Magnetic Response of Aromatic Rings Under Rotation: Aromatic Shielding Cone of Benzene Upon Different Orientations of the Magnetic Field

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The induced shielding cone is one of the most characteristic aspects of aromatic species. Herein, we explore its behavior under different orientations of the applied magnetic field by evaluating the overall and dissected ?- and ?-electron contributions. Our results shed light onto the orientation dependence behavior of the shielding cone, unraveling a characteristic pattern upon rotation of the aromatic ring. This pattern decreases the long range of the magnetic response, such that it resembles the behavior under constant molecular tumbling in solution. © 2017 Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim benzene density functional theory calculations

magnetic properties

shielding cone

?-electrons