ESTATE

Summary

Electro-topological state indices combine electronic and graph-topological information about a compound. They were introduced by Lowel H. Hall and Lemont B. Kier in the 1990s.

Theory

The Estate index $S_i = I_i + {}_i$ of the *i*-th atom is the sum of its intrinsic state I_i and a perturbation term ${}_i$. The intrinsic state is calculated as

$$I_i = \frac{(\frac{2}{N_i})^2 \delta_i^v + 1}{\delta_i}$$

,

where N_i is the principal quantum number for the valence shell of the atom, and δ_i^v and ${}_i$ are molecular connectivity delta values. ${}_i = {}_i \ h_i$ equals the number of neighbors in the structure graph, and $\delta_i^v = Z_i^v - h_i = \sigma_i + \pi_i + n_i - h_i$. Here, ${}_i$ is the number of electrons in orbitals, h_i is the number of bonded hydrogens, Z_i^v is the number of valence electrons, ${}_i$ is the number of electrons in orbitals, and n_i is the number of electrons in lone pairs. The difference ^{v} is proportional to valence state electronegativity. The perturbation state is a sum over the intrinsic states of the atoms neighbors, weighted by their squared topological distance:

$$\Delta I_i = \sum_{j \neq i} \frac{I_i - I_j}{r_{ij}^2}$$

.

Estate indices have later been extended to hydrogen atoms and bonds.

Descriptors

EState indices are separated on atom/bond type. In addition to indices, it is also possible to select E-state counts, which correspond to counts of atom or bond types according to the respective indices.

EState indices encode electronic and topological information, and have proven useful in the establishment of QSAR and QSPR models.

Options

Aromatize structures -- Whether to aromatize compounds, and which aromatization method to use.
Atom indices -- Whether to calculate atom e-state indices (intrinsic + perturbation term).

Bond indices -- Whether to calculate bond e-state indices (intrinsic + perturbation term).
Atom counts -- Whether to include counts of atom types.
Bond counts -- Whether to include counts of bond types.

Reference

- Lowell H. Hall, Lemont B. Kier: An atom-centered index for drug QSAR models. In Bernard Testa (editor): Advance in Drug Design, vol. 22, Academic Press, 1992.
- Lowell H. Hall, Lemont B. Kier: Electrotopological state indices for atom types: A novel combination of electronic, topological, and valence state information, Journal of Chemical Information and Computer Sciences 35(6): 1039-1045, American Chemical Society, 1995. ArticleID Q5388.
- Lowell H. Hall, Lemont B. Kier, Briscoe B. Brown: Molecular similarity based on novel atom-type electrotopological state indices, Journal of Chemical Information and Computer Sciences 35(6): 1074-1080, American Chemical Society, 1995.
- Lowell H. Hall, Lemont B. Kier: Molecular Structure Description: The Electrotopological State, Academic Press, 1999.

See this page for an extensive bibliography on Estate indices.