

BOND DISSOCIATION ENERGIES AND IONIZATION ENERGIES OF RHENIUM CONTAINING SMALL MOLECULES

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Resonant two-photon ionization spectroscopy has been used to determine the bond dissociation energies (BDEs) and ionization energies (IEs) of rhenium containing small molecules. The ultraviolet spectra of these molecules display a highly congested collection of indeterminate vibronic states. Couplings among these states allow the molecule to find a path to dissociation as soon as the ground separated atom limit is exceeded in energy, allowing a precise measurement of the bond energy from the observation of a sharp predissociation threshold. Measurements provide BDE values of 5.731(3) eV (ReC), 5.359(3) eV (ReC₂), 5.635(3) eV (ReN), 5.510(3) eV (ReO), and 3.947(3) eV (ReS). The ionization energy of ReC, 8.425(15) eV, was determined from the observed onset of one-color two-photon ionization. By combining our ReC results with the ionization energy of Re (7.83352(11) eV) in a thermochemical cycle, the BDE of cationic ReC⁺ was determined as 5.140(15) eV.^a This is in excellent agreement with that measured using guided ion beam mass spectrometry, 5.13(12) eV.^b

^aKramida, A.; Ralchenko, Y.; Reader, J.; NIST ASD Team, NIST Atomic Spectra Database (version 5.9). National Institute of Standards and Technology, Gaithersburg, MD: 2019.

^bKim, J.; Cox, R. M.; Armentrout, P. B., Guided ion beam and theoretical studies of the reactions of Re⁺, Os⁺, and Ir⁺ with CO. *J. Chem. Phys.* 2016, 145 (19), 194305/1-194305/13.