Оксиды щелочных элементов

1969

Окислы щелочных элементов

(Структура)

III

(см. галогениды щел.-зем. мет.)

Рассбиди Н.Г.

Ж. структ. химии, 10, № 1, 131.

О строении молекул галогенидов щелочноземельных и окислов щелочных элементов.

Окислы азота.
Механизм

1972

Gaughan R.A.R.

Vi

Diss. Abstr. Int. 1972, 32, 6948.

(см SO_2) III

$M^+O_3^-$ M – щелочной металл

1975

$M^+NO_2^-$

образование в матрицах

178134c Mechanism of $M^+O_3^-$ and $M^+NO_2^-$ formation by photolysis of matrix samples at 15°K. Andrews, Lester; Tevault, David E. (Chem. D[illegible] Univ. Virginia, Charlottesville, Va.). *J. Mol. Spectr.* [illegible] 1975, 55(1-3), 452-[illegible] (E[illegible]). The species $M^+O_3^-$ and M^+N[illegible] are produced in matrix sam[illegible] of [illegible]li metal atoms, N_2O and O_2 [illegible] NO by Hg are phot[illegible] In [illegible]ilar studies, Milligan an[illegible] [illegible]cox (1971) proposed [illegible] me[illegible]ism involving the diff[illegible] and reaction of O^- anion [illegible] obs[illegible]ations are better expl[illegible]ned by photolysis of N_2O in the presence of $M^+O_2^-$ with O atom transfer to give $M^+O_3^-$ and the an[illegible]gous reaction with M^+NO to give $M^+NO_2^-$.

(+1) нитр. $M^+NO_2^-$

C.A. 1975. 82 N26

☒

Electron gas 1977

89: 33394x Electron-gas model for open shell-closed shell interactions. II. Application to the alkali monoxides. Clugston, Michael J.; Gordon, Roy G. (Dep. Chem., Harvard Univ., Cambridge, Mass.). *J. Chem. Phys.* 1977, 66(1), 244-7 (Eng). In the preceding paper, the electron-gas method of calcg. interat. forces was extended to the case of an open shell atom interacting with a closed shell atom. This theory is applied to the calcn. of the bond distance, dissocn. energy, and vibrational frequency for the Π states of the alkali monoxides. Better than 10% agreement was attained with the data, which is either from expt. or from other a priori calcns. The electronic reasons behind the calcd. decreased sepn. in total energy between the Σ and Π states is lower for RbO. One does not predict this change because the Σ states are inaccurate by a few tenths of an eV, owing to a small degree of covalent bonding not calculable using electron-gas methods. As in the preceding paper, in these systems the electron-gas method will be useful for the calcn. of Π states but will not be reliable for Σ states. The Π states involve mainly closed shells in the region of overlap, and this explains the success of the closed shell model in describing these states.

C.A. 1978, 89, N4

MO_2

1982

М-щелочной металл

До;

19 Б800. Хемилюминесцентная реакция между димерами щелочных металлов и молекулами кислорода. Figger H., Kowalski A., Zhu X. H. Chemiluminescen reaction between alkali dimers and oxygen molecules. «Ber. Bunsenges. phys. Chem.», 1982, 86, № 5, 470 (англ.)

Изучена хемилюминесценция (ХЛ), возникающая при пересечении сверхзвукового пучка димеров щел. металлов (ДЩМ) с тепловым пучком молекул кислорода. На основании данных спектрального анализа ХЛ сделан вывод о протекании четырехцентровой р-ции $M_2+O_2 \rightarrow MO_2^*+M$; $\rightarrow MO_2+M^*$, где M — атом щел. металла. Получен более низкий (по сравнению с лит. данными) предел значения энергии связи MO_2. Высказаны соображения в пользу гарпунного механизма р-ции. Предлагается аналогичное объяснение экспериментов по наблюдению ХЛ в скрещенных молек. пучках между ДЩМ и молекулами хлора.

А. А. Иогансен

Х. 1982, 19, № 19

$M_2 + O_2 \rightarrow MO_2 + M^*$ | Оп. 17410 | 1983

M – щелочн. металл

Figger H., Schrepp W., et al.,

химическ.

J. Chem. Phys., 1983, 79, N3, 1320–1325

MO_2 (Ом. 17410) 1983

М – щелочн. металл

спектр хемилюминесценции

99: 79468j **Chemiluminescent reaction between alkali dimers and oxygen molecules.** Figger, H.; Schrepp, W.; Zhu, Xu Hui (Max-Planck-Inst. Quantenopt., D-8046 Garching, Fed. Rep. Ger.). *J. Chem. Phys.* 1983, 79(3), 1320–5 (Eng). The reaction of alkali dimers with O mols. was studied in a crossed-beam expt. Weak luminescence from the crossing zone was obsd. It was predominantly emitted by the electronically excited products of the reactions $M_2 + O_2 \rightarrow MO_2 + M^{\bullet}$ and $M_2 + O_2 \rightarrow MO_2^{-} + M$ ($^{\bullet}$ = electronic excitation). Lower limits for the dissocn. energies between M and O_2 in the product mols. were derived from the cut-off wavelengths of the continuous chemiluminescence spectra obsd. They are consistent with the values calcd. using an ionic model for the product mol. MO_2.

C.A. 1983, 99, N10

MO

1985

M-щелочной мет.

Langhoff S.R., Bauschlicher Ch.W., Jr., et al.

(De, re, ωe, теор. расчёт)

Comp. Ab Initio Quantum Chem. Exp. Small Mol., Proc. Symp. 1984 (Pub. 1985), 357–407.

(см. MX; III)

МО

1986

Langhoff S.R., Bauschlicher Ch.W., Jr.,

(De, Re, We теор. расчет)

J. Chem. Phys. 1986, 84 (8), 4474-80.

М-щелочной метал-

Theoretical study of the alkali and alkaline earth oxides.

диатомс

C.A. 1986, 104, N22, 195684