1 File Structure

1.1 .inp

Inp files contain the input values for westersim.

The first line contains a string for the name of the molecule.

The first section, after the molecule name, is Controls. This section sets global variables for westersim.

NFOLD	integer	The fold value for the rotor
S	float	Total spin value
TK	float	Temperature in Kelvin
RUNmode	flag	ESF for energy, simulation, and fit. Defines which westerfit programs will run.
mcalc	integer	defines the size of the torsional basis
vtmax	integer	maximum value of vt
Jmax	float	maximum value of J
vmin	float	minimum frequency value in GHz
vmax	float	maximum frequency value in Ghz

The second section is the values of all the second order coefficients. It's in a pseudo-fixed-width format delimited by semicolons. The first column is the name of the coefficient. The second is its value in MHz (except F, V_3, and ρ, which are in wavenumbers, wavenumbers, and unitless, respectively). The third is currently an on/off flag that can be 0.0 or 1.0, but in the future should have scaling factors for fitting.

A	MHz
B	MHz
C	MHz
Dab	MHz
ϵzz	MHz
ϵxx	MHz
ϵzz	MHz
ϵxz	MHz
χzz	MHz
χxmy	MHz
χxz	MHz
F	cm^{-1}
ρ	dimensionless
V_n	cm^{-1}
η	MHz

The third section is the operators. They are defined by a value, a scaling factor (again, currently functioning as an on/off flag), values a-h, and stg (stage).

A-h are the values to be substituted into the parameters listed above the operator section.

Stage is set to 0 for dipole operators and 1 for Hamiltonian operators. -n indicates that the parameter value is the product of the parameter value in that line and the line n lines above, and uses the same stage as the above line.

1.2 .eng

Eng files contain the energy listings produced by westersim.

1	2	3	4	5	6	7
J	N	K_a	K_c	m	σ	E

1.3 .lne and .cat

Lne files contain the line lists used by westerfit. Cat files contain the line lists produced by westersim.

1	2	3	4	5	6	7	8	9	10	11	12
J_u	N_u	K_{au}	K_{cu}	m_u	J_l	N_l	K_{al}	K_{cl}	m_l	freq	unc