FTIR DETECTION OF P_4O_{10} FROM COMBUSTION OF ELEMENTAL PHOSPHORUS

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The emission spectra of gaseous combustion products of elemental phosphorus in air and in inert atmospheres with added oxygen were measured using Fourier transform infrared spectroscopy. Features corresponding to three fundamental and one overtone vibrational modes of P_4O_{10} were assigned. To our knowledge, this is the first assignment to P_4O_{10} of infrared emissions in a reacting system. In conjunction with the experimental measurements, the structures, vibrational frequencies, and vibrational intensities of P_4O_{10} and P_4O_6 were computed using *ab initio* electronic structure methods. The calculations were performed at the Hartree-Fock level using a double zeta plus polarization basis set. The predicted vibrational spectra are in good agreement with the observed spectra and with previous absorption measurements of P_4O_{10} and P_4O_6.

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