FeH_2

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129: 267115d **Theoretical investigation of fine-structure effects in the bending and symmetric stretching vibronic spectrum of FeH_2 and FeD_2.** Martini, Heike; Marian, Christel M.; Peric, Miljenko (Institute of Physical and Theoretical Chemistry, University of Bonn, D-53115 Bonn, Germany). *Mol. Phys.* 1998, 95(1), 27-42 (Eng), Taylor & Francis Ltd.. Two-dimensional potential energy surfaces were detd. for the 25 spatial and spin components of the low-lying electronic $^5\Delta g$, $^5\Pi_g$, and $^5\Sigma_g^+$ states of Fe dihydride along the bending and sym. stretching coordinates. Spin-free electronic energies and elec. dipole moments were obtained by an averaged coupled-pair functional employing a 1-component relativistic Hamiltonian. Diagonal and off-diagonal spin-orbit coupling matrix elements were evaluated at the ab initio level for a variation of the sym. stretching coordinate while the dependence on the bending angle was estd. from the variation of the angular momentum

(cretmp)

(H)

C.A. 1999, 129, N20

matrix elements. Vibronic energy levels were calcd. sep. for each multiplet component; for the treatment of Renner–Teller coupling in the large amplitude bending motion an effective Hamiltonian was used in which the sym. stretching motion is sepd. off and integrated over. The Renner–Teller coupling is negligible in the $X^5\Delta_g$ state and its vibronic energy level scheme is dominated by spin–orbit coupling effects. The spatial components of the excited $^5\Sigma_g$ state, however, exhibit a considerable energy sepn. upon bending. Close to the $^5\Sigma_{\Lambda 2}$ component the authors locate the $5g^+$ electronic state which has large spin–orbit coupling matrix elements with both $^5\Sigma_g$ components.

FeH_2

1999

130: 243722u **The infrared spectrum of FeH_2, studied in the gas phase by laser magnetic resonance.** Korsgen, Helga; Urban, Wolfgang; Brown, John M. (Institut fur Angewandte Physik, D-53115 Bonn, Germany). *J. Chem. Phys.* **1999**, 110(8), 3861-3869 (Eng), American Institute of Physics. The IR spectrum of the FeH_2 radical in the gas phase was studied in detail between 1605-1730 cm^{-1}, by the technique of CO laser magnetic resonance. The mol. is formed in an elec. discharge through a mixt. of H_2 and $Fe(CO)_5$ in He. Many resonances are obsd. and assigned to transitions in the fundamental band of the antisym. stretching vibration 3_0^1 and in the assocd. hot band $2_1^1 3_0^1$. In the latter case, each vibrational level is split into 2 vibronic components. The measurements are used to det. the parameters of an effective Hamiltonian which is capable of modeling the data to within exptl. error. The values detd. for the band origin and zero-point vibrational const. are: $\nu_3 = 1674.7203(3)$ cm^{-1} and $B_0 = 3.07523(5)$ cm^{-1}. The data show that the mol. is linear in its ground state and are consistent with an assignment of this state as $^5\Delta_g$.

ИК спектр, ν_3, B_0

C.A. 1999, 130, N18