PEPISCO_species v1.0

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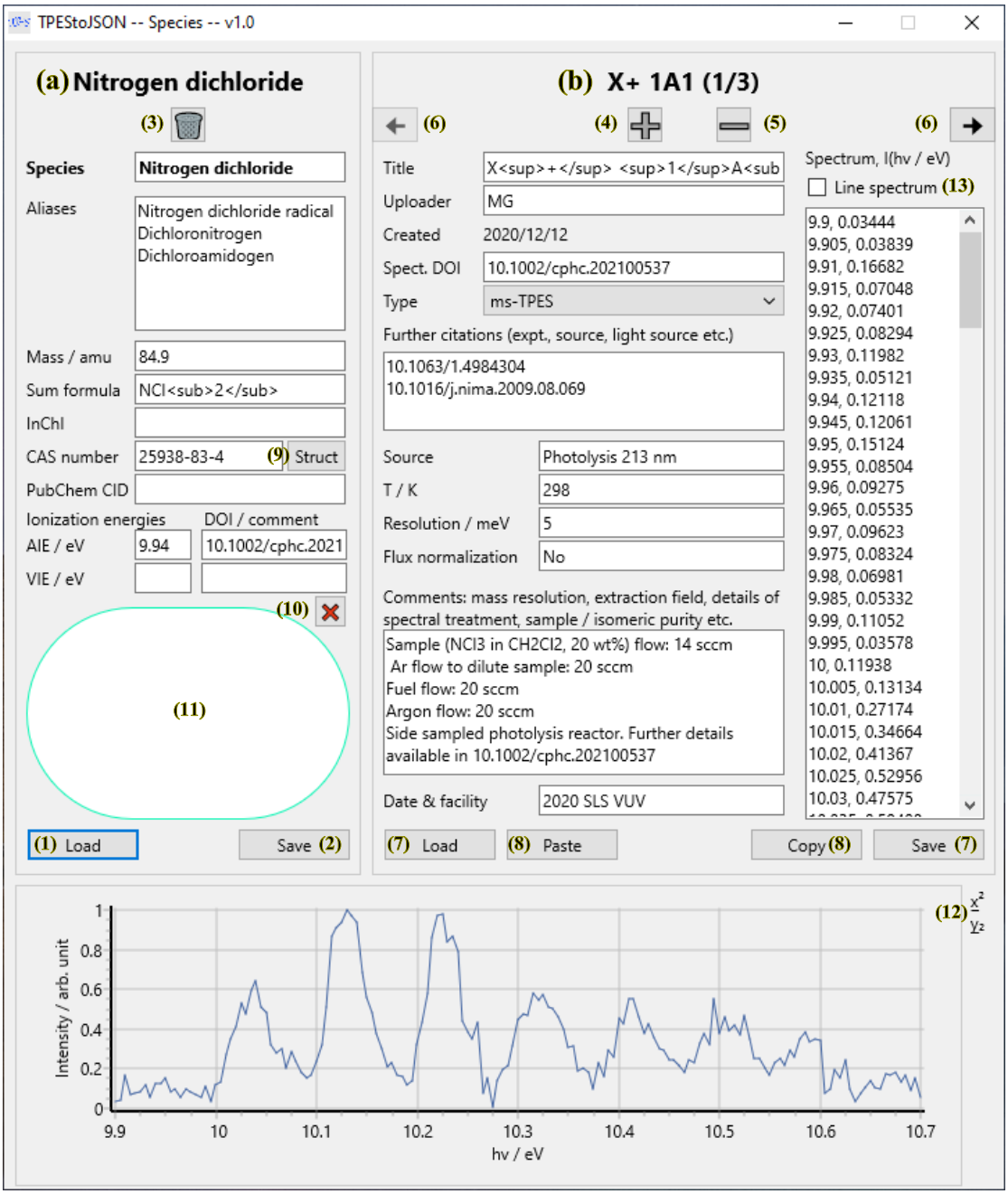
This manual is meant to support you contributing spectra to the Photoelectron Photoion Spectral Compendium hosted at https://pepisco.psi.ch. The helper program `PEPISCO_species.exe` creates `.json` files with species and spectral information, which will be included in the database after being e-mailed to pepisco@psi.ch. The file, saved by clicking on (2), contains the species information together with all the spectra associated with the species. Thank you for your contribution!



1. Creating new species, adding and removing spectra, moving spectra between species

1.1 Species panel (a)

`Load (1)`	Opens a species including multiple experimental spectra and simulations from a `.json` file
`Save (2)`	Saves a species including multiple experimental spectra and simulations to a `.json` file to be submitted to the TPES database
`Bin (3)`	Clears the species to start editing a new one

1.2 Spectrum panel (b)

`+ button (4)`	Adds a new spectrum (measurement or simulation) to the current species
`– button (5)`	Deletes the current spectrum from the species dataset
`←/→ buttons (6)`	Step through the spectra associated with the current species
`Save and Load (7)`	Saves the current spectrum into a standalone `.json` file from which it can be loaded into, *e.g.*, the current spectrum of a different species. Helpful to move erroneously placed spectra between species, but not needed otherwise: when the species is saved, all the spectra are saved into the file, as well.
`Copy and Paste (8)`	The same as `Save` and `Load` but with the help of the `Clipboard`.

2. Adding species details, spectral metadata and data

2.1 Species panel (a)

These data are used to search for the species in the database, based on the given name(s), formula, species identifiers and ionization energies. The more data given here, the easier it will be for the species to be found.

Species	Unique, most common name of a compound/molecule, e.g., `Nitrogen dichloride`
Aliases	Other, commonly used English species names in physical chemistry context. Consult PubChem if needed
Mass	Molar mass without units, preferably to two significant figures. (84.91 for NCl_2)
Sum formula	$C_zH_yO_xN_v$ – Use the subscript button (12) or `Alt + y` to format the entry (subscripts are only rendered in the live database)
InChI	IUPAC International Chemical Identifier, consult PubChem or generate using ChemDraw. *Example:* `InChI=1S/C2H6O/c1-2-3/h3H,2H2,1H3` for ethanol

CAS number	CAS Registry Number, consult PubChem. *Example:* `64-17-5` for ethanol
PubChem CID	PubChem Compound ID, consult PubChem. *Example:* `702` for ethanol
Ionization energies / eV	Adiabatic (`AIE`) and/or vertical (`VIE`) ionization energies, preferably based on assigned experimental spectra, given in eV without unit. Please give DOI if literature reference is available, otherwise details to help put the values into context.
Struct button (9)	Attempts to download a molecular structure to display in the field (11). If a structure is unavailable, please delete the image by clicking on (10). By right clicking in the field (11), a custom image (preferred resolution 150 × 150 or slightly larger) can be pasted into the field.

2.2 Spectral information (b)

Title	Give a title to the spectrum in the database. Do not give the name of the species but focus on how to describe the spectrum best, possibly specifying the ion states involved, as in the image above. You can use buttons (12) for sub- and superscripts or `Alt + x` or `y` (only rendered in the live database). It is best practice to specify the type of the spectrum (`TPES`, `PIS`, or `ms-TPES`) and give the energy range.
Uploader	This is going to be your signature below the spectrum in the database. Initials are preferred, i.e., `US` for `Urs Schweizer`
Spect. DOI	DOI (without DOI or http link), where the spectrum was published. Leave empty if unpublished. Example: `10.1021/jp501117n`
Type	Select the type of spectrum/simulation etc. from the dropdown menu
Further citations	Add DOIs of the beamline, instrument, experiment etc. Examples: `10.1063/1.3082016, 10.1016/j.nima.2009.08.069`
Source	Briefly describe the source of the sample, especially important for reactive species, such as radicals. Examples: `effusive inlet, supersonic molecular beam, pyrolysis reactor, photolysis reactor 213 nm, McKenna burner, jet stirred reactor, liquid vaporization, catalytic reactor, or fluorine discharge`
T / K	Source temperature in kelvin, without unit
Resolution / meV	Combined photon energy and electron kinetic energy resolution, giving the effective energy resolution of the spectrum in meV without unit
Flux normalization	Was the spectrum normalized to the photon flux? Add yes/no or more details and/or DOI. Examples: `flux from AXUV photodiode, PMT, details about response functions, or literature flux from 10.1016/j.nima.2009.08.069`
Comments	Describe at bit more in detail how the reactive intermediate (e.g., radical) or stable species was measured. Example: `3-methyl benzyl bromide heated to 50 °C diluted at 70 mbar in argon (20 sccm), expansion through a 150 um pinhole and subsequent pyrolysis. Mass resolution 100, extraction field 120 V/cm`

Date & Facility	Describe when and where the spectrum was obtained. Example: `2020/05 SLS/VUV`

Spectrum	Insert the spectrum given in two columns with photon energies in *x*, and intensities in *y* as ASCII values. The columns can be separated by space, tab, or comma. Copy from Excel or Origin and paste the data in this field.
	Example:
	`6.995 0`
	`7.000 0.5`
	`7.005 1`
	`7.010 0.5`
	`7.015 0`

Line spectrum (13)	The (*x*,*y*) values given in the spectrum will not be connected, but lines will be plotted for the transitions. Taking the previous example, the corresponding spectrum could be given as `7.005 1` Zero *y* values, if given, will be removed. Useful for Franck–Condon simulations (see below).

2.3 Including Franck–Condon simulations (b)

When adding an FC simulation (after adding a new spectrum by clicking on button (4), select FC simulation in **Type**), the meaning of certain fields change correspondingly. A few notes regarding FC simulations follow.

Title	Describe the simulation briefly, using the states, transitions and symmetries simulated. It is encouraged to save the simulation of each state separately. Example: $X^+\ ^2A_2 \leftarrow X\ ^1A_1$
Further citations	Describe the tools used to obtain the simulation. Give DOI if available or name/version of the program. Examples: `Gaussian 16, Revision C.01, Q-Chem 4.3, FCFit, PESCAL, eZspectrum, ezFCF`
Level(s) of theory	Describe the methods/functional(s) and basis set(s) used in the *ab initio* geometry optimization and frequency calculations. Example: `(EOM-IP-)CCSD/cc-pVTZ or B3LYP/6-311G(d,p)`
Vib. T / K	Vibrational temperature of the simulation in K, without unit
Conv. FWHM / meV	Full width half maximum of the Gaussian function used to convolute the line spectrum in meV without unit. Note that Gaussian16 required half width half maximum (HWHM) in cm^{-1}. Please convert to FWHM in meV [FWHM / meV = 2 × HWHM / (cm^{-1}) / 8065 × 1000]. Leave empty in case of a line spectrum.
0–0 transition / eV	Specify where the 0–0 transition is located in the simulated spectrum in eV without units. This could be a calculated ionization energy or the measured one if the simulation is shifted to fit the experiment; without this value, the simulation is difficult to interpret.

Comments	More details, *e.g.*, Duschinsky or parallel approximation, convergence issues, large-amplitude vibrations or internal rotations, relevant calculation parameters etc. Example: `including the Duschinsky rotation in the double harmonic approximation`
Data & Facility	When and where was the simulation carried out? Example: `2021/05 PSI, merlin6 cluster`