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IL QC QSPR - Preliminary Results

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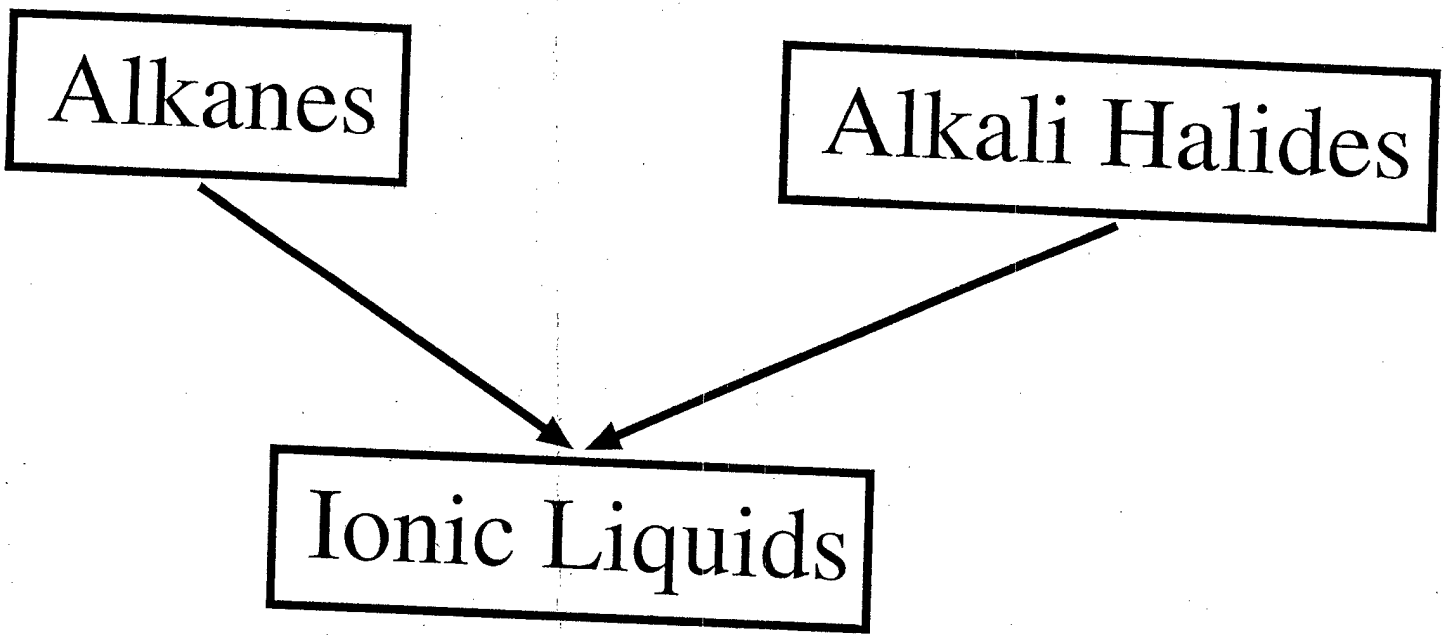
Propellants Branch

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

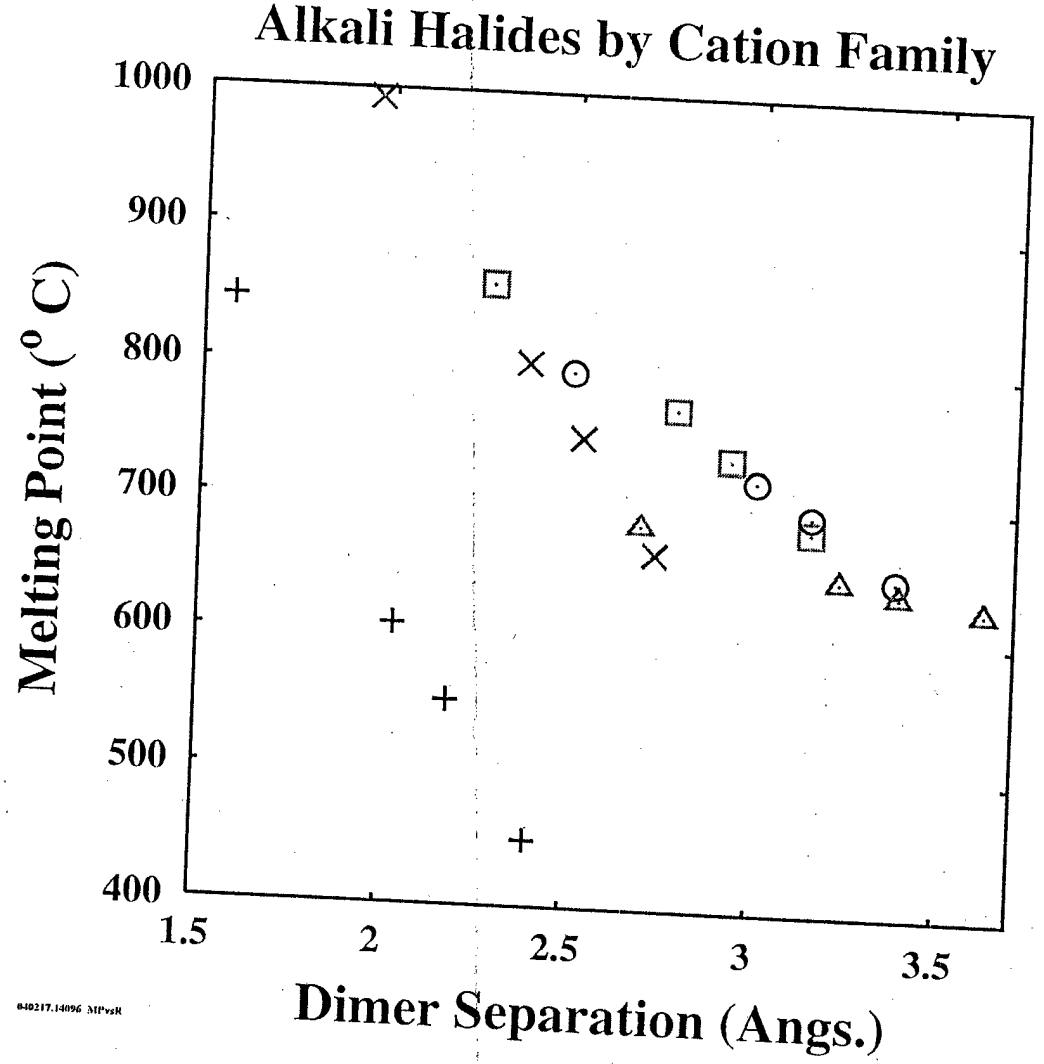
- Pair:

  Separation
  Binding Energy

Constraints/Goals

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

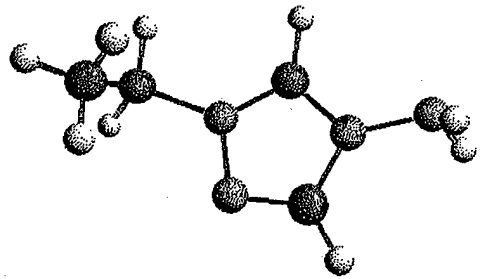
Cation Families Summarized

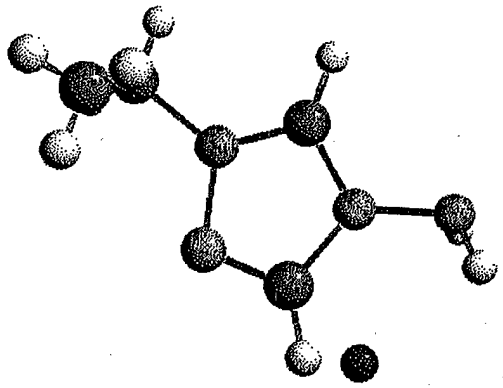


Structures

1-Ethyl-4-amino-1,2,4-triazolium Cation

B3LYP 6-311++G(d,p): Crystal (with Br^-):

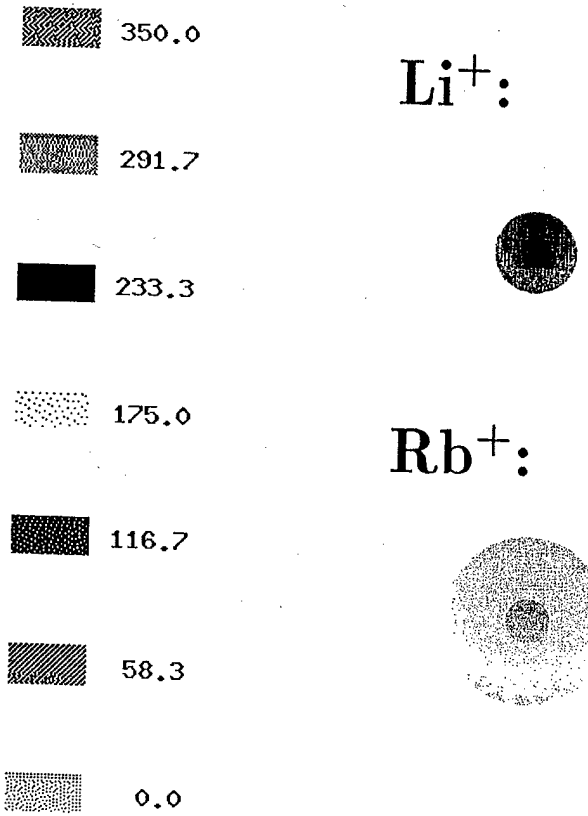




Surface Electrostatic Potential

Color Map:

kcal/mol



V at 0.001 au Electron Density:

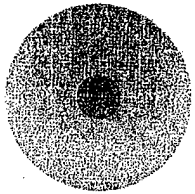
Li^+:

Na^+:

K^+:

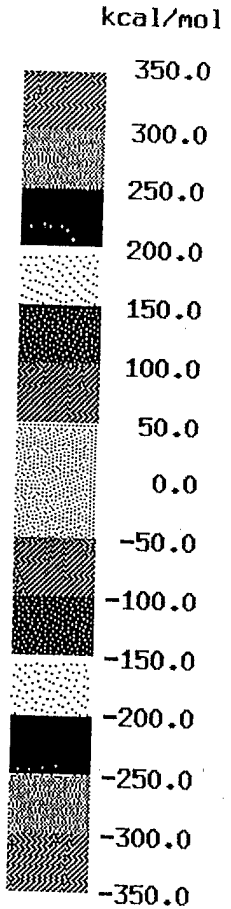
Rb^+:

Cs^+:

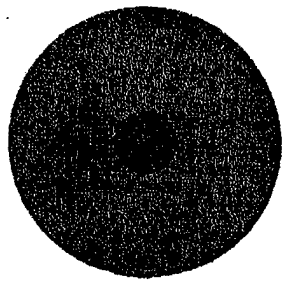


Surface Electrostatic Potential

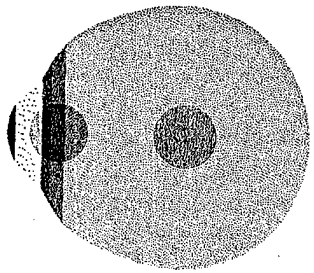
Li^+:



I^-:

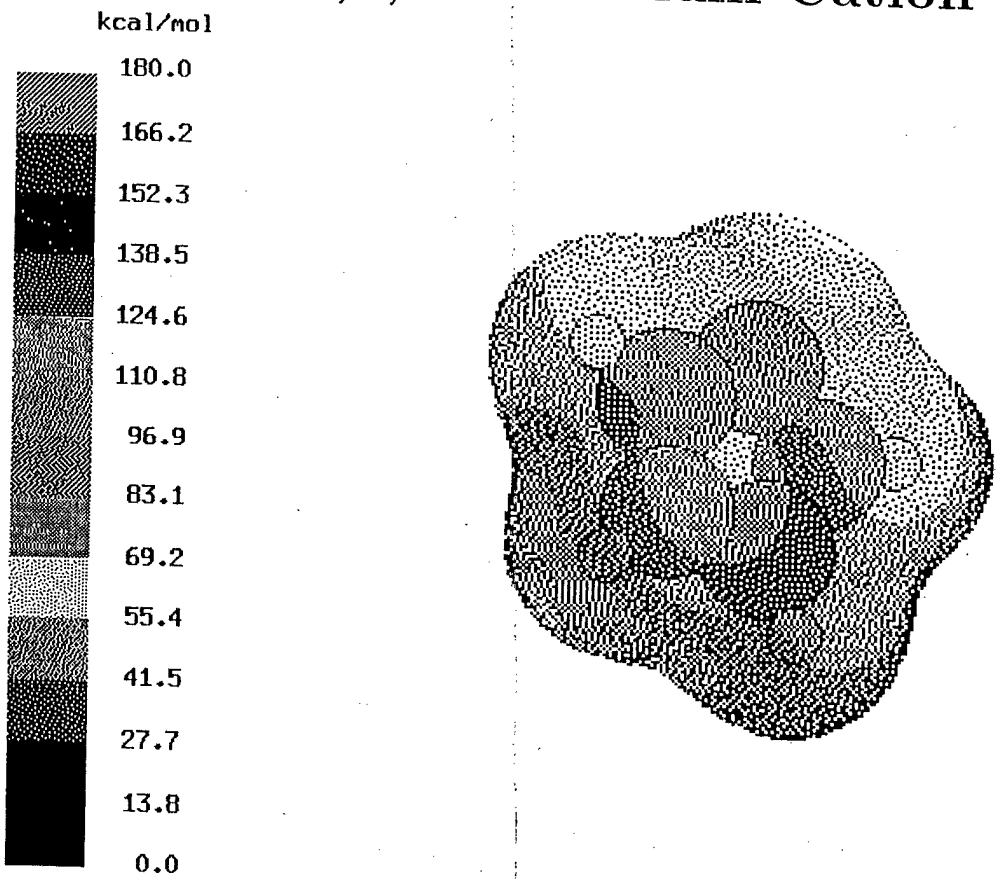


LiI:



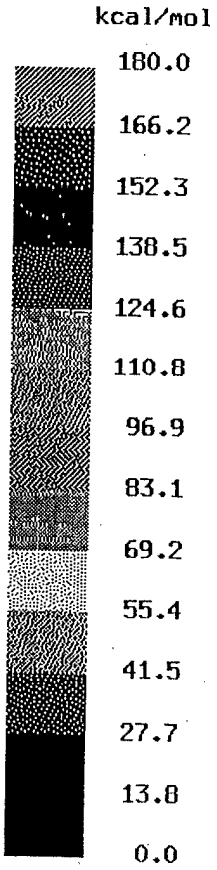
Surface Electrostatic Potential

1,2,4-Triazolium Cation



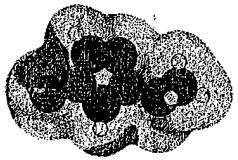
Surface Electrostatic Potential

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



n=0:

n=2:



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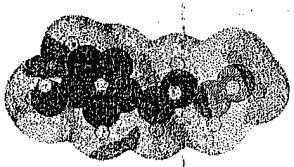

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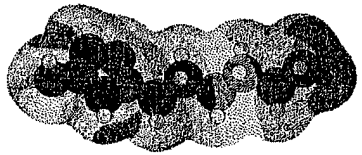

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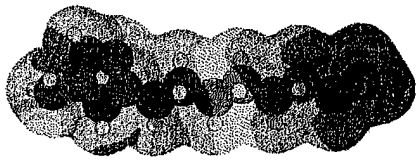


Descriptors

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)

$$\text{Asphericity} = \frac{I_2 - I_0}{\bar{I}}$$

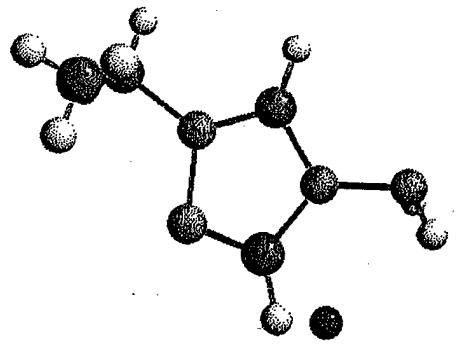
$$\text{Blateness} = \frac{I_1 - I_0}{I_2 - I_0}$$

Separation and Interaction Energy

1-Ethyl-4-amino-1,2,4-triazolium Bromide

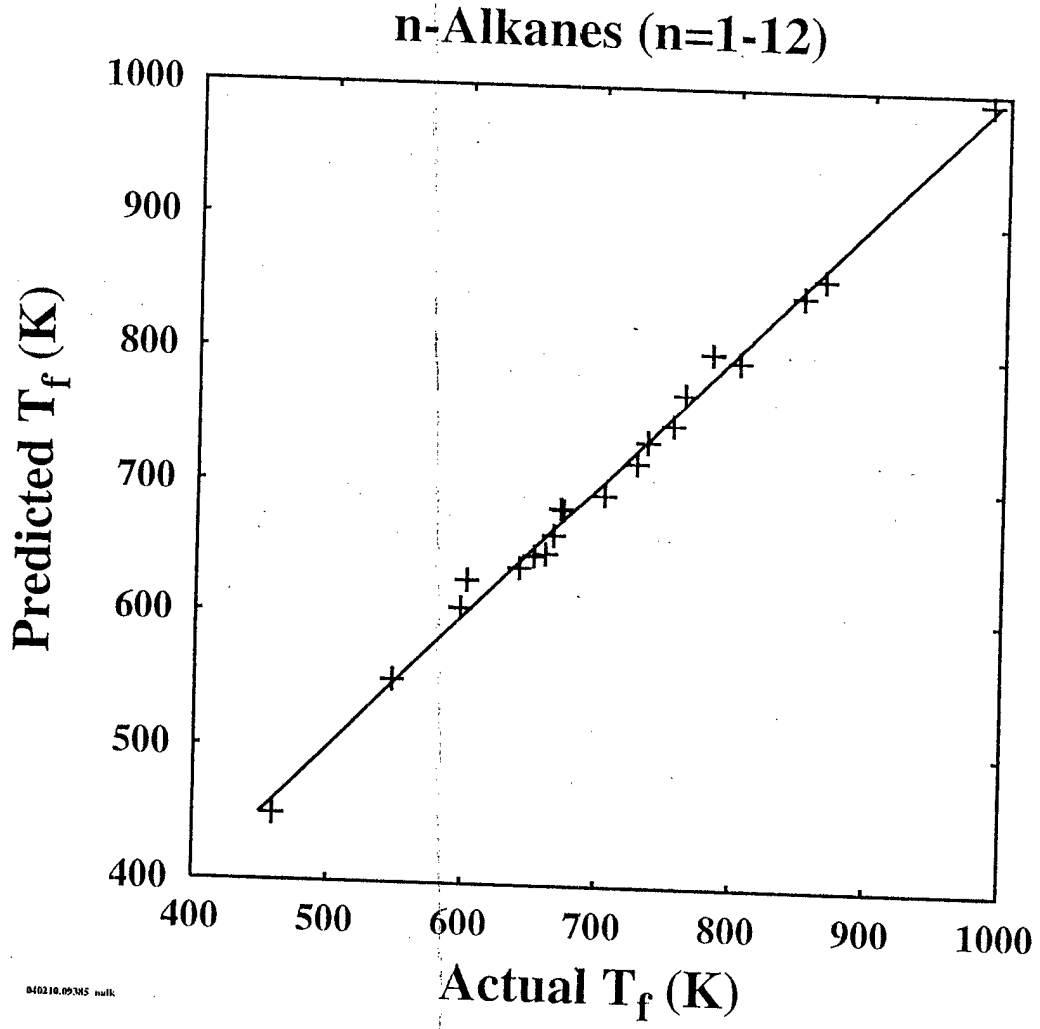
B3LYP 6-31+G(d):

Crystal:

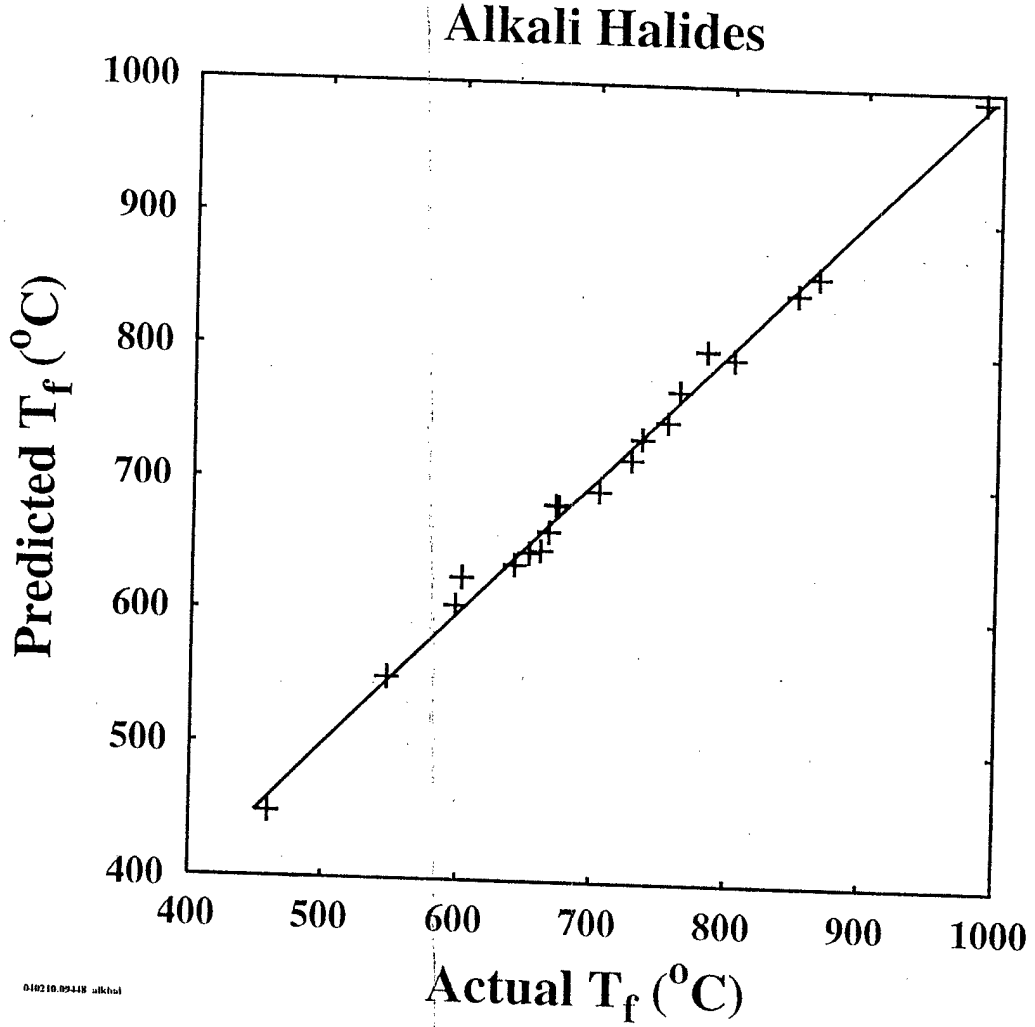


Binding Energy

QSPR Correlation



QSPR Correlation



Concluding (Open) Question

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

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J. Boatz

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