Last update: 16th June, 2021

GRRM program function comparison table

Function (Job-type / Option)	GRRM1.22	GRRM-Basic	GRRM11	GRRM-Neo11	GRRM14	GRRM17	GRRM20
Path search by ADD following (ADDF) method a	✔	✔	✔	✔	✔	✔	✔
Normal mode analysis (FREQ)	✔	✔	✔	✔	✔	✔	✔
Zero-point vibrational energy correction	✔	✔	✔	✔	✔	✔	✔
Thermochemistry calculation (G, H, S and so on)	✔	✔	✔	✔	✔	✔	✔
Minimum point optimization (MIN)	✔	✔	✔	✔	✔	✔	✔
Saddle-point optimization (SADDLE)	✔	✔	✔	✔	✔	✔	✔
IRC following (IRC)	✔	✔	✔	✔	✔	✔	✔
Double-ended minimum search by SCW	✔	✔	✔	✔	✔	✔	✔
Double-ended saddle-point optimization by 2PSHS	✔	✔	✔	✔	✔	✔	✔
Geometry refinement calculation (ReStruct)	✔	✔	✔	✔	✔	✔	✔
Energy refinement calculation (ReEnergy)	✔	✔	✔	✔	✔	✔	✔
Random structure generation b	✔	✔	✔	✔	✔	✔	✔
Structure selection, part selection	✔	✔	✔	✔	✔	✔	✔
Frozen atoms c	✔	✔	✔	✔	✔	✔	✔
ONIOM	✔	✔	✔	✔	✔	✔	✔
MicroIteration	✖	✖	✔	✔	✔	✔	✔
Limited search EQOnly	✔	✔	✔	✔	✔	✔	✔
FirstOnly	✔	✔	✔	✔	✔	✔	✔
NoBondRearrange	✔	✔	✔	✔	✔	✔	✔
BondCondition	✖	✖	✔	✔	✔	✔	✔
Large ADD Following (LADD)	✔	✔	✔	✔	✔	✔	✔
NLowest	✔	✔	✔	✔	✔	✔	✔
Excited-state analysis, Minimum state of each spin multiplicity	✔	✔	✔	✔	✔	✔	✔
General excited-state analysis	✖	✖	✔	✔	✔	✔	✔
Automated analysis of minimum on seam of crossing (MSX)	✖	✖	✔	✔	✔	✔	✔
Automated analysis of conical intersections on potential surfaces	✖	✖	✔	✔	✔	✔	✔
Path search by AFIR method							
MC-AFIR	✖	✖	✖	✖	✔	✔	✔
SC-AFIR	✖	✖	✖	✖	✖	✔	✔
DS-AFIR	✖	✖	✖	✖	✖	✔	✔
Interface for changing AFIR search method from the outside	✖	✖	✖	✖	✖	✖	✔
LUP path optimization	✖	✖	✖	✖	✔	✔	✔
RePath	✖	✖	✖	✖	✔	✔	✔
Periodic boundary conditions (PBCs)	✖	✖	✖	✖	✖	✖	✔
Kinetic simulation	✖	✖	✖	✖	✖	✖	✔
Kinetics-based navigation using RCMC	✖	✖	✖	✖	✖	✖	✔
Intra-node parallel exploration	✖	✔	✔	✔	✔	✔	✔
Inter-node parallel exploration (NeoGRRM)	✖	✔	✖	✔	✖	✖	✖
Inter-node parallel exploration (MPI)	✖	✖	✖	✖	✖	✔	✔
General interface with external ab initio programs	Expandable	Expandable	Not expendable	Not expendable	Expandable	Expandable	Expandable
Included interface	GAUSSIAN	GAUSSIAN	GAUSSIAN	GAUSSIAN	GAUSSIAN	GAUSSIAN	GAUSSIAN
			MOLPRO	MOLPRO	MOLPRO	MOLPRO	MOLPRO
					GAMESS	GAMESS	GAMESS
						TURBOMOL	TURBOMOL
						SIESTA	SIESTA
							ORCA
Commercialized version	✖	✔	✖	✔	✖	✖	✔

a Name of Job-type ADD-Following(ADDF) automatic exploration is GRRM until GRRM14, ADDF in GRRM17 or later.

b Name of this option is MaxRUN in GRRM1.22(GRRM-Basic), NRUN in other versions.

c In the structure input, movable structure first, and immediately before the fixed structure to be entered after that, enter FIELD in GRRM1.22 (GRRM-Basic) and Frozen Atoms in others to classify.

(Detailed options and the functions to change the default parameter values are omitted)