

README for SI files from: Experimental energy levels of $^{12}\text{C}^{14}\text{N}$ through MARVEL analysis

July 2020

SI_2020_CNMARVEL.pdf

This pdf file contains additional details on the data, including:

- Vibronic resolution of table 2 and 3 from the main text.
- Vibronic resolution of the differences in energies between MARVEL and MOLLIST.

12C-14N_MARVEL.inp

The input file for the MARVEL procedure. Transitions not validated are shown with a - in front of their frequencies.

Column	Notation	
1	$\tilde{\nu}$	Transition frequency (in cm^{-1})
2	$\Delta\tilde{\nu}$	Estimated uncertainty in transition frequency (in cm^{-1})
3	State'	Electronic state of upper energy level; also includes parity and Ω for Π and Δ states
4	ν'	Vibrational quantum number of upper level
5	J'	Total angular momentum of upper level
6	State''	Electronic state of lower energy level; also includes parity and Ω for Π and Δ states
7	ν''	Vibrational quantum number of lower level
8	J''	Total angular momentum of lower level
9	ID	Unique ID for transition, with reference key for source and counting number

12C-14N_MARVEL.energies

The output file of empirical energies and uncertainties for $^{12}\text{C}^{14}\text{N}$. Spectroscopic networks are separated by empty lines, with the main SN appearing first in the file.

Column	Notation	Description
1	State	Electronic state of the energy level; also includes parity and Ω for Π and Δ states
2	ν	Vibrational quantum number of the state
3	J	Total angular momentum of the state
4	E	Energy in cm^{-1} of the state
5	ΔE	Uncertainty in cm^{-1} of the state
6	No.	Number of transitions from the input file that contribute to the energy of the state

12C-14N_Mollist-Marvelised.states

ExoMol format of the MARVELised .states file for CN. Index numbers are kept as the same from the original file, such that they match transitions from the 12C-14N_Mollist.trans file found on the ExoMol website.

Column	Notation	Description
1	<i>i</i>	State counting number
2	<i>E</i>	State energy in cm^{-1} (Marvel energy here if used)
3	<i>g</i>	Total statistical weight, equal to $g_{ns}(2J + 1)$
4	<i>J</i>	Total angular momentum
5	ΔE	MARVEL uncertainty in the state energy in cm^{-1} , P for predicted energy levels
6	<i>v</i>	State vibrational quantum number
7	State	Electronic state
8	<i>F</i>	Spin multiplet component of the state
9	<i>e/f</i>	Rotationless parity
10	M/P	M = MARVEL, P = Predicted from MOLLIST