vibrational frequencies were obsd. to decrease from ScC2 to a min. in CrC2 and then increases slightly in MnC2 and FeC2. The trends of the electron affinities and vibrational frequencies for the MC2 species correlate well with the corresponding monoxides, suggesting that the chem. bonding in M-C2 is analogous to that in M-O. The M-C2 bonding was thus interpreted to be quite ionic, and MC2 can be qual. viewed as M2+C22-, analogous to M2+O2-.

F: VC3-
P: 3

2000

132:257572 Vibrationally resolved photoelectron spectroscopy of the first row transition metal and C3 clusters: MC3- (M=Sc, V, Cr, Mn, Fe, Co, and Ni). Wang, Lai-Sheng; Li, Xi Department of Physics, Washington State University Richland, WA 99352, USA J. Chem. Phys., 112(8), 3602-3608 (English) 2000 American Institute of Physics Properties) 76 The authors report photoelectron spectra of the MC3- clusters for M = Sc, V, Cr, Mn, Fe, Co, and Ni at 2 photon energies, 355 and 266 nm. Vibrational structure is resolved for the ground and excited state detachment transitions for all the clusters except for CoC3- and NiC3-. Electron affinity (EA) and vibrational frequencies for the MC3 clusters are obtained. Complicated low-lying excited state features are

C.A. 2000.

obsd. for all the species. The trend of the EA across the 3d series for the MC3 clusters is similar to that of the MC2 species. The vibrational frequency increases from ScC3 to TiC3 and then decreases monotonically to the right of the 3d series. Preliminary d. functional theory calcns. are performed on all the MC3 and MC3- clusters at several initial geometries and spin multiplicities. The ground states of all the MC3 and MC3- species have C2v ring structures. The calcd. M-C stretching frequency for all the MC3 species is in good agreement with the exptl. measurement, lending credence to the obtained C2v structure. ~~transition metal carbon cluster~~

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late early 3d transition-
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