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Quantum Chemical Estimation of the Acidities of Some Inorganic Nitrogen Acids

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Abstract

The class of inorganic nitrogen acids encompasses a number of important chemical compounds, including ammonia, hydrazine, and their derivatives. Whereas a large number of computational studies have examined the acidities of organic nitrogen acids, relatively few have been directed at inorganic nitrogen compounds. The present work follows a previous study of inorganic oxo acids [54th Sanibel Symposium] and examines the acidities, as represented by pK_a values, of a diverse set of inorganic nitrogen acids supplemented by some related organic acids. Calculations were performed at the semiempirical RM1 level and the density functional theory B3LYP/6-31+G** level with and without the SM8-water solvent model of Marenich et al. [*J. Chem. Theory Comput.* **2007,** *3,* 2011]. The abilities of both atomic charge descriptors and energy descriptors to model the acidities of these compounds is reported.

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