MOPAC2009™

the next generation quantum chemistry tool for property prediction

- **Fast optimizations up to 15,000 atoms, e.g. proteins**
- **NEW PM6 parameterization from experimental & *ab initio***
- **More accurate H-bond and dispersion energies***
- **ALL main group elements & transition metals (83)**
- **Major improvements over PM3 and AM1**
- **Crystals, surfaces & polymers with periodic boundaries**
- **FREE to academics**

*A Transferable H-Bonding Correction for Semiempirical Quantum-Chemical Methods, Martin Korth, Michal Pitonak, Jan Rezac, and Pavel Hobza, *J. Chem. Theory Comput.* **2010,** *6,* 344352

MOPAC2009™

• Giant molecule capability

MOPAC2009's linear-scaling algorithm, MOZYME, allows geometry optimizations on closed shell systems of up to 15,000 atoms (e.g. proteins). Conventional MOPAC is limited to about 1,500 atoms.

No. of atoms	Time for 1 SCF (minutes)		Memory (megabytes)	
	MOZYME	MOPAC	MOZYME	MOPAC
400	0.2	2.3	17	101
1,500	2.3	222.6	78	1,424
15,000	230.3	*222,600.0	1,026	*142,400

**estimated*

• NEW parameterization (PM6)

The most widely used semiempirical quantum chemistry package, MOPAC®, has been completely rewritten from the ground up with a new and more accurate parameterization (PM6) for all the main group elements and transition metals. Experimental and *ab initio* data from over 9,000 compounds were used to develop the new PM6 method. This compares with only 39 compounds used to develop the original MNDO method, about 200 compounds used for AM1, and about 500 compounds used for PM3. The original AM1 and PM3 methods have been used in numerous commercial semiempirical packages over the past 20 years. MOPAC2009™ with PM6 represents the first major improvement in methodology to MOPAC®, since PM3 was published in 1989.[1]

Year	Method	# compounds used for parameterization	
1977	MNDO	39	experimental
1985	AM1	~200	experimental
1989	PM3	~500	experimental
2007	**PM6**	**> 9,000**	**experimental & *ab initio***

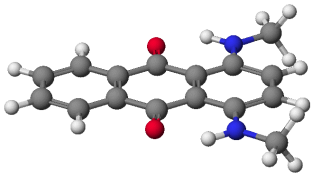
• More accurate heats of formation from PM6

Method	Average unsigned error (kcal/mol)	Largest error (kcal/mol)
PM6	**4.79**	**-42.2**
B3LYP 6-31G(d)	5.19	35.8
PM3	6.26	135.6
HF 6-31G(d)	7.37	72.5
AM1	10.01	111.9

Comparison of errors in heats of formation for a set of 1,373 compounds containing only C, H, O, N, F, Cl, S, P and Br.

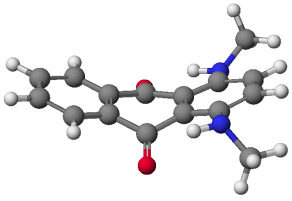
MOPAC® is the most cited semiempirical program and has far more published accuracy data than any comparable program.[1] MOPAC® has been used to check for and correct errors in the published experimental heats of formation tables on the NIST website.[2,3]

• More accurate geometries from PM6



PM6 & DFT ✓

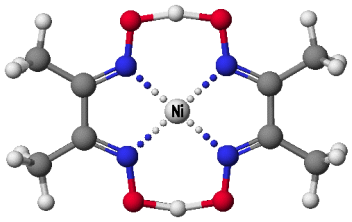
PM6 optimizes anthraquinones to the correct planar fused-ring structure, consistent with DFT geometries (left). Most semiempirical methods, such as AM1 and PM3, produce erroneous non-planar fused rings (right). PM6 also optimizes the amines attached to aromatic rings to the correct planar geometry.

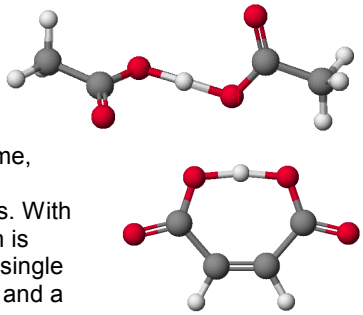


PM3 & AM1 ✗

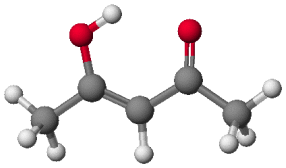
• More accurate hydrogen bonds from PM6

PM6 positions the bridging hydrogen approximately equidistant between the oxygen atoms in dicarboxylic acid anions such as hydrogen diacetate and hydrogen maleate anions and, similarly, in nickel dimethylglyoxime, consistent with experimental observations and DFT geometries. With AM1 and PM3 the hydrogen atom is incorrectly displaced indicating a single bond to one of the oxygen atoms and a normal hydrogen bond to the other.





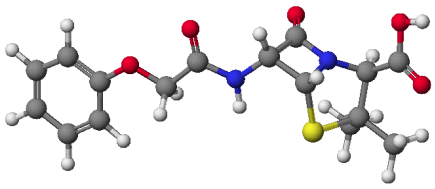
• PM6 offers major improvements over AM1 & PM3



Semiempirical gas-phase calculations using PM3 incorrectly predict that the free energy of the enol tautomer of acetylacetone is higher than the keto tautomer. PM6 correctly predicts that the enol form is the lower energy tautomer in the gas phase, consistent with DFT results and experimental observation.

• Fast descriptor generation for QSAR

New algorithms in MOPAC2009™ facilitate fast property prediction for screening libraries of drug-sized molecules for a wide range of properties, including pKa. The speed of MOPAC2009™ and improved accuracy of PM6 are particularly valuable for generating electronic descriptors for quantitative structure-property relationships (QSAR).

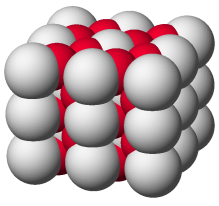


• ALL main group elements & transition metals parameterized with PM6

PM6 in MOPAC2009™ includes parameters for a wider range of elements than any other semiempirical quantum chemistry program. All main group elements and transition metals up to Bismuth are now parameterized in PM6. Further, MOPAC2009™ includes new elements for PM3 & AM1.

PM6: (83) H, He, Li, Be, B, C, N, O, F, Ne, Na, Mg, Al, Si, P, S, Cl, Ar, K, Ca, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Ga, Ge, As, Se, Br, Kr, Rb, Sr, Y, Zr, Nb, Mo, Tc, Ru, Rh, Pd, Ag, Cd, In, Sn, Sb, Te, I, Xe, Cs, Ba, La, Lu, Hf, Ta, W, Rh, Os, Ir, Pt, Au, Hg, Tl, Pb, Bi, + 15 lanthanide sparkles[4]

• Crystals, surfaces & polymers with periodic boundaries



MOPAC2009™ can handle extended solids including straight-chain polymers such as bucky tubes (one-dimensional), surfaces (two-dimensional), and crystals (three-dimensional) with periodic boundary conditions. This approach eliminates the problems of edge effects and facilitates the calculation of properties on extended systems that cannot be handled adequately by other quantum chemistry packages.