

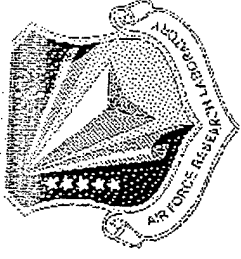
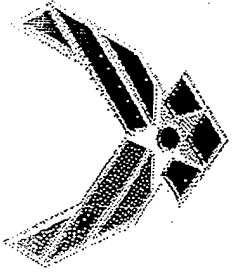
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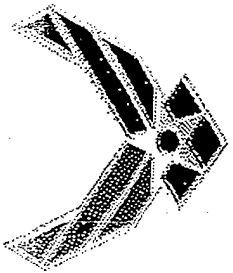
IL QC QSPR - Preliminary Results

Jeffrey D. Mills

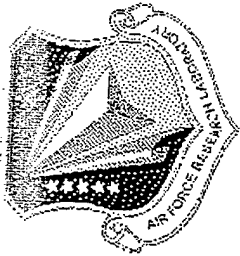
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AFRL/PRSP

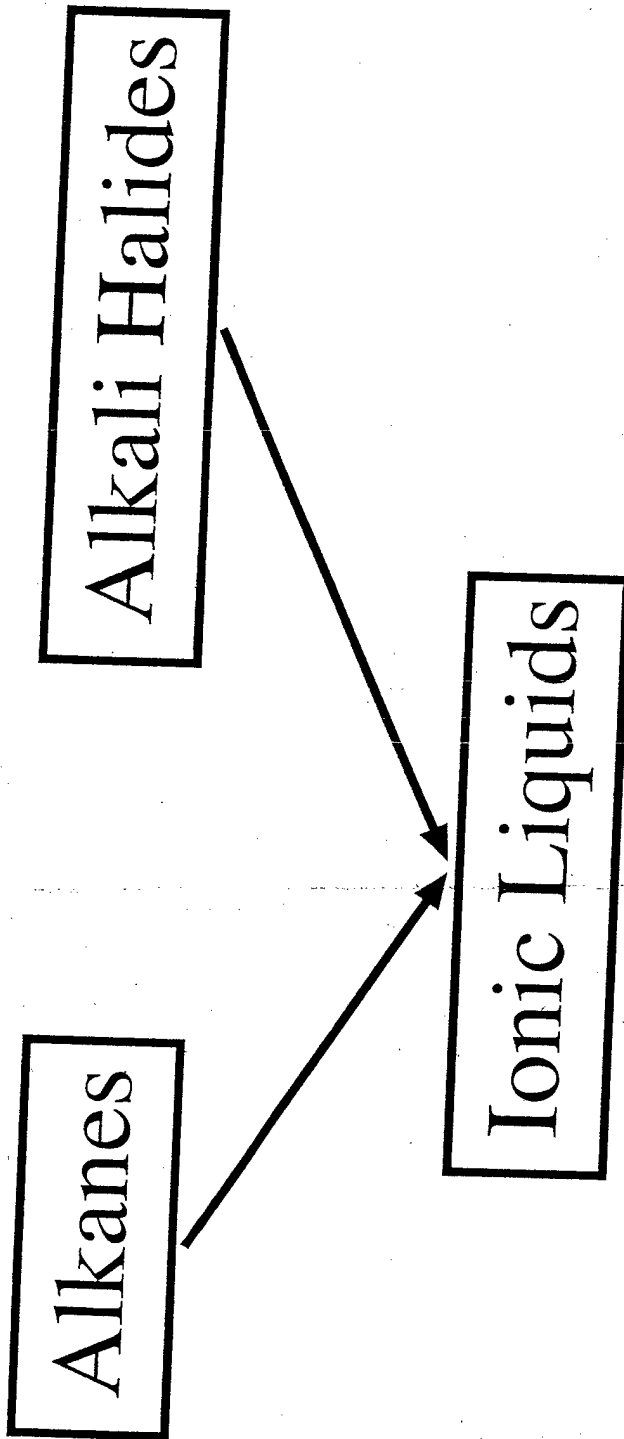
Air Force Research Laboratory
Space and Missile Propulsion Division
Propellants Branch

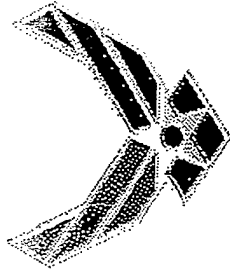


QSPR

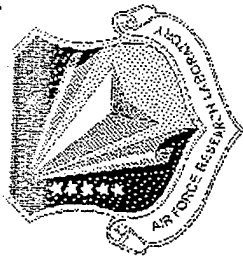


Quantitative Structure-Property Relationships Property (Descriptor)





Property (Descriptor)

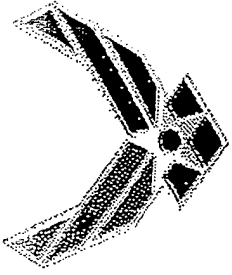


Properties:

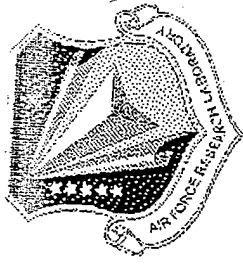
Melting Point
Density (liquid)
(Decomp. Temp.)
(Impact Sensitivity)
(Density (Solid))
(Others ??)

QC Descriptors:

- Single Particle:
Surface Electrostatic
Potential
Surface Size and Shape
- Pair:
Separation
Binding Energy



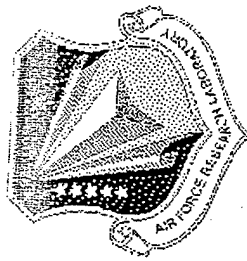
Constraints/Goals



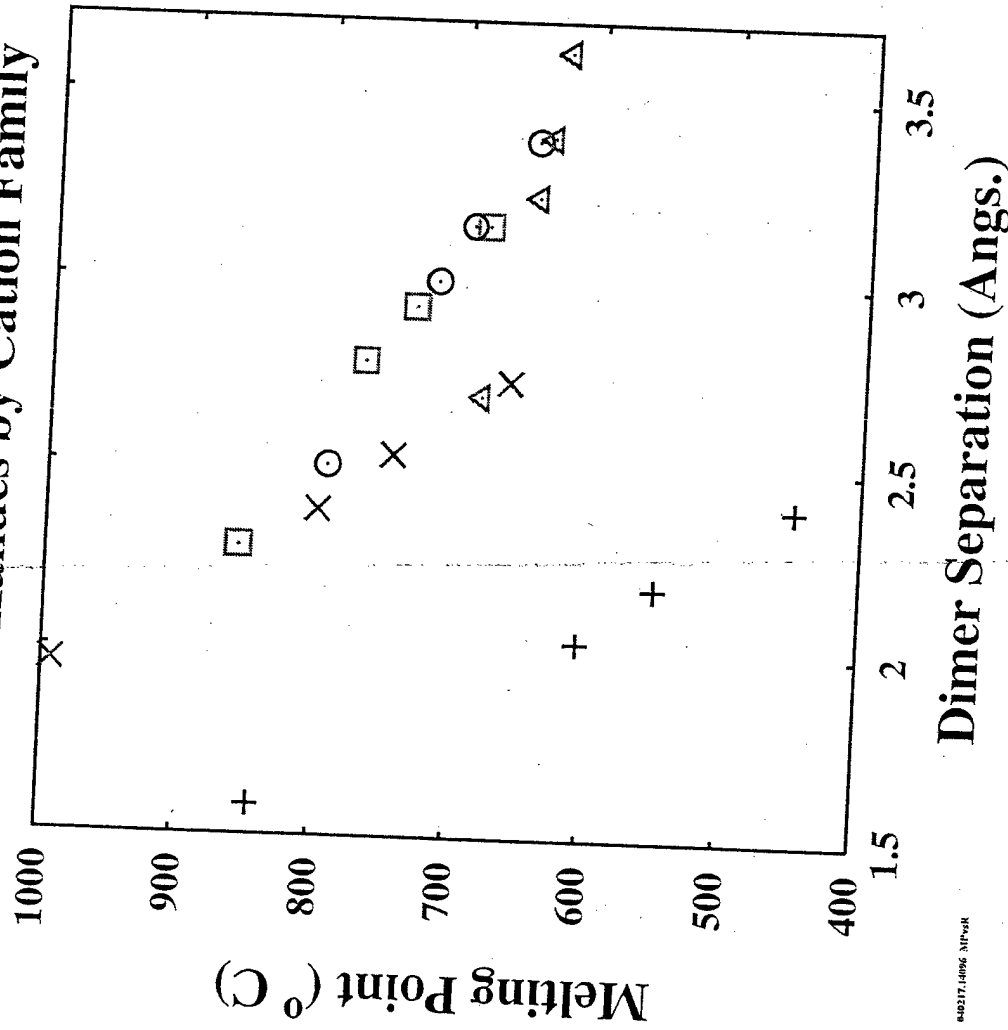
1. Predictive (not just summarize or interpolate)
2. "Universal" Descriptors (Ionic and Nonionic)
3. Allow Ion Interchangability
4. Physically Meaningful and Chemically Ignorant
 - a. No "Kitchen-Sink" Fits
 - b. Charge Symmetry



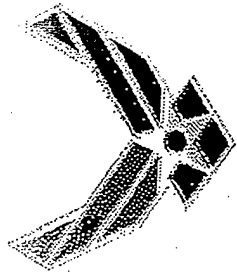
Cation Families Summarized



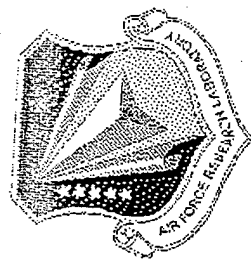
Alkali Halides by Cation Family



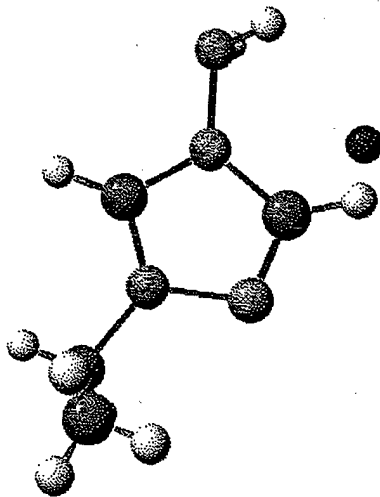
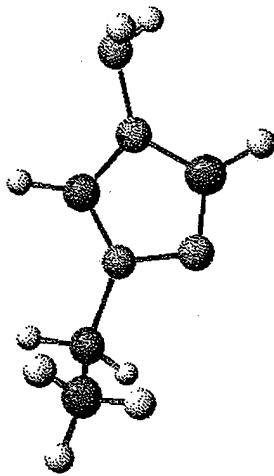
640317-1-696 31P/5K

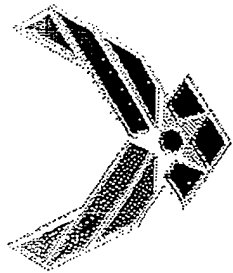


Structures

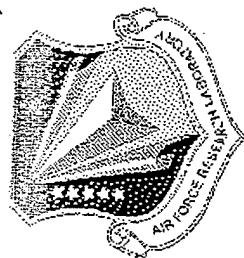


1-Ethyl-4-amino-1,2,4-triazolium Cation
B3LYP 6-311++G(d,p): Crystal (with Br⁻):







Surface Electrostatic Potential




Color Map: V at 0.001 au Electron Density:

kcal/mol


 350.0

 291.7

 233.3

 175.0

 116.7

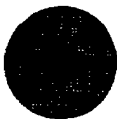
 58.3

 0.0

Li⁺:



Na⁺:



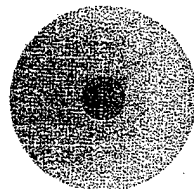
K⁺:

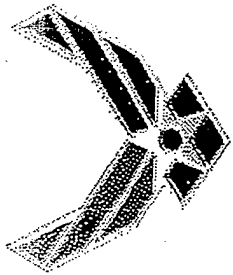


Rb⁺:

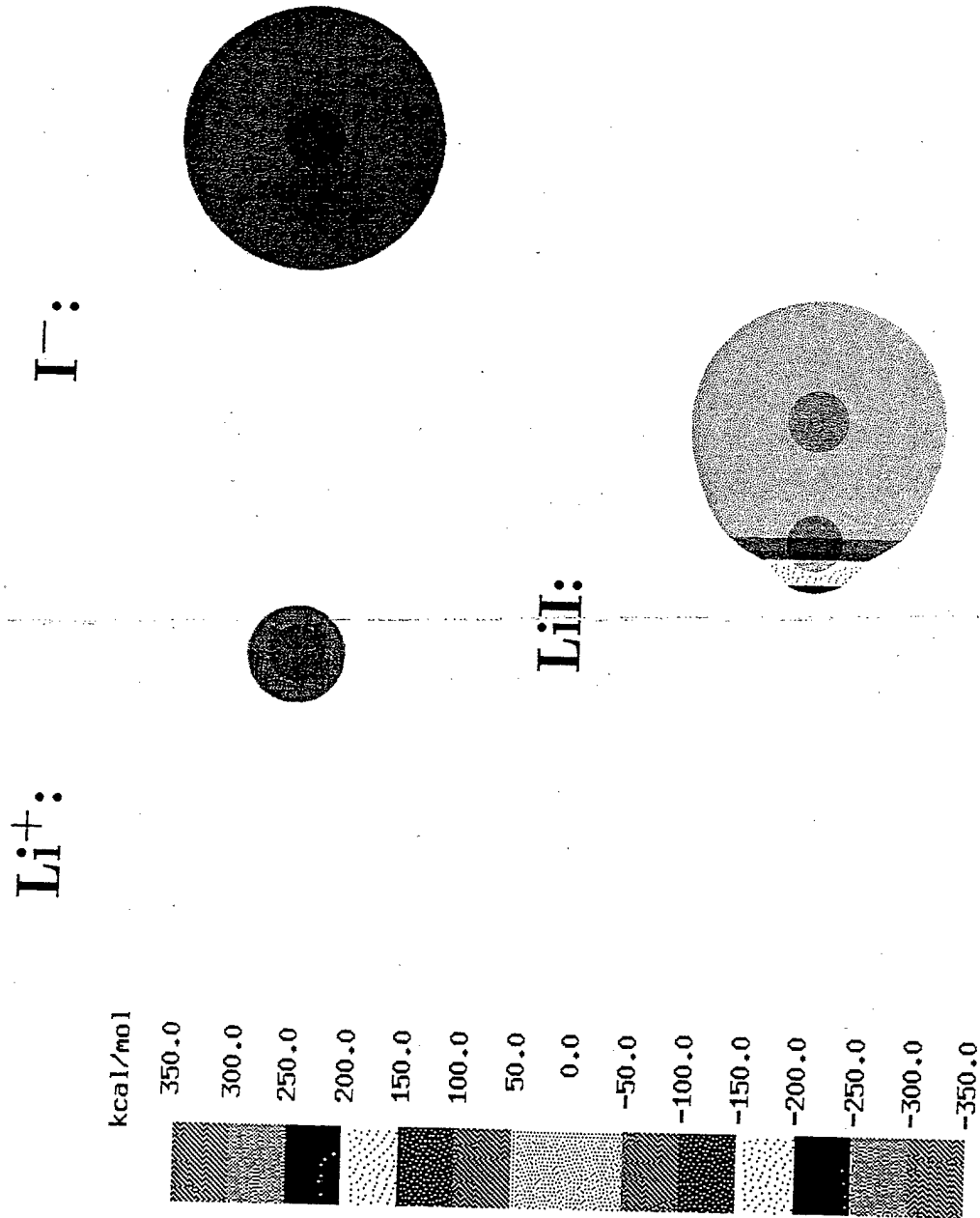
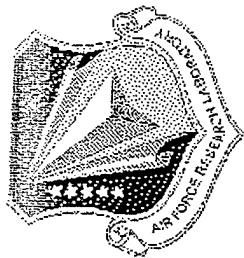


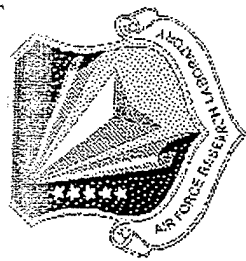
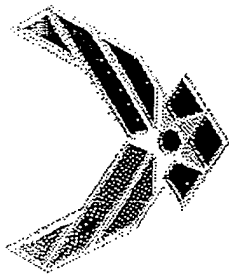
Cs⁺:





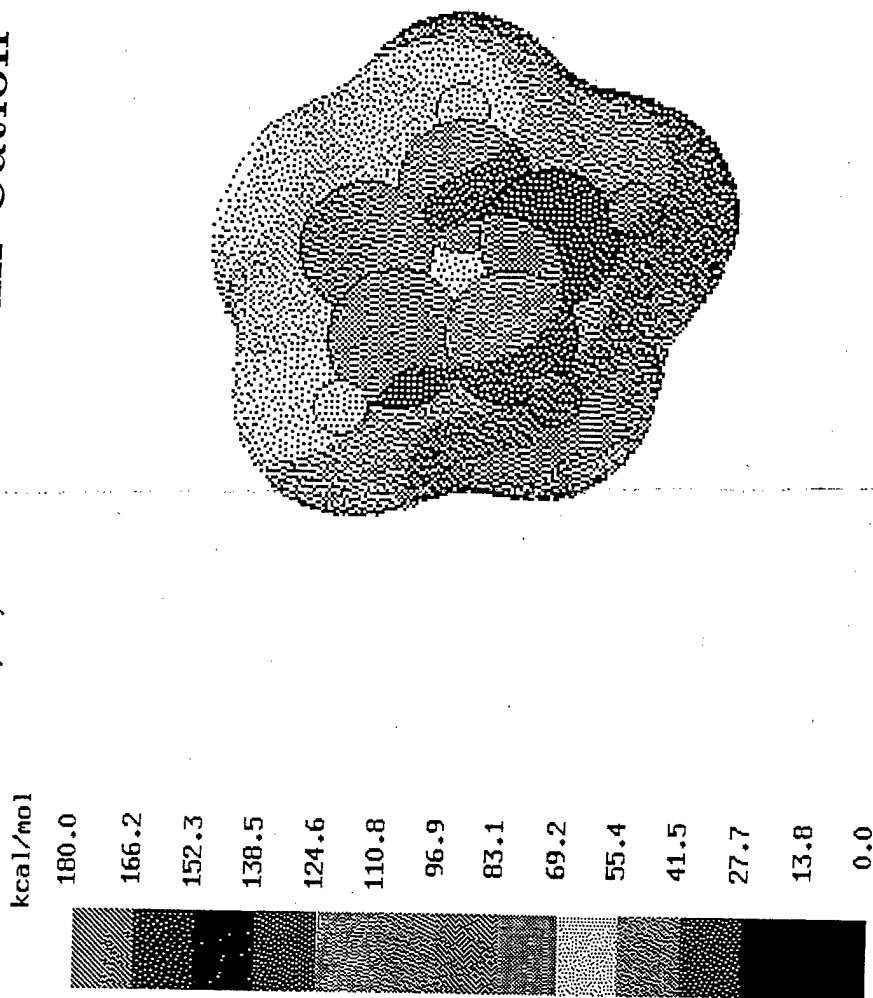
Surface Electrostatic Potential

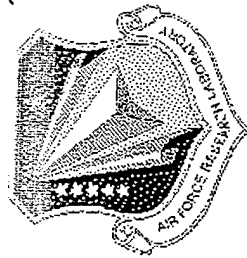




Surface Electrostatic Potential

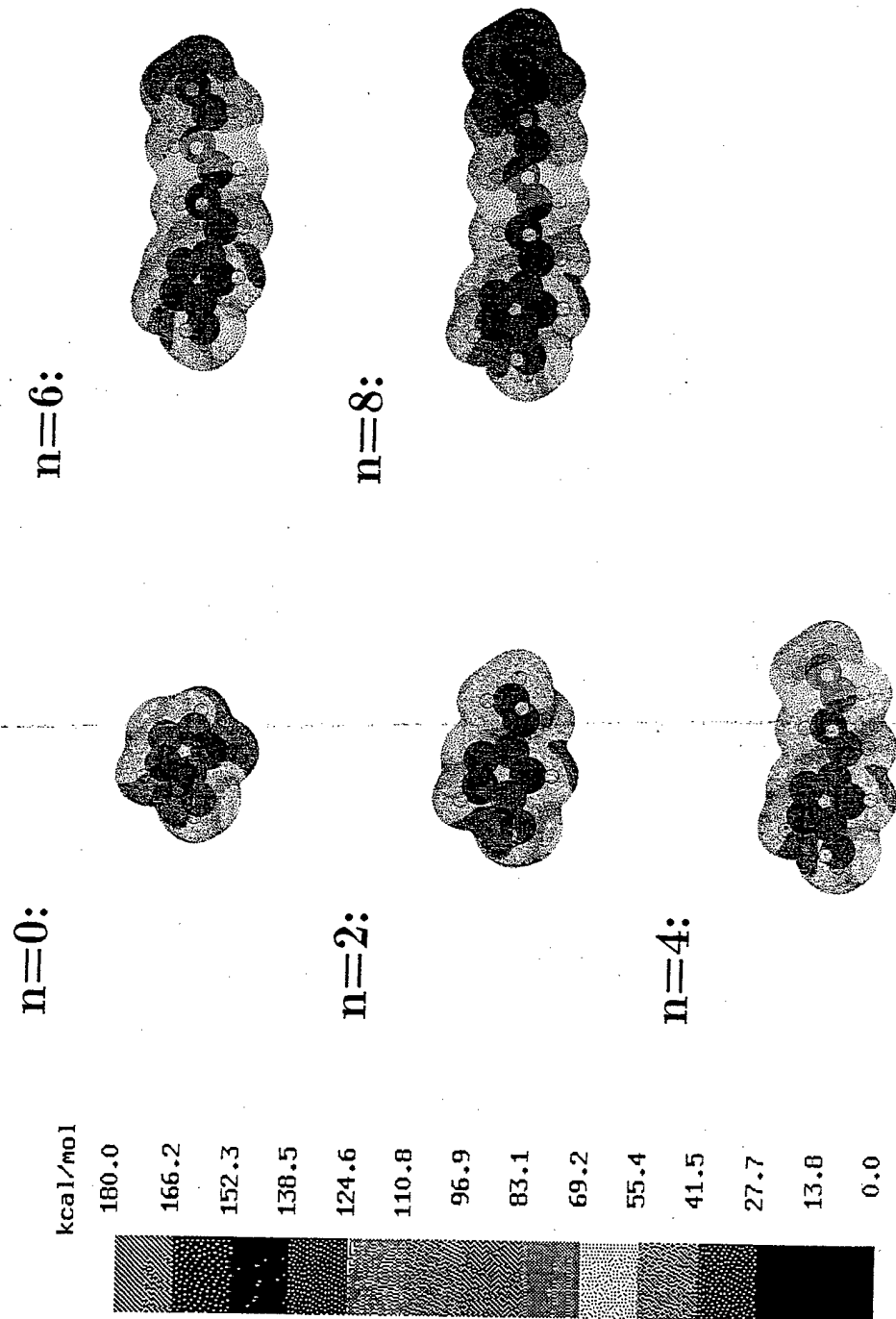
1,2,4-Triazolium Cation

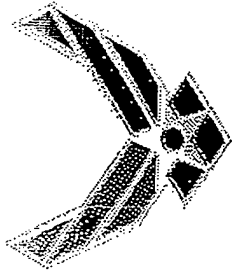




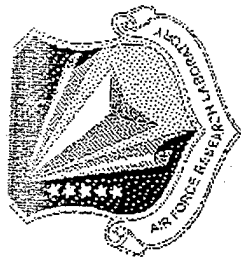
Surface Electrostatic Potential

1-R_n-4-amino-1,2,4-triazolium Cation, n=even:





Descriptors



Electrostatic Potential:

$$\Pi = \frac{1}{A} \sum_i |V_i - \bar{V}| A_i$$

Size:

$$A = \sum_i A_i$$

Shape:

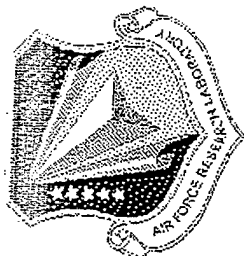
(I_0, I_1, I_2) - PA Moments of Extensia (ordered)

$$\text{Asphericity} = \frac{I_2 - I_0}{I_1}$$

$$\text{Blateness} = \frac{I_1 - I_0}{I_2 - I_0}$$

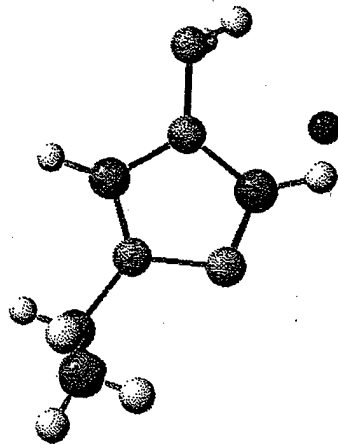


Separation and Interaction Energy



1-Ethyl-4-amino-1,2,4-triazolium Bromide
B3LYP 6-31+G(d):

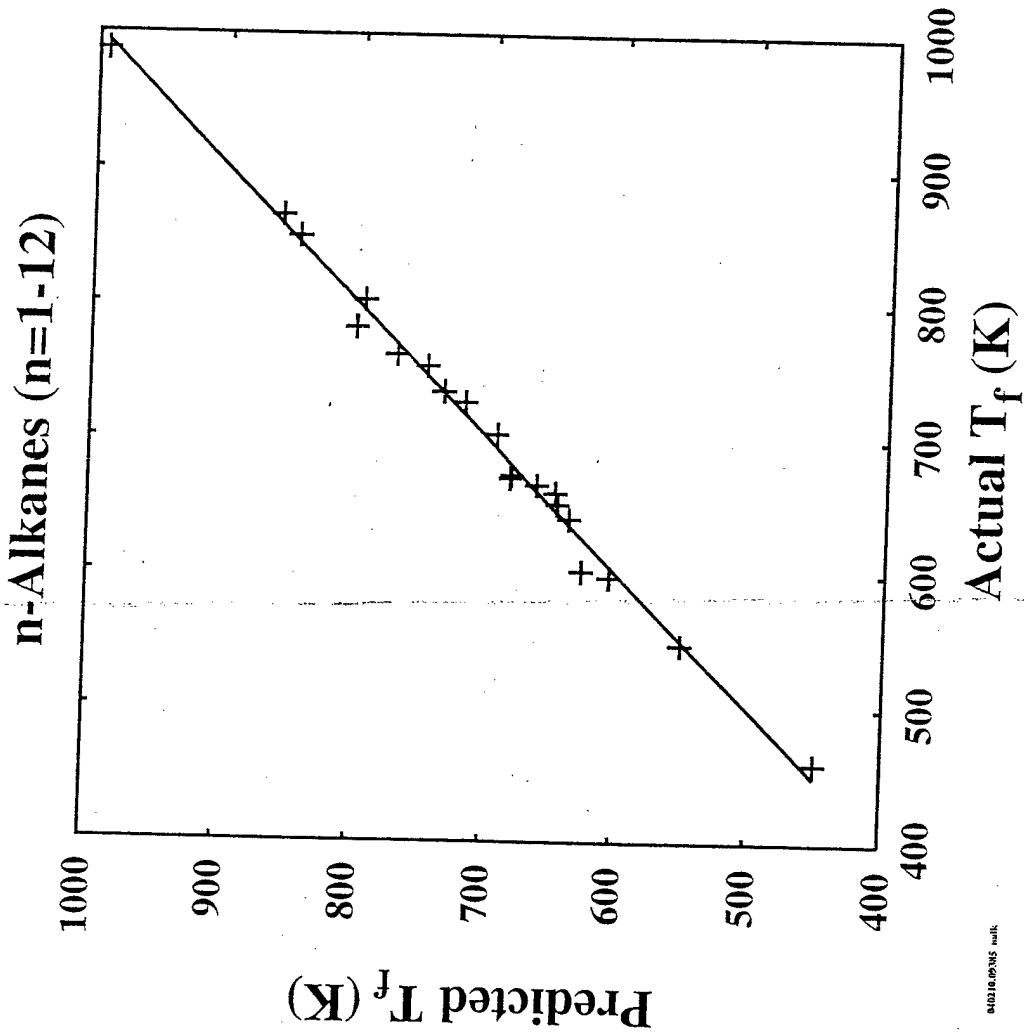
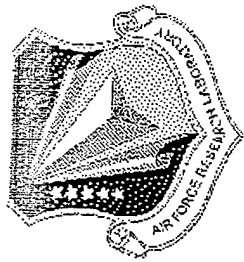
Crystal:



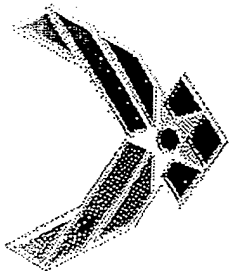
Binding Energy



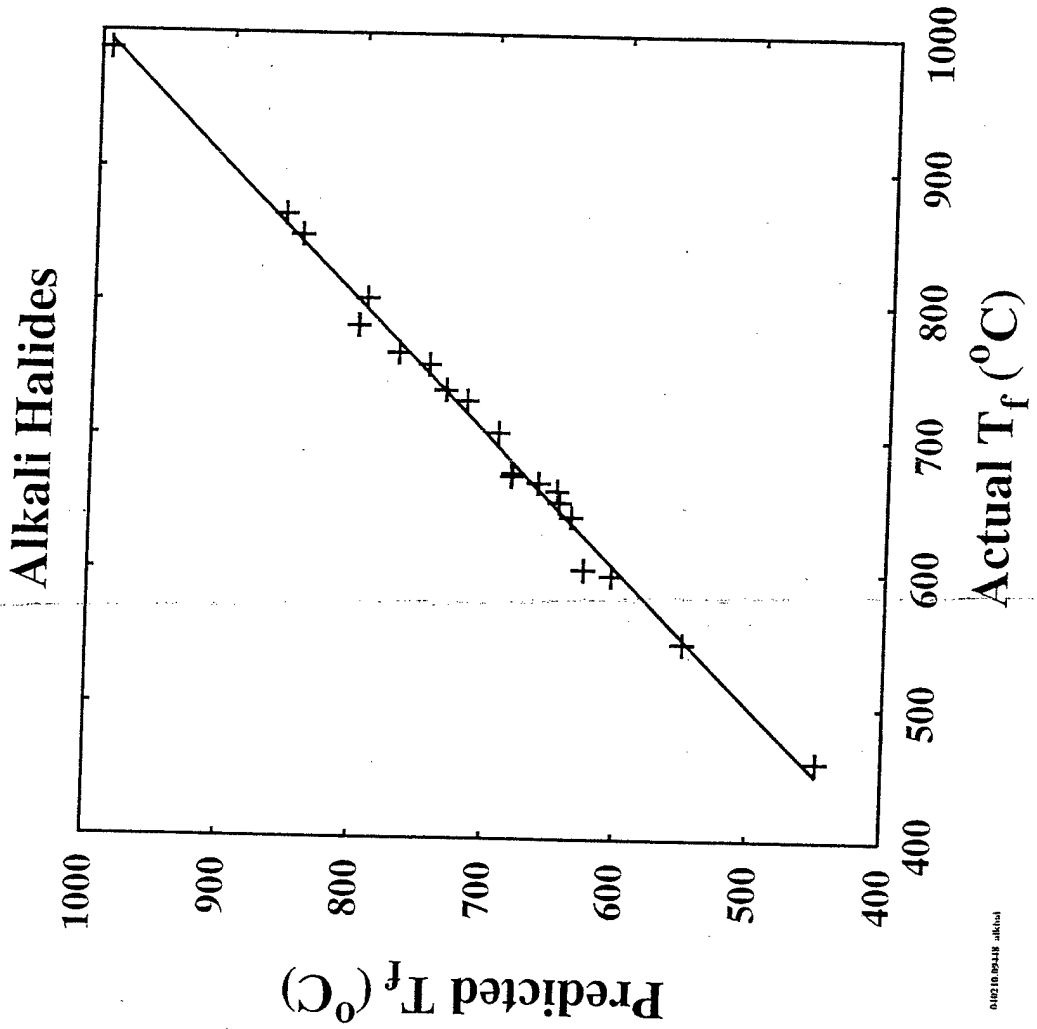
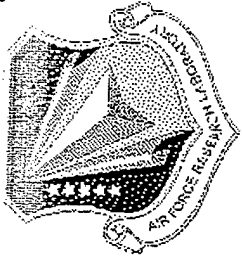
QSPR Correlation



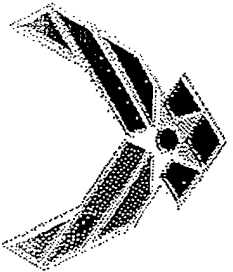
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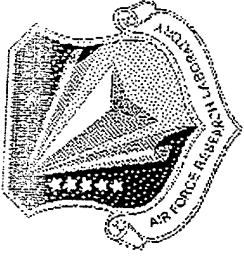
QSPR Correlation



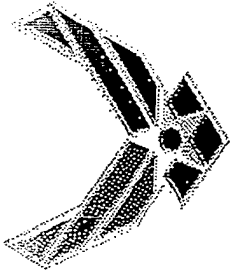
0102100000 alkhal



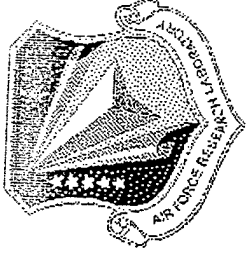
Concluding (Open) Question



Can QC QSPR aid the IL synthesist or will it merely follow?



Acknowledgements



Peter Politzer

J. Boatz

DoD HPCMP - ASC

G. Drake, L. Hall