Al — N

AlH_3NH_3

BH_3NH_3

и др.

спектр

1965

21 Б85. Колебательные спектры и силовые постоянные некоторых соединений типа $X_3Z \leftarrow NR_3$. Sawodny W., Goubeau J. Schwingungsspektren und Kraftkonstanten einiger Verbindungen des Typs $X_3Z \leftarrow NR_3$. «Z. phys. Chem.» (BRD), 1965, 44, № 3—4, 227—241 (нем.; рез. англ.)

Приведена таблица частот и интенсивностей в ИК-спектрах и спектрах комб. расс. комплексных соединений типа $X_3Z \leftarrow NR_3$ ($Z = B$, Al; $X = H$, CH_3, F, Cl, Br; $R = H$, CH_3). Таблица составлена на основании оригинальных измерений авторов и литературных данных. Частоты в области 1600—2700 *см*$^{-1}$ относятся к обертонам и составным частотам и в таблицу не включены. На основании сопоставления частот предложено их отнесение к типам симметрии группы C_{3v} и к валентным деформационным колебаниям. Выделены частоты внутренних колебаний метильных групп. Приводятся значения длин связей, использованные для вычисления силовых постоянных в естественных колебательных координатах. Составлена таблица их численных значений, обсуждаемых в связи с особенностями строения отдельных комплексов.

М. Ковнер

Ф-825

X·1965·21

$AlX_3 \cdot n NH_3$

$X = Br, J$

$n = 0, 1, 3, 5, 6;$

Pino V. C. 1966

An. Real soc. esp. fis. y quim., 1966, B62, № 1, 17.

Исследование соединений $AlX_3 \cdot n NH_3$ методом ИК-спектроскопии. (см. $X = Cl$.)

1968

Горение Al

23049g Differences between the combustion of aluminum droplets in air and in an oxygen–argon mixture. Prentice, J. L.; Nelson, L. S. (Michelson Lab., U.S. Nav. Weapons Center, China Lake, Calif.). *J. Electrochem. Soc.* 1968, 115(8), 809–12 (Eng). Small spherical liq. drops of Al were prepd. by focusing a Nd laser on Al foil and the free fall and light emission of the droplets were observed by time exposure photography and a photomultiplier. The droplets spin and jet in air but not in O–Ar mixts. They radiate less intensely but fall more rapidly in air than in O–Ar mixts. This variation in behavior is attributed to the accumulation of a condensed phase product during combustion in air, possibly a compd. of Al–O–N.

J. L. Weininger

(возм. образование Al–O–N)

C. A. 1969. 70. 6

NOAlCl

1972

2 Д559. **Изучение кристалла нитрозила хлоралюмината по спектрам комбинационного рассеяния.** Barbier Pierre, Mairesse Gaëtan, Wallart Francis, Wignacourt Jean-Pierre. Étude du cristal de chloroaluminate de nitrosyle par spectroscopie Raman. «C. r. Acad. sci.», 1972, C275, № 9, 475—478 (франц.)

Исследованы спектры комб. рас. NOAlCl (I) при т-рах 80, 198 и 470° К. Дано следующее отнесение полос в спектре твердого I: колебания иона $AlCl_4^-$ $\nu_1(A)=359$, $\nu_2(E)=133$, $\nu_3(F_2)=482$, $\nu_4(F_2)=203—228$ $см^{-1}$; ион NO^+ $\nu_1'(\Sigma^+)=2246$ $см^{-1}$. Сделан вывод, что I кристаллизуется в пространственной группе *Pnma*. Электроотрицат. группа NO^+ приводит к деформации иона $AlCl_4^-$. Приведены таблицы частот. Библ. 7. Э. В. Б.

Vi

Ржф-73-2

$AlCl_3 \cdot NH_3$ 1973

[illegible]

5 Б110. Конфигурация связей алюминия в $AlCl_3 \cdot NH_3$. Электронографическое исследование. Hargittai Magdolna, Hargittai István, Spiridonov Victor P. Aluminium bond configuration in $AlCl_3 \cdot NH_3$: an electron diffraction study. «J. Chem. Soc. Chem. Communs», 1973, № 19, 750—751 (англ.)

Симмет. молек.

Методом газовой электронографии изучена структура молекулы $AlCl_3 \cdot NH_3$. В предположении о шахматном расположении фрагментов $AlCl_3$ и NH_3 найдены след. значения межъядерных расстояний (A) и углов: Al—N 1,996±0,019, Al—Cl 2,100±0,005, ClAlCl 116,35±0,4°. Полученные параметры фиксируют конфигурацию связей у атома алюминия в молекуле; аналогичные параметры для характеристики конфигурации связей у атома азота надежно не получены. Найденные данные сопоставляются с результатами исследований родственных молекул.

В. Спиридонов

Х. 1974 N 5 ☒ (+1) [illegible]

$AlCl_3 \cdot NH_3$

1973

(электронография)

(r_{Al-N})

20372c Aluminum. bond configuration in the aluminum chloride-ammonia 1:1 adduct. Electron diffraction study. Hargittai, Magdolna; Hargittai, Istvan; Spiridonov, Victor P. (Cent. Res. Inst. Chem., Hung. Acad. Sci., Budapest, Hung.). *J. Chem. Soc., Chem. Commun.* 1973, (19), 750-1 (Eng). Detn. of Al bond configuration in $AlCl_3 \cdot NH_3$ revealed r(Al–N) = 1.996 Å, indicating strong linkage.

C.A. 1974. 80. N4

Гурвич.

$AlCl_3 \cdot NH_3$ Жч-8011 1974

(∂i)

Жч-8011

9 Б226. Спектроскопическое исследование комплекса $AlCl_3 \cdot NH_3$. Cyvin S. J., Cyvin B. N., Hargittai I. Spectroscopic studies of the $AlCl_3 \cdot NH_3$ complex. «J. Mol. Struct.», 1974, 23, № 3, 385—397 (англ.)

Проведен расчет нормальных колебаний комплекса $AlCl_3 \cdot NH_3$. Проведен расчет гипотетич. комплекса с плоским фрагментом $AlCl_3$ и рассмотрено изменение спектра при отклонении от плоскостной структуры. В кач-ве нулевого приближения использованы силовые поля составляющих молекул. Обсуждена роль кинематич. факторов в изменении спектров компонент при переходе в комплекс. Проведен расчет частот, форм колебаний, а также среднеквадратичных амплитуд колебаний.

А. П. Курбакова

х. 1975 №9

$AlCl_3 \cdot NH_3$ 1974

(сил. пост.)

√36716v Spectroscopic studies of the aluminum chloride.ammonia complex. Cyvin, S. J.; Cyvin, B. N.; Hargittai, I. (Div. Phys. Chem., Univ. Trondheim, Trondheim, Norway). *J. Mol. Struct.* 1974, 23(3), 385–97 (Eng). A normal coordinate anal. for the $AlCl_3.NH_3$ complex was performed. Calcns. for a hypothetical complex with a planar $AlCl_3$ ligand are included. A deviation from planarity was found in the realistic complex. Force fields for free NH_3 and $AlCl_3$ mols. are employed in the construction of an initial approx. force field. The theory of kinematic coupling was used to study the frequency shifts from free to complexed ligands. A final force field was developed to reproduce exactly a set of obsd. frequencies from the literature. Calcns. on mean amplitudes and perpendicular amplitude correction coeffs. are reported.

C.A. 1975, 22, N6

$AlCl_3 \cdot NH_3$

1974

$GaCl_3 \cdot$
$\cdot NH_3$

163565v Electron diffraction study of the coordination compounds ammonia-aluminum chloride and ammonia-gallium chloride in the gas phase. Hargittai, Magdolna; Hargittai, Istvan; Spiridonov, V. P. (Cent. Res. Inst. Chem., Hung. Acad. Sci., Hung.). *Fiz. Mat. Metody Koord. Khim., Tezisy Dokl., Vses. Soveshch., 5th* 1974 (Pub. 1974), 149–50 (Russ). "Shtiintsa": Kishinev, USSR. $AlCl_3.NH_3$ and $GaCl_3.NH_3$ mols. have ethane-like configuration with staggered arrangement of donor and acceptor groups. The mol. distances are N–H [1.030], 1.024; M–N 1.996, 2.057; and M–Cl 2.100, 2.142 Å for $AlCl_3.NH_3$ and $GaCl_3.NH_3$, resp.; angles are also given. Data are compared with related compds.

структ.
парам.

C. A. 1975. 82 N 24

(+1)

40520.1413 TE.Ch	молек. геометр 40892 02 $AlCl_3 \cdot NH_3$ x	1974 15-4903

Hargittai Istvan, Hargittai Magdolna.
On the bond angle in $AlCl_3$.
"J. Chem. Phys.", 1974, 60, N 6, 2563

(англ.)

0110

ВИНИТИ

жч-8031 / ВФ-2260-XV / 1975

$AlCl_3 \cdot NH_3$

геометр. структ.

х 1975 №10

10 Б71. Электронографическое исследование и расчеты методом ППДП/2 комплекса трихлорида алюминия с аммиаком. Hargittai Magdolna, Hargittai István, Spiridonov Victor P., Pelissier Michel, Labarre Jean-François. Electron diffraction study and CNDO/2 calculations on the complex of aluminium trichloride with ammonia, $Cl_2Al \cdot NH_3$. «J. Mol. Struct.», 1975, 24, № 1, 27—39 (англ.)

Методом газовой электронографии изучена структура молекулы $AlCl_3 \cdot NH_3$ (I). Найдены след. значения основных межъядерных расстояний (r_a, Å) и углов ($\angle\alpha$): Al—Cl 2,100±0,005, Al—N 1,996±0,019, Cl...Cl 3,569±±0,011, Cl...N 3,165±0,012, ∠Cl—Al—Cl 116,9°. Расчеты методом ППДП/2 свидетельствуют в пользу шахматной конформации I, принятой в электронографическом структурном анализе. Полученные данные сопоставлены с данными для родственных соединений, обсуждены изменения конформации молекул при комплексообразовании.

В. Спиридонов

$Cl_3Al \cdot NH_3$ ЖЦ-8031 1975

1975

структ. парам.

50133j Electron diffraction study and CNDO/2 calculations on the complex of aluminum trichloride with ammonia. Hargittai, Magdolna; Hargittai, Istvan; Spiridonov, Victor P.; Pelissier, Michel; Labarre, Jean F. (Cent. Res. Inst. Chem., Hung. Acad. Sci., Budapest, Hung.). *J. Mol. Struct.* 1975, 24(1), 27–39 (Eng). The mol. geometry of the complex $Cl_3Al.NH_3$ was studied by electron diffraction. CNDO/2 calcns. confirmed the assumption of a staggered C_{3v} structure. The interat. distances are: Al-Cl 2.100 ± 0.005, Al-N 1.996 ± 0.019, Cl...Cl 3.569 ± 0.01, and Cl...N 3.165 ± 0.012 Å. The Cl-Al-Cl bond angle is 116.9°. The data indicate strong linkage of donor and acceptor. Variations in the bond configurations of the donor and acceptor are compared with those of the respective free mols.

ВФ-2260-XV

С.А1975 82 N8

$AlBr_3 \cdot NH_3$ Cyvin S. J. 1976

„Spectrosc. Lett" 1976,
9, N 2, 131-137 (англ).

ср. амплит.
колебан.

(см $GaCl_3 \cdot NH_3$; III

$AlCl_3 \cdot N_2$

1976

(Di)

Shirk James S.

J. Chem Phys 1976,
64(2) 910-11 (eng)

(см $AlCl_3$; $\overline{\underline{III}}$)

$Al(NO_3)_3$

1976

85: 86472v Anhydrous aluminum nitrate. Shirokova, G. N.; Zhuk, S. Ya.; Rosolovskii, V. Ya. (USSR). *Zh. Neorg. Khim.* 1976, 21(6), 1464-9 (Russ). $Al(NO_3)_3$ was prepd. from the reaction of $NO_2[Al(NO_3)_4]$ with $AlCl_3$ and then sepd. from excess $AlCl_3$ by vacuum sublimation at 50°. The multiple sublimation of $NO_2[Al(NO_3)_4]$ is an ineffective method for prepg. anhyd. $Al(NO_3)_3$. The soly., thermal decompn., and ir spectra of $Al(NO_3)_3$ were studied. $Al(NO_3)_3$ is a highly volatile compd. with a high degree of covalence of the bands of the bidentate groups with the central metal atom.

И.К.
спектр

C.A. 1976 85 N12

$Br_3Al\cdot NH_3$ оттиск 5377 1977

Br_3GaNH_3

1Б81. Электронографическое исследование структуры молекулярных соединений $Br_3Al\cdot NH_3$ и $Br_3Ca\cdot NH_3$ в паровой фазе. Hargittai Magdolna, Hargittai I., Spiridonov V. P., Ivanov A. A. Electron diffraction investigation of the molecular structures of the addition compounds $Br_3Al\cdot NH_3$ and $BrGa\cdot NH_3$ in the vapour phase. «J. Mol. Struct.», 1977, 39, № 2, 225—230 (англ.)

молекул. структ.

Методом газовой электронографии установлено, что структура $Br_3Al\cdot NH_3$ и $Br_3Ga\cdot NH_3$ сходна со структурой аналогичных хлоридных комплексов. Измеренные значения межъядерных расстояний составляют: $R_{Al-N}=1{,}997\pm0{,}019$, $R_{Ga-N}=2{,}081\pm0{,}023$, $R_{Al-Br}=2{,}264\pm0{,}005$, $R_{Ga-Br}=2{,}288\pm0{,}005$, $R_{Br\ldots Br}=3{,}834\pm0{,}008$A для $Br_3Al\cdot NH_3$ и $R_{Br\ldots Br}=3{,}884\pm0{,}008$A для $Br_3Ga\cdot NH_3$. Углы Br—Al—Br и Br—Ga—Br составляют 116,1° и 116,6° соответственно. Резюме

(+)

Х. 1978 N1

$Br_3Al \cdot NH_3$ 0

1977

$Br_3\,GaNH_3$

Структ. параметры

r_e

87: 76672n Electron diffraction investigation of the molecular structures of the addition compounds aluminum bromide-ammonia ($Br_3Al.NH_3$) and gallium bromide.ammonia ($Br_3Ga.NH_3$) in the vapor phase. Hargittai, Magdolna; Hargittai, I.; Spiridonov, V. P.; Ivanov, A. A. (Cent. Res. Inst. Chem., Hung. Acad. Sci., Budapest, Hung.): *J. Mol. Struct.* 1977, 39(2), 225-30 (Eng). According to an electron-diffraction anal., the mol. geometries of the addn. compds. $Br_3Al.NH_3$ and $Br_3Ga.NH_3$ closely resemble those of their chlorine analogs. The coordination linkages and the acceptor parts are characterized by the internuclear distances (in Å): Al-N, 1.997 ± 0.019; Ga-N, 2.081 ± 0.023; Al-Br, 2.264 ± 0.005; Ga-Br, 2.288 ± 0.005; Br...Br(Al), 3.834 ± 0.008; Br...Br(Ga), 3.884 ± 0.008. With the estd. harmonic corrections, the bond angles Br-M-Br are 116.1 and 116.6° for M = Al and Ga, resp.

оттиск 5374

C.A. 1977. 87 n10

(+1) ☒

AlF_3-NH_3
$AlCl_3$-NH_3
AlF_3-N_2

1978

Curtis L. A.

From Energy Res. Abstr. 1979, 4(8), Abstr No. 19832.

кв. мех.
расчет
структуры,
$И_0$

см. Al_2F_6 – III

NH_4AlCl_4 оттиск 6234 1978

Mairesse G.
et al

ЯМР,
Раман спектр
кристал.
структ.

Can. J. Chem.
1978, 56, 764-71.

X-Ray, Raman infrared, NMR
studies of the crystal structure..

1978

$AlCl_3 \cdot NH_3$
(тв)

Семененко К. Н.
и др.

И. К. спектр
ν_1

Координац. химия,
1978, 4 (11), 1649-52.

(см. $AlCl_3 \cdot NH_3$; I)

$AlF_3 \cdot N_2$
$AlF_3 \cdot NH_3$

1979

Curtiss L. A.

мол.
структ.
U_0
кв. мех.
расчет

U. S. Dep. Commer. Nat. Bur. Stand. Spec. Pub., 1979, N 561/1, 791-807

См. Al_2F_6 / $\overline{III}$

$AlCl_3 \cdot NH_3$

1979

Curtiss L. A.

мол.
структ.
Ио
кв. мех.
расчет

U. S. Dep. Commer. Nat. Bur. Stand. Spec. Pub., 1979, N 561/1, 491-807

Cu AlaF6 i III

$AlCl_3 \cdot NH_3$; $AlBr_3 \cdot NH_3$ оттиск N 8 в папке Hargittai 1979

$GaCl_3 \cdot NH_3$

$GaBr_3 \cdot NH_3$

молекул. структ.

(+1) ☒

Х. 1979 N 23

23 Б100. Изучение молекулярной структуры донорно-акцепторных комплексов галогенидов алюминия и галлия с аммиаком методами газовой электронографии и масс-спектрометрии. Hargittai M., Tamás J., Bihari M., Hargittai I. On the molecular structure of the donor-acceptor complexes of aluminium and gallium halides with ammonia as studied by electron diffraction and mass spectrometry. «Acta chim. Acad. sci. hung.», 1979, 99, № 2, 127—135 (англ.)

Изучены масс-спектры (МС) соединений $MX_3 \cdot NH_3$ (**I**), где M=Al, Ga и X=Cl, Br (энергия электронов 50 эВ, т-ра ионного источника 100 и 150° для хлоридов и бромидов соотв.). Наличие в МС молек. ионов (МИ) указывает на стабильность **I**. Относит. интенсивность МИ уменьшается при замене Al на Ga или Cl на Br. Основным процессом фрагментации для соединений Al является отрыв атома галогена, для соединений Ga — молекулы аммиака. На основании выполненных ранее электронографич. исследований I (см. РЖХим, 1975, 10Б71, 1976, 13Б102, 1978, 1Б81) и лит. данных сопоставлены геометрич. параметры молекул I, MX_3 и M_2X_6. Относит. прочность связи M—N по сравнению с прочностью связей M—X в соединениях I выше, когда M=Al и X=Cl. Г. В. Гиричев

cos

NH_4AlCl_4 $\bar{X}$ - 10303 1980

фотоэл. спектр, Эi структура

93: 104376p The photoelectron spectroscopic characterization of vapors above heated alkali tetrafluoroaluminates, alkali tetrachloroaluminates, and ammonium tetrachloroaluminate. Lassiter, Thomas W.; Allen, J. D., Jr.; Schweitzer, Geo. K. (Dep. Chem., Univ. Tennessee, Knoxville, TN 37916 USA). *J. Electron Spectrosc. Relat. Phenom.* 1980, 19(4), 321-6 (Eng). The high-temp. He(I) photoelectron spectra of gas-phase alkali tetrafluoroaluminates, alkali tetrachloroaluminates, and ammonium tetrachloroaluminate were obtained. The identities of the vapor-phase entities were assigned from data derived by electron diffraction, mass spectrometry, and matrix-isolation and IR spectroscopies. The ionization energies obsd. in the spectra were assigned mol.-orbital origins through the use of theor. calcns. and comparisons with analogous compds.

☒ (42) $MAlF_4$ M = щел. мет.

$MAlCl_4$

C.A. 1980. 93 N10

$N(SCl)_2AlCl_4$ 1980

Schnepel, F. M.,
et al.

Ji ; сил. пост.

Spectrochim. Acta,
Part A 1980, 36A (10),
895-8.

(см. $N(SCl)_2AsF_6$; III).

$Al \ldots NH_3$ 1982

Jordan K.D., Kurtz H.A.
Metal Bond and Interact.
High Temp. Syst. Emphasis.
Alkali Metals. Symp. 181
Meet. Amer. Chem. Soc., Atlanta, Ga, March 31 – Apr. 3,
1981. Washington, D.C., 1982,
377-393

теорет.
расчет
структуры,
энергии
связи,
теплот.
реакций

(см. $Li \ldots OH_2$; $\underline{\overline{III}}$)

$AlCl_3 \cdot NH_3$ (г) 1982

спектр

Rytter E., Hvisten-dahl J., et al.,
J. Mol. Struct.,
1982, 79, 323-328.

(см. AlCl (2); III)

NH_4AlF_4 От. 16503 1983

Couzi M., Loyrance P. L., et al.

Ber. Bunsenges. phys. Chem., 1983, 87, N3, 232-235.

Раман спектр, структурн. фазовый переход.

$AlNH_3$

Om. 17279

1983

Smith S. F., Chandrasekhar J., et al.,

J. Phys. Chem., 1983, 87, N 11, 1898 - 1902.

структ,
ab initio
расчет,
Ae;

Al_4NH_3

1984

Bagus P.S., Herman K., et al.

расчёт структ., E.

J. Chem. Phys., 1984, <u>80</u>, N 9, 4378–4386.

(см. Al_4CO; $\underline{\overline{III}}$)

$NH_3 \cdot AlCl_3$ От. 16601 1983

$NH_3 \cdot AlF_3$

98: 169613m **Raman spectra, ab initio molecular orbital calculations, vibrational analysis, and thermodynamic functions for ammonia:AlX_3 (X = F,Cl,Br).** Papatheodorou, G. N.; Curtiss, L. A.; Maroni, V. A. (Argonne Natl. Lab., Argonne, IL 60439 USA). *J. Chem. Phys.* 1983, 78(6, Pt. 1), 3303–15 (Eng). Raman spectra of gaseous NH_3:$AlCl_3$ and NH_3:$AlBr_3$ were recorded at 400°. The obsd. Raman frequencies in combination with reported IR frequencies for NH_3:$AlCl_3$ and ab initio MO calcns. on NH_3:$AlCl_3$ and NH_3:AlF_3 were used to derive force consts. for all 3 NH_3:AlX_3 complexes (X = F, Cl, Br) based on an adjusted valence force field (AVFF) concept. The resulting force const. calcns. produced complete sets of A_1 and E mode frequencies for each complex. Statistical mech. analyses were then performed using the A_1 and E mode frequencies together with estd. values for the torsional mode of each complex and published enthalpy data. From these analyses, the relative thermodn. stability of each complex was detd. At 700 and 1000 K, NH_3:$AlCl_3$ more stable than NH_3:$AlBr_3$. The reaction of gaseous NH_3 with solid AlF_3 to form NH_3:AlF_3 is not favored in this temp. range, which provides an explanation for the lack of success in prior efforts to produce NH_3:AlF_3.

СКР, сил.пост. термод.ф-ии

f.2

C. A. 1983, 98, N20. NH_3AlF_3, NH_3AlBr_3

$NH_3 : AlF_3$
$NH_3 : AlCl_3$
$NH_3 : AlBr_3$

От. 16601 1983

9 Д539. Спектры комбинационного рассеяния, расчеты молекулярных орбиталей методом ab initio, колебательный анализ и термодинамические функции $NH_3 : AlX_3 (X=F, Cl, Br)$. Raman spectra, ab initio molecular orbital calculations, vibrational analysis, and thermodynamic functions for $NH_3 : AlX_3$ (X=F, Cl, Br). Papatheodorou G. N., Curtiss L. A., Maroni V. A. «J. Chem. Phys.», 1983, 78, № 6, Pt 1, 3303—3315 (англ.)

Изучены спектры комб. рас. (10—3500 $см^{-1}$) комплексов $NH_3 : AlX_3$ (**I**), где X=Cl и Br, в газовой фазе при т-ре 400° С и возбуждении лазерной линией 514,5 нм. Сопоставлены спектры комб. рас. и ИК-поглощения **I**. Методом ab initio рассчитаны значения энергии молекулярных орбиталей в **I**. Проведен анализ норм. колебаний и определены величины констант вал. силового поля **I**. Идентифицированы полосы колебаний

м.п., ν_i,
сил. пост., ΔH

ф. 1983, 18, N9

I типов симметрии a_1 и e. Обсуждена относит. термодинамич. стабильность перечисленных комплексов I. Показано, что при т-ре 700 и 1000 K комплекс I с $X=Cl$ более стабилен, нежели комплекс с $X=Br$. Сделан вывод, что комплексы I обладают этаноподобной структурой, содержащей связи Al—N, причем вращение групп NH_3 вокруг этой связи в комплексах является практически свободным. Библ. 37. И. В. А.

$Al(NH_2)_2^+$

От. 21454 1985

9Д134. Неэмпирическое исследование дикоординированных катионов алюминия и сопоставления с их борсодержащими аналогами. An ab initio study of di-coordinate aluminum cations and comparison with their boron analogs. Coffer Jeffrey L., Petersen John D., Bennett Dennis W. «J. Mol. Struct.», 1985, 122, № 1—2, Suppl.: «Theochem», 23, № 1—2, 115—121 (англ.)

Неэмпирическим методом ССП МО ЛКАО в базисах ОСТ-4ГФ, ОСТ-6ГФ, ОСТ-4-31ГФ и ОСТ-6-31ГФ исследовано электронное строение, гипотетич. катионов $A(NX_2)_2^+$, X=H, CH_3; A=Al (**I** и **II**) и B (**III**, **IV**). Оптимизировались длины связей A—N и углы N—A—N. Барьеры вращения (в базисе ОСТ-6ГФ) найдены равными 1,13; 1,27; 17,6 и 21,0 ккал/моль для **I**—**IV** соответственно; уменьшение барьеров при переходе от **III** и **IV** к **I** и **II**, видимо, обусловлено малостью π-компоненты связи Al—N в сравнении со связью B—N. Для **I**—**IV** наиболее стабильны линейные конфигурации с

геометр., стр.,
Ио

(+3)

Ф 1985, 18, N9.

шахматной конформацией групп NX_2. В **I** и **II** положительный заряд в гораздо большей степени локализован на центральном атоме, чем в **III** и **IV**. Проведенные в том же приближении расчеты трикоординированных систем $A(NX_2)_3$ показали, что, хотя дикоординационные соединения Al, видимо, стабильны и могут существовать в виде интермедиатов, являющихся очень сильными льюисовскими кислотами, маловероятно, чтобы их можно было получить исходя из трехкоординационных соединений. Обсуждено влияние величины базиса на результаты расчетов. В. Л. Лебедев

$AlCl_3 NH_3$
$AlCl_3 ND_3$

От 22380 1985

7 Б1265. ИК-спектры паров при высокой температуре, расчет молекулярных орбиталей и нормальных колебаний $AlCl_3NH_3$ и $AlCl_3ND_3$. High temperature infrared vapour spectra, molecular orbital calculations and vibrational analysis of $AlCl_3NH_3$ and $AlCl_3ND_3$. Sjøgren Carl E., Rytter E. «Spectrochim. Acta», 1985, **A41**, № 11, 1277—1286 (англ.)

В области 50—1800 и 2300—3500 см$^{-1}$ в кюветах для газ. образцов с алмазными окошками при 350—664 К измерены ИК-спектры поглощения и излучения паров $AlCl_3NH_3$ (**I**) и $AlCl_3ND_3$ (**II**). На основе анализа колебательно-вращат. полос, расчета нормальных колебаний для шахматной конформации и сравнения с лит. КР-спектрами сделано отнесение полос. Неэмпирич. квантовохим. расчетами в приближении Хартри-Фока подтверждено наличие заторможенного внутр. вращения в **I**, **II**. Показано, что шахматная конформация более стабильна, чем затененная. Обсуждены закономерности в силовых константах. Н. Л. Арюткина

Vi;

Х. 1986, 19, N 7.

$AlCl_3 \cdot NH_3$ От 22380 1985

$AlCl_3 \cdot ND_3$

103: 203030c **High temperature infrared vapor spectra, molecular orbital calculations and vibrational analysis of trichloroamminealuminum and trichloroammine-d_3-aluminum.** Sjoegren, Carl E.; Rytter, E. (Dep. Chem., Univ. Oslo, 0315 Blindern, Norway). *Spectrochim. Acta, Part A* 1985, 41A(11), 1277–86 (Eng). The IR spectra of $AlCl_3NH_3$ and $AlCl_3ND_3$ vapors were recorded in the 50–1800 and 2300–3500 cm^{-1} regions with an evacuable Fourier transform spectrometer by transmission and emission techniques. Evacuable cells of Ni, having windows of type IIa diamond and sealed with O-rings of Au were employed. All IR active fundamentals were assigned and a valence force field based upon the present IR frequencies was derived. An indirect observation of the inactive torsional mode rules out the possibility of free internal rotation around the Al–N bond and this conclusion was supported by an ab initio calcn. The spectra were interpreted in terms of a staggered C_{3v} structure and anal. of IR band contours and Raman polarization measurements reported in the literature were used as an aid to the assignment of fundamentals.

(ИК спектр)

C.A.1985, 103, N 24

$AlPS_4$

(Om 22665)

1985

103: 186064x Vibrational spectrum and normal coordinate analysis of aluminum tetrathiophosphate polymeric chains. Wibbelmann, C.; Cyvin, B. N.; Cyvin, S. J. (Norges Tek. Hoegsk., Univ. Trondheim, Trondheim, Norway). *Z. Naturforsch., A: Phys., Phys. Chem., Kosmophys.* 1985, 40A(9), 909-12 (Ger). $AlPS_4$ forms edge-sharing tetrahedral chains which are isosteric to SiS_2. The Raman and IR spectra were recorded and assigned on the basis of D_{2d} symmetry of the free mol. Splitting of several bands due to the lower site symmetry in the crystal lattice were treated subsequently using a correlation diagram. The frequencies of internal vibrations were calcd. using a simple model consisting of chain fragments of various lengths.

(ИК, СКР, Di)

C.A. 1985, 103, N22

От. 22665   1985

$(AlPS_4)_n$

Wibbelmann C.,
Cyvin B.N., Cyvin S.

(сил.пост.)
ν_i

Z. Naturforsch.,
1985, A40, N9,
909 – 912.

NH_4AlF_4 оп·24192 1986

Bentrup U., Stodolski R.,
et al.

ИК
спектр

Z. Chem., 1986, 26, N5,
187 – 188.

$AlBr_3NH_3$ 1986

Rytter E., Einarsrud
M. A., et al.

ИК спектр,
см. посл.

Spectrochim. Acta.
Part A 1986, <u>42A</u>(11),
1317–22.

(см. $GaBr_3$; <u>III</u>)

ом 28513 1987

$Cl_3Al\cdot NH_3$

$Cl_3Al\cdot ND_3$

15 Б1324. Колебательные спектроскопические расчеты для молекул $Cl_3Al\cdot NH_3$ и $Cl_3Al\cdot ND_3$. Vibrational spectroscopic calculations for $Cl_3Al\cdot NH_3$ and $Cl_3Al\cdot ND_3$ molecules. Sebestyén Attila. «Acta chim. hung.», 1987, 124, № 6, 845—850 (англ.)

По совокупности эксперим. данных, полученных методами газ. электронографии и колебат. спектроскопии, МНК для молекул $Cl_3Al\cdot NH_3$ (I) и $Cl_3Al\cdot ND_3$ (II) рассчитан набор силовых постоянных I. С полученным силовым полем вычислены средние амплитуды колебаний для разных типов межатомных расстояний в I и II при 0, 298 и 522 K (последняя — т-ра эксперимента). Существенные отличия в эксперим. и рассчитанных величинах амплитуды l(Al—N) объясняются большим сдвигом частоты вал. кол. ν(Al—N) в спектрах крист. I и II (использованных в расчетах силового поля) по сравнению со спектрами газ. в-в (~на 100 см$^{-1}$).

Г. М. Курамшина

М.Л.

Х. 1988, 19, N15

$Cl_3Al \cdot NH_3$
$Cl_3Al \cdot ND_3$

Om·28513

1987

(сил. пост., ν_i)

108: 176004s Vibrational spectroscopic calculations for aluminum chloride.ammonia and aluminum chloride.perdeuterated ammonia molecules. Sebestyen, Attila (Dep. Gen. Inorg. Chem., Veszprem Univ. Chem. Eng., H-8201 Veszprem, Hung.). *Acta Chim. Hung.* 1987, 124(6), 845–50 (Eng). Normal coordinate analyses for the $Cl_3Al.NH_3$ and $Cl_3Al.ND_3$ mols. were performed on the basis of vibrational gas spectra and electron diffraction structural data by the least squares refinements, using an algorithm of generalized matrix inversion. The mean amplitudes of vibration along with their frame contributions were also calcd. Potential barriers to internal rotation were then detd. from the assigned torsional frequency, ν_τ, from the calcd. mean square amplitudes of vibration, $\langle l^2\sigma$bb and from the torsional angle difference, $\langle \Delta\tau \rangle$, between the sym. and distorted equil. structures. Results obtained in the various ways are compared.

C·A·1988, 108, N 20

NH_4AlF_4 От. 26698а" 1987

"

Smith David.

теор. расчёт, вращ. потенц. ф-ии

J. Chem. Phys. 1987, <u>86</u>(7), 4055-65.

(см. NH_4ZnF_3; <u>III</u>)

$F_n AlH_m NH_2$ 1988

Reed Alan E.,
Schleyer Paul v. R.

теор.
расчет
структурн.
параметр.,
стабильн.

Inorg. Chem. 1988,
<u>27</u> (22), 3969-87.

(См. F_2BNH_2; III)

H_2AlNH_2 1990

Lyman M.M.,
Interrante L.V. et al.
геометрия, Gov. Rep. Announ-
расчёт ce. Index (U.S.). 1990
90 (13), Abstr. No
033,222. (см. $(CH_3)_2AlNH_2$; III

$S_4N_4Al^-$ 1990

Rzepa Henry S.,
Woollins J. Derek.

структура, Polyhedron 1990,
расчёт 9 (1), 107–11.

(см. S_4N_4 и др.; III)

NH_4AlH_4 1990

Баранов Л. Я.,
Чаркин О. П.

Ж. неорган. химии. 1990.

м. п. 35, N 11. С. 2888–2898.

(См. NH_4BH_4; III)

NF_4AlF_4

1990

Baranov L. Ya.,
Charkin O. P.
Zh. Neorg. Khim.
1990, 35 (11), 2899–
2905.
(см. NF_4BF_4; III)

расчёт
структ.,
D_0

Al^+N_2 Оm. 37 063 1991

He L.X., Hammond T.D.,
Winstead C.B., Cole J.L., –
J. Chem. Phys., 1991, 95,
N10, 7183 – 7193
Electric- field - enchanced

молекул.
констр.,
расчет

laser-induced plasma spectroscopy of jet-cooled metal-based ion-molecule complexes.

$AlH_3 \cdot NH_3$

1992

4 Д63. Алан аммиака. Ammonia alane / Marsh Craig M. B., Hamilton Tracy P., Xie Yaoming, Schaefer Henry F. (III) // J. Chem. Phys. .— 1992 .— 96 , № 7 .— С. 5310—5317 .— Англ.

Методами конфигурац. взаимодействия и связанных кластеров в расширенных базисах исследованы молекулы AlH_3/NH_3 (I), AlH_3 и NH_3. Определена энергия диссоциации I, равная 26 ккал/моль. Показано, что поскольку сохраняется дативная природа связи Al—N, группы AlH_3 и NH_3 не испытывают существенных изменений при образовании I. Рассчитаны параметры равновесной геометрии, частоты гармонич. колебаний, ИК-интенсивности, атомные заряды и дипольный момент I.

М-Л·

Ф. 1993, N 4

$AlNO_3$

1992

200845a **IR and Raman spectra of silver nitrate at low peratures.** Shen, Z. X.; Sherman, W. F.; Kuok, M. H.; Tang, H (Dep. Phys., Natl. Univ. Singapore, Singapore, Singapore *J. Raman Spectrosc.* 1992, 23(9), 509-14 (Eng). The IR of $AgNO_3$ were recorded using single-crystal samples and ured radiation. More detailed information was obtained than reported in previous studies using polycryst. samples. The very IR absorption bands of the ν_3 and ν_2 modes were studied by ured reflection measurements. Raman spectra of $AgNO_3$ were recorded and used to provide supplementary data. Better ments for the components of the fundamental modes were ned using the polarized spectra, and some isotope and combination were also obsd. and assigned. The present data allow a better standing of the splittings of the fundamental modes. The temp. phase showed a softening of the ν_3 and ν_4 modes as the stals were cooled below the transition temp. (140 K), and this a limited (*P*, *T*) range of stability for this phase.

(ν_i)

C.A. 1992, <u>117</u>, N20

AlH_3NH_3 Chaillet Max, 1994
Dargelos A. et al.

ab initio
расчёт
структ.
и энергии
связи

New. J. Chem. 1994,
18 (6), 693–700.

(См. BH_3NH_3; III)

$AlNH_2$
$AlNH_3$
$AlNH_4$

ОМ 37748 (только (Сп) 1994

2Б1047. Кратные связи алюминий—азот в малых молекулах AlNH. Структуры и колебательные частоты $AlNH_2$, $AlNH_3$ и $AlNH_4$. Aluminum—nitrogen multiple bonds in small AlNH molecules: Structures and vibrational frequencies of $AlNH_2$, $AlNH_3$, and $AlNH_4$ /Davy Randall D., Jaffrey Kent L. //J. Phys. Chem. .—1994 .—98 ,№ 36 .—С. 8930—8936 .—Англ.

Методами Хартри-Фока, конфигурац. вз-вия и в приближении связанных кластеров определены равновесные геометрич. параметры и частоты колебаний изомеров молекул $AlNH_2$, $AlNH_3$ и $AlNH_4$. Найдено, что структурные ф-лы низших по энергии изомеров можно представить в виде $Al—NH_2$, $HAl—NH_2$ и $H_2Al—NH_2$. Обсуждена формальная кратность связи Al—N в различных соед., к-рая может варьироваться от 1 до 3. А. В. Немухин

М.Л.

Х.1995, N2

$AlNH_2$
$AlNH_3$
$AlNH_4$

87 748 (отна ст.) 1994

121: 164357q Aluminum–Nitrogen Multiple Bonds in Small AlNH Molecules: Structures and Vibrational Frequencies of $AlNH_2$, $AlNH_3$, and $AlNH_4$. Davy, Randall D.; Jaffrey, Kent L. (Department of Chemistry, Liberty University, Lynchburg, VA 24506 USA). *J. Phys. Chem.* 1994, 98(36), 8930–6 (Eng). Ab-initio mol.-electronic-structure methods were used to study aluminum–nitrogen analogs of the simplest alkyne and alkene mols. and their isomers, and the exptl. studied $AlNH_3$. Geometries, relative energies, and harmonic vibrational frequencies of isomers having the formulas $AlNH_2$, $AlNH_3$, and $AlNH_4$ were obtained at the SCF, single and double excitation CI (CISD), and coupled cluster including all single and double substitutions (CCSD) levels of theory. The lowest energy isomers were $Al–NH_2$, $HAl–NH_2$, and $H_2Al–NH_2$. The HAl–NH isomer is quasi-linear, and has a theor. bond length indicative of a triple bond. It, however, is very high energy, as evidenced by the very large neg. heat of hydrogenation, –62 kcal/mol, and the lower energy of the $Al–NH_2$ isomer. The double bond (σ bond plus N to Al π donation) is much more favorable. The strength of the Al–N bond depends strongly on the no. of hydrogens on the aluminum atom because the hydrogens increase the Lewis acid strength of the aluminum atom. The addn. and insertion products of aluminum atoms and ammonia are fully characterized, and compared to previous exptl. and theor. studies.

ν_i, структура, стабильность, теор. расч

C.A. 1994, 121, N 14

(AlN)x 1995

Lambrecht W.R.L.,

обзор энергии связи

Lee C.H. et al.

NATO ASI Ser., Ser. 3

1995, 1, 335-372.

(см. BN; D)

AlH_3NH_3 1995

Leboeuf, Martin;
Russo, Nino; et al.;

(V_0) J. Chem. Phys., 1995,
<u>103</u> (17), 7408-13.

(см. BH_3NH_3; <u>III</u>)

AlH_3NH_3 от: 38234 1995

мол. структ.,
колебат. част.,
D_0, V_{ep}.

Martin Leboeuf,
Nino Russo et al.,

J. Chem. Phys., 1995,
<u>103</u> (17), 7408 ....

A density functional

study of borane and alane
monoammoniate.

$Al_{\widehat{n}}N_{\widehat{n}}$

$n = 12, 16$

теор.
расчёт
структ.
парам.,
I, $\Delta_f H$.

1995

Stankevich I.V.
Chistyakov A.L.,
et al.

Zh. Strukt. Khim.
1995, 36 (6), 976-82.

(см. $B_{\widehat{n}}N_{\widehat{n}}$; III)

Ar-N=S 1996

теор. и экспер. иссл. в газ. фазе

Chem. Ber., 1996, 129, №11, p. 1379–1381.

$(AlN)_{12}$ 1996

Zandler M.E.

Behrman E.C. et al.

теор. расчёт структ., Vi, стаб.

THEOCHEM 1996, <u>362</u> (2), 215–24.

●

(см. $(ZnO)_n$, <u>III</u>)

$Al(N_3)_3$ 1996

Linnen C.J., Gilbert J.V.,

ИК в матрице

Int. Conf. Low Temp. Chem., 2nd 1996, 143–144.

(См. В $●(N_3)_3$; III)

H_2AlNSO

1996.

Pasinszki T.,
Veszpremi T., et al.
Chem. Phys. Lett.,
1996, 250 (5,6), 466-
470.

структур.,
теор.
расчет

(см. LiNSO; II)

1996

F: Al(NH3)+
P: 3

97. 13Б157. Применение гибридных методов, объединяющих теории функционала плотности и Хартри-Фока. Геометрии и энергии диссоциации комплексов Al{+}. Application of density functional theory/Hartree-Fock hybrid methods. Geometries and bond dissociation energies of Al{+} complexes / Stockigt D. // Chem. Phys. Lett. - 1996. - 250, N 3 - 4. - С. 387-392. - Англ.

С помощью гибридного подхода, объединяющего метод функционала плотности и неэмпирический метод ССП, рассчитаны геометрии и энергии разрыва связи в комплексах Al{+}-X (X=CH[3], NH[3], H[2]O, OH, HF, HCN, HNC, CO, CN, CH[2]O, CO[2], N[2], O[2], F[2]). Результаты, полученные при использовании функционалов B3LYP/6-311++ГФ(3df, 2p)//B3LYP/6-311++ГФ(d, p), хорошо согласуются с эксперим. данными и расчетами уровня Гауссиан-2.

РЖХ 1997

$HAlNH_2$
$AlNH_2$
$HAlNH$

От 38 886 1997

127: 72362h Reactions of Laser–Ablated Aluminum Atoms with Ammonia. Infrared Spectra of $HAlNH_2$, $AlNH_2$, and HAlNH in Solid Argon. Lanzisera, Dominick V.; Andrews, Lester (Department of Chemistry, University of Virginia, Charlottesville, VA 22901 USA). *J. Phys. Chem. A* **1997**, 101(28), 5082–5089 (Eng), American Chemical Society. Pulsed laser–ablated Al atoms react with NH_3 to give 2 major products, $HAlNH_2$ and $AlNH_2$, which are trapped in solid Ar and identified from IR spectra through isotopic substitution (^{15}N, D) and MP2 calcns. of product structures and isotopic frequencies. The bent HAlNH mol. was a minor product.

спектр
в Ar

м.н.

C. A. 1997, 127, N 5

$AlCl_3 \cdot NH_3$ 1997

126: 321641a The Chemical Vapor Deposition of Aluminum Nitride: Unusual Cluster Formation in the Gas Phase. Timoshkin, Alexey Y.; Bettinger, Holger F.; Schaefer, Henry F. III (Department of Chemistry, St. Petersburg State University, St. Petersburg, Russia 198904). *J. Am. Chem. Soc.* 1997, 119(24), 5668–5678 (Eng), American Chemical Society. An ab initio investigation of the chem. vapor deposition of AlN from the $AlCl_3NH_3$ adduct is presented. Geometries, harmonic vibrational frequencies and relative energies for the $AlCl_3NH_3$ adduct, its dissocn. products $AlCl_n$, NH_n (n = 1–3), and ring and cluster compds. [$(Cl_2AlNH_2)_n$ (n = 1, 2), $(ClAlNH)_n$ (n = 1, 2, 3, 4, 6)] are discussed. The Al–N bond lengths in the investigated compds. are strongly dependent on the coordination nos. of the aluminum and nitrogen centers, decreasing from 2.0 Å for 4–coordinated Al/N centers to 1.79 and 1.68 Å for 3– and 2–coordinated Al/N centers, resp. Thermodn. anal. shows that dissocn. of Cl_xAlNH_x (x = 2, 3) compds. with elimination of HCl and simultaneous formation of oligomeric forms is preferable to the process of dissocn. into components or simple HCl detachment. Under std. conditions gaseous 4–coordinated Al/N compds. $(ClAlNH)_6$ and $(ClAlNH)_4$ are more stable than 3–coordinated $(ClAlNH)_2$ and $(ClAlNH)_3$ compds. In 4–membered rings and clusters, the electrostatic repulsion between nearby Al–Al and N–N atoms makes reorganization to 6–membered rings extremely favorable. The suggested mechanism of AlN deposition involving cluster formation in the gas phase is discussed.

структура,
частоты
колебаний,
ab initio
расчет

C.A. 1997, 126, N24

$Al_2N_3H_5$

1997

127: 195707g About the aromaticity of $Al_2N_3H_5$. Nyulaszi, Laszlo (Department of Inorganic Chemistry, Technical University of Budapest, H–1521 Budapest, Hung.). *J. Chem. Soc., Dalton Trans.* 1997, (13), 2373–2375 (Eng), Royal Society of Chemistry. Ab initio quantum-chem. calcns. showed that the $Al_2N_3H_5$ ring is not planar, mainly as a result of the repulsion of the neighboring nitrogen lone pairs. The planar structure, which is a saddle point on the potential energy surface, however, is 1.01 kcal mol^{-1} less stable at the CCSD(T)/6–311 + G(2D)//MP2/6–311 + G(2D) + ZPE level of theory than the min.-energy structure. According to energy criteria, the aromaticity of the mol. is small at most. The geometric criteria on the other hand were shown to be useless in the prediction of aromaticity in this case.

ab initio
расчет,
стр-ра,
стабильн.

C-A. 1997, 127, N 14

$(HAlNH)_n$

1998

$n=2-4$

стр-ра
и
стабильн.,
ab initio
расчет

CA 1998, 129, №10

129: 127360e **Structure and stabilities of $(HAlNH)_n$ (n = 2−4).** Chen, Xian Yang; Li, Chong De; Wu, Tao; Yao, Tian Yang; Ju, Guan Zhi (State Key Laboratory Coordination Chemistry, Coordination Chemistry Institute, Department Chemistry, Nanjing University, Nanjing, Peop. Rep. China 210093). *Theor. Chem. Acc.* 1998, 99(4), 272−276 (Eng), Springer−Verlag. Ab initio mol. electronic structure methods were used to study the relative stability of the planar inorg. ring $(HAlNH)_n$ (n = 2−4) during homodesmotic and monomer polymn. reactions. Optimized geometries, frequencies, and energies through RHF/6−31G* are reported, and energies at the SCF optimized geometries including Moeller−Plesset 4th perturbation theory with single, double, and quadruple excitation (MP4SDQ) corrections are also reported for both reactions. Homodesmotic reactions with MP4SDQ −28.5 kcal/mol for $(AlN)_2$, 1.9 kcal/mol for $(AlN)_3$ and −0.97 kcal/mol for $(AlN)_4$. On analyzing a π−MOs diagram, only 1, 3, and 3 strongly bonding π−MOs exist for the planar 4−, 6−, and 8−membered AlN rings, resp.

$(HAl-NH)_2$

$(H_2Al-NH_2)_2$

1998

process initiated by Fe_2O_3.

128: 300233v **Structure, Spectra, and Reaction Energies of the Aluminum–Nitrogen $(HAl-NH)_2$ and $(H_2Al-NH_2)_2$ Rings and the $(HAl-NH)_4$ Cluster.** Davy, Randall D.; Schaefer, Henry F., III (Department of Chemistry, Liberty University, Lynchburg, VA 24502 USA). *Inorg. Chem.* **1998**, 37(9), 2291–2295 (Eng), American Chemical Society. Rings of four-coordinate aluminum and nitrogen are easily synthesized and well studied, as are clusters of four-coordinate Al and N. Only recently, however, have rings that are derivs. of the model compds. $(HAl-NH)_n$ ($n = 2, 3$) with three-coordinate Al and N been synthesized. Ab initio investigations of the structure, bonding, vibrational spectra, and reaction energies for the three-coordinate ring $(HAl-NH)_2$, the four-coordinate ring $(H_2Al-NH_2)_2$, and the four-coordinate cluster $(HAl-NH)_4$ are presented. Even in the absence of differences in steric factors, the four-membered ring has longer Al–N bonds than either the six-membered ring or the unassocd. aluminum amide, H_2Al-NH_2. This is due to both rehybridization and π interactions. Theor. reaction energies for formation of the $(HAl-NH)_4$ cluster from the $(H_2Al-NH_2)_2$ ring are consistent with intermol. loss of hydrogen, or the necessity of surface catalysis.

Структура
спектр,
хемим.

C.A. 1998, 128, N24

$Al_3N_3H_6$ 1998

Jemmis, Eluvathingal D., et al.,

теор. Inorg. Chem. 1998, <u>37</u>(9),
расчет 2110 - 2116
стр-ры.
стабильн

(см. $B_3N_3H_6$, <u>III</u>)

Al_nN

1998

$n=2-6$

128: 248812s **Evolution of bonding in Al_nN clusters: transition from nonmetallic to metallic character.** Nayak, S. K.; Khanna, S. N.; Jena, P. (Physics Department, Virginia Commonwealth University, Richmond, VA 23284–2000 USA). *Phys. Rev. B: Condens. Matter Mater. Phys.* **1998**, 57(7), 3787–3790 (Eng), American Physical Society. The evolution of the equil. geometry, binding energy, and electronic structure of Al_nN clusters has been studied using first-principles calcns. based on d.-functional theory. The bonding in small ($n = 2-6$) Al_nN clusters, in analogy with the electronic structure of bulk aluminum nitride, is found to be intermediate between ionic and covalent. However, the electronic structure takes on a metallic character in $Al_{12}N$ and the cluster's chem. is seen to mimic the chem. of an alkali atom. The calcns. also reveal the existence of an anomalously stable Al_3N cluster, in sharp contrast with the bulk stoichiometric compn.

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стр-ры
и стаб.

C.A. 1998, 128, N20

Al–N_2 ФГ 39616 1998

Спектр,
М.П.

130: 174617z **Electronic spectroscopy and excited state dynamics of the Al–N_2 complex.** Yang, Xin; Gerasimov, Irina; Dagdigian, Paul J. (Department of Chemistry, The Johns Hopkins University, Baltimore, MD 21218–2685 USA). *Chem. Phys.* 1998, 239(1–3), 207–221 (Eng), Elsevier Science B.V.. The weakly bound Al...N_2 complex was prepd. in a pulsed supersonic beam and studied with laser fluorescence excitation spectroscopy. Transitions to bound vibrational levels in electronic states correlating with the Al(5s, 4d) + N_2 asymptotes were obsd. Resonance fluorescence from the excited levels could not be detected. These excited levels decay nonradiatively, and the excitation

AlAr

С.А. ④ 1999, 130, N13

spectrum was obtained by monitoring emission from the lower Al at. levels. The band systems were dominated by progressions in the excited state Al–N stretch vibrational mode. Vibrational assignments were made through anal. of N isotope shifts. The rotational contours were obscured by Lorentzian line broadening from the nonradiative decay. For excitation to the Al(5s)...N_2 state the rotational structure of bands with small linewidths was consistent with a ${}^2\Sigma^+ - {}^2\Pi$ electronic transition of a linear mol., in accord with the previously calcd. linear structure of the ground state (Chaban, G., and Gordon, M.S., 1997). The excited state binding energies are 1218 ± 10 cm^{-1} for the Al(5s)...N_2 state [${}^2\Sigma^+$ symmetry] and 2705 ± 165 cm^{-1} for the Al(4d)...N_2 state of ${}^2\Delta$ symmetry. From the threshold for formation of Al(5s) from the nonradiative decay of Al-(4d)...N_2, an upper bound to the ground state dissocn. energy $D_0'' \leq 354 \pm 2$ cm^{-1} was obtained. For comparison with high–resoln. scans over Al...N_2 bands, similar scans were recorded and analyzed over several bands of the AlAr $H^2\Sigma^+ - X^2\Pi_{1/2}$ transition, which correlates with the Al 5s ← 3p at. transition. Excited–state rotational consts. were derived and employed to obtain $B_e' = 0.1128 \pm 0.0020$ cm^{-1}, and hence $R_e' = 3.05 \pm 0.03$ A. A weak predissocn., giving Al(3d), was obsd. for AlAr-($H^2\Sigma^+$).

F: AlnNn
P: 3

1999

132:69574 The structure of AlnNn (n=2-4) clusters: a DFT study. BelBruno, J. Burke. Laboratory, Department of Chemistry, Dartmouth Molecular Materia Group, Dartmouth College Hanover, NH, USA
Chem. Phys. Lett., 313(5,6), 795-804 (English) 1999 The geometry, harmonic vibrational frequencies and stability of the structural isomers of small aluminum nitride clusters were investigated. lowest energy structures are cyclic with Dnh symmetry. The caged structu Al4N4 lies higher in energy than the planar cumulenic monocyclic ring. T bond dominates the structures for many isomers so that one preferred diss channel is loss of the AlN monomer. The properties of the aluminum nitri clusters are similar to those of the BN clusters even though the aluminum have a significantly larger at. radius.

C.A.2000, 132

AlN_3
Al_3N
Al_2N_2

ФГ 39679

1999

130: 272272c **Ab Initio Investigation of Structures and Energies of Low–Lying Electronic States of AlN_3, Al_3N, and Al_2N_2.** Boo, Bong Hyun; Liu, Zhaoyang (Department of Chemistry, Chungnam National University, Taejon, 305–764 S. Korea). *J. Phys. Chem.* A **1999**, 103(9), 1250–1254 (Eng), American Chemical Society. The structures and energies of low–lying electronic states of AlN_3, Al_3N, and Al_2N_2 were evaluated at the HF, MP2, QCISD(T), CCSD, and CCSD(T) levels of theory, using several basis sets of 6–31G* (for HF), cc–pVDZ (for MP2 and QCISD(T)), and cc–pVTZ (for CCSD and CCSD(T)). The ground state of AlN_3 was predicted to be a $^1\Sigma^+$ state with a linear Al–N–N–N structure. The most stable species of Al_3N was found, however, to have D_{3h} symmetry and $^1A'_1$ ground state. For Al_2N_2, various isomers were

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С.А., 1999, 130, N20

found to be energetically favorable. A rhombic isomer with the N atoms along the short diagonal and with a $^{1}A_{g}$ electronic state is the lowest in energy at the MP2/cc−pVDZ, QCISD(T)/cc−pVDZ, CCSD/cc−pVTZ, and CCSD(T)/cc−pVTZ levels. A linear structure Al−N−N−Al with a $^{3}\Sigma g^{-}$ electronic state is the second lowest. The third stable isomer with Al atoms bonded directly to the N_2 π orbital seems to be one of the model species for the sake of the nitrogen fixation. The formation of a variety of configurations of Al_2N_2 is energetically plausible under the reaction conditions employed since the energy differences in the Al_2N_2 species are relatively small.

AlN От 39964 1999

AlN^-

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стабиль-
ность

Gutsev G. L. et al.,

J. Chem. Phys., 1999,
10, N6, 2928-35

(Ом. 40 010) 1999

Al_nN_n

(n=2-4)

Joseph J. BelBruno,

стр-ра

Chem. Phys. Lett. 1999, 313, 795-804.

The structure of Al_nN_n (n=2-4) clusters: a DFT study

F: AlNH3
P: 3

1999

132:56342 Zero kinetic energy spectroscopy of AlNH3 complex. Yang, D.-S.; Miyawaki, J.

Department of Chemistry, University of Kentucky Lexington, KY, USA Chem. Phys. Lett., 313(3,4), 514-518 (English) 1999 Pulsed field ionization-zero kinetic energy photoelectron spectrum of the jet-cooled Al-NH3 complex, AlNH3, was obsd. for the 1st time. The spectrum shows vibronic transitions from 2 spin-orbit levels of the neutral ground state, which allows the measurement of the

C.A. 2000, 132

following spectroscopic consts.: ionization potential (39{  omitted}746 cm-1), spin-orbit splitting (58 cm-1), intermol. stretching vibrational frequencies (.omega.3+=339 cm-1, .omega.3+x3+=3.1 cm-1, and .nu.3=227 cm-1), and intermol. bending frequency (.nu.6+=557 cm-1). The observation of the spin-orbit splitting confirms that the ground state of the neutral complex is the 2E state.

Эƒ.40640

2000

F: Al3N
P: 3'

132:229128 Reactions of Laser-Ablated Aluminum Atoms with Nitrogen Atoms Molecules. Infrared Spectra and Density Functional Calculations for the A Al2N, Al2N2, AlN3, and Al3N Molecules. Andrews, Lester; Zhou, Mingfei; Chertihin, George V.; Bare, William D.; Hannachi, Yacine Chemistry Department, University of Virginia Charlottesville, VA 22901, USA J. Phys. Chem. A, 104(8), 1656-1661 (English) 2000 Laser-ablated Al atoms react with

C.A. 2000, 132

dinitrogen on condensation at 10 K to form N3 radical and the subject mols., which are identified by N isotopic substitution, further reactions on annealing, and comparison wit isotopic frequencies computed by d. functional theory. The major AlN3 product is identified from 3 fundamentals and a statistically mixed N isotopic octet pattern. The Al rich Al2N and Al3N species are major prod on annealing to allow diffusion and further reaction of trapped species. This work provides the 1st exptl. evidence for mol. AlxNy species that ma involved in ceramic film growth.

2000

g. 40640

F: AlN2
P: 3
132:229128 Reactions of Laser-Ablated Aluminum Atoms with Nitrogen Atoms Molecules. Infrared Spectra and Density Functional Calculations for the A Al2N, Al2N2, AlN3, and Al3N Molecules. Andrews, Lester; Zhou, Mingfei; Chertihin, George V.; Bare, William D.; Hannachi, Yacine Chemistry Department, University of Virginia Charlottesville, VA 22901, USA J. Phys. Chem. A, 104(8), 1656-1661 (English) 2000 Laser-ablated Al atoms react with

C. A. 2000, 132

dinitrogen on condensation at 10 K to form N_3 radical and the subject mols., which are identified by N isotopic substitution, further reactions on annealing, and comparison wit isotopic frequencies computed by d. functional theory. The major AlN_3 product is identified from 3 fundamentals and a statistically mixed N isotopic octet pattern. The Al rich Al_2N and Al_3N species are major prod on annealing to allow diffusion and further reaction of trapped species. This work provides the 1st exptl. evidence for mol. Al_xN_y species that ma involved in ceramic film growth.

Al_2N_2 AlN_3 Al_2N 2000

ф.40640

F: Al2N2 \
P: 3
132:229128 Reactions of Laser-Ablated Aluminum Atoms with Nitrogen Atoms Molecules. Infrared Spectra and Density Functional Calculations for the A Al2N, Al2N2, AlN3, and Al3N Molecules. Andrews, Lester; Zhou, Mingfei; Chertihin, George V.; Bare, William D.; Hannachi, Yacine Chemistry Department, University of Virginia Charlottesville, VA 22901, USA J. Phys. Chem. A, 104(8), 1656-1661 (English) 2000 Laser-ablated Al atoms react with

C.A. 2000, 132

dinitrogen on condensation at 10 K to form N_3 radical and the subject mols., which are identified by N isotopic substitution, further reactions on annealing, and comparison wit isotopic frequencies computed by d. functional theory. The major AlN_3 product is identified from 3 fundamentals and a statistically mixed N isotopic octet pattern. The Al rich Al_2N and Al_3N species are major prod on annealing to allow diffusion and further reaction of trapped species. This work provides the 1st exptl. evidence for mol. Al_xN_y species that ma involved in ceramic film growth.

Al · NH_3 | Ūn · 40415 | 2000

Hans-Jörg Himmel Anthony J. Downs, and Tim M. Greene,

J. Am. Chem. Soc., 2000, <u>122</u>, 9793-9807

Thermal and photochemical
Reactions to Aluminium,

Gallium, and Indium Atoms
(M) in the Presence of Ammonia:
Generation and Characterization
of the Species $M \cdot NH_3$, $HMNH_2$,
MNH_2, and H_2MNH_2

$(AlN)_n$ От. 40539 2010

Wu Haisun et al.,

структура, стабилн. Science in China (Series B), 2000, <u>43</u>, N6, 634-642.

F: AlND3
P: 3

2000

132:300424 The excited electronic states and the ionization potential of the AlND3 complex.

Jakubek, Zygmunt J.; Simard, Benoit

Steacie Institute for Molecular Sciences, National Research Council Ottawa, ON K1A 0R6, Can. J. Chem. Phys., 112(4), 1733-1743 (English) 2000 [illegible]

The AlND3 complex was studied in a mol. beam by resonant one-color two-photon and two-color two-photon photoionization techniques with a resoln. of 0.3 cm-1. Six progressions of bands were obsd. in the 18100-26200 cm-1 (381-552 nm) region. One progression (.omega.e = 316 .+-. 0.8 cm-1) was assigned to the Al-ND3 stretch (.nu.3') in the B2A1 state correlating with the 3s2S term of

C-A. 2000

Al. The origin of the B2A1-X2E1/2 system was found at 18532.5 .+-. 0.7 cm-1. The second (.omega.e = 428 .+-. 2 cm-1) and third (.omega.e = 594 .+-. 12 cm-1) progressions were assigned to the Al-ND3 stretch (.nu.3') and the bend (.nu.6') in the C2E state correlating with the 3d2D term of Al. The origin of the C2E-X2E1/2 system was found at 21185 .+-. 5 cm-1. Assignments of the other three progressions with origins and harmonic wave nos. of 22667 .+-. 2 and 358 .+-. 2 cm-1; 24382 .+-. 10 and 432 .+-. 10 cm-1; and ~21871 and ~1050 cm-1 remain uncertain. The spin-orbit splitting of the X2E ground state was detd. to be 55.8 .+-. 0.7 cm-1. Several Rydberg series converging to the v3+ = 1, 2 and 3 levels of the ground state of the AlND3+ ion were obsd. The ionization potential of the AlND3 complex was measured to be 39710 .+-. 2 cm-1. The .nu.3+ fundamental in the ground state of the AlND3+ ion was found to be 325 .+-. 5 cm- 1. To aid the interpretation of our spectra, ab initio optimized structures and vibrational wave nos. for the ground states of various isotopomers of AlNH3 and AlNH3+ were calcd. Also, Al-NH3 potential curves for several low-lying excited states were calcd. In addn., the ionization potential of the AlNH3 isotopomer was measured by the one-photon photoionization efficiency technique. The value of 39760 .+-. 10 cm-1 is an improvement on that reported previously, which was 180 cm-1 smaller.

$(AlN)_x$

$x = 1, 2, 4, 6, 12$

05 1128

2001

135: 322975k **A density functional study of small $(AlN)_x$ clusters: structures, energies, and frequencies.** Chang, C.; Patzer, A. B. C.; Sedlmayr, E.; Steinke, T.; Sulzle, D. (Zentrum fur Astronomie und Astrophysik, Technische Universitat Berlin, D−10623 Berlin, Germany). *Chem. Phys.* **2001**, 271(3), 283−292 (Eng), Elsevier Science B.V. Structural properties of energetically low−lying stationary points of small aluminum/nitrogen clusters with unity stoichiometric ratio $(AlN)_x$ (x = 1,2,4,6,12) have been investigated by theor. d. functional techniques employing the Becke−Perdew−86 gradient cor. exchange correlation functional. A large no. of singlet and triplet stationary points representing local min. and transition structures of $(AlN)_x$ are completely characterized. We report energies, equil. geometric parameters, selected harmonic vibrational wave nos. along with corresponding absorption coeffs. Stability and geometric aspects of $(AlN)_{12}$ are discussed in detail by introducing a measure of sphericity.

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стр-ры и
энергии кол, ν_i

C.A. 2001, 135, N22

2001

F: Al-N2
P: 3

134:317667 **Electronic spectroscopy and excited state dynamics of aluminum atom-molecule complexes.** Dagdigian, Paul J.; Yang, Xin; Gerasimov, Irina; Lei, Jie. Department of Chemistry, The Johns Hopkins University, Baltimore, MD, USA. Editor(s): Campargue, Roger. At. Mol. Beams (2001), 367-378. Publisher: Springer-Verlag, Berlin, Germany Conference; General Review written in English.

Review with 21 refs. The authors review the electronic spectra of Al-mol. complexes including Al-H2, Al-N2 and Al-CH4.

Al_3N_3

дм. 40862

2001

135: 157927m **Theoretical Study of Structural and Vibrational Properties of Al_3N_3, Ga_3N_3, and In_3N_3.** Kandalam, Anil K.; Blanco, M. A.; Pandey, Ravindra (Department of Physics, Michigan Technological University, Houghton, MI 49931 USA). *J. Phys. Chem. B* 2001, 105(26), 6080–6084 (Eng), American Chemical Society. We report DFT–GGA study of structure, stability, and vibrational properties of Al_3N_3, Ga_3N_3, and In_3N_3. The calcd. results reveal a distinct structural difference between the most stable isomers of Al and those of Ga and In, which can be explained in terms of the evolution of the relative strengths of metal–nitrogen and metal–metal bonds in going from Al to Ga to In. The strength of the N–N bond still dominates the preferred fragmentation path for these clusters and that fragmentation occurs at a lower energy than ionization. Assignments to the frequencies of the various normal modes are made in terms of those of the MN monomers (Al_3N_3) or in terms of those of weakly bonded $(M_3)^+$ and $(N_3)^-$ subunits (Ga_3N_3 and In_3N_3)

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Di

$H_{\bar{m}} Al_{\bar{n}} N_{\bar{n}} H_{\bar{m}}$

2001

135: 157922f **Bonding behavior of polycyclic compounds $X_m \cdot Al_nN_nH_m$ (X = Cl, H).** Wu, Hai–shun; Xu, Xiao–hong; Zhang, Cong–jie; Zhang, Fu–qiang (Department of Chemistry, Shanxi Normal University, Linfen, Peop. Rep. China 041004). *Huaxue Xuebao* 2001, 59(5), 676–684 (Ch), Kexue Chubanshe. The optimized geometries, IR spectra and bonding behavior of $X_mAl_nN_nH_m$ (X = Cl, H; n = 3, 5, 7, 8, 10, 12; m = 3, 4, 5, 6) polycyclic compds. were investigated using HF and B3LYP (DFT) methods at the 6–31G* level. The structures were compared with corresponding $X_mC_{2n}H_m$ series compds. such as benzene, naphthalene, phenanthrene, pyrene, perylene and coronene. The results show that $X_mAl_nN_nH_m$ and $X_mC_{2n}H_m$ share the same geometries; the bond energy of Al–N increases and bond length decreases gradually with R increasing (R is the ratio of ligand atoms' no. to skeleton atoms' no.); the ligand atom X slightly affects the skeleton bond (Al–N or C–C).

структура,
ИК спектр,
теор. расч.

$Cl_m Al_n N_n H_m$ 2001

стр-ра, ИК спектр, теор. расчет

135: 157922f **Bonding behavior of polycyclic compounds $X_m\cdot Al_nN_nH_m$ (X = Cl, H).** Wu, Hai-shun; Xu, Xiao-hong; Zhang, Cong-jie; Zhang, Fu-qiang (Department of Chemistry, Shanxi Normal University, Linfen, Peop. Rep. China 041004). *Huaxue Xuebao* 2001, 59(5), 676-684 (Ch), Kexue Chubanshe. The optimized geometries, IR spectra and bonding behavior of $X_mAl_nN_nH_m$ (X = Cl, H; n = 3, 5, 7, 8, 10, 12; m = 3, 4, 5, 6) polycyclic compds. were investigated using HF and B3LYP (DFT) methods at the 6-31G* level. The structures were compared with corresponding $X_mC_{2n}H_m$ series compds. such as benzene, naphthalene, phenanthrene, pyrene, perylene and coronene. The results show that $X_mAl_nN_nH_m$ and $X_mC_{2n}H_m$ share the same geometries; the bond energy of Al-N increases and bond length decreases gradually with R increasing (R is the ratio of ligand atoms' no. to skeleton atoms' no.); the ligand atom X slightly affects the skeleton bond (Al-N or C-C).

(AlN)n

2001

135: 97688x Structure and stability of aluminum nitride clusters. Xu, Xiaohong; Jin, Zhihao; Wang, Yonglan (School of Materials Science and Engineering, Xi'an Jiaotong University, Xi'an, Peop. Rep. China 710049). *Xi'an Jiaotong Daxue Xuebao* 2001, 35(2), 183–186 (Ch), Xi'an Jiaotong Daxue Xuebao Bianjibu. The d. functional theory (DFT) method was used to predict geometries, electronic states and total energies both of aluminum nitride and hydrogenated chlorinated aluminum nitride clusters. Harmonic vibrational frequencies for these clusters are given in order to support the information of detg. the ground states. Chem. bond properties in these clusters are discussed in detail. The results of calcns. show that the ground state geometric structures of these two kinds of clusters are of C_{2h} symmetry and that only Al–N bonds exist in these clusters.

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C.A. 2001, 135, N7.

(см. прил.)

$(ClAlNH)_n$
$(n = 1-10)$

2001

стр-ра,
D_0 ν_i, терм.
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135: 142506z **$(ClAlNH)_n$ cluster formation in the gas phase for the chemical vapor deposition of AlN thin films.** Xu, X.-H.; Wu, H.-S.; Zhang, F.-Q.; Zhang, C.-J.; Jin, Z.-H. (Department of Chemistry, Shanxi Normal University, Linfen, Peop. Rep. China 041004). *THEOCHEM* 2001, 542, 239-246 (Eng), Elsevier Science B.V. In this paper, both ab initio and d. functional theory methods have been used to predict geometries, electronic states and total energies of $(ClAlNH)_n$ $(n = 1-10)$ clusters. Harmonic vibrational frequencies for these clusters are given in order to aid in the characterization of the ground states. In addn., the thermodn. properties of the oligomerization processes $(ClAlNH)_m \rightarrow {}^m/_n(ClAlNH)_n$ are discussed in detail. These results show that the ground state geometric structures of $(ClAlNH)_n(n = 1-10)$ clusters are $C_s(n = 1)$, $D_{2h}(v = 2)$, $D_{3h}(n = 3)$, $T_d(n = 4)$, $C_s(n = 5)$, $D_{3d}(n = 6)$, $C_s(n = 7)$, $S_4(n = 8)$, $D_{3h}(n = 9)$ and $C_{2h}(n = 10)$ symmetry, resp. The stabilities of the $(ClAlNH)_n$ clusters with even n (n = 2, 4, 6, 8, 10) are greater than that with odd n (n = 1, 3, 5, 7, 9).

C. A. 2001, 135, N10

$H_{\bar{m}}AlNH_{\bar{n}}$

$m, n = 0-3$

2001

135: 97683s **Compounds featuring a bond between a Group 13 (M) and a Group 15 element (N or P) and with the formulae H_m-MNH_n and H_mMPH_n: structural aspects and bonding.** Himmel, Hans-Jorg; Downs, Anthony J.; Green, Jennifer C.; Greene, Tim M. (Inorganic Chemistry Laboratory, University of Oxford, Oxford, UK OX1 3QR). *J. Chem. Soc., Dalton Trans.* 2001, (5), 535–545 (Eng), Royal Society of Chemistry. Following studies of the thermal and photoactivated reactions of the Group 13 metal atoms Al, Ga or In (M) with NH_3 or PH_3 in solid argon matrixes, the properties of the obsd. or potential reaction products are discussed. These are mols. with the general formula H_mMEH_n, where M = Al, Ga or In, E = N or P, and m, n = 0–3. All the mols. have been characterized structurally, energetically and vibrationally by D. Functional Theory (DFT) calcns. The following products have been identified exptl. by their IR spectra: the adducts $M{\cdot}EH_3$, the metal(II) insertion products $HMEH_2$, the metal(III) derivs. H_2MNH_2 and

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C.A. 2001, 135, N7.

$H_mAlPH_{\bar{n}}$, $H_{\bar{m}}GaNH_{\bar{n}}$, $H_mGaPH_{\bar{n}}$, $H_mInNH_{\bar{n}}$, $H_{\bar{m}}InPH_{\bar{n}}$

H_2MPH, and the metal(I) amides MNH_2. The observation of most of the IR–active fundamentals for different isotopic forms of the mols. MNH_2 and H_2MNH_2 allowed normal coordinate anal. calcns. to be performed, thereby endorsing the vibrational assignments and affording reliable force consts. Obsd. and hypothetical H_mMEH_n mols. have been compared with particular ref. to structural and energetic differences according to whether $E = N$ or P. Questions of bonding have been addressed through calcns. of barriers to rotation of planar mols. and of barriers to inversion for mols. contg. pyramidal MPH_2 moieties. π–Type interactions play only a minor part in the bonding of planar mols. like H_2MNH_2. The much larger barrier to inversion of PH_3 compared with NH_3 results in pyramidal MPH_2 but planar MNH_2 fragments. With the help of an appropriate MO scheme it is possible to rationalize how the inversion barrier changes when one hydrogen of PH_3 is replaced by an MH_m group.

Al_nN_n Оп 41 351 2002

$n=4,5,6$ Anil K. Kandalam et al.,

стр-ра, теорет. расчет J. Phys. Chem. B 2002, 106, 1945-1953.

Al_2N_4

AlN_n

(n=4-7)

ab initio расчет

От. 41466

2002

Edmond P. F. Lee et al.,

J. Phys. Chem. 2002, A106, 8680-95.