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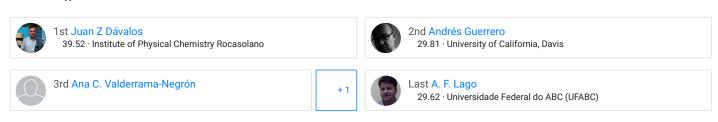
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## Energetics and structural properties of neutral and deprotonated phenyl carbinols

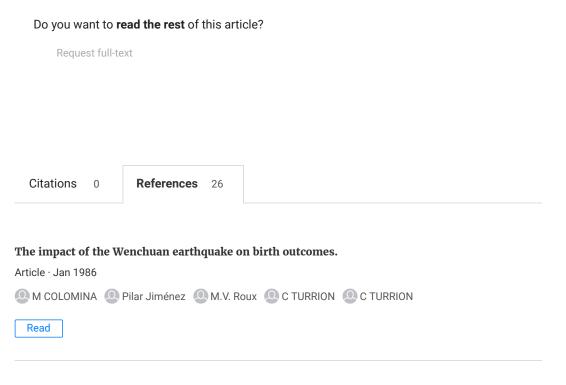
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## **Abstract**

Theoretical and experimental studies on the energetics, structure and other physicochemical properties of neutral 1-phenylethanol (10H), diphenylmethanol (20H) and triphenylmethanol (30H) and their corresponding deprotonated anions (oxyanions, formed by deprotonation of the OH group) are reported in this work. The standard enthalpies of formation in the gas phase at 298.15 K, (g) have been determined. Quantum chemical calculations, at the DFT (particularly M05-2X method) and in some cases at the ab initio (G3) levels, have shed light on structural and electronic effects on the thermodynamic stability and intrinsic acidity of the studied compounds. These calculations confirmed the excellent consistency of the experimental results.



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