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131:134938 Equation of state and thermodynamic properties of pure D2O and H2O mixtures in and beyond the critical region. Kiselev, S. B.; Abdulagat Harvey, A. H. (Physical and Chemical Properties Division, National Instit Standards and Technology, Boulder, CO 80303, USA). Int. J. Thermophys., 563-588 (English) 1999 A parametric crossover model is adapted to represent the thermodn. properties of pure D2O in the extended crit. region. The crossover equat state for D2O incorporates scaling laws asymptotically close to the crit. and is transformed into a regular classical expansion far from the crit. An isomorphic generalization of the

C.A. ~~1999~~, 131

law of corresponding states is applie the prediction of thermodn. properties and the phase behavior of D2O + H2 mixts. over a wide region around the locus of vapor-liq. crit. points. A comparison is made with exptl. data for pure D2O and for the D2O + H2O mi The equation of state yields a good representation of thermodn. property the range of temps. 0.8Tc(x) .ltoreq. T .ltoreq. 1.5T(x) and densities 0.35.rho.c(x) .ltoreq. .rho. .ltoreq. 1.65.rho.c(x).

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132:143715 The 3.nu.2 Band of D216O. Bykov, A.; Naumenko, O.; Sinitsa, L.; Voronin, B.; Winnewisser, B. P. Institute of Atmospheric Optics, SB R Tomsk, Russia J. Mol. Spectrosc., 199(2), 158-165 (English) 2000 The 3.nu.2 overtone band of D oxide, D2O, centered at 3474.3193 cm-1, was measured with high resoln. in a 4-m base-length White cell attached t Fourier transform spectrometer. The anal. of the spectrum led to the assignment of 347 transitions in this band, defining rovibrational energy levels in the (030) state up to Ka = 7 for J .ltoreq.9, and lower Ka leve for J .ltoreq. 16. The (030) state was treated as an isolated state, following a Pade-Borel approxn. in the effective Hamiltonian. Of the 115 energy levels included in the anal., 80% were reproduced by the 21 adjust parameters to within 0.0008 cm-1, and the largest error was 0.0017 cm-1.

C. A. 2000, 132

F: D2O
P: 3

2000

132:172686 High-Resolution Study of the First Hexad of D2O. Wang, Xiang-huai; Ulenikov, O. N.; Onopenko, G. A.; Bekhtereva, E. S.; He, Shen gui; Hu, Shui-ming; Lin, Hai; Zhu, Qing-shi Open Laboratory of Bond Selective Chemistry, Department of Chemical Physics, University of Scienc and Technology of China Hefei 230026, Peop. Rep. China J. Mol. Spectrosc., 200(1), 25-33 (English) 2000 The high-resoln. FTIR spectra of the D2O mol. were recorded and assigned in the 4200-5700 cm-1 region where the vibration-rotation bands 2.nu.1, 2.nu.3, .nu.1 + .nu.3, .nu.1 + 2.nu.2, 2.nu.2 + .nu.3, and 4.nu.2 located. The presence of numerous and very strong accidental perturbatio between the states of the hexad makes it necessary to take into account n only ordinary resonance interactions of the Fermi, Darling-Dennison, and/ Coriolis types, but interactions between

C-A 2000, 132

the states (.nu.1.nu.2.nu.3) and (.nu.1 .-+. 2.nu.2 .+-. 2.nu.3 .+-. 1) as well. Parameters of all 6 vibrational states of the hexad were obtained from the fit of exptl. ener values.

7

F: D2O
P: 3
132:172687 High-Resolution Fourier Transform Spectrum of the D2O Molecule the Region of the Second Triad of Interacting Vibrational States. He, She gui; Ulenikov, O. N.; Onopenko, G. A.; Bekhtereva, E. S.; Wang, Xiang-hua Hu, Shui-ming; Lin, Hai; Zhu, Qing-shi Open Laboratory of Bond Selective Chemistry, Department of Chemical Physics, University of Science

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and Technology of China Hefei 230026, Peop. Rep. China J. Mol. Spectrosc., 200(1), 34-39 (English) The high-resoln. FTIR spectrum of D2O was recorded at 3200-4200 cm-1, where the bands of the 2nd triad of interacting vibrational states are located. As a result of the theor. anal., both the rotational-vibrationa structure of the (011) vibrational state was improved, and the rotational energies of the (110) and (030) vibrational states were detd. up to rotational quantum nos. Jmax = 15 and 14, resp.

D_2O 2001

135: 99069v **Frequency Measurement of Pure Rotational Transitions of D_2O from 0.5 to 5 THz.** Matsushima, Fusakazu; Matsunaga, Motomi; Qian, Guang−Yuan; Ohtaki, Yuichiro; Wang, Rong−Long; Takagi, Kojiro (Department of Physics, Toyama University, Toyama, Japan 930−8555). *J. Mol. Spectrosc.* **2001**, 206(1), 41−46 (Eng), Academic Press. Frequencies of pure rotational transitions of D_2O were measured in the region 0.5−5 THz with a high−precision far−IR spectrometer using a tunable radiation source. Measured frequencies of ~150 spectral lines, 30 of them being newly measured lines, provide an excellent frequency std. for the far−IR region together with previous measurements on $H_2{}^{16}O$, $H_2{}^{17}O$, and $H_2{}^{18}O$. Mol. parameters of Watson's A−reduced Hamiltonian were obtained to reproduce the obsd. frequencies. (c) 2001 Academic Press.

чисто вращ. спектр

C.A. 2001, 135, N7

DO_2

2001

135: 159307h **Improved Molecular Constants for the Ground State of DO_2.** Chance, K. V.; Ramsay, D. A.; Fink, E. H. (Harvard–Smithsonian Center for Astrophysics, Cambridge, MA 02138 USA). *J. Mol. Spectrosc.* **2001**, 207(1), 123 (Eng), Academic Press. Mol. consts. for the ground state of DO_2 are redetd. using a combined anal. of previously published microwave measurements and combination differences from a rotational anal. of the 000−000 band of the $\tilde{A}^2A' \rightarrow \tilde{X}^2A''$ electronic transition in the 7000 cm^{-1} region. (c) 2001 Academic Press.

м.п. в
основном
электрон.
состоянии

Д2О (кол.-вр. спектр высокого разреш.) 2001

135: 172391a **High resolution vibration–rotation spectrum of the D_2O molecule in the region near the $2\nu_1 + \nu_2 + \nu_3$ absorption band.** Zheng, Jing–Jing; Ulenikov, O. N.; Onopenko, G. A.; Bekhtereva, E. S.; He, Sheng–Gui; Wang, Xiang–Huai; Hu, Shui–Ming; Lin, Hai; Zhu, Qing–Shi (Open Laboratory of Bond – Selective Chemistry, University of Science and Technology of China, Hefei, Peop. Rep. China 230026). *Mol. Phys.* 2001, 99(11), 931–937 (Eng), Taylor & Francis Ltd. The high resoln. Fourier transform spectrum of the D_2O ($\nu = \nu_1 + \nu_2/2 + \nu_3 = 3.5$) polyad was analyzed within the framework of the Hamiltonian model taking into account resonance interactions between the seven states (310), (211), (112), (013), (230), (131) and (032). Transitions belonging to the $2\nu_1 + \nu_2 + \nu_3$, $3\nu_1 + \nu_2$ and $3\nu_2 + 2\nu_3$ bands were assigned in the exptl. recorded spectrum. This provided the possibility of obtaining spectroscopic parameters of the "visible" states (211), (310) and (032) and of estg. the band centers, and the rotational and resonance interaction parameters of the "dark" states (112) and (131).