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Using isoelectronic reasoning to examine the constancy of bond dissociation enthalpy ratios.

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It has been shown both computationally and experimentally that the bond dissociation enthalpy ratio $\frac{D_m^\circ(XYX)}{2D_m^\circ(XY)}$, where X= O, S, Se (group 16) and Y= C, Si, Ge (group 14) is nearly constant at 0.8. Computations also show that the corresponding ratios when Y= N+, P+, As+ (group 15) or Y= B-, Al-, Ga- (group 13) are nearly constant at 0.7 and 0.9 respectively. We have extended these calculations to the isoelectronic systems HXYXH, where X= N, P, As (group 15) and Y=C, Si, Ge (group 14) or Y= N+, P+, As+ (group 15) to determine whether our earlier observations or the constancy and relative magnitudes of the bond dissociation enthalpy of the ratios still hold. The dependency of the ratios on the geometries of the HXYXH and HXY molecules is also being examined. It would be particularly advantageous if our isoelectronic reasoning is valid because many of the systems that we are now examining computationally are difficult to study in the laboratory.