Quick Start Guide for MULTIMODE User Parameters Change Only These

Input Parameter	Meaning	Comments
NATOM	Number of atoms	--
ICOUPL	n in nMR of V (3 or 4)	n-mode representation of potential
ICOUPC	n in nMR I_{eff} (2 or 3)	"Coriolis term", if 0 ignore this term
ISCFCI	Number of VCI States (eigen values and vectors)	May override CUT (see below) if ISCFCI states are reached first
NROTTR	(3N-6)-|NROTTR| = nmode	0 or < -1. If <-1 exclude |NROTTR| lowest-freq modes; if 0 use all modes
NMAX	Level of mode-coupling in VCI (2-4)	NMAX is negative so excitation = -NMAX; usually -2 to -4
CUT	Max VCI energy (cm^{-1})	May override ISCFCI for output if CUT is reached first
IPRINT	0 minimal. Usually < 0	Print |IPRINT| VCI coefs per state
MATSIZ	0 or 1	If 1 output H-matrix size and stop; if 0 normal run
XMODQ	1.0 1.0 ... 1.0 nomde entries	Scaling for normal coordinate leave 1.0
MAXSUM	N_1 N_2 ... $N_{\|NMAX\|}$ |NMAX| entries	Max sum of excitations for n-mode (n=1,2,...|NMAX|) coupling basis
MAXBAS	Max quanta per mode for 1-mode excitation Max quanta per mode for 2-mode excitation ... Max quanta per mode for |NMAX|-mode excitation	|NMAX| lines, NMODE numbers in each line Approx 8 Approx 7 ... Decrease with n-mode to keep the H-matrix from growing too large
NCYCLE	Number of cycles for iterative diagonalizer	NCYCLE=0 diagonalize the whole matrix directly. Use iterative for matrices > 50K
NBF MBF NVF MVF	No. of primitive HO functions No. of Gauss-Hermite points No. of contracted numerical functions No. of HEG quadrature points ...	One line for each mode Default value NBF=4+MAXBAS, 1-mode Default value MBF=NBF+4 Default value NVF=MAXBAS, 1-mode Default value MVF=NBF. In general MVF<=NBF
Masses	Atomic mass units (C is 12.0)	--
Equilib	x, y, z in bohr	Dimension NATOM*3