

SpaceMol

Database of Molecules in Space

Version 1.0

<https://irsa.ipac.caltech.edu/data/SpaceMol/overview.html>

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1 SpaceMol Summary

SpaceMol is a searchable database of molecular transitions detected in space. Each entry is searchable by all parameters given in Table 1. This consists of parameters related to the target (e.g. name, type), transition (e.g. rest wavelength, Einstein A), measured values (e.g. flux, width), and observation (e.g. instrument, program ID, date). SpaceMol additionally provides notes on transitions that include observation IDs, irregular situations, and changes from publications. Measurements of the molecular transitions are either from publications or are performed by the SpaceMol Team.

Category	Items
Target	Name, Type, Right Ascension, Declination
Transition Properties	Species, Transition Description, Rest Wavelength ^a , Rest Wavenumber ^a , Upper and Lower Energy Levels, Upper and Lower Statistical Weights, Einstein A, Transition References
Measured Values	Line Flux ^{a,b} , Amplitude ^{a,b} , Velocity ^{a,b} , Width ^{a,b} , Indication of Substructure, Number of Velocity Components, Linked Snapshot of Spectrum, Snapshot File Type, Measurement References, Measurement Notes
Observation Parameters	Observatory, Instrument, Program ID, Observation Date, Multi-epoch flag, Spectral Resolution ^b , Beam Size, Map Dimensions

^a Includes uncertainty ^b Includes units

Table 1: SpaceMol Database Contents

SpaceMol is expected to include spectroscopic data from three Herschel instruments (HIFI, SPIRE, and PACS) and two SOFIA instruments (EXES and GREAT). Together these instruments span a wide wavelength range, 5–670 μm , covering MIR, FIR, and sub-mm wavelengths, and resolving powers of 10^3 – 10^7 (Figure. 1, Table 2) that enable studies of a broad range of environments and phenomena: galaxies, dense and diffuse gas, supernova remnants, protostars, protoplanetary disks, debris disks, and the solar system; shocks, dynamics, structure, and chemistry.

This is the first data drop of SpaceMol, containing data from the SOFIA/EXES, Herschel/HIFI and SPIRE instruments only. The next data drop is anticipated for Spring 2027.

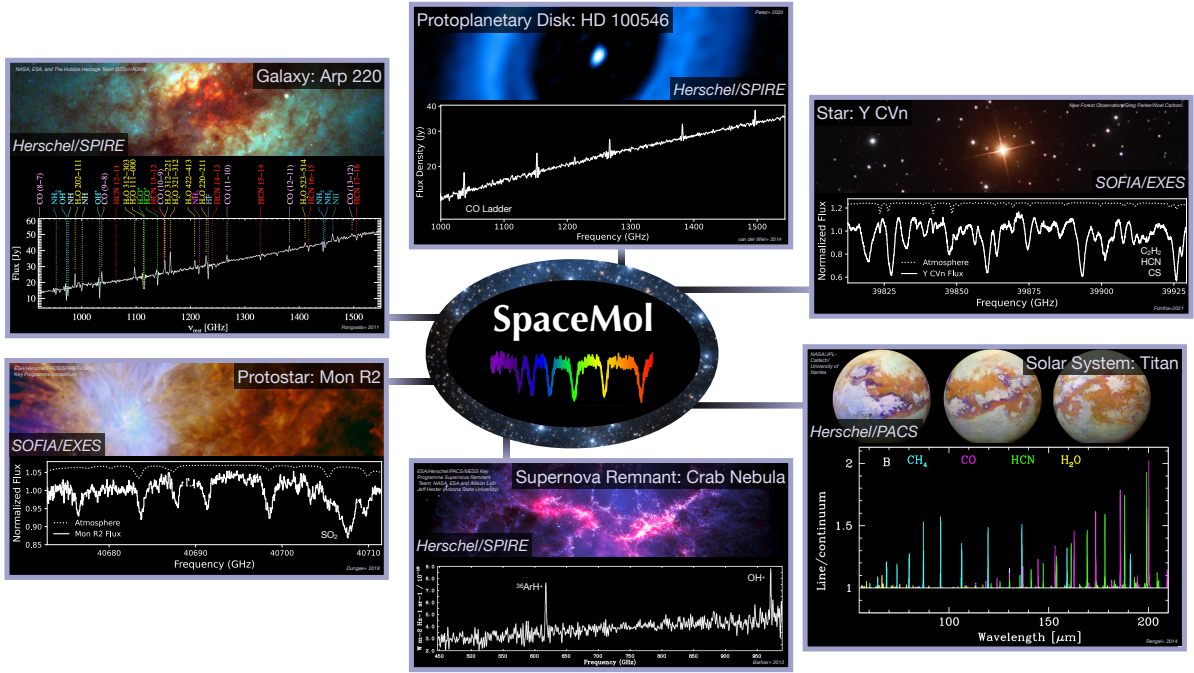


Figure 1: SpaceMol provides access to observed molecular transitions, arising in different astrophysical environments, and the transition characteristics over a wide bandwidth.

Observatory	Instrument	λ (μm)	R	Beam Size (arcsec)
SOFIA	EXES	5–28	10^5	3.5
SOFIA	GREAT	63–611	10^7	13–40
Herschel	PACS	55–210	10^3	9–13
Herschel	HIFI	157–625	10^7	11–44
Herschel	SPIRE	194–671	10^3	17–42

Note: Instruments in grey will be included in future releases

Table 2: Specifications of missions and instruments included in SpaceMol

2 Additional Information

A breakdown by instrument of the current contents of the SpaceMol Database is given in Table 3, a list of the currently available molecules in Table 4, and a list of currently available target types in Table 5.

Inquiries and feedback are welcome! (all emails are appended by “@nasa.gov”)

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Observatory/Instrument	# Programs	# Molecular Lines
SOFIA/EXES	22	1809
Herschel/HIFI	13	2556
Herschel/SPIRE	12	974
Total	47	5339

Table 3: Breakdown of Current SpaceMol Contents By Instrument

Species	Isotopologues	# Molecular Lines
AlO	—	2
C2H	—	44
C2H2	—	112
	(13)CCH2	13
C3	—	14
CF+	—	1
CH	—	31
CH+	—	30
	(13)CH+	9
CH3OCH3	—	1
CH3OCHO	—	2
CH3OH	—	733
CH4	—	6
CN	—	32
CO	—	307
	(13)C(18)O	2
	(13)CO	173
	C(17)O	22
	C(18)O	109
CO+	—	1

CO ₂	—	90
	OC(17)O	30
	OC(18)O	122
	O(13)C(17)O	2
	O(13)C(18)O	42
CS	—	101
	(13)CS	2
	C(34)S	7
H ₂	—	37
H ₂ Cl ⁺	—	5
	H ₂ (37)Cl ⁺	1
H ₂ CO	—	126
H ₂ CS	—	6
H ₂ O	—	1620
	D ₂ O	8
	HD(18)O	4
	HDO	124
	H ₂ (17)O	32
	H ₂ (18)O	111
H ₂ O ⁺	—	17
H ₂ S	—	91
	H ₂ (33)S	9
	H ₂ (34)S	27
H ₃ O ⁺	—	6
HCl	—	18
	H(37)Cl	10
HCN	—	178
	H(13)CN	25
	HC(15)N	1
	DCN	3
HCO ⁺	—	64
	H(13)CO ⁺	11
	DCO ⁺	2
HDS	—	1
HF	—	6
HNC	—	47
	HN(13)C	4
N ₂ H ⁺	—	20
NH	—	1
	ND	1
NH ₂	—	1
NH ₃	—	39

	NH2D	2
	(15)NH3	1
NO	—	10
O2	—	3
OH	—	9
OH+	—	31
PN	—	2
PO	—	7
SH+	—	14
SiO	—	68
	(29)SiO	3
	(30)SiO	8
SiS	—	3
SO	—	77
SO2	—	79
	OS(18)O	1
UID	UID	325

UID refers to unidentified transitions

Table 4: Molecules Currently Available in SpaceMol

Active Galaxies
AGB Stars
Circumstellar Disks
Evolved Stars
Galaxy Clusters
Giants
Herbig-Haro Objects
HII Regions
Hot Cores
Interstellar Medium
Molecular Clouds
Planetary Nebulae
Planets
Protoplanetary Disks
Protostars
RSG Stars
Star Formation
Star Forming Clouds
Starburst Galaxies
Supernova Remnants
T Tauri Stars
White Dwarfs
Young Stellar Objects

Table 5: Target Types Currently Available in SpaceMol