Potential importance of neutral-neutral reactions involving the CH_2 radical

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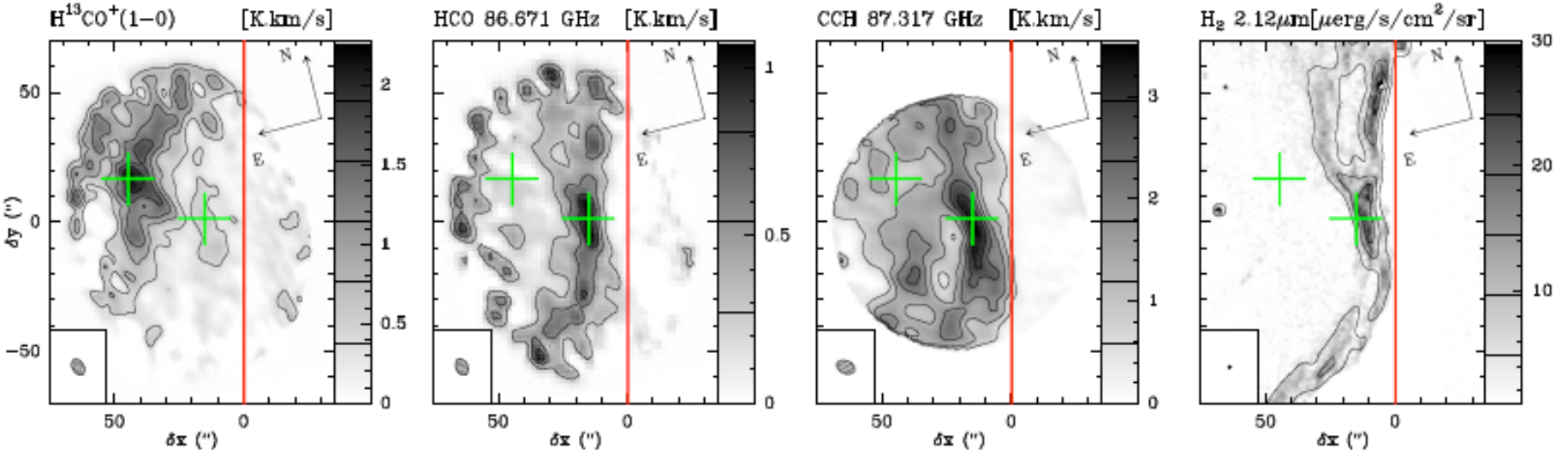
New observational facts (1)



High angular observations of $H^{13}CO^+$, HCO, CCH and H_2 at PdB

➔ Detection of HCO in the Horsehead nebula (Gerin et al. AstroPh 1108.1470)

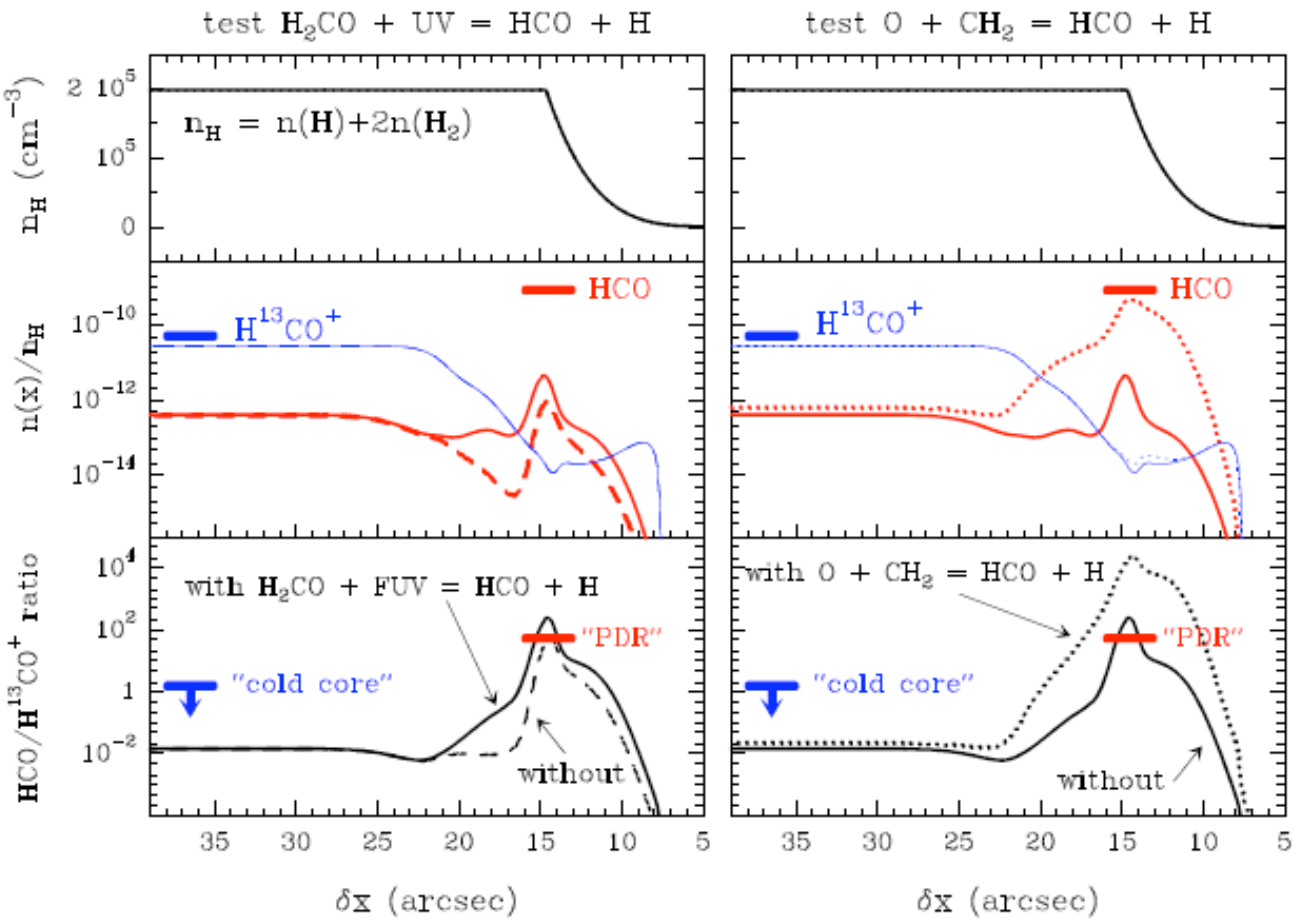
HCO

- HCO detected with a large fractional abundance
- Test of the HCO channel in the photodissociation of H_2CO
- Test of the $O+CH_2$ reaction
- Available in the UMIST chemical network
- Measured at high temperature
- Theoretical study?

Table 4. Inferred column densities and abundances with respect to molecular hydrogen, *e.g.* $\chi(X) = N(X)/N(H_2)$.

Molecule	Method	HCO peak	DCO^+ peak
$N(H_2)$ [cm^{-2}]	1.2 mm cont.	1.9×10^{22}	2.9×10^{22}
$N(HCO)$ [cm^{-2}]	$T_{ex} = 5$ K	3.2×10^{13}	4.6×10^{12}
$N(H^{13}CO^+)$ [cm^{-2}]	Full excitation	5.8×10^{11}	5.0×10^{12} •
$N(HCO^+)$ [cm^{-2}]	$^{12}C/^{13}C$=60	3.5×10^{13}	2.3×10^{14}
$\chi(HCO)$		1.7×10^{-9}	1.6×10^{-10} †
$\chi(H^{13}CO^+)$		3.1×10^{-11}	1.7×10^{-10}
$\chi(HCO^+)$		1.9×10^{-9}	7.9×10^{-9}

• Pety et al. (2007a) † 1.7×10^{-9} if HCO arises only from the cloud surface ($A_V \simeq 3$).



UMIST data base results on neutral-neutral reactions with CH_2

- $CH_2 + O \rightarrow CO + H2$ 8.00E-11 0.00 0.0 1900 - 2600
  within 25% Lit. Search
- $CH_2 + O \rightarrow CO + H + H$ 1.33E-10 0.00 0.0 10 - 2500
  within 25% Lit. Search
- $CH_2 + O \rightarrow HCO + H$ 5.01E-11 0.00 0.0 1200 - 1812
  within 25% Measurement (not in OSU)

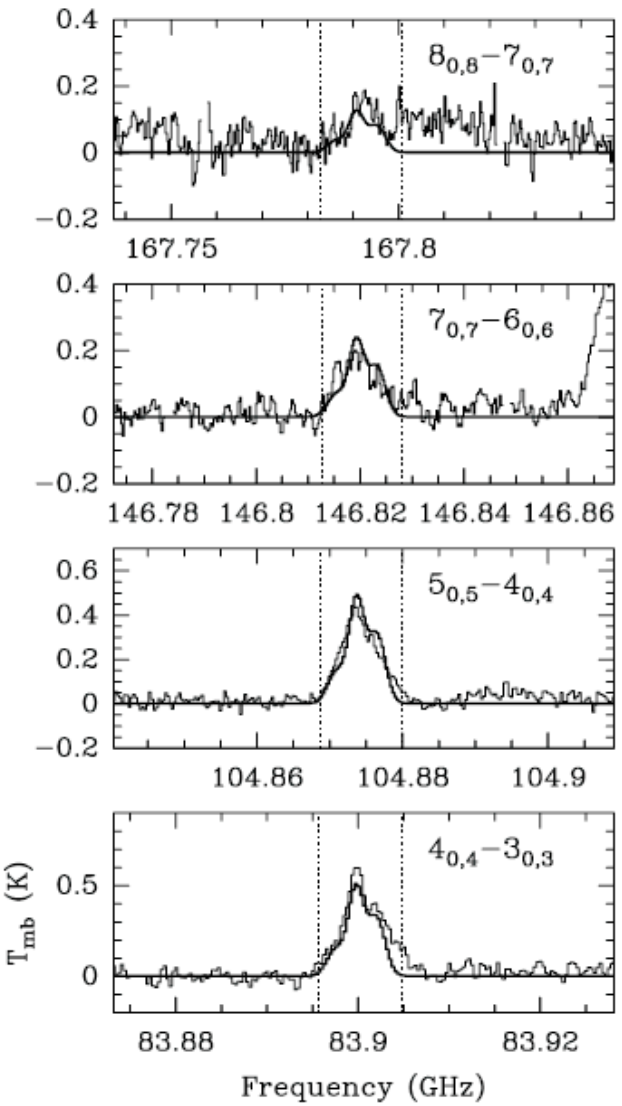
Photodissociation of H_2CO :

Theoretical calculations by Yin et al. (Science 2006) and Troe, JPC A 111, 3868 (2007) : HCO channel available for $\lambda > 310$ nm

New observational facts (2)

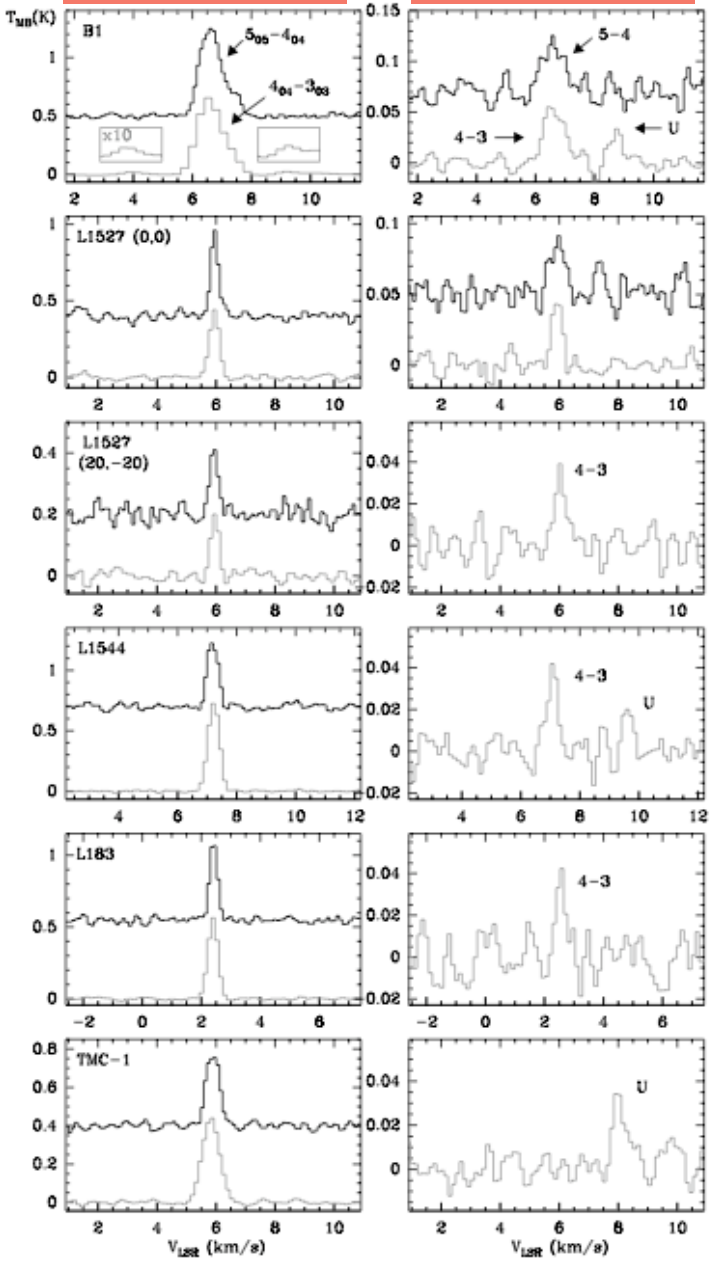
- Detection of HCNO in dense cold cores (Marcelino et al. ApJL 09)
- Detection of HOCN towards SgB2 (Brunken et al. ApJ submitted)

HOCN



HNCO

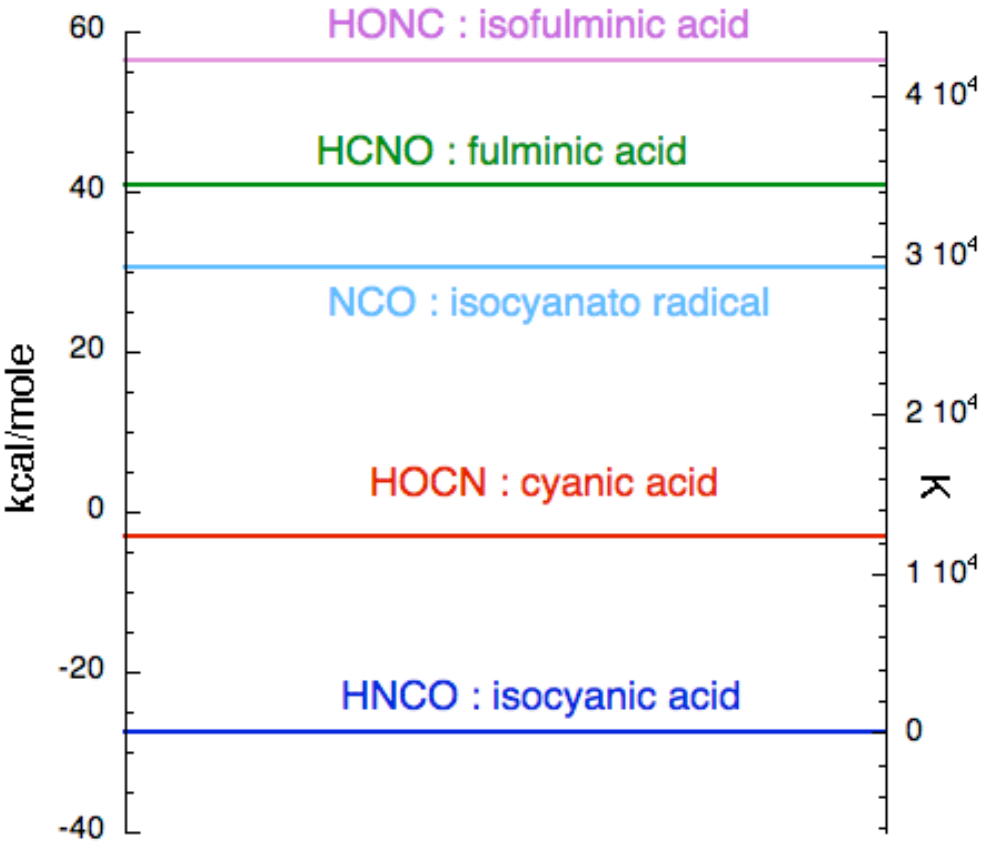
HCNO



HNCO isomers

- HNCO detected in numerous regions
- Detection of HOCN towards SgB2 (together with laboratory frequencies)
- Detection of HCNO in cold clouds
- Geometry and stability revisited by Mladenovic & Lewerenz (2008) : HCNO is linear, HOCN is planar

Formation enthlapies from theoretical calculations at "subchemical" accuracy (Schuurman et al. 2004)



Chemical pathways to HCNO and HOCN ?
I. Ionic channels

- No obvious parent molecule candidate
- $HCNH^+ + O$? No reaction
- $NCO^+ + OH \rightarrow HNCO^+$
- $NCO + H_3^+ \rightarrow HNCO^+$, $HOCN^+$, not $HCNO^+$ (3380 K)
- $HNCO^+$, $HOCN^+$ & $HCNO^+$ react with H_2 giving H_2NCO^+, $HNCOH^+$, $HCNOH^+$, H_2CNO^+
- DR channels : $H_2NCO^+ \rightarrow HNCO$
  $HNCOH^+ \rightarrow HNCO$ (and HOCN)
  $H_2CNO^+ \rightarrow HCNO$
  $HCNOH^+ \rightarrow HCNO$

	kcal/mol
NCO^+	308
$HNCO^+$	243
$HOCN^+$	267
$HCNO^+$	302
H_2NCO^+	167
$HNCOH^+$	186 ±?
$HCNOH^+$	246
H_2CNO^+	254

theoretical values (Mebel et al. 1996, Hop et al. 89)

Chemical pathways to HCNO and HOCN ?
II. Neutral-neutral channels

- $CN + O_2 \rightarrow NCO + O$ (studied by Sims et al. 1994 at low temperature
- $NCO + H_2 \rightarrow HNCO + H$ measured between 591-913K $k = 1.4(-11) \exp(-1082/T)$ (Perry et al. 1985, JCP 82, 5485)
- $CH_2 + NO \rightarrow HCNO + H$ (Glarborg 1998, CF 115, 1) no activation barrier found by Roggenbuck & Temps, 1998, CPL 285, 422)

Chemical modelling attempt of H, N, C and O chemical family

T= 10K, $n(H_2) = 10^5$ cm^{-3}

HNCO

fabric: 8.797312E-15 destru: 8.797312E-15 abond: 1.001162E-04

Processus de fabrication de hnco :

h2nco+ + electr = hnco h 7.3580E-15 cm-3 s-1 7.3494E-11 s-1
83.64 % 785

hncoh+ + electr = hnco h 1.1891E-15 cm-3 s-1 1.1877E-11 s-1
13.52 % 790

Processus de destruction de hnco :

o + hnco = hno co 5.2994E-15 cm-3 s-1 5.2932E-11 s-1
60.24 % 636

h + hnco = nh2 co 3.3346E-15 cm-3 s-1 3.3308E-11 s-1
37.91 % 631

Chemical modelling attempt of H, N, C and O chemical family

HCNO

fabric: 4.339648E-17 destru: 4.339648E-17 abond: 1.276732E-06

Processus de fabrication de hcno :

ch2 + no = hcno h 3.5644E-17 cm-3 s-1 2.8848E-11 s-1
82.14 % 621

ch2 + hno = hcno h2 6.6585E-18 cm-3 s-1 5.3890E-12 s-1
15.34 % 624

Processus de destruction de hcno :

h + hcno = hcn oh 4.1154E-17 cm-3 s-1 3.3308E-11 s-1
94.83 % 632

Chemical modelling attempt of H, N, C and O chemical family

HOCN

fabric: 4.237854E-17 destru: 4.237854E-17 abond: 4.840400E-07

Processus de fabrication de hocn :

hncoh+ + electr = hocn h 4.1002E-17 cm-3 s-1 8.4708E-11 s-1
96.75 % 789

Processus de destruction de hocn :

o + hocn = oh nco 2.5621E-17 cm-3 s-1 5.2932E-11 s-1
60.46 % 640

h + hocn = nco h2 1.6122E-17 cm-3 s-1 3.3308E-11 s-1
38.04 % 633

Some quantitative comparison

from Marcelino et al. 2009

Source	N (HCNO) 10^{10} cm^{-2}	N (HNCO) 10^{12} cm^{-2}	$n(H_2)$ 10^5 cm^{-3}	R HNCO/HCNO
B1	21(1)/17	9(1)/8.0	6	42/47
L1527	6(1)/4.5	2.2(6)/1.8	5	37/40
L1527-B	5(1)/4.0	0.9(5)/0.8	5	18/20
L1544	8(3)/6.3	5(1)/4.1	0.7	62/66
L183	6(2)/5.0	3.4(3)/2.5	0.5	57/50
TMC-1	≤1.3/≤1.4	5.7(4)/4.5	0.3	>390/>320
Orion-KL		**9000(2000)**		**>1100**

Prediction of NCO

$n(H_2)$ 10^4 cm^{-3} T=10K	NO 10^{-7}	HNCO 10^{-10}	HCNO 10^{-11}	HOCN 10^{-13}	NCO 10^{-8}	R
0.1	0.005	0.004	0.04	0.47	0.02	0.8
0.3	0.01	0.01	0.08	1.30	0.07	1.5
1.0	8.6	18	6.30	38.0	6.6	29
3.0	7.4	18	3.10	12.0	4.5	58
10	5.1	9.3	1.20	2.0	2.0	72
30	3.2	3.4	0.58	0.31	0.8	58
50	2.5	2.0	0.41	0.13	0.5	49
100	1.7	0.9	0.25	0.04	0.3	36

- satisfactory agreement with observations
- several guesses need to be critically analysed
- further observations needed of the 3 isomers (IRAM 2009)

Conclusions

- ✓ possible role of CH_2 ($X\ ^3B_1$) in interstellar chemistry
  - HCO formation route in PDR : CH_2 + O ? spin conservation
  - HCNO formation route : CH_2 + NO ?
- ✓ further observations of the 3 HNCO isomers: HNCO (quasi-linear) HOCN (quasilinear), HCNO (linear $^1\Sigma^+$) in various environments
- ✓ $HOCNH^+$ DR branching ratios critical for the HNCO/HOCN ratio
- ✓ experimental and/or theoretical check?
- ✓ Grain formation path ? Discrimination between the isomers?