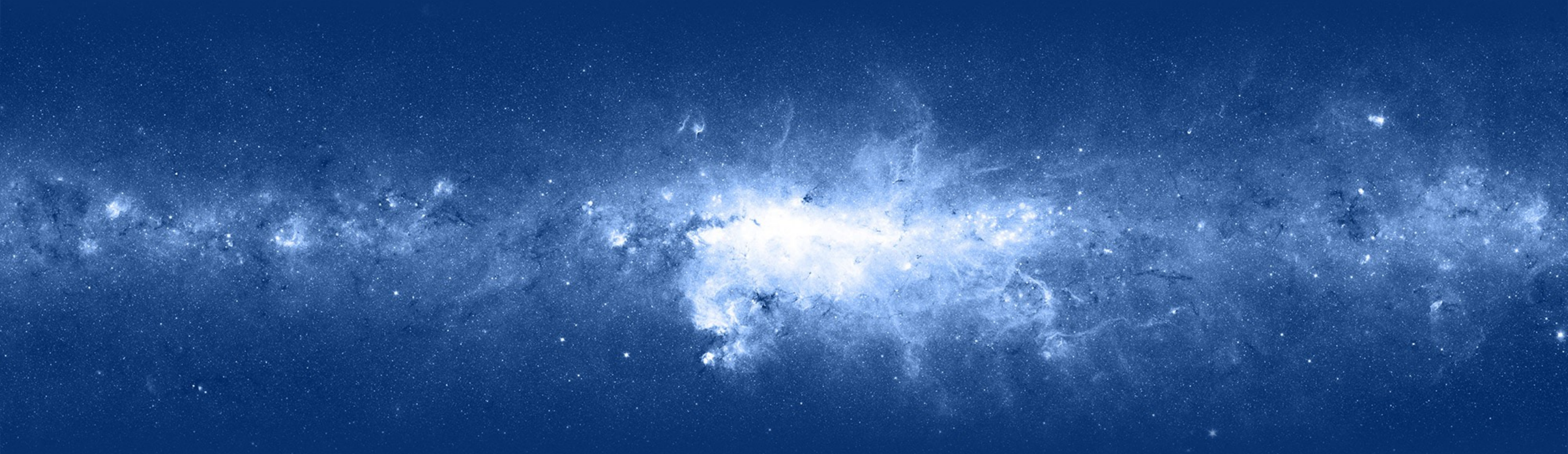


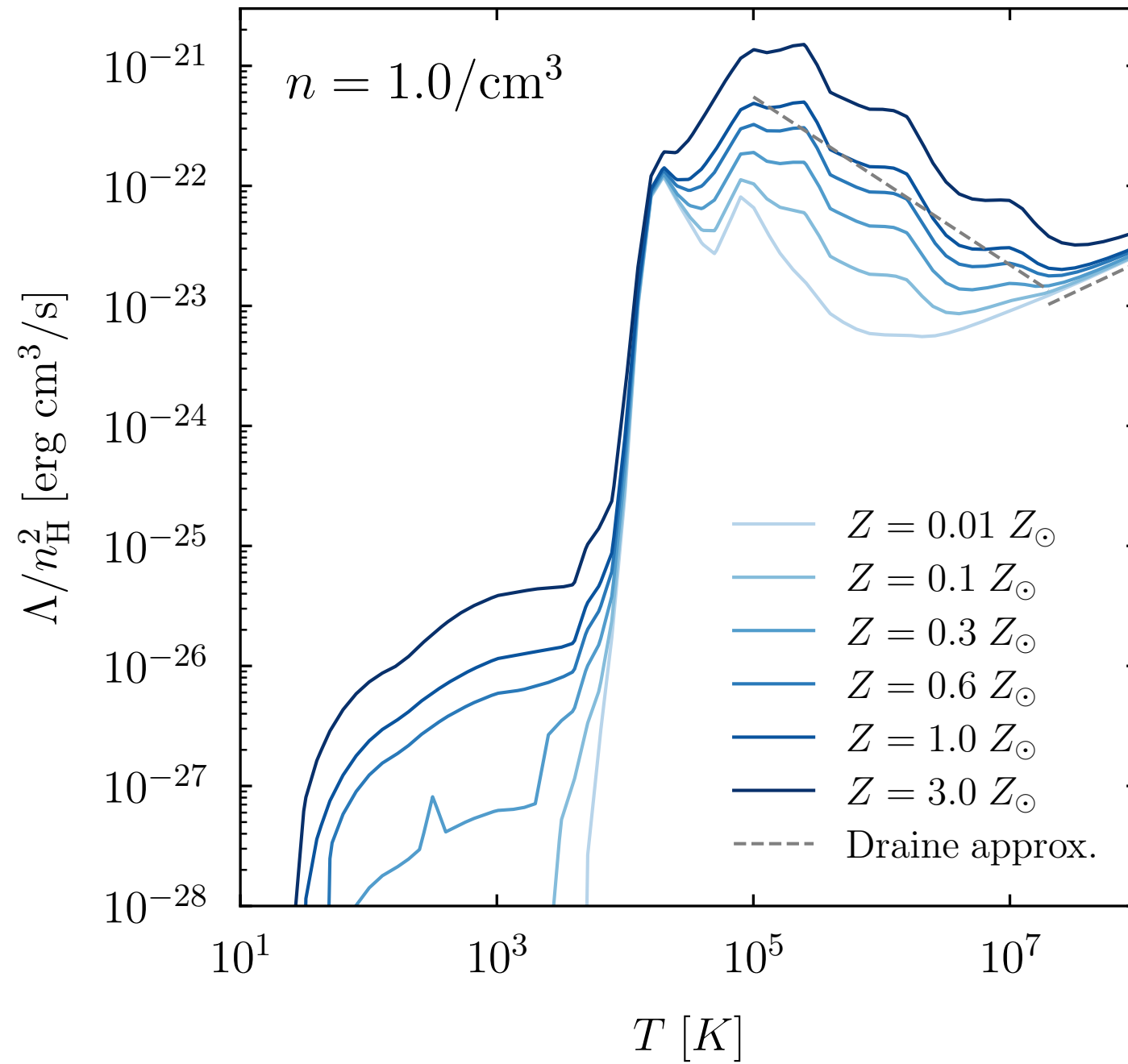
ASTR 670: Interstellar medium and gas dynamics

Prof. Benedikt Diemer

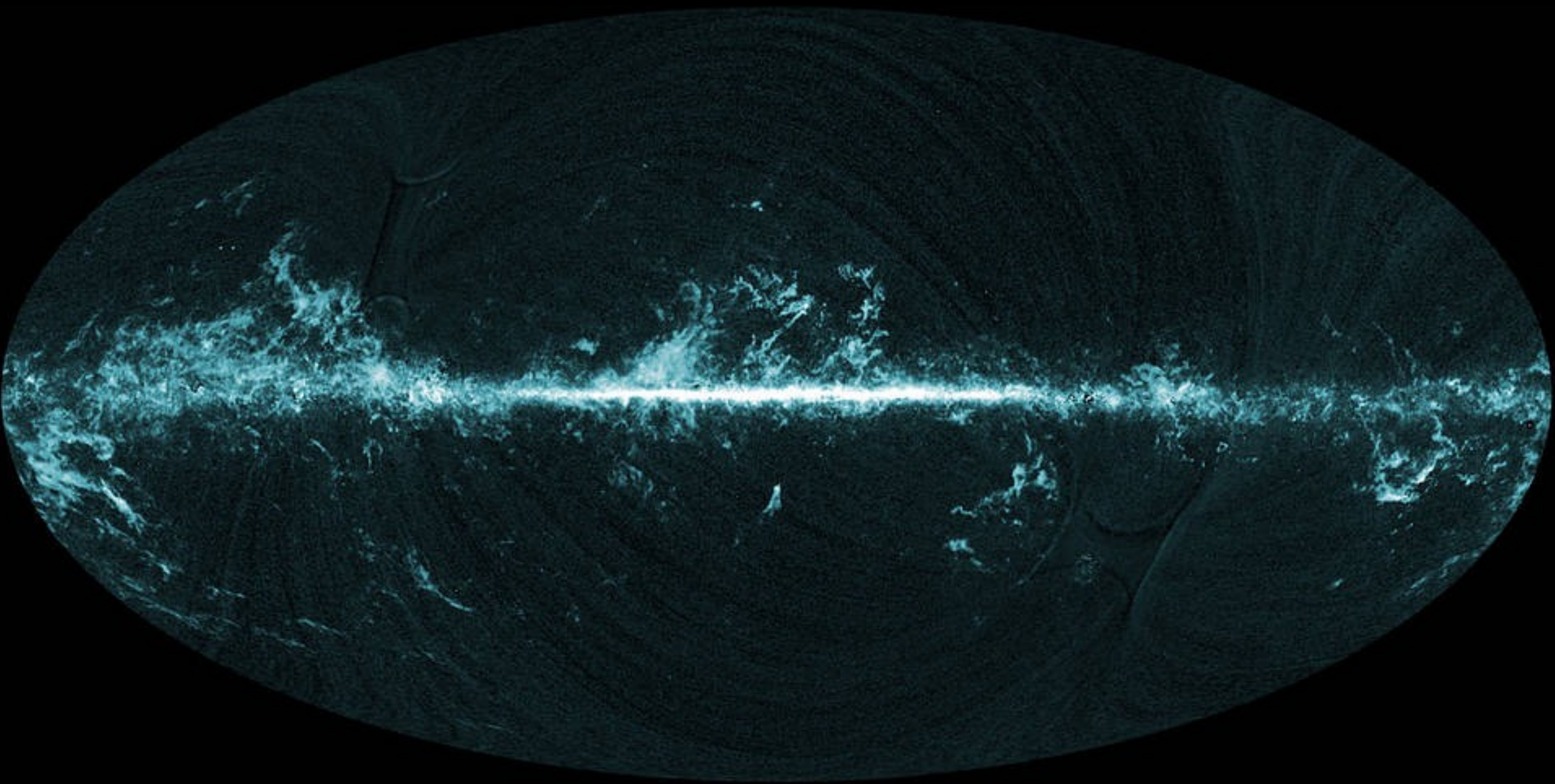


Chapter 7 • Atomic physics III: Molecules

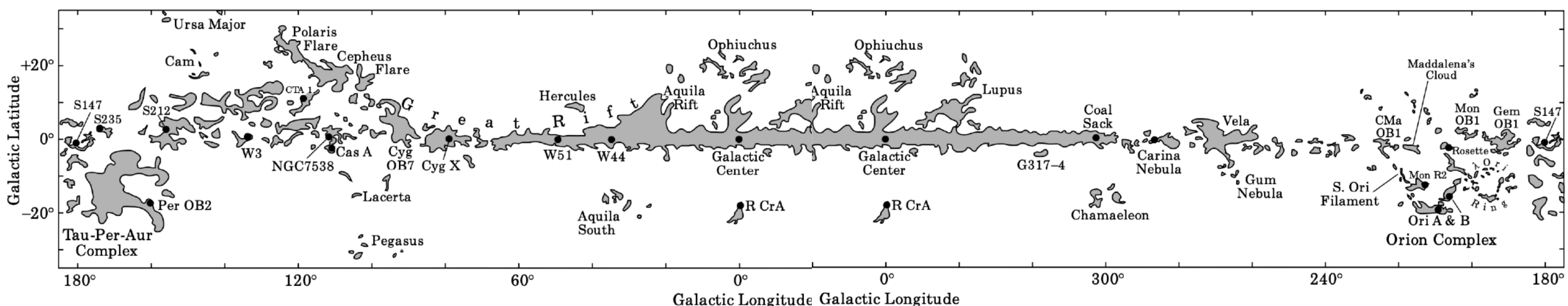
Recap: Cooling curves



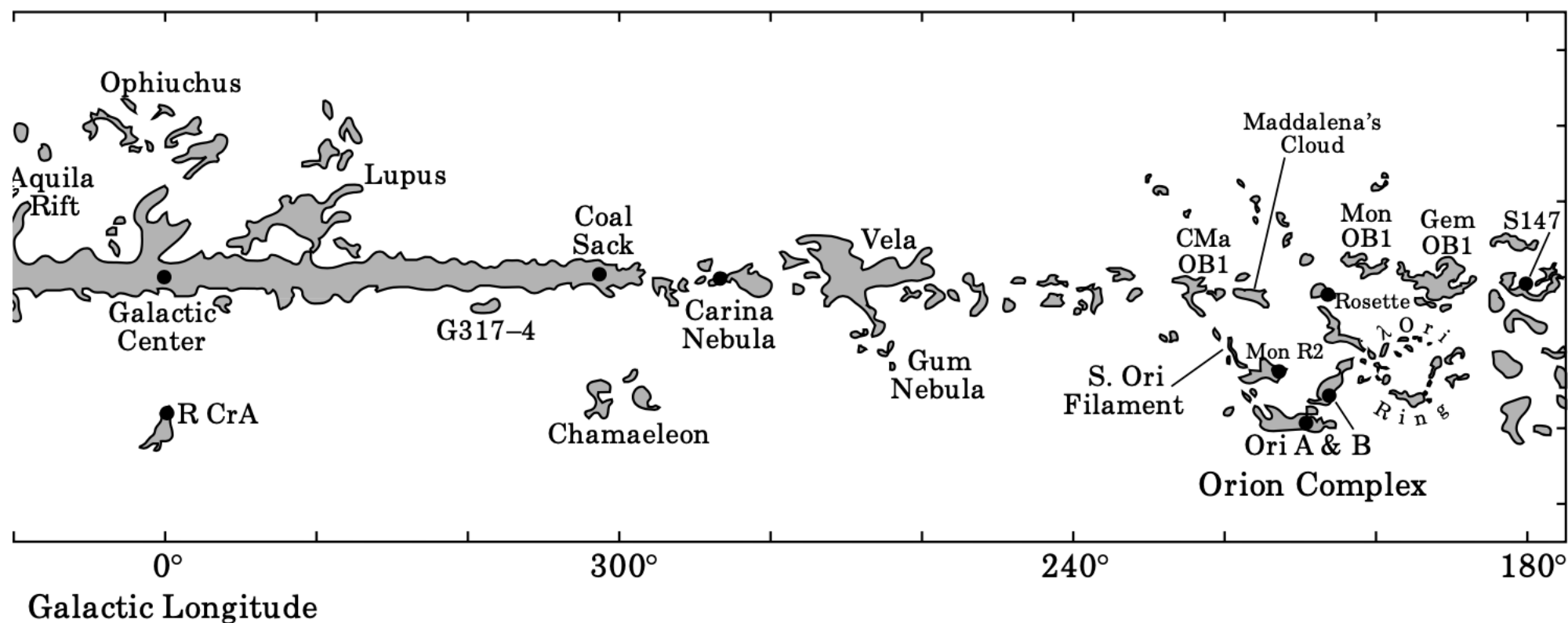
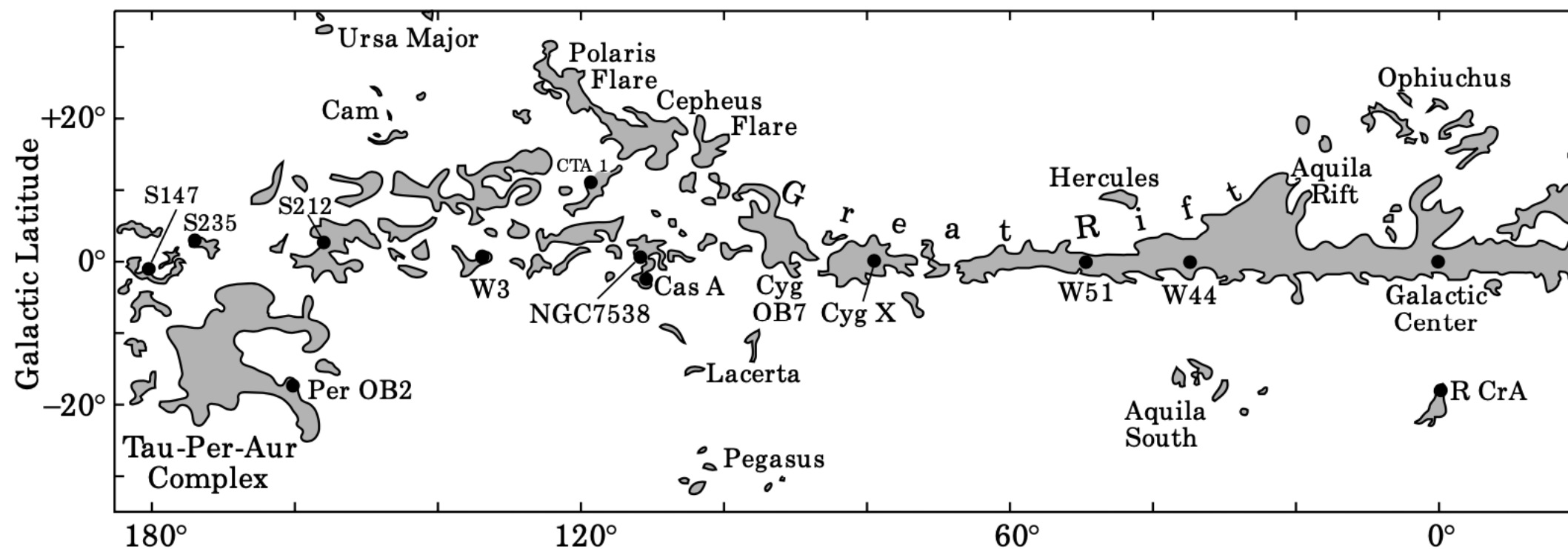
Molecular gas (CO)



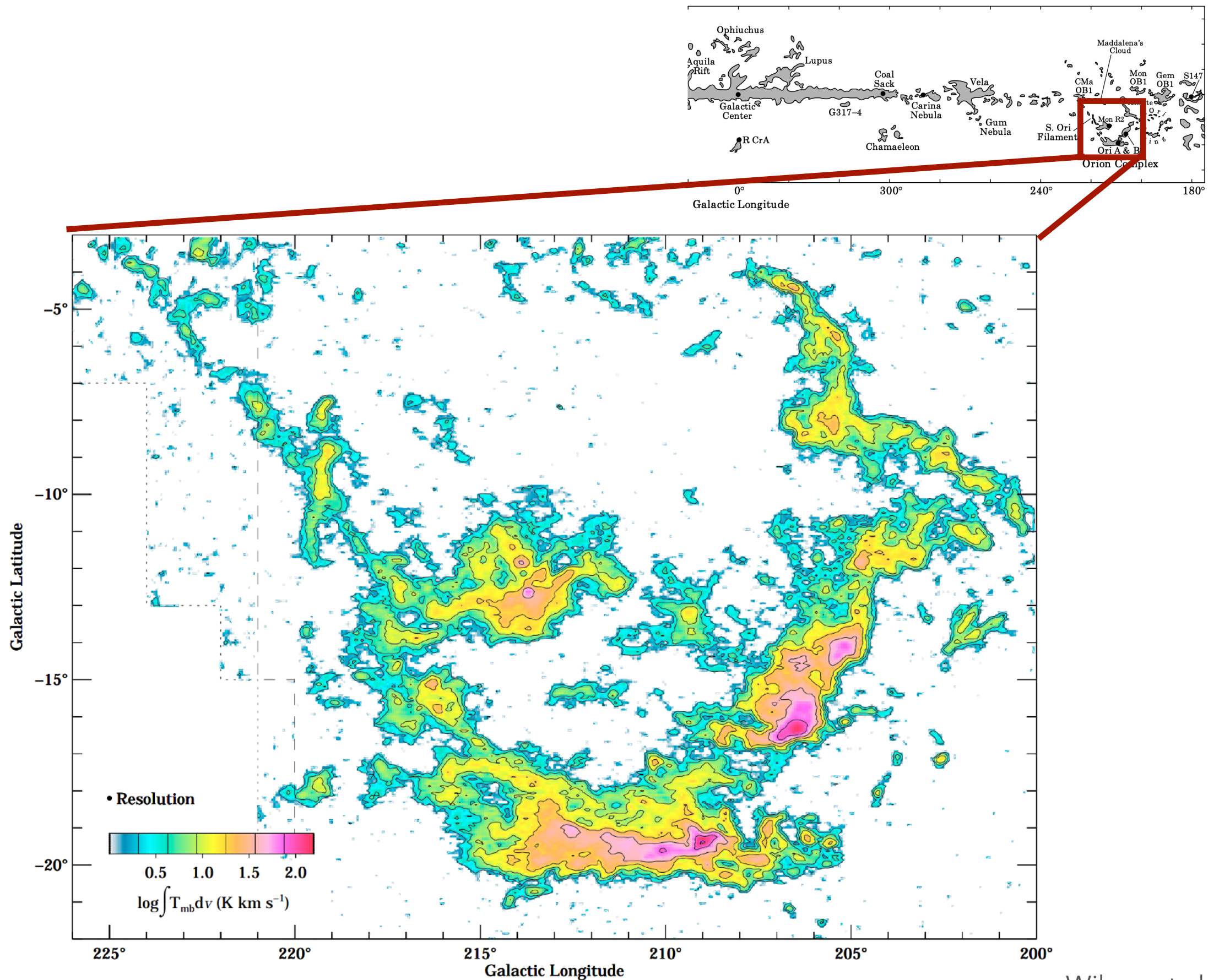
Molecular clouds in the Milky Way



Molecular clouds in the Milky Way

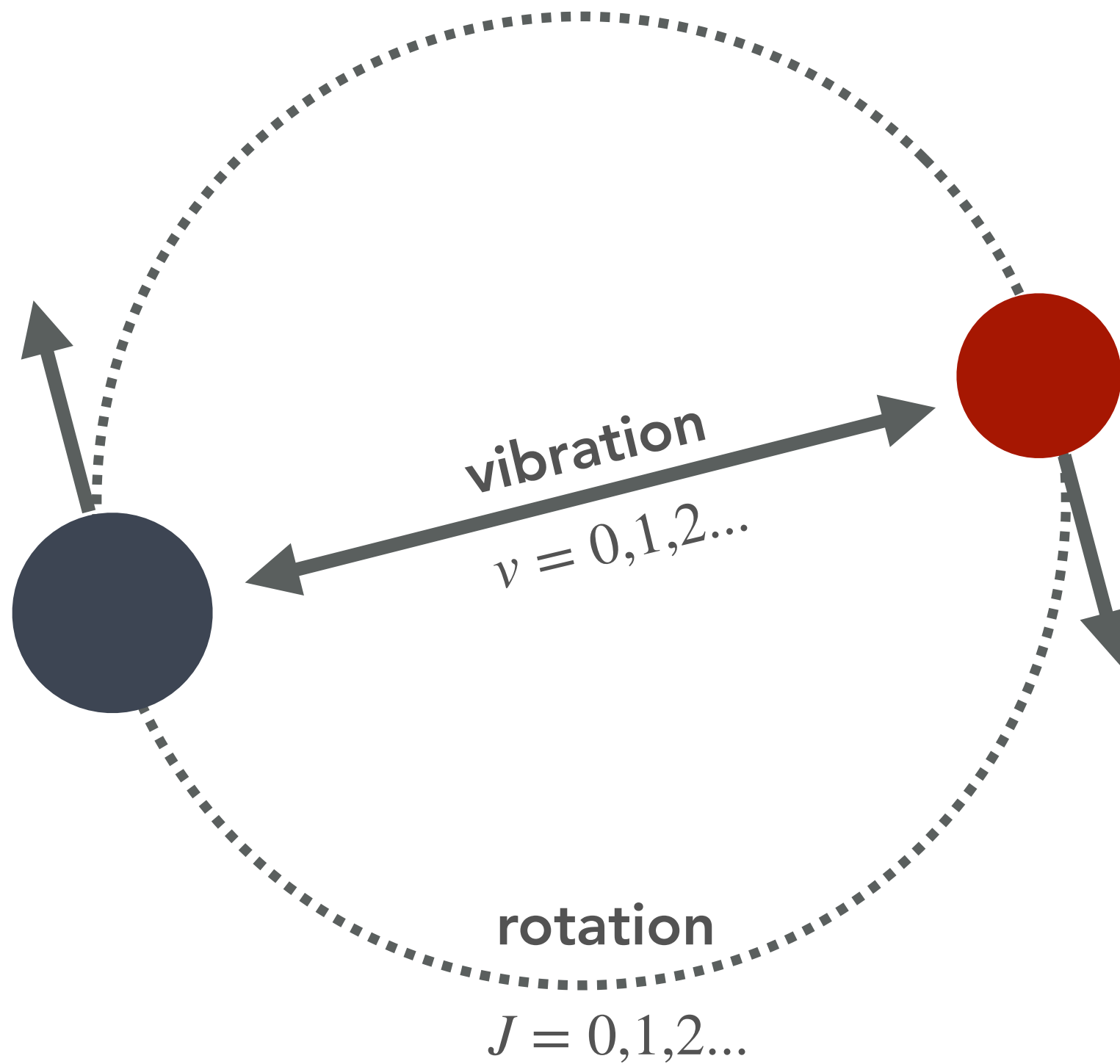


Molecular clouds in the Milky Way

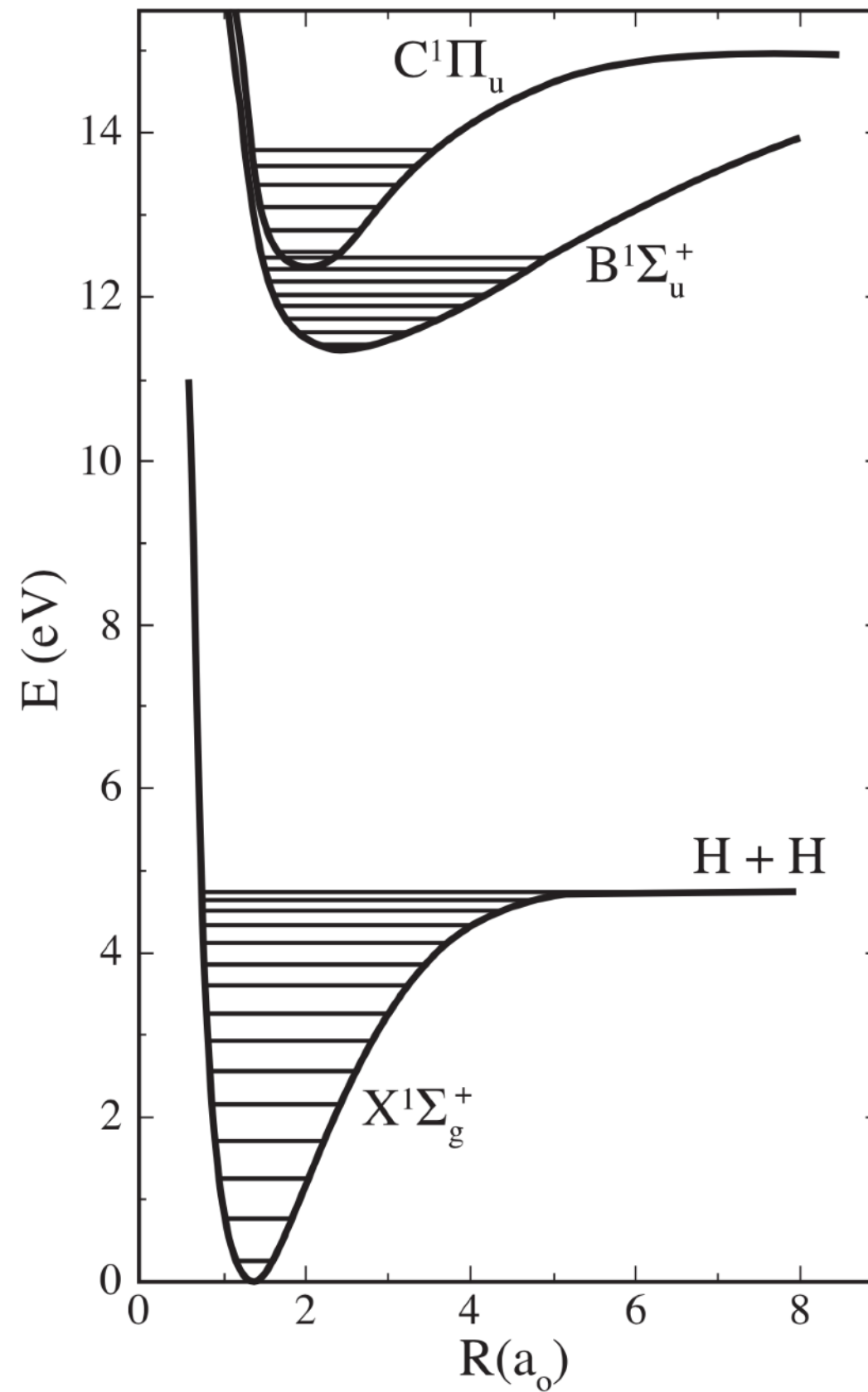


§7.1 • Vibrational and rotational energy levels

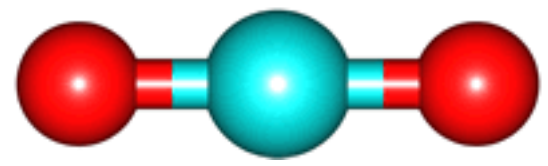
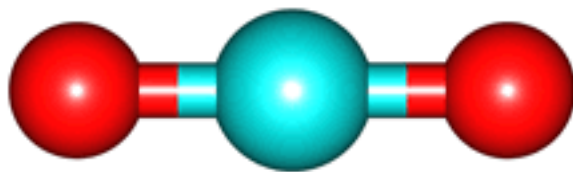
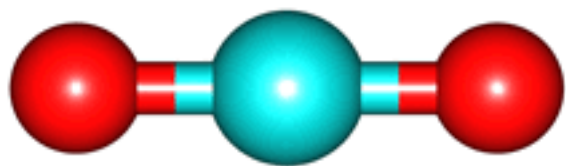
Energy levels



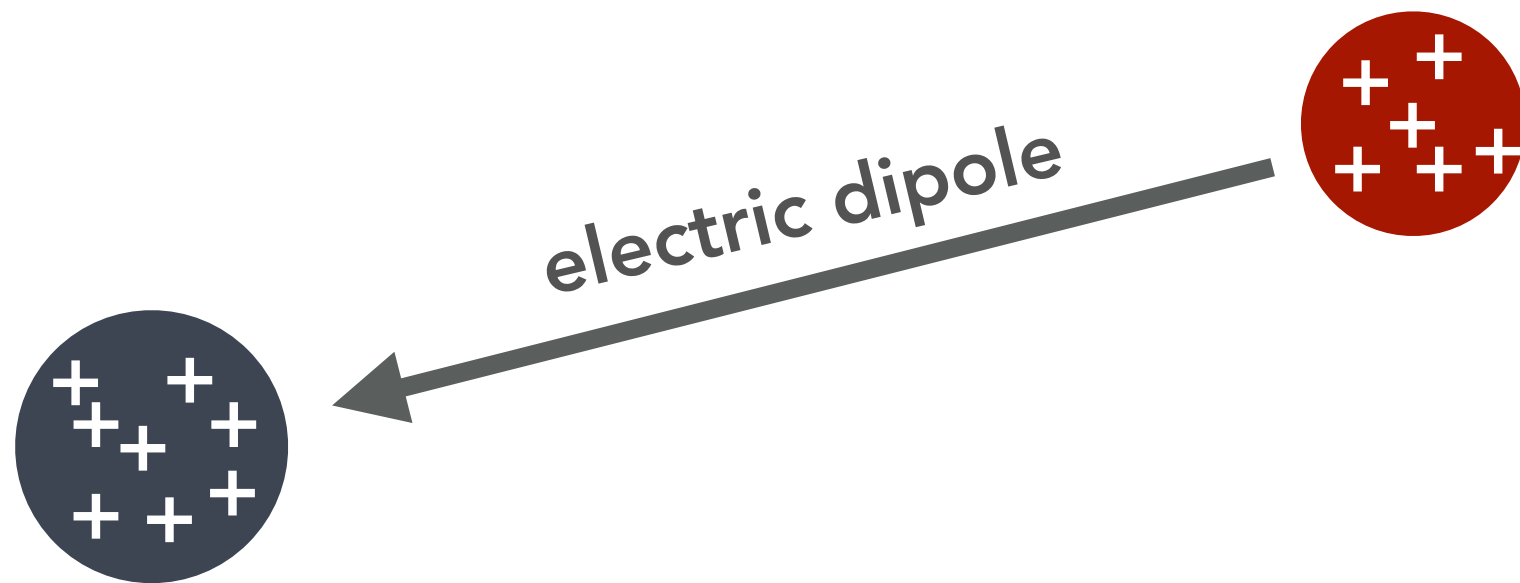
Potentials of H₂ molecule



Molecules with more atoms

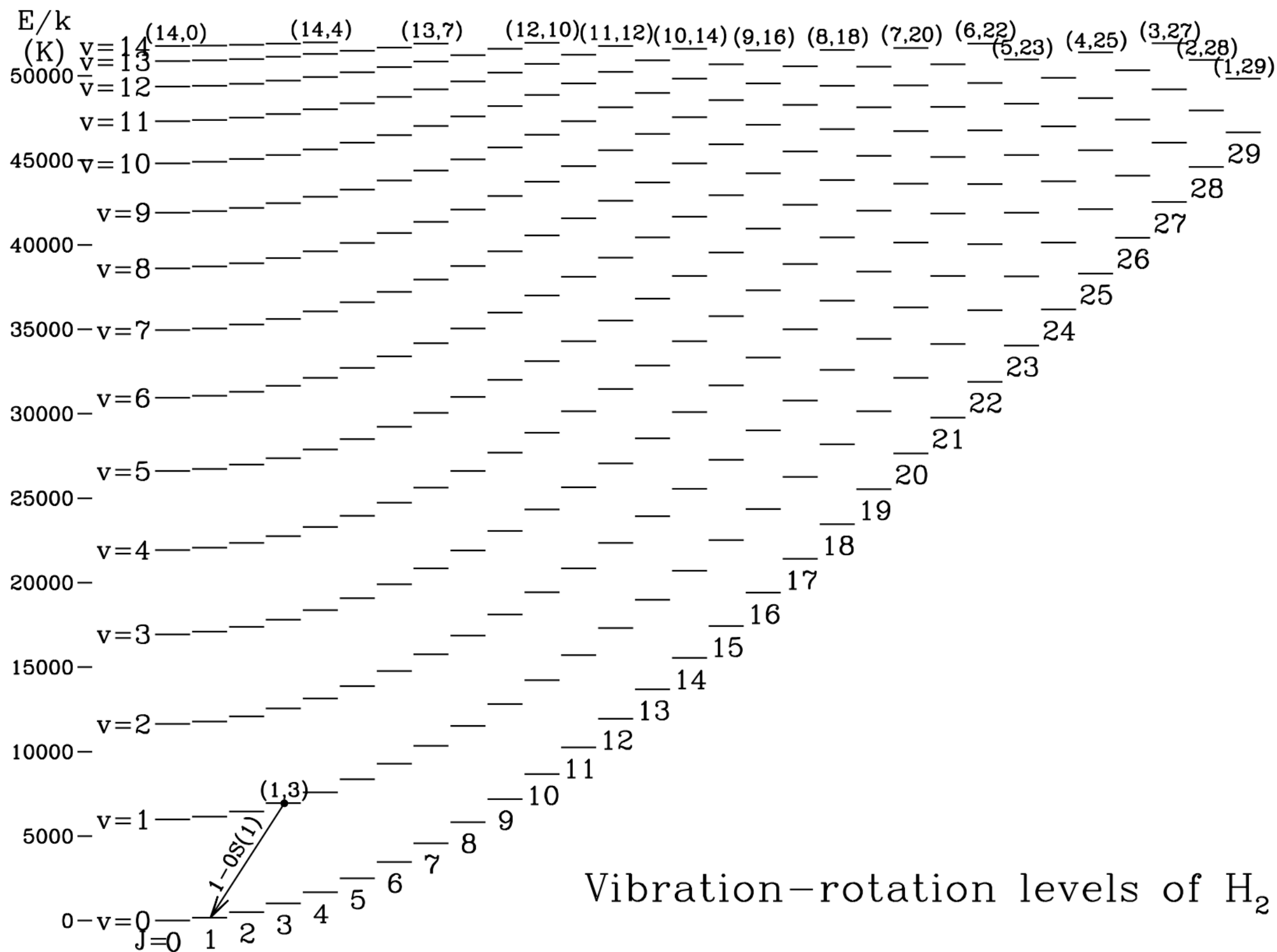


Electric dipole



§7.2 • Molecular Hydrogen (H₂)

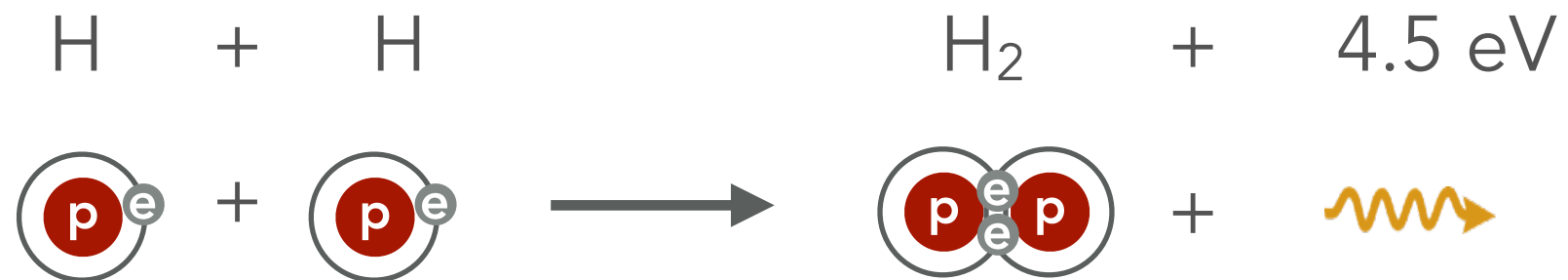
Energy levels of molecules



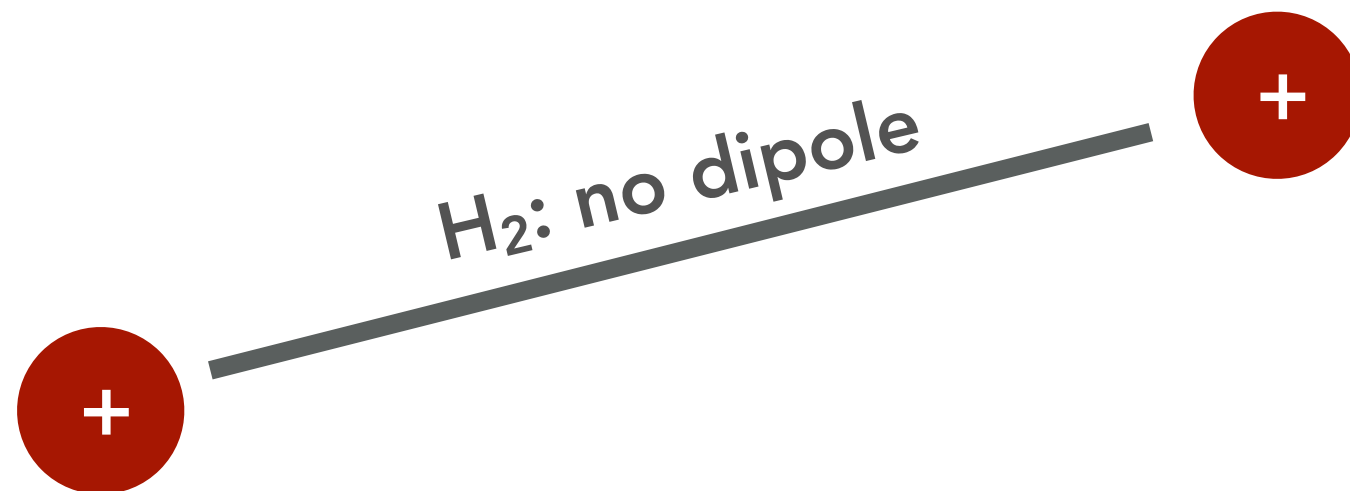
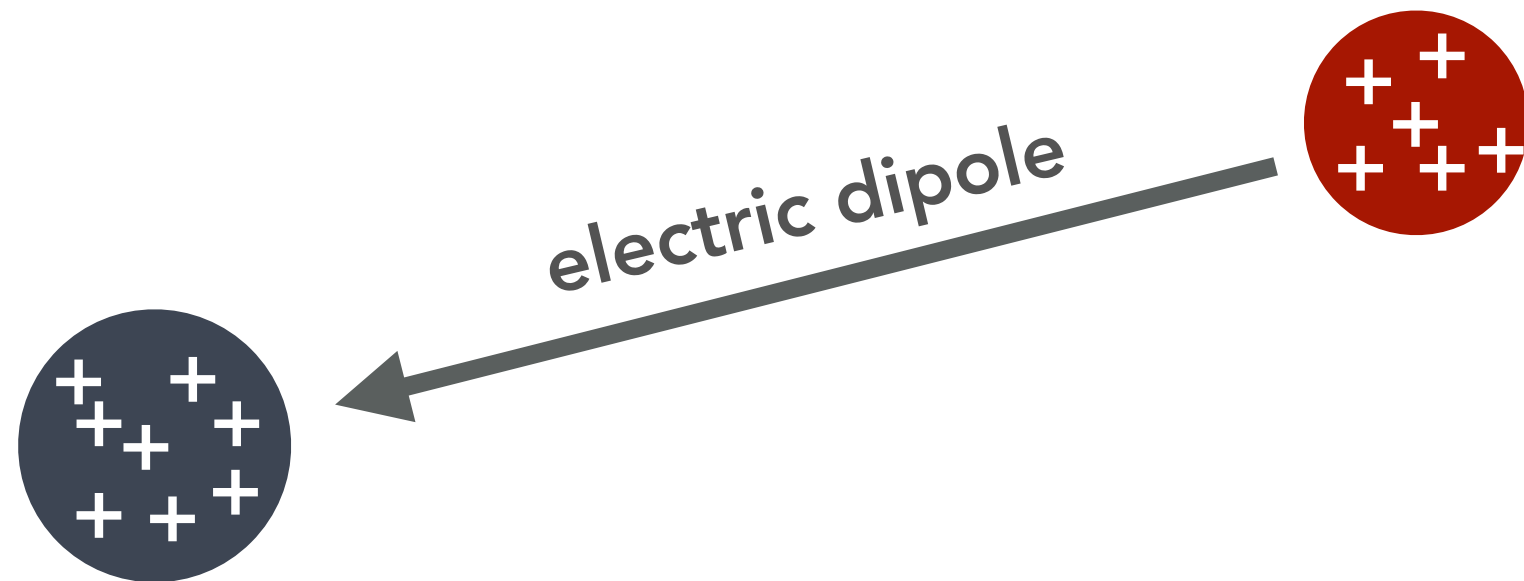
Vibration-rotation levels of H_2

H₂ formation

In principle:

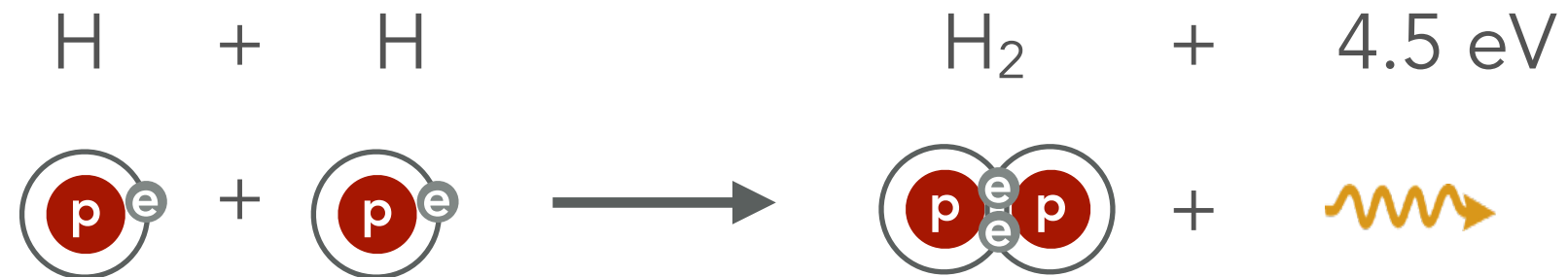


Electric dipole

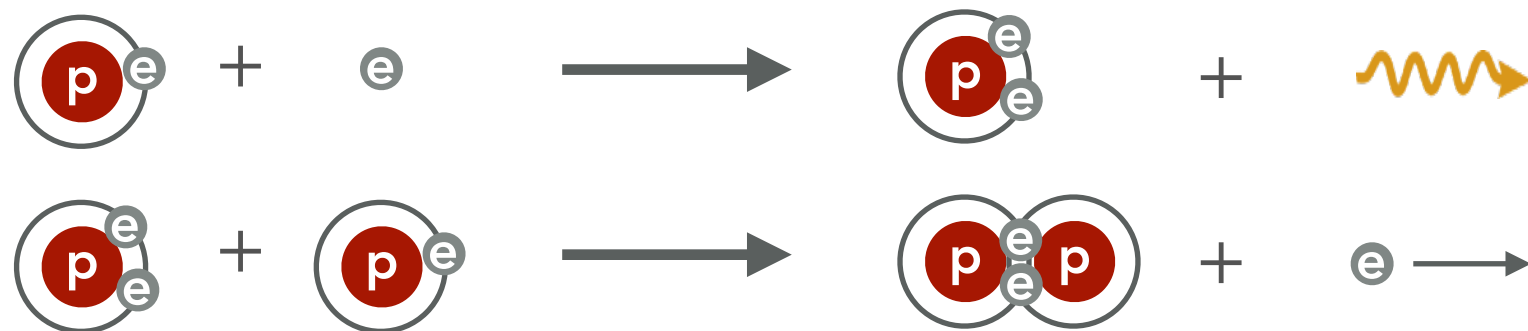
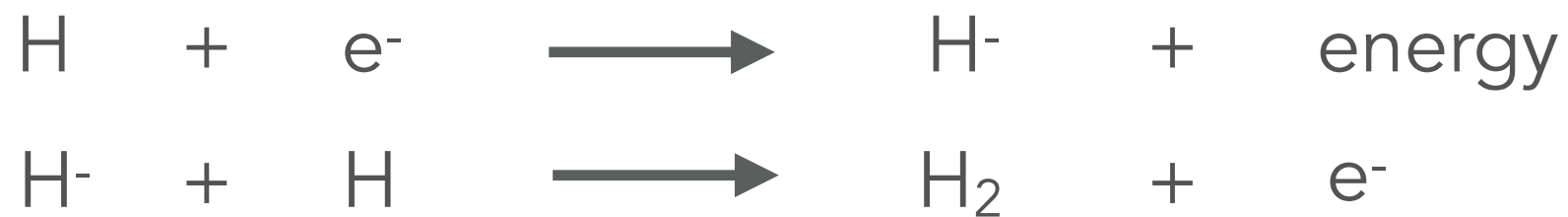


H₂ formation

In principle:



Associative detachment:



H₂ formation

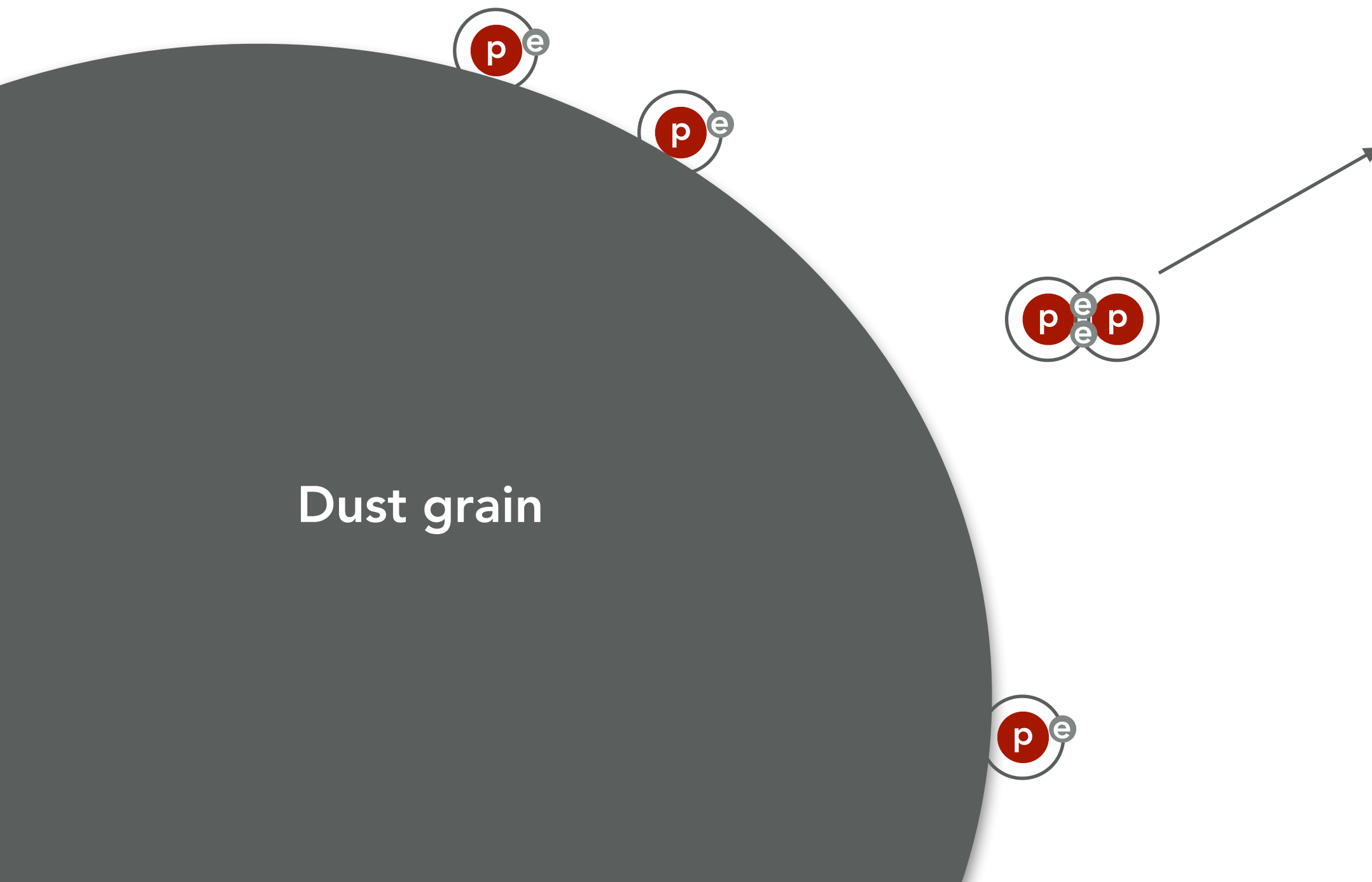


Photo-dissociation of H₂

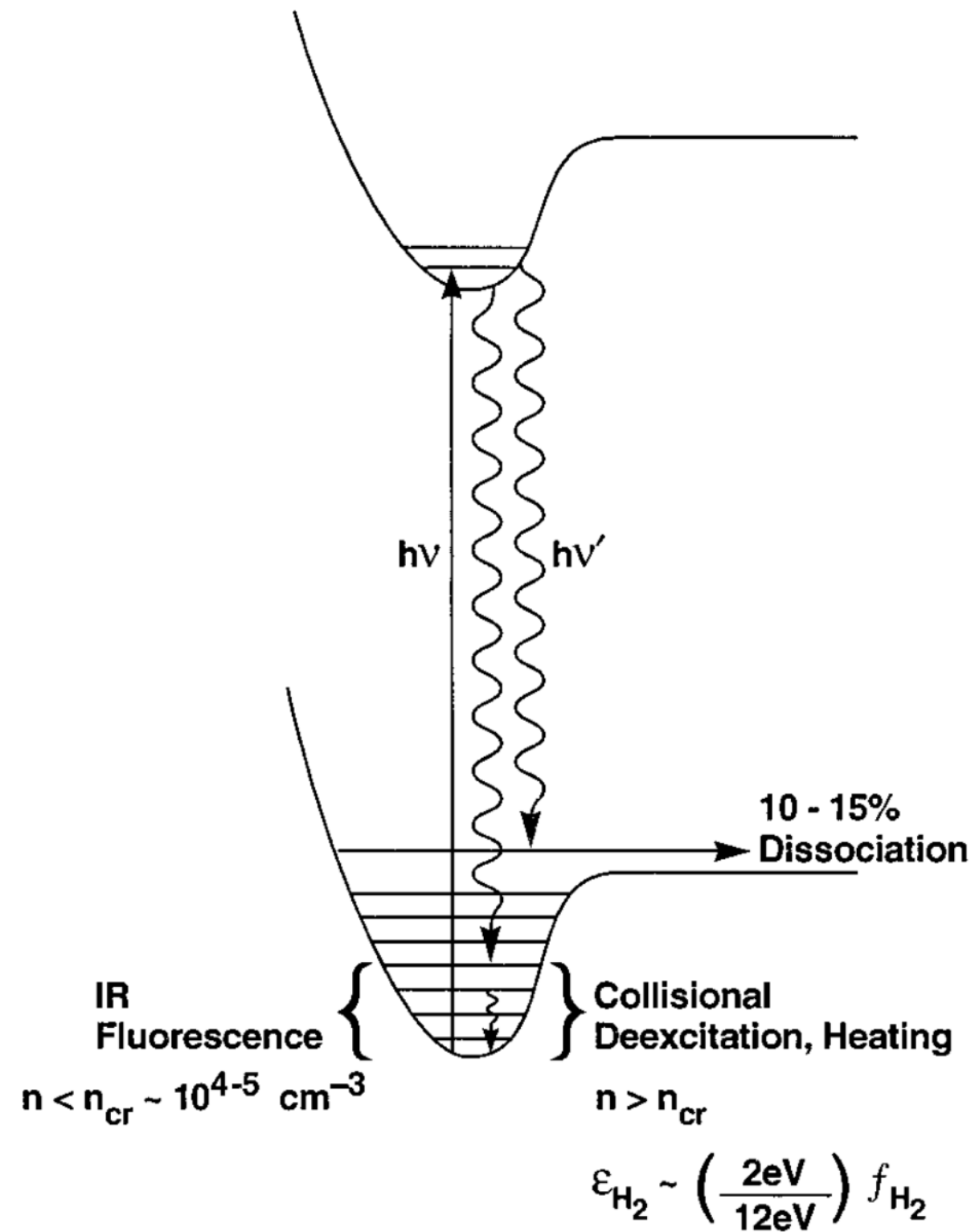


Photo-dissociation of H₂

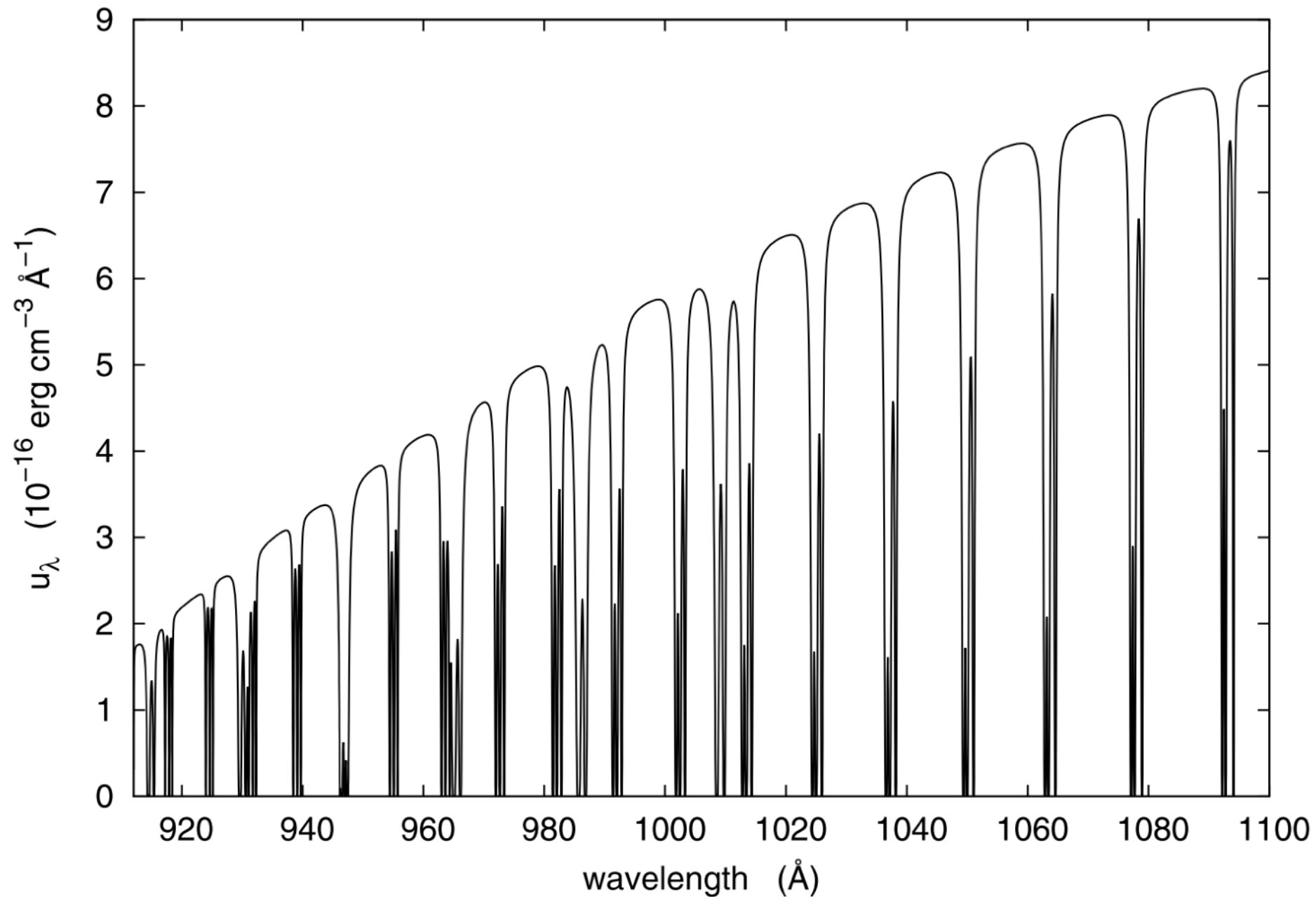
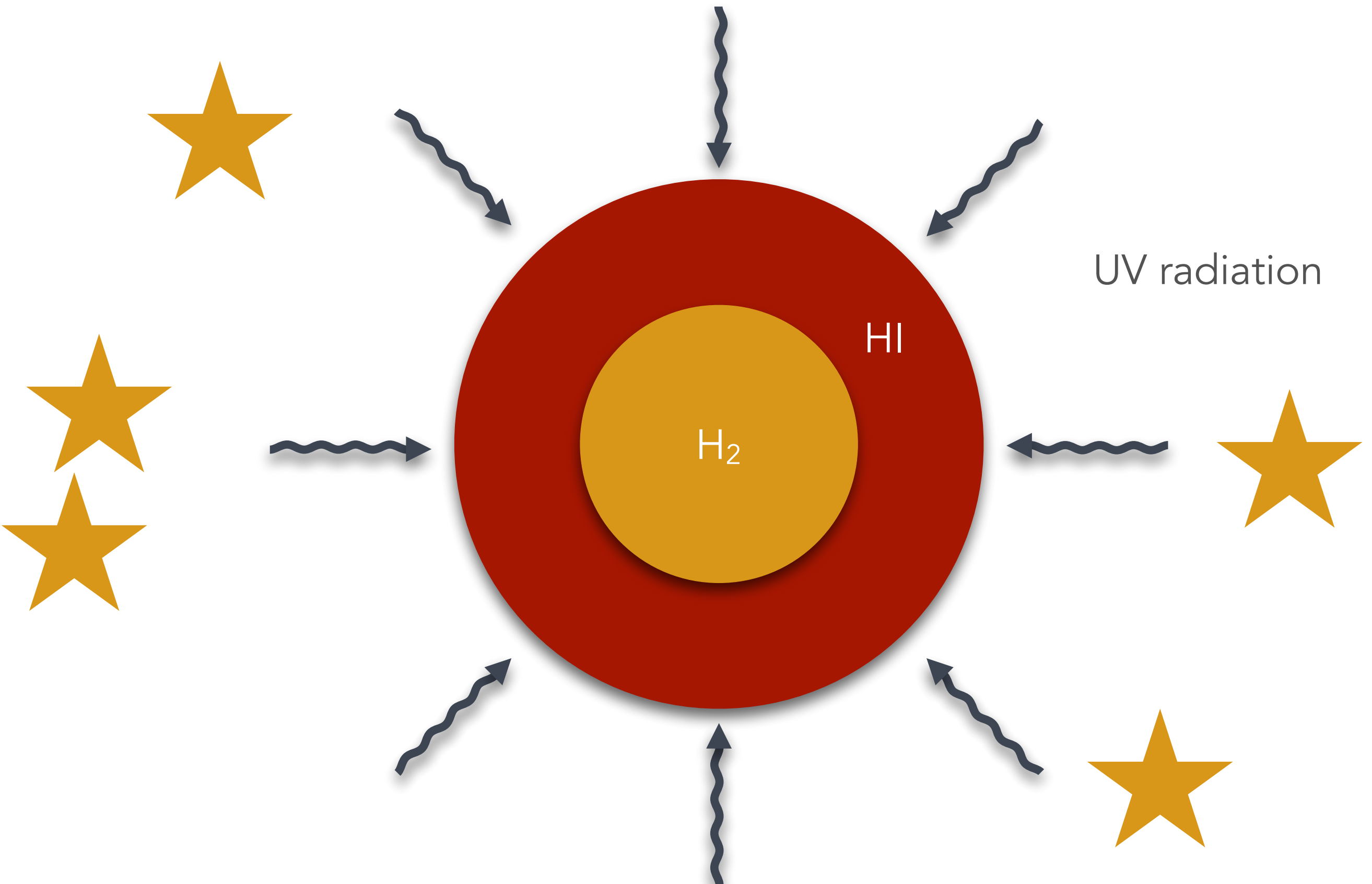
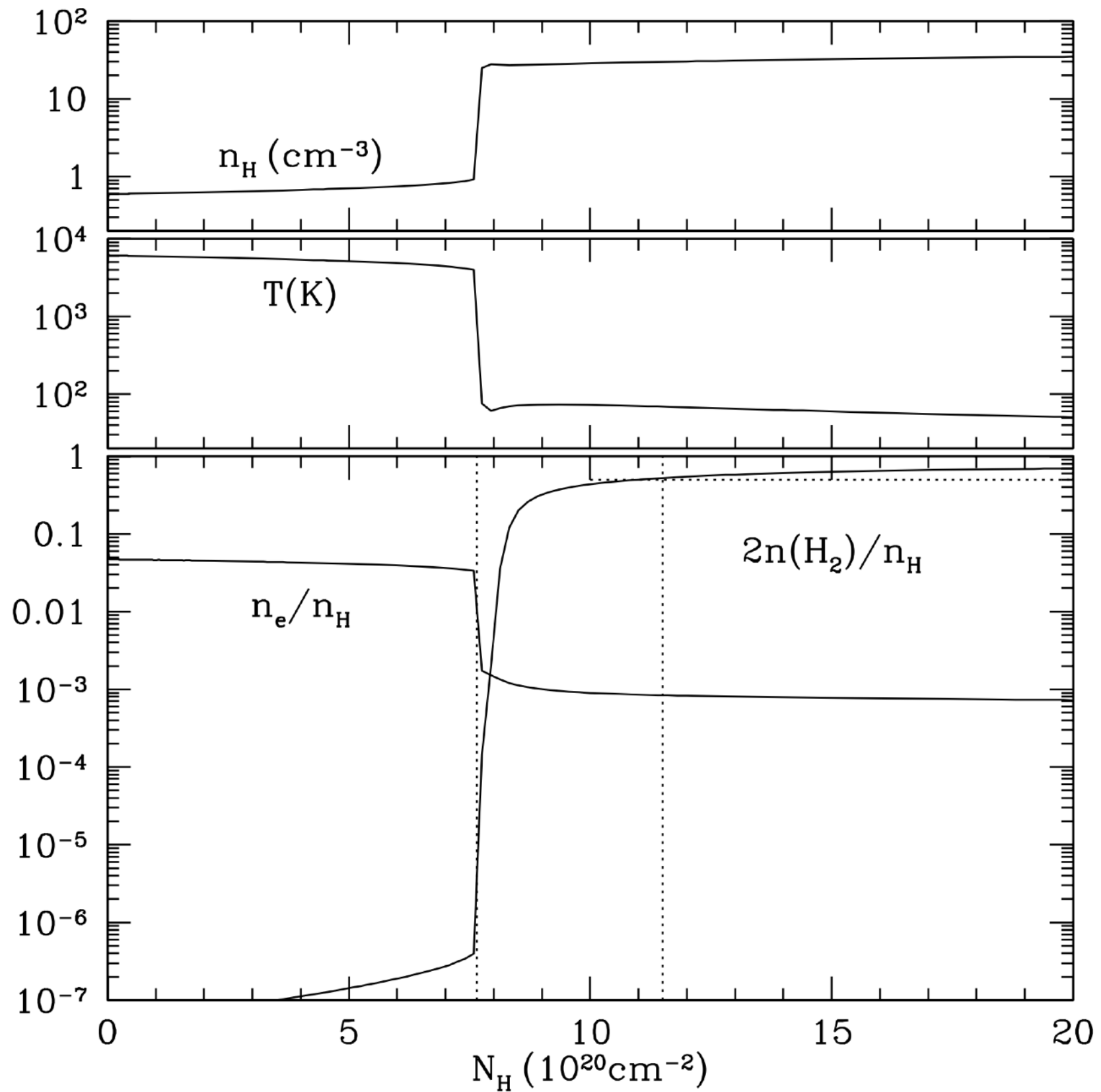


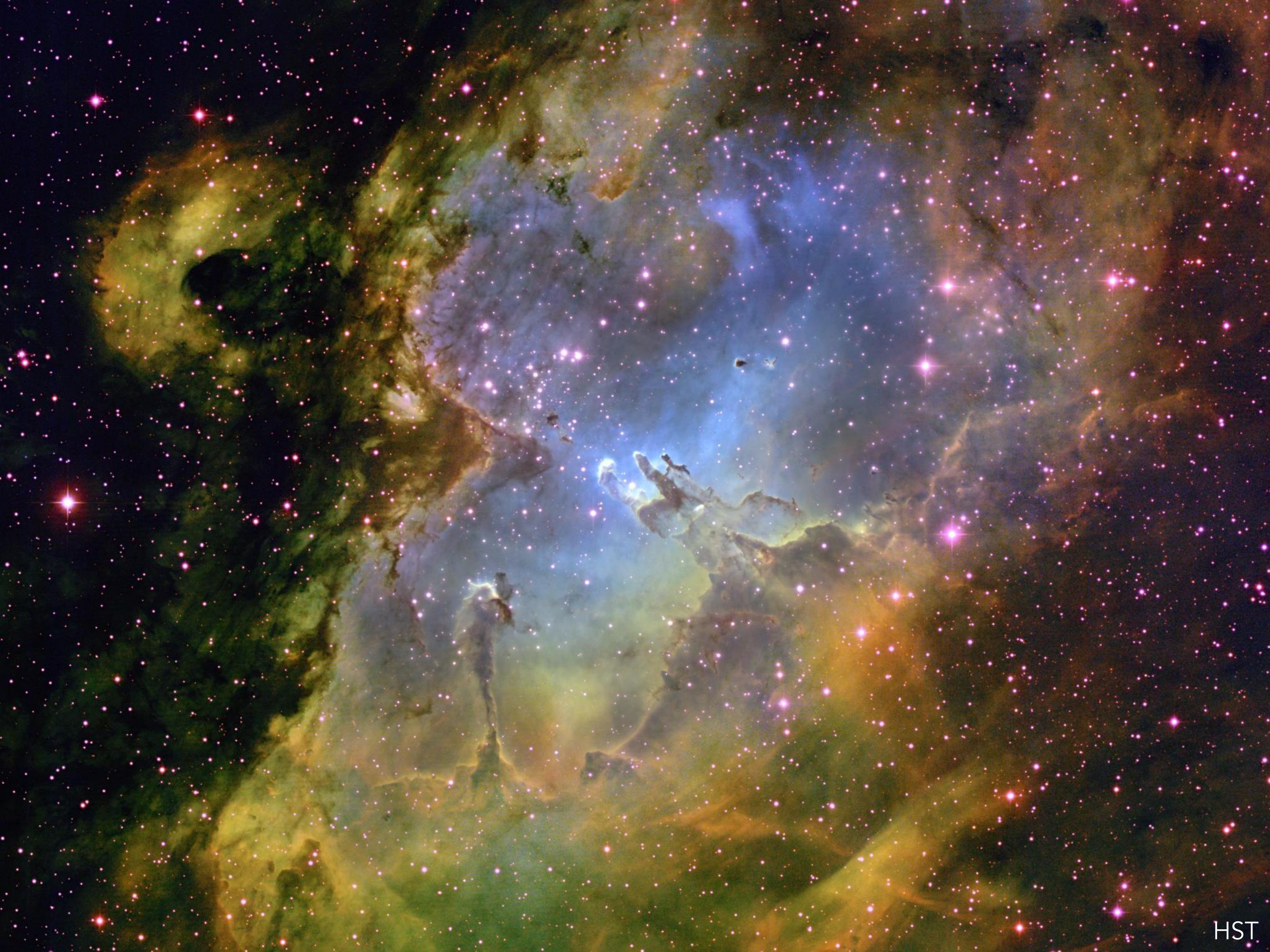
Figure 2. Absorbed far-UV spectrum showing partially overlapping Lyman–Werner band absorption lines, for beamed radiation into a cloud, at a total hydrogen gas column density of $3.74 \times 10^{20} \text{ cm}^{-2}$, for a free-space radiation intensity $I_{\text{UV}} = 35.5$, gas density $n = 10^3 \text{ cm}^{-3}$, and metallicity $Z' = 1$ ($\alpha G/2 = 1$).

Model of molecular cloud

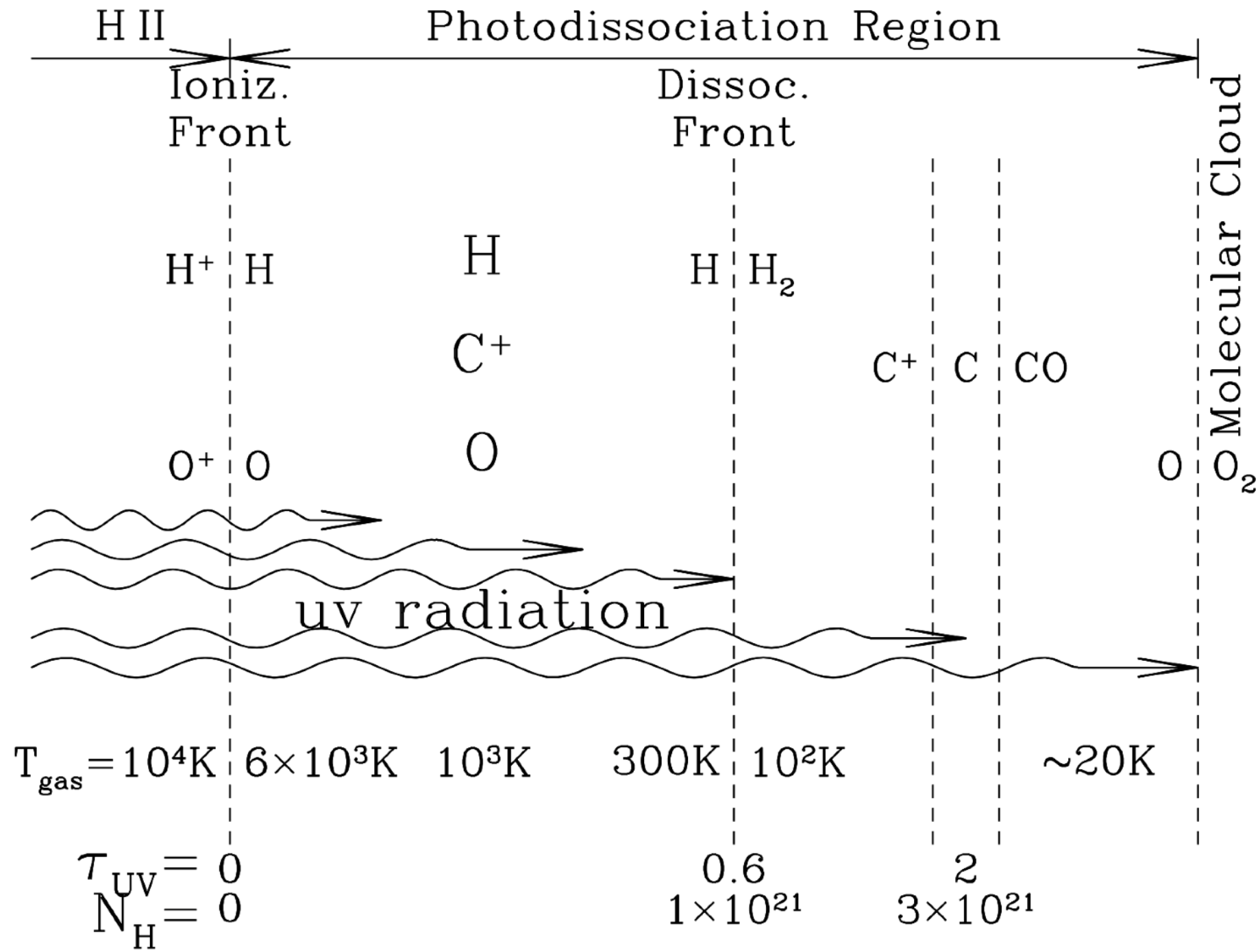


HI/H₂ transition

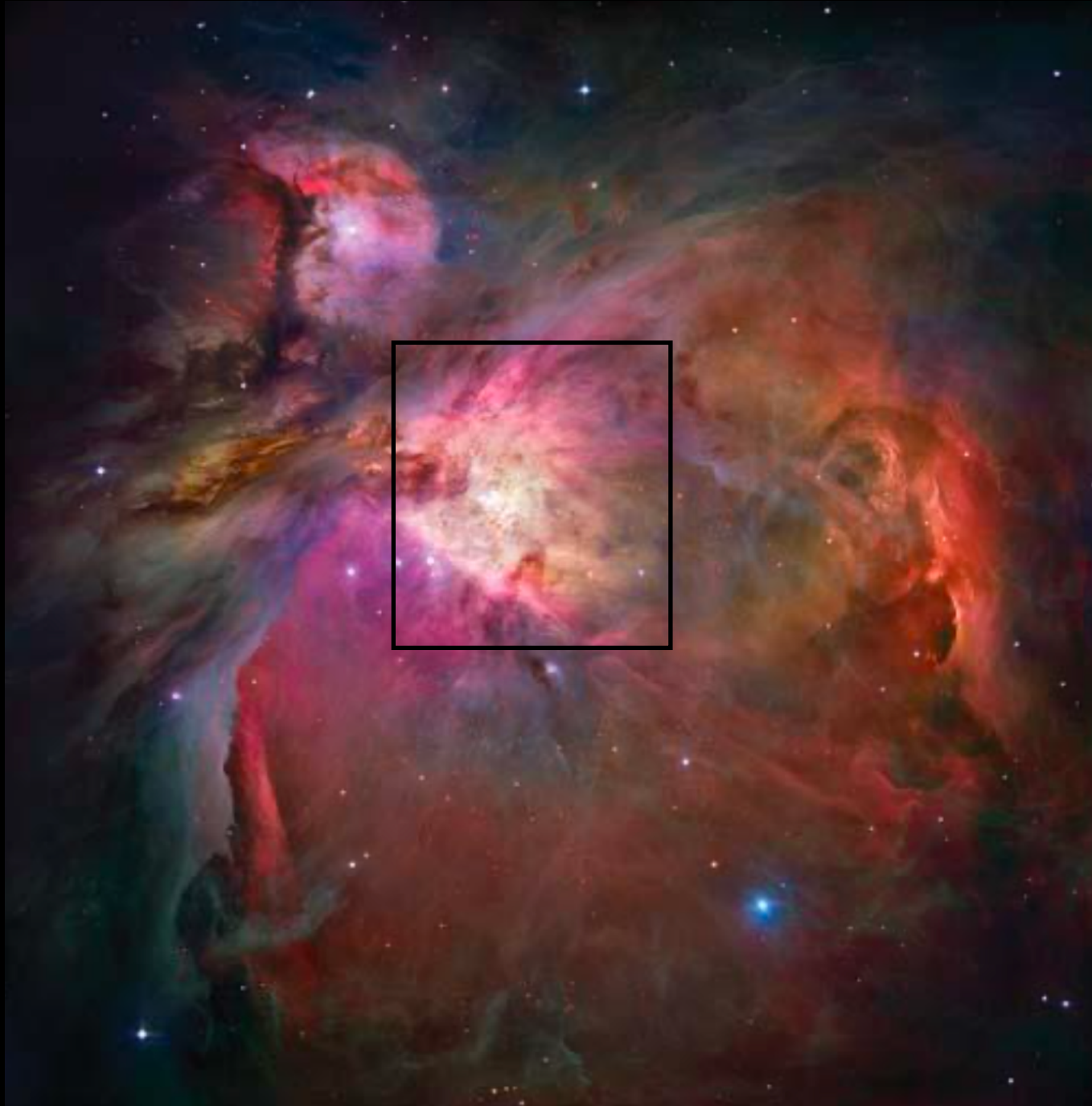




Photodissociation region

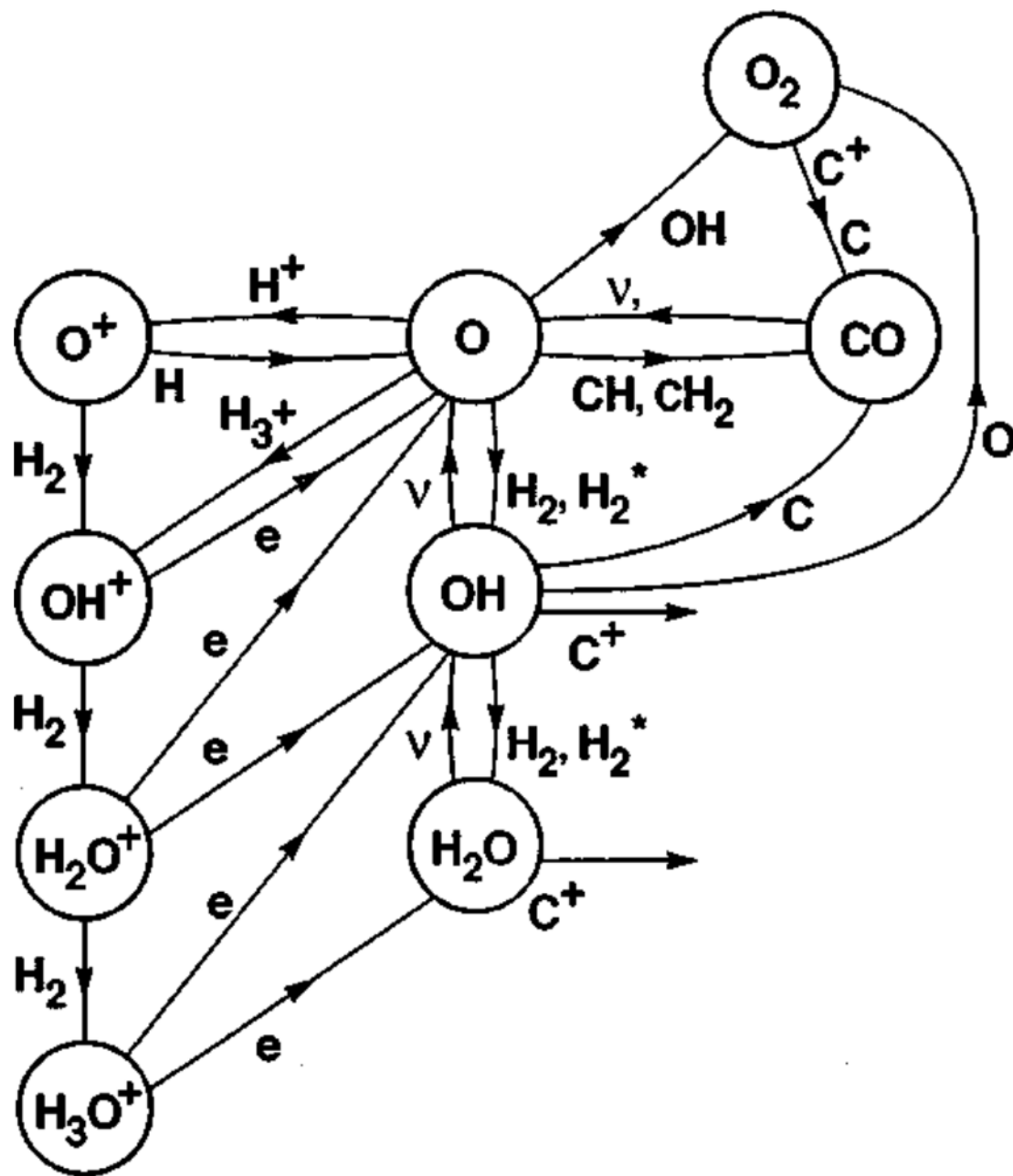


Orion nebula

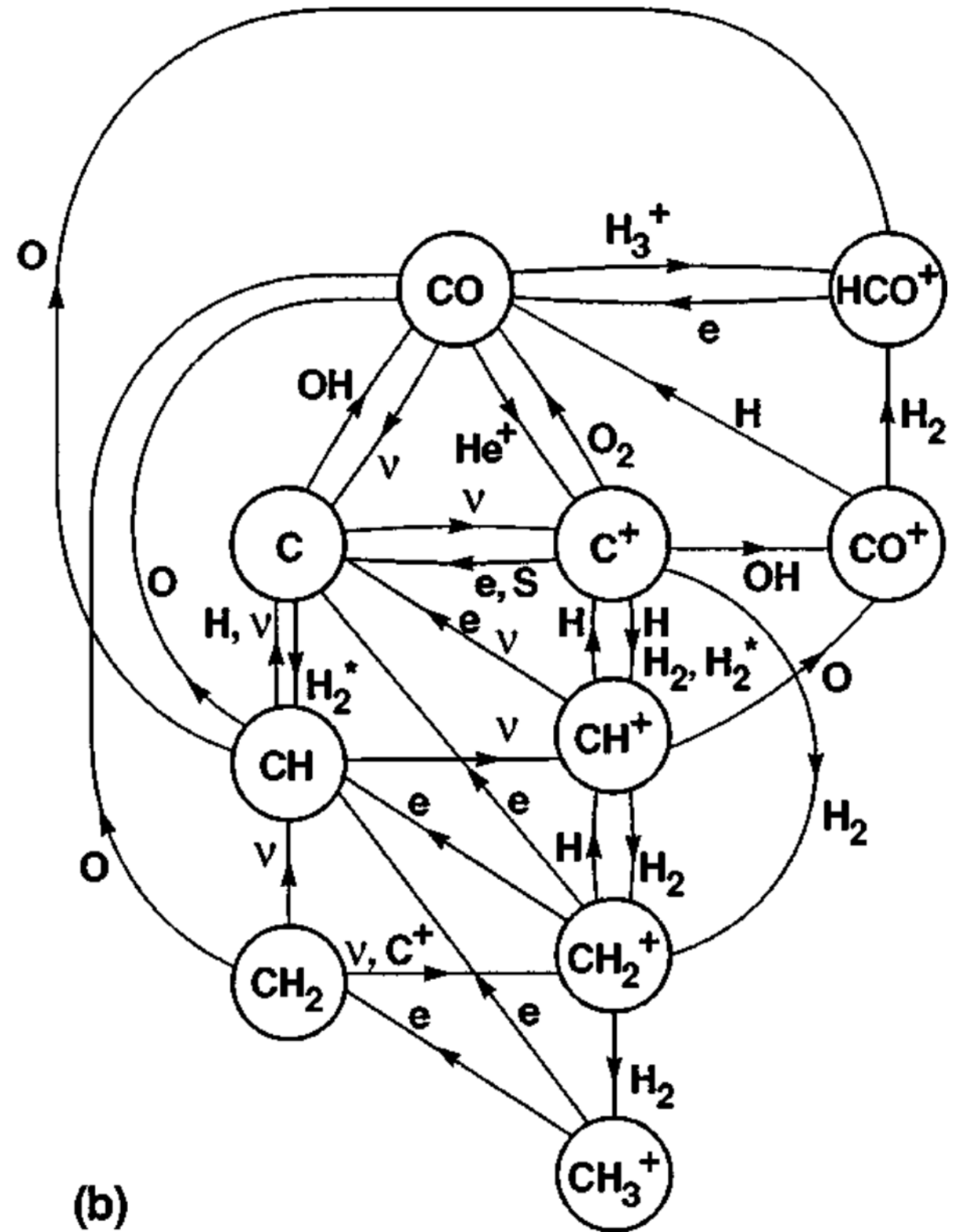


§7.3 • Carbon Monoxide (CO)

Pathways to CO

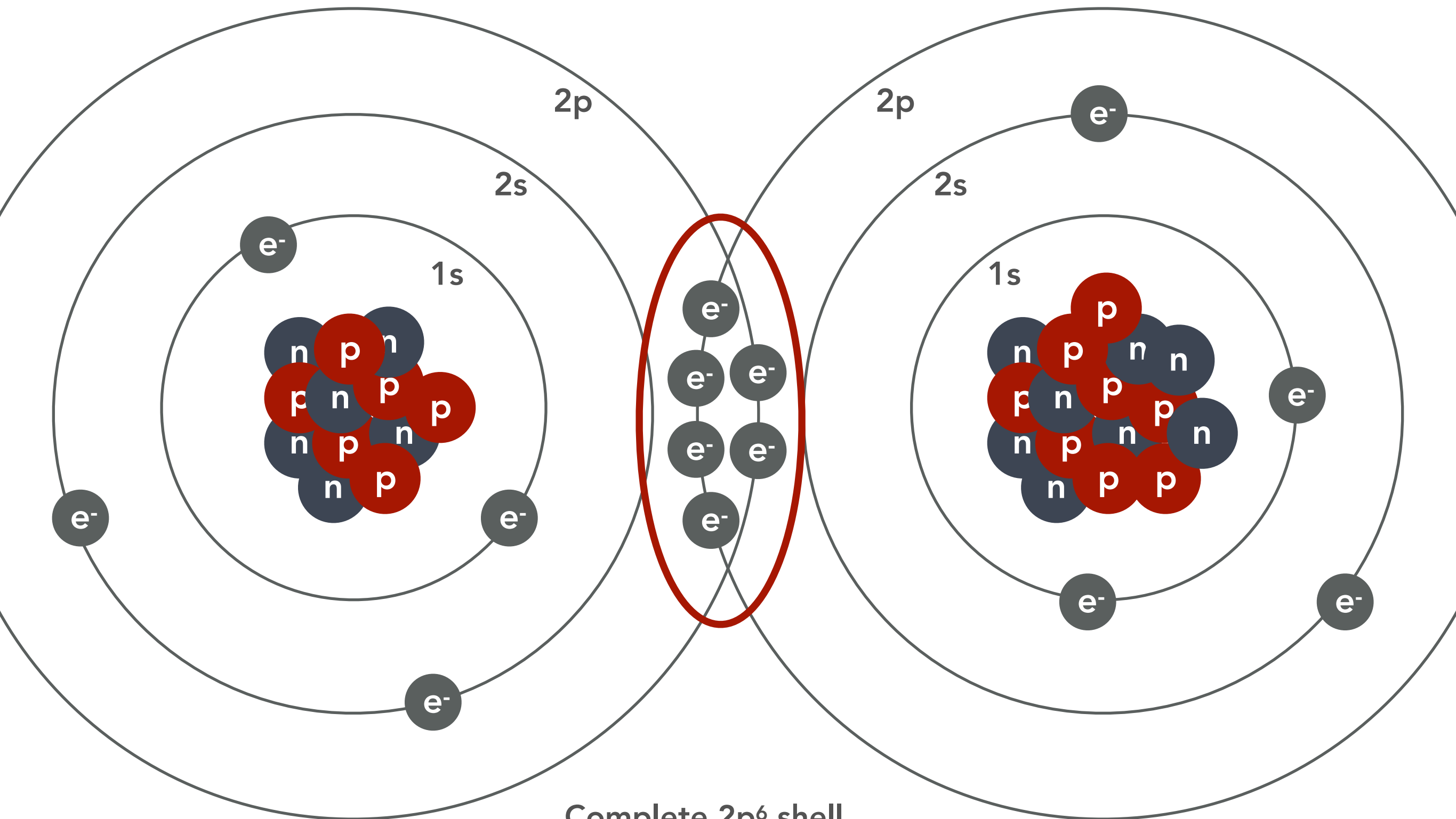


(a)



(b)

The CO molecule

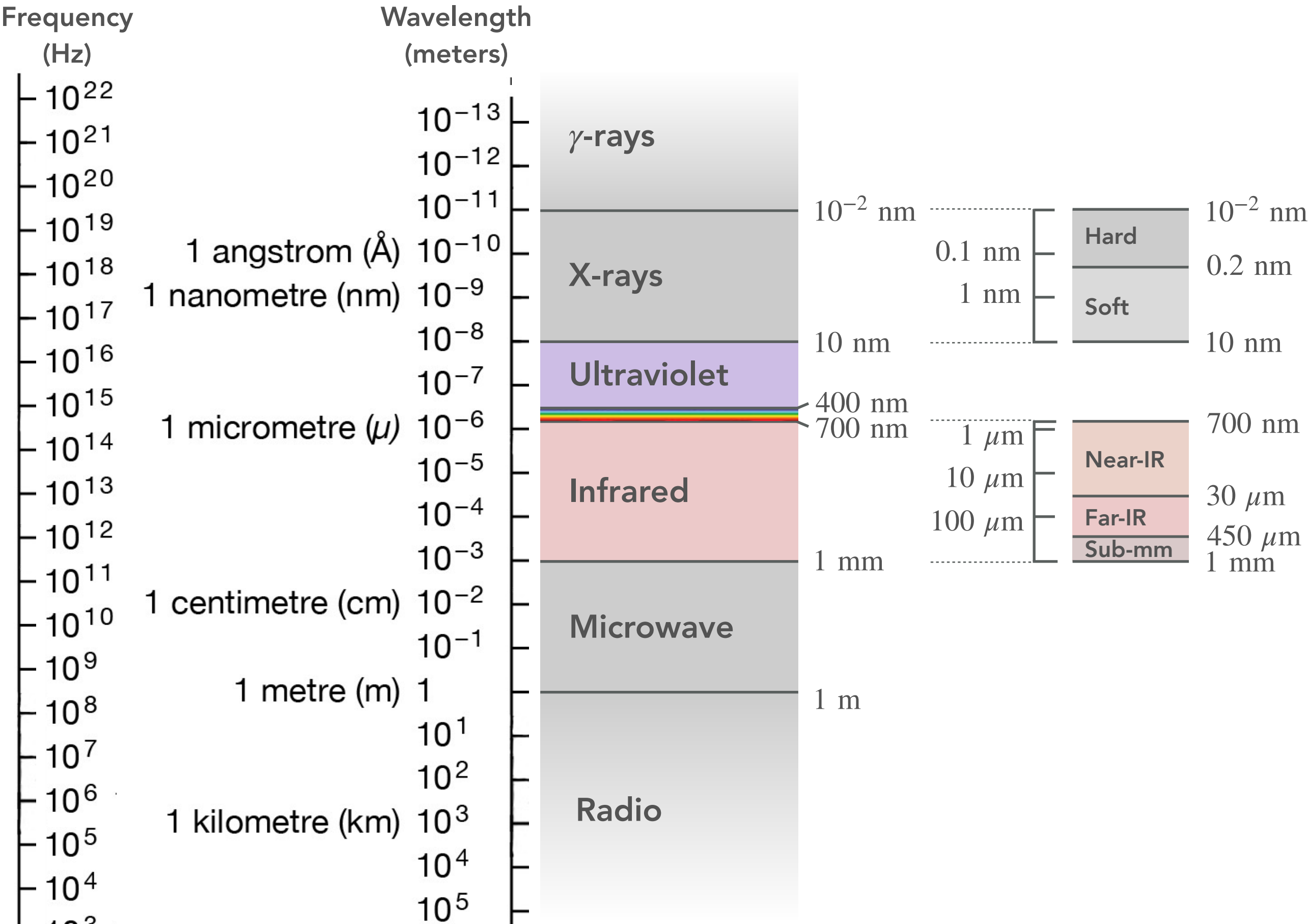


Carbon ground state:
 $1s^2 2s^2 2p^2$

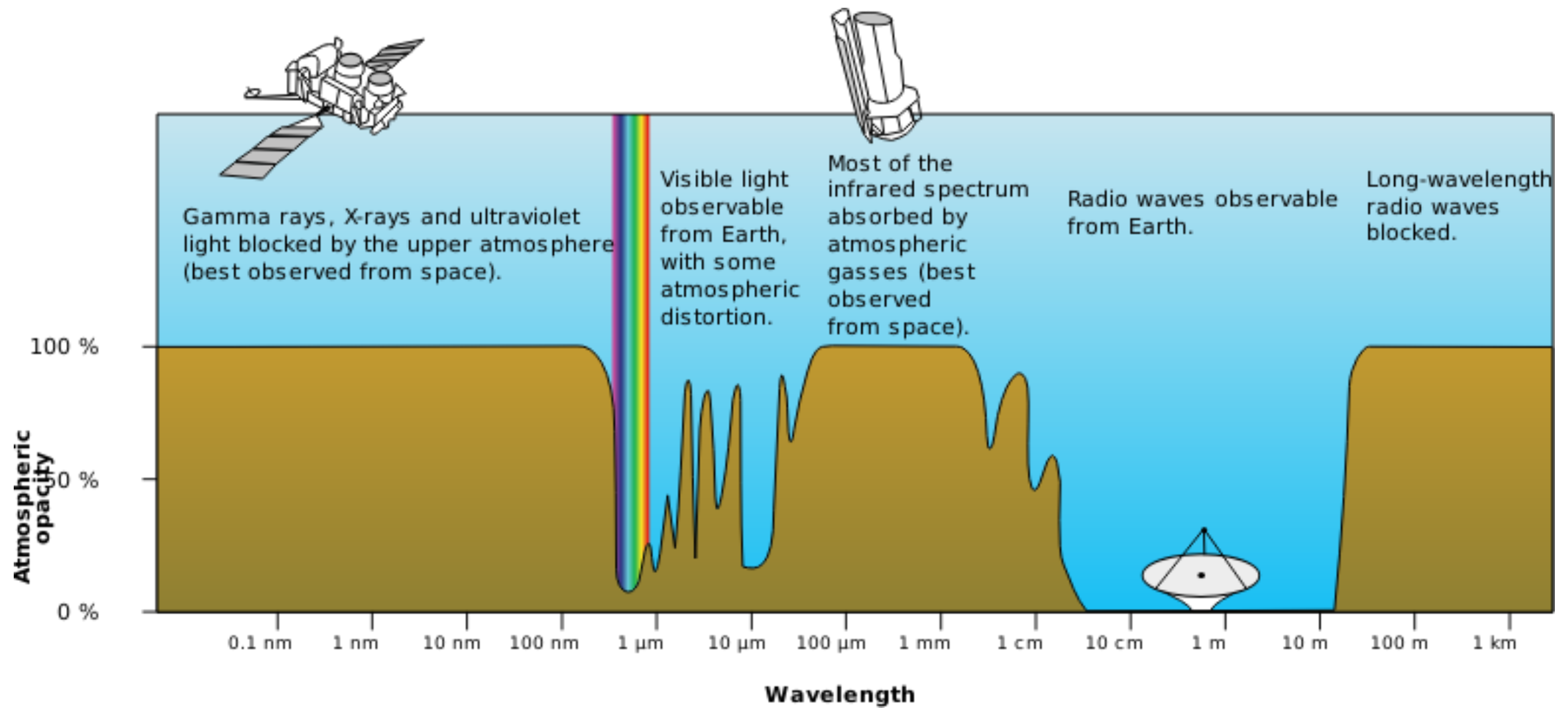
Complete $2p^6$ shell,
ground state has $J = 0$

Oxygen ground state:
 $1s^2 2s^2 2p^4$

EM spectrum in astronomy



Atmospheric windows



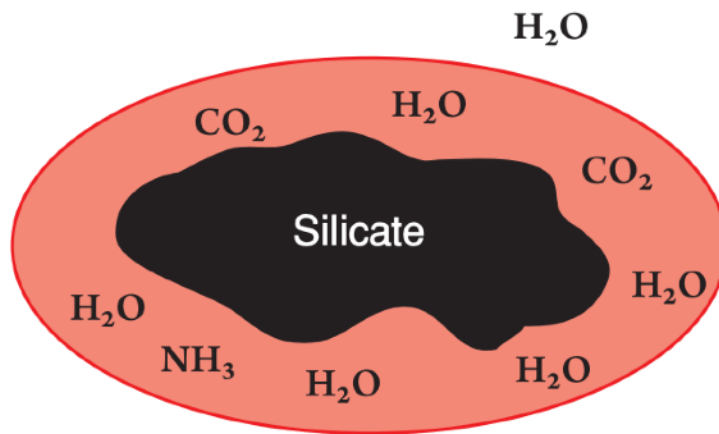
Atacama Large mm/sub-mm Array (ALMA)



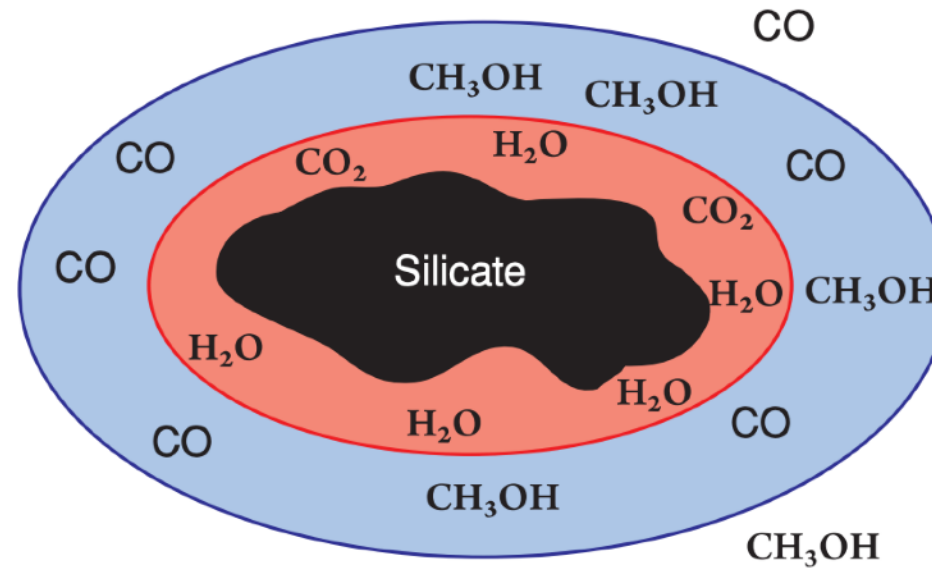
Molecular chemistry beyond H₂

Ices

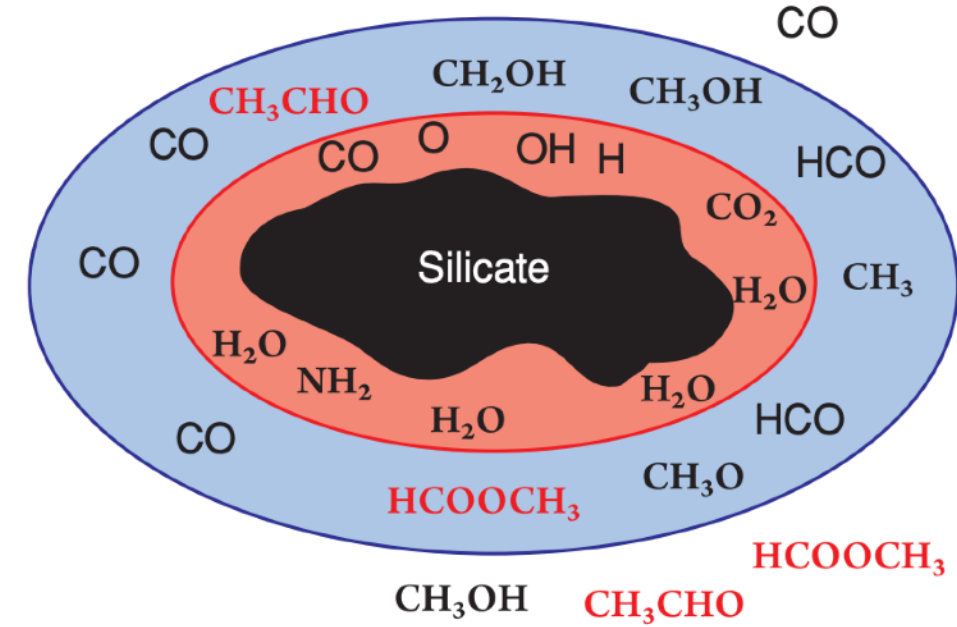
(a) Early ice formation



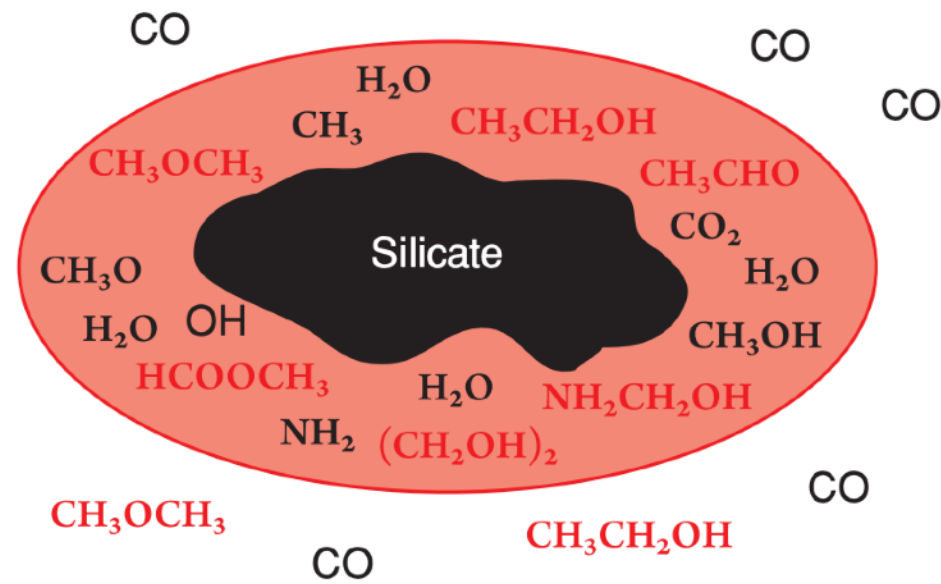
(b) Cloud core ice formation



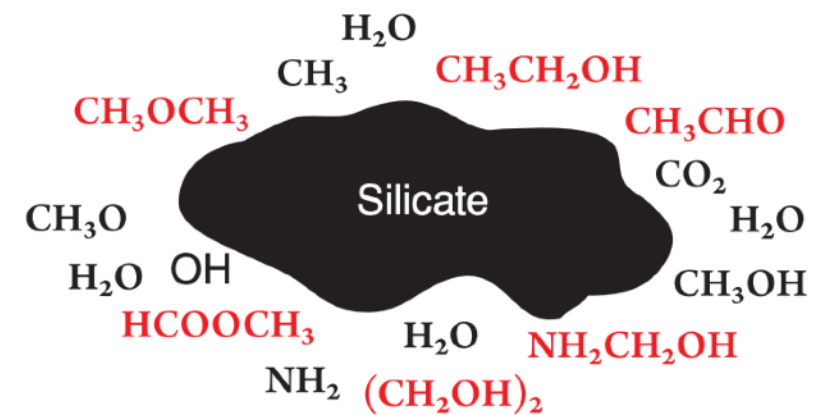
(c) Cold ($<20\text{ K}$) UV-processing



(d) Lukewarm protostellar envelope $>20\text{ K}$



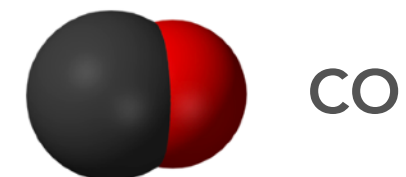
(e) Protostellar hot core $>100\text{ K}$



Molecules detected in space: 2 atoms

Molecule ◆	Designation ◆
AlCl	Aluminium monochloride ^{[13][14]}
AlF	Aluminium monofluoride ^{[13][15]}
AlO	Aluminium monoxide ^[16]
—	Argonium ^{[17][18]}
C ₂	Diatomic carbon ^{[19][20]}
—	Fluoromethyldynium
CH	Methyldyne radical ^{[22][23]}
CN	Cyano radical ^{[13][23][25][26]}
CO	Carbon monoxide ^{[13][29][30]}
CP	Carbon monophosphide ^[26]
CS	Carbon monosulfide ^[13]
FeO	Iron(II) oxide ^[32]
—	Helium hydride ion ^{[33][34]}
H ₂	Molecular hydrogen ^[5]
HCl	Hydrogen chloride ^[35]
HF	Hydrogen fluoride ^[37]
HO	Hydroxyl radical ^[13]
KCl	Potassium chloride ^{[13][14]}

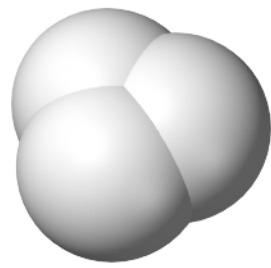
Molecule ◆	Designation ◆
NH	Imidogen radical ^{[39][40]}
N ₂	Molecular nitrogen ^{[41][42]}
NO	Nitric oxide ^[43]
NS	Nitrogen sulfide ^[13]
NaCl	Sodium chloride ^{[13][14]}
—	Magnesium monohydride cation
O ₂	Molecular oxygen ^[44]
PN	Phosphorus mononitride ^{[45][46]}
PO	Phosphorus monoxide ^[47]
SH	Sulfur monohydride ^[48]
SO	Sulfur monoxide ^[13]
SiC	Carborundum ^{[13][50]}
SiN	— ^[51]
SiO	Silicon monoxide ^[13]
SiS	Silicon monosulfide ^[13]
TiO	Titanium(II) oxide ^[52]



Molecules detected in space: 3 atoms

Molecule	Designation
AlNC	Aluminium isocyanide ^[13]
AlOH	Aluminium hydroxide ^[55]
C ₃	Tricarbon ^{[56][57]}
C ₂ H	Ethynyl radical ^{[13][25]}
CCN	Cyanomethyldyne ^[58]
C ₂ O	Dicarbon monoxide ^[59]
C ₂ S	Thioxoethenylidene ^[60]
C ₂ P	— ^[61]
CO ₂	Carbon dioxide ^[62]
CaNC	Calcium isocyanide ^[63]
FeCN	Iron cyanide ^[64]
—	Protonated molecular hydrogen
H ₂ C	Methylene radical ^[65]
—	Chloronium
H ₂ O	Water ^[67]
HO ₂	Hydroperoxyl ^[69]
H ₂ S	Hydrogen sulfide ^[13]
HCN	Hydrogen cyanide ^{[13][25][70]}
HNC	Hydrogen isocyanide ^{[71][72]}
HCO	Formyl radical ^[73]

Molecule	Designation
HCP	Phosphaethyne ^[75]
HCS	Thioformyl ^[76]
—	Diazenylium ^{[74][24][77]}
HNO	Nitroxyl ^[78]
—	Isoformyl
HSC	Isothioformyl ^[76]
KCN	Potassium cyanide ^[13]
MgCN	Magnesium cyanide ^[13]
MgNC	Magnesium isocyanide ^[13]
NH ₂	Amino radical ^[79]
N ₂ O	Nitrous oxide ^[80]
NaCN	Sodium cyanide ^[13]
NaOH	Sodium hydroxide ^[81]
OCS	Carbonyl sulfide ^[82]
O ₃	Ozone ^[83]
SO ₂	Sulfur dioxide ^{[13][84]}
c-SiC ₂	c-Silicon dicarbide ^{[13][50]}
SiCSi	Disilicon carbide ^[85]
SiCN	Silicon carbonitride ^[86]
SiNC	^[87]
TiO ₂	Titanium dioxide ^[52]

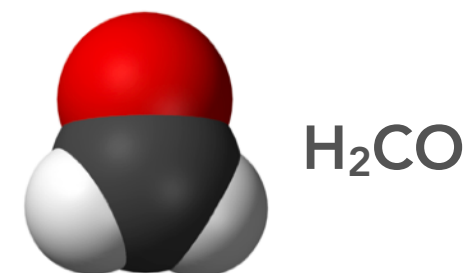


H₃⁺

Molecules detected in space: 4 atoms

Molecule	Designation
CH ₃	Methyl radical ^[89]
<i>i</i> -C ₃ H	Propynylidyne ^{[13][90]}
<i>c</i> -C ₃ H	Cyclopropynylidyne ^[92]
C ₃ N	Cyanoethynyl ^[93]
C ₃ O	Tricarbon monoxide ^[90]
C ₃ S	Tricarbon sulfide ^{[13][60]}
—	Hydronium
C ₂ H ₂	Acetylene ^[96]
H ₂ CN	Methylene amidogen ^[97]
H ₂ CO	Formaldehyde ^[88]
H ₂ CS	Thioformaldehyde ^[98]
HCCN	— ^[99]
HCCO	Ketenyl ^[100]
—	Protonated hydrogen cyanide

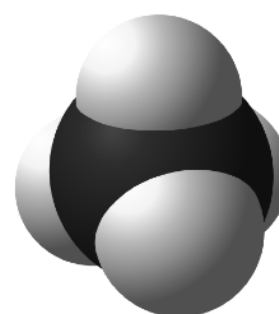
Molecule	Designation
—	Protonated carbon dioxide
HCNO	Fulminic acid ^[102]
HOCN	Cyanic acid ^[103]
CNCN	Isocyanogen ^[104]
HOOH	Hydrogen peroxide ^[105]
HNCO	Isocyanic acid ^[84]
HNCS	Isothiocyanic acid ^[106]
NH ₃	Ammonia ^{[13][107]}
HSCN	Thiocyanic acid ^[108]
SiC ₃	Silicon tricarbon ^[13]
HMgNC	Hydromagnesium isocyanide ^[109]
HNO ₂	Nitrous acid ^[110]



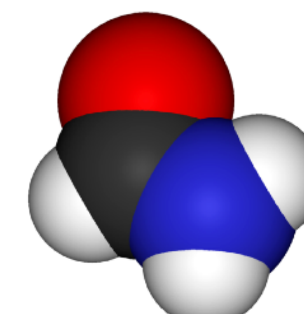
Molecules detected in space: 5/6 atoms

Molecule	Designation
—	Ammonium ion ^{[112][113]}
CH ₄	Methane ^[114]
CH ₃ O	Methoxy radical ^[115]
c-C ₃ H ₂	Cyclopropenylidene ^{[25][116][117]}
l-H ₂ C ₃	Propadienylidene ^[117]
H ₂ CCN	Cyanomethyl ^[118]
H ₂ C ₂ O	Ketene ^[84]
H ₂ CNH	Methylenimine ^[119]
HNCNH	Carbodiimide ^[120]
—	Protonated formaldehyde
C ₄ H	Butadiynyl ^[13]
HC ₃ N	Cyanoacetylene ^{[13][25][74][123][124]}
HCC-NC	Isocyanoacetylene ^[125]
HCOOH	Formic acid ^{[126][123]}
NH ₂ CN	Cyanamide ^{[127][128]}
NH ₂ OH	Hydroxylamine ^[129]
—	Protonated cyanogen
HC(O)CN	Cyanoformaldehyde ^[131]
C ₅	Linear C ₅ ^[132]
SiC ₄	Silicon-carbide cluster ^[50]
SiH ₄	Silane ^[133]

Molecule	Designation
c-H ₂ C ₃ O	Cyclopropenone ^[135]
E-HNCHCN	E-Cyanomethanimine ^[136]
C ₂ H ₄	Ethylene ^[137]
CH ₃ CN	Acetonitrile ^{[84][138][139]}
CH ₃ NC	Methyl isocyanide ^[138]
CH ₃ OH	Methanol ^{[84][140]}
CH ₃ SH	Methanethiol ^[141]
l-H ₂ C ₄	Diacetylene ^{[13][142]}
—	Protonated cyanoacetylene
HCONH ₂	Formamide ^[134]
C ₅ H	Pentynylidyne ^{[13][60]}
C ₅ N	Cyanobutadiynyl radical ^[143]
HC ₂ CHO	Propynal ^[144]
HC ₄ N	— ^[13]
CH ₂ CNH	Ketenimine ^[116]
C ₅ S	— ^[145]



CH₄

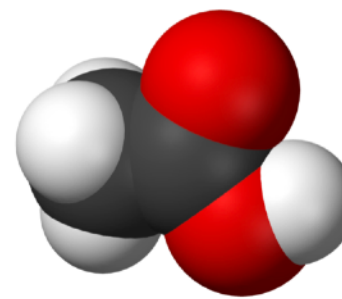
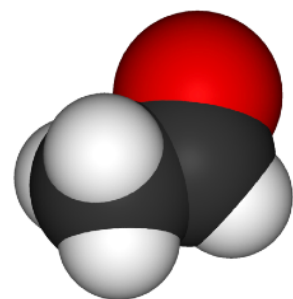


HCONH₂

Molecules detected in space: 7/8 atoms

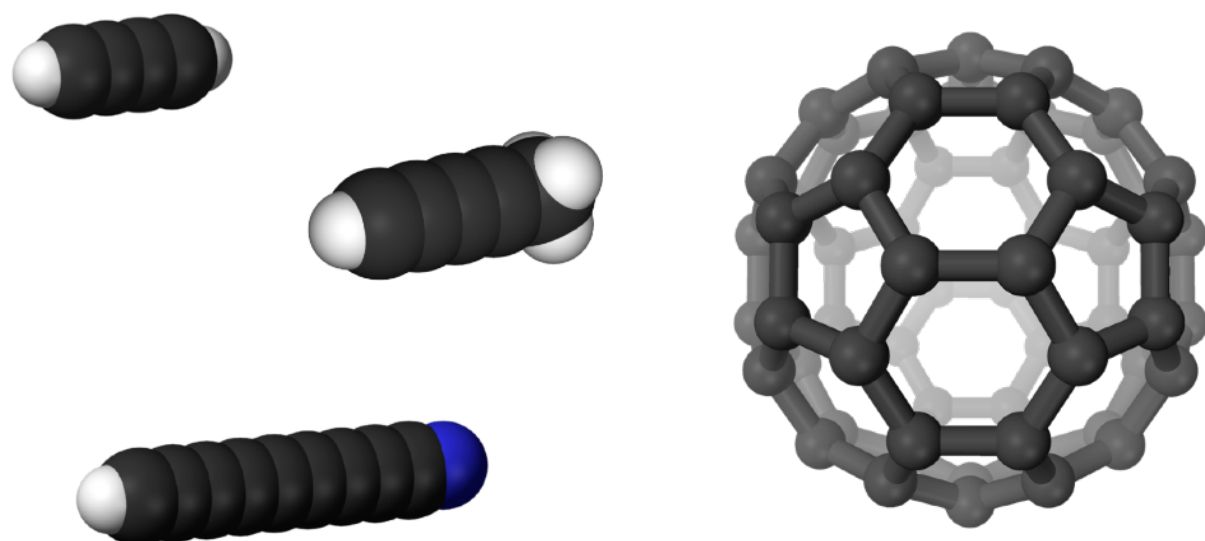
Molecule ◆	Designation ◆
c-C ₂ H ₄ O	Ethylene oxide ^[147]
CH ₃ C ₂ H	Methylacetylene ^[25]
H ₃ CNH ₂	Methylamine ^[148]
CH ₂ CHCN	Acrylonitrile ^{[84][138]}
H ₂ CHCOH	Vinyl alcohol ^[146]
C ₆ H	Hexatriynyl radical ^{[13][60]}
HC ₄ CN	Cyanodiacetylene ^{[84][124][138]}
HC ₄ NC	Isocyanodiacetylene ^[150]
HC ₅ O	— ^[151]
CH ₃ CHO	Acetaldehyde ^{[13][147]}
CH ₃ NCO	Methyl isocyanate ^[152]
HOCH ₂ CN	Glycolonitrile ^[153]

Molecule ◆	Designation ◆
H ₃ CC ₂ CN	Methylcyanoacetylene ^[155]
HC ₃ H ₂ CN	Propargyl cyanide ^[156]
H ₂ COHCHO	Glycolaldehyde ^[157]
HCOOCH ₃	Methyl formate ^{[84][123][157]}
CH ₃ COOH	Acetic acid ^[154]
H ₂ C ₆	Hexapentaenylidene ^{[13][142]}
CH ₂ CHCHO	Propenal ^[116]
CH ₂ CCHCN	Cyanoallene ^{[116][155]}
CH ₃ CHNH	Ethanimine ^[158]
C ₇ H	Heptatrienyl radical ^[159]
NH ₂ CH ₂ CN	Aminoacetonitrile ^[160]
(NH ₂) ₂ CO	Urea ^[161]



Molecules detected in space: 9/10+ atoms

Molecule	Designation
$\text{CH}_3\text{C}_4\text{H}$	Methyldiacetylene ^[162]
CH_3OCH_3	Dimethyl ether ^[163]
$\text{CH}_3\text{CH}_2\text{CN}$	Propionitrile ^{[13][84][138]}
CH_3CONH_2	Acetamide ^{[116][134][128]}
$\text{CH}_3\text{CH}_2\text{OH}$	Ethanol ^[164]
C_8H	Octatetraynyl radical ^[165]
HC_7N	Cyanoheptatriyne or Cyanotriacetylene ^{[13][107][168][169]}
CH_3CHCH_2	Propylene (propene) ^[170]
$\text{CH}_3\text{CH}_2\text{SH}$	Ethyl mercaptan ^[171]
CH_3NHCHO	N-methylformamide ^[128]



Atoms	Molecule	Designation
10	$(\text{CH}_3)_2\text{CO}$	Acetone ^{[84][172]}
10	$(\text{CH}_2\text{OH})_2$	Ethylene glycol ^{[173][174]}
10	$\text{CH}_3\text{CH}_2\text{CHO}$	Propanal ^[116]
10	$\text{CH}_3\text{OCH}_2\text{OH}$	Methoxymethanol ^[175]
10	$\text{CH}_3\text{C}_5\text{N}$	Methylcyanodiacetylene ^[116]
10	$\text{CH}_3\text{CHCH}_2\text{O}$	Propylene oxide ^[176]
11	HC_8CN	Cyanotetraacetylene ^{[13][168]}
11	$\text{C}_2\text{H}_5\text{OCHO}$	Ethyl formate ^[177]
11	$\text{CH}_3\text{COOCH}_3$	Methyl acetate ^[178]
11	$\text{CH}_3\text{C}_6\text{H}$	Methyltriacetylene ^{[116][162]}
12	C_6H_6	Benzene ^[142]
12	$\text{C}_3\text{H}_7\text{CN}$	<i>n</i> -Propyl cyanide ^[177]
12	$(\text{CH}_3)_2\text{CHCN}$	<i>iso</i> -Propyl cyanide ^{[179][180]}
13	$\text{C}_6\text{H}_5\text{CN}$	Benzonitrile ^[181]
13	HC_{10}CN	Cyanopentaacetylene ^[168]
60	C_{60}	Buckminsterfullerene (C ₆₀ fullerene) ^[182]
70	C_{70}	C ₇₀ fullerene ^[182]

Reading

Draine

- §5.1
- §31.1-4, §31.7