MOPAC2009™

the next generation quantum chemistry tool for property prediction

- **Optimize systems of up to 15,000 atoms, e.g. proteins**
- **NEW PM6 parameterization from experimental *& ab initio***
- **More accurate* heats of formation and geometries**
- **ALL main group elements & transition metals**
- **Serious errors from PM3 and AM1 corrected**
- **Crystals, surfaces & polymers with periodic boundaries**
- **FREE to academics**

*compared to AM1, PM3 and some *ab initio* methods (see over)

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***

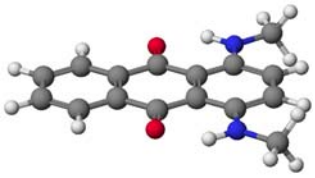
• More accurate heats of formation from PM6

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.

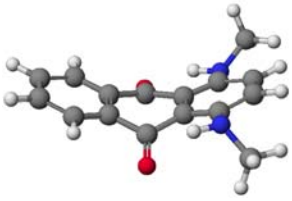
MOPAC® is the most cited semiempirical program and has far more published accuracy data than any comparable program.[1] MOPAC® has been used to check for and correct errors in the published experimental heats of formation tables on the NIST website.[2,3]

• More accurate geometries from PM6



PM6 & DFT ✓

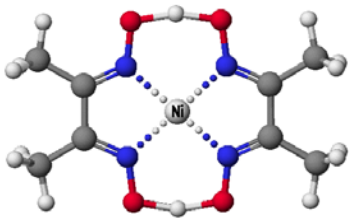
PM6 optimizes anthraquinones to the correct planar fused-ring structure, consistent with DFT geometries (left). Most semiempirical methods, such as AM1 and PM3, produce erroneous non-planar fused rings (right). PM6 also optimizes the amines attached to aromatic rings to the correct planar geometry.

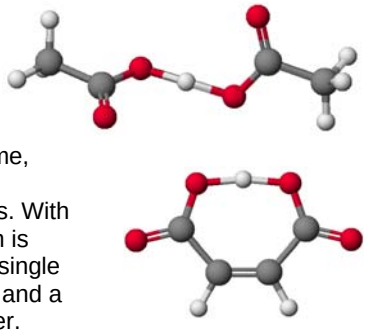


PM3 & AM1 ✗

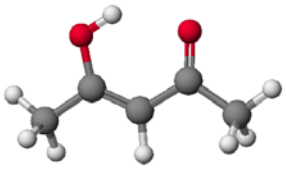
• More accurate hydrogen bonds from PM6

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.





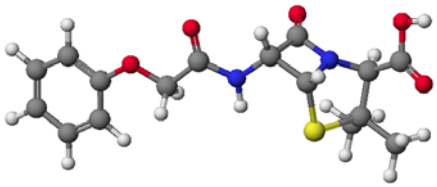
• PM6 method corrects major errors in AM1 & PM3



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 are now parameterized in PM6. Further, MOPAC2009™ includes new elements for PM3 & AM1.

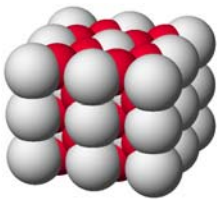
PM6: (69) H, He, Li, Be, B, C, N, O, F, Ne, Na, Mg, Al, Si, P, S, Cl, Ar, K, Ca, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Ga, Ge, As, Se, Br, Kr, Rb, Sr, Y, Zr, Nb, Mo, Tc, Ru, Rh, Pd, Ag, Cd, In, Sn, Sb, Te, I, Xe, Cs, Ba, La, Lu, Hf, Ta, W, Rh, Os, Ir, Pt, Au, Hg, Th, Pb, Bi

For comparison, available AM1 and PM3 parameterization from a third-party package:

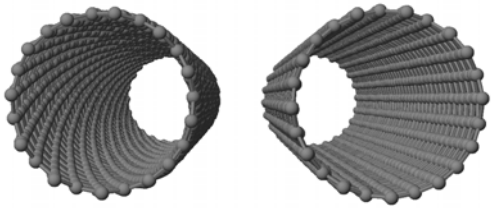
PM3: (32) *H, Li, Be, B, C, N, O, F, Na, Mg, Al, Si, P, S, Cl, Ca, Zn, Ga, Ge, As, Se, Br, Cd, In, Sn, Sb, Te, I, Hg, Tl, Pb, Bi.*

AM1: (18) *H, B, C, N, O, F, Mg, Al, Si, P, S, Cl, Zn, Ge, Br, Sn, I, Hg*

• 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.



• MOPAC2009™ specifications

Properties

Thermodynamic properties (heats of formation, entropies, free energies, heat capacities), vibrational (IR) spectra (including isotope effects), dipole moments, ionization potentials, partial charges, bond orders, static and frequency-dependent polarizabilities and hyperpolarizabilities, pKa, molecular orbitals, band gaps, electron densities, electrostatic potentials, transition states, intrinsic reaction coordinates, dynamic reaction coordinates, excited state geometries and energetics, compressibility, density, and thermodynamic properties of crystals.

Types of calculations

Open and closed-shell Hartree-Fock methods: Restricted (RHF), Unrestricted (UHF), Restricted open-shell (ROHF), singlet, doublet, triplet, quartet, quintet, sextet, etc. (ground and excited states)
Geometry optimization: Eigenvector following (EF), BFGS, NLLSQ, SIGMA
Locating Transition states: Saddle, Path, Grid
Refining Transition states: Transition State Eigenvector Following (TS), NLLSQ, SIGMA
Vibrational frequency calculation
Solvent effects: Conductor-like Screening Model (COSMO) including d-orbitals and excited states
Configuration interaction (CI) includes dynamic and static Jahn-Teller, symmetry analysis
Periodic boundary conditions: 1, 2, & 3 dimensional translation vectors (Tv)

Hamiltonians

PM6: (69) 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, Th, Pb, Bi
PM3: (42) H, He, Li, Be, B, C, N, O, F, Ne, Na, Mg, Al, Si, P, S, Cl, Ar, K, Ca, Zn, Ga, Ge, As, Se, Br, Kr, Rb, Sr, Cd, In, Sn, Sb, Te, I, Xe, Cs, Ba, Hg, Th, Pb, Bi
AM1: (42) H, He, Li, Be, B, C, N, O, F, Ne, Na, Mg, Al, Si, P, S, Cl, Ar, K, Ca, Zn, Ga, Ge, As, Se, Br, Kr, Rb, Sr, Mo, In, Sn, Sb, Te, I, Xe, Cs, Ba, Hg, Th, Pb, Bi, + 15 lanthanide sparkles[4]
MNDO: (17) H, B, C, N, O, F, Na, Al, Si, P, S, Cl, Zn, Br, Cd, I, Hg
RM1[5]: (10) H, C, N, O, P, S, F, Cl, Br, I

User Interface

MOPAC2009™ is command driven and is designed to work with a wide range of third-party graphical user interfaces (GUI)s. The original MOPAC® file format has been preserved so that MOPAC2009™ can work with third-party GUIs that have been developed to interface to the public domain version of MOPAC®. MOPAC2009™ also reads and writes other file formats such as PDB and Gaussian®.

Platforms

MOPAC2009™ is available to download for Windows®, LINUX and Macintosh. For source code, please contact MrMOPAC@OpenMOPAC.net

• FREE to academics

MOPAC2009™ is available for free to bona-fide academics for teaching and not-for-profit R&D. Academics may download MOPAC2009 at http://www.MOPAC2009.com

MOPAC2009™ prices (Windows®)	Academic	Government	Industry
1 permanent license	free	$2,500	$5,000
5 permanent licenses	-	$5,000	$10,000
Annual site license	-	$5,000	$10,000

For commercial and government sales, please contact CAChe Research LLC, USA
URL: http://www.cacheresearch.com/mopac.html Email: mopac@cacheresearch.com

1. Stewart, J. J. P. (1989). J. Comp. Chem. 10(2): 209-220; 221-264.
2. Stewart, J. J. P. (2004). J. Mol. Modelling 10: 6-12.
3. Stewart, J. J. P. (2004). J. Phys. Chem. Ref. Data 33(3): 713-724.
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