

# Mechanism of Thermal Decomposition of Bisphenol C Polycarbonate: Nature of Its Fire Resistance

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# Flammability Rating

Polymers	H. R. Capacity (J/g*K)	Total heat released (kJ/g)	Char yield (%) at 930°C	T <sub>onset</sub> (°C)
PE	1558	40.4	0	456
PS	1199	37.4	0	387
Nylon 66	648	28.1	0	413
PPO	553	22.4	23.4	439
PET	393	17.3	7.8	409
PC	382	19.3	16.7	481
PMMA	376	23.4	0	245
Kevlar	292	15.2	31.8	555
POM	261	14.2	0	345
PEEK	163	12.9	46.0	557
Polyphenyl sulfone	156	12.3	41.5	538
ULTEM	121	11.8	49.2	
PHA	42	10.3	56.1	586
PI	29	8.5	50.1	533
PBZT	24	5	57.8	693
BPC PC	18	5.7	53.0	455

# BPC PC Pyrolysis: Key Experimental Observations<sup>1,2</sup>

$$T_{\text{onset}} = 450^{\circ} \text{C}$$

Char Yield = 50 % (mass)

$$\Delta H_{\text{decomp.}} = -20 \text{ kcal/mol}$$

Decomposition Products: HCl, CO<sub>2</sub>

1. Stewart, J. *Ph.D. Dissertation*; University of Massachusetts, Amherst; **1999**.
2. Ramirez M. L. *M.S. Thesis*; University of Puerto Rico; **2000**.

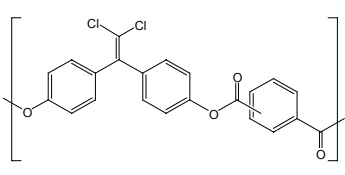
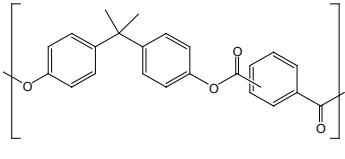
# Identification of BPC PC Decomposition Pathways by means of Quantum Chemistry

Method: B3LYP/6-31G(d)<sup>3</sup>

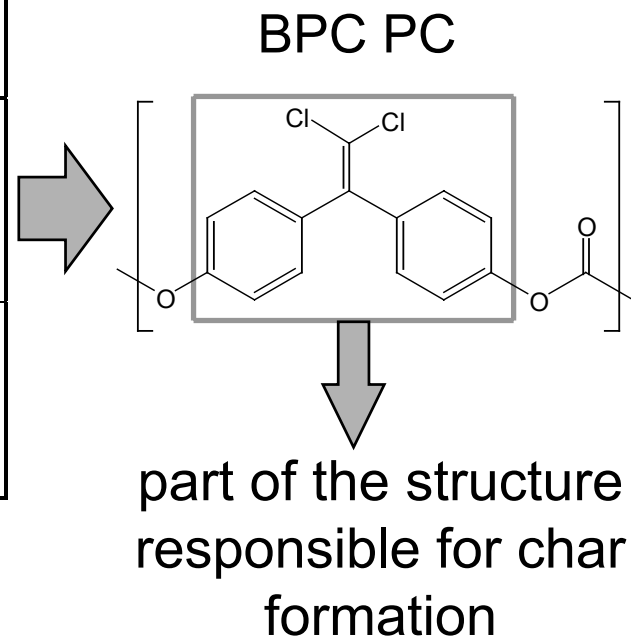
Computation Routine: Selection of model compounds  
Search for transition states and intermediates  
Optimization of molecular structures, calculation of energies and vibrational frequencies  
Verification of identified reaction paths

3. Becke, A. D. *J. Chem. Phys.* **1993**, 98: 5648.

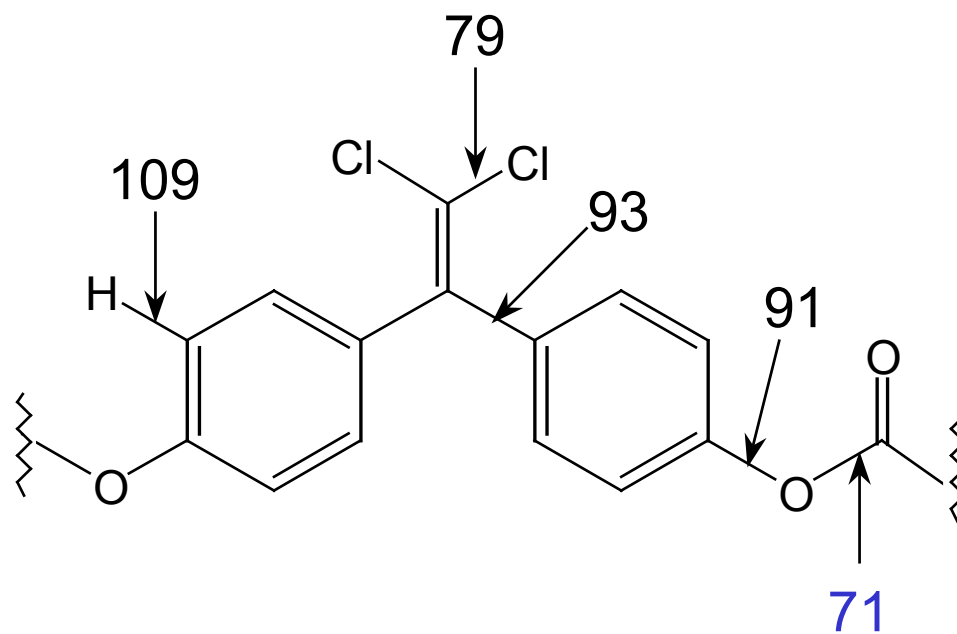
# Selection of Model Compound

Structure	Heat Release Capacity J/(g*K)	Char Yield % (mass) at 930°C
	18	50
	486	2

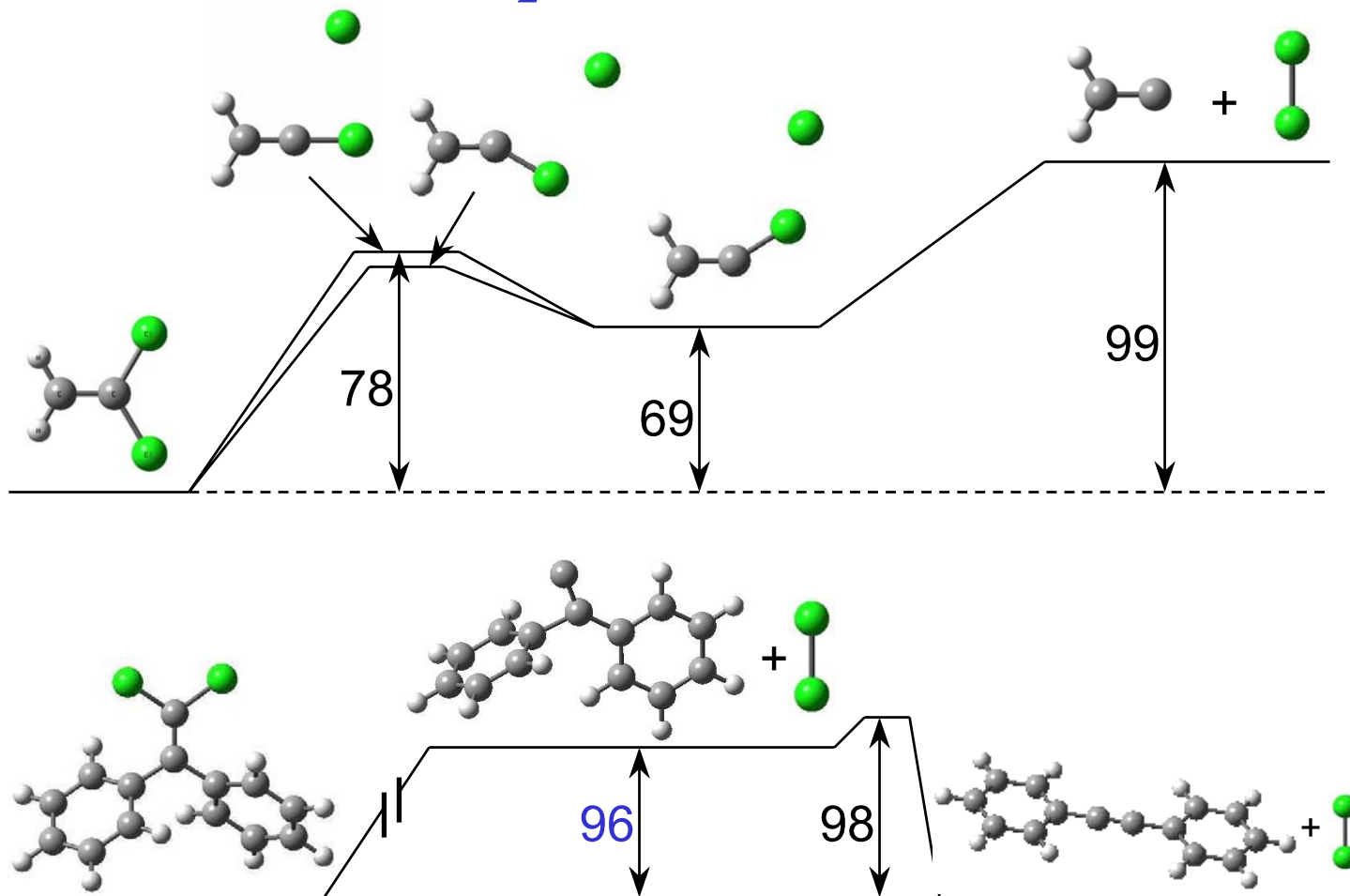
Stewart, J. *Ph.D. Dissertation.*



## Calculated Bond Energies (kcal/mol)

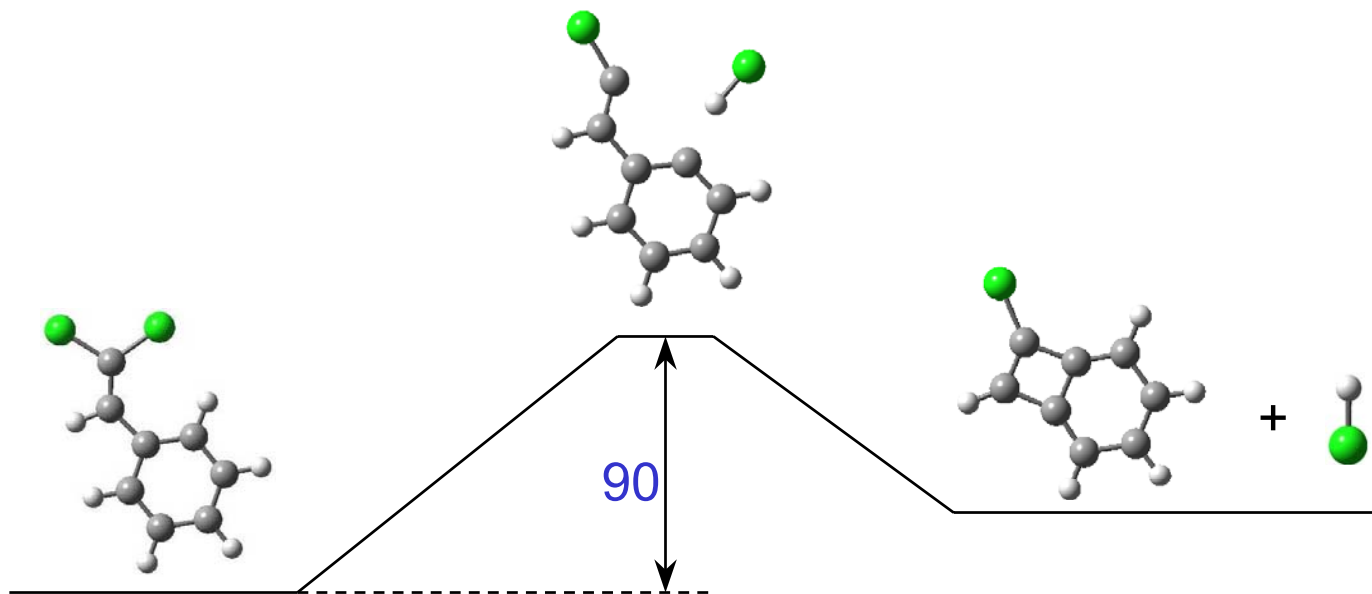


# Cl<sub>2</sub> Elimination



Energy values are in kcal/mol

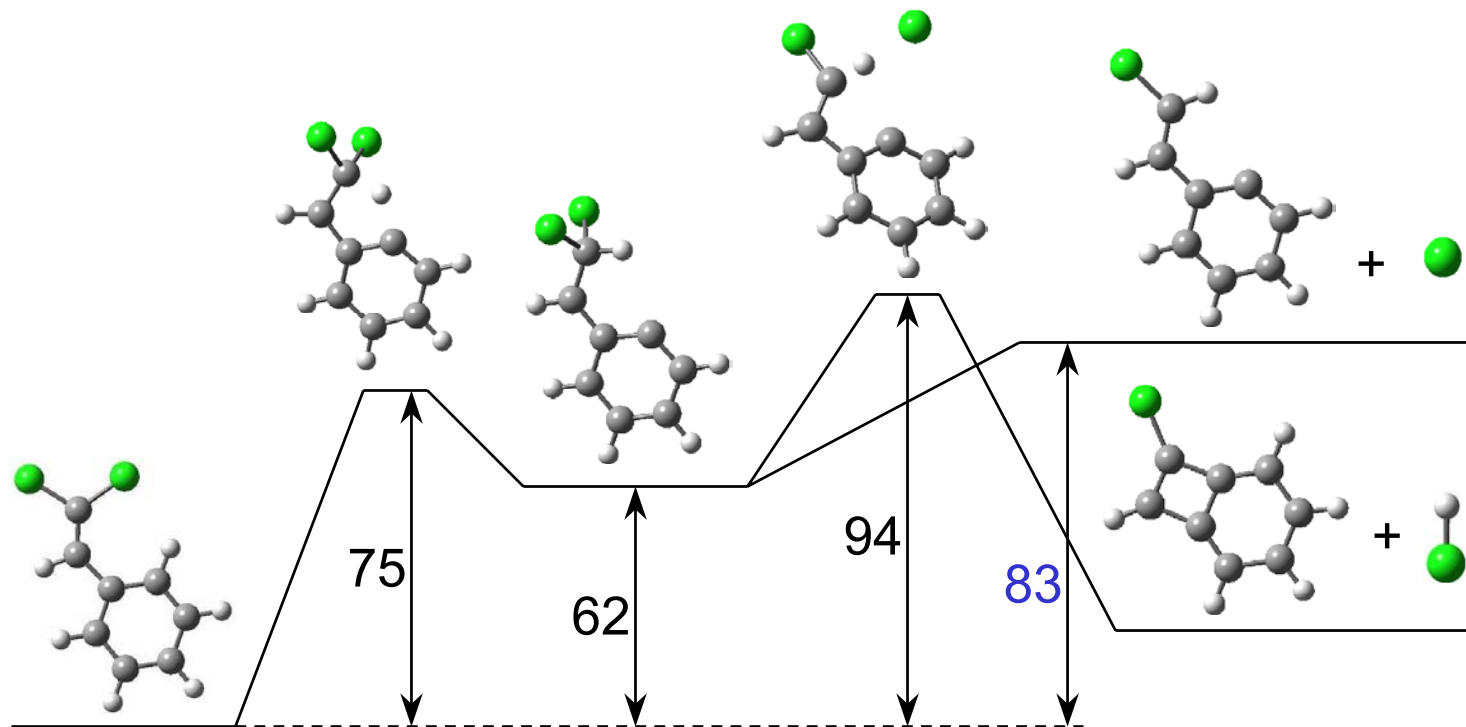
# HCl Elimination



Energy values are in kcal/mol

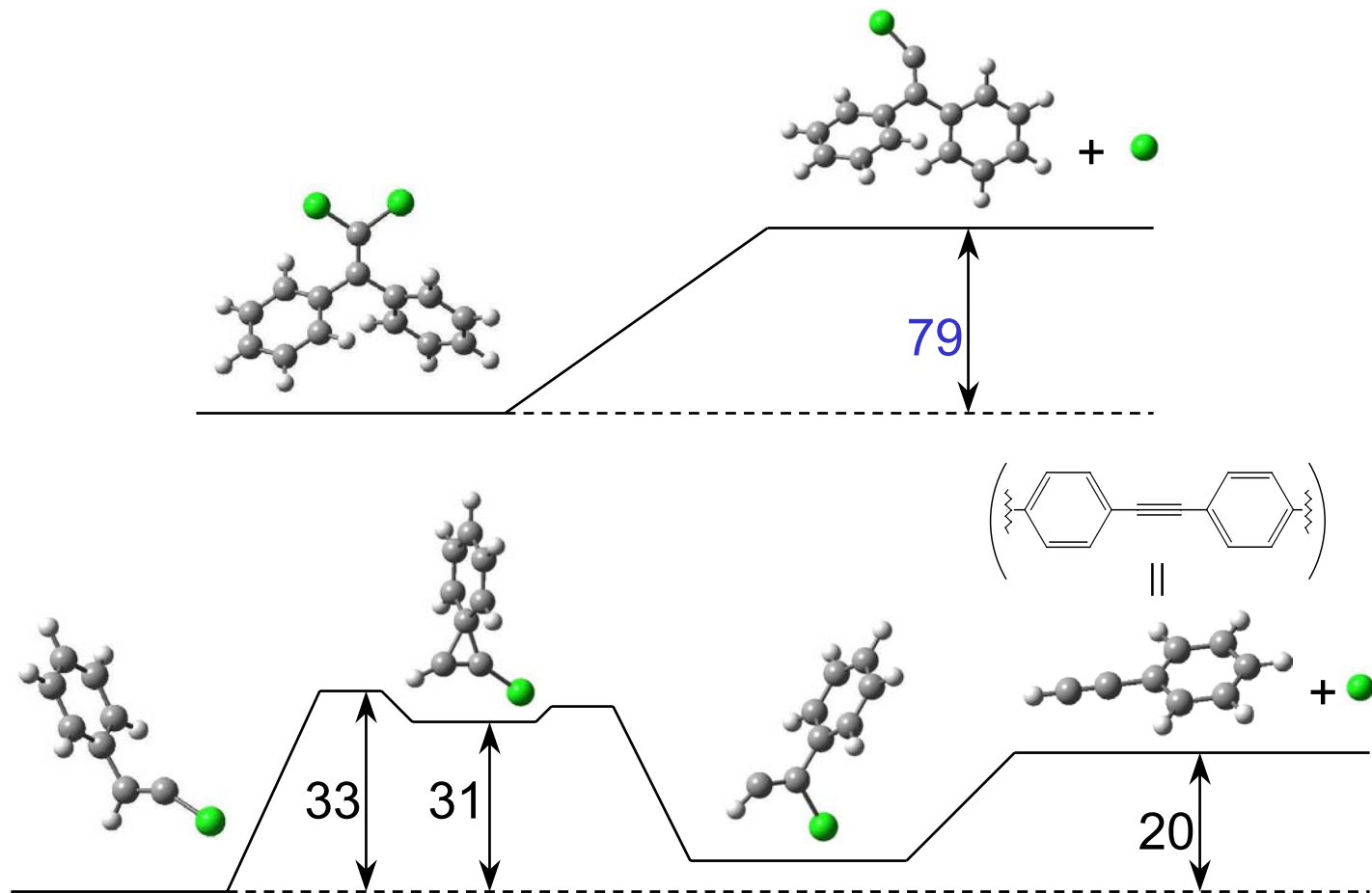


# H-atom Shift



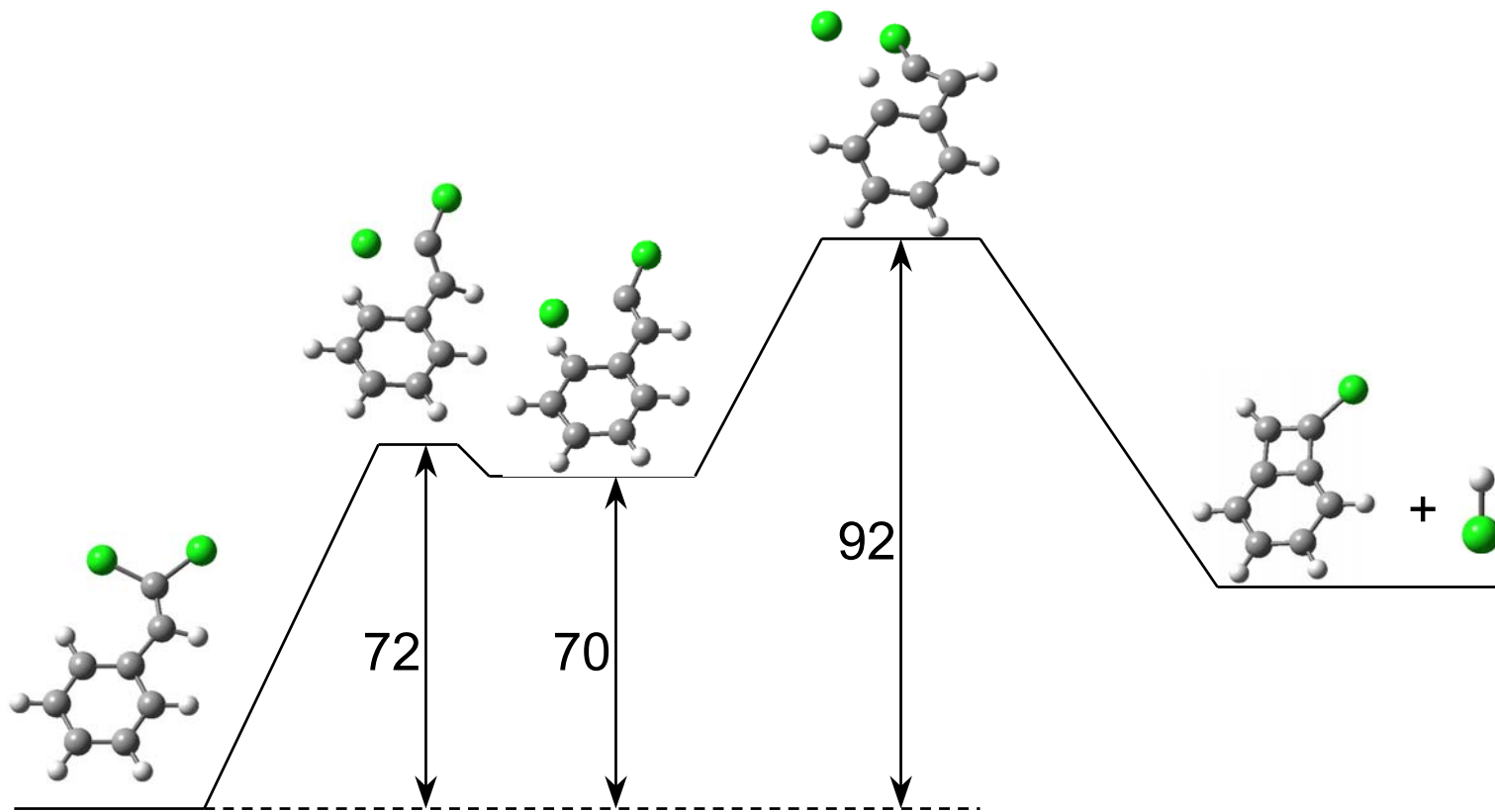
Energy values are in kcal/mol

# Cl-atom Elimination



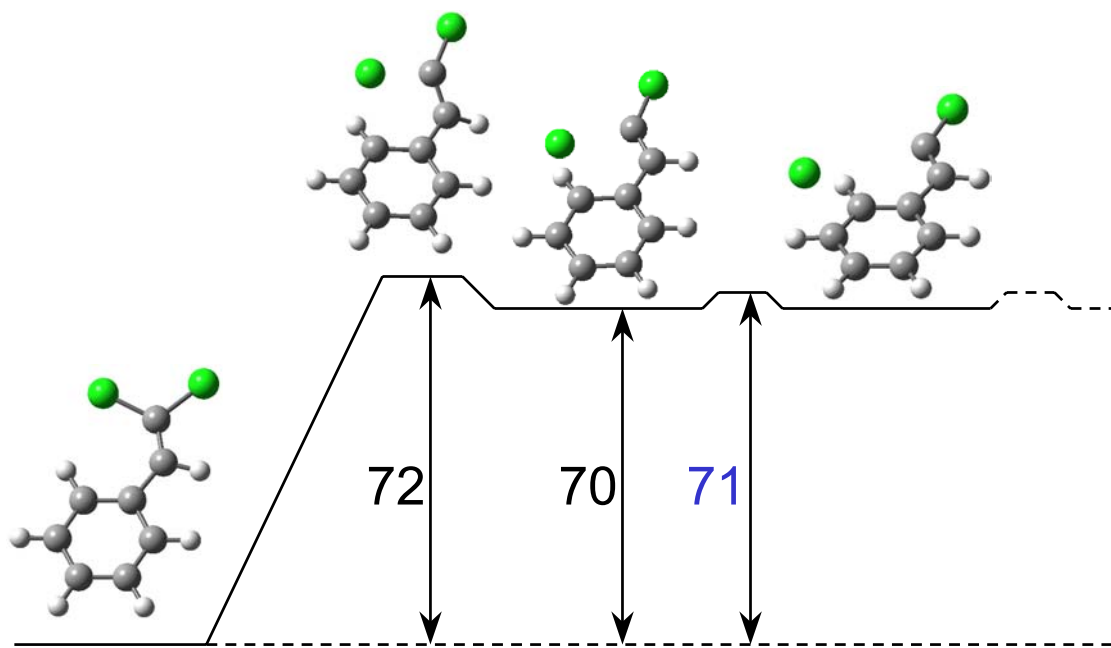
Energy values are in kcal/mol

# Cl-atom Shift



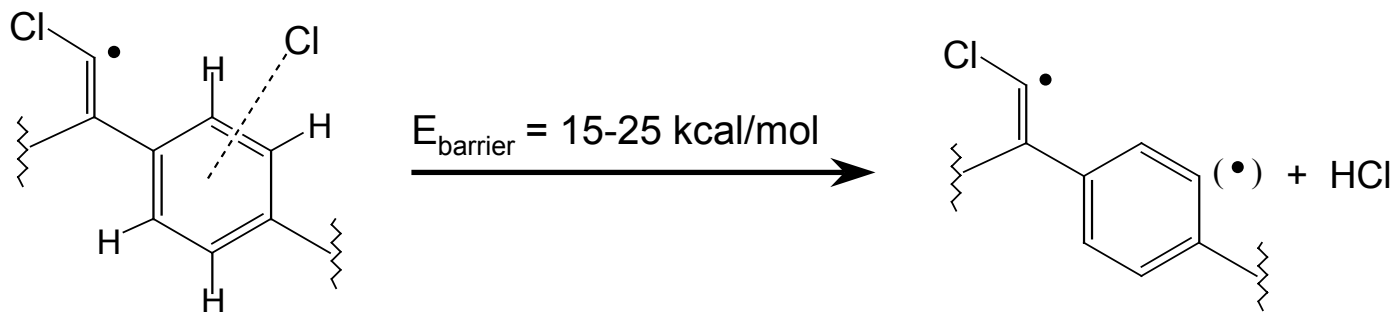
Energy values are in kcal/mol

# Cl-atom Shift



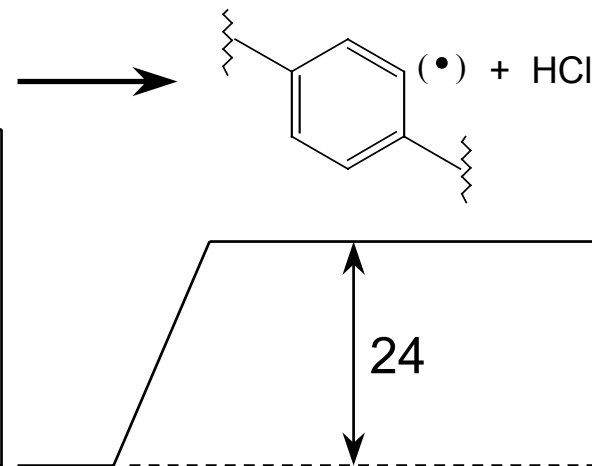
Energy values are in kcal/mol

# Phenol-Cl Intermediate



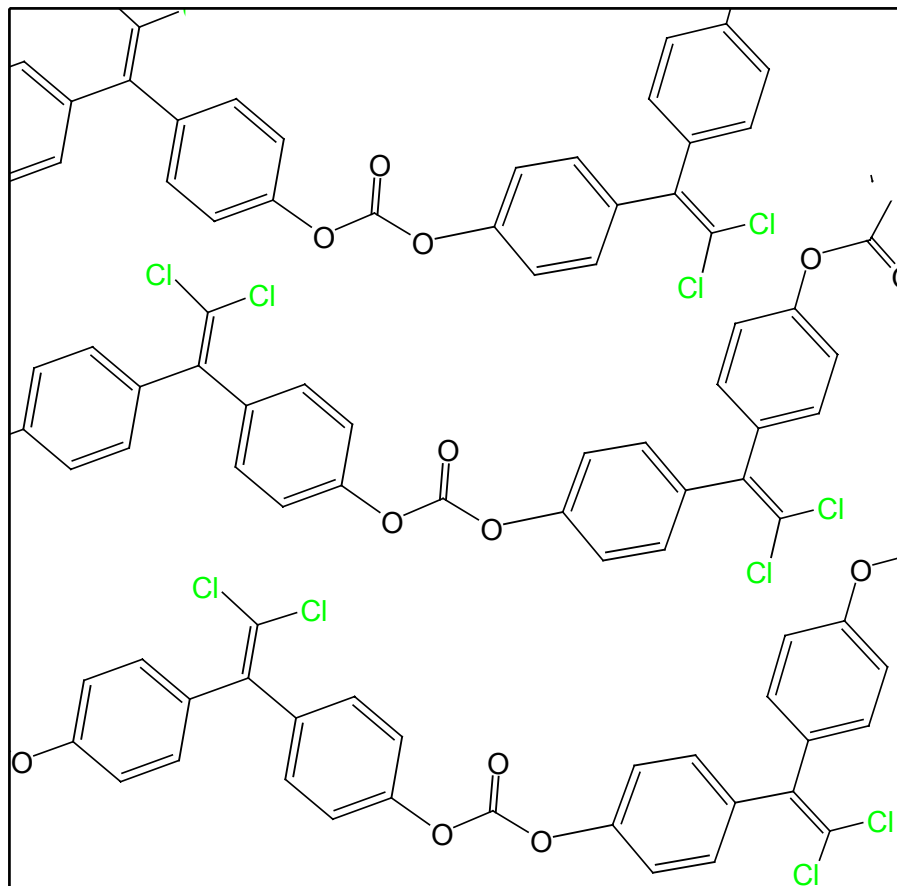
Cl forms complexes with other phenol rings

Bn-Cl BE*	10	6	6

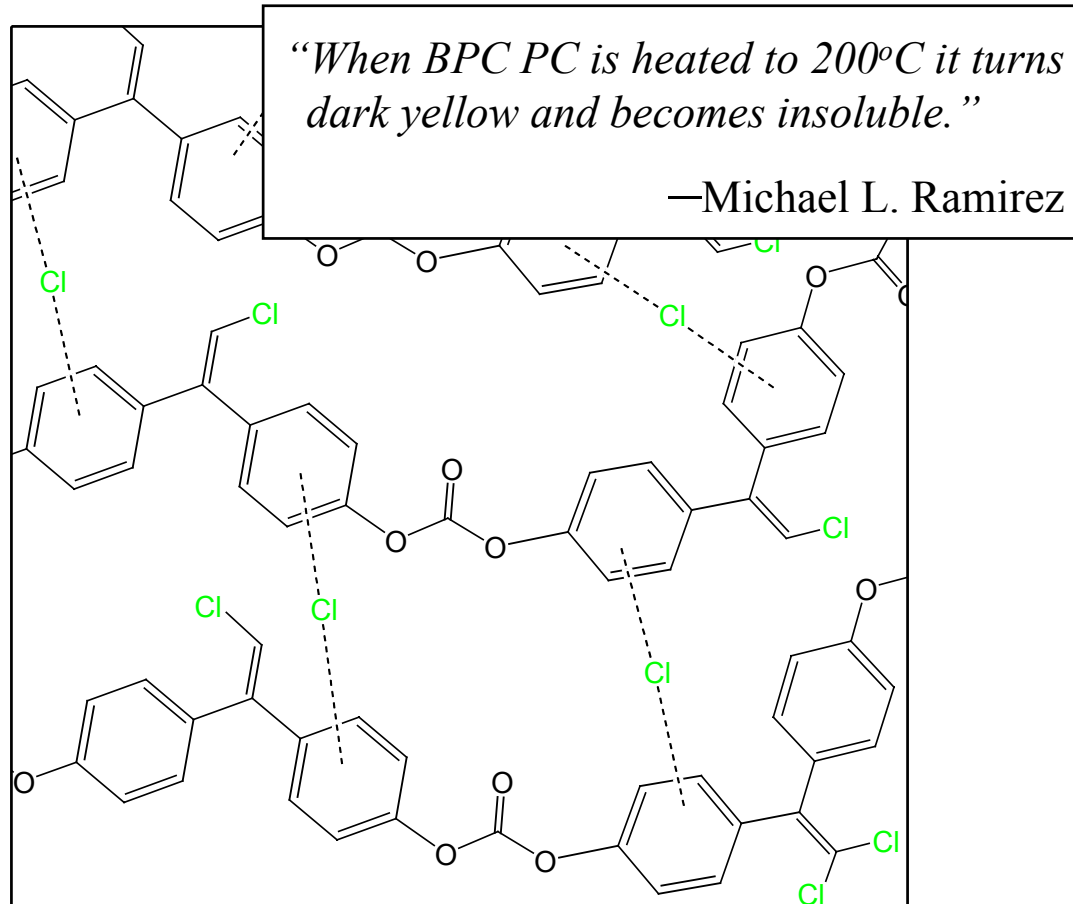


\* Benzene-Cl bond energy in kcal/mol

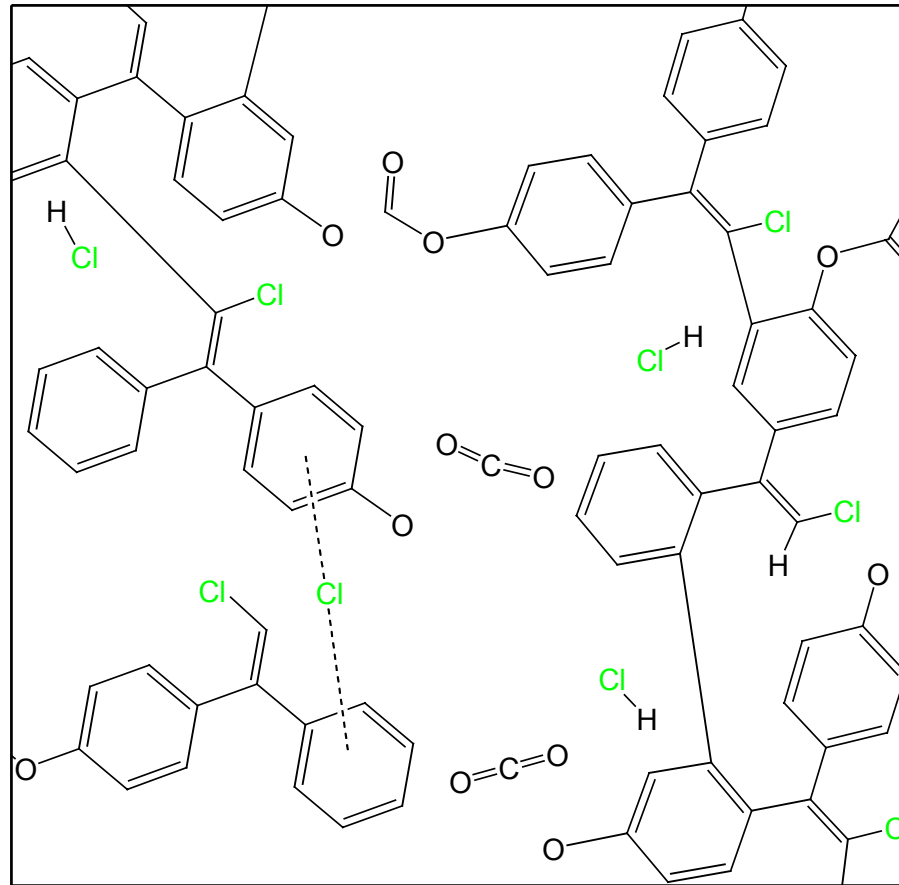
# Mechanism of Decomposition of BPC PC



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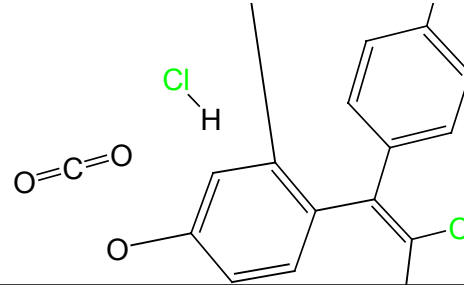
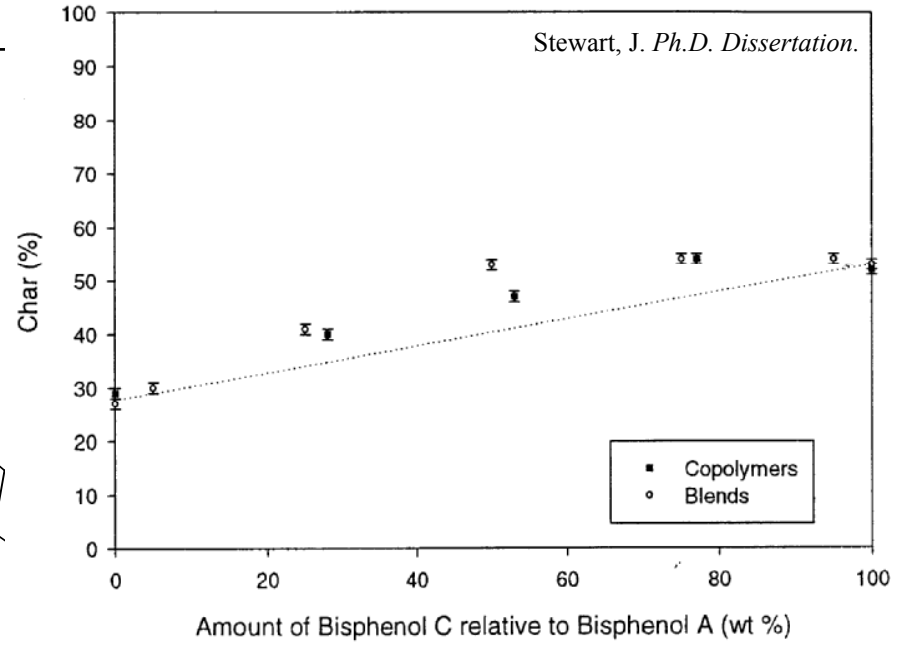
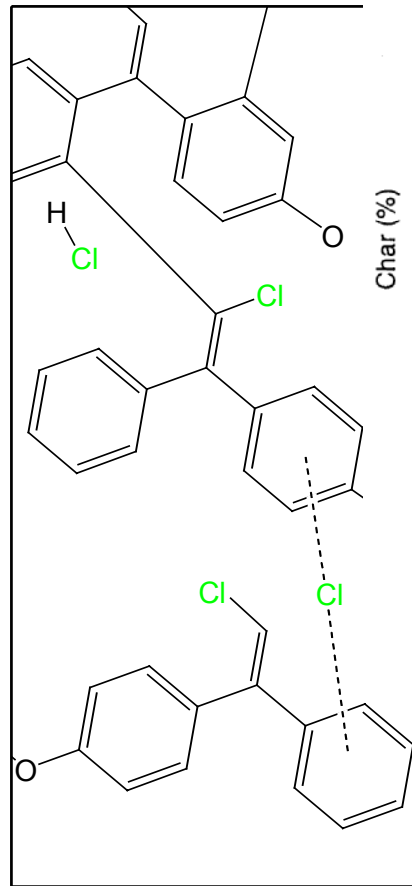


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