
KO_2

ν_1 (H_2O_2, Li_2O_2, Na_2O_2, K_2O_2, Rb_2O_2, MgO_2, CaO_2, SrO_2, BaO_2, KO_2, RbO_2) (1969) IX 705 10 9 11

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ЕСТЬ Ф. Н.

10 7

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Na, K

Smardzewski R.R., Andrews L.,

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NaO_2; KO_3^-; $K_2^+O_3^-$; KO_2; RbO_3^-; $Rb_2^+O_3^-$;
RbO_2; CsO_3^-; $Cs_2^+O_3^-$; CsO_2

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075 076 089 ВИНИТИ

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0749 ПМК

689 700 741

ВИНИТИ

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1976

Andrews L.

(Vi)

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(cit. $Li^+O_2^-$; III)

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поперечн-
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образ O_2^-

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KO_2 | Отпеск 12781 | 1981

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KO_2

1993

120: 176723y Spectral analysis of potassium and alkaline-earth metal peroxides, potassium superoxide and its melts with nitrates. Brunere, V.; Kalina, Yu. (Riga Tech. Univ., Riga, Latvia). *Latv. Kim. Z.* 1993, (3), 276–80 (Russ). The IR spectra of K, Ca, Sr, and Ba peroxides, K superoxide and its melts with K, Rb and Cs nitrates were studied on the frequency range 100–400 cm^{-1}. The absorption max. of Ca, Sr, Ba, and K peroxides are at 316, 234, 220 and (124, 180) cm^{-1}, resp., and that of KO_2 at 168 cm^{-1}. In the cases of alk.-earth metal peroxides, K superoxide and peroxide, the shift of absorption band towards the smaller wavenumbers in succession $CaO_2 \rightarrow SrO_2 \rightarrow BaO_2 \rightarrow KO_2 \rightarrow K_2O_2$ is obsd. Changes in the pattern of spectra of K superoxide melts with nitrates give evidence to the structural changes related to formation of peroxonitrates.

(ИК спектр)

(+6) RbO_2, CaO_2, SrO_2, CsO_2, BaO_2, K_2O_2 (KOH, g. Silabk)

C.A. 1994, 120, N 14.

KO_2

1993

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(cer. Na_2O; I)

$Li_2O(g)$

KO_2

Tremblay B., Mancerou L., Roy P., Le-Quere A-M., Roy D., 1994

Chem. Phys. Lett., 1994, 228, №4-5, 410-16

Vibrational spectra and structure of the KO_2 complex in solid argon. A far-infrared study.

$\angle OKO = 37 \pm 2°$

$r_{K-O} = 2,10 \pm 0,14$ Å

ν_i для изотопозамещенных KO_2.

сил. пост.

$I_{O-O} = 1,33$ Å.

$\nu_1 = 1108.9$

$\nu_2 = 306.98$

$\nu_3 = 304.3$

$f_{KO} = 0,675$ мдин/Å

$f_{KO,KO} = -0,131$

$f_{O-O} = 5,784$

KO_2

1994

18 Б1193. **Колебательные спектры и структура комплекса KO_2 в твердом аргоне. Исследование в дальней ИК-области.** Vibrational spectra and structure of the KO_2 complex in solid argon. A far-infrared study / Tremblay Benoît, Manceron Laurent, Roy Pascale, LeQuére Anne-Marie, Roy Denis // Chem. Phys. Lett. / .— 1994 .— **228** , № 4 - 5 .— С. 410—416 .— Англ.

Исследованы ИК-спектры матрично-изолированной молекулы KO_2. Проведено изотопное замещение по K и O. Впервые измерена полоса ν_3: 304,3 $см^{-1}$ для основного изотопомера. В предположении определенного расстояния O—O, равного 1,33 Å, подобраны значения других геометрич. параметров, согласующиеся с наблюдаемыми полосами в спектрах. Найденные значения расстояния K—O 2,10±0,14 Å и угла O—K—O 37°±2° заметно отличаются от результатов теор. оценок.

А. В. Немухин

М.П.

Х. 1996, N 18

KO_2

1994

121: 266735d **Vibrational spectra and structure of the KO_2 complex in solid argon. A far-infrared study.** Tremblay, Benoit; Manceron, Laurent; Roy, Pascale; LeQuere, Anne-Marie; Roy, Denis (LURE, Batiment 209D, Universite Paris Sud, 91405 Orsay, Fr.). *Chem. Phys. Lett.* 1994, 228(4-5), 410-16 (Eng). The observation of new fundamental frequencies for the potassium superoxide KO_2 is reported for different isotopic species: ν_3 of $^{39}K^{16}O_2$, $^{39}K^{18}O_2$ and $^{39}K^{16}O^{18}O$, and ν_2 of $^{41}K^{16}O_2$, $^{41}K^{18}O_2$, $^{41}K^{16}O^{18}O$ and $^{39}K^{17}O^{18}O$. Using these values and a fixed O–O internuclear distance, we calcd. the geometry and force consts. from a harmonic force field. We estd. an O–K–O angle of 37°±2°, and a K–O internuclear distance of the order of 2.10±0.14 Å. These values disagree with previous theor. detns.

Uk & A2,

Di, $2K\text{-}O = 2{,}10 \pm 0{,}14 Å$.

$\angle OKO = 37 \pm 2°$

C.A. 1994, 121, N 22

KO_2 0m 39371 1998

were calcd. to 15 meV and the ...

128: 145583p **A Study of the $\tilde{X}^2A_2$ State of KO_2 Using Ab Initio and Density Functional Theory: The Equilibrium Geometry and Vibrational Frequencies.** Lee, Edmond P. F.; Wright, Timothy G. (Chemistry Department, University of Southampton, Southampton, UK SO17 1 BJ). *J. Phys. Chem. A* **1998**, 102(6), 1036–1040 (Eng), American Chemical Society. Geometry optimization and harmonic vibrational frequency calcns. at the CASSCF, CISD, UMP2, QCISD, CCSD(T), and B3LYP levels of theory were performed on the ground $\tilde{X}^2A_2$ state of KO_2. Various augmented effective core potential and all–electron basis sets were employed, with the largest being the LANL2DZ effective core potential augmented by [6s6p3d1f], the all–electron basis set, [11s10p5d3f] for potassium, and aug–cc–pVTZ for oxygen. These calcns. lead to the conclusion that the C_{2v} $\tilde{X}^2A_2$ state of KO_2 has an equil. bond angle of 32.3 ± 0.5°, a K–O bond length of 2.410 ± 0.005 Å, and an O–O bond length of 1.341 ± 0.001 Å. The B3LYP d. functional method is also employed for NaO_2 and LiO_2, and it appears that this method does not suffer from symmetry breaking; a similar conclusion is reached for the QCISD method. Isotopic shifts for all three mols. are also reported and compared to available exptl. values.

ab initio, $\tilde{X}^2A_2$ спектр. параметр.

C.A. 1998, 128 N12

KO_2 | Dm. 41368 | 2002

Edmond P.F. Lee et al.,

$(\tilde{X}^2A_2)$ Chem. Phys. Lett.,

энергия 2002, 363, 139–144.

ионизации, The ionization energy

до & KO_2 ($\tilde{X}^2$ [redacted] A_2) and dis-

sociation energies of KO_2 and KO_2^+.