

CIMTYP chooses a Cluster-In-Molecule (CIM) calculation.

- = NONE skip CIM computation, i.e., perform a canonical calculation (default).
- = SECIM perform a single-environment CIM (SECIM) computation.
- = DECIM perform a dual-environment CIM (DECIM) computation.
- = GSECIM perform a generalized SECIM (GSECIM) computation. The \$CIMFRG must be included as well.

See also \$CIMINP and, optionally, \$CIMFRG and \$CIMATM. If CIMTYP is given, SUBMTD in \$CIMINP is required. Only RUNTYP=ENERGY and SCFTYP=RHF or ROHF work when CIMTYP is given. See SUBMTD in \$CIMINP for more details.

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RELWFN Selects all-electron scalar relativity treatment. See the \$RELWFN input group for more information, including nuclear derivative availability.

- = NONE use the basic Schrodinger equation (default)
- = LUT-IOTC local unitary transformation modification of IOTC, due to H.Nakai, J.Seino, Y.Nakajima. This is the fastest and most numerically reliable scalar relativity method, so it is preferred over RESC, DK, or IOTC.
- = IOTC infinite-order two-component method of M. Barysz and A.J. Sadlej.
- = DK Douglas-Kroll transformation, available at the 1st, 2nd, or 3rd order.
- = RESC relativistic elimination of small component, the method of T. Nakajima and K. Hirao, available at 2nd order only.
- = NESC normalised elimination of small component, the method of K. Dyall, 2nd order only.

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RUNTYP specifies the type of computation, for example at a single geometry point:

- = ENERGY Molecular energy. (default)
- = GRADIENT Molecular energy plus gradient.
- = HESSIAN Molecular energy plus gradient plus