An Improved Method for Calculating Ligand Solid Angles

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A new approach has been developed to numerically calculate solid angles of the ligands in organometallic complexes. The novelty of the method is in using atomic radii corresponding to the distance where the Morse potential becomes zero, rather than in using the "typical" atomic van der Waals radii corresponding to the minimum of the Morse function. The calculated values include the ligand solid angles, the corresponding cone angles (rather than Tolman cone angles), the ligand special overlaps, ligand overshadowing, and the molecular solid angle. In addition, the calculated solid and cone angles are normalized to a Metal-Ligand distance of 2.28 Å to allow facile comparison of ligand steric demands in complexes of different metals with different compositions of coordination spheres. The new approach has been implemented in the program Solid-G and solid angles parameters with standard deviations have been computed for most common ligands such as cyclopentadienyl and tri-substituted phosphines. The new approach allos to evaluate the conformational flexibility of the ligands.

Keywords: solid angle, **organometallic complexes**, **ligands**