CORRESPONDENCE

Comment on "The Extent of the Relationship between the Graph-Theoretical and the Geometric Shape Coefficients of Chemical Compounds"

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Received September 12, 1995

In a recent paper[1] in this Journal, Bath and al. determined the correlation between the 2D and the 3D representations of molecules applying a quantitative method, which I had proposed previously,[2] to subsets of the Cambridge Structural Database. They reported poor correlation coefficients (in a regression sense) between the 2D and the 3D shape coefficients and inferred that the 2D−3D correlation assumption was incorrect.

The geometrical shape coefficient computed by Bath et al. is that of the convex hull of the atomic positions, but this important detail is only available to the reader in the original work of Bath.[3] The implication of this is that all molecules, even alkyl derivatives, have a convex shape with no cavities. This unrealistic model leads to surprisingly significant correlation coefficients, as high as 0.4.[1] A more useful model, such as the van der Waals body, would have been preferable, but the associated computation of the shape coefficients is not trivial and numeric evaluation using triangulated molecular solids is probably necessary.

Bath et al. write that my basic assumption was that there exists a "strong relationship" between the 2D and the 3D shapes, and their paper tends to assume that I support the idea of a strong 2D−3D correlation. The scope of my work[2] was indeed to propose a quantitative method, but the hypothesis of a strong correlation did not appear in my paper. In fact, it appears that, aside from the Sheffield group, no one has attempted quantitative measurements of this correlation.

A reasonable conclusion is that the 2D representations of molecules do indeed contain useful information concerning 3D shapes, but, as Bath et al. stated, such information is not sufficient; 3D descriptors are also necessary before the 3D shapes can be reliably described.

REFERENCES AND NOTES

(1) Bath, P. A.; Poirrette, A. R.; Willett, P. The Extent of the Relationship between the Graph-Theoretical and the Geometrical Shape Coefficients of Chemical Compounds. *J. Chem. Inf. Comput. Sci.* **1995**, *35*, 714−716.
(2) Petitjean, M. Applications of the Radius-Diameter Diagram to the Classification of Topological and Geometrical Shapes of Chemical Compounds. *J. Chem. Inf. Comput. Sci.* **1992**, *32*, 331−337.
(3) Bath, P. A. Similarity Searching in the Cambridge Structural Database. Ph.D. Thesis, University of Sheffield, September, 1994; Section 4.2.3 (pp 46−47).

CI950118C

Response to Comment on "The Extent of the Relationship between the Graph-Theoretical and the Geometrical Shape Coefficients of Chemical Compounds"

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Received September 12, 1995

The rationale for our study[1] was suggested by Petitjean himself,[2] when he states that "Thus, for a given family of compounds, the topology-geometry correlation, sometimes called the topology−topography correlation, may be thought of as an ordinary correlation (in the regression sense) between the graph-theoretical coefficient $I(T)$ and the geometrical coefficient $I(G)$ and computed as the ordinary correlation coefficient $r[I(G)I(T)]$" and, later, that "Comparisons between the two diagrams are possible...". No such correlations or comparisons were presented in his paper, and we felt that the 2D and 3D data available in the Cambridge Structural Database provided a unique opportunity to investigate the extent of the relationship, if any: hence the experiments that were reported in our paper, which showed that while such relationships existed they were not strong. We are thus in full agreement with the final sentence of Petitjean's note, in which he emphasizes the continuing need for appropriate 3-D descriptors to be developed.

REFERENCES AND NOTES

(4) Bath, P. A.; Poirrette, A. R.; Willett, P.; Allen, F. H. The Extent of the Relationship between the Graph-Theoretical and the Geometrical Shape Coefficients of Chemical Compounds. *J. Chem. Inf. Comput. Sci.* **1995**, *35*, 714−716.
(5) Petitjean, M. Applications of the Radius-Diameter Diagram to the Classification of Topological and Geometrical Shapes of Chemical Compounds. *J. Chem. Inf. Comput. Sci.* **1992**, *32*, 331−337.

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