MainWindow

File Edit

Levels, Fit and Spectrum

Datasets | Energy Levels | Fitting | Spectrum

Molecule and Grid | States | Operators | Hamiltonian

Molecule and isotopologues:

CO

12C16O
12C17O
12C18O
13C16O
13C17O
13C18O

Grid: (•) Equidistant ( ) Non-equidistant

Number of points: 800

Rmin: 0.83

Rmax: 3.0

Solver: (•) Sinc ( ) Fourier ( ) FD5

Selected isotopologues: 12C16O

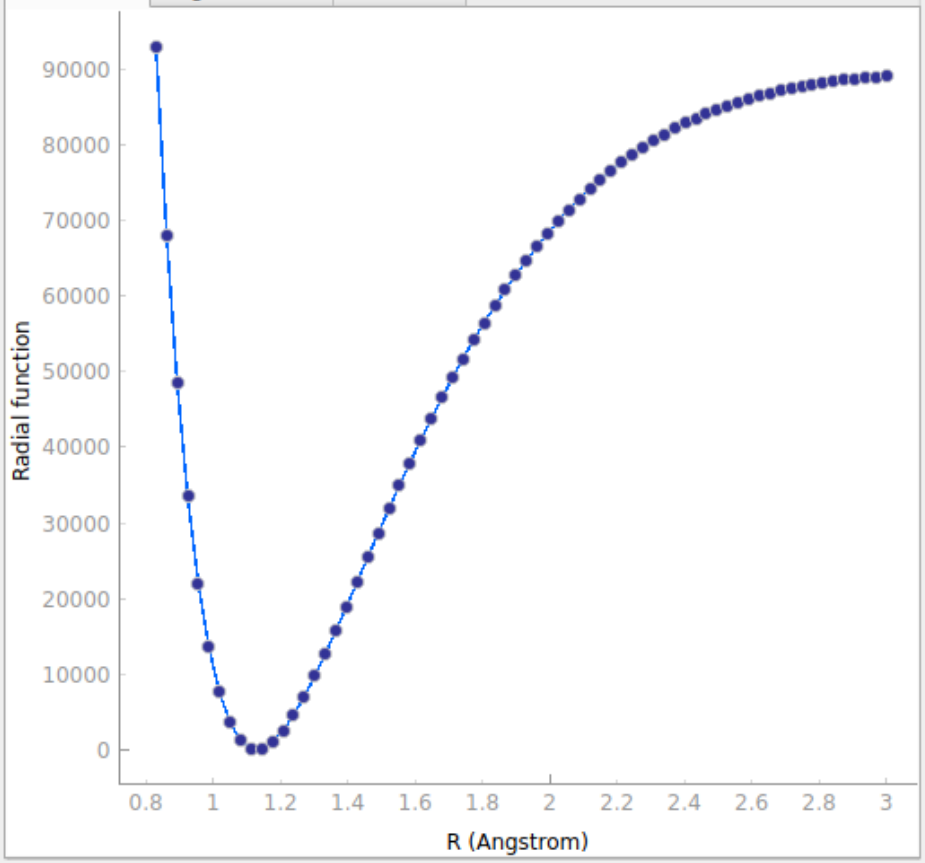
Isotopologue 12C16O:
Reduced mass = 6.856208638002872

Atomic Symbol = C
Mass number = 12
Relative Atomic Mass = 12.0000000(00)
Isotopic Composition = 0.9893(8)

Ref J: Ref Energy:

Plots

Rad. func | Eigenvectors | All funcs



Data Viewer and Editor

Input Data | Output Data

Parameters | Obs. Energies | Obs. Waven | Obs. Intensity

	1	2	3	4	5	6	7	8
1	1.00000	0.00000	0.00000	1081.61130	1.00000	0.10000	1.00000	1.00000
2	2.00000	1.00000	0.00000	3224.96434	1.00000	0.10000	1.00000	1.00000
3	3.00000	2.00000	0.00000	5341.74923	1.00000	0.10000	1.00000	1.00000
4	4.00000	3.00000	0.00000	7432.13410	1.00000	0.10000	1.00000	1.00000
5	5.00000	4.00000	0.00000	9496.16376	1.00000	0.10000	1.00000	1.00000
6	6.00000	5.00000	0.00000	11533.90907	1.00000	0.10000	1.00000	1.00000