ASn

1973

As_3^-

As_2^-

As^-

(A.P)

ΔHf

13 Б870. Отрицательные ионы при высокой температуре: электронный удар в парах As_4. Bennett S. L., Margrave J. L., Franklin J. L., Hudson J. E. High temperature negative ions: electron impact of As_4 vapor. «J. Chem. Phys.», 1973, **59**, № 11, 5814—5819 (англ.)

В интервале т-р 380—420° при испарении мышьяка из камеры Кнудсена с помощью масс-спектрометра обнаружены образующиеся за счет диссоциативной ионизации отриц. ионы As_3^-; As_2^-; As^- с Пт появления 80,7±2,3; 70,2±2,3; 83,0±2,3 ккал/моль соотв. Определены избыточные энергии ионов As_3^-, As_2^-, As^-, соотв. равные 10,6±0,8; 18,3±0,7; 11,4±0,6 ккал/моль. Установлено, что найденные ионы образуются при электронном ударе за счет процессов $As_4+e\rightarrow As_n^-+As_{4-n}$ ($n=1,2,3$). Образование As^- за счет процесса $As_4+e\rightarrow As^-+As_2+As$ маловероятно. С помощью лит. данных вычислены ΔH^0 (обр., 298° К) газ. As_2^-, As_3^- и As_3, соотв. равные 43,1±4,5; 38,3±4,3; 57,6±3,9 ккал/моль и сродства к электрону As_2 и As_3, равные 2,4±4,1 и 19,3±8,2 ккал/моль.

М. В. Коробов

Bennett #4-38БD

(+1)

☒

X. 1974. N 13

(см. As_2; I)

As_3 оттиск 5757 1977

(Аē)

Lowe J.P.

J.Amer. Chem. Soc.,
1977, 99,(17),5557-70.

As_8 1981

Trinquier G., et al.

Chem. Phys. Lett., 1981, 80, N3, 552–557.

кв. мех. рас., геом. сил. пост., D_0

(см. N_4; III)

As_7^{3-} 1986

Cyvin B.N., Cyvin S.J.,
et al.

сил. пост., ν;

Z. Naturforsch., A: Phys.;
Phys. Chem., Kosmophys.
1986, 41A(3), 549-52.

(см. P_7^{3-}; III)

As_3 1991

Balasubramanian K.,
Sumathi K., et al.

J. Chem. Phys. 1991.

м.п.

<u>95</u>, N5.C. 3494-3505.

●

(см. P_3, $\overline{\underline{III}}$)

As_3 11Д108 1991

Katircioglu S., Erkoç S.,

м.л. Chem. Phys. Lett., 1991,
182, N 5, c. 451–454.

Структурная стабильность и энергетика микрокластеров As, Sb и Bi. Расчеты с ис-

Р.Ж.Ф. N 11, 1991

пользованием эмпирической многочастичной функции потенциальной энергии.

$As_{\overline{x}}$ 1991

$(x = 1-4)$

Meier U., Peyerimhoff S.D. et al.

Chem. Phys. 1991. 150, N3. С. 331–351.

м. п.

(см. ● $Ga_{\overline{x}}$; III)

As_n

1992

120: 38719a **Ion/molecule reactions of metal and semiconductor clusters: ionization potentials and electron affinities.** Bach, S. B.; Bruce, J. E.; Cheeseman, M. A.; Ramanathan, R.; Watson, C. H. (Dep. Chem., Univ. Florida, Gainesville, FL USA). *Report* 1992, 39; Order No. AD-A251618, 22 pp. (Eng). Avail. NTIS. From *Gov. Rep. Announce. Index* (*U. S.*) 1992, 92(19), Abstr. No. 252,552. Electron affinities and ionization potentials of As, C, P, Ag, Au, and Cu clusters were estd. precisely based on charge-transfer bracketing expts. involving cluster ions and neutral mols. of known electron affinities and ionization potentials.

(Ae, I, оценка)

☒

C_n, P_n, Ag_n, Au_n, Cu_n

㊺

C.A. 1994, 120, N 4

Азп

1993

Bach S.B.H., Bruil J.E.,
et al.,

(J,Ae) On Clusters Clustering
1993, 59-68.

(См. Сп і III)

As_m
$m<6$

1993

120: 38743d **Structure and ionization potentials of clusters containing heavy elements. I. Homonuclear group V clusters up to hexamers.** Igel-Mann, G.; Stoll, H.; Preuss, H. (Inst. Theor. Chem., Univ. Stuttgart, W-7000 Stuttgart, 80 Germany). *Mol. Phys.* 1993, 80(2), 325-39 (Eng). Homonuclear clusters X_m of heavy group V atoms (X = As, Sb) up to m = 6 have been studied with valence ab initio self consistent field/configuration integration calcns. using energy-adjusted pseudopotentials. Several structures have been investigated and results are given for bond lengths (R_e), atomization energies (D_e) and vertical ionization potentials of the ground states. Comparison with exptl. and other theor. values is made where possible.

ab initio рас-
чет структу-
ры и Э

(+) ☒ Sb_m $(m<6)$

C.A. 1994, 120, N4

As_n **Оп. 37754** 1994

$n = 2, 4, 12, 20$

Mingzuo Shen and
Henry F. Schaefer <u>III</u>

J. Chem. Phys., 1994, <u>101</u>,
N3, 2261 – – – (только 1 стр.!)

Dodecahedral ● and smaller

arsenic clusters: As_n, $n = 2, 4, 12, 20$

As_{20} 1994

Shen Mingzuo,
Schaerfer <u>III</u> Henry F.

стабильн. и структ.

J. Chem. Phys. 1994,
<u>101</u> (3), 2267-72.

(см. As_2, As_4, As_{12}; III)

As_{12} 1994

Shen Mingzuo,
Schaerfer III Henry F.

теорет. расчёт J. Chem. Phys. 1994, 101 (3), 2267-72.

(см. As_2, ~~As_4~~, ~~As_{12}~~, III)

As_6

1994

120: 117266d **Valence isomers of benzene and their relationship to the isoelectronic isomers of arsenic molecule (As_6).** Warren, D. Scott; Gimarc, Benjamin M.; Zhao, Ming (Dep. Chem. Biochem., Univ. South Carolina, Columbia, SC 29208 USA). *Inorg. Chem.* 1994, 33(4), 710–15 (Eng). The authors report the results of geometry-optimized ab initio SCF-MO calcns. for As_6 in structural forms corresponding to the five valence isomers of benzene, C_6H_6, with which As_6 is valence-isoelectronic. The authors used Scuseria's 752+P polarized basis set for arsenic. The resulting energy ordering of As_6 isomeric structures is very similar to what the authors found previously for P_6 isomers but quite different from that known for the C_6H_6 valence isomers. For As_6 as for P_6, prismane and benzvalene structures have the lowest energies while the planar hexagon (benzene) has the highest. The range of energies of the five structures is small, around 45 kcal/mol, somewhat larger than for the P_6 isomers but far smaller than for C_6H_6. Calcd. bond distances are easily identified with exptl. examples of AsAs single, double, and arom. bonds. The energy of $2As_6$ lies only 30 kcal/mol above that of $3As_4$. Calcd. energy change of homodesmotic reactions involving As_4 and As_6 give ests. of strain energies and resonance energies. The strain energies range from 2 kcal/mol for Dewar benzene to 33

структура
и
стабильн.,
теор. расч.

С.А. 1994, 120, N 10

kcal/mol for prismane. These are uniformly lower than comparable calcd. strain energies of P_6 isomers and much lower than strain energies of the valence isomers of C_6H_6. The authors' est. of the resonance energy of planar hexagonal As_6 is 17.6 kcal/mol, somewhat larger than that for the same structure for P_6 and smaller than the calcd. resonance energy of benzene, C_6H_6. Using calcd. strain and resonance energies for As_6 isomers, the authors obtain an est. of 60 kcal/mol for the As:As double bond energy. As with carbon and phosphorus, the homoat. double bond is weaker than two homoat. single bonds, and it is this result that establishes the basic energy ordering of As_6 isomers. Calcd. charge densities for As_6 isomers are uniformly smaller than those for comparable P_6 structures. Weaker bonds, smaller strain energies, and lower charge densities are properties that are consistent with the fact that valence AO's of larger principal quantum no. are more diffuse.

As_8

1997

Rodionov A.N., Zhukovskii Yu.F. et al.,

кв.-хим-расчет

J. Mol. Struct., 1997, <u>410–411</u>, 361–364.

Formation of As_8 dimers in molecular solid-state arsenic

As_3 От. 39557 1998

As_5 Lippa T.P. et al.,

J. Chem. Phys., 1998,

М.Л. <u>109</u>, N2, 10727-10731

As_3^- Эт 39557
Lippa T.P. et al., 1998

фотоэлектр. спектр., м.п., D_0
J. Chem. Phys. 1998, <u>109</u>(24), 10727-731

(см. As^-; <u>III</u>)

As_5^- От 39557 1998

Lippa T.P. et al.,

фотоэлектр.
спектр,
М.П., D_0

J. Chem. Phys. 1998,
<u>109</u>(24), 10727-731

(См. As^-; <u>III</u>)

F: Asn
P: 3

1999

132:227699 Energetics and stability of Gam, Asn, and GamAsn microclusters calculation. Erkoc, Sakir; Turker, Lemi Department of Physics, Middle East Technical University Ankara 06531, Turk. Physica E (Amsterdam), 5(1&2), 7-15 (English) 1999 Calcns. based on PM3 type semiempirical MO method have been performed to investigate the energetics and structural stabilities of Gam, Asn, and Ga microclusters. It has been found that both two- and three-dimensional geometries are realizable as stable structures.

C.A. 2000, 132

A53 OM 91443 2002

Haechol Choi et al.,

J. Phys. Chem. 2002, A106, 5777-87

геометр.,
колебан.
св-ва
нижних
электр.-
сост.;
ab initio расчет