THE DISSOCIATION ENERGY OF THE HOOO RADICAL

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The dissociation of the hydrogen trioxyl radical (HOOO) to OH and O_2 has been studied theoretically using coupled cluster methods. The calculated dissociation energy for the *trans*-HOOO isomer is 2.4 kcal/mol including zero-point corrections. The minimum energy path to dissociation has been explored and an exit barrier has been revealed, thereby rationalizing the apparent disagreement between theory and experiment on the magnitude of the bond energy.