

The steps for updating a new line list

The steps for updating a new line list to the exoweb server

1. Use code (Jupyter Notebook) to check the .states file (if there is no lifetime, use the ExoCross program to add the lifetime into the .states file)
2. Upload line list files (the .states and .trans files) to the exoweb server.
3. Create def file (read the paper and use code (Jupyter Notebook) to get information).
4. Upload the .def file to the exoweb server.

Code GitHub: https://github.com/Beryl-Jingxin/update_new_linelists.git

The steps for updating a new line list to the ExoMol website

<https://exomol.com/admin/>

1. Chems
 - 1) Molecules
 - 2) Isotopologues
2. Data
 - 1) Add data set
 - 2) Add link
 - 3) Add data collections
3. Pages → Activities → ExoMol updates

EXMOL.def	# ID
(23Na) (16O) (1H)	# IsoFormula
23Na-16O-1H	# Iso-slug
OYT5	# Isotopologue dataset name
20201201	# Version number with format YYYYMMDD
HEMHJVSXTPQXMS-UHFFFAOYSA-M	# Inchi key of molecule
3	# Number of atoms
23	# Isotope number 1
Na	# Element symbol 1
16	# Isotope number 2
O	# Element symbol 2
0	# Isotope number 3
1	# Element symbol 3
H	# Isotopologue mass (Da) and (kg)
39.9971 .6641674712e-25	# Symmetry group
C	# Number of irreducible representations
2	# Irreducible representation ID
Sigma+	# Irreducible representation label
6	# Nuclear spin degeneracy
2	# Irreducible representation ID
Sigma-	# Irreducible representation label
6	# Nuclear spin degeneracy
3500.00	# Maximum temperature of linelist
0	# No. of pressure broadeners available
0	# Dipole availability (1=yes, 0=no)
0	# No. of cross section files available
0	# No. of k-coefficient files available
0	# Lifetime availability (1=yes, 0=no)
0	# Lande g-factor availability (1=yes, 0=no)
7927877	# No. of states in .states file
1	# No. of quanta cases
ltcs	# Quantum case label
9	# No. of quanta defined
Gamma	# Quantum label 1
A2 %2s	# Format quantum label 1
Symmetry	# Description quantum label 1
v1	# Quantum label 2
I3 %3d	# Format quantum label 2
v1 vibrational quantum number	# Description quantum label 2
v2lin	# Quantum label 3
I3 %3d	# Format quantum label 3
v2lin vibrational quantum number	# Description quantum label 3
L	# Quantum label 4
I3 %3d	# Format quantum label 4
L vibrational quantum number	# Description quantum label 4
v3	# Quantum label 5
I3 %3d	# Format quantum label 5
v3 vibrational quantum number	# Description quantum label 5
Cl	# Quantum label 6
F4.2 %f.2	# Format quantum label 6
Contribution coefficient	# Description quantum label 6
n1	# Quantum label 7
I3 %3d	# Format quantum label 7
I2 vibrational quantum number	# Description quantum label 7
n2	# Quantum label 8
I3 %3d	# Format quantum label 8
n2 vibrational quantum number	# Description quantum label 8
n3	# Quantum label 9
I3 %3d	# Format quantum label 9
n3 vibrational quantum number	# Description quantum label 9
496639230921	# Total number of transitions
90	# No. of transition files
9000.00	# Maximum wavenumber (in cm ⁻¹)
16000.00	# Higher energy with complete set of transitions (in cm ⁻¹)
4000.00	# Maximum temperature of partition function
1.00	# Step size of temperature
0	# Cooling function availability (1=yes, 0=no)
0.0840	# Default value of Lorentzian half-width for all lines (in cm ⁻¹ /bar)
0.500	# Default value of temperature exponent for all lines
1	# Uncertainty availability (1=yes, 0=no)