

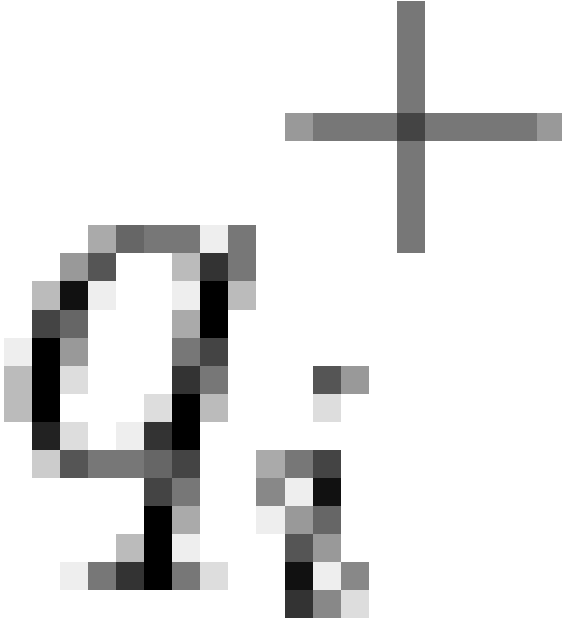
MERA descriptors

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Authors:

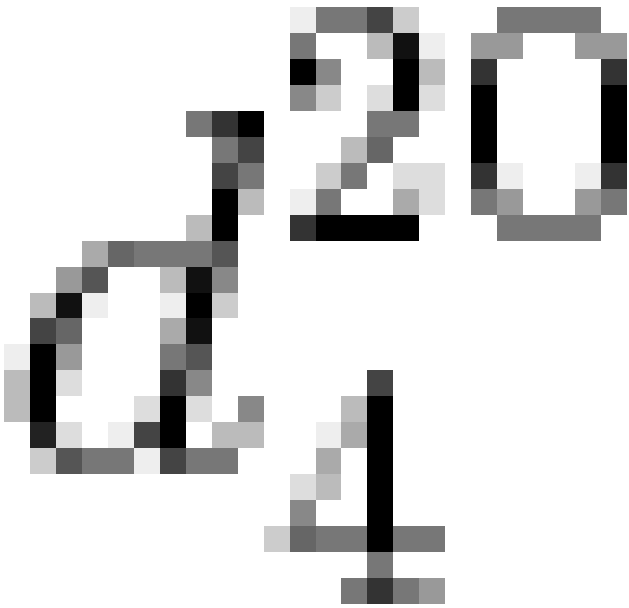
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Mera descriptors summary

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

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

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

d204	 <p>density of compound</p>
DMo	dipole moment, D
SPH	<p>sphericity, the ratio of surface of sphere (S_S) with the volume equal to the molecular volume, and</p> $SPH = \frac{S_S}{S_M}$ <p>the molecular surface (S_M):</p>
VOIN1	sum of atomic volumes, \AA^3
VOIN1R	$VOIN1R = VOIN1/VME$
VOIN2	sum of volumes of double overlaps of atomic spheres, \AA^3
VOIN2R	<p>part of double overlaps in the molecular volume,</p> $VOIN2R = \frac{VOIN2}{VME}$
VOIN3	sum of volumes of triple overlaps of atomic spheres, \AA^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	<p>proportion of molecule in the space of principal rotational invariants,</p> $PI12 = \frac{IR1}{IR2}$
PI13	<p>proportion of molecule in the space of principal rotational invariants,</p> $PI13 = \frac{IR1}{IR3}$
PI23	<p>proportion of molecule in the space of principal rotational invariants,</p> $PI23 = \frac{IR2}{IR3}$
DISS1	<p>dissymmetry about the first principal rotational invariant. The dissymmetry is calculated as the third</p> $DISS1 = \left \sum_{i=1}^N x_i^3 \right $ <p>moment (skewness), i.e.</p> <p>(N – number of atoms; x_i is the first coordinate of i^{th} atom in the space of principal rotational invariants), Å³</p>
DISS2	<p>dissymmetry about the second principal rotational invariant,</p> $DISS2 = \left \sum_{i=1}^N y_i^3 \right $ <p>(N – number of atoms; y_i is the second coordinate of i^{th} atom in the space of principal rotational invariants), Å³</p>

DISS3	<p>dissymmetry about the third principal rotational invariant,</p> $DISS3 = \left \sum_{i=1}^N z_i^3 \right $ <p>(N – number of atoms; z_i is the third coordinate of i^{th} atom in the space of principal rotational invariants), Å³</p>
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Further reading

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