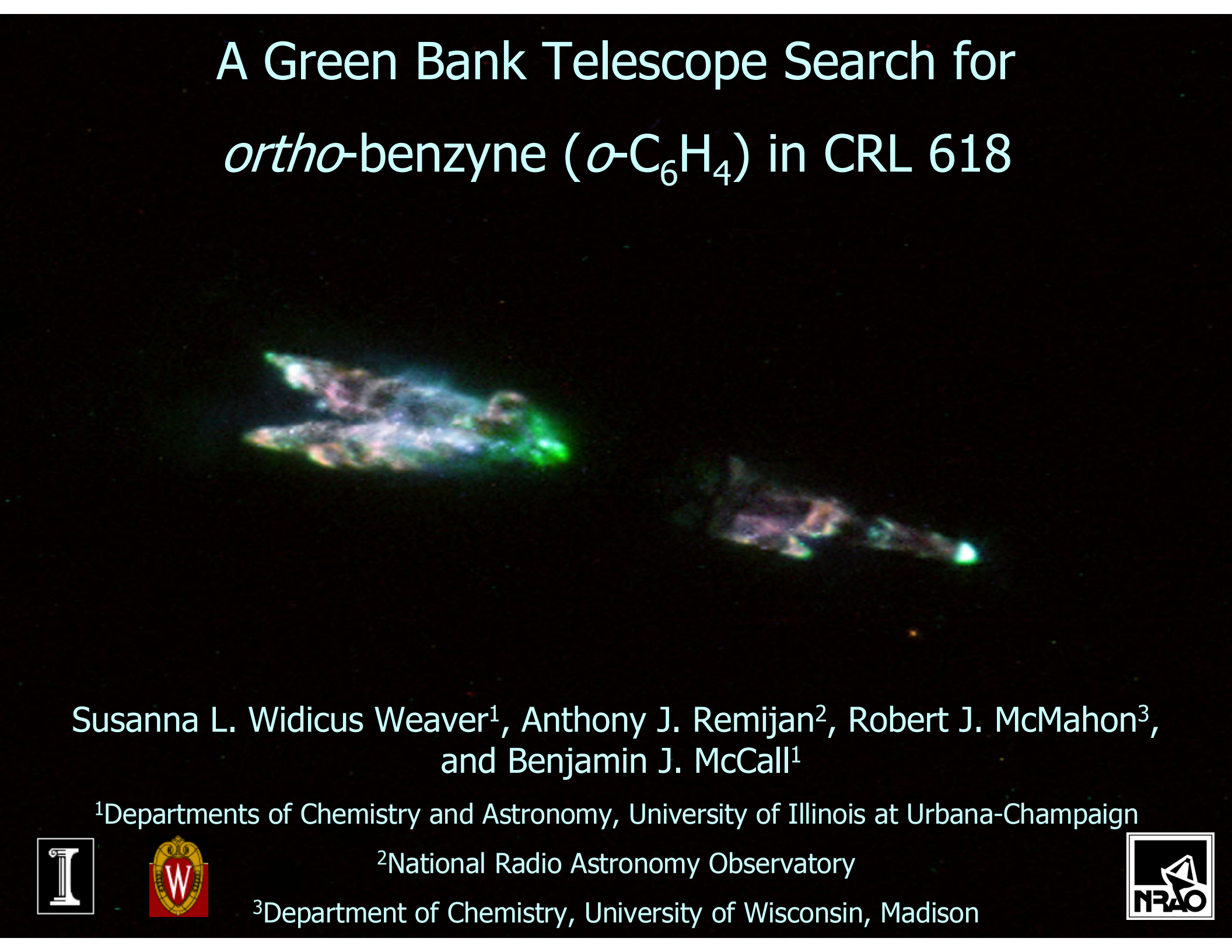
A Green Bank Telescope Search for *ortho*-benzyne (*o*-C_6H_4) in CRL 618



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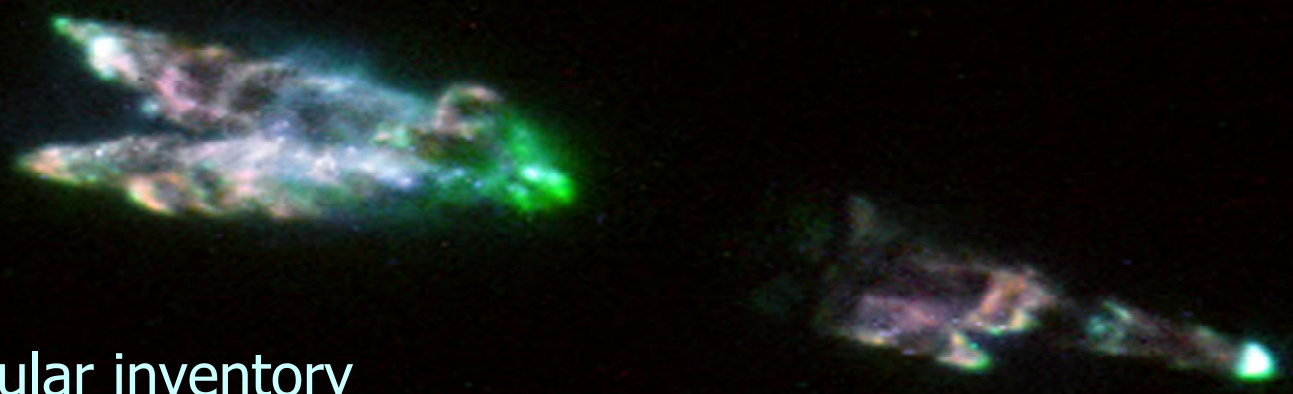
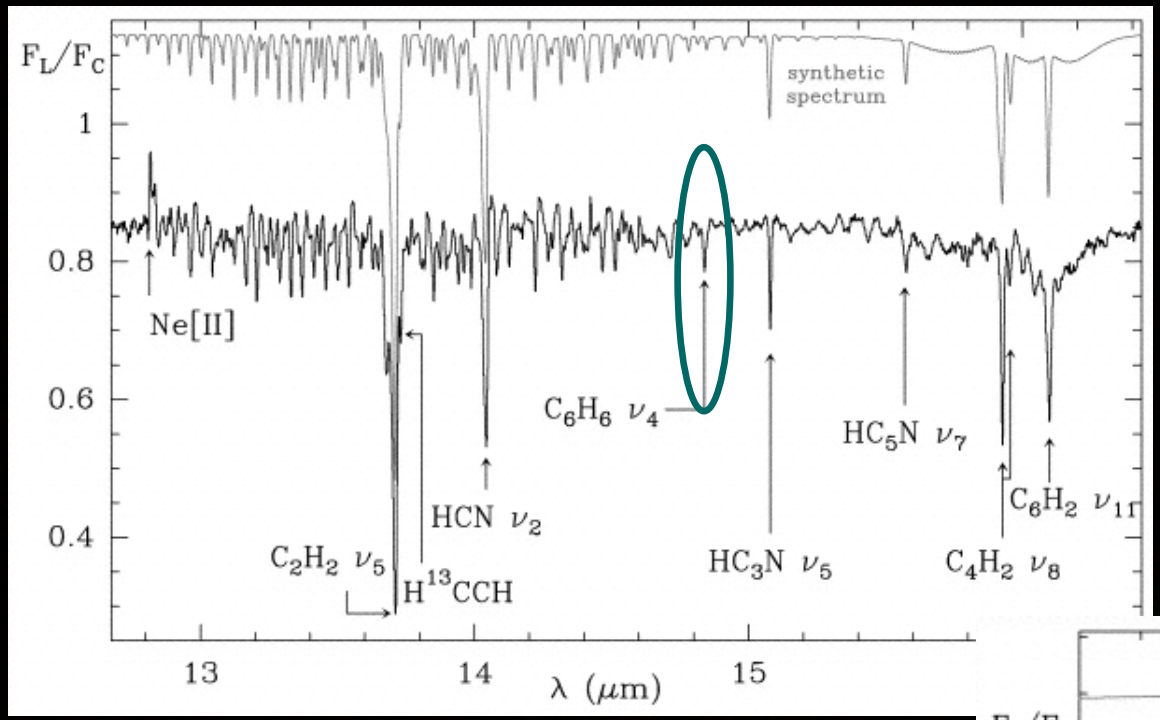
CRL 618

- Proto-planetary nebula (PPN)
- Thick molecular envelope surrounding B0 star and ultracompact HII region

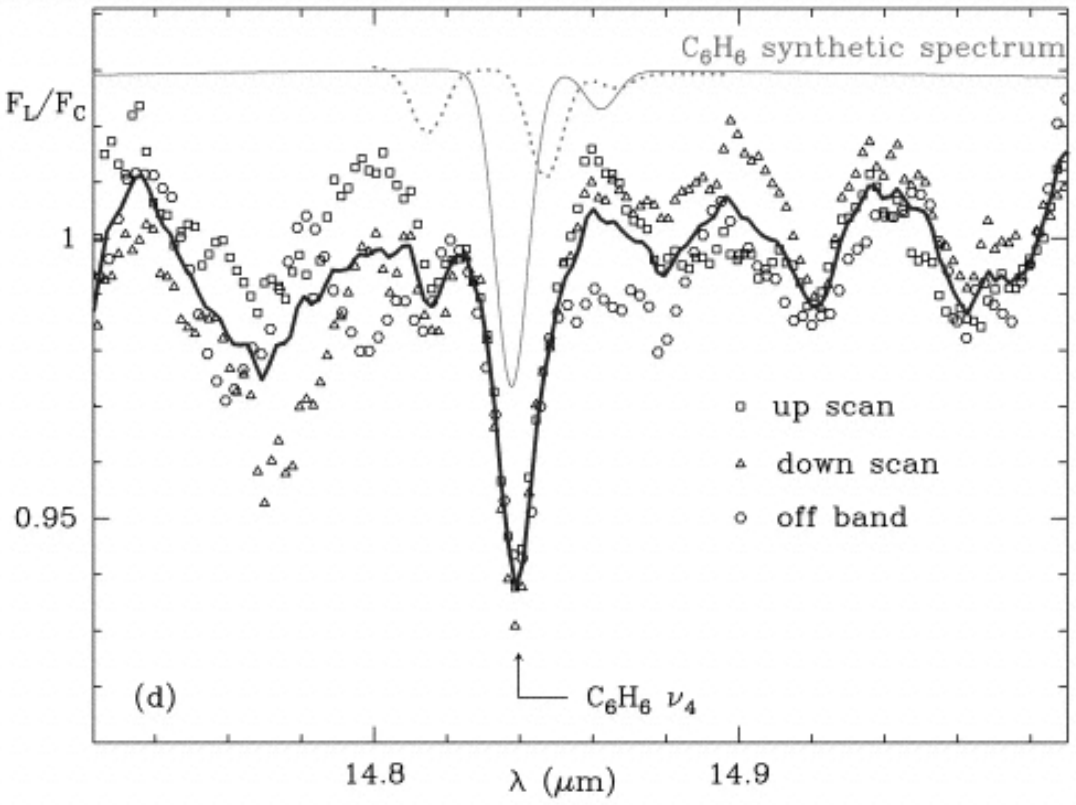


- Rich molecular inventory
  - Cernicharo & coworkers have detected O-bearing species such as H_2O, OH, and H_2CO (1989, *A & A* 222, L1; 2000, ApJ 530, L129).
  - Cernicharo et al. (2001, *ApJL* 546, L127) observed one vibrational band of C_6H_6.
  - Remijan et al. (2005, *ApJ* 626, 233) observed CH_3CN, HC_3N, and HC_5N.
  - Pardo et al. (2007, *ApJ* 661, 250) assigned over 3100 transitions to 33 molecular species, their isomers, and their excited vibrational states.

Benzene Detection in CRL 618

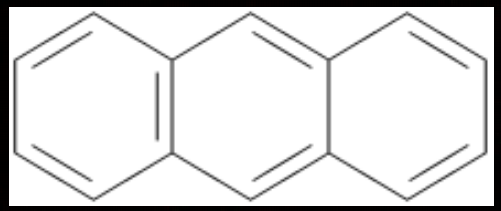


Cernicharo et al. 2001, *ApJL* 546, L123

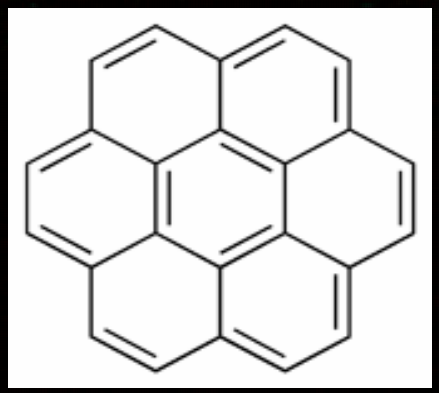


Benzene and PAHs

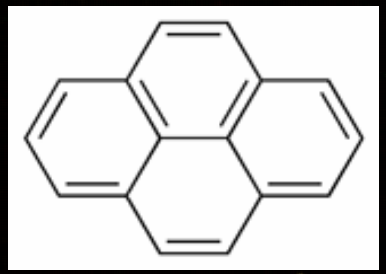
- Benzene is the main building block of polycyclic aromatic hydrocarbons (PAHs).
- PAHs as band carriers?
  - unidentified infrared bands (UIRs)
  - diffuse interstellar bands (DIBs)
- PAHs are typically planar molecules that contain only C and H
- PAH C atoms usually arranged in 5- or 6-member rings:



anthracene

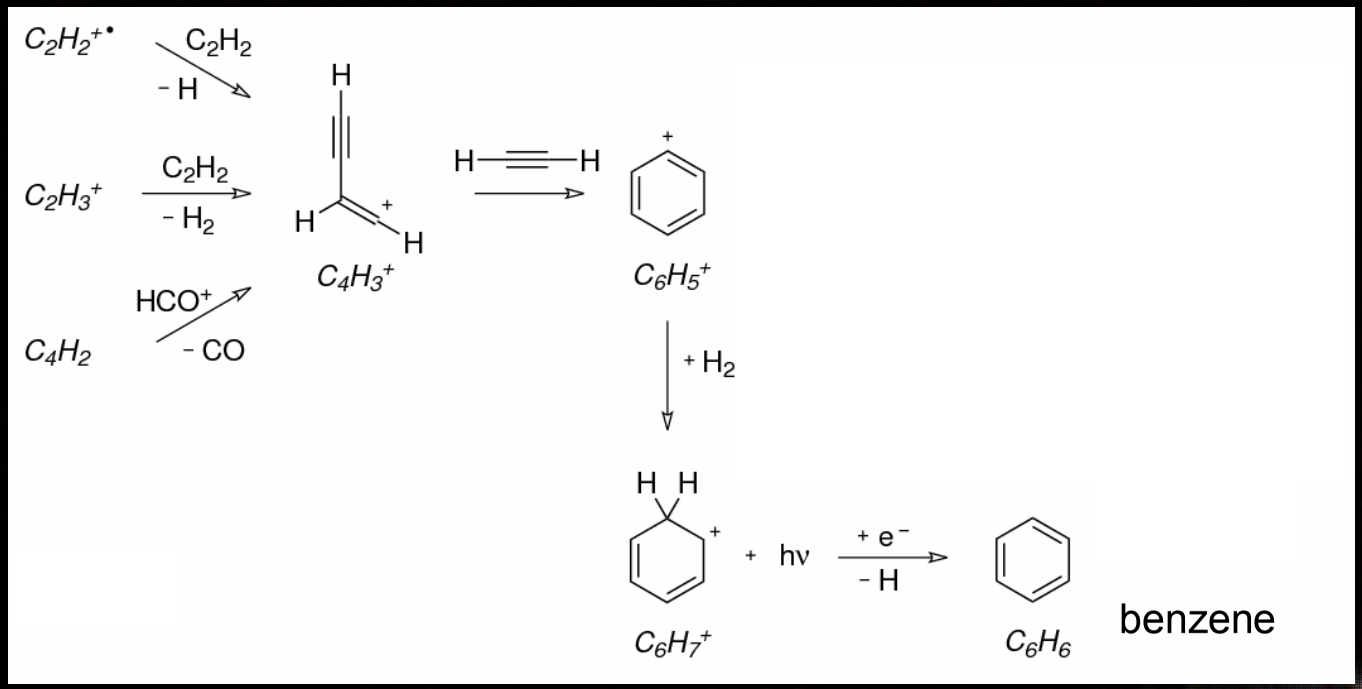


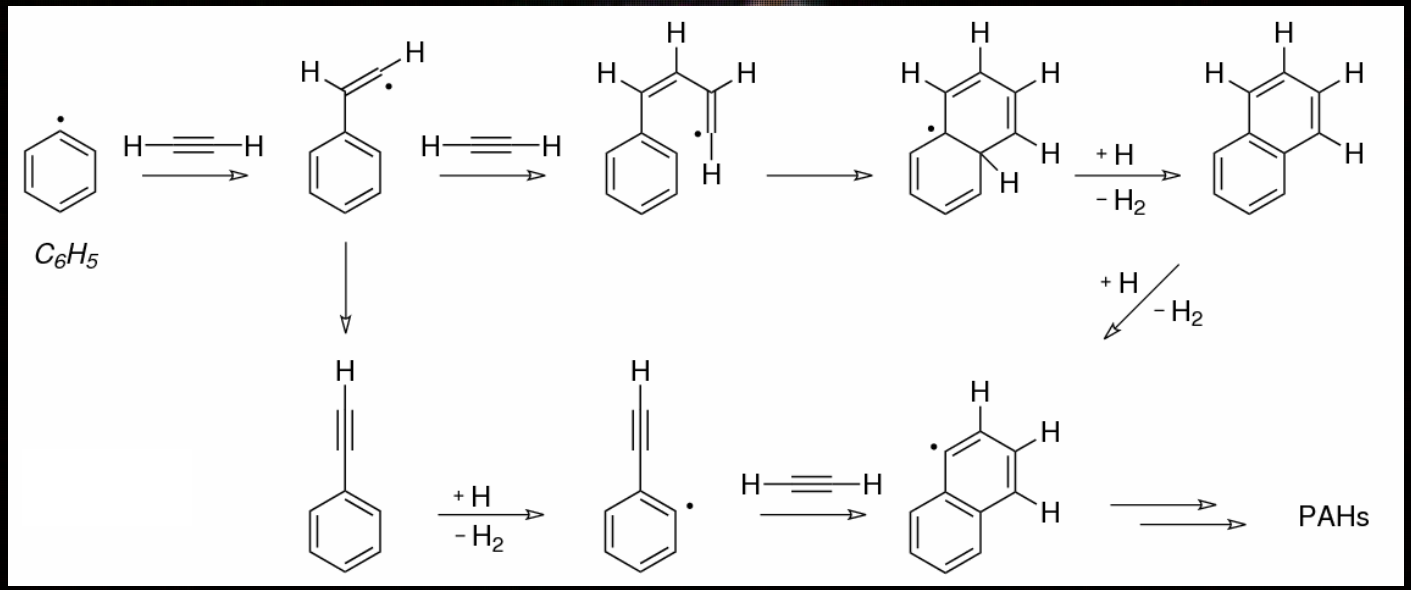
coronene



pyrene

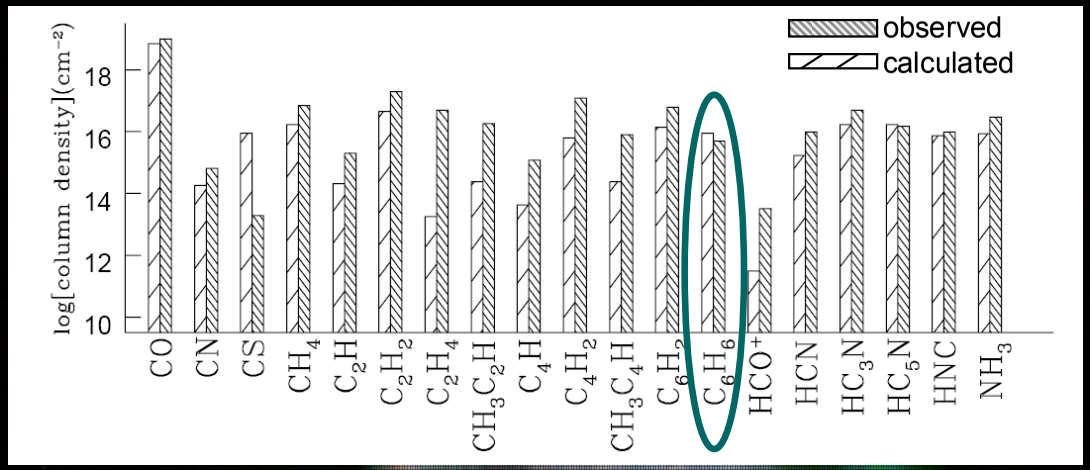
Benzene and PAH Chemistry





Woods et al. 2002, *ApJL* 574, L167; Woods et al. 2003, *A & A* 402, 189;
Kaiser et al. 2003, *A & A* 406, 385; Kazakov & Frenklach 1998, *Combust. Flame* 112, 270

Chemical Models of CRL 618



$C_6H_6 \sim 10^{16}$ cm^{-2}

o-$C_6H_4 \sim C_6H_6 \sim 10^{16}$ cm^{-2}

$C_6H_5 \leq 4 \times 10^{15}$ cm^{-2}

McMahon et al. 2003, *ApJL* 530, L61

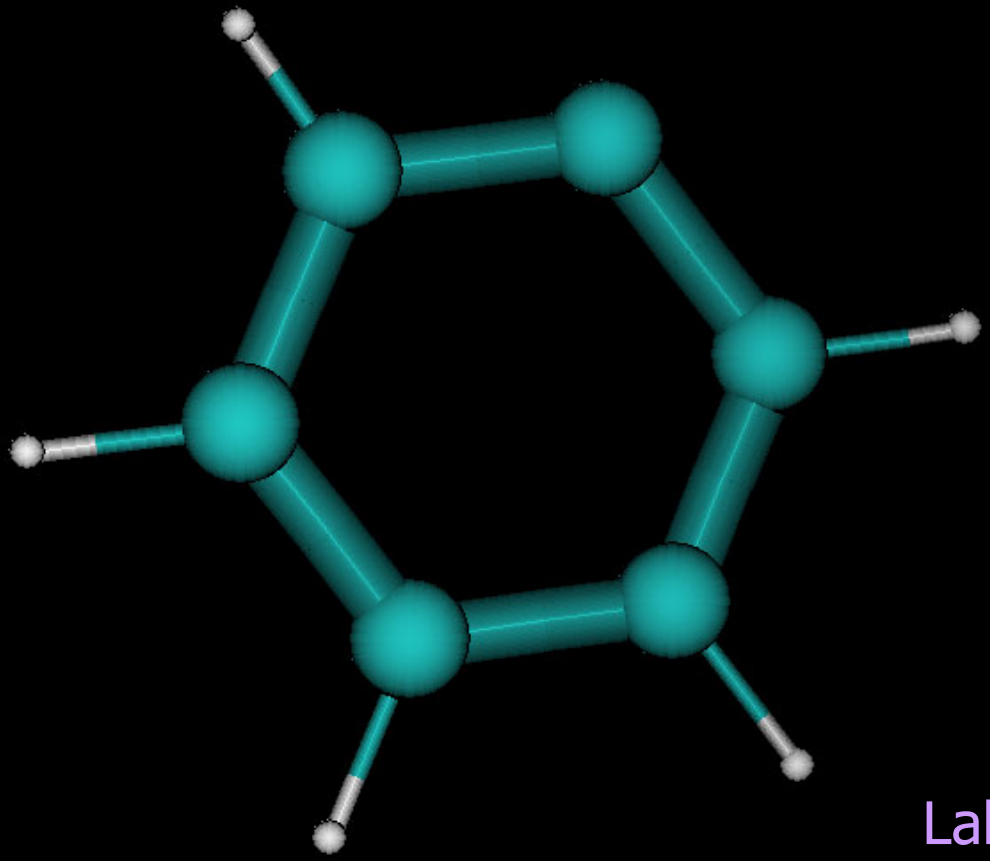
Table 1. Comparison of fractional abundances of potentially observable species at different times. The density, temperature and extinction at these times can be readily calculated from the equations in Section 2.

Species	X(clump) $t = 2550$ yr	$\frac{X(\text{clump})}{X(\text{interclump})}$ $t = 2550$ yr	X(clump) $t = 6300$ yr	$\frac{X(\text{clump})}{X(\text{interclump})}$ $t = 6300$ yr	X(clump) $t = 10\,050$ yr	$\frac{X(\text{clump})}{X(\text{interclump})}$ $t = 10\,050$ yr
Benzene	2.6×10^{-8}	90	2.6×10^{-8}	90	2.6×10^{-8}	90
Benzyne	1.9×10^{-8}	7.1	1.9×10^{-8}	7.1	1.9×10^{-8}	7.1

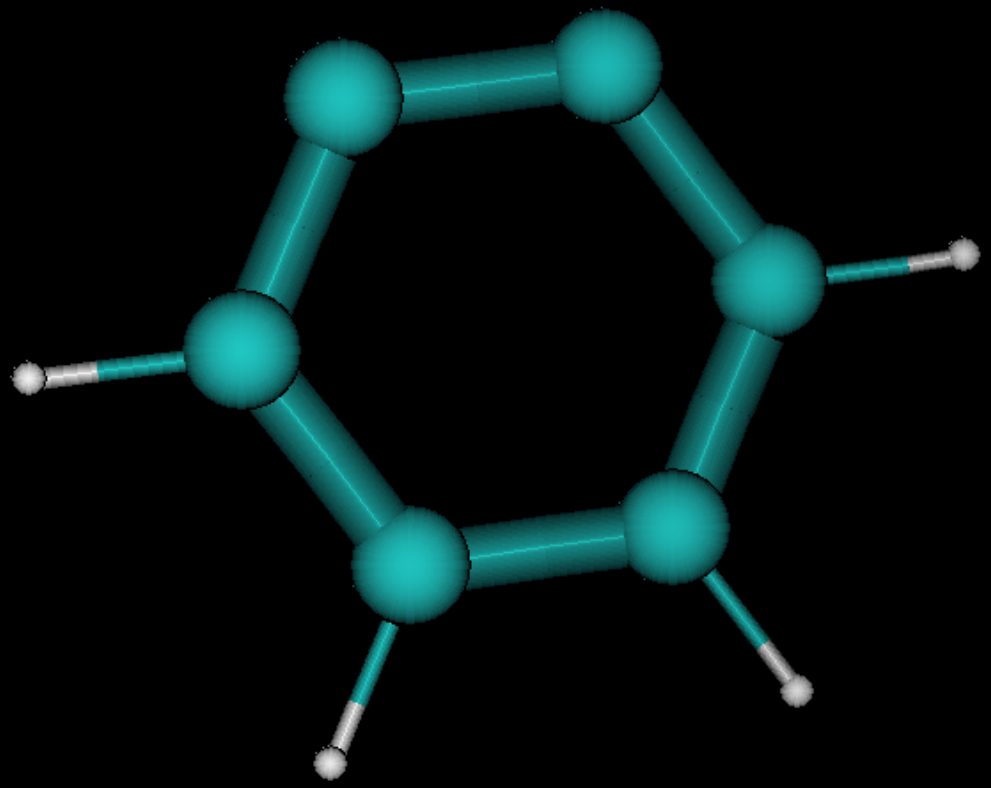
Woods et al. 2002, *ApJL* 574, L167; Woods et al. 2003, A & A 402, 189;
Redman et al. 2003, *MNRAS* 345, 1291

How do we begin the search for more aromatics?

Search for benzene derivatives and small PAHs with permanent dipole moments!



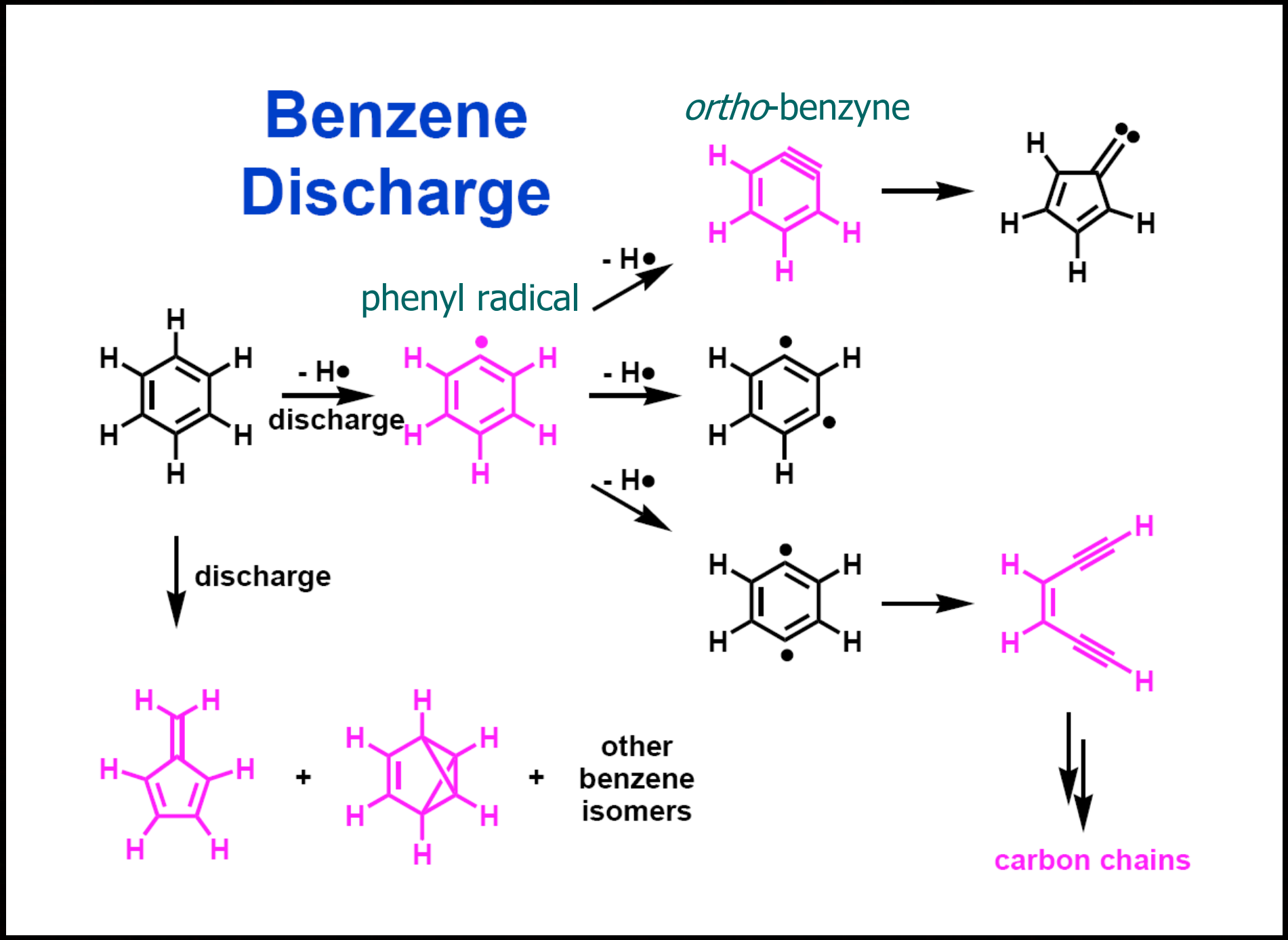
phenyl radical



ortho-benzyne

Laboratory rotational spectra are required!

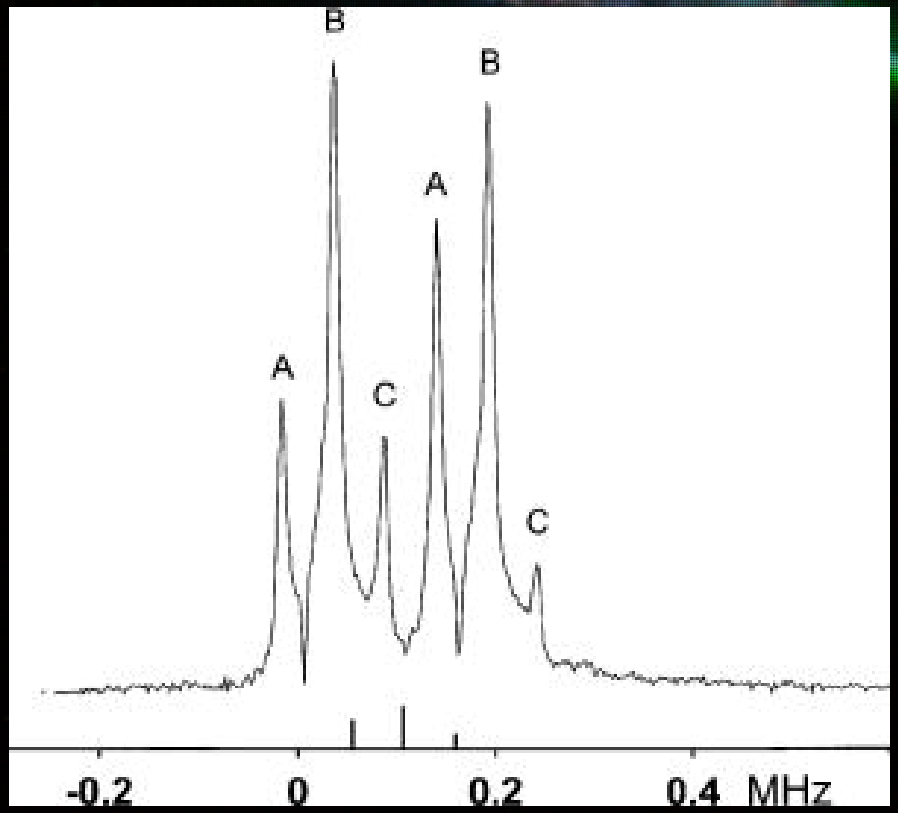
o-C_6H_4 and C_6H_5 Laboratory Chemistry

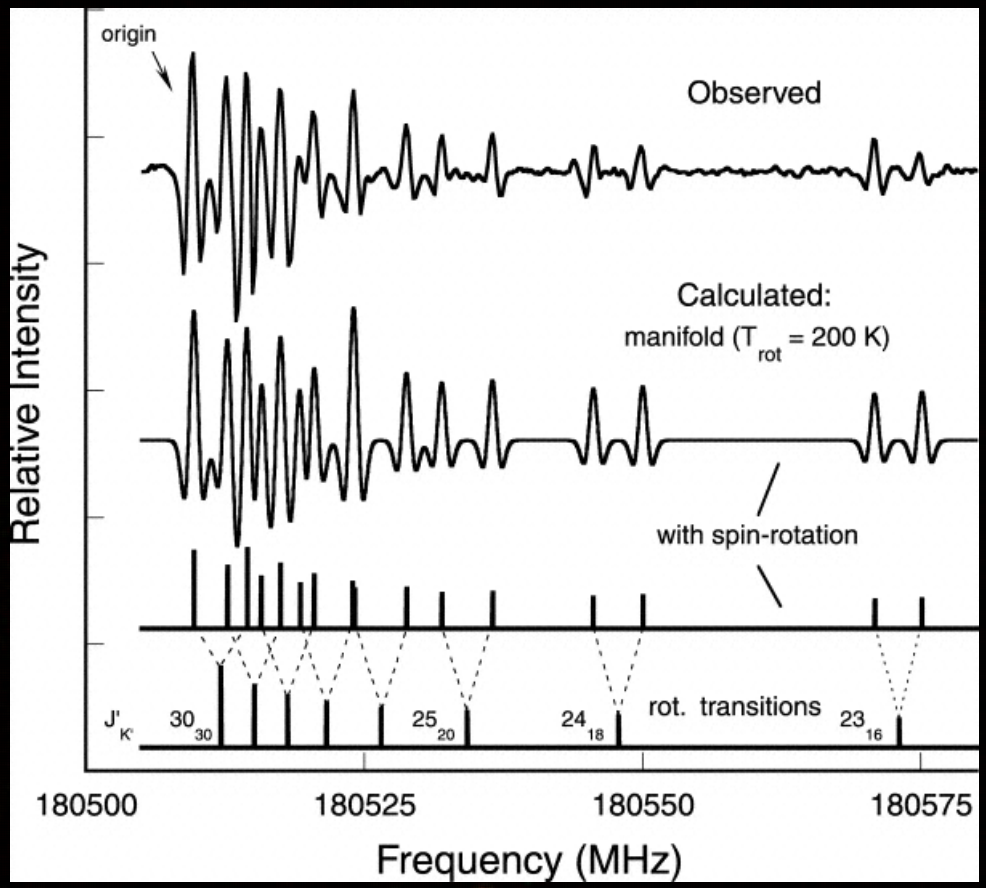


Spectroscopic studies of *o*-C_6H_4 and C_6H_5

The rotational spectrum of *o*-benzyne

Brown et al. 1981, *JACS* 103, 1981
Robertson et al. 2003, *JMS* 217, 123
Kukolich et al. 2003, *JCP* 119, 4353



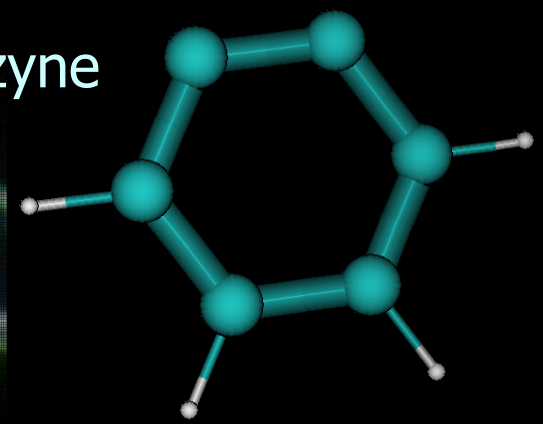


The rotational spectrum of the phenyl radical

McMahon et al. 2003, *ApJL* 530, L61

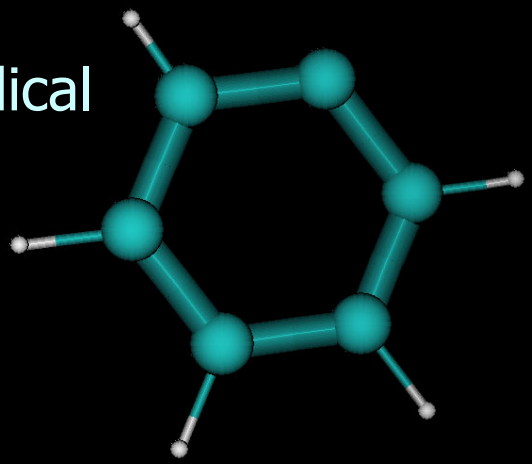
To search for *o*-C_6H_4 or C_6H_5?

ortho-benzyne



- μ = 1.4 D
- no hyperfine splitting
- strong spectrum, fewer lines

phenyl radical



- μ = 0.9 D
- hyperfine splitting
- weak spectrum, but many lines

The search for *o*-C_6H_4 with the GBT

Ku-band (12.0-15.4 GHz)

K-band (18.0-26.5 GHz)

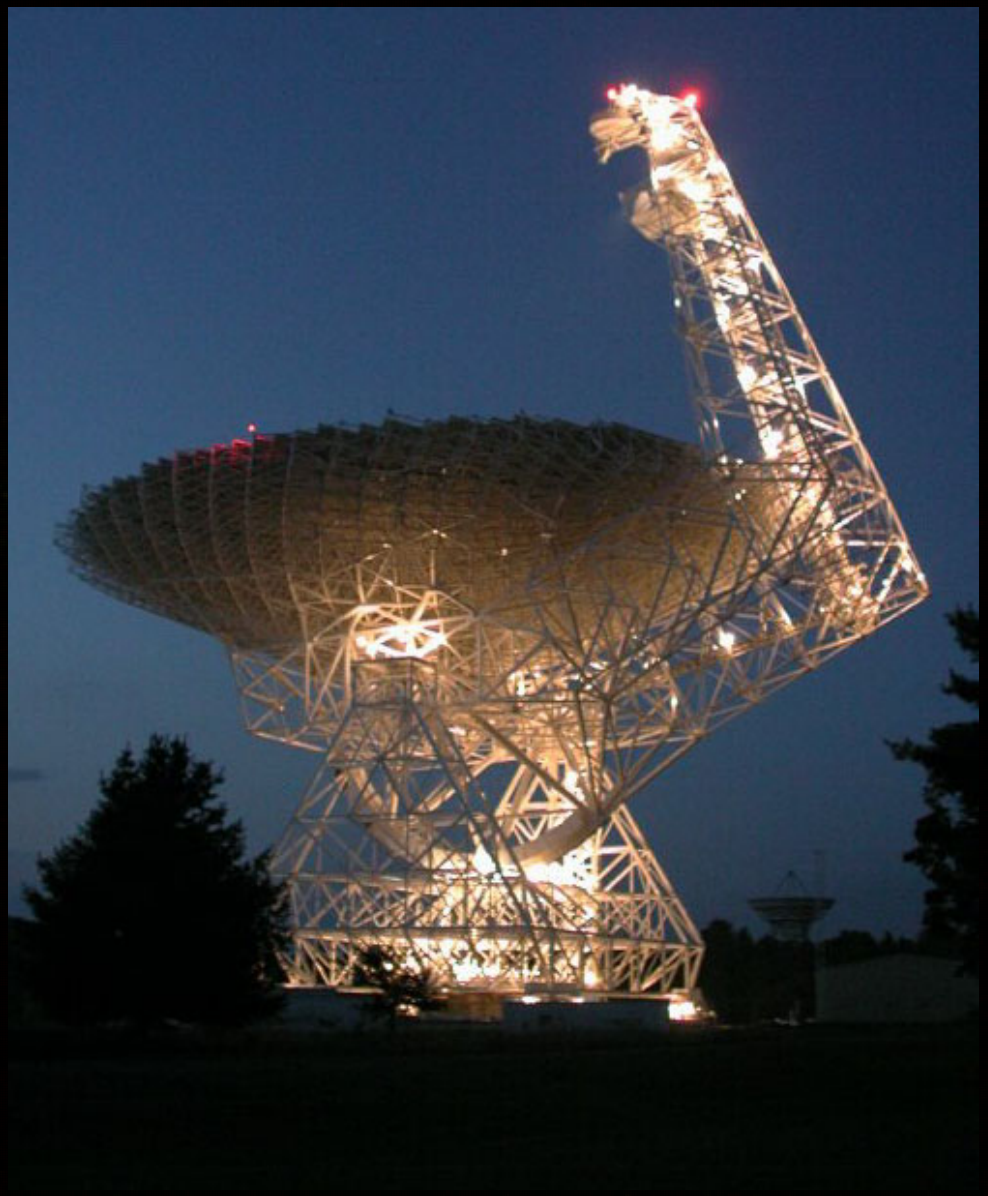
Q-band (38.2-49.8 GHz)

Sept 2006 to Jan 2007

OFF(2 min)-ON(2 min)

4 x 200 MHz windows

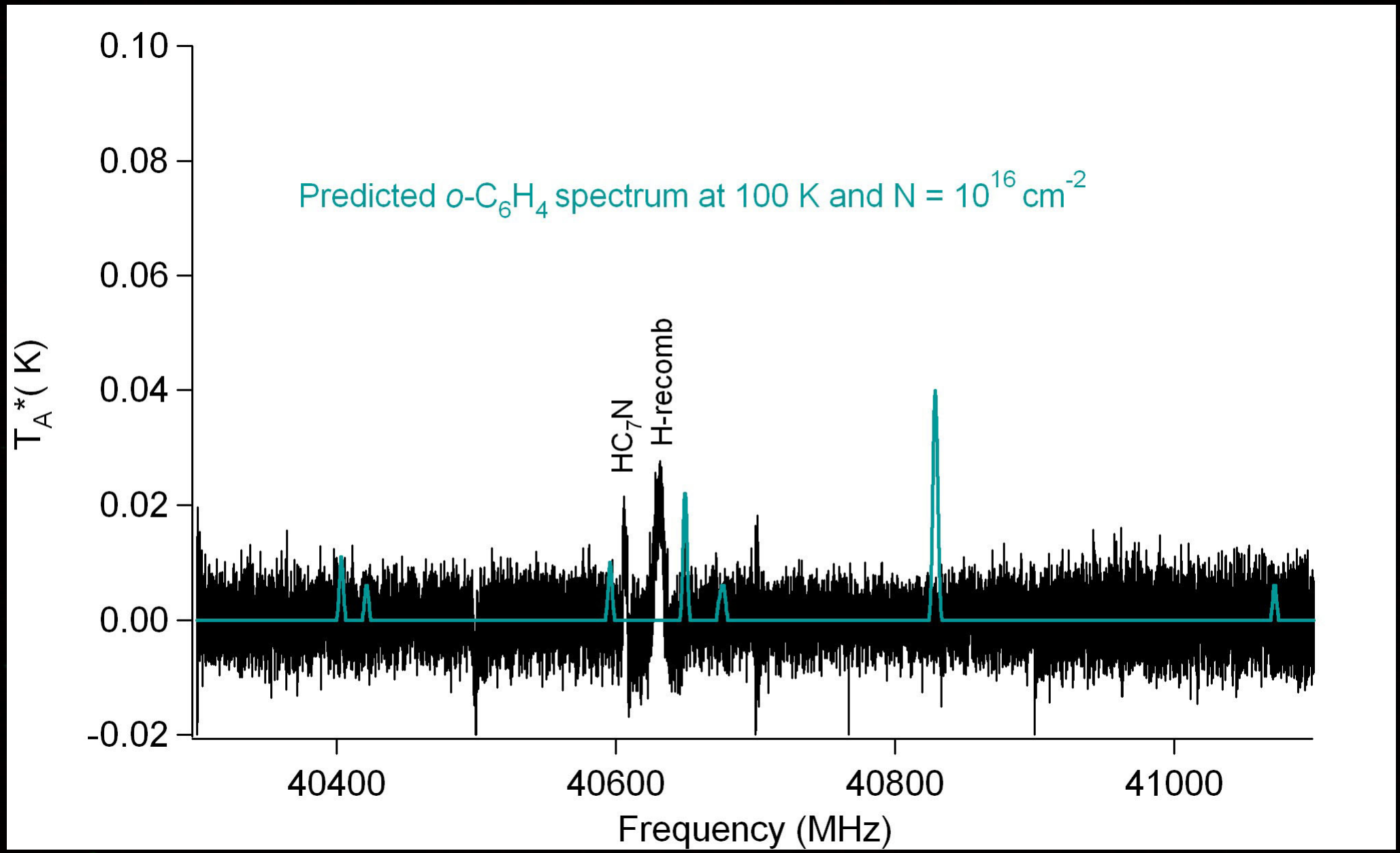
Spectral resolution ~24.4 kHz



o-C_6H_4 Upper Limits in CRL 618

	Transition	Frequency (MHz)	Ag_u (s^{-1})	E_u (K)	RMS (mK)	N_T Upper Limit (cm^{-2})
Ku	$4_{2,2}$ - $4_{1,3}$	13250.8230	6.08×10^{-7}	5.28	1.48	4.94×10^{15}
	$3_{3,1}$-$3_{2,2}$	13680.0050	3.59×10^{-7}	3.70	1.76	1.04×10^{16}
	$6_{5,1}$ - $6_{4,2}$	14608.9021	1.28×10^{-6}	12.37	1.45	3.01×10^{16}
	$3_{1,2}$ - $3_{0,3}$	14619.6969	2.40×10^{-7}	2.96	1.45	1.37×10^{16}
	$2_{0,2}$ - $1_{1,1}$	14753.9974	4.23×10^{-7}	1.19	1.45	7.02×10^{15}
K	$3_{0,3}$ - $2_{1,2}$	21770.7375	1.60×10^{-6}	2.26	2.47	6.93×10^{15}
	$4_{2,3}$ - $4_{1,4}$	21963.3591	7.93×10^{-7}	4.67	2.47	1.46×10^{16}
	$11_{8,3}$ - $11_{7,4}$	22142.0552	5.35×10^{-6}	37.44	2.18	2.62×10^{15}
	$9_{5,4}$ - $9_{4,5}$	22143.1890	4.10×10^{-6}	24.25	2.18	3.00×10^{15}
	$3_{1,3}$ - $2_{0,2}$	22216.3288	2.88×10^{-6}	2.26	2.18	3.45×10^{16}
	$7_{5,3}$ - $7_{4,4}$	23578.9636	5.35×10^{-6}	15.55	2.51	2.76×10^{15}
	$2_{2,1}$ - $1_{1,0}$	24109.5097	1.40×10^{-6}	1.77	1.76	6.74×10^{15}
	$3_{1,2}$ - $2_{2,1}$	24842.4030	8.22×10^{-7}	2.96	2.13	7.88×10^{15}
Q	$8_{2,6}$ - $8_{1,7}$	40403.3815	1.64×10^{-5}	16.25	6.42	3.58×10^{15}
	$8_{3,6}$ - $8_{2,7}$	40421.4144	9.83×10^{-6}	16.25	6.42	5.80×10^{15}
	$5_{1,4}$ - $4_{2,3}$	40595.9260	1.40×10^{-5}	6.62	5.92	3.43×10^{15}
	$22_{13,9}$ – $22_{12,10}$	40649.5538	1.13×10^{-4}	137.89	5.92	1.59×10^{15}
	$7_{1,6}$ - $7_{0,7}$	40674.4124	5.21×10^{-6}	11.45	5.92	9.73×10^{15}
	$7_{2,6}$ - $7_{1,7}$	40677.1133	8.69×10^{-6}	11.45	5.92	5.38×10^{15}
	$6_{0,6}$ - $5_{1,5}$	40828.1686	4.05×10^{-5}	7.23	6.21	1.13×10^{15}
	$6_{1,6}$ - $5_{0,5}$	40829.9929	2.43×10^{-5}	7.23	6.21	1.88×10^{15}
	$3_{3,0}$ - $2_{2,1}$	41071.9441	8.57×10^{-6}	3.74	9.40	7.57×10^{15}

The search for *o*-C_6H_4 with the GBT



Conclusions and Future Work

The *o*-benzyne N_T upper limit in CRL 618 is 1 x 10^{15} cm^{-2}.

The phenyl radical upper limit is 4 x 10^{15} cm^{-2} .

(McMahon et al. 2003, *ApJL* 530, L61)

Both are below the expected value of 10^{16} cm^{-2}!

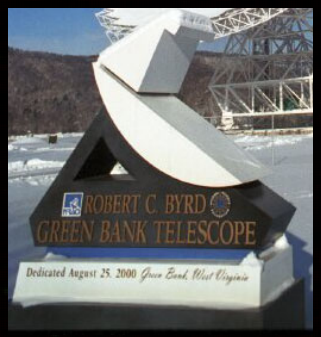
Clearly more work needs to be done:

- Confirmation of C_6H_6
- Searches for *o*-C_6H_4 in other sources
- Searches for C_6H_5
- New chemical models

Acknowledgements

National Radio Astronomy Observatory

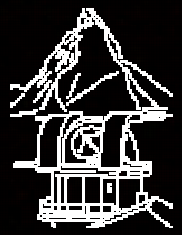
Green Bank Telescope Staff (especially Carl Bignell)



UIUC Astronomy & LAI/CARMA

NSF

CDMS



Michael Remijan