**SUPPORTING INFORMATION**

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**Ionization, intrinsic basicity and intrinsic acidity of unsaturated diols of astrochemical interest: 1,1- and 1,2-ethenediol. A theoretical survey.**

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**CONTENTS**

**Table S1.** Comparison of experimental rotational constants and the calculated values at the CCSD(T)/CBS+CV and G4 levels of theory for (Z)-1,2-ethenediol

**Figure S1.** Linear correlations between ΔHgas,acid and the ΔGgas,acid and between ΔHgas,bas and the ΔGgas,bas for 1,1- and 1,2-ethenediol.

**Figure S2.** Linear correlation between the stabilities of the different conformations of 1,2-ethenediol and their protonated and deprotonated forms calculated using enthalpies (ΔH) or electronic energies + ZPE.

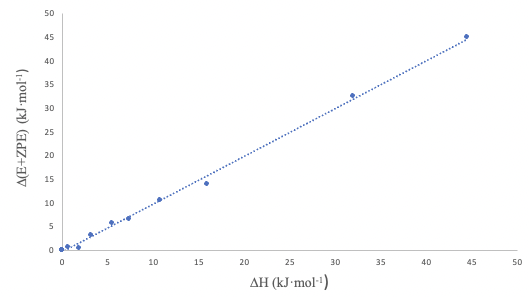
**Figure S3.** The two conformers obtained by the deprotonation of the *syn-syn* (E) 1,2-ethenediol.

**Table S1.** Comparison of experimental rotational constants and the calculated values at the CCSD(T)/CBS+CV and G4 levels of theory for (Z)-1,2-ethenediol. All values in MHz.

|  |  |  |  |
| --- | --- | --- | --- |
| Constant | Experimentala | CCSD(T)/CBS+CVa | G4 |
| A | 19507.2 | 19597.9 | 19502.7 |
| B | 6312.1 | 6298.6 | 6292.1 |
| C | 4772.4533 | 4766.8 | 4792.9 |

a Values taken form ref. 15

**Figure S1.** Linear correlations between ΔHgas,acid and the ΔGgas,acid and between ΔHgas,bas and the ΔGgas,bas for 1,1- and 1,2-ethenediol. These correlations obey the equations: ΔGgas,acid = 1.0246 ΔHgas,acid - 34.006 (r2 = 0.989) and ΔGgas,bas = 0.8557 ΔHgas,bas + 107.58 (r2 = 0.983). All values in kJ·mol-1.

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**Figure S2.** Linear correlation between the stabilities of the different conformations of 1,2-ethenediol and their protonated and deprotonated forms calculated using enthalpies (ΔH) or electronic energies + ZPE. These correlation obey the equation: Δ(E+ZPE) = 1.0056 ΔH – 0.329 (r2 = 0.997). All values in kJ·mol-1.



**Figure S3.** The two conformers obtained by the deprotonation of the *syn-syn* (E) 1,2-ethenediol. As shown the C1 form is the most stable one.