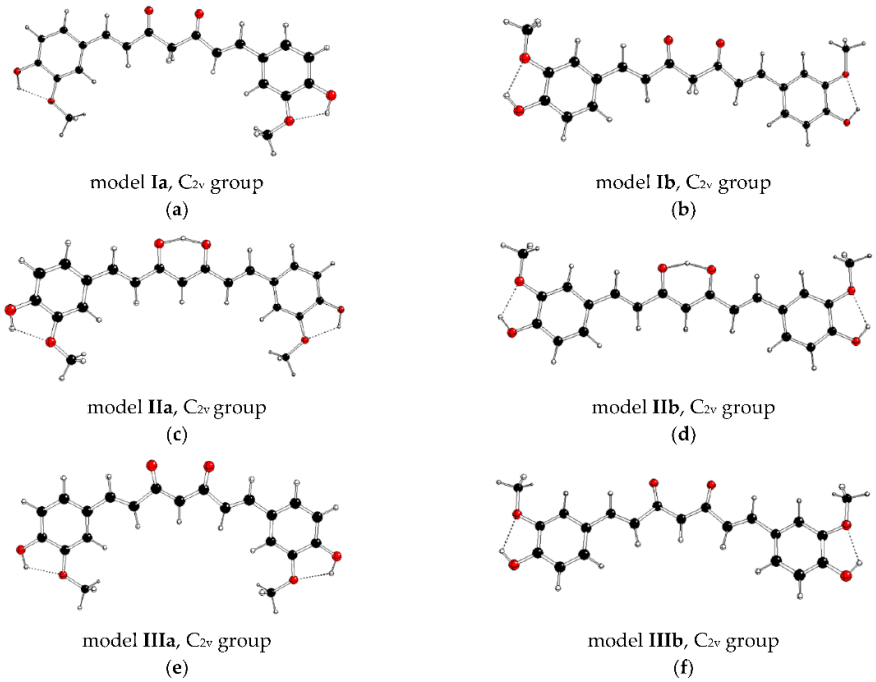
Pseudo-Jahn-Teller Effect and Photoprotective Potential of Curcumin

Dagmar Štellerová, Vladimír Lukeš, Martin Breza

Institute of Physical Chemistry and Chemical Physics, Slovak University of Technology in Bratislava, Bratislava, Slovakia

This work presents a theoretical investigation of curcumin, an organic dye produced by *Curcuma longa* species. Molecular and electronic structures of its keto–keto, enol–keto, and enolate forms were analyzed. Curcumin tautomers together with their deprotonated forms of C_{2v} symmetry and of its subgroups were identified in gas phase using density functional theory (M062X hybrid functional). Lower-symmetric stable geometries were clarified by Pseudo-Jahn-Teller (PJT) effect, applying PJT vibronic interactions between the ground electron state and selected excited states. Theoretical results indicate significance of PJT effect which may alter aforementioned states during photodynamic processes producing stable enol and keto curcumin structures. PJT effect may play an essential role and open new opportunities for understanding photoprotection and bioactivity of natural dyes.



Optimized C_{2v} structures of neutral keto–keto (a, b), enol–keto (c, d), and anionic enolate (e, f) forms of curcumin.