MOPAC 5.022mn

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MOPAC 5.022mn is an enhanced version of MOPAC 5 with the following noteworthy features:

- very portable
- conveniently structured for use in molecular dynamics or parameter optimization
- well documented with installation instructions and a test suite
- includes the following molecular orbital methods (in both restricted and UHF forms):
    - MNDO, AM1, PM3
    - PDDG/MNDO, PDDG/PM3 (developed by Jorgensen and coworkers)
    - RM1 (developed in Recife)
    - PM6 (developed by Stewart)
    - AM1-D, PM3-D (developed by Hillier and coworkers)
    - PMOv1, PMO2, and PMO2a (developed at Minnesota)
    - option to add dispersion (in either the form used by Wu and Yang, Grimme, and McNamara and Hillier or the form used by Tang and Toennies and Misquitta and Stone) to MNDO, RM1, or PM6 or to change the form of dispersion in AM1 and PM3
    - option to use a different beta for each pair of atomic numbers, rather than the standard procedure by which $\beta_{AB} = (\beta_A + \beta_B)/2$
    - option to use specific reaction parameters (SRPs)
    - option to include *p* orbitals on hydrogen atoms
    - various options to add molecular mechanics damped dispersion, including the D3 and Misquitta-Stone formulas
- includes semianalytic gradients for all the above methods with an option to represent the Slater-type orbitals as STO-6G for higher precision.
- includes CM2 (a class IV charge model) as well as Mulliken population analysis
- includes a more general version of configuration interaction than in the original version of MOPAC 5
- includes the eigenvector following (EF) method for geometry optimization of minima and transition states (donated by Frank Jensen)

The program is available at the Data Repository for University of Minnesota (DRUM):
https://conservancy.umn.edu/drum

Publications of results obtained with the *MOPAC* - version 5.022mn software should cite the program and the DOI given at the DRUM.