VAMDC demonstration

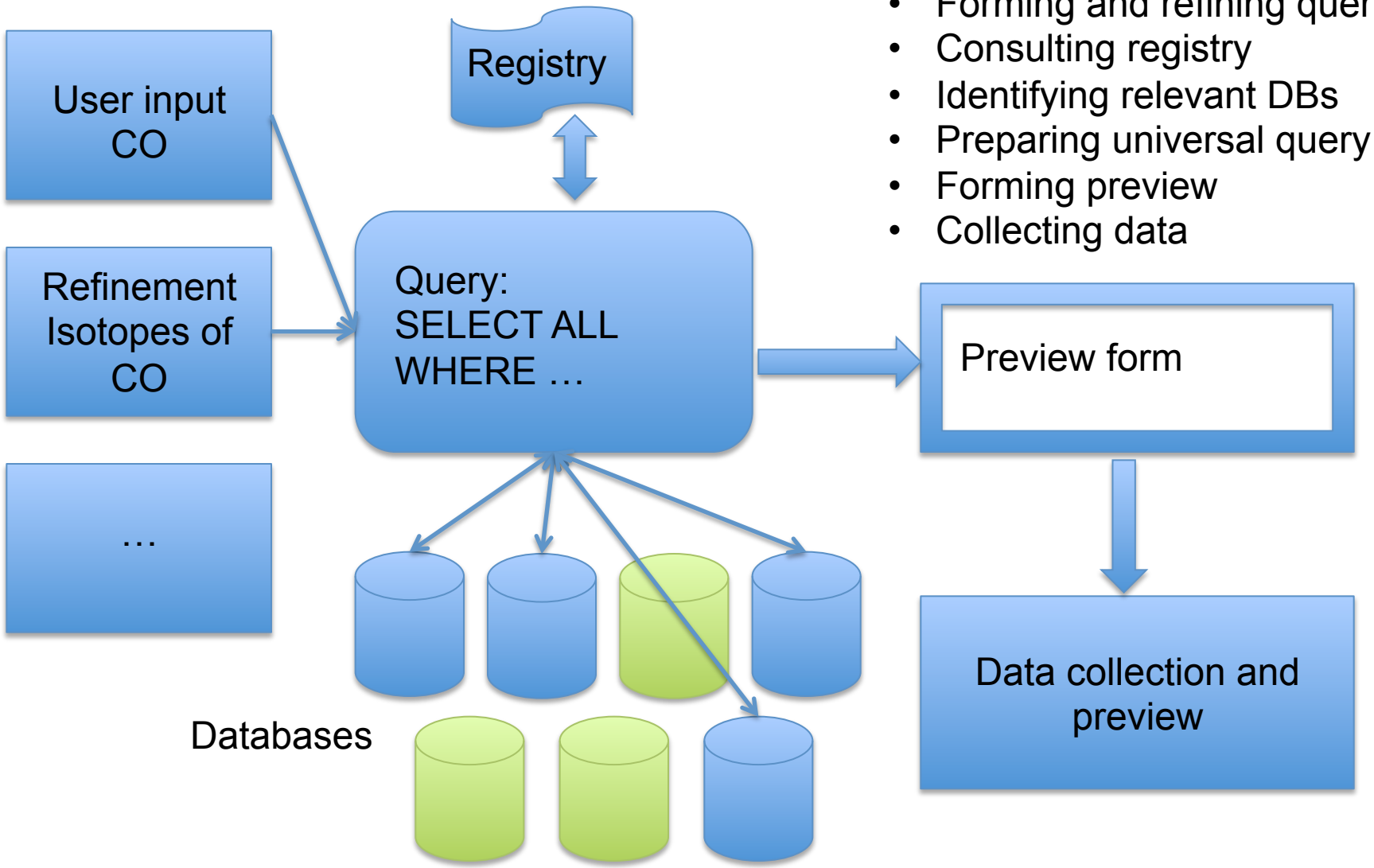
1. Current (VSS1) functionality and preview of VSS2:

- Universal query language
- Multiple search through several heterogeneous DBs
- Unit transformation
- Query response following VAMDC standard (XSAMS)
- XSAMS views and table conversion

2. Use cases

Search for molecular data

- Forming and refining query
- Consulting registry
- Identifying relevant DBs
- Preparing universal query
- Forming preview
- Collecting data



Query Parameters

- Atoms
- Molecules
- Transitions
- Collisions
- Free Form

Resource	Query Parameters
TOPbase : VAMDC-TAP interface	atomioncharge radtranswavelength atomnuclearcharge atomsymbol
Carbon Dioxide Spectroscopic Databank (VAMDC-TAP)	radtranswavenumber
TIPbase : VAMDC-TAP interface	atomioncharge atomnuclearcharge atomsymbol
HITRAN-UCL resource	radtranswavenumber radtranswavelength moleculeinchikey moleculestoichiometricformula moleculechemicalname radtransprobabilitya
Lund laboratory spectroscopy database	radtranswavenumber radtranswavelength atomstateenergy radtransprobabilitylog10weightedoscillatorstrength atomnuclearcharge atomsymbol atomioncharge
Spectr-W3	atomnuclearcharge radtranswavelength atomioncharge radtransprobabilityoscillatorstrength atomsymbol

Query Parameters

Atoms

Molecules

Transitions

Collisions

Free Form

Molecules X Close

Chemical Name:

Stoichiometric Formula: CO

Molecule Ion Charge:

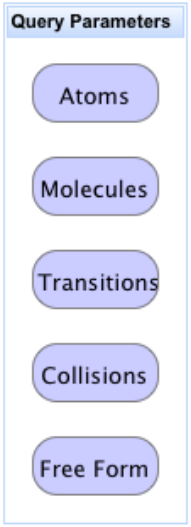
Molecule InChI:

InChI Key:

CO2
CO
COS
COF2
CO+
COFe
CONi

Clear

Resource	Query Parameters
TOPbase : VAMDC-TAP interface	atomioncharge radtranswavelength atomnuclearcharge atomsymbol
Carbon Dioxide Spectroscopic Databank (VAMDC-TAP)	radtranswavenumber
TIPbase : VAMDC-TAP interface	atomioncharge atomnuclearcharge atomsymbol
HITRAN-UCL resource	radtranswavenumber radtranswavelength moleculeinchikey **moleculestoichiometricformula** moleculechemicalname radtransprobabilitya
Lund laboratory spectroscopy database	radtranswavenumber radtranswavelength atomstateenergy radtransprobabilitylog10weightedoscillatorstrength atomnuclearcharge atomsymbol atomioncharge
Spectr-W3	atomnuclearcharge radtranswavelength atomioncharge radtransprobabilityoscillatorstrength



Molecules X Close

Chemical Name:

Stoichiometric Formula: CO

Molecule Ion Charge: Range

Molecule InChI:

InChI Key:

Formula	InChI	InChI Key
☑ (12C)(16O)	InChI=1S/CO /c1-2/i1+0,2+0	UGFAIRIUMAVXCW-ZCWHFVSRSA-N
☐ (13C)(16O)	InChI=1S/CO /c1-2/i1+1,2+0	UGFAIRIUMAVXCW-CRWWGTSDSA-N
☐ (12C)(18O)	InChI=1S/CO /c1-2/i1+0,2+2	UGFAIRIUMAVXCW-FNPQUGRCSA-N
☐ (12C)(17O)	InChI=1S/CO /c1-2/i1+0,2+1	UGFAIRIUMAVXCW-DZEMCFCNSA-N
☐ (13C)(18O)	InChI=1S/CO /c1-2/i1+1,2+2	UGFAIRIUMAVXCW-RGIGPVFXSA-N
☐ (13C)(17O)	InChI=1S/CO /c1-2/i1+1,2+1	UGFAIRIUMAVXCW-ZDOIIHCHSA-N

Select All

Clear Cancel Preview

TOPbase : VAMDC-TAP interface	atomioncharge radtranswavelength atomnuclearcharge atomsymbol
Carbon Dioxide Spectroscopic Databank (VAMDC-TAP)	radtranswavenumber
TIPbase : VAMDC-TAP interface	atomioncharge atomnuclearcharge atomsymbol
HITRAN-UCL resource	radtranswavenumber radtranswavelength moleculeinchikey **moleculestoichiometricformula** moleculechemicalname radtransprobabilitya
Lund laboratory spectroscopy database	radtranswavenumber radtranswavelength atomstateenergy radtransprobabilitylog10weightedoscillatorstrength atomnuclearcharge atomsymbol atomioncharge
Spectr-W3	atomnuclearcharge radtranswavelength atomioncharge radtransprobabilityoscillatorstrength atomsymbol
GSMA S&MPO Reims	moleculeinchi radtranswavenumber radtranswavelength moleculeinchikey moleculechemicalname
Ethylene Database	radtranswavenumber radtranswavelength radtransprobabilitylinestrength moleculeinchikey **moleculestoichiometricformula**

Query Parameters

- Atoms
- Molecules
- Transitions
- Collisions
- Free Form

Molecules

Chemical Name:

Stoichiometric Formula: CO

Molecule Ion Charge: Range

Molecule InChI:

InChI Key:

Formula	InChI	InChI Key
☑ (12C)(16O)	InChI=1S/CO /c1-2/i1+0,2+0	UGFAIRIUMAVXCW-ZCWHFVSRSA-N
☐ (13C)(16O)	InChI=1S/CO /c1-2/i1+1,2+0	UGFAIRIUMAVXCW-CRWWGTSDSA-N
☐ (12C)(18O)	InChI=1S/CO /c1-2/i1+0,2+2	UGFAIRIUMAVXCW-FNPQUGRCSA-N
☐ (12C)(17O)	InChI=1S/CO /c1-2/i1+0,2+1	UGFAIRIUMAVXCW-DZEMCFCNSA-N
☐ (13C)(18O)	InChI=1S/CO /c1-2/i1+1,2+2	UGFAIRIUMAVXCW-RGIGPVFXSA-N
☐ (13C)(17O)	InChI=1S/CO /c1-2/i1+1,2+1	UGFAIRIUMAVXCW-ZDOIIHCHSA-N

Select All

XSAMS Query: SELECT ALL WHERE MoleculeInchiKey='UGFAIRIUMAVXCW-ZCWHFVSRSA-N'

Resource Title	Status	Species	States	Radiative	Collisions	Non Radiative	Sources
☑ HITRAN-UCL resource	OK	0	172	100	0	0	0
☐ Ethylene Database	NO CONTENT	0	0	0	0	0	0
☑ TAP-XSAMS for GhoSST database	OK	1	0	0	0	0	1
☑ BASECOL: VAMDC-TAP interface	OK	6	0	0	11	0	0
☑ Cologne Database for Molecular Spectroscopy: VAMDC-TAP service	OK	2	186	182	0	0	4

Cancel Get data

Refine the Submitted Query

Query results: atomic and molecular states

(Switch to display of radiative transitions.)

Specie	Ion charge	State energy	Description	Quantum numbers	More information
Carbon Monoxide - CO		0.0 1/cm		Label=X^1\Sigma^+, v=0, J=0, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		3.845033 1/cm		Label=X^1\Sigma^+, v=0, J=1, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		11.534953 1/cm		Label=X^1\Sigma^+, v=0, J=2, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		23.069466 1/cm		Label=X^1\Sigma^+, v=0, J=3, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		38.448131 1/cm		Label=X^1\Sigma^+, v=0, J=4, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		57.67036 1/cm		Label=X^1\Sigma^+, v=0, J=5, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		80.735419 1/cm		Label=X^1\Sigma^+, v=0, J=6, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		107.642427 1/cm		Label=X^1\Sigma^+, v=0, J=7, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		138.390355 1/cm		Label=X^1\Sigma^+, v=0, J=8, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		172.978029 1/cm		Label=X^1\Sigma^+, v=0, J=9, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		211.404127 1/cm		Label=X^1\Sigma^+, v=0, J=10, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		253.667181 1/cm		Label=X^1\Sigma^+, v=0, J=11, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		299.765576 1/cm		Label=X^1\Sigma^+, v=0, J=12, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		349.69755 1/cm		Label=X^1\Sigma^+, v=0, J=13, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		403.461194 1/cm		Label=X^1\Sigma^+, v=0, J=14, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		461.054454 1/cm		Label=X^1\Sigma^+, v=0, J=15, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		522.475129 1/cm		Label=X^1\Sigma^+, v=0, J=16, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		587.720871 1/cm		Label=X^1\Sigma^+, v=0, J=17, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		656.789186 1/cm		Label=X^1\Sigma^+, v=0, J=18, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		729.677434 1/cm		Label=X^1\Sigma^+, v=0, J=19, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		806.382828 1/cm		Label=X^1\Sigma^+, v=0, J=20, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		886.902435 1/cm		Label=X^1\Sigma^+, v=0, J=21, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		971.233178 1/cm		Label=X^1\Sigma^+, v=0, J=22, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		1059.371831 1/cm		Label=X^1\Sigma^+, v=0, J=23, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		1151.315024 1/cm		Label=X^1\Sigma^+, v=0, J=24, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		1247.059241 1/cm		Label=X^1\Sigma^+, v=0, J=25, F1=, F2=, parity=, symmetry=	Detail
Carbon Monoxide - CO		1346.60082 1/cm		Label=X^1\Sigma^+, v=0, J=26, F1=, F2=, parity=, symmetry=	Detail

Available data for selected state

Specie

Structural formula: CO

Stoichiometric formula: CO

Molecule name: Carbon Monoxide

InChI: 1S/CO/c1-2/i1+0,2+0 (UGFAIRIUMAVXCW-ZCWHFVSRSA-N)

State

State description:

State energy above ground state: 38.448131 1/cm

Total statistical weight: 9

Quantum description of state as closed-shell, diatomic molecule: Label=X^1\Sigma^+, v=0, J=4, F1=, F2=, parity=, symmetry=

Closed-shell, diatomic molecules

- case prefix: dcs
- case ID: 1

`ElecStateLabel`

XML Element
`dcs:ElecStateLabel`

Description
`ElecStateLabel` is a label identifying the electronic state: X, A, a, B, etc..

Attributes
None

Restrictions
string

v

XML Element
`dcs:v`

Description
v is the vibrational quantum number.

Attributes
None

Restrictions
non-negative integer

J

XML Element
`dcs:J`

Query results: radiative transitions

(Switch to display of states.)

Specie	Ion charge	λ/ν/n/E	Probability	Initial state	Final state
Carbon Monoxide - CO		ν=115271.2021 MHz	A=7.20378864479e-08 1/cm $\log_{10}$gf=-5.0105	- 0.0 1/cm	- 3.845033 1/cm
Carbon Monoxide - CO		ν=230538.0 MHz	A=6.91079000503e-07 1/cm $\log_{10}$gf=-4.1197	- 3.845033 1/cm	- 11.534953 1/cm
Carbon Monoxide - CO		ν=345795.9899 MHz	A=2.49670085538e-06 1/cm $\log_{10}$gf=-3.6118	- 11.534953 1/cm	- 23.069466 1/cm
Carbon Monoxide - CO		ν=461040.7681 MHz	A=6.12668117242e-06 1/cm $\log_{10}$gf=-3.2657	- 23.069466 1/cm	- 38.448131 1/cm
Carbon Monoxide - CO		ν=576267.931 MHz	A=1.22134274135e-05 1/cm $\log_{10}$gf=-3.0118	- 38.448131 1/cm	- 57.67036 1/cm
Carbon Monoxide - CO		ν=691473.076 MHz	A=2.13750692698e-05 1/cm $\log_{10}$gf=-2.8193	- 57.67036 1/cm	- 80.735419 1/cm
Carbon Monoxide - CO		ν=806651.8008 MHz	A=3.42239824576e-05 1/cm $\log_{10}$gf=-2.6716	- 80.735419 1/cm	- 107.642427 1/cm
Carbon Monoxide - CO		ν=921799.7039 MHz	A=5.13419191151e-05 1/cm $\log_{10}$gf=-2.559	- 107.642427 1/cm	- 138.390355 1/cm
Carbon Monoxide - CO		ν=1036912.3846 MHz	A=7.33007011041e-05 1/cm $\log_{10}$gf=-2.4751	- 138.390355 1/cm	- 172.978029 1/cm
Carbon Monoxide - CO		ν=1151985.4434 MHz	A=0.000100638923207 1/cm $\log_{10}$gf=-2.4156	- 172.978029 1/cm	- 211.404127 1/cm
Carbon Monoxide - CO		ν=1267014.4817 MHz	A=0.000133903406762 1/cm $\log_{10}$gf=-2.3773	- 211.404127 1/cm	- 253.667181 1/cm
Carbon Monoxide - CO		ν=1381995.1022 MHz	A=0.000173532853014 1/cm $\log_{10}$gf=-2.3581	- 253.667181 1/cm	- 299.765576 1/cm
Carbon Monoxide - CO		ν=1496922.9091 MHz	A=0.000220040322442 1/cm $\log_{10}$gf=-2.3561	- 299.765576 1/cm	- 349.69755 1/cm
Carbon Monoxide - CO		ν=1611793.5079 MHz	A=0.00027390476357 1/cm $\log_{10}$gf=-2.3699	- 349.69755 1/cm	- 403.461194 1/cm
Carbon Monoxide - CO		ν=1726602.5057 MHz	A=0.000335356678509 1/cm $\log_{10}$gf=-2.3987	- 403.461194 1/cm	- 461.054454 1/cm
Carbon Monoxide - CO		ν=1841345.5116 MHz	A=0.000404993044566 1/cm $\log_{10}$gf=-2.4413	- 461.054454 1/cm	- 522.475129 1/cm
Carbon Monoxide - CO		ν=1956018.1363 MHz	A=0.000482878531678 1/cm $\log_{10}$gf=-2.4973	- 522.475129 1/cm	- 587.720871 1/cm
Carbon Monoxide - CO		ν=2070615.9924 MHz	A=0.000569495347659 1/cm $\log_{10}$gf=-2.5659	- 587.720871 1/cm	- 656.789186 1/cm
Carbon Monoxide - CO		ν=2185134.6949 MHz	A=0.000664985100589 1/cm $\log_{10}$gf=-2.6467	- 656.789186 1/cm	- 729.677434 1/cm
Carbon Monoxide - CO		ν=2299569.8609 MHz	A=0.000769499240577 1/cm $\log_{10}$gf=-2.7393	- 729.677434 1/cm	- 806.382828 1/cm
Carbon Monoxide - CO		ν=2413917.1097 MHz	A=0.000883246473397 1/cm $\log_{10}$gf=-2.8433	- 806.382828 1/cm	- 886.902435 1/cm

Query Parameters

- Atoms
- Molecules
- Transitions
- Collisions
- Free Form

Atoms X Close

Atomic (elemental) symbol:			
Atom Inchi:			
Atom Inchi Key:			
Atom Mass Number:	Range		
Atom Ion Charge:	Range		
Atom Nuclear Charge:	Range		

Clear Cancel Preview

Resource	Query Parameters
TOPbase : VAMDC-TAP interface	atomioncharge radtranswavelength atomnuclearcharge atomsymbol
Carbon Dioxide Spectroscopic Databank (VAMDC-TAP)	radtranswavenumber
TIPbase : VAMDC-TAP interface	atomioncharge atomnuclearcharge atomsymbol
HITRAN-UCL resource	radtranswavenumber radtranswavelength moleculeinchikey moleculestoichiometricformula moleculechemicalname radtransprobabilitya
Lund laboratory spectroscopy database	radtranswavenumber radtranswavelength atomstateenergy radtransprobabilitylog10weightedoscillatorstrength atomnuclearcharge atomsymbol atomioncharge
Spectr-W3	atomnuclearcharge radtranswavelength atomioncharge radtransprobabilityoscillatorstrength

Query Parameters

- Atoms
- Molecules
- Transitions
- Collisions
- Free Form

Transitions X Close

RadTransWavelength:
From
To
Units Å

RadTransFrequency:
From
To
Units Hz

RadTransEnergy:
From
To
Units eV

RadTransWavenumber:
From
To
Units 1/cm

Initial State Energy:
From
To
Units eV

RadTransProbabilityA:
From
To
Units 1/s

Resource	Query Parameters
TOPbase : VAMDC-TAP interface	atomioncharge radtranswavelength atomnuclearcharge atomsymbol
Carbon Dioxide Spectroscopic Databank (VAMDC-TAP)	radtranswavenumber
TIPbase : VAMDC-TAP interface	atomioncharge atomnuclearcharge atomsymbol
HITRAN-UCL resource	radtranswavenumber radtranswavelength moleculeinchikey moleculestoichiometricformula moleculechemicalname radtransprobabilitya
Lund laboratory spectroscopy database	radtranswavenumber radtranswavelength atomstateenergy radtransprobabilitylog10weightedoscillatorstrength atomnuclearcharge atomsymbol atomioncharge
Spectr-W3	atomnuclearcharge radtranswavelength atomioncharge radtransprobabilityoscillatorstrength atomsymbol
GSMA S&MPO Reims	moleculeinchi radtranswavenumber radtranswavelength moleculeinchikey moleculechemicalname

Query Parameters

Atoms

Molecules

Transitions

Collisions

Free Form

Collisions X Close

Process Name: in

Process Description:

Process Code:

IAEA Process Code:

- Inelastic scattering
- interchange
- Interaction with General Electromagnetic Field
- Interaction with time-varying fields
- Interchange Reactions - Heavy Particle

Clear Ca

Resource	Query Parameters
TOPbase : VAMDC-TAP interface	atomioncharge radtranswavelength atomnuclearcharge atomsymbol
Carbon Dioxide Spectroscopic Databank (VAMDC-TAP)	radtranswavenumber
TIPbase : VAMDC-TAP interface	atomioncharge atomnuclearcharge atomsymbol
HITRAN-UCL resource	radtranswavenumber radtranswavelength moleculeinchikey **moleculestoichiometricformula** moleculechemicalname radtransprobabilitya
Lund laboratory spectroscopy database	radtranswavenumber radtranswavelength atomstateenergy radtransprobabilitylog10weightedoscillatorstrength atomnuclearcharge atomsymbol atomioncharge
Spectr-W3	atomnuclearcharge radtranswavelength atomioncharge radtransprobabilityoscillatorstrength

.eu/vamdc-portal-level2/xsamsForm.seam;j...Method=home.xhtml;navigator.defaultQueryBuilder()&cid=168#

Query Parameters

- Species
- Processes

Include in result

Select All Select None

- Species
  - Atoms
    - States
  - Molecules
    - States
      - Quantum Numbers
  - Particles
  - Solids
- Processes
  - Transitions
  - Collisions

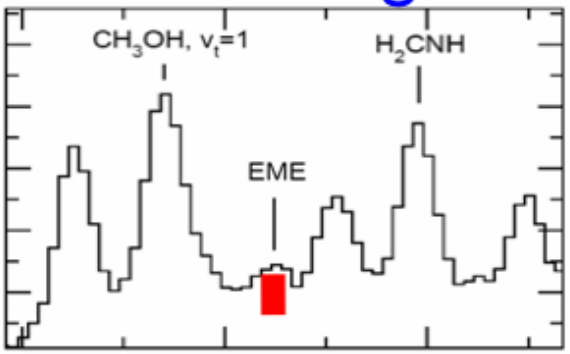
Query generator

```
SELECT ALL WHERE
```

VSS2 Rebuild Preview

Resource	Query Parameters
BASECOL: development VAMDC-TAP interface	atomsymbol collisioncode inchikey moleculeinchikey moleculestoichiometricformula moleculestateenergy moleculestatenuclearspinisomer sourceyear temperature
KIDA: VAMDC-TAP interface	moleculeioncharge moleculechemicalname moleculeinchi moleculeinchikey moleculeioncharge moleculestoichiometricformula atomsymbol
TOPbase : VAMDC-TAP interface	atomioncharge radtranswavelength atomnuclearcharge atomsymbol
Carbon Dioxide Spectroscopic Databank (VAMDC-TAP)	radtranswavenumber
TIPbase : VAMDC-TAP interface	atomioncharge atomnuclearcharge atomsymbol
	radtranswavenumber

Understanding the Language of Interstellar Molecules

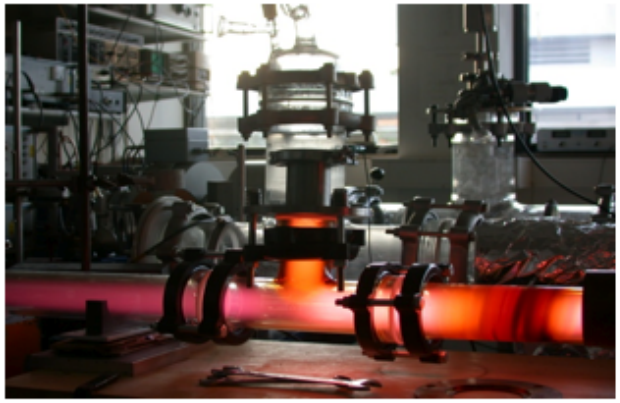


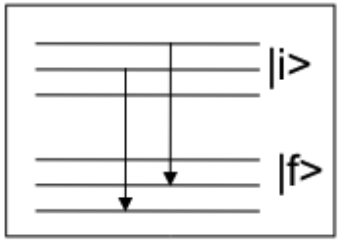
Observations
+
Modelling

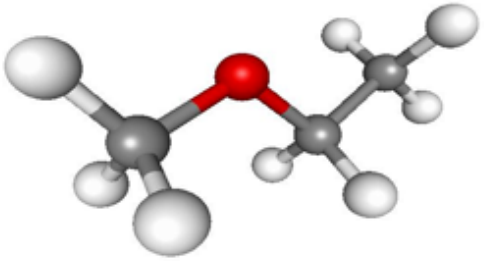
CDMS + JPL
BASECOL + KIDA

Laboratory expriments

Quantum Chemistry







Courtesy of Stephan Schlemmer

SPECTCOL Tool

- Handles
  - VAMDC-XSAMS files from different databases
  - Matching and Cross-Federation of Spectroscopic data and Collisional Data From Different Databases
- Spectroscopic Data
  - Species, Energy Tables, Frequencies, Einstein Coefficients (CDMS for now), Sources
- Collisional Data
  - Species, Energy Tables (not the same), Rate Coefficients

Cross-federation and matching tool

BASECOL

Rate Coefficients

Rotational Excitation of ortho-cyclopropendyle by He (Chandra & al., 2000)

Number of temperature columns : 4

I	J	Temperature (K)... 30	60	90	120
2	1	8.032e-12	8.321e-12	8.281e-12	8.16e-12
3	1	2.091e-11	2.096e-11	2.091e-11	2.098e-11
3	2	1.609e-12	1.895e-12	2.102e-12	2.17e-12
4	1	1.251e-11	1.33e-11	1.454e-11	1.581e-11
4	2	8.396e-12	8.54e-12	8.632e-12	8.6e-12
4	3	1.329e-11	1.33e-11	1.341e-11	1.357e-11
5	1	2.067e-12	2.334e-12	2.485e-12	2.526e-12
5	2	2.55e-11	2.346e-11	2.287e-11	2.284e-11
5	3	8.323e-12	8.103e-12	7.968e-12	7.822e-12
5	4	2.784e-12	3.241e-12	3.485e-12	3.607e-12
6	1	4.456e-12	3.715e-12	3.559e-12	3.529e-12
6	2	1.497e-12	1.363e-12	1.357e-12	1.331e-12
6	3	1.348e-11	1.381e-11	1.477e-11	1.582e-11
6	4	2.135e-11	2.109e-11	2.097e-11	2.098e-11
6	5	6.256e-12	6.754e-12	6.977e-12	7.066e-12
7	1	7.275e-12	6.789e-12	7.051e-12	7.442e-12
7	2	5.075e-13	5.046e-13	5.221e-13	5.291e-13
7	3	1.23e-11	1.193e-11	1.189e-11	1.19e-11
7	4	5.586e-12	6.061e-12	6.513e-12	6.91e-12
7	5	1.763e-12	2.053e-12	2.257e-12	2.382e-12
7	6	1.572e-11	1.647e-11	1.68e-11	1.708e-11
8	1	1.858e-11	1.498e-11	1.399e-11	1.366e-11
8	2	2.586e-12	2.673e-12	2.715e-12	2.728e-12
8	3	7.54e-12	7.841e-12	8.159e-12	8.324e-12
8	4	1.614e-11	1.449e-11	1.4e-11	1.388e-11

Rotational Excitation of ortho-cyclopropendyle by He (Chandra & al., 2000)

Reference : JPL

N	g	Energy in cm^{-1}	Level details...
1	9	1.6332	Ka=0 Kc=1 N=1 epsilon=-1 tau=-1
2	15	1.6332	Ka=1 Kc=0 N=1 epsilon=1 tau=1
3	15	2.2451	Ka=1 Kc=2 N=2 epsilon=-1 tau=-1
4	15	4.4798	Ka=2 Kc=1 N=2 epsilon=1 tau=1
5	21	4.4798	Ka=0 Kc=3 N=3 epsilon=-1 tau=-3
6	21	6.3153	Ka=1 Kc=2 N=3 epsilon=1 tau=-1
7	21	8.3875	Ka=2 Kc=1 N=3 epsilon=-1 tau=1
8	21	4.4798	Ka=1 Kc=4 N=4 epsilon=-1 tau=-3
9	21	11.155	Ka=3 Kc=0 N=3 epsilon=1 tau=3
10	27	8.3875	Ka=2 Kc=3 N=4 epsilon=1 tau=-1
11	21	6.3153	Ka=0 Kc=5 N=5 epsilon=-1 tau=-5
12	21	8.3875	Ka=3 Kc=2 N=4 epsilon=-1 tau=1
13	21	12.6262	Ka=4 Kc=1 N=4 epsilon=1 tau=3
14	27	11.155	Ka=1 Kc=4 N=5 epsilon=1 tau=-3
15	27	13.4194	Ka=1 Kc=6 N=6 epsilon=-1 tau=-5
16	27	13.5296	Ka=2 Kc=3 N=5 epsilon=-1 tau=-1
17	33	13.4194	Ka=3 Kc=2 N=5 epsilon=1 tau=1
18	27	8.3875	Ka=4 Kc=1 N=5 epsilon=-1 tau=3
19	27	12.6262	Ka=2 Kc=5 N=6 epsilon=1 tau=-3
20	27	17.3465	Ka=5 Kc=0 N=5 epsilon=1 tau=5
21	27	11.155	Ka=0 Kc=7 N=7 epsilon=-1 tau=-7
22	27	13.4194	Ka=3 Kc=4 N=6 epsilon=-1 tau=-1
23	27	13.5296	Ka=4 Kc=3 N=6 epsilon=1 tau=1
24	27	20.2037	Ka=1 Kc=6 N=7 epsilon=1 tau=-5
25	33	17.3465	Ka=1 Kc=8 N=8 epsilon=-1 tau=-7
26	33	19.5679	Ka=5 Kc=2 N=6 epsilon=-1 tau=-3
27	33	22.3944	Ka=6 Kc=1 N=6 epsilon=1 tau=5
28	39	19.5679	Ka=2 Kc=5 N=7 epsilon=-1 tau=-3
29	33	13.4194	Ka=2 Kc=7 N=8 epsilon=1 tau=-5
30	33	20.2037	Ka=3 Kc=4 N=7 epsilon=1 tau=-1
31	33	24.6162	Ka=0 Kc=9 N=9 epsilon=-1 tau=-9
32	33	26.8337	Ka=4 Kc=3 N=7 epsilon=-1 tau=1
33	33	17.3465	Ka=5 Kc=2 N=7 epsilon=1 tau=3
34	33	19.5679	Ka=3 Kc=6 N=8 epsilon=-1 tau=-3
35	33	22.3944	Ka=6 Kc=1 N=7 epsilon=-1 tau=5
36	33	28.5113	Ka=7 Kc=0 N=7 epsilon=1 tau=7
37	33	13.4194	Ka=1 Kc=8 N=9 epsilon=1 tau=-7
38	33	20.2037	Ka=4 Kc=5 N=8 epsilon=1 tau=-1
39	33	24.6162	Ka=1 Kc=10 N=10 epsilon=-1 tau=-9
40	33	31.083	Ka=5 Kc=4 N=8 epsilon=-1 tau=1
41	39	24.6162	Ka=2 Kc=7 N=9 epsilon=-1 tau=-5
42	39	26.8337	Ka=6 Kc=3 N=8 epsilon=1 tau=3
43	39	31.083	Ka=2 Kc=9 N=10 epsilon=1 tau=-7
44	33	17.3465	Ka=7 Kc=2 N=8 epsilon=-1 tau=5
45	33	22.3944	Ka=0 Kc=11 N=11 epsilon=-1 tau=-11
46	33	28.5113	Ka=3 Kc=6 N=9 epsilon=1 tau=-3

Theoretical Energy Levels

CDMS

Einstein Coefficients

Einstein coefficients A_ij for c-C3H2

Reference : JPL

i	j	A_ij....
2	1	4.2263065752e-07
3	1	2.55334550477e-05
4	2	7.46365079557e-05
4	3	3.80296644732e-06
5	3	7.67030052301e-05
6	4	7.44204214473e-05
6	5	1.0907409924e-05
7	3	6.49147849116e-05
7	6	3.51497796146e-06
8	5	0.0001800850413
9	4	0.000281274770668
9	5	4.09019577389e-07
9	7	1.07159096204e-06
10	6	0.000239338358103
10	8	2.46408072369e-05
10	9	3.8977132555e-07
11	8	0.000346901479579
12	5	8.90722201873e-05
12	7	0.000342485688259
12	10	1.67297462027e-05
13	6	0.000130700524776
13	8	1.45695026515e-07
13	9	0.000799273098548
13	12	7.57505463427e-06
14	10	0.000442683072
14	11	4.3505634887e-05
15	13	7.18729155496e-09
16	11	0.000593376026698
16	8	0.000125491181256
16	12	0.000457272678169
17	14	3.66887521178e-05
18	15	4.89008576098e-10
18	10	0.0002941249067
19	11	1.86320242591e-07
19	13	0.000177015839039
19	16	1.54060633156e-05
20	8	9.11569309474e-07
20	12	0.000661124626506
20	14	1.05257205244e-06
21	17	4.07161990011e-06
21	14	0.000742320443638

Experimental Energy TABLE

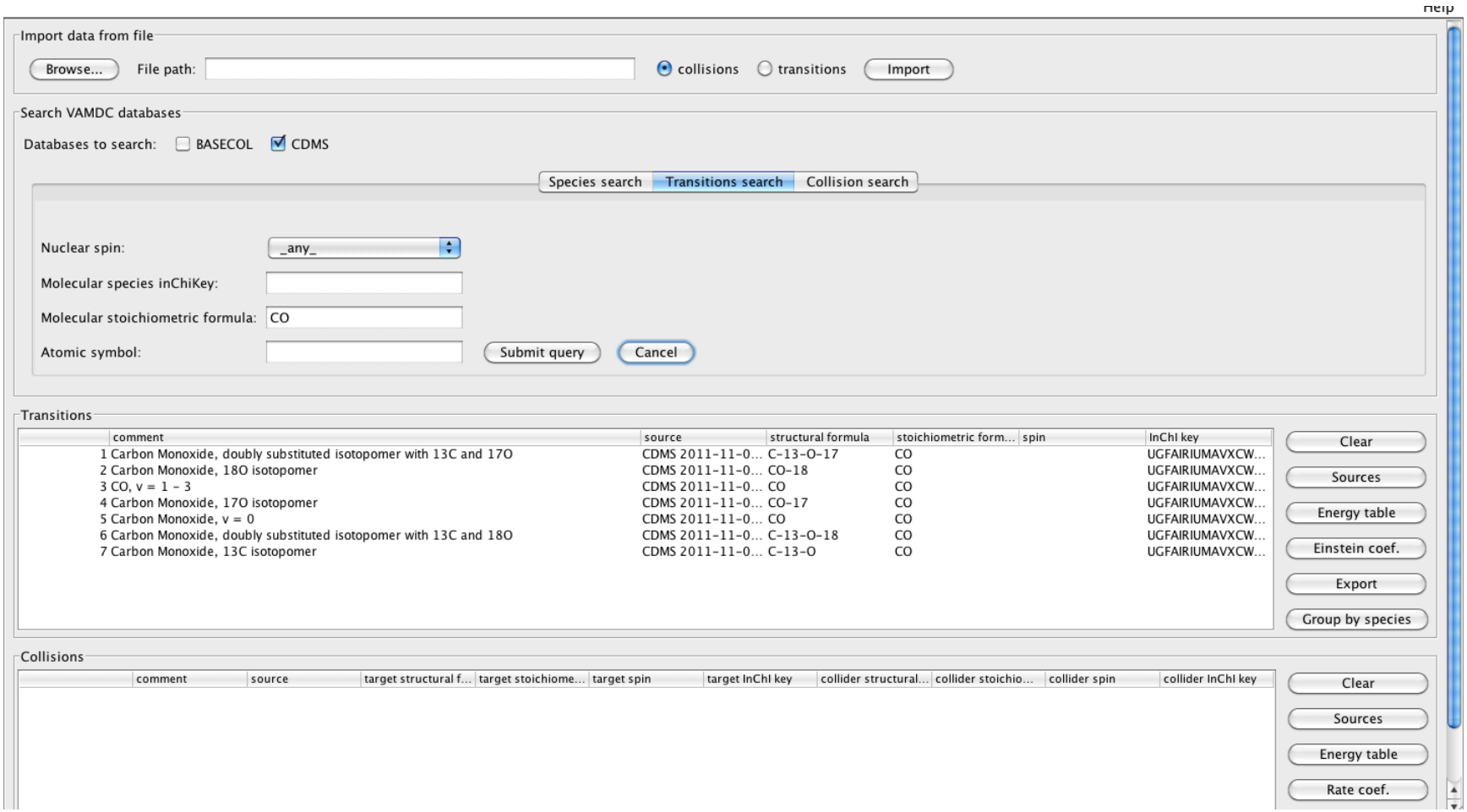
Rotational Excitation of ortho-cyclopropendyle by He (Chandra & al., 2000)

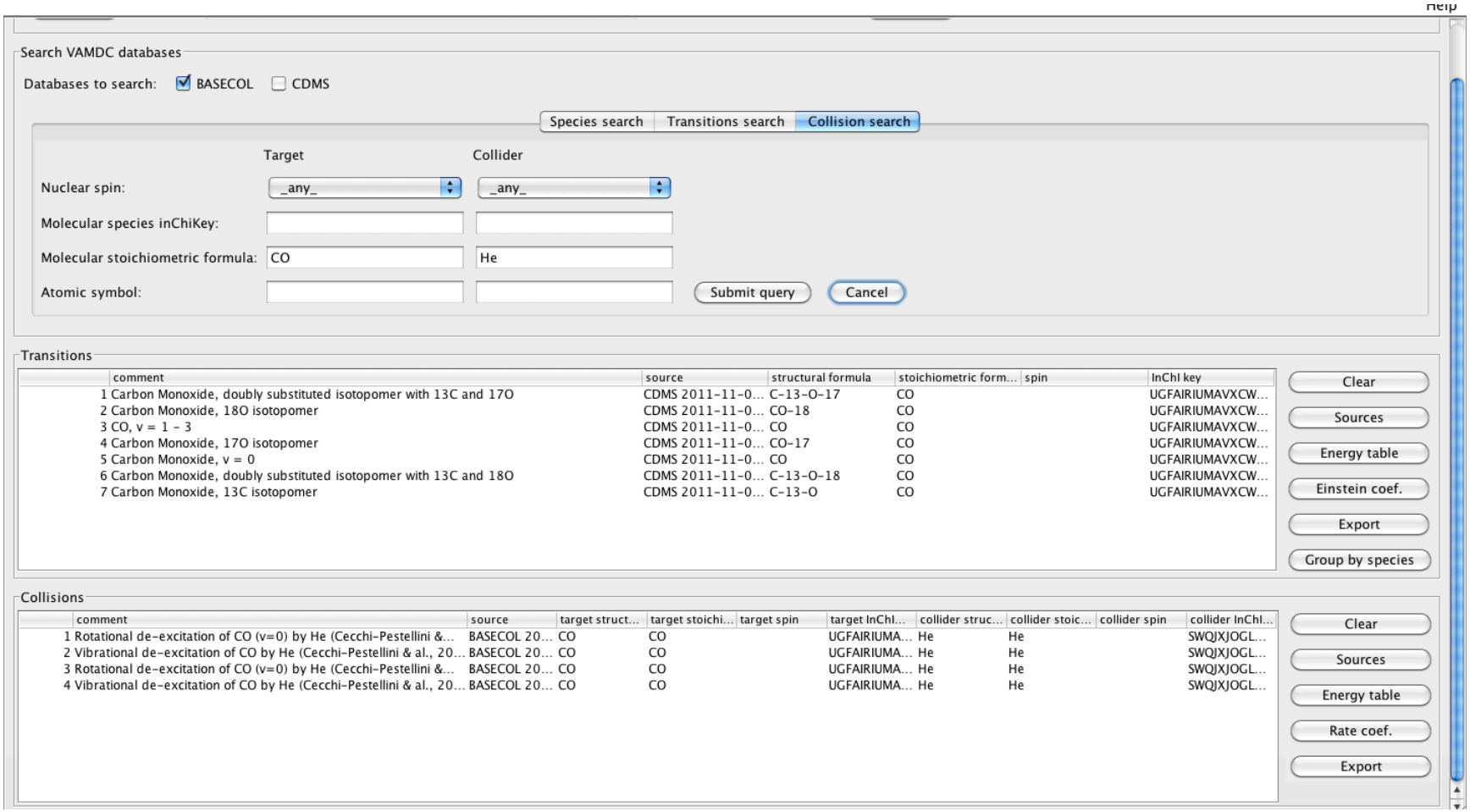
Reference : JPL

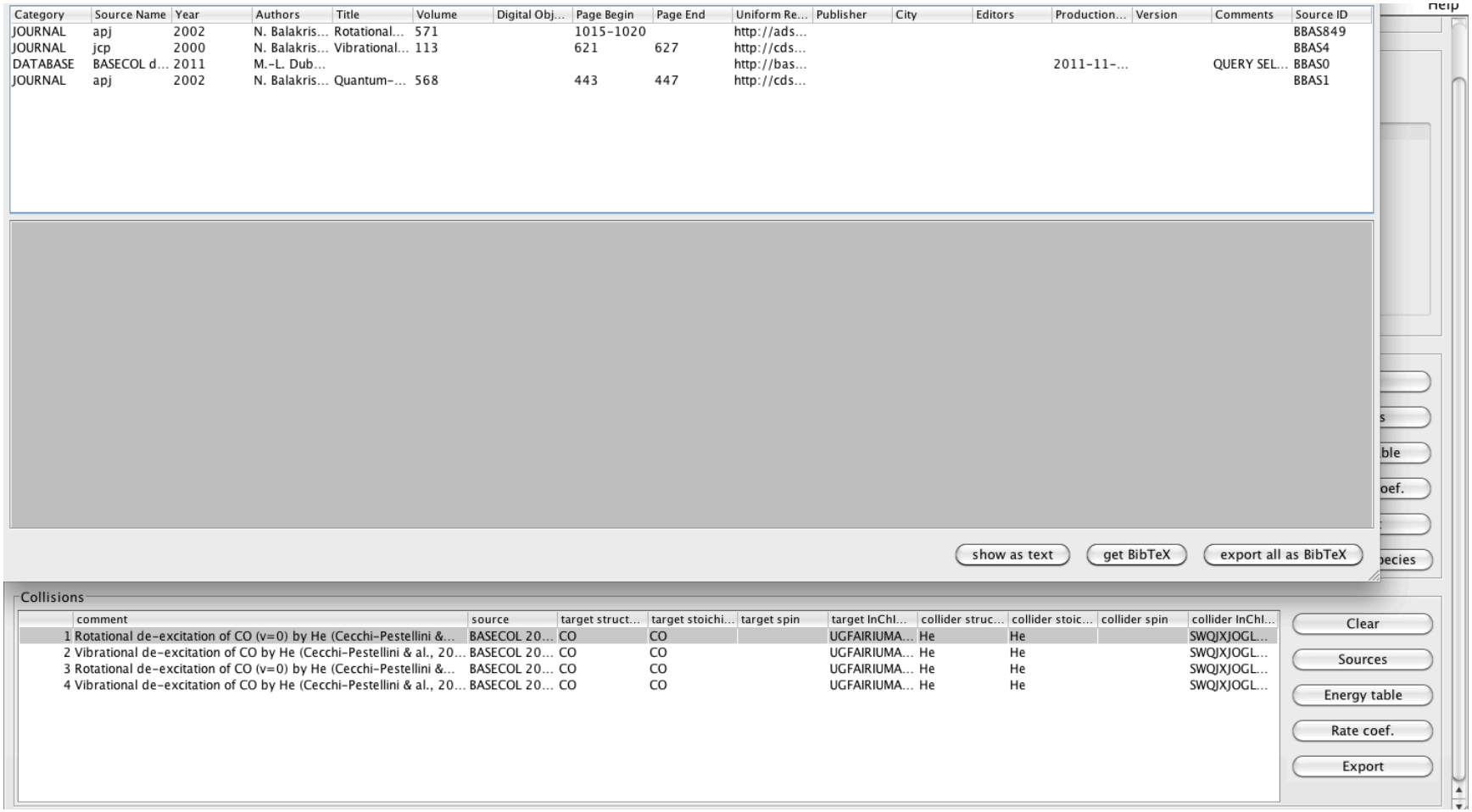
N	g	Energy in cm^{-1}	Level details...
1	9	1.6332	Ka=0 Kc=1 N=1 epsilon=-1 tau=-1
2	15	1.6332	Ka=1 Kc=0 N=1 epsilon=1 tau=1
3	15	2.2451	Ka=1 Kc=2 N=2 epsilon=-1 tau=-1
4	15	4.4798	Ka=2 Kc=1 N=2 epsilon=1 tau=1
5	21	4.4798	Ka=0 Kc=3 N=3 epsilon=-1 tau=-3
6	21	6.3153	Ka=1 Kc=2 N=3 epsilon=1 tau=-1
7	21	8.3875	Ka=2 Kc=1 N=3 epsilon=-1 tau=1
8	21	4.4798	Ka=1 Kc=4 N=4 epsilon=-1 tau=-3
9	21	11.155	Ka=3 Kc=0 N=3 epsilon=1 tau=3
10	27	8.3875	Ka=2 Kc=3 N=4 epsilon=1 tau=-1
11	21	6.3153	Ka=0 Kc=5 N=5 epsilon=-1 tau=-5
12	21	8.3875	Ka=3 Kc=2 N=4 epsilon=-1 tau=1
13	21	12.6262	Ka=4 Kc=1 N=4 epsilon=1 tau=3
14	27	11.155	Ka=1 Kc=4 N=5 epsilon=1 tau=-3
15	27	13.4194	Ka=1 Kc=6 N=6 epsilon=-1 tau=-5
16	27	13.5296	Ka=2 Kc=3 N=5 epsilon=-1 tau=-1
17	33	13.4194	Ka=3 Kc=2 N=5 epsilon=1 tau=1
18	27	8.3875	Ka=4 Kc=1 N=5 epsilon=-1 tau=3
19	27	12.6262	Ka=2 Kc=5 N=6 epsilon=1 tau=-3
20	27	17.3465	Ka=5 Kc=0 N=5 epsilon=1 tau=5
21	27	11.155	Ka=0 Kc=7 N=7 epsilon=-1 tau=-7
22	27	13.4194	Ka=3 Kc=4 N=6 epsilon=-1 tau=-1
23	27	13.5296	Ka=4 Kc=3 N=6 epsilon=1 tau=1
24	27	20.2037	Ka=1 Kc=6 N=7 epsilon=1 tau=-5
25	33	17.3465	Ka=1 Kc=8 N=8 epsilon=-1 tau=-7
26	33	19.5679	Ka=5 Kc=2 N=6 epsilon=-1 tau=-3
27	33	22.3944	Ka=6 Kc=1 N=6 epsilon=1 tau=5
28	39	19.5679	Ka=2 Kc=5 N=7 epsilon=-1 tau=-3
29	33	13.4194	Ka=2 Kc=7 N=8 epsilon=1 tau=-5
30	33	20.2037	Ka=3 Kc=4 N=7 epsilon=1 tau=-1
31	33	24.6162	Ka=0 Kc=9 N=9 epsilon=-1 tau=-9
32	33	26.8337	Ka=4 Kc=3 N=7 epsilon=-1 tau=1
33	33	17.3465	Ka=5 Kc=2 N=7 epsilon=1 tau=3
34	33	19.5679	Ka=3 Kc=6 N=8 epsilon=-1 tau=-3
35	33	22.3944	Ka=6 Kc=1 N=7 epsilon=-1 tau=5
36	33	28.5113	Ka=7 Kc=0 N=7 epsilon=1 tau=7
37	33	13.4194	Ka=1 Kc=8 N=9 epsilon=1 tau=-7
38	33	20.2037	Ka=4 Kc=5 N=8 epsilon=1 tau=-1
39	33	24.6162	Ka=1 Kc=10 N=10 epsilon=-1 tau=-9
40	33	31.083	Ka=5 Kc=4 N=8 epsilon=-1 tau=1
41	39	24.6162	Ka=2 Kc=7 N=9 epsilon=-1 tau=-5
42	39	26.8337	Ka=6 Kc=3 N=8 epsilon=1 tau=3
43	39	31.083	Ka=2 Kc=9 N=10 epsilon=1 tau=-7
44	33	17.3465	Ka=7 Kc=2 N=8 epsilon=-1 tau=5
45	33	22.3944	Ka=0 Kc=11 N=11 epsilon=-1 tau=-11
46	33	28.5113	Ka=3 Kc=6 N=9 epsilon=1 tau=-3

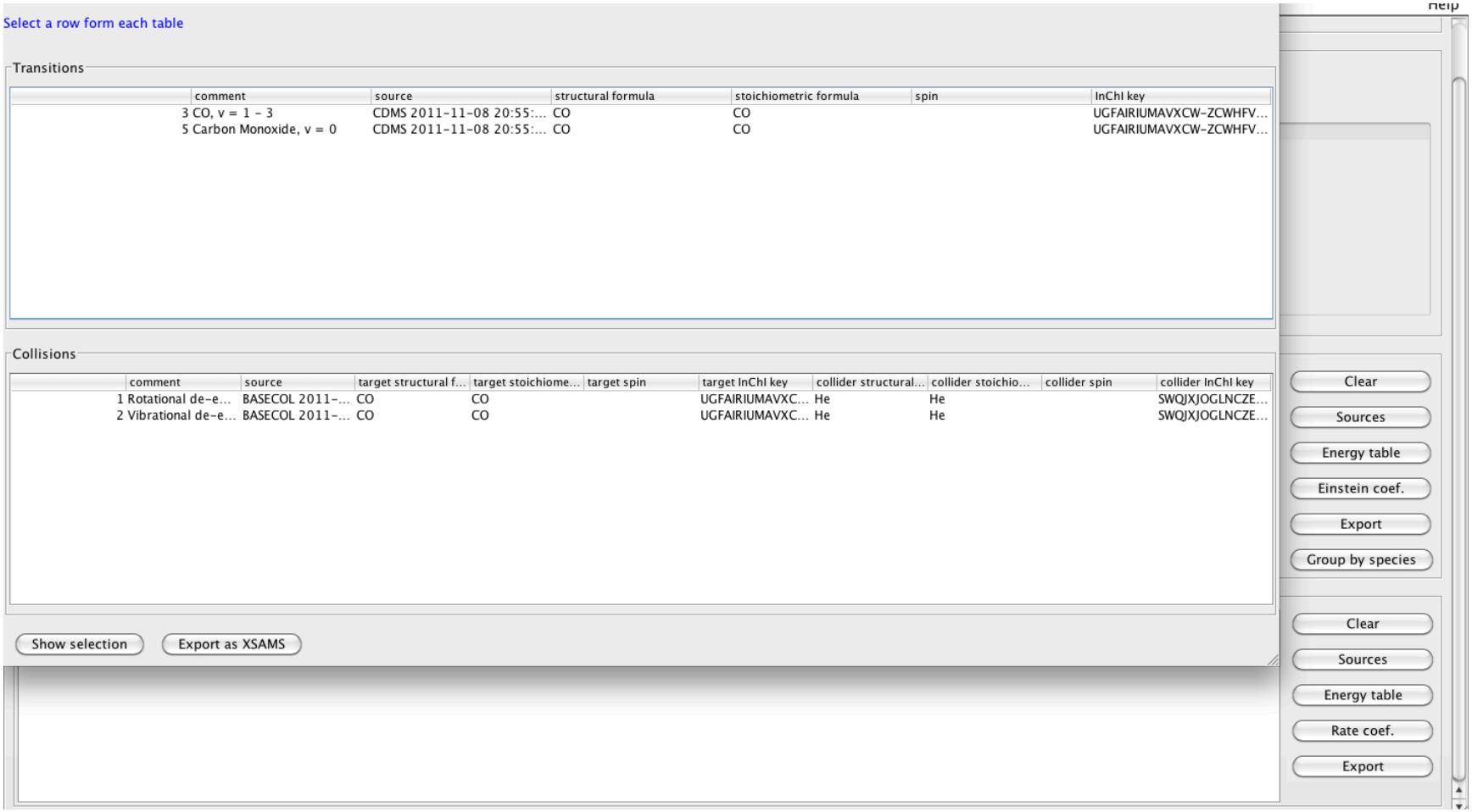
Demo

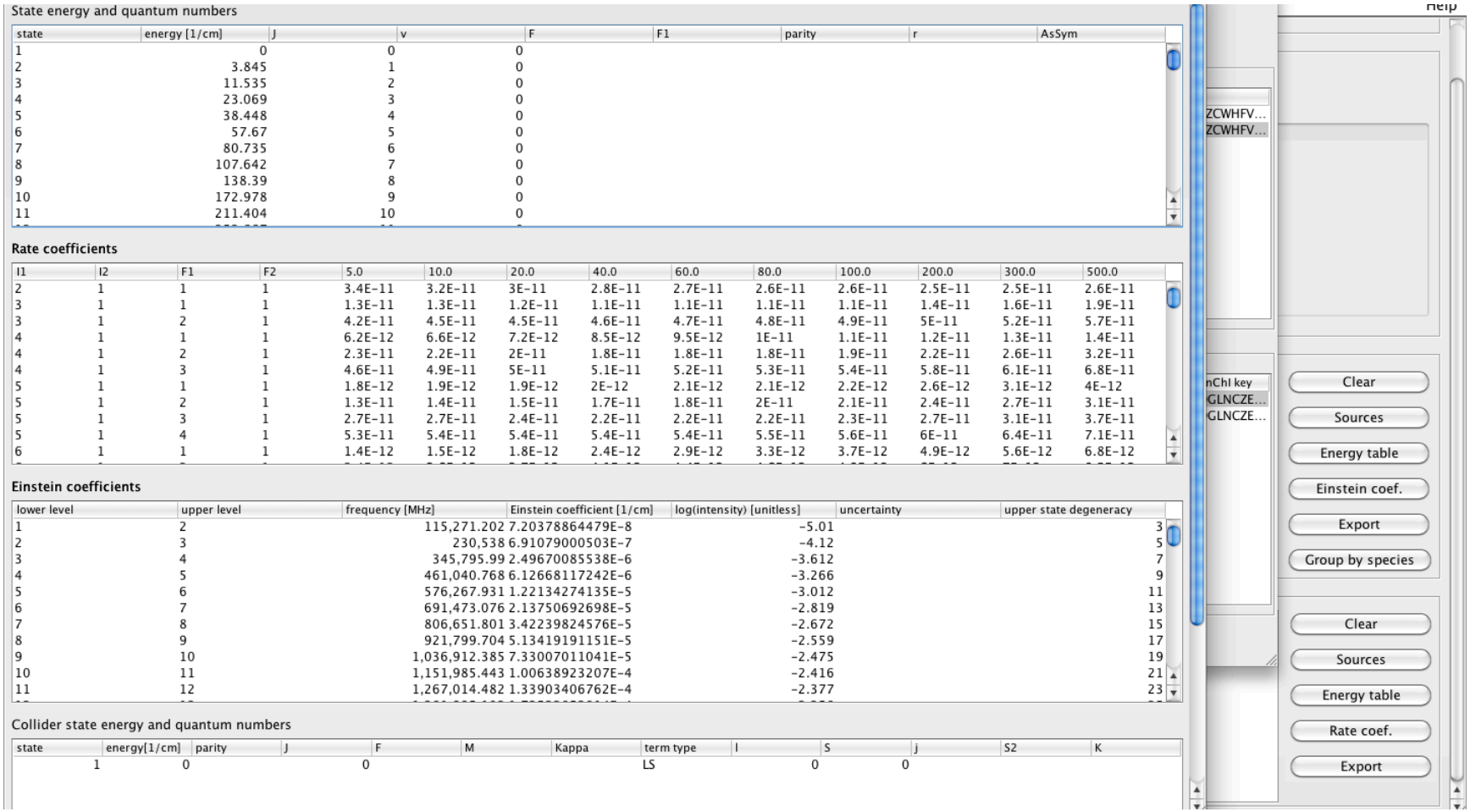
- Query CDMS for transitions on a species
- Query BASECOL for collisions on same species
  - USE OF STOECHIOMETRIC FORMULA
- Group results by same species
- Select the spectroscopic and collisional sets to be combined
- Extract them in ASCII or XSAMS (to be re-fed in style sheet to provide customized output)

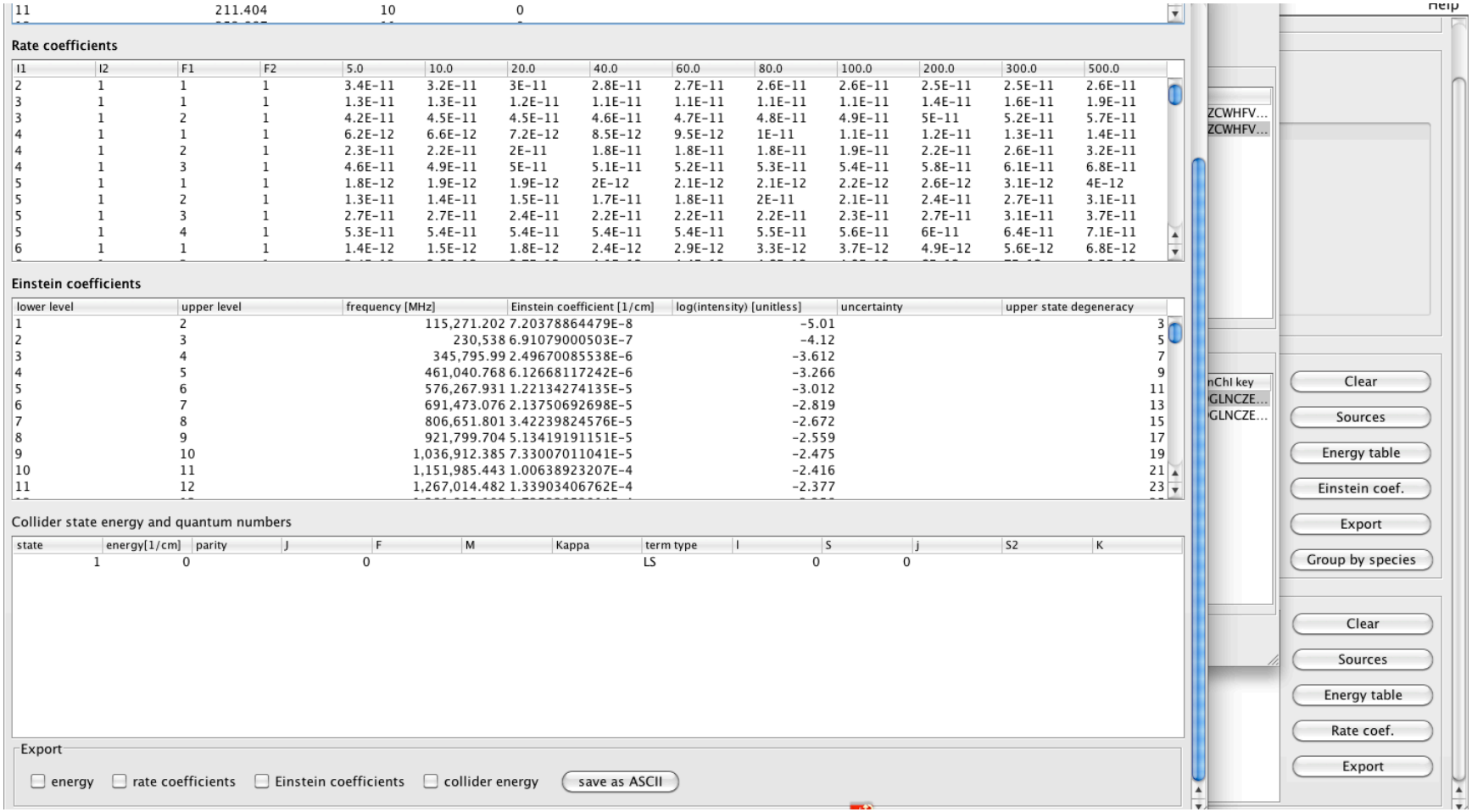

Help
Import data from file
Browse...
File path:
collisions
transitions
Import
Search VAMDC databases
Databases to search:
BASECOL
CDMS
Species search
Transitions search
Collision search
Nuclear spin:
any
Molecular species inChiKey:
Molecular stoichiometric formula:
CO
Atomic symbol:
Submit query
Cancel
Transitions
comment
source
structural formula
stoichiometric form...
spin
InChI key
1 Carbon Monoxide, doubly substituted isotopomer with 13C and 17O
CDMS 2011-11-0... C-13-O-17
CO
UGFAIRIUMAVXCW...
2 Carbon Monoxide, 18O isotopomer
CDMS 2011-11-0... CO-18
CO
UGFAIRIUMAVXCW...
3 CO, v = 1 - 3
CDMS 2011-11-0... CO
CO
UGFAIRIUMAVXCW...
4 Carbon Monoxide, 17O isotopomer
CDMS 2011-11-0... CO-17
CO
UGFAIRIUMAVXCW...
5 Carbon Monoxide, v = 0
CDMS 2011-11-0... CO
CO
UGFAIRIUMAVXCW...
6 Carbon Monoxide, doubly substituted isotopomer with 13C and 18O
CDMS 2011-11-0... C-13-O-18
CO
UGFAIRIUMAVXCW...
7 Carbon Monoxide, 13C isotopomer
CDMS 2011-11-0... C-13-O
CO
UGFAIRIUMAVXCW...
Clear
Sources
Energy table
Einstein coef.
Export
Group by species
Collisions
comment
source
target structural f...
target stoichiome...
target spin
target InChI key
collider structural...
collider stoichio...
collider spin
collider InChI key
Clear
Sources
Energy table
Rate coef.


Help
Search VAMDC databases
Databases to search: BASECOL CDMS
Species search
Transitions search
Collision search
Target
Collider
Nuclear spin:
any
any
Molecular species inChiKey:
Molecular stoichiometric formula:
CO
He
Atomic symbol:
Submit query
Cancel
Transitions
comment
source
structural formula
stoichiometric form...
spin
InChI key
1 Carbon Monoxide, doubly substituted isotopomer with 13C and 17O
CDMS 2011-11-0... C-13-O-17
CO
UGFAIRIUMAVXCW...
2 Carbon Monoxide, 18O isotopomer
CDMS 2011-11-0... CO-18
CO
UGFAIRIUMAVXCW...
3 CO, v = 1 - 3
CDMS 2011-11-0... CO
CO
UGFAIRIUMAVXCW...
4 Carbon Monoxide, 17O isotopomer
CDMS 2011-11-0... CO-17
CO
UGFAIRIUMAVXCW...
5 Carbon Monoxide, v = 0
CDMS 2011-11-0... CO
CO
UGFAIRIUMAVXCW...
6 Carbon Monoxide, doubly substituted isotopomer with 13C and 18O
CDMS 2011-11-0... C-13-O-18
CO
UGFAIRIUMAVXCW...
7 Carbon Monoxide, 13C isotopomer
CDMS 2011-11-0... C-13-O
CO
UGFAIRIUMAVXCW...
Clear
Sources
Energy table
Einstein coef.
Export
Group by species
Collisions
comment
source
target struct...
target stoichi...
target spin
target InChI...
collider struc...
collider stoic...
collider spin
collider InChI...
1 Rotational de-excitation of CO (v=0) by He (Cecchi-Pestellini &...
BASECOL 20...
CO
CO
UGFAIRIUMA...
He
He
SWQJXJOGL...
2 Vibrational de-excitation of CO by He (Cecchi-Pestellini & al., 20...
BASECOL 20...
CO
CO
UGFAIRIUMA...
He
He
SWQJXJOGL...
3 Rotational de-excitation of CO (v=0) by He (Cecchi-Pestellini &...
BASECOL 20...
CO
CO
UGFAIRIUMA...
He
He
SWQJXJOGL...
4 Vibrational de-excitation of CO by He (Cecchi-Pestellini & al., 20...
BASECOL 20...
CO
CO
UGFAIRIUMA...
He
He
SWQJXJOGL...
Clear
Sources
Energy table
Rate coef.
Export


Help
Category Source Name Year Authors Title Volume Digital Obj... Page Begin Page End Uniform Re... Publisher City Editors Production... Version Comments Source ID
JOURNAL apj 2002 N. Balakris... Rotational... 571 1015-1020 http://ads... BBAS849
JOURNAL jcp 2000 N. Balakris... Vibrational... 113 621 627 http://cds... BBAS4
DATABASE BASECOL d... 2011 M.-L. Dub... http://bas... 2011-11-... QUERY SEL... BBAS0
JOURNAL apj 2002 N. Balakris... Quantum-... 568 443 447 http://cds... BBAS1
show as text
get BibTeX
export all as BibTeX
Collisions
comment source target struct... target stoichi... target spin target InChI... collider struc... collider stoic... collider spin collider InChI...
1 Rotational de-excitation of CO (v=0) by He (Cecchi-Pestellini &... BASECOL 20... CO CO UGFAIRIUMA... He He SWQJXJOGL...
2 Vibrational de-excitation of CO by He (Cecchi-Pestellini & al., 20... BASECOL 20... CO CO UGFAIRIUMA... He He SWQJXJOGL...
3 Rotational de-excitation of CO (v=0) by He (Cecchi-Pestellini &... BASECOL 20... CO CO UGFAIRIUMA... He He SWQJXJOGL...
4 Vibrational de-excitation of CO by He (Cecchi-Pestellini & al., 20... BASECOL 20... CO CO UGFAIRIUMA... He He SWQJXJOGL...
Clear
Sources
Energy table
Rate coef.
Export


Help
Select a row form each table
Transitions
comment
source
structural formula
stoichiometric formula
spin
InChI key
3 CO, v = 1 - 3
CDMS 2011-11-08 20:55:...
CO
CO
UGFAIRIUMAVXCW-ZCWHFV...
5 Carbon Monoxide, v = 0
CDMS 2011-11-08 20:55:...
CO
CO
UGFAIRIUMAVXCW-ZCWHFV...
Collisions
comment
source
target structural f...
target stoichiome...
target spin
target InChI key
collider structural...
collider stoichio...
collider spin
collider InChI key
1 Rotational de-e...
BASECOL 2011-...
CO
CO
UGFAIRIUMAVXC...
He
He
SWQJXJOGLNCZE...
2 Vibrational de-e...
BASECOL 2011-...
CO
CO
UGFAIRIUMAVXC...
He
He
SWQJXJOGLNCZE...
Clear
Sources
Energy table
Einstein coef.
Export
Group by species
Show selection
Export as XSAMS
Clear
Sources
Energy table
Rate coef.
Export


State energy and quantum numbers
state energy [1/cm] J v F F1 parity r AsSym
1 0 0 0
2 3.845 1 0
3 11.535 2 0
4 23.069 3 0
5 38.448 4 0
6 57.67 5 0
7 80.735 6 0
8 107.642 7 0
9 138.39 8 0
10 172.978 9 0
11 211.404 10 0
Rate coefficients
I1 I2 F1 F2 5.0 10.0 20.0 40.0 60.0 80.0 100.0 200.0 300.0 500.0
2 1 1 1 3.4E-11 3.2E-11 3E-11 2.8E-11 2.7E-11 2.6E-11 2.6E-11 2.5E-11 2.5E-11 2.6E-11
3 1 1 1 1.3E-11 1.3E-11 1.2E-11 1.1E-11 1.1E-11 1.1E-11 1.1E-11 1.4E-11 1.6E-11 1.9E-11
3 1 2 1 4.2E-11 4.5E-11 4.5E-11 4.6E-11 4.7E-11 4.8E-11 4.9E-11 5E-11 5.2E-11 5.7E-11
4 1 1 1 6.2E-12 6.6E-12 7.2E-12 8.5E-12 9.5E-12 1E-11 1.1E-11 1.2E-11 1.3E-11 1.4E-11
4 1 2 1 2.3E-11 2.2E-11 2E-11 1.8E-11 1.8E-11 1.8E-11 1.9E-11 2.2E-11 2.6E-11 3.2E-11
4 1 3 1 4.6E-11 4.9E-11 5E-11 5.1E-11 5.2E-11 5.3E-11 5.4E-11 5.8E-11 6.1E-11 6.8E-11
5 1 1 1 1.8E-12 1.9E-12 1.9E-12 2E-12 2.1E-12 2.1E-12 2.2E-12 2.6E-12 3.1E-12 4E-12
5 1 2 1 1.3E-11 1.4E-11 1.5E-11 1.7E-11 1.8E-11 2E-11 2.1E-11 2.4E-11 2.7E-11 3.1E-11
5 1 3 1 2.7E-11 2.7E-11 2.4E-11 2.2E-11 2.2E-11 2.2E-11 2.3E-11 2.7E-11 3.1E-11 3.7E-11
5 1 4 1 5.3E-11 5.4E-11 5.4E-11 5.4E-11 5.4E-11 5.5E-11 5.6E-11 6E-11 6.4E-11 7.1E-11
6 1 1 1 1.4E-12 1.5E-12 1.8E-12 2.4E-12 2.9E-12 3.3E-12 3.7E-12 4.9E-12 5.6E-12 6.8E-12
Einstein coefficients
lower level upper level frequency [MHz] Einstein coefficient [1/cm] log(intensity) [unitless] uncertainty upper state degeneracy
1 2 115,271.202 7.20378864479E-8 -5.01 3
2 3 230,538 6.91079000503E-7 -4.12 5
3 4 345,795.99 2.49670085538E-6 -3.612 7
4 5 461,040.768 6.12668117242E-6 -3.266 9
5 6 576,267.931 1.22134274135E-5 -3.012 11
6 7 691,473.076 2.13750692698E-5 -2.819 13
7 8 806,651.801 3.42239824576E-5 -2.672 15
8 9 921,799.704 5.13419191151E-5 -2.559 17
9 10 1,036,912.385 7.33007011041E-5 -2.475 19
10 11 1,151,985.443 1.00638923207E-4 -2.416 21
11 12 1,267,014.482 1.33903406762E-4 -2.377 23
Collider state energy and quantum numbers
state energy[1/cm] parity J F M Kappa term type I S j S2 K
1 0 0 LS 0 0
Help
ZCWHFV...
ZCWHFV...
nChI key
GLNCZE...
GLNCZE...
Clear
Sources
Energy table
Einstein coef.
Export
Group by species
Clear
Sources
Energy table
Rate coef.
Export


11 211.404 10 0
Rate coefficients
I1 I2 F1 F2 5.0 10.0 20.0 40.0 60.0 80.0 100.0 200.0 300.0 500.0
2 1 1 1 3.4E-11 3.2E-11 3E-11 2.8E-11 2.7E-11 2.6E-11 2.6E-11 2.5E-11 2.5E-11 2.6E-11
3 1 1 1 1.3E-11 1.3E-11 1.2E-11 1.1E-11 1.1E-11 1.1E-11 1.1E-11 1.4E-11 1.6E-11 1.9E-11
3 1 2 1 4.2E-11 4.5E-11 4.5E-11 4.6E-11 4.7E-11 4.8E-11 4.9E-11 5E-11 5.2E-11 5.7E-11
4 1 1 1 6.2E-12 6.6E-12 7.2E-12 8.5E-12 9.5E-12 1E-11 1.1E-11 1.2E-11 1.3E-11 1.4E-11
4 1 2 1 2.3E-11 2.2E-11 2E-11 1.8E-11 1.8E-11 1.8E-11 1.9E-11 2.2E-11 2.6E-11 3.2E-11
4 1 3 1 4.6E-11 4.9E-11 5E-11 5.1E-11 5.2E-11 5.3E-11 5.4E-11 5.8E-11 6.1E-11 6.8E-11
5 1 1 1 1.8E-12 1.9E-12 1.9E-12 2E-12 2.1E-12 2.1E-12 2.2E-12 2.6E-12 3.1E-12 4E-12
5 1 2 1 1.3E-11 1.4E-11 1.5E-11 1.7E-11 1.8E-11 2E-11 2.1E-11 2.4E-11 2.7E-11 3.1E-11
5 1 3 1 2.7E-11 2.7E-11 2.4E-11 2.2E-11 2.2E-11 2.2E-11 2.3E-11 2.7E-11 3.1E-11 3.7E-11
5 1 4 1 5.3E-11 5.4E-11 5.4E-11 5.4E-11 5.4E-11 5.5E-11 5.6E-11 6E-11 6.4E-11 7.1E-11
6 1 1 1 1.4E-12 1.5E-12 1.8E-12 2.4E-12 2.9E-12 3.3E-12 3.7E-12 4.9E-12 5.6E-12 6.8E-12
Einstein coefficients
lower level upper level frequency [MHz] Einstein coefficient [1/cm] log(intensity) [unitless] uncertainty upper state degeneracy
1 2 115,271.202 7.20378864479E-8 -5.01 3
2 3 230,538 6.91079000503E-7 -4.12 5
3 4 345,795.99 2.49670085538E-6 -3.612 7
4 5 461,040.768 6.12668117242E-6 -3.266 9
5 6 576,267.931 1.22134274135E-5 -3.012 11
6 7 691,473.076 2.13750692698E-5 -2.819 13
7 8 806,651.801 3.42239824576E-5 -2.672 15
8 9 921,799.704 5.13419191151E-5 -2.559 17
9 10 1,036,912.385 7.33007011041E-5 -2.475 19
10 11 1,151,985.443 1.00638923207E-4 -2.416 21
11 12 1,267,014.482 1.33903406762E-4 -2.377 23
Collider state energy and quantum numbers
state energy[1/cm] parity J F M Kappa term type I S j S2 K
1 0 0 LS 0 0
Export
energy
rate coefficients
Einstein coefficients
collider energy
save as ASCII
Help
ZCWHFV...
ZCWHFV...
nChI key
GLNCZE...
GLNCZE...
Clear
Sources
Energy table
Einstein coef.
Export
Group by species
Clear
Sources
Energy table
Rate coef.
Export