

# REPORT DOCUMENTATION PAGE

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MEMORANDUM FOR IN-HOUSE PUBLICATIONS

FROM: PROI (TI) (STINFO)

30 Apr 98

SUBJECT: Authorization for Release of Technical Information, Control Number: AFRL-PR-ED-TP-1998-095  
**J. Harper, J. Sheehy, J. Mills and Bill Larson** "Quantitative Analysis of the Condensation of  $B_n C_{n-1}$   
Clusters ( $n = 2-12, J = 0,1,2$ ) in Solid Argon" **HEDM Conference Presentation** (Statement A)

# Quantitative Analysis of the Condensation of

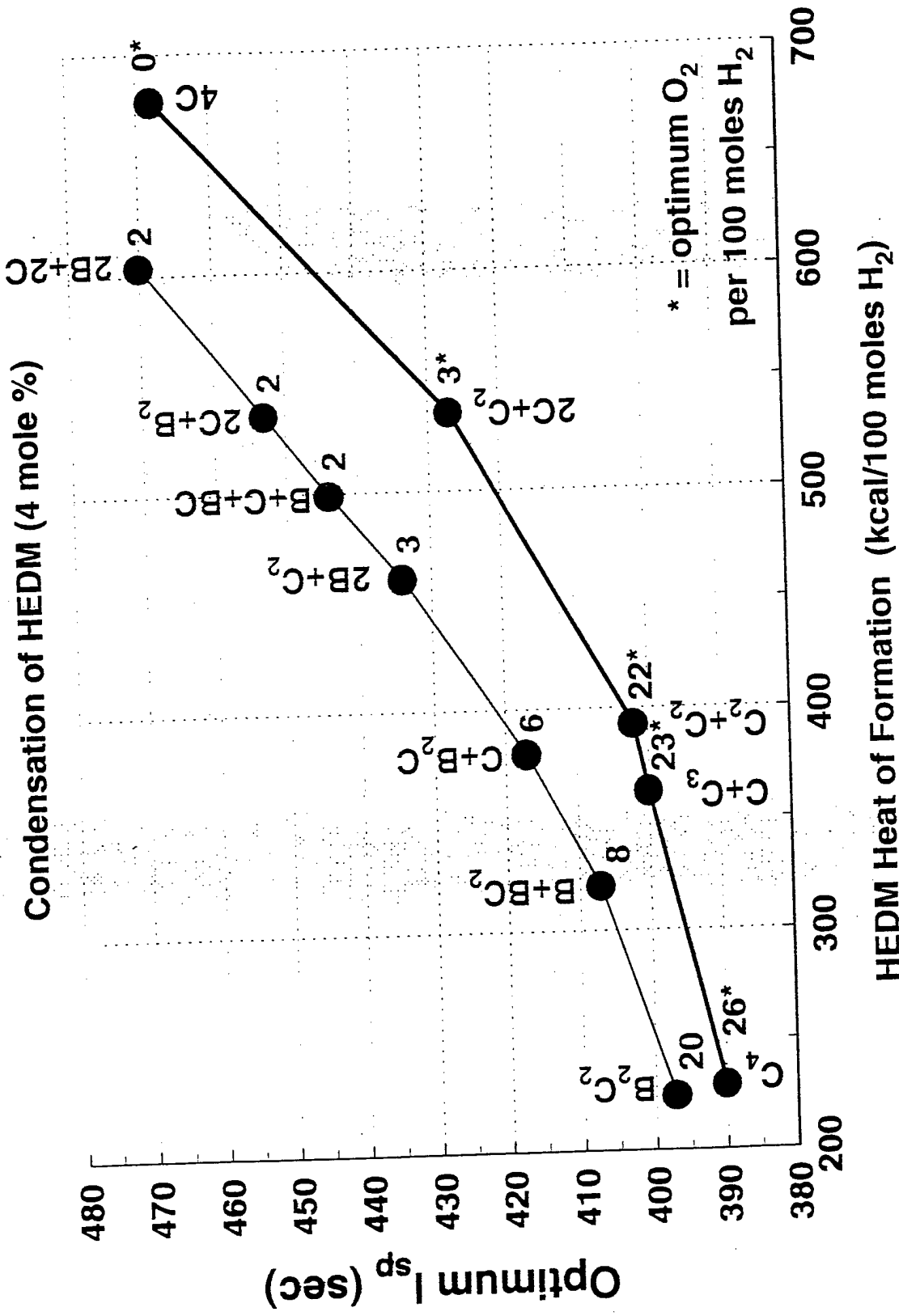
$B_J C_{n-J}$  Clusters ( $n = 2-12$ ,  $J = 0, 1, 2$ ) in

Solid Argon

J. Harper, J. A. Sheehy, J. D. Mills and C.W. Larson

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AFOSR HEDM Contractors' Conference  
Monterey, California  
20-22 May 1998



## Objective - 5% atoms in cryogenic matrix

### Approach

1. FTIR spectroscopy of  $B_nC_{n-j}$  clusters isolated in 10 K argon matrix
2. Ab-initio calculations of cluster
  - (a) normal mode frequencies and frequency shifts of their isotopomers
  - (b) infrared absorption intensities ( $\text{km mol}^{-1}$ )
3. Measurement of cluster distributions produced upon deposition and after annealing . Absolute column densities (molecules  $\text{cm}^{-2}$ ) from Beer's Law

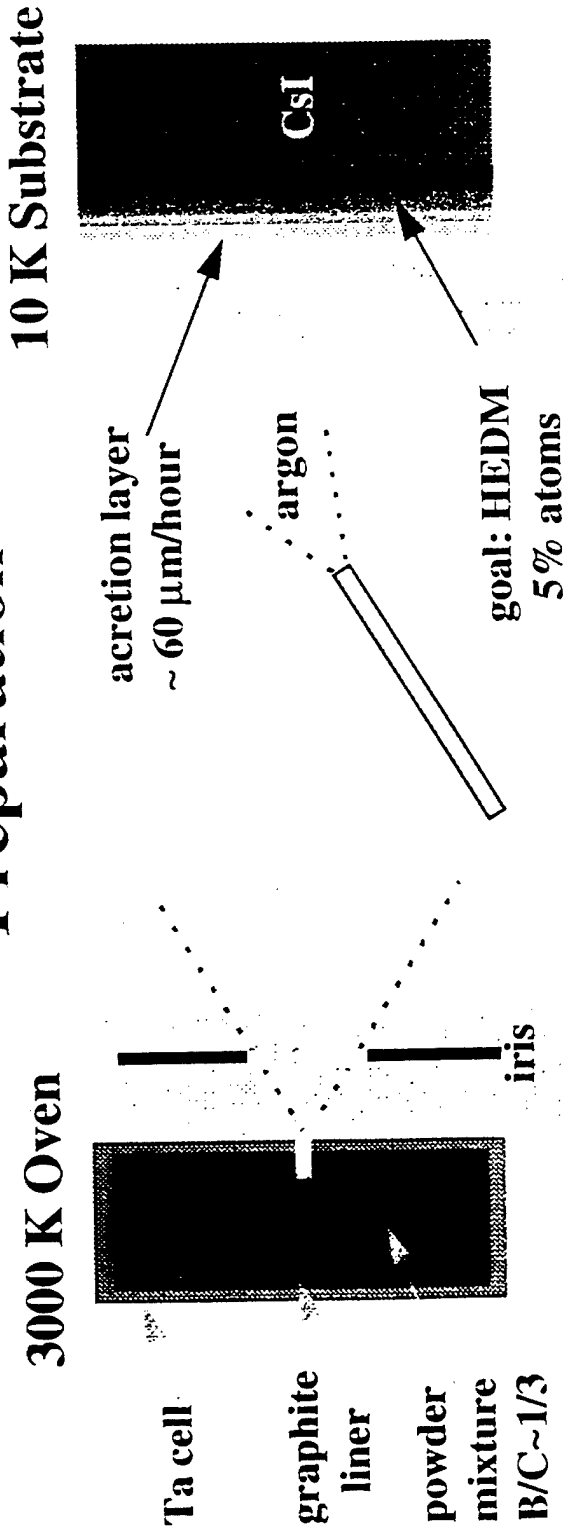
$$\langle \rho_l \rangle = \frac{A_{\text{exp}}}{I_{\text{theory}}} N$$

$$A_{\text{exp}} = - \int_{\nu} \ln \left[ \frac{E_t(\nu)}{E_0(\nu)} \right] d\nu$$

# Summary of $C_n$ and $B_J C_{n-J}$ clusters identified or analyzed

cyclic- $C_n$	n	J			
		linear- $C_n$ J=0	J=1	J=2	J=3
	2	$C_2$	BC	$B_2$	$B_3$ $B_3C$
$cC_4$	3	$C_3$	$BC_2$	$B_2C$	$B_3C_2$
$cC_6$	4	$C_4$	$BC_3$	$B_2C_2$ $B_2C_3$	$B_3C_3$
	5	$C_5$	$BC_4$	$B_2C_4$	$B_3C_4$
	6	$C_6$	$BC_5$	$B_2C_5$	$B_3C_5$
$cC_8$	7	$C_7$	$BC_6$	$B_2C_6$	$B_3C_6$
	8	$C_8$	$BC_7$	$B_2C_7$	$B_3C_7$
	9	$C_9$	$BC_8$	$B_2C_8$	$B_3C_8$
$cC_{10}$	10	$C_{10}$	$BC_9$	$B_2C_9$	$B_3C_9$
	11	$C_{11}$	$BC_{10}$	$B_2C_{10}$	$B_3C_{10}$
	12	$C_{12}$	$BC_{11}$	$B_2C_{11}$	
$cC_{12}$	13	$C_{13}$	$BC_{12}$		

# Preparation



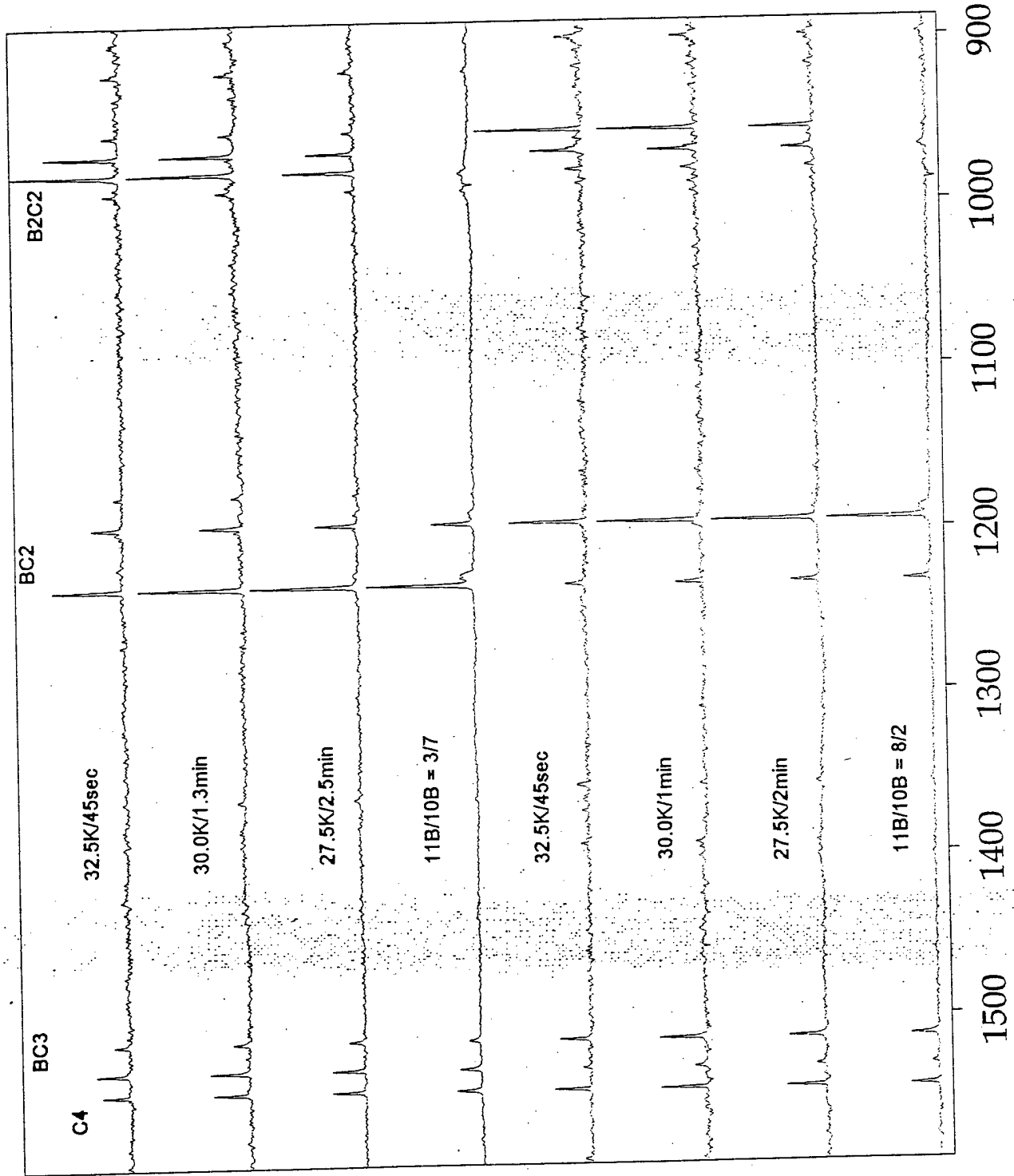
# Annealing

a0	10 K	a3	32.5 K, 60 s	a6	40.0 K, 20 s
a1	27.5 K, 120 s	a4	35.0 K, 45 s	sublimation	
a2	30.0 K, 90 s	a5	37.5 K, 20 s	rate ~ 1 μm/s	

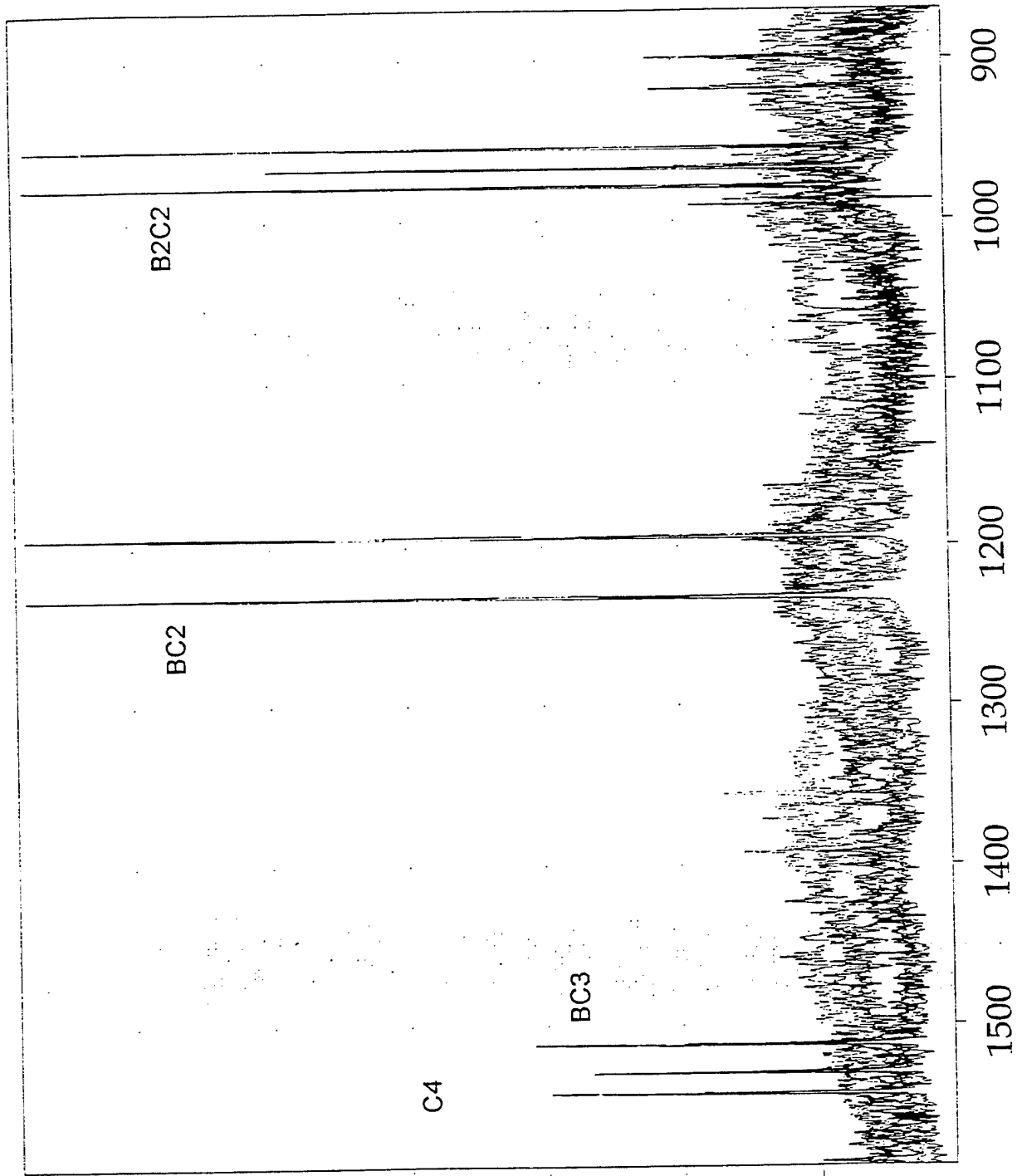
# Precision matched pair of matrices

Green Matrix	$^{11}\text{B}/^{10}\text{B} = 80/20$	enhanced $^{11}\text{B}_j\text{C}_{n-j}$
Red Matrix	$^{11}\text{B}/^{10}\text{B} = 27/73$	enhanced $^{10}\text{B}_j\text{C}_{n-j}$

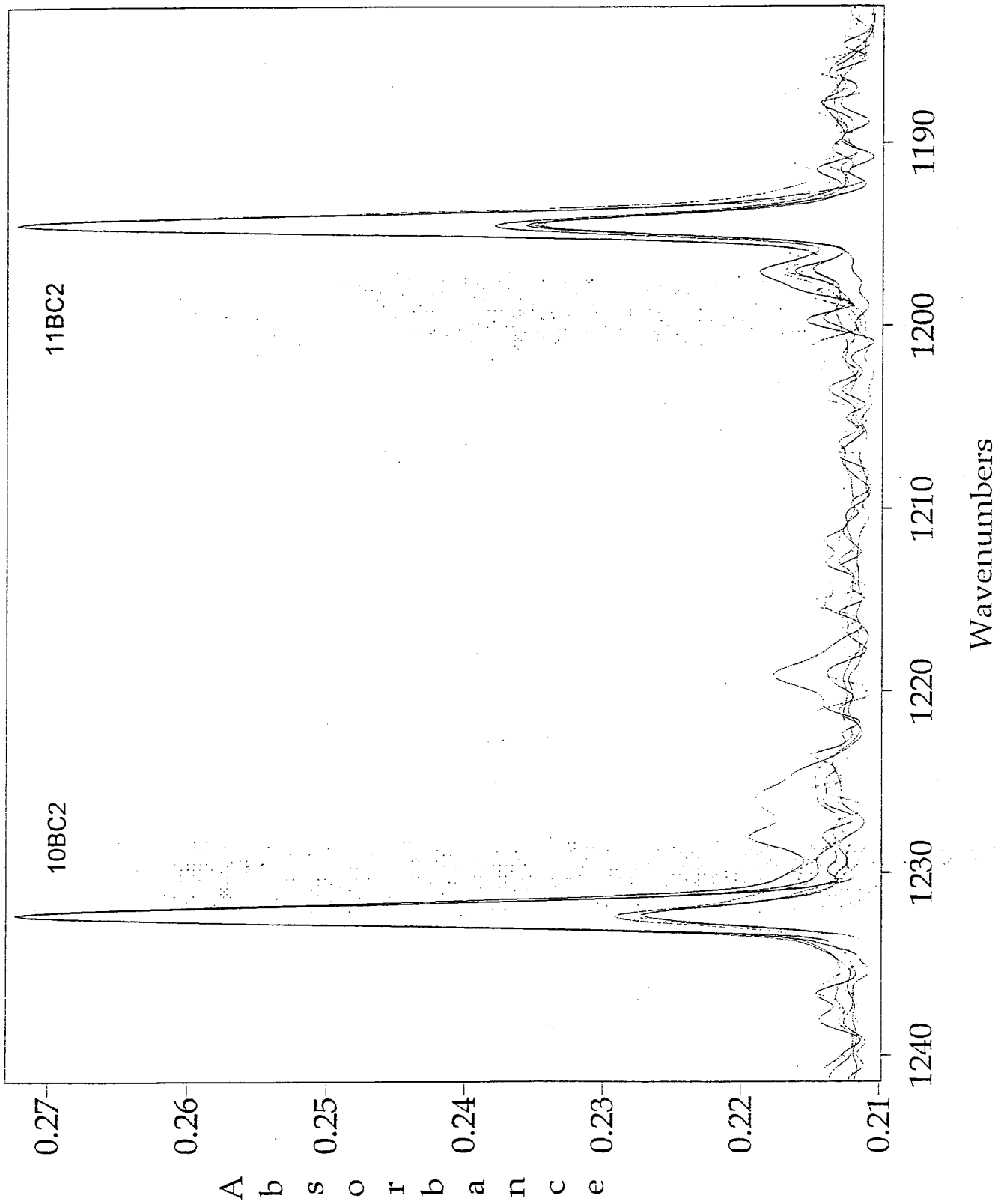
A s o r b a n c e

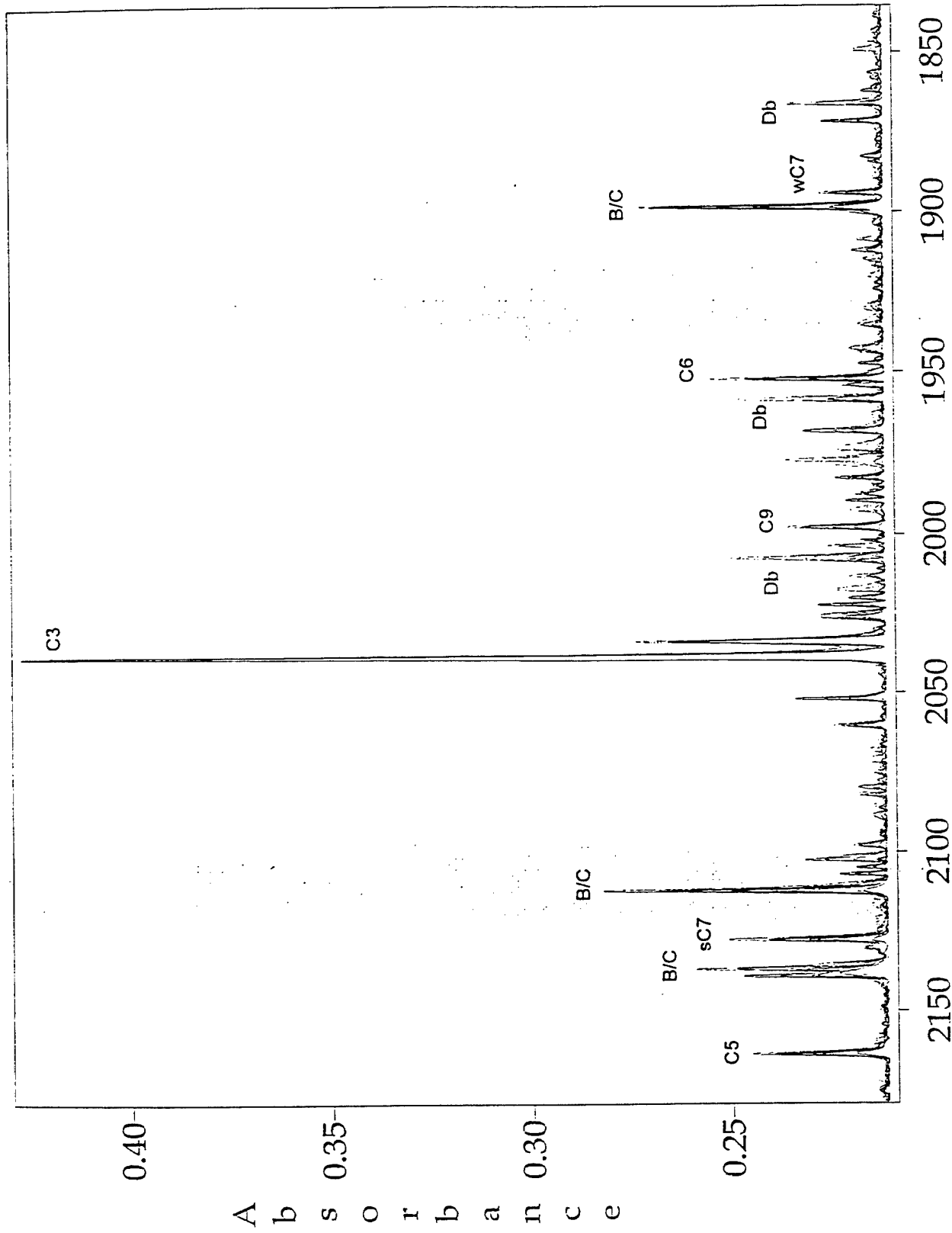


A 0.43-  
b 0.42-  
s 0.41-  
o 0.41-  
r 0.41-  
b 0.40-  
a 0.40-  
n 0.39-  
c 0.39-  
e 0.38-

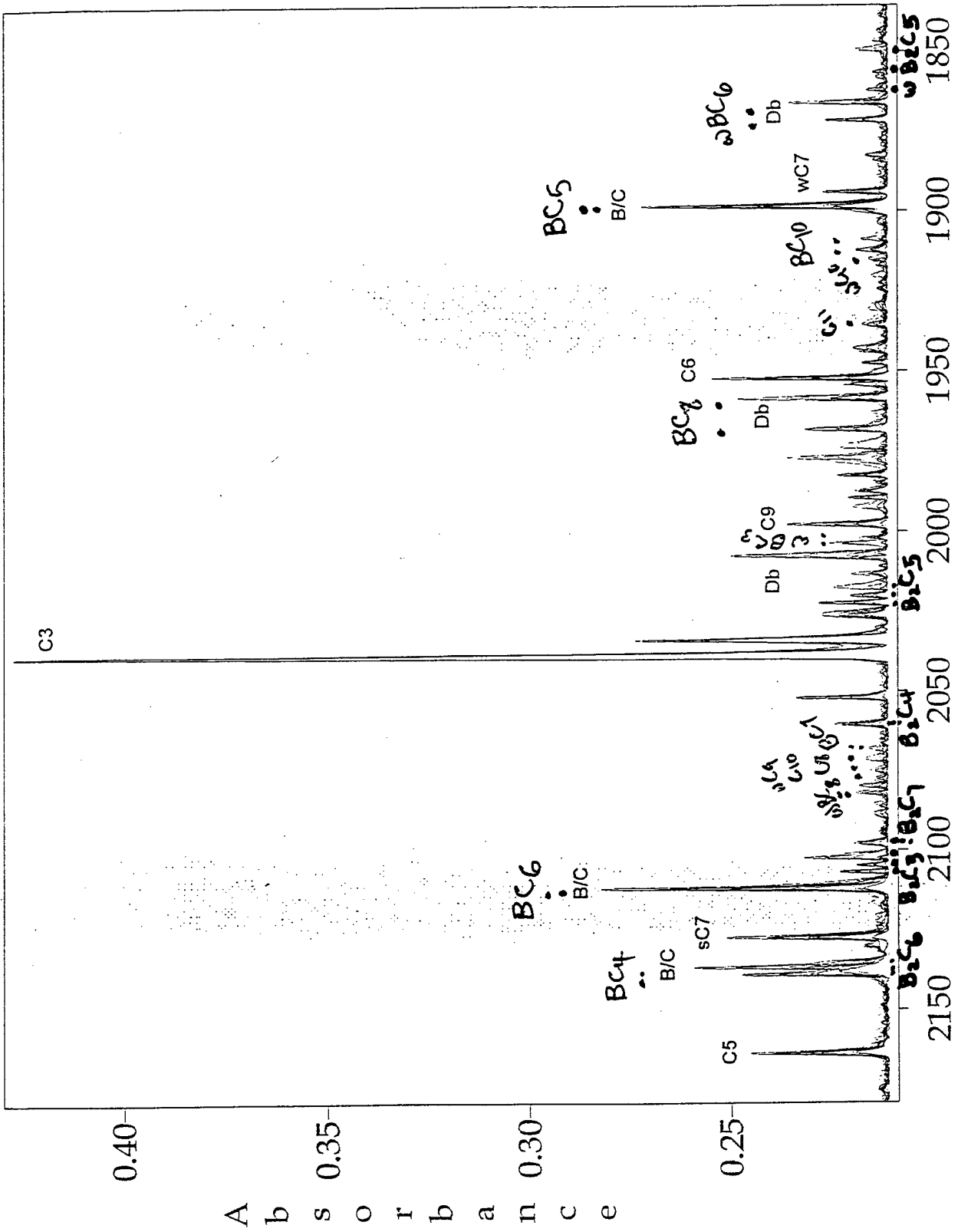


Wavenumbers





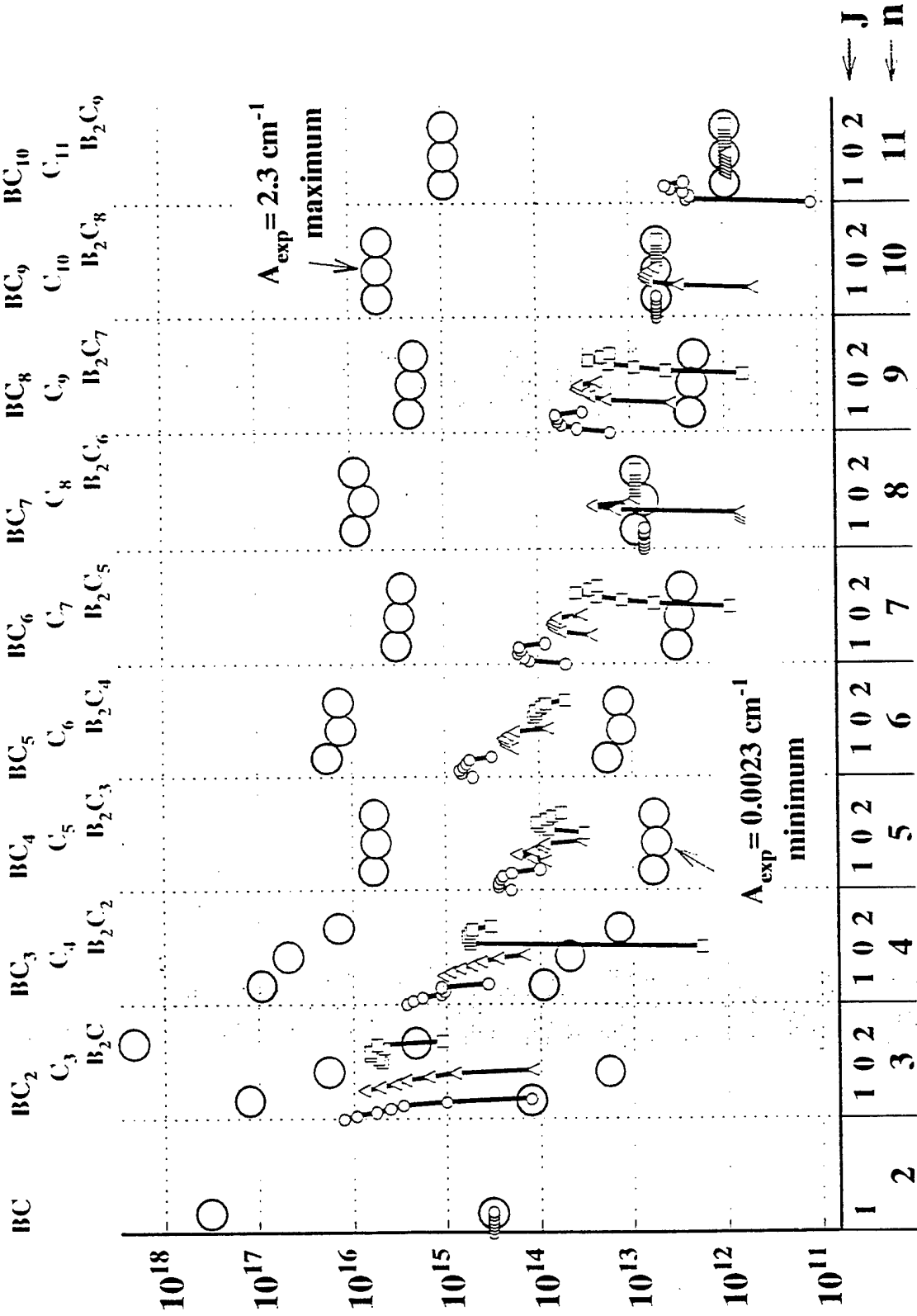
Wavenumbers



Wavenumbers

Column density (molecules  $\text{cm}^{-2}$ )

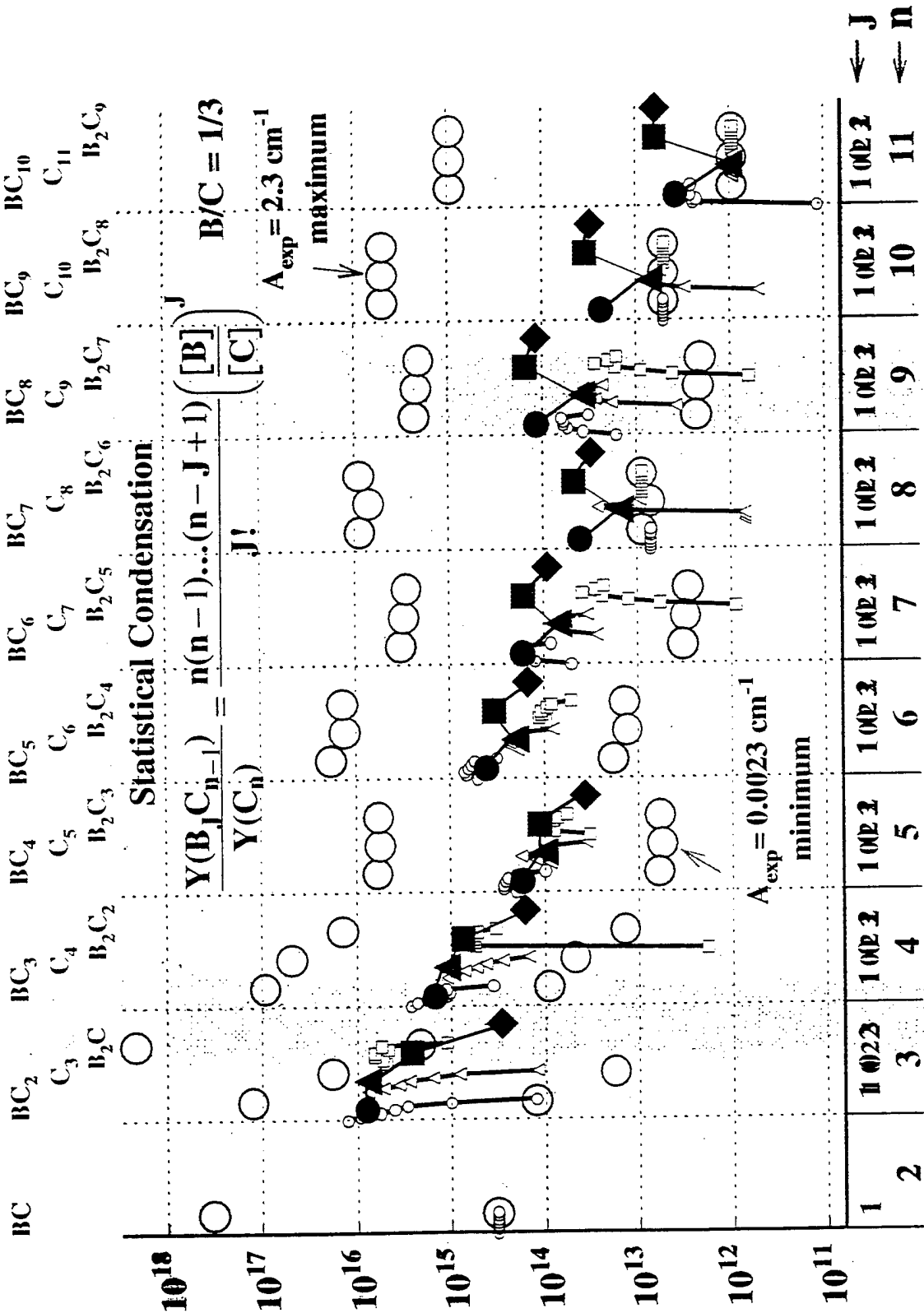
GREEN



Cluster  $B_J C_{n-J}$

Column density (molecules cm<sup>-2</sup>)

GREEN



Cluster  $B_J C_{n-J}$

## Conclusions

1.  $C_3$  is linear but  $BC_2$ ,  $B_2C$  and  $B_3$  are cyclic.
2.  $n > 3$ ;  $J = 0$ , 1, 2 clusters are linear. Boron atoms cap the ends of linear chains.
3.  $J = 0$ , 1, 2 substitution in  $n \geq 5$  clusters does not significantly affect IR intensities.
4. For  $n \geq 5$  the absorption intensity of even  $n$  clusters is two to three times smaller than that of odd  $n$  clusters.
5.  $B_2C_2$  grew most dramatically upon annealing.  $BC$  was not detected. Its upper limit column density is comparable to that of  $n = 4$  clusters.  $B_2C_2$  sources may be  $2BC$  or  $B + BC_2$  but  $C + B_2C$  does not form  $B_2C_2$ .
6.  $n = 3, 4$ ;  $J = 0$ , 1 clusters disappear upon annealing but  $J = 2$  clusters either grow or remain unchanged. Capping the ends of clusters with boron seems to render them inert to further condensation.
7. Statistical cluster distributions are apparent in  $n = 4$  and 5 clusters.  $B_2C$  yields are too high and  $B_2C_{n-2}$  yields are too low in larger  $n \geq 6$  clusters.
8.  $n \geq 5$  clusters grow upon annealing and larger clusters grow more than smaller clusters.