The ODM*x* Methods: New Consistent Semiempirical Methods

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Recently we have introduced two new NDDO-based semiempirical quantum-chemical (SQC) methods ODM2 and ODM3 (ODM*x*), which include orthogonalization and dispersion corrections along with penetration integrals and core–valence interactions as integral parts.[1] These corrections are important for improving the underlying NDDO model[2] and for obtaining more accurate SQC methods.[3-4] The ODM*x* methods build upon the NDDO-based SQC methods OM*x*[3] with D3-dispersion corrections including three-body terms for Axilrod–Teller–Muto dispersion interactions (D3T). In the new methods, the historical convention of assuming that the SCF atomization energy is equal to the atomization enthalpy at 298 K is abandoned. In addition, the ODM*x* methods are parametrized not only with regard to ground-state properties, but also vertical excitation energies, because of the frequent use of general-purpose SQC methods for excited-state calculations and dynamics simulations.

Mean Absolute Errors

		MNDO	OM2	OM2-D3T	ODM2
Heats of formation (CHNO set)	kcal/mol	6.36	3.05	5.10	2.64
Noncovalent interaction energies (S66x8 set)	kcal/mol	9.48	1.93	0.79	0.75
Vertical excitation energies (Thiel's set)	eV	1.44	0.46	0.46	0.35
Atomization energies w/o ZPVE at 0 K (TAE140 set)	kcal/mol	20.13	14.93	14.27	4.89
corrected		11.90	4.81	4.64	

The ODMx methods perform consistently better than other SQC methods for a broad range of properties ranging from ground-state to excited-state properties and noncovalent interactions. They manifest the successes in SQC method improvement since 1977, when the first successful general-purpose SQC method MNDO was introduced.

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[2] X. Wu, P. O. Dral, A. Koslowski, W. Thiel, *J. Comput. Chem.* **2019,** *40*, 638–649.
[3] P. O. Dral, X. Wu, L. Spörkel, A. Koslowski, W. Weber, R. Steiger, M. Scholten, W. Thiel, *J. Chem. Theory Comput.* **2016,** *12*, 1082–1096.
[4] P. O. Dral, X. Wu, L. Spörkel, A. Koslowski, W. Thiel, *J. Chem. Theory Comput.* **2016,** *12*, 1097–1120.