



MOPAC 6

Impressum

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The Old Vicarage
132 Bedford Road
Kempston
BEDFORD, MK42 8BQ
www.ceposinsilico.com

Manual

Timothy Clark

Layout

www.eh-bitartist.de





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1 INTRODUCTION

CEPOS Mopac 6 is a modified version of Mopac version 6 (QCPE 455) that is supplied as open source free of charge as an economic alternative to commercial semiempirical molecular orbital packages for ParaSurf™ users. Mopac 6 does not include many modern options and Hamiltonians (in particular, it does not include methods that use d-orbitals) but it is adequate for MNDO, AM1 and PM3 calculations. We recommend that the EF geometry optimizer always be used as the default BFGS optimizer often exits at high values of the gradient norm.



2 CEPOS MODIFICATIONS

2.1 File names

CEPOS Mopac has been modified to assign the file names automatically without using a run script. Thus, it can be called using the command

```
mopac6.exe <filename>(.dat)
```

<filename> is the name of the input file, which may optionally also have the extension **.dat**.

The above command produces the following files, independent of whether the extension **.dat** is used or not:

Table 1: The SDF data blocks that ParaFit™ transforms after a superposition calculation.

| | | |
|-------------------------------|---|---|
| <filename>.out | Output file | <i>See the following Mopac manual for definitions</i> |
| <filename>.arc | Mopac archive file | |
| <filename>.log | Mopac log file | |
| <filename>.syb | Mopac Sybil file | |
| <filename>_m.sdf | .sdf file suitable for input to ParaSurf™ | |

2.2 SDF-file

CEPOS Mopac writes an additional output file, named **<filename>_m.sdf** that is suitable as input for ParaSurf™. This file complies with the SDF file (version 2000) convention and contains the following additional tags used by ParaSurf™:

<HAMILTONIAN>

This tag defines the semiempirical Hamiltonian used. Possible values are MNDO, AM1 or PM3.

<MOPACBASICS>

This block is equivalent to the VAMPBASICS block written by VAMP and includes the heat of formation (kcal mol⁻¹), the HOMO and LUMO energies (eV), and the x-, y-, and z-components of the dipole-moment vector (Debye).

<TOTAL COULSON CHARGE>

Gives the sum of the Coulson charges on the atoms (= the total molecular charge).

**<ORBITAL VECTORS>**

Lists the molecular orbitals as the AO-coefficients in the same format as VAMP.

<DENSITY MATRIX ELEMENTS>

Lists the one-atom elements of the density matrix for non-hydrogen atoms.

<CHARGE ON HYDROGENS>

Lists the Coulson charges on the hydrogen atoms.

<CALCULATION STATUS>

Indicates whether the calculation concluded successfully.

The formats of these blocks are defined in the ParaSurf[™] manual.

2.3 Cartesian Coordinates

In order to make calculations on overlaid structures possible without Mopac reorienting and shifting the coordinate system, CEPOS Mopac uses exactly the input Cartesian coordinates if the keywords **1scf** and **XYZ** are used together.



3 INSTALLATION

CEPOS Mopac is provided for free download in several zipped archives:

3.1 Executables

`mopac_exe_files.zip`

contains three executables for 32-bit Windows systems (`mopac6_Win32.exe`), 32-bit Linux systems (`mopac6_Linux.exe`) and Silicon Graphics Irix (`mopac6_Irix.exe`). These files need only be copied onto your machine and the directory in which they reside added to the paths.

3.2 Source files

`mopac_source.zip`

contains the Mopac Fortran Source files and makefiles for Windows (`mopac.mak`), the GNU g77 compiler under Linux (`makefile`) and for the f90 compiler under Irix (`Makefile_Irix`). It is only necessary to download this archive if you wish to install Mopac on a system other than those given above or if you wish to modify the code. Changes made by CEPOS are commented using the tag `Cepos`.

3.3 Example files

`mopac_examples_Windows.zip` and `mopac_examples_Unix.zip`

The only difference between these two archives is that the former is readable on Windows systems and the latter on Unix-based systems such as Linux and Irix. They contain the input examples given in the Mopac 6 manual and output calculated using CEPOS Mopac 6. These files are useful for checking the results on your machine.



4 MOPAC 6 MANUAL

The original manual for Mopac 6 written by Jimmy Stewart is available online at:

<http://www.chm.tu-dresden.de/edv/mopac6/mop.html>.