Spectcol

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Spectcol overview

- Java application

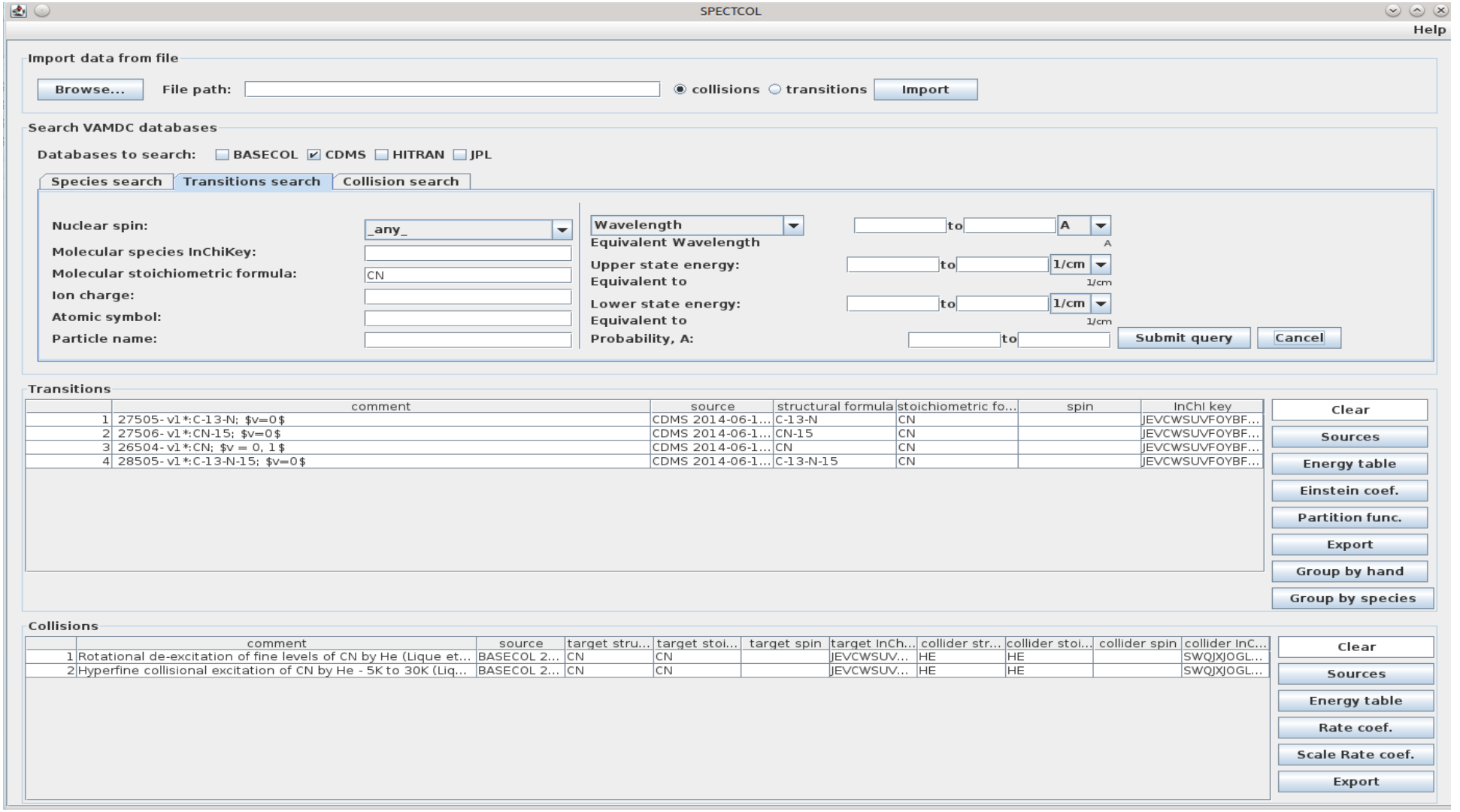
- Dedicated to spectroscopic and collisional data manipulation and combination

- Uses the VAMDC infrastructure to query several databases :
    - Basecol for collisional data
    - JPL, CDMS and Hitran for spectroscopic data

- Uses XSAMS format to read data

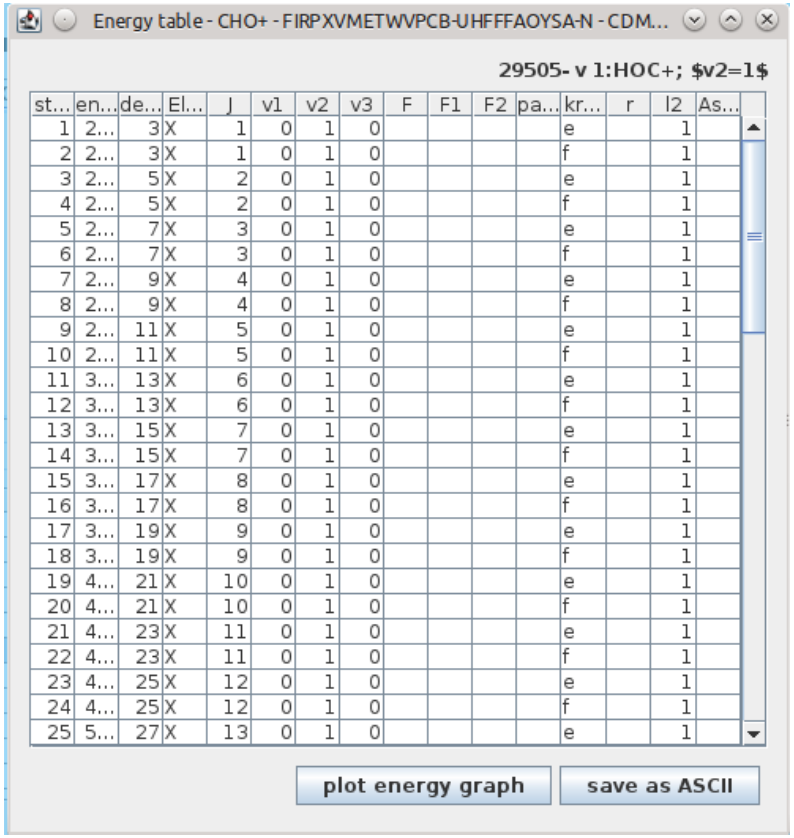
- Provides export functionnalities to other formats

Main window


SPECTCOL
Help
Import data from file
Browse...
File path:
collisions
transitions
Import
Search VAMDC databases
Databases to search:
BASECOL
CDMS
HITRAN
JPL
Species search
Transitions search
Collision search
Nuclear spin:
any
Molecular species InChiKey:
Molecular stoichiometric formula:
CN
Ion charge:
Atomic symbol:
Particle name:
Wavelength
to
A
Equivalent Wavelength
Upper state energy:
1/cm
Equivalent to
Lower state energy:
Probability, A:
Submit query
Cancel
Transitions
comment
source
structural formula
stoichiometric fo...
spin
InChI key
1 27505- v1*:C-13-N; $v=0$ CDMS 2014-06-1... C-13-N CN JEVCWSUVFOYBF...
2 27506- v1*:CN-15; $v=0$ CDMS 2014-06-1... CN-15 CN JEVCWSUVFOYBF...
3 26504- v1*:CN; $v = 0, 1$ CDMS 2014-06-1... CN CN JEVCWSUVFOYBF...
4 28505- v1*:C-13-N-15; $v=0$ CDMS 2014-06-1... C-13-N-15 CN JEVCWSUVFOYBF...
Clear
Sources
Energy table
Einstein coef.
Partition func.
Export
Group by hand
Group by species
Collisions
comment
source
target stru...
target stoi...
target spin
target InCh...
collider str...
collider stoi...
collider spin
collider InC...
1 Rotational de-excitation of fine levels of CN by He (Lique et... BASECOL 2... CN CN JEVCWSUV... HE HE SWQJXJOGL...
2 Hyperfine collisional excitation of CN by He - 5K to 30K (Liq... BASECOL 2... CN CN JEVCWSUV... HE HE SWQJXJOGL...
Clear
Sources
Energy table
Rate coef.
Scale Rate coef.
Export

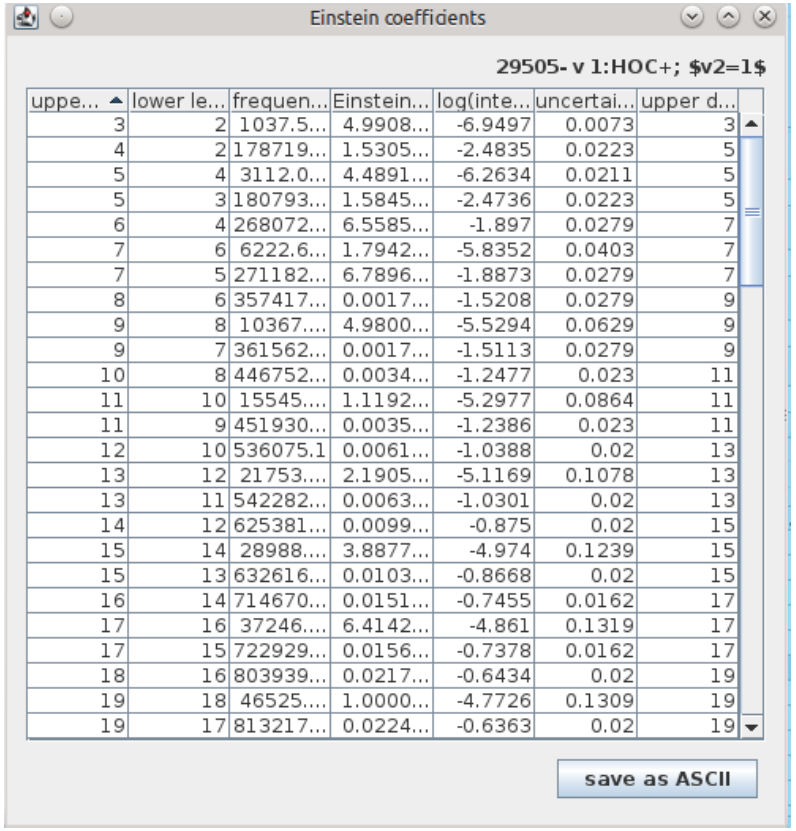
Data visualization (1/2)

Energy table



st...	en...	de...	El...	J	v1	v2	v3	F	F1	F2	pa...	kr...	r	l2	As...
1	2...	3	X	1	0	1	0					e		1	
2	2...	3	X	1	0	1	0					f		1	
3	2...	5	X	2	0	1	0					e		1	
4	2...	5	X	2	0	1	0					f		1	
5	2...	7	X	3	0	1	0					e		1	
6	2...	7	X	3	0	1	0					f		1	
7	2...	9	X	4	0	1	0					e		1	
8	2...	9	X	4	0	1	0					f		1	
9	2...	11	X	5	0	1	0					e		1	
10	2...	11	X	5	0	1	0					f		1	
11	3...	13	X	6	0	1	0					e		1	
12	3...	13	X	6	0	1	0					f		1	
13	3...	15	X	7	0	1	0					e		1	
14	3...	15	X	7	0	1	0					f		1	
15	3...	17	X	8	0	1	0					e		1	
16	3...	17	X	8	0	1	0					f		1	
17	3...	19	X	9	0	1	0					e		1	
18	3...	19	X	9	0	1	0					f		1	
19	4...	21	X	10	0	1	0					e		1	
20	4...	21	X	10	0	1	0					f		1	
21	4...	23	X	11	0	1	0					e		1	
22	4...	23	X	11	0	1	0					f		1	
23	4...	25	X	12	0	1	0					e		1	
24	4...	25	X	12	0	1	0					f		1	
25	5...	27	X	13	0	1	0					e		1	

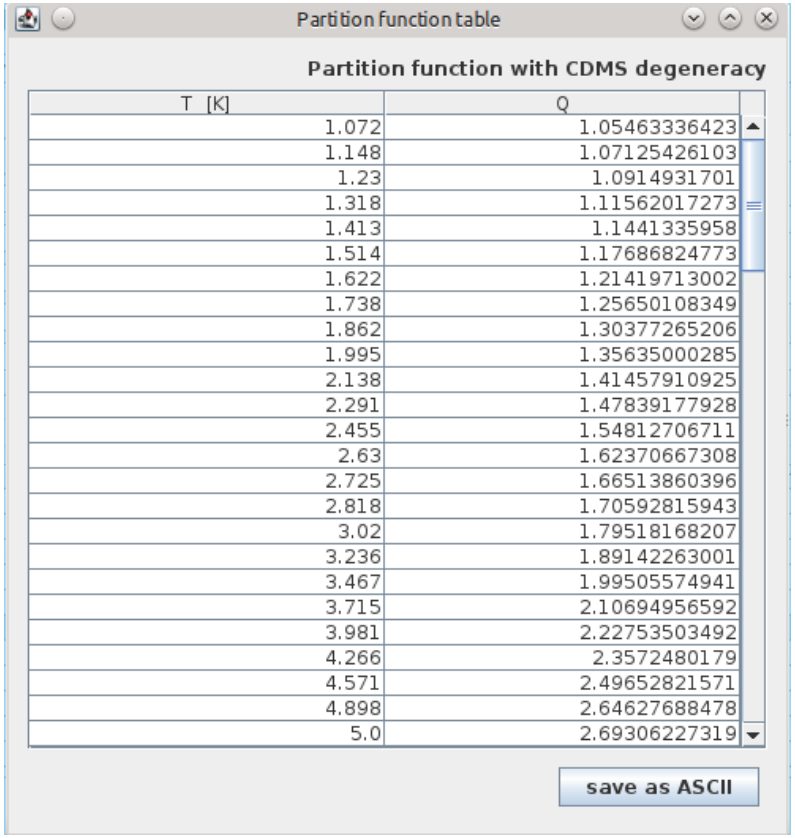
Einstein coefficients



uppe...	lower le...	frequen...	Einstein...	log(inte...	uncertai...	upper d...
3	2	1037.5...	4.9908...	-6.9497	0.0073	3
4	2	178719...	1.5305...	-2.4835	0.0223	5
5	4	3112.0...	4.4891...	-6.2634	0.0211	5
5	3	180793...	1.5845...	-2.4736	0.0223	5
6	4	268072...	6.5585...	-1.897	0.0279	7
7	6	6222.6...	1.7942...	-5.8352	0.0403	7
7	5	271182...	6.7896...	-1.8873	0.0279	7
8	6	357417...	0.0017...	-1.5208	0.0279	9
9	8	10367....	4.9800...	-5.5294	0.0629	9
9	7	361562...	0.0017...	-1.5113	0.0279	9
10	8	446752...	0.0034...	-1.2477	0.023	11
11	10	15545....	1.1192...	-5.2977	0.0864	11
11	9	451930...	0.0035...	-1.2386	0.023	11
12	10	536075.1	0.0061...	-1.0388	0.02	13
13	12	21753....	2.1905...	-5.1169	0.1078	13
13	11	542282...	0.0063...	-1.0301	0.02	13
14	12	625381...	0.0099...	-0.875	0.02	15
15	14	28988....	3.8877...	-4.974	0.1239	15
15	13	632616...	0.0103...	-0.8668	0.02	15
16	14	714670...	0.0151...	-0.7455	0.0162	17
17	16	37246....	6.4142...	-4.861	0.1319	17
17	15	722929...	0.0156...	-0.7378	0.0162	17
18	16	803939...	0.0217...	-0.6434	0.02	19
19	18	46525....	1.0000...	-4.7726	0.1309	19
19	17	813217...	0.0224...	-0.6363	0.02	19

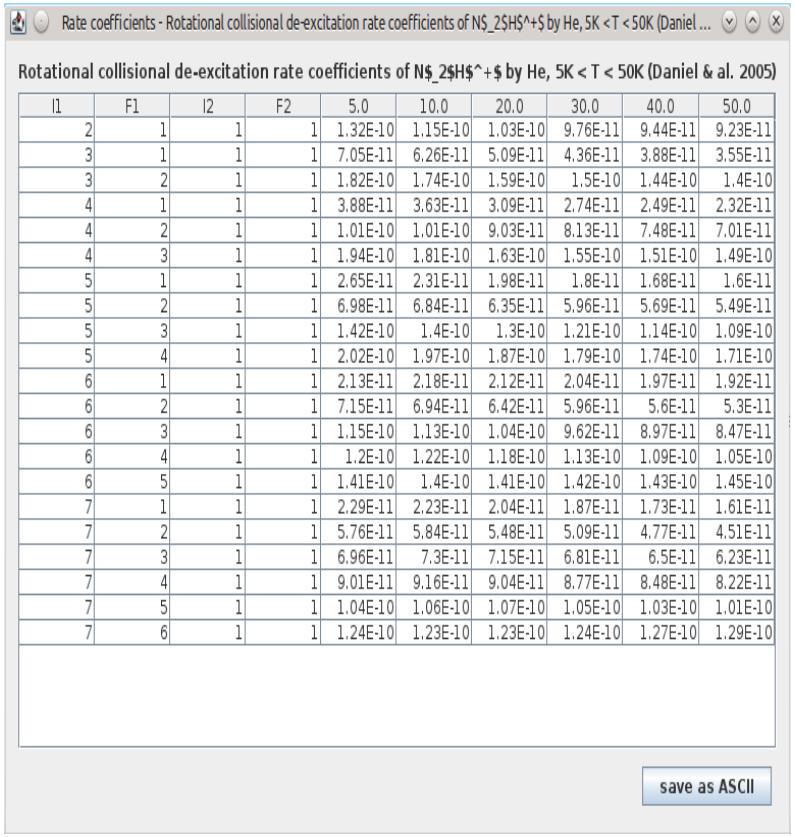
Data visualization (2/2)

Partition function



T [K]	Q
1.072	1.05463336423
1.148	1.07125426103
1.23	1.0914931701
1.318	1.11562017273
1.413	1.1441335958
1.514	1.17686824773
1.622	1.21419713002
1.738	1.25650108349
1.862	1.30377265206
1.995	1.35635000285
2.138	1.41457910925
2.291	1.47839177928
2.455	1.54812706711
2.63	1.62370667308
2.725	1.66513860396
2.818	1.70592815943
3.02	1.79518168207
3.236	1.89142263001
3.467	1.99505574941
3.715	2.10694956592
3.981	2.22753503492
4.266	2.3572480179
4.571	2.49652821571
4.898	2.64627688478
5.0	2.69306227319

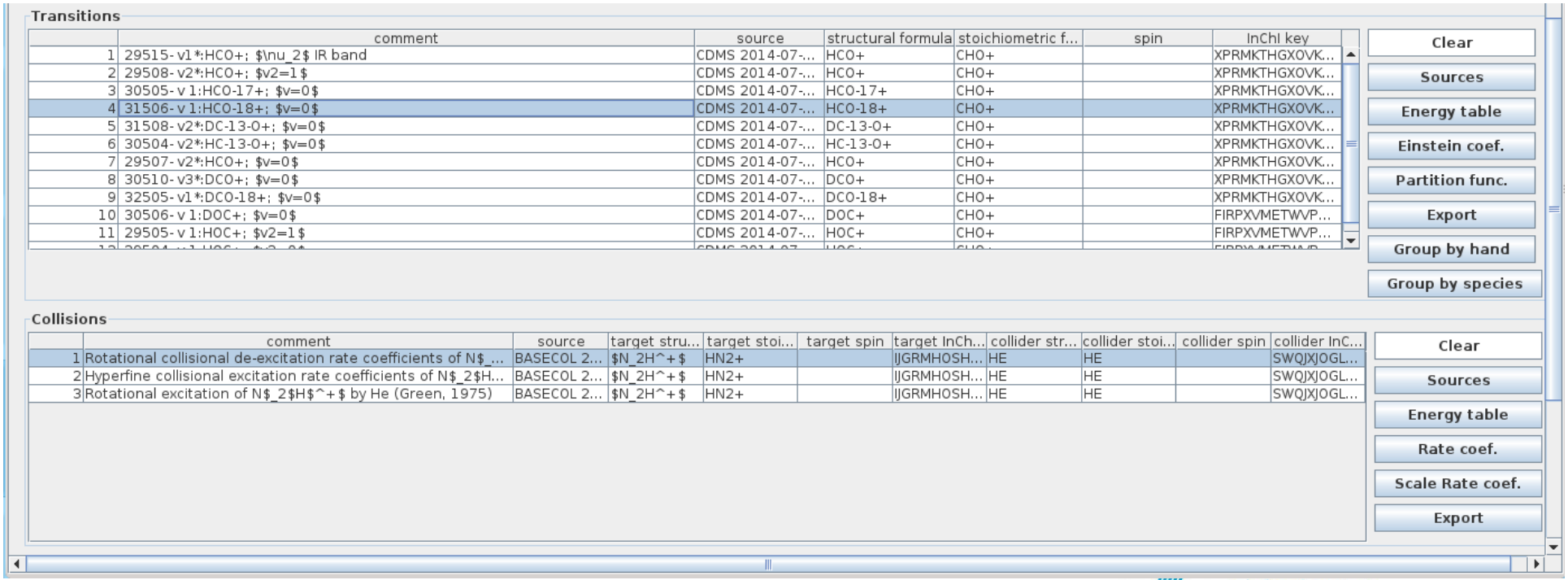
Rate coefficients



I1	F1	I2	F2	5.0	10.0	20.0	30.0	40.0	50.0
2	1	1	1	1.32E-10	1.15E-10	1.03E-10	9.76E-11	9.44E-11	9.23E-11
3	1	1	1	7.05E-11	6.26E-11	5.09E-11	4.36E-11	3.88E-11	3.55E-11
3	2	1	1	1.82E-10	1.74E-10	1.59E-10	1.5E-10	1.44E-10	1.4E-10
4	1	1	1	3.88E-11	3.63E-11	3.09E-11	2.74E-11	2.49E-11	2.32E-11
4	2	1	1	1.01E-10	1.01E-10	9.03E-11	8.13E-11	7.48E-11	7.01E-11
4	3	1	1	1.94E-10	1.81E-10	1.63E-10	1.55E-10	1.51E-10	1.49E-10
5	1	1	1	2.65E-11	2.31E-11	1.98E-11	1.8E-11	1.68E-11	1.6E-11
5	2	1	1	6.98E-11	6.84E-11	6.35E-11	5.96E-11	5.69E-11	5.49E-11
5	3	1	1	1.42E-10	1.4E-10	1.3E-10	1.21E-10	1.14E-10	1.09E-10
5	4	1	1	2.02E-10	1.97E-10	1.87E-10	1.79E-10	1.74E-10	1.71E-10
6	1	1	1	2.13E-11	2.18E-11	2.12E-11	2.04E-11	1.97E-11	1.92E-11
6	2	1	1	7.15E-11	6.94E-11	6.42E-11	5.96E-11	5.6E-11	5.3E-11
6	3	1	1	1.15E-10	1.13E-10	1.04E-10	9.62E-11	8.97E-11	8.47E-11
6	4	1	1	1.2E-10	1.22E-10	1.18E-10	1.13E-10	1.09E-10	1.05E-10
6	5	1	1	1.41E-10	1.4E-10	1.41E-10	1.42E-10	1.43E-10	1.45E-10
7	1	1	1	2.29E-11	2.23E-11	2.04E-11	1.87E-11	1.73E-11	1.61E-11
7	2	1	1	5.76E-11	5.84E-11	5.48E-11	5.09E-11	4.77E-11	4.51E-11
7	3	1	1	6.96E-11	7.3E-11	7.15E-11	6.81E-11	6.5E-11	6.23E-11
7	4	1	1	9.01E-11	9.16E-11	9.04E-11	8.77E-11	8.48E-11	8.22E-11
7	5	1	1	1.04E-10	1.06E-10	1.07E-10	1.05E-10	1.03E-10	1.01E-10
7	6	1	1	1.24E-10	1.23E-10	1.23E-10	1.24E-10	1.27E-10	1.29E-10

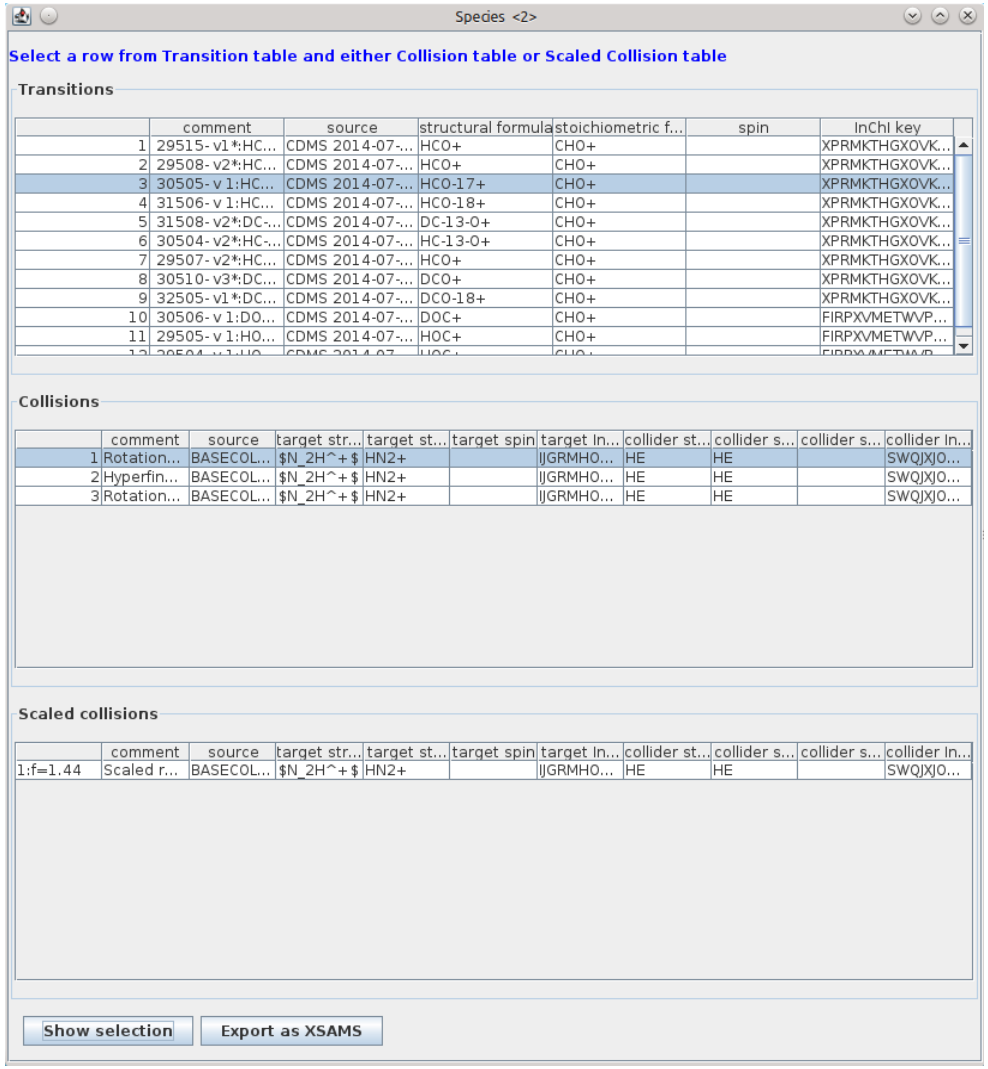
Combining spectroscopic and collisional data

- We have the possibility to do a matching of levels between isoelectronic molecules
- In the example below we have spectroscopic data for **HCO^+**, collisional data for **N_2H^+ - He**
- **HCO^+** and **N_2H^+** are isoelectronic → **N_2H^+- He ~ HCO^+- He**

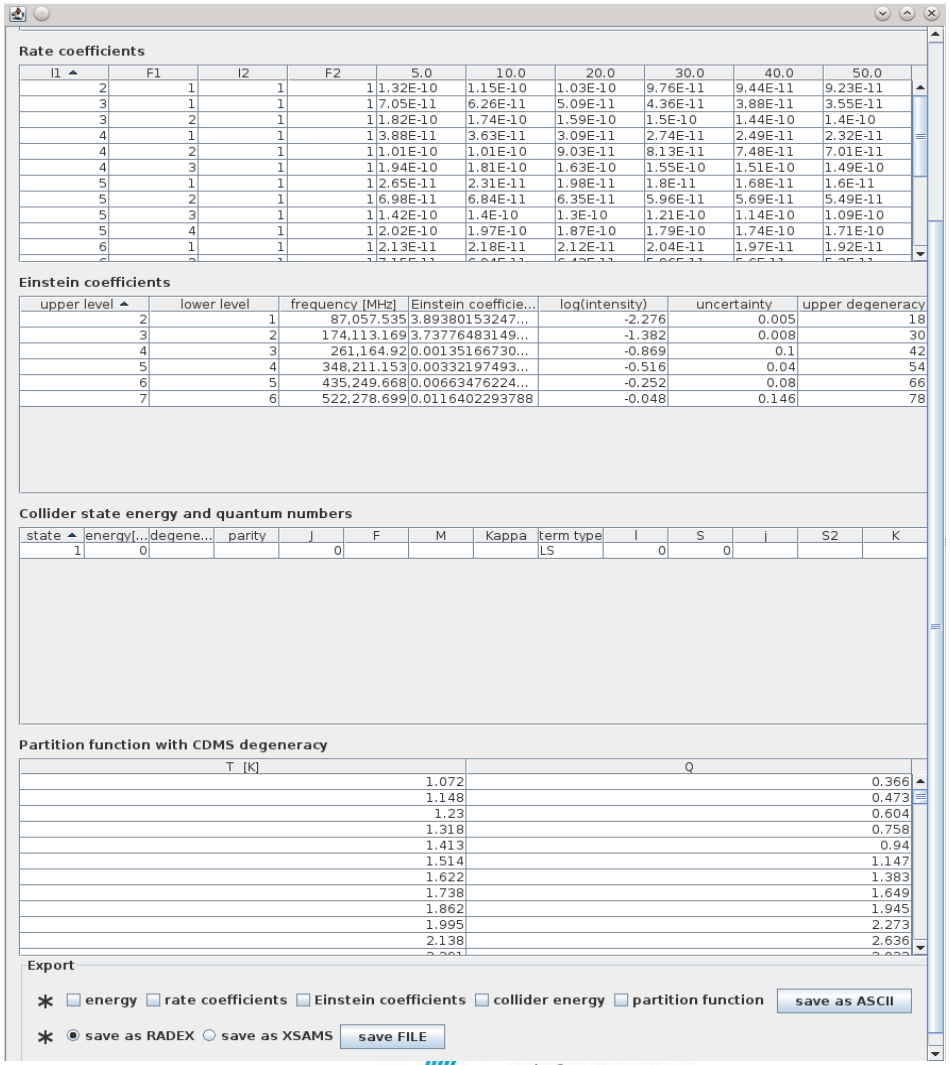


Combining spectroscopic and collisional data

1. Dataset selection



2. Levels matching



Export data in a RADEX file

```
! Molecule
 CHO+
! MASS
 29.0
! Number of Energy Level
 7
! LEVEL + ENERGY(CM-1) + WEIGHT + QUANTUM NOS.  ElecStateLabel_J_v1_v2_v3_F_F1_F2_parity_kronigParity_r_l2_AsSym
 1»              0.0»     1»   X_0_0_0_0_ _ _ _ _ _ _ _
 2»         2.975009»     3»   X_1_0_0_0_ _ _ _ _ _ _ _
 3»         8.924961»     5»   X_2_0_0_0_ _ _ _ _ _ _ _
 4»        17.849722»     7»   X_3_0_0_0_ _ _ _ _ _ _ _
 5»        29.749095»     9»   X_4_0_0_0_ _ _ _ _ _ _ _
 6»        44.622814»    11»   X_5_0_0_0_ _ _ _ _ _ _ _
 7»        62.470547»    13»   X_6_0_0_0_ _ _ _ _ _ _ _
! NUMBER OF RADIATIVE TRANSITIONS
 6
! TRANS + UP + LOW + EINSTEINA(s^-1) + FREQ(GHz)+ E_up(K)
  1»      2»       1»     4.1868569558E-5»          8.91885247E1»         4.2805884892E0
  2»      3»       2»    4.01927531801E-4»         1.783750563E2»         1.2841670504E1
  3»      4»       3»    0.00145336567852»         2.675576259E2»         2.5683053237E1
  4»      5»       4»    0.00357205286939»          3.56734223E2»         4.2804453237E1
  5»      6»       5»    0.00713528253952»         4.459028721E2»          6.420548777E1
  6»      7»       6»     0.0125158127422»          5.35061581E2»         8.9885679137E1
! NUMBER OF COLLISION PARTNERS
 1
! COLLISION PARTNER
 1
! COLLISIONS BETWEEN
 , Scaled rate coefficients - (factor = 1.44) - Rotational collisional de-excitation rate coefficients of N$_2$H$^+$ by He, 5K < T < 50K (Daniel & al. 2005)
! NUMBER OF COLLISIONAL TRANSITIONS
 21
! NUMBER OF COLLISION TEMPERATURES
 6
! COLLISION TEMPERATURES
 5.0»   10.0»    20.0»    30.0»    40.0»    50.0»
! TRANS + UP + LOW + RATE COEFFS(cm^3 s^-1)
     1»    2»       1»    1.9008E-10  1.656E-10 1.4832E-10 1.40544E-10 1.35936E-10 1.3291199999999997E-10
     2»    3»       1»    1.0152E-10 9.0144E-11 7.3296E-11 6.2784E-11 5.5871999999999995E-11  5.112E-11
     3»    3»       2»    2.6208E-10 2.5055999999999996E-10 2.2895999999999998E-10 2.1599999999999998E-10 2.0736E-10  2.016E-10
     4»    4»       1»    5.5871999999999995E-11 5.2271999999999995E-11 4.449599999999999E-11 3.9455999999999997E-11 3.5856E-11 3.3408E-11
     5»    4»       2»    1.4544E-10 1.4544E-10 1.30032E-10 1.17072E-10 1.07712E-10 1.0094399999999999E-10
     6»    4»       3»    2.7936E-10 2.6064E-10 2.3472E-10 2.2320000000000002E-10 2.1743999999999997E-10 2.1456E-10
     7»    5»       1»    3.8159999999999994E-11 3.3264E-11 2.8511999999999998E-11  2.592E-11 2.4191999999999997E-11  2.304E-11
     8»    5»       2»    1.0051199999999999E-10 9.8496E-11  9.144E-11 8.5824E-11 8.1936E-11 7.9056E-11
     9»    5»       3»    2.0448E-10  2.016E-10 1.8719999999999998E-10 1.7423999999999998E-10 1.6415999999999998E-10 1.5696E-10
    10»    5»       4»    2.9088E-10 2.8368E-10 2.6927999999999997E-10 2.5776E-10 2.5055999999999996E-10 2.4624E-10
    11»    6»       1»    3.0672E-11 3.1392E-11 3.0528E-11 2.9376E-11 2.8368E-11 2.7648E-11
    12»    6»       2»    1.0296E-10 9.9936E-11 9.244799999999998E-11 8.5824E-11 8.063999999999999E-11 7.631999999999999E-11
    13»    6»       3»     1.656E-10 1.6271999999999998E-10 1.4976E-10 1.38528E-10 1.29168E-10 1.21968E-10
    14»    6»       4»     1.728E-10 1.7567999999999998E-10 1.6992E-10 1.6271999999999998E-10 1.5696E-10  1.512E-10
    15»    6»       5»    2.0304E-10  2.016E-10 2.0304E-10 2.0448E-10 2.0592E-10 2.0879999999999997E-10
    16»    7»       1»    3.2976E-11 3.2112E-11 2.9376E-11 2.6928E-11 2.4912000000000002E-11 2.3184E-11
    17»    7»       2»    8.2944E-11 8.409599999999999E-11 7.891199999999999E-11 7.3296E-11 6.868799999999999E-11 6.494399999999999E-11
    18»    7»       3»    1.00223999999999999E-10 1.0512000000000001E-10 1.0296E-10 9.8064E-11 9.3599999999999999E-11 8.971199999999998E-11
    19»    7»       4»    1.29744E-10 1.31904E-10 1.30176E-10 1.26288E-10 1.22112E-10 1.1836799999999998E-10
```