MERA descriptors

See also full list of MERA descriptors as well as MERSY descriptors

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Mera descriptors summary

Descriptor name	Description
VME	molecular volume, Å^3
SME	molecular surface, Å^2
SMEP	weighted positively charged surface, $SMEP = \sum_i q_i^+ SME_i^+$ (sum for positively charged atoms; q_i^+ is atomic charge)

SMEN	weighted negatively charged surface, $SMEP = \sum_i q_i^- SME_i^-$ (sum for negatively charged atoms; q_i^- is atomic charge)
SMED	*SMEP SMEN*
SMEPR	fraction of positively charged area, $\frac{SMEP}{SME}$

SMENR	fraction of negatively charged area, $\frac{SMEN}{SME}$
SMEDR	*SMEPR SMENR*
ESMEP	weighted average positively charged area, $ESMEP = \frac{\sum_i q_i^+ SME_i^+}{\sum_i q_i^+}$
ESMEN	weighted average negatively charged area, $ESMEN = \frac{\sum_i q_i^- SME_i^-}{\sum_i q_i^-}$
ESMED	*ESMEP ESMEN*
QSMEP	weighted average positive charge of surface, $QSMEP = \frac{\sum_i q_i^+ SME_i^+}{\sum_i SME_i^+}$
QSMEN	weighted average positive charge of surface, $QSMEN = \frac{\sum_i q_i^- SME_i^-}{\sum_i SME_i^-}$
QSMED	*QSMEP QSMEN*

d204	density of compound d_4^{20}
DMo	dipole moment, *D*
SPH	sphericity, the ratio of surface of sphere (S_S) with the volume equal to the molecular volume, and the molecular surface (S_M): $$SPH = \frac{S_S}{S_M}$$
VOIN1	sum of atomic volumes, Å^3
VOIN1R	VOIN1R = VOIN1/VME
VOIN2	sum of volumes of double overlaps of atomic spheres, Å^3
VOIN2R	part of double overlaps in the molecular volume, $$VOIN2R = \frac{VOIN2}{VME}$$
VOIN3	sum of volumes of triple overlaps of atomic spheres, Å^3

VOIN3R	part of triple overlaps in the molecular volume, $$VOIN3R = \frac{VOIN3}{VME}$$
VOIN4	sum of volumes of quadruple overlaps of atomic spheres, Å^3
VOIN4R	part of quadruple overlaps in the molecular volume, $$VOIN4R = \frac{VOIN4}{VME}$$
VOIN5	sum of volumes of fivefold overlaps of atomic spheres, Å^3
VOIN5R	part of fivefold overlaps in the molecular volume, $$VOIN5R = \frac{VOIN5}{VME}$$
VOIN6	sum of volumes of sixfold overlaps of atomic spheres, Å^3
VOIN6R	part of sixfold overlaps in the molecular volume, $$VOIN6R = \frac{VOIN6}{VME}$$
HIMERA	pKA
MI1	the minimal principal moment of inertia, a.u.
MI2	the middle principal moment of inertia, a.u.
MI3	the maximal principal moment of inertia, a.u.
IR1	the minimal principal inertial radius, Å
IR2	the middle principal inertial radius, Å
IR3	the maximal principal inertial radius, Å
SI12	the minimal principal inertial section, $SI12 = \pi \cdot IR1 \cdot IR2$, Å^2
SI13	the middle principal inertial section, $SI13 = \pi \cdot IR1 \cdot IR3$, Å^2
SI23	the maximal principal inertial section, $SI23 = \pi \cdot IR2 \cdot IR3$, Å^2

PI12	proportion of molecule in the space of principal rotational invariants, $$PI12 = \frac{IR1}{IR2}$$
PI13	proportion of molecule in the space of principal rotational invariants, $$PI13 = \frac{IR1}{IR3}$$
PI23	proportion of molecule in the space of principal rotational invariants, $$PI23 = \frac{IR2}{IR3}$$
DISS1	dissymmetry about the first principal rotational invariant. The dissymmetry is calculated as the third moment (skewness), i.e. $$DISS1 = \left\| \sum_{i=1}^{N} x_i^3 \right\|$$ (N – number of atoms; x_i is the first coordinate of i^{th} atom in the space of principal rotational invariants), Å^3
DISS2	dissymmetry about the second principal rotational invariant, $$DISS2 = \left\| \sum_{i=1}^{N} y_i^3 \right\|$$ (N – number of atoms; y_i is the second coordinate of i^{th} atom in the space of principal rotational invariants), Å^3

DISS3	dissymmetry about the third principal rotational invariant, $$DISS3 = \left| \sum_{i=1}^{N} z_i^3 \right|$$ (N – number of atoms; z_i is the third coordinate of i^{th} atom in the space of principal rotational invariants), Å^3

Further reading

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