



# **MOPAC Manual**

## ***ADF Modeling Suite 2018***

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## INTRODUCTION

MOPAC [1 (page 5)] is a general-purpose semiempirical molecular orbital package for the study of solid state and molecular structures and reactions. A good trade-off between speed and accuracy is achieved through a minimal basis and parameterization against experimental data, with parameters for most elements.

As of the 2018 release of the Amsterdam Modeling Suite, MOPAC has become an engine in the new AMS driver setup. If you have not done so yet, we highly recommend you to first read the General section of the AMS Manual. In practice the inclusion of MOPAC into AMS means that MOPAC can now be used for many applications that were previously not supported:

- Elastic tensor and related properties (e.g. Bulk modulus)
- Linear transit and PES scan
- Lattice optimization (also under pressure)
- Constrained geometry optimizations
- Molecular dynamics simulations
- Phonon calculations
- ...

Please refer to the AMS manual for a complete overview.

Note that the MOPAC engine is not parallelized in the 2018 release. However, for embarrassingly parallel calculations (e.g. elastic properties) it can be run in parallel by the AMS driver, see AMS manual on double parallelism.



## INPUT KEYWORDS

This manual documents the input for the MOPAC engine used together with the AMS driver. If you are not yet familiar with the AMS driver setup, we highly recommend reading the introductory section in the AMS manual.

The MOPAC engine is selected and configured in the AMS input with:

```
Engine MOPAC
... keywords documented in this manual ...
EndEngine
```

This page documents all keywords of the MOPAC engine input, basically the contents of the `Engine MOPAC` block in the AMS input file.

```
Model [ ... ]
UnpairedElectrons int
Sparkles [True | False]
Properties
  BondOrders [True | False]
End
Mozyme [True | False]
Solvation [None | COSMO-CRS | COSMO-Water]
```

The most important keyword in the MOPAC engine input is the model selection:

### Model

**Type** Multiple Choice

**Default value** PM7

**Options** [AM1, MNDO, MNDOD, PM3, RM1, PM6, PM6-D3, PM6-DH+, PM6-DH2, PM6-DH2X, PM6-D4H4, PM6-D3H4X, PM7, PM7-TS]

**Description** Selects the model Hamiltonian to use in the calculation. AM1 Use the AM1 Hamiltonian MNDO Use the MNDO Hamiltonian MNDOD Use the MNDO-d Hamiltonian RM1 Use the RM1 Hamiltonian PM3 Use the MNDO-PM3 Hamiltonian PM6 Use the PM6 Hamiltonian PM6-D3 Use the PM6 Hamiltonian with Grimme's corrections for dispersion PM6-DH+ Use the PM6 Hamiltonian with corrections for dispersion and hydrogen-bonding PM6-DH2 Use the PM6 Hamiltonian with corrections for dispersion and hydrogen-bonding PM6-DH2X Use PM6 with corrections for dispersion and hydrogen and halogen bonding PM6-D3H4 Use PM6 with Rezac and Hobza's D3H4 correction PM6-D3H4X Use PM6 with Brahmshatriya, et al.'s D3H4X correction PM7 Use the PM7 Hamiltonian PM7-TS Use the PM7-TS Hamiltonian (only for barrier heights)

The default PM7 model [2 (page 5)] is the latest parametrization for MOPAC and should be the most accurate for most calculations.

**UnpairedElectrons****Type** Integer

**Description** If this key is present, a spin-unrestricted calculation with the specified number of unpaired electrons is performed. If this key is not present the number of unpaired electrons is determined automatically (0 for systems with an even number of electrons, 1 for radicals), and a restricted or unrestricted calculation is performed accordingly.

**Sparkles****Type** Bool**Default value** False

**Description** Represent lanthanides by their fully ionized 3+ sparkles. That is, they have no basis set, and therefore cannot have a charge different from +3. When using sparkles, the geometries of the lanthanides are reproduced with good accuracy, but the heats of formation and electronic properties are not accurate.

**Properties****BondOrders****Type** Bool**Default value** False

**Description** Whether or not bond orders are calculated based on the final molecular orbitals.

**Mozyne****Type** Bool**Default value** False

**Description** Replace the standard SCF procedure with a localized molecular orbital (LMO) method. The time required for an SCF cycle when Mozyne is used scales linearly with system size.

**Solvation****Type** Multiple Choice**Default value** None**Options** [None, COSMO-CRS, COSMO-Water]

**Description** Configures the solvation model. Select COSMO-Water to specify the COSMO solvation method, COSMO-CRS for use with COSMO-RS.

Finally it is possible to pass any other keywords directly to the MOPAC program [*1* (page 5)]. The full list of keywords can be found on the [standalone MOPAC manual](http://openmopac.net/manual/index.html) (<http://openmopac.net/manual/index.html>).

Keywords string

**Keywords****Type** String

**Description** A string containing all the desired custom MOPAC keywords. Basically for anything not directly supported through AMS.

These keywords are just literally passed through to MOPAC program which the AMS MOPAC engine wraps, without any checking in AMS. One should therefore be very careful with this, as it is very easy to set up completely nonsensical calculations in this way. E.g. it obviously does not make sense to let the MOPAC program do a geometry optimization, when the AMS driver is really just trying to get energy and gradients for a single geometry.



## REFERENCES

The MOPAC engine in the 2018 of the Amsterdam Modeling Suite is a wrapper around the standalone MOPAC2016 program developed by Dr. Jimmy Stewart.

1. MOPAC2016, James J.P. Stewart, Stewart Computational Chemistry, Colorado Springs, CO, USA, <http://OpenMOPAC.net> (2016)
2. James J.P. Stewart, *Optimization of parameters for semiempirical methods VI: more modifications to the NDDO approximations and re-optimization of parameters*, *J. Mol. Modeling* 19, 1-32 (2013) (<https://doi.org/10.1007/s00894-012-1667-x>)

A full list of references for the MOPAC package can be found on the [official MOPAC references page](http://openmopac.net/Manual/references.html) (<http://openmopac.net/Manual/references.html>).