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С помощью масс-спектрометра в равновесном паре над палладнем зарегистрированы молекулы Pd₂ Их потенциал появления найден равным 7,7±0,3 эв. Отношение парциальных давлений Ppd/Ppd составляет 3,3⋅10⁵, 2,5⋅10⁵ и 1,4⋅10⁵ при 1975, 2025 и 2085° К соответственно. Расчет проведен в предположении, что сечение нонизации Pd₂ в 1,6 раза больше сечения для Pd. Ю. Ходеев

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F: Pd2+

Studies the Theoretical 133:301515 Coordination and Stability of Divalent Cations in ZSM-5. Rice, Mark J.; Chakraborty, Arup K.; Bell, Alexis T. Chemical and Materials Sciences Divisions Lawrence Berkeley National Laboratory Departments of Chemical Engineering and Chemistry, University of California Berkeley, CA 94720-1462, USA J. Phys. Chem. B, 104(43), 9987-9992 (English) 2000. The coordination of divalent metal cations to ZSM-5 has been investigated using gradient-cor. d. functional theory Coordination at both isolated charge-exchange sites and pairs of charge- exchange sites was considered for Co2+, Cu2+, Fe2+, Ni2+, Pd2+, Pt2+, Ru2+, Rh2+, and Zn2+. Thermodn. calcns. of the stability of M2+ to redn. to M0 and demetalation to form MOx particles were also carried out. The results indicate that Cu2+, Co2+, Fe2+, and Ni2+ are coordinated preferentially to five-membered rings contg. two Ai atoms, which are located on the walls of the sinusoidal channels, whereas Pd2+, Pt2+, Ru2+, Rh2+, and Zn2+ are coordinated preferentially to six-membered rings located on the walls of the sinusoidal channels. Examn. of the stability of dimer cations of the form [M-O-M]2+ shows that such structures are not generally stable to hydrolysis, with the possible exception of [Cu-O- Cu]2+. The findings of these calcns. are in good general agreement with exptl. results.

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132:212842 Theoretical Studies in Palladium and Platinum Molecular Chemis Dedieu, Alain Laboratoire de Chimie Quantique, UMR 7551 CNRS/ULP Universite Louis Pasteur Strasbourg 67000, Fr. Chem. Rev. (Washington, D. C.), 100(2), 543-600 (English) 2000 The quantum chem. studies of Pd and Pt mol. systems carried out since 19 are reviewed with 482 refs. to complement earlier comprehensive reviews. covered include; mononuclear systems; polynuclear systems; reactivity of Pt complexes; and catalytic cycles.

C.A. 2000, 132