Spectroscopy and Energetics of Diatomic PtH, PtH^+ and PtH^-

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Hybrid CCSD(T)/spin-orbit-CI methods are used to obtain potential-energy functions leading to rovibrational levels for several low-lying electronic states. Ideal-gas thermodynamic functions are computed from the energy levels. For quantitative energetics, nondynamical correlation is extended to the CCSDT(Q) level. We obtain vibrational zero-point energies and spin-orbit stabilization energies, which lead to predictions for observable quantities: ionization energy IE(PtH) = (9.44 ± 0.07) eV, electron affinity EA(PtH) = (1.65 ± 0.04) eV, and dissociation energies D_0(Pt–H) = (329.6 ± 3.9) kJ mol^{-1}, D_0(Pt^+–H) = (279.3 ± 5.7) kJ mol^{-1}, and D_0(Pt^-–H) = (285.0 ± 2.4) kJ mol^{-1}. Combined with the ideal-gas state functions, $\Delta_f H^\circ_{298.15}$(PtH) = (448.3 ± 4.4) kJ mol^{-1} (all uncertainties expanded by k = 2). Results are compared with available experimental measurements.