An Ionic Liquid Dependent Mechanism for Base Catalyzed $\beta$-Elimination Reactions from QM/MM Simulations
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Figure S1. Selected CM3 atomic charges (e units) for the transition structure in [BMIM][BF4] (blue), $[\mathrm{BMIM}]\left[\mathrm{PF}_{6}\right]$ (black), and methanol (pink) for the $\beta$-elimination of 1,1,1-tribromo-2,2-bis(3,4-dimethoxyphenyl)ethane with pyrrolidine from the QM/MM/MC calculations.


Figure S2. Solute-solvent energy pair distributions for $\beta$-elimination of 1,1,1-tribromo-2,2-bis(3,4-dimethoxyphenyl)ethane with piperidine (in red) and pyrrolidine (in black) for the
reactants (dashed line) and transition state (solid line) in methanol at $25^{\circ} \mathrm{C}$. The ordinate records the number of solvent molecules that interact with the solutes and their interaction energy on the abscissa. Units for ordinate are number of molecules per $\mathrm{kcal} / \mathrm{mol}$.


Figure S3. Typical snapshot of a transition state for the $\beta$-elimination with piperidine in [ BMIM$]\left[\mathrm{BF}_{4}\right]$ from the $\mathrm{QM} / \mathrm{MM} / \mathrm{MC}$ calculations. A single BMIM cation is illustrated to highlight the $\pi-\pi$ interaction with the solute.

## $[$ BMIM $]\left[\mathrm{BF}_{4}\right]$ Reactant Complex Figures



Figure S4 - The reactant complex of 1,1,1-tribromo-2,2-bis(3,4-dimethoxyphenyl)ethane with piperidine in the ionic liquid [BMIM][BF4]. For solvent effect data see Table S1.


Figure $\mathbf{S 5}$ - The reactant complex of 1,1,1-tribromo-2,2-bis(3,4-dimethoxyphenyl)ethane with pyrrolidine in the ionic liquid $[\mathrm{BMIM}]\left[\mathrm{BF}_{4}\right]$. For solvent effect data see Table S 2 .

## $[$ BMIM $]\left[\mathrm{BF}_{4}\right]$ Transition Structure Figures



Figure S6 - The transition structure of 1,1,1-tribromo-2,2-bis(3,4-dimethoxyphenyl)ethane with piperidine in the ionic liquid $[\mathrm{BMIM}]\left[\mathrm{BF}_{4}\right]$. For solvent effect data see Table S3.


Figure S7 - The transition structure of 1,1,1-tribromo-2,2-bis(3,4-dimethoxyphenyl)ethane with pyrrolidine in the ionic liquid $[\mathrm{BMIM}]\left[\mathrm{BF}_{4}\right]$. For solvent effect data see Table S 4 .

Table S1: Piperidine reactant-complex in $\left.\left[\mathrm{BMIM}^{2}\right] \mid \mathrm{BF}_{4}\right]$ - solvent effect data
Interactions $<4$ Angstroms
Interactions > 4 Angstroms

| BMIM <br> Cation | Average Distance ( $\AA$ ) | Interaction | BMIM <br> Cation | Average Distance <br> (A) | Interaction |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 213 | 3.75 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{C}_{\text {anion }}$ | 102 | 4.99 | $\mathrm{H}_{4}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 102 | 3.39 | $\mathrm{H}_{4}$ with $\mathrm{Br}_{\text {bonded }}$ | 213 | 4.76 | $\mathrm{H}_{4}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 102 | 3.13 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\text {bonded }}$ | 102 | 5.07 | $\mathrm{H}_{4}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 102 | 3.21 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\text {bonded }}$ | 210 | 4.05 | $\mathrm{H}_{2}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 102 | 3.47 | $\mathrm{H}_{\text {Me }}$ with $\mathrm{Br}_{\text {bonded }}$ | 213 | 4.24 | $\mathrm{H}_{2}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 102 | 3.62 | $\mathrm{H}_{\text {Me }}$ with $\mathrm{Br}_{\text {bonded }}$ | 102 | 4.25 | $\mathrm{H}_{\text {Me }}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 213 | 2.99 | $\mathrm{H}_{\text {Me }}$ with $\mathrm{Br}_{\text {bonded }}$ | 102 | 4.55 | $\mathrm{H}_{\text {Me }}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 213 | 3.55 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\text {bonded }}$ | 102 | 4.81 | $\mathrm{H}_{\text {Me }}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 213 | 3.55 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\text {bonded }}$ | 213 | 4.63 | $\mathrm{H}_{\text {Me }}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 162 | 3.2 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 213 | 4.69 | $\mathrm{H}_{\text {Me }}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 162 | 3.35 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 213 | 4.79 | $\mathrm{H}_{\text {Me }}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 162 | 3.54 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 15 | 3.9 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 210 | 3.67 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 15 | 4.01 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 213 | 3.68 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\text {bonded }}$ | 15 | 4.79 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| All Interactions < 5 Angstroms |  |  | 162 | 4.53 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 162 | 4.7 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| $\begin{gathered} \mathrm{BF}_{4} \\ \text { Anion } \end{gathered}$ | Average Distance <br> ( $\AA$ ) | Interaction | 184 | 4.62 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 205 | 4.07 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 164 | 3.31 | $\mathrm{F}_{\text {BF4 }}$ with $\mathrm{H}_{\text {transfer }}$ | 205 | 5.04 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 210 | 4.07 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 210 | 4.03 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 210 | 4.44 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 210 | 4.59 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 162 | 4.97 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{C}_{\text {anion }}$ |
|  |  |  | 98 | 4.34 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{C}_{\text {anion }}$ |
|  |  |  | 98 | 4.55 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{C}_{\text {anion }}$ |
|  |  |  | 98 | 4.78 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{C}_{\text {anion }}$ |
|  |  |  | 162 | 4.48 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{C}_{\text {anion }}$ |
|  |  |  | 213 | 4.83 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{C}_{\text {anion }}$ |

Table S2: Pyrrolidine reactant-complex in $[$ BMIM $]\left[B_{4} 4\right.$ - solvent effect data
Interactions < 4 Angstroms
Interactions > 4 Angstroms

| BMIM Cation | Average Distance (A) | Interaction | BMIM Cation | Average Distance <br> (A) | Interaction |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 170 | 3.72 | $\mathrm{H}_{4}$ with $\mathrm{Br}_{\text {bonded }}$ | 101 | 4.03 | $\mathrm{H}_{4}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 164 | 3.75 | $\mathrm{H}_{4}$ with $\mathrm{Br}_{\text {bonded }}$ | 170 | 4.31 | $\mathrm{H}_{4}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 170 | 2.91 | $\mathrm{H}_{5}$ with $\mathrm{Br}_{\text {bonded }}$ | 170 | 4.61 | $\mathrm{H}_{4}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 170 | 2.91 | $\mathrm{H}_{5}$ with $\mathrm{Br}_{\text {bonded }}$ | 164 | 4.99 | $\mathrm{H}_{4}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 164 | 3.57 | $\mathrm{H}_{5}$ with $\mathrm{Br}_{\text {bonded }}$ | 170 | 4.27 | $\mathrm{H}_{5}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 101 | 3.19 | $\mathrm{H}_{\text {Me }}$ with $\mathrm{Br}_{\text {bonded }}$ | 164 | 4.91 | $\mathrm{H}_{2}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 101 | 3.19 | $\mathrm{H}_{\text {Me }}$ with $\mathrm{Br}_{\text {bonded }}$ | 170 | 4.9 | $\mathrm{H}_{5}$ with $\mathrm{C}_{\text {anion }}$ |
| 101 | 3.29 | $\mathrm{H}_{\text {Me }}$ with $\mathrm{Br}_{\text {bonded }}$ | 101 | 4.43 | $\mathrm{H}_{\text {Me }}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 101 | 3.52 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\text {bonded }}$ | 101 | 4.43 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 101 | 3.52 | $\mathrm{H}_{\text {Me }}$ with $\mathrm{Br}_{\text {bonded }}$ | 101 | 4.72 | $\mathrm{H}_{\text {Me }}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 101 | 3.61 | $\mathrm{H}_{\text {Me }}$ with $\mathrm{Br}_{\text {bonded }}$ | 170 | 4.55 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 170 | 2.95 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 170 | 4.56 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 170 | 2.95 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 170 | 4.63 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 170 | 3.19 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 170 | 4.64 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 170 | 3.19 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 170 | 4.71 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 170 | 3.51 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 170 | 4.72 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 170 | 3.51 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 170 | 4.74 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 164 | 3.03 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 170 | 4.74 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 164 | 3.62 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 170 | 4.99 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| All Interactions < 5 Angstroms |  |  | 170 | 4.99 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 187 | 4.82 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{C}_{\text {anion }}$ |
| $\mathrm{BF}_{4}$ Anion | Average Distance <br> (A) | Interaction | 164 | 4.94 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{C}_{\text {anion }}$ |
|  |  |  | 101 | 4.99 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{C}_{\text {anion }}$ |
| 227 | 3.71 | $\mathrm{F}_{\text {BF4 }}$ with $\mathrm{H}_{\text {transfer }}$ |  |  |  |
| 227 | 4.26 | $\mathrm{F}_{\text {BF4 }}$ with $\mathrm{H}_{\text {transfer }}$ |  |  |  |
| 227 | 4.49 | $\mathrm{F}_{\mathrm{BF} 4}$ with $\mathrm{H}_{\text {transfer }}$ |  |  |  |

Table S3: Piperidine TS in $[$ BMIM $]\left[B_{4}\right]$ - solvent effect data
Interactions < 4 Angstroms
Interactions > 4 Angstroms

| BMIM <br> Cation | Average Distance <br> (A) | Interaction | BMIM <br> Cation | Average Distance <br> (A) | Interaction |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 210 | 3.28 | $\mathrm{H}_{2}$ with $\mathrm{Br}_{\text {bonded }}$ | 102 | 4.99 | $\mathrm{H}_{4}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 102 | 2.72 | $\mathrm{H}_{4}$ with $\mathrm{Br}_{\mathrm{LG}}$ | 213 | 4.78 | $\mathrm{H}_{5}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 102 | 2.79 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\mathrm{LG}}$ | 102 | 4.33 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 102 | 3.16 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\mathrm{LG}}$ | 176 | 4.46 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 213 | 2.78 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ | 213 | 4.3 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 213 | 3.12 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ | 213 | 4.32 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 213 | 3.82 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ | 213 | 4.74 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 213 | 3.9 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ | 213 | 4.91 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 210 | 3.38 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\text {bonded }}$ | 213 | 4.99 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 210 | 3.79 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\text {bonded }}$ | 15 | 4.45 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 102 | 3.38 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\text {bonded }}$ | 15 | 4.74 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {LG }}$ |
| 102 | 3.57 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\text {bonded }}$ | 210 | 4.83 | $\mathrm{H}_{\text {Me }}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 213 | 3.05 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 102 | 4.3 | $\mathrm{H}_{\text {Me }}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 15 | 3.48 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 102 | 5.14 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 15 | 3.49 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 15 | 4.11 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 15 | 3.86 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 15 | 4.72 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 15 | 3.87 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 184 | 4.63 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 213 | 3.91 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 184 | 4.65 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| $\text { All Interactions < } 5 \text { Angstroms }$ |  |  | 210 | 4.89 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 213 | 4.03 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| $\mathrm{BF}_{4}$ Anion | Average Distance <br> ( $\AA$ ) | Interaction | 213 | 4.62 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 210 | 4.29 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{C}_{\text {anion }}$ |
| 61 | 3.2 | $\mathrm{F}_{\mathrm{BF} 4}$ with $\mathrm{H}_{\text {transfer }}$ | 176 | 4.37 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{C}_{\text {anion }}$ |
| 61 | 4.43 | $\mathrm{F}_{\text {BF4 }}$ with $\mathrm{H}_{\text {transfer }}$ | 176 | 4.51 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{C}_{\text {anion }}$ |
| 61 | 4.77 | $\mathrm{F}_{\mathrm{BF} 4}$ with $\mathrm{H}_{\text {transfer }}$ | 102 | 4.33 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{C}_{\text {anion }}$ |
|  |  |  | 184 | 4.71 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{C}_{\text {anion }}$ |

## Table S4: Pyrrolidine TS in $\left[\right.$ BMIM $\left.^{2}\right]$ BF $\left._{4}\right]$ - solvent effect data

Interactions < 4 Angstroms
Interactions > 4 Angstroms

| BMIM <br> Cation | Average Distance <br> ( $\AA$ ) | Interaction | BMIM <br> Cation | Average Distance <br> (A) | Interaction |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 170 | 3.6 | $\mathrm{H}_{5}$ with $\mathrm{Br}_{\mathrm{LG}}$ | 170 | 4.58 | $\mathrm{H}_{2}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 164 | 2.58 | $\mathrm{H}_{4}$ with $\mathrm{Br}_{\text {bonded }}$ | 170 | 4.89 | $\mathrm{H}_{4}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 164 | 3.94 | $\mathrm{H}_{4}$ with $\mathrm{Br}_{\text {bonded }}$ | 102 | 4.46 | $\mathrm{H}_{4}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 164 | 3.73 | $\mathrm{H}_{4}$ with $\mathrm{Br}_{\text {bonded }}$ | 164 | 4.5 | $\mathrm{H}_{5}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 102 | 2.98 | $\mathrm{H}_{4}$ with $\mathrm{Br}_{\text {bonded }}$ | 102 | 4.31 | $\mathrm{H}_{2}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 102 | 3.29 | $\mathrm{H}_{4}$ with $\mathrm{Br}_{\text {bonded }}$ | 102 | 4.59 | $\mathrm{H}_{5}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 170 | 2.81 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ | 164 | 4.95 | $\mathrm{H}_{4}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 170 | 3.04 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ | 170 | 4.47 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 170 | 3.22 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ | 170 | 4.71 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 170 | 3.48 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 170 | 4.97 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 170 | 3.74 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 170 | 5.03 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 117 | 3.33 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 164 | 4.12 | $\mathrm{H}_{\text {Me }}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 117 | 3.55 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 164 | 4.31 | $\mathrm{H}_{\text {Me }}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 117 | 3.84 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 102 | 4.37 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 164 | 3.53 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\text {bonded }}$ | 170 | 4.28 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 164 | 3.68 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\text {bonded }}$ | 170 | 5.03 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 102 | 3.17 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\text {bonded }}$ | 117 | 4.46 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 102 | 3.72 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\text {bonded }}$ | 117 | 4.79 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| All Interactions < 5 Angstroms |  |  | 117 | 4.79 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 117 | 4.98 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| $\mathbf{B F}_{4}$ <br> Anion | Average Distance <br> ( $\AA$ ) | Interaction | 208 | 4.5 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 102 | 4.02 | $\mathrm{H}_{\text {Me }}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 166 | 3.42 | $\mathrm{F}_{\text {BF4 }}$ with $\mathrm{H}_{\text {transfer }}$ | 102 | 4.56 | $\mathrm{H}_{\text {Me }}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 166 | 4.14 | $\mathrm{F}_{\mathrm{BF} 4}$ with $\mathrm{H}_{\text {transfer }}$ | 102 | 4.73 | $\mathrm{H}_{\text {Me }}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 166 | 4.71 | $\mathrm{F}_{\text {BF4 }}$ with $\mathrm{H}_{\text {transfer }}$ | 102 | 4.99 | $\mathrm{H}_{\text {Me }}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 122 | 4.96 | $\mathrm{F}_{\text {BF4 }}$ with $\mathrm{H}_{\text {transfer }}$ | 102 | 5.09 | $\mathrm{H}_{\text {Me }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 164 | 4.37 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{C}_{\text {anion }}$ |
|  |  |  | 170 | 4.79 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{C}_{\text {anion }}$ |
|  |  |  | 117 | 4.57 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{C}_{\text {anion }}$ |
|  |  |  | 117 | 4.81 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{C}_{\text {anion }}$ |

## [BMIM $]\left[\mathrm{PF}_{6}\right]$ Reactant Complex Figures



Figure S8 - The reactant complex of 1,1,1-tribromo-2,2-bis(3,4-dimethoxyphenyl)ethane with piperidine in the ionic liquid [BMIM][PF $\left.{ }_{6}\right]$. For solvent effect data see Table S5.


Figure S9 - The reactant complex of 1,1,1-tribromo-2,2-bis(3,4-dimethoxyphenyl)ethane with pyrrolidine in the ionic liquid $[\mathrm{BMIM}]\left[\mathrm{PF}_{6}\right]$. For solvent effect data see Table S6.

## [BMIM $]$ PF $\left.{ }_{6}\right]$ Transition Structure Figures



Figure S10 - The transition structure of 1,1,1-tribromo-2,2-bis(3,4-dimethoxyphenyl)ethane with piperidine in the ionic liquid $[\mathrm{BMIM}]\left[\mathrm{PF}_{6}\right]$. For solvent effect data see Table S 7 .


Figure S11 - The transition structure of 1,1,1-tribromo-2,2-bis(3,4-dimethoxyphenyl)ethane with pyrrolidine in the ionic liquid $[\mathrm{BMIM}]\left[\mathrm{PF}_{6}\right]$. For solvent effect data see Table S 8.

Table S5: Piperidine reactant-complex in [BMIM]|PF ${ }_{6}$ - - solvent effect data
Interactions < 4 Angstroms
Interactions > 4 Angstroms

| BMIM <br> Cation | Average Distance ( $\AA$ ) | Interaction | BMIM <br> Cation | Average Distance ( $\AA$ ) | Interaction |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 218 | 3.35 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\text {bonded }}$ | 216 | 4.02 | $\mathrm{H}_{5}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 218 | 3.8 | $\mathrm{H}_{\text {Me }}$ with $\mathrm{Br}_{\text {bonded }}$ | 102 | 4.16 | $\mathrm{H}_{5}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 218 | 3.86 | $\mathrm{H}_{\text {Me }}$ with $\mathrm{Br}_{\text {bonded }}$ | 118 | 4.54 | $\mathrm{H}_{5}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 216 | 3.57 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 218 | 4.99 | $\mathrm{H}_{4}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 216 | 3.85 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 218 | 4.11 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 102 | 3.35 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 218 | 4.06 | $\mathrm{H}_{\text {Me }}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 102 | 3.58 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 218 | 4.65 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 102 | 3.75 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 15 | 4.79 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 102 | 3.93 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 102 | 4.34 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 109 | 3.48 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 102 | 4.55 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| All Interactions < 5 Angstroms |  |  | 102 | 4.62 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 109 | 4.44 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 109 | 4.48 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| $\mathrm{PF}_{6}$ <br> Anion | Average Distance <br> (A) | Interaction | 109 | 4.51 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 109 | 4.54 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 299 | 4.51 | $\mathrm{F}_{\text {PF6 }}$ with $\mathrm{H}_{\text {transfer }}$ | 109 | 4.59 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 299 | 4.67 | $\mathrm{F}_{\text {PF6 }}$ with $\mathrm{H}_{\text {transfer }}$ | 216 | 4.17 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 152 | 4.7 | $\mathrm{F}_{\text {PF6 }}$ with $\mathrm{H}_{\text {transfer }}$ | 216 | 4.46 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 216 | 4.83 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 216 | 4.96 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 118 | 4.47 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{C}_{\text {anion }}$ |
|  |  |  | 118 | 4.61 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{C}_{\text {anion }}$ |
|  |  |  | 109 | 4.5 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{C}_{\text {anion }}$ |
|  |  |  | 109 | 4.49 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{C}_{\text {anion }}$ |
|  |  |  | 98 | 4.85 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{C}_{\text {anion }}$ |

Table S6: Pyrrolidine reactant-complex in $\left[\right.$ BMIIM $\left.^{2}\right] \mathrm{PF}_{6}$ - solvent effect data
Interactions < 4 Angstroms
Interactions > 4 Angstroms

| BMIM Cation | Average Distance <br> ( $\AA$ ) | Interaction | BMIM <br> Cation | Average Distance <br> (A) | Interaction |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 109 | 3.09 | $\mathrm{H}_{2}$ with $\mathrm{Br}_{\text {bonded }}$ | 216 | 4.68 | $\mathrm{H}_{4}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 216 | 3.02 | $\mathrm{H}_{5}$ with $\mathrm{Br}_{\text {bonded }}$ | 216 | 4.85 | $\mathrm{H}_{4}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 118 | 3 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\text {bonded }}$ | 216 | 4.14 | $\mathrm{H}_{5}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 118 | 3.61 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\text {bonded }}$ | 216 | 4.29 | $\mathrm{H}_{5}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 118 | 3.98 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\text {bonded }}$ | 118 | 4.17 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 109 | 3.13 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\text {bonded }}$ | 118 | 4.72 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 102 | 3.65 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 109 | 4.48 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 102 | 3.66 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 109 | 4.54 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 102 | 3.69 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 109 | 4.95 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 102 | 3.77 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 28 | 4.78 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 99 | 3.68 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 99 | 4.36 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 99 | 3.97 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 102 | 4.14 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 213 | 3.7 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{C}_{\text {anion }}$ | 102 | 4.29 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| All Interactions < 5 Angstroms |  |  | 102 | 4.44 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 102 | 4.55 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 102 | 4.82 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| $\begin{gathered} \hline \mathrm{PF}_{6} \\ \text { Anion } \end{gathered}$ | Average Distance <br> ( $\AA$ ) | Interaction | 109 | 4.76 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 118 | 4.44 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 222 | 3.54 | $\mathrm{F}_{\text {PF6 }}$ with $\mathrm{H}_{\text {transfer }}$ | 118 | 4.84 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 222 | 4.05 | $\mathrm{F}_{\text {PF6 }}$ with $\mathrm{H}_{\text {transfer }}$ | 216 | 4.59 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 222 | 4.78 | $\mathrm{F}_{\text {PF6 }}$ with $\mathrm{H}_{\text {transfer }}$ | 216 | 4.78 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 109 | 4.02 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{C}_{\text {anion }}$ |
|  |  |  | 216 | 4.36 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{C}_{\text {anion }}$ |
|  |  |  | 213 | 4.39 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{C}_{\text {anion }}$ |
|  |  |  | 99 | 4.39 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{C}_{\text {anion }}$ |
|  |  |  | 102 | 4.75 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{C}_{\text {anion }}$ |

Table S7: Piperidine TS in $[$ BMIM $]\left[\mathrm{PF}_{6}\right]$ - solvent effect data
Interactions < 4 Angstroms
Interactions > 4 Angstroms

| BMIM <br> Cation | Average Distance <br> (A) | Interaction | BMIM <br> Cation | Average Distance (A) | Interaction |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 216 | 3.37 | $\mathrm{H}_{4}$ with $\mathrm{Br}_{\text {bonded }}$ | 102 | 4.47 | $\mathrm{H}_{4}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 102 | 3.65 | $\mathrm{H}_{4}$ with $\mathrm{Br}_{\text {bonded }}$ | 216 | 4.08 | $\mathrm{H}_{4}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 102 | 2.76 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ | 15 | 4.25 | $\mathrm{H}_{2}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 102 | 3.29 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ | 15 | 4.17 | $\mathrm{H}_{4}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 102 | 3.54 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ | 102 | 4.37 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 15 | 3.44 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ | 102 | 4.64 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 15 | 3.86 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ | 102 | 4.76 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 109 | 3.95 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {LG }}$ | 102 | 4.87 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 216 | 2.88 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ | 216 | 4.33 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 216 | 3.63 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ | 216 | 4.85 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 118 | 3.87 | $\mathrm{H}_{\text {Me }}$ with $\mathrm{Br}_{\mathrm{LG}}$ | 15 | 4.43 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 15 | 2.98 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 109 | 4.77 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 15 | 3.1 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 109 | 4.91 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 15 | 3.43 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 118 | 4.39 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 15 | 3.99 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 118 | 4.55 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 102 | 3.72 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 118 | 4.45 | $\mathrm{H}_{\text {Me }}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 216 | 3.92 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 118 | 4.67 | $\mathrm{H}_{\text {Me }}$ with $\mathrm{Br}_{\text {bonded }}$ |
| All Interactions < 5 Angstroms |  |  | 118 | 5.05 | $\mathrm{H}_{\text {Me }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 15 | 4.79 | $\mathrm{H}_{\text {Me }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 118 | 4.26 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{C}_{\text {anion }}$ |
| $\begin{gathered} \text { PF }_{6} \\ \text { Anion } \end{gathered}$ | Average Distance <br> ( $\AA$ ) | Interaction | 118 | 4.61 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{C}_{\text {anion }}$ |
|  |  |  | 109 | 4.49 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{C}_{\text {anion }}$ |
| 152 | 4.43 | $\mathrm{F}_{\text {PF6 }}$ with $\mathrm{H}_{\text {transfer }}$ | 109 | 4.5 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{C}_{\text {anion }}$ |
| 152 | 4.63 | $\mathrm{F}_{\text {PF6 }}$ with $\mathrm{H}_{\text {transfer }}$ | 109 | 4.49 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{C}_{\text {anion }}$ |
| 152 | 4.81 | $\mathrm{F}_{\text {PF6 }}$ with $\mathrm{H}_{\text {transfer }}$ |  |  |  |

Table S8: Pyrrolidine TS in [BMIM] $\left.] \mathrm{PF}_{6}\right]$ - solvent effect data
Interactions $<4$ Angstroms Interactions $>4$ Angstroms

| BMIM <br> Cation | Average Distance <br> (A) | Interaction | BMIM <br> Cation | Average Distance (A) | Interaction |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 109 | 3.09 | $\mathrm{H}_{2}$ with $\mathrm{Br}_{\text {bonded }}$ | 216 | 4.14 | $\mathrm{H}_{4}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 216 | 3.01 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ | 216 | 4.29 | $\mathrm{H}_{4}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 102 | 3.65 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ | 216 | 4.68 | $\mathrm{H}_{3}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 102 | 3.66 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ | 118 | 4.44 | $\mathrm{H}_{2}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 102 | 3.69 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 118 | 4.83 | $\mathrm{H}_{2}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 102 | 3.77 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 102 | 4.14 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 99 | 3.68 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 102 | 4.29 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 99 | 3.96 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ | 102 | 4.55 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 118 | 3 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\text {bonded }}$ | 216 | 4.59 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 109 | 3.13 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\text {bonded }}$ | 216 | 4.78 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 28 | 3.61 | $\mathrm{H}_{\text {Me }}$ with $\mathrm{Br}_{\text {bonded }}$ | 118 | 4.72 | $\mathrm{H}_{\text {Me }}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 213 | 3.7 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{C}_{\text {anion }}$ | 109 | 4.94 | $\mathrm{H}_{\text {Me }}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 109 | 4.01 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{C}_{\text {anion }}$ | 99 | 4.36 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| All Interactions < 5 Angstroms |  |  | 102 | 4.44 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 109 | 4.76 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 118 | 4.78 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| $\begin{gathered} \text { PF }_{6} \\ \text { Anion } \end{gathered}$ | Average Distance <br> (A) | Interaction | 102 | 4.82 | $\mathrm{H}_{\mathrm{Bu}}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 109 | 4.48 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 222 | 3.54 | $\mathrm{F}_{\text {PF6 } 6}$ with $\mathrm{H}_{\text {transfer }}$ | 109 | 4.56 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 222 | 4.05 | $\mathrm{F}_{\text {PF6 }}$ with $\mathrm{H}_{\text {transfer }}$ | 118 | 4.17 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 222 | 4.78 | $\mathrm{F}_{\text {PF6 }}$ with $\mathrm{H}_{\text {transfer }}$ | 118 | 4.78 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 213 | 4.36 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{C}_{\text {anion }}$ | 102 | 4.75 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{C}_{\text {anion }}$ |
|  |  |  | 213 | 4.36 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{C}_{\text {anion }}$ |
|  |  |  | 213 | 4.39 | $\mathrm{H}_{\mathrm{Me}}$ with $\mathrm{C}_{\text {anion }}$ |

## Methanol Reactant-Complex Figures




Figure S12 - The reactant complex of 1,1,1-tribromo-2,2-bis(3,4-dimethoxyphenyl)ethane with piperidine in methanol. For solvent effect data see Table S9.



Figure S13 - The reactant complex of 1,1,1-tribromo-2,2-bis(3,4-dimethoxyphenyl)ethane with pyrrolidine in methanol. For solvent effect data see Table S10.

## Methanol Transition Structure Figures



Figure S14 - The transition structure of 1,1,1-tribromo-2,2-bis(3,4-dimethoxyphenyl)ethane with piperidine in methanol. For solvent effect data see Table S11.


Figure S15 - The transition structure of 1,1,1-tribromo-2,2-bis(3,4-dimethoxyphenyl)ethane with pyrrolidine in methanol. For solvent effect data see Table S12.

Table S9: Piperidine reactant-complex in methanol-solvent effect data
Interactions < 4 Angstroms Interactions $>4$ Angstroms

| Methanol | Average distance ( $\AA$ ) | Interaction | Methanol | Average distance <br> (A) | Interaction |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 71 | 3.3 | $\mathrm{O}_{\text {MeOH }}$ with $\mathrm{H}_{\text {transfer }}$ | 90 | 5.42 | $\mathrm{O}_{\text {MeOH }}$ with $\mathrm{H}_{\text {transfer }}$ |
|  |  |  | 55 | 5.55 | $\mathrm{O}_{\text {MeOH }}$ with $\mathrm{H}_{\text {transfer }}$ |
|  |  |  | 199 | 5.91 | $\mathrm{O}_{\text {MeOH }}$ with $\mathrm{H}_{\text {transfer }}$ |
|  |  |  | 99 | 5.97 | $\mathrm{O}_{\text {MeOH }}$ with $\mathrm{H}_{\text {transfer }}$ |
|  |  |  | 54 | 4.99 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 58 | 5.32 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 59 | 4.64 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 66 | 5.83 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 70 | 5.76 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 70 | 5.88 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 71 | 4.37 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 71 | 4.75 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 82 | 4.98 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 82 | 5.44 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 92 | 5.48 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 97 | 4.36 | $\mathrm{H}_{\text {Meor }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 101 | 5.4 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 101 | 5.45 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 104 | 4.74 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 104 | 5.53 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 104 | 5.66 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 114 | 5.87 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 118 | 5.07 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 118 | 5.86 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 166 | 5.88 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 213 | 4.94 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 70 | 4.37 | $\mathrm{H}_{\mathrm{MeOH}}$ with $\mathrm{C}_{\text {anion }}$ |
|  |  |  | 55 | 4.46 | $\mathrm{H}_{\mathrm{MeOH}}$ with $\mathrm{C}_{\text {anion }}$ |
|  |  |  | 199 | 4.94 | $\mathrm{H}_{\mathrm{MeOH}}$ with $\mathrm{C}_{\text {anion }}$ |
|  |  |  | 114 | 5.86 | $\mathrm{H}_{\mathrm{MeOH}}$ with $\mathrm{C}_{\text {anion }}$ |
|  |  |  | 68 | 5.88 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{C}_{\text {anion }}$ |

Table S10: Pyrrolidine reactant-complex in methanol-solvent effect data
Interactions $<4$ Angstroms Interactions $>4$ Angstroms

| Methanol | Average Distance <br> (A) | Interaction | Methanol | Average Distance <br> ( $\AA$ ) | Interaction |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 79 | 3.2 | $\mathrm{O}_{\text {MeOH }}$ with $\mathrm{H}_{\text {transfer }}$ | 20 | 5.24 | $\mathrm{O}_{\text {MeOH }}$ with $\mathrm{H}_{\text {transfer }}$ |
|  |  |  | 29 | 5.65 | $\mathrm{O}_{\text {MeOH }}$ with $\mathrm{H}_{\text {transfer }}$ |
|  |  |  | 252 | 5.71 | $\mathrm{O}_{\text {MeOH }}$ with $\mathrm{H}_{\text {transfer }}$ |
|  |  |  | 20 | 4.31 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 20 | 5.41 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 36 | 5.01 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 36 | 5.62 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 56 | 5.29 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 56 | 5.29 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 56 | 5.83 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 62 | 4.76 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 62 | 5.82 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 69 | 5.93 | $\mathrm{H}_{\mathrm{MeOH}}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 79 | 4.58 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 79 | 5.2 | $\mathrm{H}_{\mathrm{MeOH}}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 81 | 5.05 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 81 | 5.62 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 84 | 4.72 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 103 | 5.11 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 104 | 5.28 | $\mathrm{H}_{\mathrm{MeOH}}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 213 | 5.57 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 20 | 4.96 | $\mathrm{H}_{\mathrm{MeOH}}$ with $\mathrm{C}_{\text {anion }}$ |
|  |  |  | 79 | 4.98 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{C}_{\text {anion }}$ |

## Table S11: Piperidine TS in methanol - solvent effect data

Interactions < 4 Angstroms
Interactions > 4 Angstroms

| Methanol | Average Distance <br> ( $\AA$ ) | Interaction | Methanol | Average Distance <br> ( $\AA$ ) | Interaction |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 105 | 3.23 | $\mathrm{O}_{\text {MeOH }}$ with $\mathrm{H}_{\text {transfer }}$ | 79 | 4.82 | $\mathrm{O}_{\text {MeOH }}$ with $\mathrm{H}_{\text {transfer }}$ |
| 70 | 2.16 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {LG }}$ | 38 | 5.11 | $\mathrm{O}_{\text {MeOH }}$ with $\mathrm{H}_{\text {transfer }}$ |
| 181 | 2.55 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\mathrm{LG}}$ | 116 | 5.3 | $\mathrm{O}_{\text {MeOH }}$ with $\mathrm{H}_{\text {transfer }}$ |
| 83 | 2.65 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\mathrm{LG}}$ | 16 | 5.52 | $\mathrm{O}_{\text {MeOH }}$ with $\mathrm{H}_{\text {transfer }}$ |
| 240 | 3.14 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {LG }}$ | 85 | 5.09 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {LG }}$ |
| 240 | 3.17 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ | 141 | 5.09 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {LG }}$ |
| 83 | 3.18 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ | 146 | 5.17 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 141 | 3.49 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ | 58 | 5.43 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
| 116 | 3.76 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ | 137 | 5.84 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {LG }}$ |
| 105 | 3.94 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ | 38 | 4.06 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 105 | 3.99 | $\mathrm{H}_{\mathrm{MeOH}}$ with $\mathrm{Br}_{\text {bonded }}$ | 38 | 4.06 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
| Continuation of Right Hand Column |  |  | 58 | 4.57 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 58 | 4.57 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 70 | 4.13 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 70 | 4.23 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 79 | 4.05 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 79 | 4.98 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 83 | 5.28 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 85 | 5.74 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 16 | 4.72 | $\mathrm{H}_{\mathrm{MeOH}}$ with $\mathrm{C}_{\text {anion }}$ | 97 | 5.16 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 105 | 4.77 | $\mathrm{H}_{\mathrm{MeOH}}$ with $\mathrm{C}_{\text {anion }}$ | 137 | 5.57 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 38 | 4.87 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{C}_{\text {anion }}$ | 141 | 5.75 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 70 | 5.02 | $\mathrm{H}_{\mathrm{MeOH}}$ with $\mathrm{C}_{\text {anion }}$ | 146 | 5.06 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 240 | 5.32 | $\mathrm{H}_{\mathrm{MeOH}}$ with $\mathrm{C}_{\text {anion }}$ | 181 | 4.67 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 79 | 5.67 | $\mathrm{H}_{\mathrm{MeOH}}$ with $\mathrm{C}_{\text {anion }}$ | 181 | 5.04 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
| 116 | 5.69 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{C}_{\text {anion }}$ | 240 | 4.72 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 181 | 4.12 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{C}_{\text {anion }}$ |
|  |  |  | 83 | 4.67 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{C}_{\text {anion }}$ |

Table S12: Pyrrolidine TS in methanol - solvent effect data
Interactions < 4 Angstroms Interactions $>4$ Angstroms

| Methanol | Average Distance <br> (A) | Interaction | Methanol | Average Distance <br> ( $\AA$ ) | Interaction |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 70 | 3.11 | $\mathrm{O}_{\text {MeOH }}$ with $\mathrm{H}_{\text {transfer }}$ | 194 | 4.88 | $\mathrm{O}_{\text {MeOH }}$ with $\mathrm{H}_{\text {transfer }}$ |
| 103 | 2.91 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {LG }}$ | 20 | 5.38 | $\mathrm{O}_{\text {MeOH }}$ with $\mathrm{H}_{\text {transfer }}$ |
| 103 | 3.6 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ | 58 | 5.88 | $\mathrm{O}_{\text {MeOH }}$ with $\mathrm{H}_{\text {transfer }}$ |
|  |  |  | 107 | 4.28 | $\mathrm{H}_{\mathrm{MeOH}}$ with $\mathrm{Br}_{\text {LG }}$ |
|  |  |  | 82 | 5.61 | $\mathrm{H}_{\mathrm{MeOH}}$ with $\mathrm{Br}_{\text {LG }}$ |
|  |  |  | 87 | 5.74 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\mathrm{LG}}$ |
|  |  |  | 58 | 5.47 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {LG }}$ |
|  |  |  | 20 | 4.47 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 43 | 4.82 | $\mathrm{H}_{\mathrm{MeOH}}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 70 | 4.04 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 70 | 4.25 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 77 | 5.99 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 87 | 5.36 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 103 | 4.19 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 107 | 4.37 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 194 | 4.92 | $\mathrm{H}_{\mathrm{MeOH}}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 194 | 5.68 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 240 | 4.85 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{Br}_{\text {bonded }}$ |
|  |  |  | 58 | 4.07 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{C}_{\text {anion }}$ |
|  |  |  | 70 | 4.8 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{C}_{\text {anion }}$ |
|  |  |  | 103 | 4.84 | $\mathrm{H}_{\text {MeOH }}$ with $\mathrm{C}_{\text {anion }}$ |
|  |  |  | 20 | 5.09 | $\mathrm{H}_{\mathrm{MeOH}}$ with $\mathrm{C}_{\text {anion }}$ |

# M062X/6-31+G(d,p) DFT Calculations 

## Optimization - Gas Phase

## Piperidine

$\mathrm{N}-\mathrm{N}=2.589456619393 \mathrm{D}+02 \mathrm{E}-\mathrm{N}=-1.100702934398 \mathrm{D}+03 \mathrm{KE}=2.495426026897 \mathrm{D}+02$ $1 \backslash 1 \backslash G I N C-D M C 125 \backslash F O p t \backslash R M 062 X \backslash 6-31+G(d, p) \backslash C 5 H 11 N 1 \backslash A U B C R A \backslash 11-M a y-2012 \backslash 0 \backslash \backslash$ \# opt=(noeigen, Z-Matrix) M062X/6-31+G(d,p) <br>Title Card Required<br>0,1\N , -1.1810722899,2.4488467391,-0.4190424729\C,-1.4884700963,2.6483280415 , -1.8335084946\C, -0.4124671137, 3.5612306429, 0.1348919849\H,-2.04466630 $89,2.3338752059,0.1063762843 \backslash C,-2.1704947966,3.9869260865,-2.138641202$ $6 \backslash H,-2.1019742581,1.8090574352,-2.176570676 \backslash \mathrm{H},-0.5377405545,2.59426226$ $49,-2.3829939194 \backslash C,-1.3408220834,5.148219141,-1.5834332978 \backslash \mathrm{H},-3.166612$ $4269,3.9959618219,-1.6735712676 \backslash \mathrm{H},-2.3191675836,4.0966945154,-3.219273$ $4012 \backslash \mathrm{C},-1.0534911678,4.934804479,-0.094483673 \backslash \mathrm{H},-0.3875652709,5.200983$ $9359,-2.1287137074 \backslash \mathrm{H},-1.8519831833,6.10298792,-1.7468573781 \backslash \mathrm{H},-1.99548$ $44365,4.9894767189,0.4697088913 \backslash \mathrm{H},-0.4002395016,5.7254037611,0.2930146$ $231 \backslash \mathrm{H},-0.2546728257,3.3760012235,1.2022403889 \backslash \mathrm{H}, 0.5777511301,3.5409408$ 705,-0.3423921754 <br>Version=EM64L-G09RevC.01 \State=1-A\HF=-251.795295\R $M S D=2.601 e-09 \backslash R M S F=2.124 e-05 \backslash$ Dipole=-0.2939879,0.4253379,-0.0365725\Qu adrupole=1.011199,-2.3685985,1.3573995,1.7654562,-0.6182169,0.7726535\} $\mathrm{PG}=\mathrm{C} 01$ [X(C5H11N1)] <br>@

## Pyrrolidine

$\mathrm{N}-\mathrm{N}=1.899551888848 \mathrm{D}+02 \mathrm{E}-\mathrm{N}=-8.720204546404 \mathrm{D}+02 \mathrm{KE}=2.106103932093 \mathrm{D}+02$ $1 \backslash 1 \backslash G I N C-D M C 177 \backslash F O p t \backslash R M 062 X \backslash 6-31+G(d, p) \backslash C 4 H 9 N 1 \backslash A U B C R A \backslash 26-J u n-2012 \backslash 0 \backslash \ \#$ opt=(noeigen,z-matrix) M062X/6-31+g(d,p) <br>Title Card Required $\backslash \backslash 0,1 \backslash N$, $-0.6636315433,-2.5305868744,-0.8580323574 \backslash C,-0.7661249353,-2.717393384$ $3,-2.3069820328 \backslash C,-1.6727563374,-3.4450019038,-0.3190729624 \backslash \mathrm{H}, 0.258197$ $3918,-2.8290324958,-0.5469779727 \backslash C,-1.0387405857,-4.222245235,-2.54627$ $64622 \backslash \mathrm{H}, 0.1324553357,-2.3506857427,-2.8091330729 \backslash \mathrm{H},-1.6137949845,-2.11$ $91848091,-2.6626757766 \backslash \mathrm{H},-0.1045926637,-4.7507374095,-2.7595014863 \backslash \mathrm{H},-$ $1.7055524898,-4.3862331469,-3.3970861885 \backslash \mathrm{C},-1.651703514,-4.7113668859$, $-1.2094665293 \backslash \mathrm{H},-1.0255622252,-5.4866342889,-0.7576937128 \backslash \mathrm{H},-2.6509415$ $423,-5.1359900417,-1.3386764896 \backslash \mathrm{H},-1.483997421,-3.6504771224,0.7374218$ $677 \backslash \mathrm{H},-2.6478898886,-2.9484104219,-0.392437156 \backslash \backslash V e r s i o n=E M 64 \mathrm{~L}-\mathrm{G0} 9 \mathrm{RevC}$. $01 \backslash$ State $=1-A \backslash H F=-212.4903584 \backslash R M S D=3.455 e-09 \backslash R M S F=3.369 e-05 \backslash D i p o l e=0.12$ 1609,-0.5471409,-0.1450257\Quadrupole=2.1108988,-2.8769759, 0.7660771, -$0.3566251,0.2579623,-1.6784545 \backslash \mathrm{PG}=\mathrm{C01}$ [X(C4H9N1)]<br>@

## 1,1,1-tribromo-2,2-bis(3,4-dimethoxyphenyl)ethane

$\mathrm{N}-\mathrm{N}=4.184677292895 \mathrm{D}+03 \mathrm{E}-\mathrm{N}=-2.908435597814 \mathrm{D}+04 \mathrm{KE}=8.651819724450 \mathrm{D}+03$ $1 \backslash 1 \backslash G I N C-D M C 34 \backslash F O p t \backslash R M 062 X \backslash 6-31+G(d, p) \backslash C 18 H 19 B r 304 \backslash A U B C R A \backslash 13-M a y-2012 \backslash$ $0 \backslash \ \#$ opt $=($ noeigen, Z-Matrix) M062X/6-31+G(d,p) <br>Title Card Required<br>0, $1 \backslash C, 0.9225174599,0.9173932152,-0.0289477469 \backslash C,-0.4763301914,1.01078585$ $65,0.0421160207 \backslash \mathrm{C}, 1.7073840359,2.0529272114,-0.1208725914 \backslash \mathrm{H}, 1.38690395$ $82,-0.0598421674,0.0051363906 \backslash C,-1.3166134945,-0.2480546912,0.18519100$ $71 \backslash C,-1.0684749252,2.2627215423,0.0620275105 \backslash C,-1.6605708113,-0.883646$ $5772,-1.1833667631 \backslash \mathrm{C},-0.7359031087,-1.1967068812,1.2239121084 \backslash \mathrm{H},-2.300$ $0871242,0.0554942511,0.562775403 \backslash \mathrm{Br},-2.8506550859,0.3119483696,-2.1538$ $616862 \backslash \mathrm{Br},-2.5916151511,-2.5690672128,-0.9385300177 \backslash \mathrm{Br},-0.1262943262$, -
$1.1976613613,-2.3413986897 \backslash C,-1.0789699209,-0.9885160107,2.5498267493 \backslash$ C, $0.193395019,-2.2015191768,0.9175457781 \backslash C,-0.4946362786,-1.7490041701$ , 3. $5706736335 \backslash \mathrm{H},-1.7927290301,-0.2116036699,2.8102488684 \backslash \mathrm{C}, 0.426766460$ $8,-2.7425144978,3.2690934884 \backslash \mathrm{H},-0.7766305861,-1.55760818,4.5989271752 \backslash$ C, $0.7682781922,-2.9724526651,1.9162457736 \backslash 0,1.0471935942,-3.5355300492$ , 4.1757285727\0,1.6674182873,-3.9615915408,1.6916010088\H, 0.4516528116 ,-2.3989537051,-0.1126206335\C, 2.0350420596,-4.2040730818, 0.3491064184 $\backslash \mathrm{H}, 2.7632710356,-5.0137704199,0.3800630535 \backslash \mathrm{H}, 2.4930389217,-3.314899729$ $1,-0.1042679038 \backslash \mathrm{H}, 1.1691219502,-4.5088855829,-0.251328057 \backslash \mathrm{C}, 0.73414145$ $47,-3.3286952735,5.536655477 \backslash \mathrm{H}, 1.3285308806,-4.0512820733,6.0947735358$ $\backslash H,-0.3313988468,-3.5039144358,5.728966676 \backslash \mathrm{H}, 0.9998253355,-2.312928828$ $5,5.8538670364 \backslash \mathrm{C},-0.2852978191,3.4217478784,-0.0192812903 \backslash \mathrm{H},-2.1481372$ $414,2.3530084925,0.1368729209 \backslash \mathrm{C}, 1.0962320306,3.3305742306,-0.118414 \backslash \mathrm{H}$, $-0.7710682067,4.3898126072,-0.0017070823 \backslash 0,1.9435126872,4.3836827187$, $0.198989246 \backslash 0,3.0611610638,2.0472778556,-0.1975526632 \backslash \mathrm{C}, 3.6981104683,0$ $.7866628761,-0.1722475562 \backslash \mathrm{H}, 4.7661304478,0.9878978603,-0.2471626008 \backslash \mathrm{H}$, $3.3791495723,0.1672528601,-1.0203229424 \backslash \mathrm{H}, 3.4872136591,0.2556619081,0$. $7642999539 \backslash \mathrm{C}, 1.3772481873,5.6765274932,-0.1647145952 \backslash \mathrm{H}, 2.2125434465,6$. $3721703964,-0.235579814 \backslash \mathrm{H}, 0.836372859,5.8468636213,0.7740481391 \backslash \mathrm{H}, 0.69$ $73562704,5.8336107327,-1.0109368209 \backslash \backslash V e r s i o n=E M 64 L-G 09 R e v C .01 \backslash$ State=1$A \backslash H F=-8713.2396515 \backslash \mathrm{RMSD}=6.089 \mathrm{e}-09 \backslash \mathrm{RMSF}=2.601 \mathrm{e}-05 \backslash \mathrm{Dipole}=0.1539064,0.45$ 62838, 0.7956221 \Quadrupole=-5.155626,3.7437062,1.4119198,-6.9081271,-4 $.8862378,0.9049399 \backslash \mathrm{PG}=\mathrm{C01}[\mathrm{X}(\mathrm{C} 18 \mathrm{H} 19 \mathrm{Br} 304)] \backslash \backslash @$

Piperidine + 1,1,1-tribromo-2,2-bis(3,4-dimethoxyphenyl)ethane
$\mathrm{N}-\mathrm{N}=5.554019254784 \mathrm{D}+03 \mathrm{E}-\mathrm{N}=-3.240905718350 \mathrm{D}+04 \quad \mathrm{KE}=8.901116988697 \mathrm{D}+03$ $1 \backslash 1 \backslash G I N C-D M C 86 \backslash F T S \backslash R M 062 X \backslash 6-31+G(d, p) \backslash C 23 H 30 B r 3 N 104 \backslash A U B C R A \backslash 06-M a y-2012$ \1<br>\# opt=(TS, noeigen, Z-Matrix) freq=noraman M062X/6-31+G(d,p) <br>Title Card Required $\backslash \backslash 0,1 \backslash C \backslash C, 1, B 1 \backslash C, 1, B 2,2, A 1 \backslash C, 1, B 3,3, A 2,2, D 1,0 \backslash H, 1, B 4,4, A 3$ $, 3, D 2,0 \backslash B r, 2, B 5,1, A 4,4, D 3,0 \backslash B r, 2, B 6,1, A 5,4, D 4,0 \backslash B r, 2, B 7,1, A 6,4, D 5,0 \backslash C$, $3, B 8,1, A 7,4, D 6,0 \backslash C, 3, B 9,1, A 8,4, D 7,0 \backslash C, 9, B 10,3, A 9,1, D 8,0 \backslash H, 9, B 11,3, A 10$, $1, D 9,0 \backslash C, 11, B 12,9, A 11,3, D 10,0 \backslash H, 11, B 13,9, A 12,3, D 11,0 \backslash C, 10, B 14,3, A 13,1$, $\mathrm{D} 12,0 \backslash 0,13, \mathrm{~B} 15,11, \mathrm{~A} 14,9, \mathrm{D} 13,0 \backslash 0,15, \mathrm{~B} 16,10, \mathrm{~A} 15,3, \mathrm{D} 14,0 \backslash \mathrm{H}, 10, \mathrm{~B} 17,3, \mathrm{~A} 16,1$ , D15, $0 \backslash \mathrm{C}, 17, \mathrm{~B} 18,15, \mathrm{~A} 17,10, \mathrm{D} 16,0 \backslash \mathrm{H}, 19, \mathrm{~B} 19,17, \mathrm{~A} 18,15, \mathrm{D} 17,0 \backslash \mathrm{H}, 19, \mathrm{~B} 20,17, \mathrm{~A}$ $19,15, \mathrm{D} 18,0 \backslash \mathrm{H}, 19, \mathrm{~B} 21,17, \mathrm{~A} 20,15, \mathrm{D} 19,0 \backslash \mathrm{C}, 16, \mathrm{~B} 22,13, \mathrm{~A} 21,11, \mathrm{D} 20,0 \backslash \mathrm{H}, 23, \mathrm{~B} 23$ $, 16, \mathrm{~A} 22,13, \mathrm{D} 21,0 \backslash \mathrm{H}, 23, \mathrm{~B} 24,16, \mathrm{~A} 23,13, \mathrm{D} 22,0 \backslash \mathrm{H}, 23, \mathrm{~B} 25,16, \mathrm{~A} 24,13, \mathrm{D} 23,0 \backslash \mathrm{C}, 4$ , $\mathrm{B} 26,1, \mathrm{~A} 25,3, \mathrm{D} 24,0 \backslash \mathrm{C}, 4, \mathrm{~B} 27,1, \mathrm{~A} 26,3, \mathrm{D} 25,0 \backslash \mathrm{C}, 27, \mathrm{~B} 28,4, \mathrm{~A} 27,1, \mathrm{D} 26,0 \backslash \mathrm{H}, 27, \mathrm{~B}$ $29,4, A 28,1, D 27,0 \backslash C, 29, B 30,27, A 29,4, D 28,0 \backslash 0,29, B 31,27, A 30,4, D 29,0 \backslash C, 31$, $\mathrm{B} 32,29, \mathrm{~A} 31,27, \mathrm{D} 30,0 \backslash 0,31, \mathrm{~B} 33,29, \mathrm{~A} 32,27, \mathrm{D} 31,0 \backslash \mathrm{H}, 33, \mathrm{~B} 34,31, \mathrm{~A} 33,29, \mathrm{D} 32,0 \backslash$ $\mathrm{H}, 28, \mathrm{~B} 35,4, \mathrm{~A} 34,1, \mathrm{D} 33,0 \backslash \mathrm{C}, 34, \mathrm{~B} 36,31, \mathrm{~A} 35,29, \mathrm{D} 34,0 \backslash \mathrm{H}, 37, \mathrm{~B} 37,34, \mathrm{~A} 36,31, \mathrm{D} 35$ $, 0 \backslash H, 37, B 38,34, A 37,31, D 36,0 \backslash H, 37, B 39,34, A 38,31, D 37,0 \backslash C, 32, B 40,29, A 39,2$ $7, D 38,0 \backslash H, 41, B 41,32, A 40,29, D 39,0 \backslash H, 41, B 42,32, A 41,29, D 40,0 \backslash H, 41, B 43,32$, $\mathrm{A} 42,29, \mathrm{D} 41,0 \backslash \mathrm{~N}, 1, \mathrm{~B} 44,4, \mathrm{~A} 43,28, \mathrm{D} 42,0 \backslash \mathrm{C}, 45, \mathrm{~B} 45,1, \mathrm{~A} 44,4, \mathrm{D} 43,0 \backslash \mathrm{C}, 45, \mathrm{~B} 46,1$, $\mathrm{A} 45,4, \mathrm{D} 44,0 \backslash \mathrm{H}, 45, \mathrm{~B} 47,1, \mathrm{~A} 46,4, \mathrm{D} 45,0 \backslash \mathrm{C}, 46, \mathrm{~B} 48,45, \mathrm{~A} 47,1, \mathrm{D} 46,0 \backslash \mathrm{H}, 46, \mathrm{~B} 49,45$ , $\mathrm{A} 48,1, \mathrm{D} 47,0 \backslash \mathrm{H}, 46, \mathrm{~B} 50,45, \mathrm{~A} 49,1, \mathrm{D} 48,0 \backslash \mathrm{C}, 49, \mathrm{~B} 51,46, \mathrm{~A} 50,45, \mathrm{D} 49,0 \backslash \mathrm{H}, 49, \mathrm{~B} 52$ $, 46, \mathrm{~A} 51,45, \mathrm{D} 50,0 \backslash \mathrm{H}, 49, \mathrm{~B} 53,46, \mathrm{~A} 52,45, \mathrm{D} 51,0 \backslash \mathrm{C}, 52, \mathrm{~B} 54,49, \mathrm{~A} 53,46, \mathrm{D} 52,0 \backslash \mathrm{H}, 5$ $2, B 55,49, A 54,46, D 53,0 \backslash H, 52, B 56,49, A 55,46, D 54,0 \backslash H, 55, B 57,52, A 56,49, D 55$, $0 \backslash H, 55, B 58,52, A 57,49, D 56,0 \backslash H, 47, B 59,45, A 58,1, D 57,0 \backslash H, 47, B 60,45, A 59,1, D$ $58,0 \backslash \backslash \mathrm{~B} 1=1.40400988 \backslash \mathrm{~B} 2=1.49630682 \backslash \mathrm{~B} 3=1.50139324 \backslash \mathrm{~B} 4=1.72836326 \backslash \mathrm{~B} 5=1.932$ $21401 \backslash B 6=2.31228381 \backslash B 7=1.94350682 \backslash B 8=1.39205206 \backslash B 9=1.40536115 \backslash B 10=1.40$ $045659 \backslash \mathrm{~B} 11=1.08699899 \backslash \mathrm{~B} 12=1.38963209 \backslash \mathrm{~B} 13=1.08377389 \backslash \mathrm{~B} 14=1.38519674 \backslash \mathrm{~B} 15$ $=1.35796831 \backslash B 16=1.35499256 \backslash B 17=1.08189255 \backslash B 18=1.41692585 \backslash B 19=1.0894481$
$3 \backslash B 20=1.09638361 \backslash B 21=1.09678311 \backslash B 22=1.40948016 \backslash B 23=1.08961911 \backslash B 24=1.09$ $748199 \backslash \mathrm{~B} 25=1.09718818 \backslash \mathrm{~B} 26=1.40517985 \backslash \mathrm{~B} 27=1.3922381 \backslash \mathrm{~B} 28=1.38175146 \backslash \mathrm{~B} 29=$ $1.08662712 \backslash \mathrm{~B} 30=1.4097265 \backslash \mathrm{~B} 31=1.36800474 \backslash \mathrm{~B} 32=1.39226912 \backslash \mathrm{~B} 33=1.35869482 \backslash$ $B 34=1.08357311 \backslash B 35=1.08630144 \backslash B 36=1.41124474 \backslash B 37=1.0895993 \backslash B 38=1.09697$ $884 \backslash B 39=1.09687882 \backslash B 40=1.42514056 \backslash B 41=1.09056217 \backslash B 42=1.09538041 \backslash B 43=1$. $09632824 \backslash \mathrm{~B} 44=2.83914146 \backslash \mathrm{~B} 45=1.48853372 \backslash \mathrm{~B} 46=1.49222766 \backslash \mathrm{~B} 47=1.02513804 \backslash \mathrm{~B}$ $48=1.52271746 \backslash \mathrm{~B} 49=1.09370271 \backslash \mathrm{~B} 50=1.09513036 \backslash \mathrm{~B} 51=1.53094948 \backslash \mathrm{~B} 52=1.09868$ $537 \backslash \mathrm{~B} 53=1.09390839 \backslash \mathrm{~B} 54=1.53033886 \backslash \mathrm{~B} 55=1.0979484 \backslash \mathrm{~B} 56=1.09359973 \backslash \mathrm{~B} 57=1.0$ $9875843 \backslash \mathrm{~B} 58=1.09386382 \backslash \mathrm{~B} 59=1.09118444 \backslash \mathrm{~B} 60=1.09463895 \backslash \mathrm{~A} 1=118.9792527 \backslash \mathrm{~A} 2$ $=113.88642537 \backslash A 3=107.36847657 \backslash A 4=117.67110463 \backslash A 5=113.07376179 \backslash A 6=116.6$ $2433608 \backslash A 7=120.48189393 \backslash A 8=121.1967123 \backslash A 9=120.93662617 \backslash A 10=119.8637343$ $4 \backslash A 11=120.54815059 \backslash A 12=119.22867552 \backslash A 13=121.39782093 \backslash A 14=125.14865267 \backslash$ $A 15=123.99997205 \backslash A 16=118.83356237 \backslash A 17=116.74391667 \backslash A 18=105.80889521 \backslash A 1$ $9=111.17291388 \backslash A 20=111.23606429 \backslash A 21=117.23366117 \backslash A 22=106.05615359 \backslash A 23=$ $111.32429674 \backslash A 24=111.2102013 \backslash A 25=117.43904286 \backslash A 26=124.97015939 \backslash A 27=121$ $.52969354 \backslash A 28=120.10072207 \backslash A 29=120.20324047 \backslash A 30=119.98612769 \backslash A 31=119.0$ $0698206 \backslash A 32=116.01459834 \backslash A 33=120.76976937 \backslash A 34=120.56656304 \backslash A 35=117.369$ $22562 \backslash A 36=106.07273947 \backslash A 37=111.10267121 \backslash A 38=111.23523453 \backslash A 39=112.76969$ $74 \backslash A 40=106.5048689 \backslash A 41=110.6531802 \backslash A 42=110.18697495 \backslash A 43=103.64811472 \backslash A$ $44=106.92338261 \backslash A 45=117.91681884 \backslash A 46=99.58963587 \backslash A 47=110.79771446 \backslash A 48=$ $107.11755173 \backslash A 49=106.12044765 \backslash A 50=110.73135998 \backslash A 51=109.31180158 \backslash A 52=10$ $8.81192216 \backslash A 53=110.46078169 \backslash A 54=109.24286899 \backslash A 55=110.31327873 \backslash A 56=109$. $75037648 \backslash A 57=111.01143674 \backslash A 58=106.95734405 \backslash A 59=106.42528891 \backslash D 1=-143.95$ $364474 \backslash D 2=117.27057946 \backslash D 3=181.23252484 \backslash D 4=64.55714993 \backslash D 5=-48.45694481 \backslash$ $D 6=61.95776622 \backslash D 7=-113.70890848 \backslash D 8=181.09143606 \backslash D 9=-1.36404881 \backslash D 10=0.9$ $1409272 \backslash D 11=179.95885141 \backslash D 12=-181.09674202 \backslash D 13=-179.66537974 \backslash D 14=180.0$ $6856871 \backslash D 15=1.81521102 \backslash D 16=2.21158135 \backslash D 17=-179.88324743 \backslash D 18=60.8363944$ $6 \backslash D 19=-60.66860538 \backslash D 20=-2.62837268 \backslash D 21=-178.93213295 \backslash D 22=62.20251721 \backslash D$ $23=-59.92856517 \backslash \mathrm{D} 24=49.82136286 \backslash \mathrm{D} 25=-131.47281923 \backslash \mathrm{D} 26=-181.84816969 \backslash \mathrm{D} 2$ $7=-0.44763665 \backslash D 28=0.52894918 \backslash D 29=179.99478415 \backslash D 30=0.07791056 \backslash D 31=180.2$ $5822645 \backslash \mathrm{D} 32=180.24328404 \backslash \mathrm{D} 33=-0.81504888 \backslash \mathrm{D} 34=-179.32247068 \backslash \mathrm{D} 35=179.579$ $41077 \backslash D 36=60.76315471 \backslash D 37=-61.42086547 \backslash D 38=100.1944545 \backslash D 39=-178.609439$ $3 \backslash D 40=62.25020497 \backslash D 41=-59.48664747 \backslash D 42=-14.23351217 \backslash D 43=-70.5523069 \backslash D 4$ $4=-199.39849392 \backslash D 45=44.11916372 \backslash D 46=171.59865574 \backslash D 47=48.10195614 \backslash D 48=-$ $67.28238844 \backslash D 49=55.62633009 \backslash D 50=-65.59466013 \backslash D 51=178.03639375 \backslash D 52=-55$. $07018756 \backslash D 53=65.31113261 \backslash D 54=-177.34112775 \backslash D 55=-66.06279083 \backslash D 56=176.23$ $730118 \backslash$ D57=-55.39397971\D58=60.14240886<br>Version=EM64L-G09RevC. 01 \Stat $e=1-A \backslash H F=-8965.0088398 \backslash R M S D=1.886 e-09 \backslash R M S F=1.803 e-04 \backslash D i p o l e=-2.197316$, $4.413267,-1.7831354 \backslash$ Quadrupole=1.4753629, 13.1554134, -14.6307763, -4.791 $1883,3.4326199,-3.7461425 \backslash \mathrm{PG}=\mathrm{C01}[\mathrm{X}(\mathrm{C} 23 \mathrm{H} 30 \mathrm{Br} 3 \mathrm{~N} 104)] \backslash \backslash @$

## Pyrrolidine $+1,1,1$-tribromo-2,2-bis(3,4-dimethoxyphenyl)ethane

Please see frequency calculation data.

## Frequency Calculation - Gas Phase

## Piperidine

Sum of electronic and zero-point Energies=
-251. 635342
Sum of electronic and thermal Energies=
-251. 629754
Sum of electronic and thermal Enthalpies=
Sum of electronic and thermal Free Energies=
-251.628810
$-251.663999$
$1 \backslash 1 \backslash G I N C-D M C 27 \backslash$ Freq $\backslash$ RM0 62X $\backslash 6-31+G(d, p) \backslash C 5 H 11 N 1 \backslash A U B C R A \backslash 30-M a y-2012 \backslash 0 \backslash \backslash \#$ freq=noraman M062X/6-31+G(d,p) <br>Title Card Required<br>0,1\N,0.002425, -$1.463718,-0.179512 \backslash C, 1.212257,-0.751709,0.225887 \backslash C,-1.209676,-0.755685$ $, 0.226071 \backslash \mathrm{H}, 0.00254,-1.592455,-1.188722 \backslash \mathrm{C}, 1.256262,0.710381,-0.232876 \backslash$ $\mathrm{H}, 2.080869,-1.304965,-0.145428 \backslash \mathrm{H}, 1.256981,-0.78686,1.323844 \backslash \mathrm{C},-0.00249$ $2,1.452419,0.225529 \backslash \mathrm{H}, 1.317293,0.740126,-1.330151 \backslash \mathrm{H}, 2.158437,1.199587$, $0.15271 \backslash \mathrm{C},-1.25864,0.706178,-0.233046 \backslash \mathrm{H},-0.002736,1.514297,1.323247 \backslash \mathrm{H}$, $-0.004175,2.481533,-0.149302 \backslash \mathrm{H},-1.319417,0.735423,-1.330363 \backslash \mathrm{H},-2.16257$ $, 1.192474,0.15214 \backslash \mathrm{H},-2.076552,-1.311918,-0.144837 \backslash \mathrm{H},-1.253908,-0.79071$ $7,1.324051 \backslash \backslash V e r s i o n=E M 64 L-G 09 R e v C .01 \backslash$ State=1-A $\backslash H F=-251.795295 \backslash R M S D=3.5$ $82 e-09 \backslash \mathrm{RMSF}=2.132 e-05 \backslash$ ZeroPoint=0.1599535 C Thermal=0.1655409\Dipole=-0. $0007591,0.4581114,-0.2425113 \backslash$ DipoleDeriv=-0.6381003, 0.0003507, 0.000042 $4,0.0004164,-0.8366985,-0.0141057,0.0000204,0.0372253,-0.2218972,0.419$ $2142,0.1448433,0.0562911,0.0912595,0.3850056,-0.0103555,0.157488,0.000$ $9008,0.2653104,0.4199112,-0.1447136,-0.0562606,-0.0911166,0.3841461,-0$ $.0105346,-0.1575016,0.0003677,0.2652677,0.0707097,-0.0004211,-0.000154$ $4,-0.0004237,0.3352042,0.0906266,0.0000315,-0.0426609,-0.0197965,0.046$ $0161,0.0108926,0.0101627,-0.0243174,-0.0630564,0.0187321,-0.0165787,0$. $0307219,0.1401194,-0.1298637,0.0741535,0.0293037,0.0855881,-0.0465719$, $-0.027724,0.0823495,-0.0392339,0.0422338,0.0361197,-0.021112,0.0258271$ $,-0.0392358,0.0093028,-0.0079184,-0.0540252,0.0140946,-0.1761616,0.048$ $6186,-0.0000333,-0.0000182,-0.0000911,0.0964257,-0.0074693,-0.0000657$, $0.0246921,0.1403794,0.0330296,0.0204953,-0.0153648,0.0218982,0.0105083$ , -0.0161151, 0.0432477,0.0141972,-0.1866898,-0.1526537, -0.0832231, -0.04 $13849,-0.089403,-0.0232672,-0.0207336,-0.0779987,-0.0431704,0.0367481$, $0.0459311,-0.0106684,-0.0102935,0.0244805,-0.0629077,0.018703,0.016395$ $2,0.0308842,0.1400773,-0.0049679,-0.0000655,0.0000172,-0.0000615,0.050$ $5204,0.0169528,0.0001296,-0.0512852,-0.1813863,0.0195105,0.0003246,-0$. $0000486,0.0003136,-0.188624,0.0425436,-0.0001398,0.077388,0.0395456,0$. $0332025,-0.0203707,0.0155164,-0.0217763,0.0103794,-0.0161401,-0.043209$ $6,0.0139886,-0.1867038,-0.1532797,0.082796,0.0414072,0.0890817,-0.0227$ $805,-0.0206037,0.0780801,-0.0428827,0.0367967,-0.1293773,-0.0744717,-0$ $.0291828,-0.0859497,-0.0470997,-0.0277864,-0.0821352,-0.0394585,0.0422$ $897,0.0359796,0.0212234,-0.02586,0.0393372,0.0095134,-0.0080716,0.0539$ $124,0.0142312,-0.176133 \backslash \operatorname{Pol}$ ar $=68.2370342,0.0026542,65.3657129,-0.00120$ $77,0.3857186,59.6895903 \backslash \mathrm{PG}=\mathrm{C01}[\mathrm{X}(\mathrm{C} 5 \mathrm{H} 11 \mathrm{~N} 1)] \backslash \mathrm{NImag}=0 \backslash \backslash$

## Pyrrolidine

Sum of electronic and zero-point Energies=

$$
\begin{aligned}
& -212.359716 \\
& -212.354696 \\
& -212.353752 \\
& -212.388611
\end{aligned}
$$

Sum of electronic and thermal Energies=
Sum of electronic and thermal Enthalpies=
Sum of electronic and thermal Free Energies=
$1 \backslash 1 \backslash A S N \_A L T I X-A L T I X 8 \backslash F r e q \backslash R M 062 X \backslash 6-31+G(d, p) \backslash C 4 H 9 N 1 \backslash A U B C R A \backslash 02-J u l-201$
$2 \backslash 0 \backslash \ \#$ freq=noraman $M 062 X / 6-31+g(d, p) \backslash \backslash$ Title Card Required $\backslash \backslash 0,1 \backslash N, 0.00$ $0461,-1.262588,0.206099 \backslash C,-1.151004,-0.45242,-0.197154 \backslash C, 1.151858,-0.4$ $51485,-0.195599 \backslash \mathrm{H},-0.000294,-1.363763,1.218698 \backslash \mathrm{C},-0.775555,1.024889,0$. $072576 \backslash \mathrm{H},-2.054333,-0.776299,0.32551 \backslash \mathrm{H},-1.312546,-0.61074,-1.270352 \backslash \mathrm{H}$, $-1.161195,1.345845,1.045032 \backslash \mathrm{H},-1.195432,1.697032,-0.680641 \backslash \mathrm{C}, 0.77429,1$ $.026175,0.07065 \backslash \mathrm{H}, 1.16193,1.351537,1.040736 \backslash \mathrm{H}, 1.190551,1.696449,-0.686$ $275 \backslash \mathrm{H}, 2.054244,-0.773415,0.329845 \backslash \mathrm{H}, 1.316322,-0.611486,-1.268083 \backslash \backslash \mathrm{Vers}$ ion=IA64L-G09RevC. $01 \backslash$ State=1-A $\backslash H F=-212.4903584 \backslash R M S D=2.783 e-09 \backslash R M S F=3.3$ $62 e-05 \backslash$ ZeroPoint $=0.1306429 \backslash$ Thermal $=0.1356624 \backslash$ Dipole $=-0.0005884,0.50775$ 56, 0.2781505\DipoleDeriv=-0.531025,0.0003803,-0.0001075, 0.0000671, -0. 8 $708111,0.1156743,-0.0002707,-0.0087943,-0.2385113,0.3228678,-0.1053935$ , 0.0468977, -0.0392526,0.394399,-0.0077633,0.1409929,-0.0073845,0.28292 $71,0.3232114,0.1053269,-0.0470905,0.0389931,0.3942878,-0.007762,-0.140$ 855,-0.0075294, 0.2827467,0.081809,-0.0001663,0.0001936, -0.0000821,0.31 $2974,-0.1044576,0.0000822,0.0254552,-0.0146011,0.0111275,-0.0726902,-0$ $.0109679,-0.0115404,-0.0681267,-0.0241959,-0.043799,-0.0323814,0.13512$ $76,-0.1169655,-0.0505249,0.043018,-0.0564487,0.0088565,0.0221323,0.097$ $9875,0.0365898,0.0190594,0.029363,-0.0000839,-0.0085832,0.008916,-0.00$ $84398,-0.023783,-0.0807555,-0.0249001,-0.1614163,-0.0175702,0.0296278$, $0.0479255,0.015233,0.0103234,-0.0331424,0.0856273,-0.0860057,-0.115107$ $3,-0.0043223,0.0526466,-0.042376,0.0744685,-0.0578834,0.0611925,-0.076$ $8429,0.1059478,-0.0338645,0.0106683,0.0724323,0.0111179,0.0118515,-0.0$ $682617,-0.0235628,0.0438356,-0.0322483,0.1349263,-0.0176417,-0.0303707$ , -0.0480602,-0.0157844,0.009686,-0.0338482,-0.0857591,-0.0866639,-0.11 $40297,-0.0037779,-0.0517941,0.0422957,-0.0738429,-0.0574619,0.0612862$, $0.07688,0.1062334,-0.0348697,-0.116833,0.050282,-0.0433925,0.0559944,0$ $.0090776,0.022209,-0.0984862,0.0366662,0.0185819,0.0290885,0.0003278,0$ $.0091292,-0.0085726,-0.0086198,-0.0239789,0.0813628,-0.0249848,-0.1609$ $692 \backslash$ Polar $=55.3515982,0.0012113,54.1729747,-0.0022231,-0.2259857,48.599$ $3539 \backslash \mathrm{PG}=\mathrm{C01}[\mathrm{X}(\mathrm{C} 4 \mathrm{H} 9 \mathrm{~N} 1)] \backslash \mathrm{NImag}=0 \backslash \backslash$

## 1,1,1-tribromo-2,2-bis (3,4-dimethoxyphenyl)ethane

Sum of electronic and zero-point Energies=
Sum of electronic and thermal Energies=
Sum of electronic and thermal Enthalpies=
Sum of electronic and thermal Free Energies=
-8712.897612
-8712.871626
-8712.870682
-8712.956595
$1 \backslash 1 \backslash G I N C-D M C 160 \backslash$ Freq $\backslash$ RM0 $62 X \backslash 6-31+G(d, p) \backslash C 18 H 19 B r 304 \backslash A U B C R A \backslash 30-M a y-2012$ $\backslash 0 \backslash \ \#$ freq=noraman $M 062 X / 6-31+G(d, p) \backslash \backslash T i t l e ~ C a r d ~ R e q u i r e d \backslash \backslash 0,1 \backslash C, 1.280$ $197,1.346462,0.331935 \backslash C, 1.301755,0.410578,-0.714107 \backslash C, 2.342932,2.20800$ $4,0.537471 \backslash \mathrm{H}, 0.409339,1.399215,0.972738 \backslash \mathrm{C}, 0.105013,-0.497521,-0.947322$ $\backslash C, 2.387816,0.384375,-1.57327 \backslash C, 0.174353,-1.790385,-0.099425 \backslash C,-1.2068$ $04,0.270164,-0.870497 \backslash \mathrm{H}, 0.177747,-0.878781,-1.972643 \backslash \mathrm{Br}, 1.660585,-2.87$ $8673,-0.727399 \backslash B r,-1.448907,-2.83331,-0.311003 \backslash B r, 0.467341,-1.49845,1$. $803883 \backslash C,-1.647927,0.908481,-2.018125 \backslash C,-1.933997,0.438822,0.316873 \backslash C$, $-2.784932,1.726106,-1.993118 \backslash \mathrm{H},-1.096552,0.796093,-2.947759 \backslash \mathrm{C},-3.50452$ , 1. $895541,-0.818179 \backslash \mathrm{H},-3.100863,2.218917,-2.904591 \backslash \mathrm{C},-3.070099,1.23267$ $4,0.352968 \backslash 0,-4.616304,2.658372,-0.684698 \backslash 0,-3.822147,1.435056,1.46237$ $2 \backslash H,-1.622988,-0.074167,1.215224 \backslash \mathrm{C},-3.403127,0.79354,2.649434 \backslash \mathrm{H},-4.119$ $104,1.086639,3.416478 \backslash H,-2.396202,1.119035,2.942851 \backslash \mathrm{H},-3.409916,-0.297$ $423,2.535399 \backslash C,-5.074357,3.339598,-1.833185 \backslash \mathrm{H},-5.96183,3.889672,-1.522$ $16 \backslash \mathrm{H},-5.34025,2.635828,-2.631351 \backslash \mathrm{H},-4.318709,4.042901,-2.203797 \backslash \mathrm{C}, 3.46$
$6341,1.258563,-1.383802 \backslash \mathrm{H}, 2.411228,-0.319928,-2.399607 \backslash \mathrm{C}, 3.459491,2.16$ $5263,-0.332796 \backslash \mathrm{H}, 4.30457,1.219534,-2.068841 \backslash 0,4.445284,3.053267,-0.062$ $469 \backslash 0,2.400691,3.135134,1.525254 \backslash \mathrm{C}, 1.286759,3.21896,2.389907 \backslash \mathrm{H}, 1.52095$ $6,4.005296,3.106568 \backslash \mathrm{H}, 1.128159,2.271479,2.92072 \backslash \mathrm{H}, 0.376163,3.482063,1$. $837501 \backslash \mathrm{C}, 5.561339,3.06732,-0.92705 \backslash \mathrm{H}, 6.226238,3.841755,-0.5465 \backslash \mathrm{H}, 5.263$ $36,3.311464,-1.953908 \backslash \mathrm{H}, 6.081372,2.101657,-0.918102 \backslash \backslash V e r s i o n=E M 64 \mathrm{~L}-\mathrm{G} 09$ RevC. $01 \backslash$ State=1-A $\backslash H F=-8713.2396515 \backslash \mathrm{RMSD}=4.257 \mathrm{e}-09 \backslash \mathrm{RMSF}=2.604 \mathrm{e}-05 \backslash \mathrm{ZeroP}$ oint $=0.34204 \backslash$ Thermal $=0.3680255 \backslash$ Dipole $=0.0355102,0.7453307,-0.5550792 \backslash \mathrm{D}$ ipoleDeriv=-0.1167144,-0.0859981,-0.1091202,0.0938304,-0.1163729,-0.12 $49712,0.0371506,0.0787332,-0.1594846,-0.0624739,0.1506001,-0.016303,0$. $0303231,-0.190729,0.0671561,0.0087307,0.0645912,-0.0126305,-0.1952994$, $-0.1991813,0.013679,-0.0117051,0.6755854,0.7443299,0.1781075,0.8195221$ , 0. $887867,0.0827458,0.009612,0.0780838,0.0266976,0.1152675,0.0043344,0$ $.0893008,-0.0199904,0.050058,0.062628,0.0260363,0.0482361,-0.0298782,0$ $.3278892,-0.1412822,-0.0088637,-0.0890393,-0.0803112,-0.0143101,0.0013$ $091,-0.1041531,0.0359916,-0.0755974,0.0188961,0.004877,0.0684727,-0.05$ $79025,1.0460892,0.0420284,0.0102029,0.0588286,0.6335242,0.3166271,0.05$ $29776,0.2592324,0.7895845,0.1175397,-0.1358302,-0.0026342,-0.0454796,-$ $0.1698744,0.024656,0.112656,-0.0230377,-0.0046446,0.0208974,0.0105709$, $0.0023241,-0.0054541,-0.0192368,0.0423316,0.0028619,-0.0459075,-0.0345$ $086,-0.4380718,0.2408999,0.1207704,0.2375194,-0.2737166,-0.1009446,0.1$ $38638,-0.0961583,-0.1513497,-0.5409176,-0.2761705,-0.0650511,-0.285048$ $8,-0.2835076,-0.0488404,-0.0544506,-0.0364352,-0.0926345,-0.1323339,0$. $013273,-0.0797857,-0.0097338,-0.1416799,-0.1203798,-0.0654942,-0.11856$ $8,-0.5227143,-0.1816489,-0.0470758,0.0327502,0.0619475,-0.1207104,-0.0$ $79065,-0.0627104,0.0018905,-0.0091958,-0.2155856,-0.0008665,0.1287713$, $-0.0071335,-0.1144649,-0.1021943,-0.1734041,0.0543916,-0.1681485,-0.11$ $03697,0.0471696,-0.1109795,-0.0710225,-0.1457352,0.0281204,0.0977606,-$ $0.1356631,0.0362628,0.0456295,0.0462579,0.089219,0.0428552,0.089915,-0$ $.014618,0.0806388,-0.0067816,0.0007938,1.2483731,-0.7947446,0.1586179$, $-0.9268207,0.6293611,-0.0534739,0.106692,0.01628,-0.1772249,0.0813639$, $0.0456556,-0.0281634,0.0601741,0.0808587,0.0579891,-0.0541129,0.072373$ $,-0.0015184,0.3815244,0.0318581,-0.6760644,0.0701904,-0.0112992,0.1587$ $287,-0.8972927,0.2082496,1.112858,-1.4928345,0.8373108,-0.3191466,0.96$ $11541,-0.9314459,0.3051551,-0.2358653,0.2232989,-0.5087629,-0.6595945$, $0.0827332,0.4647664,0.1054097,-0.3332315,0.072189,0.5966054,0.0706281$, $-1.5648794,0.1600502,-0.0305301,-0.0184544,-0.0197928,0.1171537,0.0386$ $41,-0.0145538,0.0296758,0.0220347,0.3021608,-0.0263803,0.1645875,0.054$ $6842,0.3591729,-0.2781107,-0.0689007,-0.1277456,0.8210681,-0.008685,0$. $0293121,0.1182307,0.0485521,0.0680135,-0.043243,0.0672325,-0.0022129,-$ $0.0532882,-0.1091629,-0.0450572,-0.1354433,-0.0871863,0.0090619,0.0400$ $717,0.0069362,0.0195354,-0.0102081,0.0701488,0.0091606,-0.0707032,-0.0$ $22921,-0.1254503,0.0658305,-0.0032438,-0.0645525,-0.0099917,0.4991086$, $-0.1411788,0.1559138,-0.2668825,0.5486259,-0.1951696,0.5035248,-0.3881$ $031,0.6091761,-0.0725587,0.1115188,-0.0087934,0.1010736,0.0165828,0.01$ $54328,0.0529776,-0.0286786,0.0562683,0.046215,-0.0082447,-0.0024912,-0$ $.0449297,-0.0573769,-0.1064674,-0.133109,0.0186909,-0.0876554,-0.03791$ $63,-0.1318315,0.0636389,-0.0223094,-0.0413497,0.0448083,-0.074158,0.09$ $19114,-0.0200674,-0.1059175,0.049066,0.0010757,-0.1405116,-0.1712025,0$ $.1181493,-0.225632,-0.0582211,-0.0470065,0.0746853,-0.0230585,-0.01365$ $33,-0.0191956,0.0286584,-0.0939586,-0.0172629,-0.091317,0.0329891,1.21$ $48223,0.863398,0.126808,0.9439108,0.6611512,-0.0343521,0.1972667,0.009$

9912,-0.069735,-0.0124678,-0.0342917,0.0731281,-0.0132902,0.1125607,-0 $.024132,0.0971706,-0.0108597,0.0552623,-1.7784386,-0.8085922,0.1918238$ , - 0. $925912,-0.8382659,0.0258063,0.0974057,-0.0436828,-0.3825104,-0.485$ $7624,0.10095,0.2572905,-0.0029897,-0.8407247,-0.6655074,0.1581306,-0.7$ $222615,-1.171616,0.5153679,-0.2085706,-0.3687081,-0.0147644,0.3221016$, $0.0420229,-0.1801926,0.1533071,0.5943898,0.0547712,-0.0439046,-0.02857$ $73,-0.0110319,-0.0231844,-0.1229874,0.0107286,-0.0918798,-0.0227302,0$. $0110302,0.0523805,0.0825738,-0.0455932,-0.0842972,0.1305644,0.0371724$, $0.0269085,-0.0023681,-0.0958546,0.08364,0.0332864,0.0189716,0.0551354$, $0.0384747,-0.1016313,0.0299478,-0.0414326,0.9404661,0.2264269,-0.19384$ $17,0.0056341,0.3038502,-0.0339392,-0.4750378,-0.2125653,0.448609,-0.04$ $30507,-0.0822733,0.0034761,-0.1305863,-0.0161275,-0.0229507,-0.049502$, $-0.0567651,0.0589529,-0.0271683,0.0112021,-0.0830042,0.0419494,0.05071$ $49,0.0138907,0.081031,0.0941007,-0.1283253,-0.0384803,0.0014108,0.0158$ $166,0.1604756,-0.0796033,-0.0076186,0.0788444,0.0586936,0.0166707 \backslash \mathrm{Pola}$ $r=328.6635752,-3.0362978,266.7006373,-14.1109067,9.0609003,258.3118826$ $\backslash \mathrm{PG}=\mathrm{C01}[\mathrm{X}(\mathrm{C} 18 \mathrm{H} 19 \mathrm{Br} 304)] \backslash \mathrm{NImag}=0 \backslash \backslash$

Piperidine $+1,1,1$-tribromo-2,2-bis(3,4-dimethoxyphenyl)ethane

|  | 1 | 2 | 3 |
| :--- | :---: | :---: | :---: |
| Frequencies -- | A | A | A |
|  | 150.8470 | 17.5784 | 20.2658 |

Sum of electronic and zero-point Energies= -8964.507392

Sum of electronic and thermal Energies=
Sum of electronic and thermal Enthalpies=
Sum of electronic and thermal Free Energies=
$-8964.474136$
$-8964.473192$
$-8964.576397$
$1 \backslash 1 \backslash G I N C-D M C 34 \backslash$ Freq $\backslash$ RM0 $62 X \backslash 6-31+G(d, p) \backslash C 23 H 30 B r 3 N 104 \backslash A U B C R A \backslash 10-M a y-201$ $2 \backslash 1 \backslash \ \#$ freq=noraman $M 062 X / 6-31+G(d, p) \backslash \backslash i t l e ~ C a r d ~ R e q u i r e d \backslash \backslash 0,1 \backslash C \backslash C, 1$, $\mathrm{B} 1 \backslash \mathrm{C}, 1, \mathrm{~B} 2,2, \mathrm{~A} 1 \backslash \mathrm{C}, 1, \mathrm{~B} 3,2, \mathrm{~A} 2,3, \mathrm{D} 1,0 \backslash \mathrm{H}, 1, \mathrm{~B} 4,2, \mathrm{~A} 3,4, \mathrm{D} 2,0 \backslash \mathrm{Br}, 2, \mathrm{~B} 5,1, \mathrm{~A} 4,3, \mathrm{D} 3$ $, 0 \backslash B r, 2, B 6,1, A 5,3, D 4,0 \backslash B r, 2, B 7,1, A 6,3, D 5,0 \backslash C, 3, B 8,1, A 7,2, D 6,0 \backslash C, 3, B 9,1$ $, \mathrm{A} 8,2, \mathrm{D} 7,0 \backslash \mathrm{C}, 9, \mathrm{~B} 10,3, \mathrm{~A} 9,1, \mathrm{D} 8,0 \backslash \mathrm{H}, 9, \mathrm{~B} 11,3, \mathrm{~A} 10,1, \mathrm{D} 9,0 \backslash \mathrm{C}, 11, \mathrm{~B} 12,9, \mathrm{~A} 11,3, \mathrm{D}$ $10,0 \backslash H, 11, B 13,9, A 12,3, D 11,0 \backslash C, 10, B 14,3, A 13,1, D 12,0 \backslash 0,13, B 15,11, A 14,9, D$ $13,0 \backslash 0,15, \mathrm{~B} 16,10, \mathrm{~A} 15,3, \mathrm{D} 14,0 \backslash \mathrm{H}, 10, \mathrm{~B} 17,3, \mathrm{~A} 16,1, \mathrm{D} 15,0 \backslash \mathrm{C}, 17, \mathrm{~B} 18,15, \mathrm{~A} 17,10$ , D16, $0 \backslash \mathrm{H}, 19, \mathrm{~B} 19,17, \mathrm{~A} 18,15, \mathrm{D} 17,0 \backslash \mathrm{H}, 19, \mathrm{~B} 20,17, \mathrm{~A} 19,15, \mathrm{D} 18,0 \backslash \mathrm{H}, 19, \mathrm{~B} 21,17, \mathrm{~A}$ $20,15, D 19,0 \backslash C, 16, B 22,13, A 21,11, D 20,0 \backslash H, 23, B 23,16, A 22,13, D 21,0 \backslash H, 23, B 24$ $, 16, \mathrm{~A} 23,13, \mathrm{D} 22,0 \backslash \mathrm{H}, 23, \mathrm{~B} 25,16, \mathrm{~A} 24,13, \mathrm{D} 23,0 \backslash \mathrm{C}, 4, \mathrm{~B} 26,1, \mathrm{~A} 25,2, \mathrm{D} 24,0 \backslash \mathrm{C}, 4, \mathrm{~B} 2$ $7,1, \mathrm{~A} 26,2, \mathrm{D} 25,0 \backslash \mathrm{C}, 27, \mathrm{~B} 28,4, \mathrm{~A} 27,1, \mathrm{D} 26,0 \backslash \mathrm{H}, 27, \mathrm{~B} 29,4, \mathrm{~A} 28,1, \mathrm{D} 27,0 \backslash \mathrm{C}, 29, \mathrm{~B} 30$ , 27, A29, 4, D28, 0 \0, 29, B31, 27, A30, 4, D29, 0 \C, 31, B32, 29, A31, 27, D30, 0 $\mathrm{C}, ~ 31$, $\mathrm{B} 33,29, \mathrm{~A} 32,27, \mathrm{D} 31,0 \backslash \mathrm{H}, 33, \mathrm{~B} 34,31, \mathrm{~A} 33,29, \mathrm{D} 32,0 \backslash \mathrm{H}, 28, \mathrm{~B} 35,4, \mathrm{~A} 34,1, \mathrm{D} 33,0 \backslash \mathrm{C}$, $34, \mathrm{~B} 36,31, \mathrm{~A} 35,29, \mathrm{D} 34,0 \backslash \mathrm{H}, 37, \mathrm{~B} 37,34, \mathrm{~A} 36,31, \mathrm{D} 35,0 \backslash \mathrm{H}, 37, \mathrm{~B} 38,34, \mathrm{~A} 37,31, \mathrm{D} 36$ $, 0 \backslash H, 37, B 39,34, A 38,31, D 37,0 \backslash C, 32, B 40,29, A 39,27, D 38,0 \backslash H, 41, B 41,32, A 40,2$ $9, D 39,0 \backslash H, 41, B 42,32, A 41,29, D 40,0 \backslash H, 41, B 43,32, A 42,29, D 41,0 \backslash N, 1, B 44,2, A 4$ $3,4, D 42,0 \backslash C, 45, B 45,1, A 44,2, D 43,0 \backslash C, 45, B 46,1, A 45,2, D 44,0 \backslash H, 45, B 47,1, A 46$ $, 2, D 45,0 \backslash C, 46, B 48,45, A 47,1, D 46,0 \backslash H, 46, B 49,45, A 48,1, D 47,0 \backslash H, 46, B 50,45, A$ $49,1, D 48,0 \backslash C, 49, B 51,46, A 50,45, D 49,0 \backslash H, 49, B 52,46, A 51,45, D 50,0 \backslash H, 49, B 53$, $46, A 52,45, D 51,0 \backslash C, 47, B 54,45, A 53,1, D 52,0 \backslash H, 52, B 55,49, A 54,46, D 53,0 \backslash H, 52$, B56, 49, A55, 46, D54, 0 \H, 55, B57, 47, A56, 45, D55, 0 \H, 55, B58, 47, A57, 45, D56, 0\ $\mathrm{H}, 47, \mathrm{~B} 59,45, \mathrm{~A} 58,1, \mathrm{D} 57,0 \backslash \mathrm{H}, 47, \mathrm{~B} 60,45, \mathrm{~A} 59,1, \mathrm{D} 58,0 \backslash \backslash \mathrm{~B} 1=1.40400945 \backslash \mathrm{~B} 2=1.49$ $630654 \backslash \mathrm{~B} 3=1.50139284 \backslash \mathrm{~B} 4=1.72836329 \backslash \mathrm{~B} 5=1.93221335 \backslash \mathrm{~B} 6=2.31228406 \backslash \mathrm{~B} 7=1.94$ $350692 \backslash B 8=1.39205205 \backslash B 9=1.40536089 \backslash B 10=1.40045705 \backslash B 11=1.08699926 \backslash B 12=1$
$.3896329 \backslash \mathrm{~B} 13=1.08377415 \backslash \mathrm{~B} 14=1.38519665 \backslash \mathrm{~B} 15=1.35796791 \backslash \mathrm{~B} 16=1.35499257 \backslash \mathrm{~B}$ $17=1.0818931 \backslash B 18=1.41692586 \backslash B 19=1.08944785 \backslash B 20=1.09638412 \backslash B 21=1.096782$ $83 \backslash B 22=1.40948064 \backslash B 23=1.08961903 \backslash B 24=1.09748126 \backslash \mathrm{~B} 25=1.09718834 \backslash \mathrm{~B} 26=1.4$ $0518078 \backslash \mathrm{~B} 27=1.39223895 \backslash \mathrm{~B} 28=1.38175158 \backslash \mathrm{~B} 29=1.08662665 \backslash \mathrm{~B} 30=1.40972593 \backslash \mathrm{~B} 3$ $1=1.36800512 \backslash B 32=1.39226969 \backslash B 33=1.35869506 \backslash B 34=1.08357249 \backslash B 35=1.086301$ $13 \backslash B 36=1.41124463 \backslash B 37=1.08959888 \backslash B 38=1.09697931 \backslash B 39=1.09687868 \backslash B 40=1.4$ $2514063 \backslash B 41=1.09056213 \backslash B 42=1.09538062 \backslash B 43=1.09632815 \backslash B 44=2.83914096 \backslash B 4$ $5=1.48853312 \backslash B 46=1.49222793 \backslash B 47=1.02513828 \backslash B 48=1.52271739 \backslash B 49=1.093702$ $31 \backslash \mathrm{~B} 50=1.09513044 \backslash \mathrm{~B} 51=1.53094973 \backslash \mathrm{~B} 52=1.09868574 \backslash \mathrm{~B} 53=1.0939078 \backslash \mathrm{~B} 54=1.52$ $324778 \backslash \mathrm{~B} 55=1.09794822 \backslash \mathrm{~B} 56=1.09360005 \backslash \mathrm{~B} 57=1.09875801 \backslash \mathrm{~B} 58=1.09386397 \backslash \mathrm{~B} 59$ $=1.09118438 \backslash B 60=1.09463947 \backslash A 1=118.97923726 \backslash A 2=116.77858154 \backslash A 3=89.03876$ $703 \backslash A 4=117.67111296 \backslash A 5=113.07375719 \backslash A 6=116.6243254 \backslash A 7=120.48188521 \backslash A 8=$ $121.19673329 \backslash A 9=120.93663441 \backslash A 10=119.86377528 \backslash A 11=120.54814298 \backslash A 12=119$ $22869558 \backslash A 13=121.39784186 \backslash A 14=125.14865298 \backslash A 15=123.99997387 \backslash A 16=118.8$ $3355359 \backslash A 17=116.74395165 \backslash A 18=105.80891905 \backslash A 19=111.17286893 \backslash A 20=111.236$ $07099 \backslash A 21=117.2336599 \backslash A 22=106.05611137 \backslash A 23=111.324345 \backslash A 24=111.21017274$ $\backslash A 25=117.43905254 \backslash A 26=124.97018851 \backslash A 27=121.529665 \backslash A 28=120.10072109 \backslash A 29$ $=120.20329254 \backslash A 30=119.98609757 \backslash A 31=119.00698062 \backslash A 32=116.01462511 \backslash A 33=1$ $20.76978714 \backslash A 34=120.56648383 \backslash A 35=117.36922636 \backslash A 36=106.07274097 \backslash A 37=111$ $.10268411 \backslash A 38=111.23525391 \backslash A 39=112.76969537 \backslash A 40=106.50486962 \backslash A 41=110.6$ $531364 \backslash A 42=110.18702731 \backslash A 43=90.80325605 \backslash A 44=106.92339329 \backslash A 45=117.91684$ $221 \backslash A 46=99.58964598 \backslash A 47=110.79774574 \backslash A 48=107.11758538 \backslash A 49=106.12045109$ $\backslash A 50=110.731354 \backslash A 51=109.31178935 \backslash A 52=108.81196838 \backslash A 53=110.31356359 \backslash A 54$ $=109.24284124 \backslash A 55=110.31328326 \backslash A 56=109.13870152 \backslash A 57=108.57327186 \backslash A 58=1$ $06.95730197 \backslash A 59=106.42525286 \backslash D 1=142.93834769 \backslash D 2=109.02349328 \backslash D 3=38.294$ $1635 \backslash D 4=-78.38122075 \backslash D 5=168.60472817 \backslash D 6=-154.08858806 \backslash D 7=30.24474727 \backslash D$ $8=-178.90856794 \backslash D 9=-1.36405206 \backslash D 10=0.91407764 \backslash D 11=179.95888412 \backslash D 12=178$ $.90328776 \backslash D 13=-179.66540825 \backslash D 14=-179.93143547 \backslash D 15=1.81518869 \backslash D 16=2.211$ $53801 \backslash D 17=-179.88323596 \backslash D 18=60.83639322 \backslash D 19=-60.66854319 \backslash D 20=-2.628282$ $68 \backslash \mathrm{D} 21=-178.93215206 \backslash \mathrm{D} 22=62.20246674 \backslash \mathrm{D} 23=-59.9286587 \backslash \mathrm{D} 24=-94.96673463 \backslash$ $\mathrm{D} 25=83.73911824 \backslash \mathrm{D} 26=178.15184284 \backslash \mathrm{D} 27=-0.44759285 \backslash \mathrm{D} 28=0.52892757 \backslash \mathrm{D} 29=17$ $9.99480821 \backslash D 30=0.07798485 \backslash D 31=-179.74177347 \backslash D 32=-179.75675538 \backslash D 33=-0.8$ $1502442 \backslash D 34=-179.3224466 \backslash D 35=179.57942191 \backslash D 36=60.76320002 \backslash D 37=-61.4208$ $2468 \backslash D 38=100.19441631 \backslash D 39=-178.60941063 \backslash D 40=62.25022521 \backslash D 41=-59.486647$ $16 \backslash D 42=105.74790999 \backslash D 43=171.60245117 \backslash D 44=42.75622515 \backslash D 45=-73.72607321 \backslash$ $D 46=171.59866148 \backslash D 47=48.10195468 \backslash D 48=-67.28241119 \backslash D 49=55.62626658 \backslash D 50=$ $-65.59464919 \backslash D 51=178.03637481 \backslash D 52=-178.05836189 \backslash D 53=65.31119372 \backslash D 54=-1$ $77.34114285 \backslash D 55=66.67854566 \backslash D 56=-177.38558111 \backslash D 57=-55.39397857 \backslash D 58=60$. $14237944 \backslash$ VVersion=EM64L-G09RevC.01 $\operatorname{li}$ State=1-A $\backslash H F=-8965.0088398 \backslash \mathrm{RMSD}=9.4$ $51 e-09 \backslash \mathrm{RMSF}=1.803 \mathrm{e}-04 \backslash$ ZeroPoint=0.5014479 Thermal=0.5347038\Dipole=-2. $1973129,4.4132727,-1.7831362 \backslash$ DipoleDeriv=-0.4194359, 0.3611032, -0.17676 $77,0.2397301,-1.1632863,0.7218361,0.012355,0.6553419,-1.0053813,0.9504$ $165,-0.2060034,0.1905316,-0.0086408,1.7220304,-1.0040346,-0.0667126,-0$ $.7174414,1.731774,0.2996404,-0.068242,-0.2514516,0.0131501,0.0250251,-$ $0.2434745,-0.2343153,-0.1269532,0.1160644,0.0914569,0.0940463,0.319301$ $3,0.0388852,0.1036126,-0.0485111,0.2309976,0.0398922,0.016432,0.289528$ $1,-0.7281506,0.1985994,-0.5310479,1.8737114,-0.5201256,0.0191273,-0.01$ $46462,-0.0794003,-0.3895325,-0.2838348,-0.1722999,-0.2438555,-0.410726$ $2,-0.1170047,-0.1800758,-0.1706159,-0.1806094,-0.4466114,0.2044207,-0$. $152271,0.1642598,-1.3503841,0.9453383,-0.0679038,0.3911319,-0.8249366$, $-0.620046,0.2083524,0.1995165,0.1265875,-0.2375458,0.0266893,0.2354438$ ,-0.0892722,-0.2016958,-0.1345842,-0.0068539,-0.0022345,0.0189538,-0.1
$964556,-0.0115419,0.2070878,-0.0591391,-0.09359,-0.2699722,0.1171464,-$ $0.0757404,-0.0771958,-0.1470557,0.0404767,0.0987337,-0.0067023,-0.1448$ $508,-0.0609955,-0.1001491,0.1856148,0.0246469,-0.1082206,-0.1416133,-0$ $.1263982,-0.0301969,-0.0063713,-0.0596133,0.073834,-0.0468449,0.060082$ $8,0.1084371,0.0476423,-0.0651153,0.0456373,0.0580703,1.2828587,0.11088$ $62,-0.9570954,0.1367009,0.0013895,0.0586995,-0.9542865,0.0244502,0.452$ $8258,0.0808504,0.0088165,0.0082311,-0.0157164,0.1008056,0.0806512,0.04$ $31905,0.0717989,-0.0517757,1.0526384,-0.5680422,0.5443123,-0.6763711,0$ $.3323226,-0.1647102,0.7732496,-0.2311007,0.1434002,-1.5435738,-0.14289$ $63,0.9916221,-0.1013894,-0.3053867,0.1705948,0.9476611,0.2042334,-1.22$ $56628,-1.2135916,0.4454303,-0.3851211,0.5500698,-0.5827259,0.3749648$, -$0.5580942,0.4040011,-0.7670146,0.1702382,-0.0067953,-0.0271702,0.04163$ $51,0.0849665,0.0059012,-0.0649795,0.0279582,0.0525437,0.2965144,-0.016$ $5876,0.0069069,-0.1519737,0.403411,-0.2040067,0.2720859,-0.2737454,0.6$ $663108,-0.1164538,0.0944208,-0.0739362,0.0654964,0.0521895,0.0435484,-$ $0.0152247,0.0270983,0.0482917,0.021337,-0.1316196,0.0328125,-0.0474915$ , - 0.0320378, 0.0215448, -0.0889906, 0.0077236,-0.0208128, 0.0885726, 0.0078 $737,0.0873784,0.0469546,-0.0625585,-0.0832789,-0.0265122,0.0013445,-0$. $072812,0.3281398,0.0289327,-0.0693234,0.2122702,0.4035802,-0.2468763,-$ $0.4996193,-0.1606036,0.9685168,-0.1213599,0.0026959,0.1194262,0.031113$ , 0.0779014, -0.0023907, 0.0551895, 0.0138641, 0.022178, 0.0708731, 0.0800867 , -0.0531841,-0.031893,-0.1567904, 0.0778448, 0.0679257, -0.0235106, -0.040 $0755,0.0193621,-0.0577947,-0.1524748,-0.0786752,-0.0221849,-0.0401957$, $0.040398,-0.0120823,-0.0964931,-0.0676311,-0.0620224,-0.1185021,-0.045$ $9109,-0.1153059,0.0308243,-0.0008413,-0.0293041,-0.0789448,0.0582457,-$ $0.1309488,-0.0083556,0.0159534,-0.0013218,0.0557179,0.053479,0.1155891$ $,-0.0807678,-0.0286754,-0.4574728,-0.1334034,0.0007505,1.2264959,0.245$ $6761,-0.0079165,0.2577907,-0.0007908,0.0432029,0.0471122,-0.0082087,0$. $0694541,0.0994668,0.0008798,-0.0144663,0.0281436,0.1089995,0.8472167,0$ $.6937919,0.5345025,0.8533929,0.497553,0.465814,0.5473132,0.3680796,0.4$ $187778,-0.3825744,0.0467214,0.0536113,-0.1299649,-1.6160584,-0.1136588$ , 0.0394317, 0.0414464, -0.4435306, -0.0623439, 0.0504457,0.030778, -0.32351 $91,-0.1625373,-0.1143208,-0.0918539,0.0197114,-0.1791718,-1.6192948,-0$ $.5364949,-0.686732,-0.6142808,-0.7476582,-0.3975024,-0.6878906,-0.3355$ $588,-0.6269289,-0.0604849,0.0318842,-0.056025,0.0598089,0.0674548,-0.0$ $024622,-0.036997,-0.0125288,0.1153768,0.0613579,0.068155,0.0196907,0.0$ $26437,-0.1479854,-0.070211,0.0108336,-0.1022911,0.060719,1.050938,0.13$ $60877,0.3047508,-0.2410362,0.2256524,-0.1207117,0.1476274,0.0094818,0$. $383481,-0.0164875,-0.0461436,-0.0522484,-0.1169137,-0.0344526,-0.08035$ $17,-0.0744758,-0.056497,0.0411166,-0.0343634,-0.0555185,0.0052958,0.11$ $19526,-0.0408007,0.1478341,-0.0154995,0.0705259,-0.0304165,-0.0576938$, $-0.0088776,-0.0104484,0.1159531,0.0539379,0.0024184,0.1208175,-0.02581$ $06,-0.0899714,0.3232771,0.2385295,-0.0286975,0.0986733,0.76847,-0.1079$ $186,-0.0571809,-0.3686075,0.3445327,0.0600345,0.0693387,0.0283717,0.02$ $16837,-0.1597505,-0.0324265,0.0290845,-0.0684062,0.0450966,-0.1228801$, $-0.0930891,0.0359008,0.0311736,0.0374359,0.0072732,0.0068154,0.0330732$ $, 0.0387241,0.0051577,-0.0245025,-0.0679204,-0.0319394,0.0251555,-0.052$ $4707,-0.0356402,0.0660842,-0.0773992,-0.2296343,0.4960312,-0.1780032,0$ $.4008995,-1.6421603,0.3316987,-0.0800801,0.0334314,-0.2612561,0.125014$ $5,-0.0388584,-0.0218986,-0.0377119,0.2216096,-0.138734,0.0740892,-0.28$ $91148,0.3939473,0.1319102,0.1668268,0.0469206,-0.0032363,0.403756,0.16$ $82218,-0.004473,0.3080734,0.1006943,0.1345548,-0.0294022,-0.0011489,-0$
$.0376052,0.3477858,-0.0178639,0.0185755,-0.0378536,0.1274717,0.1201695$ , 0.004479,-0.0034526, 0.0140275, 0.0425739, 0.0109834, -0.0126076, 0.009102 $5,0.0343296,0.0755891,-0.0408611,-0.0085496,-0.0210622,-0.0016774,-0.0$ $573725,-0.0096743,-0.03892,0.0056593,-0.0462275,-0.0085051,0.0200308,-$ $0.031583,0.0780589,0.0153275,-0.0425532,0.0392437,0.0280048,0.0894142$, $0.0716341,-0.0199048,0.0039452,0.0532014,-0.0040471,-0.0120018,-0.0127$ $701,0.057729,-0.1152335,-0.0198892,0.0102232,-0.04227,-0.0025844,-0.00$ $1254,0.0720152,-0.0188538,0.0456727,0.0688493,-0.0033969,0.0180861,0.0$ $129446,0.0000665,0.0325636,-0.0204639,0.052515,-0.1063468,0.122293,-0$. $0226239,-0.0261417,0.0239999,0.0030376,-0.008621,-0.0182512,-0.0162688$ , 0.0842278, -0.1091296,-0.0698891, 0.0416446,-0.0063609, 0.0674829, -0.012 $9369,0.028914,0.0016435,-0.0037518,0.0241423,0.1033544,-0.018973,0.072$ $6508,-0.1318239,0.0195353,-0.0125481,0.0171561,0.03879,-0.1122291,0.00$ $88486,0.061266,-0.0488609,0.0261602,0.0412995,0.0195823,0.0401514,0.02$ $27512,0.0433058,-0.0506012,-0.0665213,-0.0113919,-0.054903,-0.0497212$, $-0.0384998,-0.0604167,-0.0273705,0.0575106,-0.0357591,-0.0013442,-0.01$ $00104,0.0571138,0.042893,-0.0076,0.0109365,0.0030494,-0.0239572,-0.019$ $4564,0.0170697,0.0136733,0.0425294,-0.0243433,0.0577174,-0.0474399,0.0$ $425702 \backslash$ Polar $=398.4257574,-2.2417104,377.3444531,5.3912355,-13.7607774$, $349.3938994 \backslash \mathrm{PG}=\mathrm{C01}[\mathrm{X}(\mathrm{C} 23 \mathrm{H} 30 \mathrm{Br} 3 \mathrm{~N} 104)] \backslash \mathrm{NImag}=1 \backslash$

Pyrrolidine $+1,1,1$-tribromo-2,2-bis (3,4-dimethoxyphenyl)ethane

## 1

A
Frequencies -- -157.9191

A
16.0541

Sum of electronic and zero-point Energies= Sum of electronic and thermal Energies= Sum of electronic and thermal Enthalpies= Sum of electronic and thermal Free Energies=
-8925.230011
$-8925.197262$
$-8925.196318$
-8925.299408
$1 \backslash 1 \backslash G I N C-D M C 44 \backslash$ Freq $\backslash$ RM0 62X $\backslash 6-31+G(d, p) \backslash C 22 H 28 B r 3 N 104 \backslash A U B C R A \backslash 17-O c t-201$ $2 \backslash 0 \backslash \ \# o p t=(c a l c a l l, t s, n o e i g e n, z-m a t r i x, m a x c y c l e=500) ~ M 062 X / 6-31+g(d, p$ ) <br>TitleCard Required<br>0,1\C,0.0381301569,-0.244716605,0.1657169472\C , 0.1371962476,-0.8956963832,-1.0687908632\C, 1.0850386491, 0.7435167688, $0.5643174879 \backslash \mathrm{C},-1.3418299932,0.1113888874,0.6366541054 \backslash \mathrm{H}, 0.4750545989$, $-1.7342731869,0.9372058677 \backslash \mathrm{Br}, 1.8879319546,-1.4348367548,-1.6750955656$ \Br, - $0.5146180795,0.4679150674,-2.8625630776 \backslash \mathrm{Br},-1.0813232835,-2.36690$ $94726,-1.3819002625 \backslash C, 1.3158429504,1.0081524993,1.912039478 \backslash C, 1.797647$ $6568,1.4838429003,-0.3937298802 \backslash C, 2.2777025531,1.9458824486,2.30495188$ $31 \backslash \mathrm{H}, 0.7119065824,0.5137241978,2.669853008 \backslash \mathrm{C}, 3.0113825115,2.645215911$, $1.3536478242 \backslash \mathrm{H}, 2.4332758909,2.134560474,3.3607912962 \backslash \mathrm{C}, 2.7524881136,2$. $4141445335,-0.0169548709 \backslash 0,3.9645281635,3.5722498103,1.6295297493 \backslash 0,3$. $4704769976,3.1588431593,-0.8916319863 \backslash \mathrm{H}, 1.5547509731,1.3550214052,-1.4$ $402087634 \backslash \mathrm{C}, 3.1893046763,2.9745181093,-2.2682661253 \backslash \mathrm{H}, 3.857922428,3.65$ $00893359,-2.8006288364 \backslash \mathrm{H}, 2.1467523948,3.2239131236,-2.4974534706 \backslash \mathrm{H}, 3.3$ $834736935,1.9400314333,-2.5768350672 \backslash C, 4.1882062966,3.8842162075,2.985$ $7742233 \backslash \mathrm{H}, 4.9594072423,4.6540842282,2.9944359323 \backslash \mathrm{H}, 4.5423477622,3.0080$ $366388,3.5437632178 \backslash \mathrm{H}, 3.2777999981,4.2722059007,3.4594836121 \backslash \mathrm{C},-1.8166$ $926781,1.3982954344,0.3325366427 \backslash \mathrm{C},-2.1905748967,-0.744273656,1.332086$ $6211 \backslash \mathrm{C},-3.0902336774,1.7981415235,0.6888865702 \backslash \mathrm{H},-1.1888769707,2.09710$
$16294,-0.2136645904 \backslash C,-3.9431063521,0.9165708032,1.3837908983 \backslash 0,-3.522$ $9120864,3.0583463075,0.3803259778 \backslash C,-3.4795017736,-0.3552047642,1.7107$ $500299 \backslash 0,-5.1789243014,1.3956258352,1.6807364862 \backslash \mathrm{H},-4.1107501564,-1.05$ $5145608,2.2454229131 \backslash H,-1.88046116,-1.758974576,1.5658712406 \backslash \mathrm{C},-6.0567$ $633264,0.5395340987,2.378854466 \backslash \mathrm{H},-6.9777979265,1.1038734643,2.5220745$ $332 \backslash \mathrm{H},-5.6443751941,0.2605932614,3.3563331053 \backslash \mathrm{H},-6.2700831982,-0.36789$ $95932,1.8005631217 \backslash \mathrm{C},-4.324710479,3.0940576871,-0.7974256246 \backslash \mathrm{H},-4.5873$ $292466,4.1395768507,-0.9618643002 \backslash \mathrm{H},-5.2364412588,2.5018373989,-0.6610$ $925917 \backslash \mathrm{H},-3.7566984817,2.7125771985,-1.6540274294 \backslash \mathrm{~N}, 0.5944631118,-2.69$ $88506459,1.4821341455 \backslash C, 0.8591520191,-2.4947823527,2.9348447997 \backslash C, 1.71$ $41888581,-3.5596345639,1.0020065689 \backslash \mathrm{H},-0.2898098608,-3.1914086647,1.32$ $65313592 \backslash \mathrm{C}, 1.4745216659,-3.8231452429,3.4171310793 \backslash \mathrm{H},-0.0636638844,-2$. $2010323866,3.4376538238 \backslash H, 1.5701059534,-1.6676688882,2.9982323902 \backslash \mathrm{H}, 0$. $7603335425,-4.397698087,4.0104865299 \backslash \mathrm{H}, 2.3411229893,-3.6263771117,4.05$ $08235624 \backslash \mathrm{C}, 1.8649480427,-4.5858826831,2.1249049291 \backslash \mathrm{H}, 1.1840523456,-5.4$ $253833688,1.95599527 \backslash \mathrm{H}, 2.87826374,-4.9887713875,2.1642405377 \backslash \mathrm{H}, 1.46343$ $51948,-3.962204247,0.0197024212 \backslash H, 2.5881203114,-2.9108743035,0.9049786$ $502 \backslash \backslash$ Version=EM64L-G09RevC. $01 \backslash$ State=1-A $\backslash \mathrm{HF}=-8925.7020629 \backslash \mathrm{RMSD}=2.629 \mathrm{e}-0$ $9 \backslash \mathrm{RMSF}=3.854 \mathrm{e}-06 \backslash$ ZeroPoint $=0.4720517 \backslash$ Thermal=0.5048008\Dipole=0.459757 $2,-3.5963892,3.9357916 \backslash$ DipoleDeriv=-0.3014356,0.0253131,-0.2173298,0.0 $704807,-0.6233035,0.5433763,-0.4306458,0.3526767,-1.6010937,0.9957656$, $-0.0059381,0.3254839,-0.1896394,0.966077,-0.6130425,0.5343607,-0.17923$ $91,2.367596,0.1364859,0.307835,0.2051994,0.2236277,0.1216156,-0.048807$ $1,0.1809477,0.048813,0.1619432,0.1826749,-0.1436754,-0.1773019,-0.0585$ $307,-0.1125426,-0.146513,-0.2021955,-0.0429958,0.112173,0.1693452,-0.2$ $430302,0.2596935,-0.4777737,1.2713559,-1.2692252,0.2393037,-0.7159228$, $0.6028014,-0.6655387,0.218136,0.0704137,0.2130211,-0.1850017,0.0202127$ , 0.1253786,-0.014422,-0.1448819,-0.5073151, 0.0769984,-0.4040419, 0.2026 $352,-0.6476853,0.7915543,-0.2492148,0.2630427,-1.4723715,-0.3408575,-0$ $.324087,-0.0368741,-0.2393698,-0.5512215,0.084853,-0.043024,-0.0338966$ , - 0. $1462608,-0.1125378,0.046798,-0.0087295,-0.0341344,-0.2403254,0.075$ $3817,-0.1768428,-0.0710794,-0.0762117,-0.2798033,-0.1022498,0.0933234$, $-0.0215872,-0.1781097,0.1023187,-0.1077205,-0.0478899,-0.1635133,-0.14$ $87538,0.0485658,-0.1464455,0.029796,-0.128113,-0.1691963,0.1336761,0.1$ $086793,0.0754214,0.044797,-0.1005083,0.0653633,-0.0809177,0.0500341,0$. $0622631,0.0805095,0.0616585,0.001664,0.9199618,0.7951032,0.5242338,0.7$ $82418,0.8070425,0.4866893,0.5304158,0.460577,0.0422179,0.0942744,-0.03$ 68531,-0.0185219,-0.0311227,0.1030259,-0.0258145,-0.0537547,-0.0519404 , -0.0684666, 0.455701, 0.3470043,-0.5765078, 0.3741775,0.4693124, -0.58282 $45,-0.7493886,-0.7611221,0.6672534,-1.1425011,-0.817521,-0.6160848,-0$. $8560892,-1.0484698,-0.617268,-0.5744707,-0.5484248,-0.8869754,-0.64560$ $88,-0.3818075,0.3767409,-0.4081293,-0.6448384,0.420065,0.5419136,0.531$ $3999,-1.2687049,0.1593889,0.0550314,0.0051319,0.0285656,0.11546,-0.012$ $8154,0.0427184,0.0271225,0.0322848,0.2553887,-0.0039574,0.0633214,0.00$ $54132,0.2691343,0.0493384,-0.1601463,-0.1580873,0.8479366,-0.0037099,-$ $0.0944745,0.0904412,-0.0952918,-0.0030393,0.092598,0.0452398,0.0463116$ , -0.0097977, -0.0746213, 0.0645034,-0.0855141, 0.05195,0.0717093,-0.04578 $36,0.0475001,0.0143827,-0.0268424,0.0700934,0.0547567,-0.0459849,0.059$ $1756,-0.091521,-0.1044772,0.0118857,0.0334029,-0.0298464,0.3928148,0.0$ $553228,0.1215023,0.0729528,0.4126658,0.1413943,0.483312,0.4495877,0.89$ $67637,-0.0361538,-0.119326,-0.0559521,-0.1200789,-0.0318119,-0.0559871$ $,-0.003367,-0.0030578,0.0474575,0.0346832,0.0400416,-0.0089964,0.10300$

86, -0.0750525,0.1264416,-0.1006691,-0.0347182,-0.0829286,-0.0665899,0. $1047518,0.114311,0.0361657,0.0303181,-0.0077549,-0.048103,-0.0858278,-$ $0.0633947,-0.143412,0.0782757,0.0392794,0.0272854,-0.0325031,0.0660697$ , 0.0040338, -0.0544436, -0.0977991, 0.0212313, 0.0934684, -0.0752597, -0.069 $4145,0.080619,-0.0454228,-0.0634797,-0.0301694,-0.101793,0.1366654,-0$. $2445496,0.1171247,-0.7409573,1.0075241,-0.3275747,0.2306767,-0.3366826$ $, 0.0559231,0.1094807,-0.030548,0.021833,-0.0469368,0.0620884,0.0246327$ , 0.0254509, 0.0535826, 0.0803921,1.5628014, -0.3551035,-0.507322,-0.46917 $41,0.0269214,0.2437403,-0.3763822,0.1568319,0.2015003,-0.7770757,0.419$ $3666,-0.2376466,0.55448,-1.0423041,0.2532334,-0.3915831,0.3751677,-0.6$ $2064,-0.2418051,-0.0578512,0.0763759,0.2972945,-0.0635,-0.1585508,-0.0$ $774277,-0.0021176,-0.1217393,-1.9874073,0.1323048,0.7143283,0.1980152$, $-0.4381396,-0.0113514,0.6437877,0.040303,-0.5612701,0.0138064,-0.03324$ $17,0.0666283,-0.0633986,0.030522,0.072552,0.0696775,0.0559287,0.079344$ $9,0.0401113,0.0652497,-0.0118322,0.1117172,-0.1497004,0.0503976,-0.009$ $7208,0.0287703,0.082515,0.7765216,0.1154083,-0.2453605,0.4823212,0.368$ $2189,-0.2264036,-0.3827571,-0.0611032,0.5225602,-0.1093744,0.0404568,0$ $.0642466,0.1079388,0.0335758,-0.0204591,0.0328235,0.0062624,0.0674412$, $0.0003774,0.0215663,-0.1068747,-0.1004767,0.0193107,0.0839184,0.028843$ $7,0.0413862,-0.1255462,0.027478,0.0054225,0.017575,-0.1560405,-0.08369$ $33,-0.0100179,-0.0043956,-0.0962875,-0.0415757,0.5736212,-0.2209507,0$. $239884,-0.0396347,0.2912029,-0.0499048,0.3329944,-0.263207,0.5666003,0$ $.0342316,0.0532983,-0.0370444,0.0995057,-0.1336159,0.0662888,-0.041884$ $7,0.0317786,0.0451553,-0.0956614,-0.0239819,-0.0398512,-0.1249679,0.01$ $64873,-0.0162276,0.0240483,0.0349214,0.0262239,-0.0170677,0.0329109,0$. $0806326,0.0015981,0.0476748,-0.0685452,-0.0055759,0.010926,-0.066318,-$ $0.2887464,0.3423036,-0.2426196,0.5000411,-1.0932972,0.882289,-0.229327$ $6,0.5370946,-0.6895667,0.1656912,-0.0045183,0.0717999,-0.0115286,0.106$ $3522,0.0306236,0.1024213,-0.1613991,0.4590871,0.3018734,-0.2660668,0.0$ $742383,-0.1284799,0.3191639,-0.0821049,-0.0508656,0.0749052,0.016255,0$ $.1829496,-0.0660311,0.0552217,-0.0440961,0.2428698,-0.060442,0.0288959$ $,-0.0968794,0.1766021,0.0850548,0.0305321,-0.0109695,0.0533573,0.00280$ $95,-0.0185011,0.0025055,-0.0330412,0.0574916,-0.0102675,0.0456319,0.03$ $59889,0.0278374,0.0511963,-0.031481,0.0188273,-0.0295611,0.0400519,0.0$ $075031,-0.0450202,0.0040317,-0.0202073,0.0530738,-0.0389754,0.0160067$, $0.0216773,0.0402848,-0.0049876,-0.063289,0.090243,-0.0289946,-0.009336$ $6,0.0559246,0.0279513,0.0452741,-0.0159814,-0.0288343,0.015318,-0.1021$ $644,-0.0221769,0.0261128,-0.0184154,-0.0468408,0.0034072,-0.0114014,0$. $0871428,0.0790302,-0.0188767,0.0234586,0.0694008,0.0586359,-0.007026,0$ $.0755764,-0.0054373,-0.0082239,-0.1118129,-0.0061192,-0.0374828,-0.044$ $2832,-0.0139203,-0.0171328,-0.0275213,0.0165038,-0.0584558,0.1011249,-$ $0.0102572,0.0426906,0.012471,0.0155321,-0.0066278,0.0172134,0.0417012$, $0.0442114,-0.0050979,-0.0347951,-0.011346,0.0977636,-0.0068209,0.01156$ $82,-0.0375076,0.0003193,0.0146184,-0.0103397,0.0006865,-0.0529505,-0.0$ $017008,0.004304,0.0128964,-0.0301168,0.0688918 \backslash \operatorname{Polar}=381.3412323,14.49$ $96403,351.8471623,-0.3923473,-19.1006198,359.484276 \backslash \mathrm{PG}=\mathrm{C} 01[\mathrm{X}(\mathrm{C} 22 \mathrm{H} 28 \mathrm{Br}$

\section*{3N1O4)]\NImag=1<br>}

## Optimization - CPCM with UFF, Water

## Piperidine

$1 \backslash 1 \backslash G I N C-D M C 182 \backslash F O p t \backslash R M 062 X \backslash 6-31+G(d, p) \backslash C 5 H 11 N 1 \backslash A U B C R A \backslash 02-J u l-2012 \backslash 0 \backslash \backslash$ \# opt=(noeigen,z-matrix) M062X/6-31+g(d,p) scrf=(cpcm, solvent=water) <br> Title Card Required $\backslash \backslash 0,1 \backslash N, 0.000628,-1.466335,-0.185433 \backslash \mathrm{C}, 1.21242,-0.7$ $52879,0.22935 \backslash \mathrm{C},-1.211789,-0.753907,0.229309 \backslash \mathrm{H}, 0.000684,-1.550831,-1.2$ $00728 \backslash \mathrm{C}, 1.256536,0.707192,-0.23241 \backslash \mathrm{H}, 2.082641,-1.304085,-0.140985 \backslash \mathrm{H}, 1$. $251154,-0.786106,1.327369 \backslash \mathrm{C},-0.000607,1.452209,0.224693 \backslash \mathrm{H}, 1.317673,0.7$ $32327,-1.329423 \backslash \mathrm{H}, 2.159858,1.193484,0.153475 \backslash \mathrm{C},-1.257144,0.706175,-0.2$ $32371 \backslash \mathrm{H},-0.000632,1.517582,1.322065 \backslash \mathrm{H},-0.001033,2.479279,-0.155578 \backslash \mathrm{H},-$ $1.31832,0.731315,-1.32938 \backslash \mathrm{H},-2.160856,1.191719,0.153553 \backslash \mathrm{H},-2.081523,-1$ $.305841,-0.141086 \backslash \mathrm{H},-1.250537,-0.787233,1.327323 \backslash$ VVersion=EM64L-G09Rev C. $01 \backslash$ State $=1-A \backslash H F=-251.7994894 \backslash \mathrm{RMSD}=8.216 \mathrm{e}-09 \backslash \mathrm{RMSF}=1.829 \mathrm{e}-05 \backslash \mathrm{Dipole}=-0$ $.000255,0.6500467,-0.3154736 \backslash$ Quadrupole=1.7266496,-3.6543625,1.9277129 $, 0.0021686,-0.0006012,1.3559757 \backslash \mathrm{PG}=\mathrm{C01}[\mathrm{X}(\mathrm{C} 5 \mathrm{H} 11 \mathrm{~N} 1)] \backslash \backslash @$

## Pyrrolidine

$\mathrm{N}-\mathrm{N}=1.899251955467 \mathrm{D}+02 \mathrm{E}-\mathrm{N}=-8.719520757723 \mathrm{D}+02 \mathrm{KE}=2.105976982248 \mathrm{D}+02$ $1 \backslash 1 \backslash G I N C-D M C 177 \backslash F O p t \backslash R M 062 X \backslash 6-31+G(d, p) \backslash C 4 H 9 N 1 \backslash A U B C R A \backslash 26-J u n-2012 \backslash 0 \backslash \ \#$ opt=(noeigen,z-matrix) M062X/6-31+g(d,p) scrf=(cpcm, solvent=water) <br>T itle Card Required <br>0,1\N, 0.0007969198,-1.6588748249,-0.0793011862\C,1 $.1539381869,-0.789813522,0.1933969036 \backslash C,-1.1532678615,-0.7909720483,0$. $193192982 \backslash \mathrm{H}, 0.0009907225,-1.8863297025,-1.0724997532 \backslash \mathrm{C}, 0.7746083629,0$. $6214031963,-0.3116393347 \backslash \mathrm{H}, 2.0568041533,-1.190952007,-0.2730869173 \backslash \mathrm{H}, 1$ $.3133778851,-0.771606302,1.2781863299 \backslash \mathrm{H}, 1.1599562578,0.7789683053,-1.3$ $231098418 \backslash \mathrm{H}, 1.1926112004,1.4052048803,0.3252968908 \backslash \mathrm{C},-0.7750834544,0.6$ $209024725,-0.311041641 \backslash \mathrm{H},-1.1614057673,0.7792818001,-1.3220464307 \backslash \mathrm{H},-1$ $.193095197,1.4039033834,0.3271604853 \backslash \mathrm{H},-2.0555395787,-1.1927318087,-0$. $273858895 \backslash \mathrm{H},-1.3132668296,-0.7733888222,1.2779134079 \backslash$ VVersion=EM64L-G0 $9 R e v C .01 \backslash$ State $=1-A \backslash H F=-212.4951649 \backslash R M S D=1.351 e-09 \backslash R M S F=2.407 e-05 \backslash$ Dipol $e=-0.0001956,0.6378066,-0.4629407 \backslash$ Quadrupole $=1.5340806,-3.2283218,1.69$ $42412,0.0024895,-0.0007587,2.2180971 \backslash \mathrm{PG}=\mathrm{CO1}[\mathrm{X}(\mathrm{C} 4 \mathrm{H} 9 \mathrm{~N} 1)] \backslash \backslash @$

## 1,1,1-tribromo-2,2-bis (3,4-dimethoxyphenyl) ethane

$\mathrm{N}-\mathrm{N}=4.179566466558 \mathrm{D}+03 \mathrm{E}-\mathrm{N}=-2.907510908956 \mathrm{D}+04 \mathrm{~K} \mathrm{E}=8.651772804862 \mathrm{D}+03$ $1 \backslash 1 \backslash G I N C-D M C 182 \backslash F O p t \backslash R M 062 X \backslash 6-31+G(d, p) \backslash C 18 H 19 B r 304 \backslash A U B C R A \backslash 02-J u l-2012$ $\backslash 0 \backslash \backslash \#$ opt=(noeigen, z-matrix) $M 062 X / 6-31+g(d, p)$ scrf=(cpcm, solvent=wate r) <br>Title Card Required<br>0,1\C,1.2769886907,1.3365632315,0.3382841604\} $\mathrm{C}, 1.27834372,0.4194893455,-0.7252927126 \backslash \mathrm{C}, 2.3374263079,2.206631549,0.5$ $26292336 \backslash \mathrm{H}, 0.4315016714,1.370211824,1.0129747334 \backslash \mathrm{C}, 0.091538075,-0.5048$ $443553,-0.9458702974 \backslash C, 2.337046706,0.425989152,-1.6207427579 \backslash C, 0.18557$ $47144,-1.7953937276,-0.0980622976 \backslash C,-1.2326145919,0.2399733198,-0.8619$ $192478 \backslash \mathrm{H}, 0.162206043,-0.8840268799,-1.9716595497 \backslash \mathrm{Br}, 1.6892339896,-2.85$ $70727678,-0.7365774825 \backslash \mathrm{Br},-1.4237222337,-2.8628894502,-0.3122487052 \backslash \mathrm{Br}$ , 0.4706795165, -1.5093676934,1.8053891978\C, -1.747273653, 0.7664699262, $2.0376954499 \backslash C,-1.9002177507,0.4993091353,0.3450215181 \backslash C,-2.8945192744$ , 1. $5707774008,-2.0238306416 \backslash \mathrm{H},-1.2477582276,0.5754372143,-2.9836184094$ $\backslash C,-3.5519290872,1.834222003,-0.8289123665 \backslash \mathrm{H},-3.2672789749,1.975673274$ $1,-2.9570841503 \backslash C,-3.0452123081,1.2819097486,0.3711758728 \backslash 0,-4.6684872$ $8,2.5945612853,-0.7040061797 \backslash 0,-3.7384057147,1.5773343902,1.5001973829$ $\backslash H,-1.5345204547,0.0753172417,1.2696650337 \backslash \mathrm{C},-3.2313923183,1.065254439$
$8,2.7249496295 \backslash \mathrm{H},-3.9049394125,1.4256785231,3.5007447546 \backslash \mathrm{H},-2.21723517$ $89,1.4366326416,2.9152078555 \backslash \mathrm{H},-3.2270211438,-0.0307182383,2.720819809$ $3 \backslash C,-5.1794452614,3.1939180943,-1.8855685179 \backslash \mathrm{H},-6.0526809869,3.7671462$ $526,-1.5783931775 \backslash \mathrm{H},-5.4771893302,2.4324050103,-2.6145358964 \backslash \mathrm{H},-4.4384$ $384488,3.8639251399,-2.3350627494 \backslash C, 3.4073173791,1.3152359399,-1.45392$ $09874 \backslash \mathrm{H}, 2.3437309622,-0.2616140487,-2.4613887805 \backslash \mathrm{C}, 3.4213009437,2.2025$ $374996,-0.3853628496 \backslash H, 4.2200471678,1.3038115848,-2.170087426 \backslash 0,4.4026$ $924878,3.1037021735,-0.1346617288 \backslash 0,2.4170065833,3.1089482306,1.538335$ $7217 \backslash \mathrm{C}, 1.3502196326,3.1220233989,2.4757932399 \backslash \mathrm{H}, 1.6112862003,3.8749014$ $899,3.2180728763 \backslash \mathrm{H}, 1.2439220503,2.1445594678,2.960227885 \backslash \mathrm{H}, 0.405670069$ $5,3.394612012,1.9911728793 \backslash \mathrm{C}, 5.486025141,3.1586573384,-1.0511546899 \backslash \mathrm{H}$, $6.1501676962,3.9393961908,-0.6841099806 \backslash \mathrm{H}, 5.1344103683,3.4157618055,-2$ $.0560708081 \backslash \mathrm{H}, 6.0222145153,2.2041538867,-1.0819090457 \backslash$ VVersion=EM64L-G $09 R e v C .01 \backslash$ State=1-A $\backslash H F=-8713.2574761 \backslash R M S D=3.190 e-09 \backslash R M S F=9.321 e-05 \backslash D i p$ ole=0.0881082,0.7702119,-0.8104511 \Quadrupole=1.2078196,-12.2400281,11 $.0322085,-2.2943268,-3.9704314,-4.0495996 \backslash \mathrm{PG}=\mathrm{C01} \quad[\mathrm{X}(\mathrm{C} 18 \mathrm{H} 19 \mathrm{Br} 304)] \backslash \backslash @$

## Piperidine + 1,1,1-tribromo-2,2-bis(3,4-dimethoxyphenyl)ethane

$\mathrm{N}-\mathrm{N}=5.572015406221 \mathrm{D}+03 \mathrm{E}-\mathrm{N}=-3.244617037878 \mathrm{D}+04 \mathrm{KE}=8.901072988224 \mathrm{D}+03$ $1 \backslash 1 \backslash G I N C-D M C 174 \backslash F T S \backslash R M 062 X \backslash 6-31+G(d, p) \backslash C 23 H 30 B r 3 N 104 \backslash A U B C R A \backslash 02-J u l-201$ $2 \backslash 0 \backslash \ \#$ opt $=(c a l c f c, t s, n o e i g e n, m a x c y c l e=600) ~ M 062 X / 6-31+g(d, p) ~ s c r f=(c p$ cm, solvent=water) <br>Title Card Required <br>0, 1 \C, -0.0440599545,0.26209012 $1,0.0447823966 \backslash C,-0.141512135,0.6105154727,-1.3560398495 \backslash C,-0.97940675$ $04,-0.7961580256,0.5688292137 \backslash C, 1.3759278408,0.037625965,0.5174547549 \backslash$ $\mathrm{H},-0.4603621019,1.5701919847,0.6137013294 \backslash \mathrm{Br},-1.939424813,0.8781010354$ $,-2.0350813893 \backslash \mathrm{Br}, 0.6867145498,-0.8485777085,-2.7086031872 \backslash \mathrm{Br}, 0.871426$ $7935,2.2021370908,-1.8423627412 \backslash C,-1.1739573549,-0.8979486462,1.945500$ $3621 \backslash C,-1.6122406411,-1.7471487845,-0.2509351271 \backslash \mathrm{C},-2.0077551754,-1.87$ $71233817,2.4946427239 \backslash \mathrm{H},-0.6521227607,-0.220284431,2.6147270118 \backslash \mathrm{C},-2.6$ $619818201,-2.7878393073,1.6726154674 \backslash \mathrm{H},-2.1374575066,-1.9168207416,3.5$ $697038118 \backslash C,-2.4461426054,-2.7216380601,0.2797163125 \backslash 0,-3.4986945686,-$ $3.7698239693,2.104259732 \backslash 0,-3.0917269003,-3.658279045,-0.4680612107 \backslash \mathrm{H}$, $-1.4244184503,-1.7497113372,-1.314424197 \backslash \mathrm{C},-2.908796504,-3.6035387043$, $-1.8749617669 \backslash \mathrm{H},-3.5168696565,-4.4072810192,-2.2875468593 \backslash \mathrm{H},-1.8580992$ $358,-3.7633005335,-2.1425561554 \backslash \mathrm{H},-3.2462874332,-2.641722843,-2.277749$ $9754 \backslash \mathrm{C},-3.6937377106,-3.8825513207,3.5052266471 \backslash \mathrm{H},-4.3792631133,-4.716$ $6898476,3.6470921059 \backslash \mathrm{H},-4.1379428234,-2.9691293327,3.9154069197 \backslash \mathrm{H},-2.7$ $4808722,-4.0917955414,4.0171311369 \backslash \mathrm{C}, 1.9033748478,-1.2649488039,0.4852$ $215221 \backslash C, 2.2080026499,1.0560140336,0.9786037186 \backslash C, 3.1994871793,-1.5321$ $43596,0.8854640072 \backslash \mathrm{H}, 1.2954369245,-2.0931593735,0.1300966284 \backslash \mathrm{C}, 4.02989$ $29475,-0.4915935158,1.3491017506 \backslash 0,3.6738766569,-2.8212012876,0.852158$ $8644 \backslash C, 3.5201196444,0.8044612343,1.392495069 \backslash 0,5.2819803331,-0.8503122$ $695,1.7295154684 \backslash \mathrm{H}, 4.1284897477,1.6276392766,1.7474144755 \backslash \mathrm{H}, 1.85728487$ $81,2.081852132,1.0098132325 \backslash \mathrm{C}, 6.1370927152,0.177119363,2.210726955 \backslash \mathrm{H}, 7$ $.0791745412,-0.3091806065,2.4588048169 \backslash H, 5.7175443743,0.6460247686,3.1$ $069679013 \backslash \mathrm{H}, 6.3066457473,0.9375869698,1.4413958709 \backslash \mathrm{C}, 4.5043466613,-3.0$ $776426974,-0.2820853659 \backslash \mathrm{H}, 4.8263336372,-4.1165672711,-0.2075167354 \backslash \mathrm{H}, 5$ $.3776239302,-2.4180251817,-0.2778173571 \backslash \mathrm{H}, 3.933113927,-2.9332028968,-1$ $.2063698342 \backslash N,-0.7359867434,2.6898871542,1.1333129143 \backslash C,-0.8891882828$, $2.5386727812,2.6026212109 \backslash \mathrm{C},-1.9375656423,3.288663142,0.4961628053 \backslash \mathrm{H}, 0$ $.0614771926,3.3018784703,0.9404558157 \backslash C,-1.2241755495,3.8645912437,3.2$ $755742479 \backslash \mathrm{H}, 0.0366738233,2.103155505,2.9896566431 \backslash \mathrm{H},-1.6996401946,1.81$
$87695446,2.757806694 \backslash \mathrm{C},-2.4820571837,4.4750164962,2.6546113084 \backslash \mathrm{H},-0.37$ $8087338,4.5548939271,3.162825073 \backslash \mathrm{H},-1.3592158178,3.6911060994,4.347322$ $9494 \backslash \mathrm{C},-2.3118025993,4.6186980597,1.1416005964 \backslash \mathrm{H},-3.3417270842,3.82524$ $47498,2.8652766164 \backslash \mathrm{H},-2.6946647603,5.4483662546,3.1061551303 \backslash \mathrm{H},-1.5243$ $403359,5.3532983087,0.9273917602 \backslash \mathrm{H},-3.2310083208,4.9878246863,0.676821$ $4918 \backslash \mathrm{H},-1.7193082763,3.4088020151,-0.5669870378 \backslash \mathrm{H},-2.7452241789,2.5548$ $581946,0.5985733256 \backslash \backslash V e r s i o n=E M 64 L-G 09 R e v C .01 \backslash$ State=1-A $\backslash H F=-8965.04107$ $97 \backslash \mathrm{RMSD}=8.677 \mathrm{e}-09 \backslash \mathrm{RMSF}=7.319 \mathrm{e}-06 \backslash \mathrm{Dipole=-0.3146663,4.4166748,3.3087443}$ \Quadrupole=2.2583965,2.4573601,-4.7157566,-0.3366064,-1.9698522, 14.64 $46833 \backslash \mathrm{PG}=\mathrm{C01}[\mathrm{X}(\mathrm{C} 23 \mathrm{H} 30 \mathrm{Br} 3 \mathrm{~N} 104)] \backslash \backslash @$

## Pyrrolidine + 1,1,1-tribromo-2,2-bis(3,4-dimethoxyphenyl)ethane

$\mathrm{N}-\mathrm{N}=5.361422603246 \mathrm{D}+03 \mathrm{E}-\mathrm{N}=-3.193434619757 \mathrm{D}+04 \mathrm{KE}=8.862180636912 \mathrm{D}+03$ $1 \backslash 1 \backslash G I N C-D M C 96 \backslash F T S \backslash R M 062 X \backslash 6-31+G(d, p) \backslash C 22 H 28 B r 3 N 104 \backslash A U B C R A \backslash 11-J u l-2012$ $\backslash 0 \backslash \ \#$ opt $=(c a l c f c, t s, n o e i g e n, m a x c y c l e=600) ~ M 062 X / 6-31+g(d, p) ~ s c r f=(c p c$ m, solvent=water) <br>Title Card Required <br>0,1\C,0.1781252622,0.3034130964 , -0.1131725581 \C, 0.1612486612, 0.6076712506, -1.5244947922\C, -0.86101890 $19,-0.6399339958,0.4281745055 \backslash C, 1.5539753013,0.0229317788,0.4382824308$ $\backslash \mathrm{H},-0.2960427522,1.6107769591,0.368653354 \backslash \mathrm{Br},-1.5956963078,1.066910910$ $2,-2.2255419928 \backslash \mathrm{Br}, 0.8398327512,-0.9607384831,-2.8220617499 \backslash \mathrm{Br}, 1.35606$ $04111,2.0660108974,-2.0173827614 \backslash C,-1.1596160805,-0.5801765877,1.78857$ $7532 \backslash C,-1.5332556763,-1.5956036208,-0.3525780371 \backslash C,-2.1285853466,-1.41$ $20499632,2.3575362946 \backslash \mathrm{H},-0.6325722657,0.1256424308,2.4266119559 \backslash \mathrm{C},-2.8$ $155386355,-2.3316953087,1.5722088729 \backslash \mathrm{H},-2.341164313,-1.3275566078,3.41$ $68612124 \backslash C,-2.5009032482,-2.4244535441,0.1991378154 \backslash 0,-3.7811498004,-3$ $.1768606007,2.0230263949 \backslash 0,-3.1919102819,-3.3608788902,-0.5060787606 \backslash \mathrm{H}$ $,-1.2832030436,-1.703478589,-1.3985451671 \backslash C,-2.8973858041,-3.477621155$ $6,-1.8901057687 \backslash \mathrm{H},-3.5541029348,-4.2579980883,-2.2716796685 \backslash \mathrm{H},-1.85197$ $50329,-3.7667013963,-2.046879798 \backslash \mathrm{H},-3.0978199548,-2.5373006953,-2.4162$ $519973 \backslash \mathrm{C},-4.0980647945,-3.1178707991,3.4049330244 \backslash \mathrm{H},-4.870944871,-3.86$ $75094927,3.5681100557 \backslash \mathrm{H},-4.4820553475,-2.1289930651,3.6782933364 \backslash \mathrm{H},-3$. $2222307615,-3.3535875089,4.0191744328 \backslash C, 2.0348532374,-1.2959228697,0.4$ $452802413 \backslash C, 2.3846045289,1.0205152004,0.9425872553 \backslash C, 3.2994565442,-1.5$ $987455104,0.918357646 \backslash \mathrm{H}, 1.4179925626,-2.1065341171,0.065009269 \backslash \mathrm{C}, 4.134$ $6228277,-0.5791008526,1.4180080531 \backslash 0,3.7352879718,-2.9021414008,0.9283$ $485355 \backslash C, 3.6625782864,0.7326768653,1.4307361756 \backslash 0,5.3545049695,-0.9718$ $206022,1.8657612675 \backslash \mathrm{H}, 4.2753846613,1.5383096089,1.8169877414 \backslash \mathrm{H}, 2.05022$ $05293,2.0535197526,0.9454031871 \backslash C, 6.2181726193,0.0345794777,2.37496341$ $66 \backslash H, 7.1321830259,-0.4768925791,2.6721664271 \backslash H, 5.7726643144,0.52812516$ $4,3.2449574994 \backslash \mathrm{H}, 6.4470767465,0.7797560617,1.605735417 \backslash \mathrm{C}, 4.6057195817$, $-3.20470562,-0.1636718145 \backslash \mathrm{H}, 4.9161346268,-4.2425130329,-0.0400673441 \backslash \mathrm{H}$ , $5.4836546936,-2.5512283858,-0.1488422524 \backslash \mathrm{H}, 4.0716362373,-3.0889391408$ , -1.1135988414 \N, -0.7946395387, 2. $7004181442,0.7468714504 \backslash \mathrm{C},-0.23096097$ $62,3.1797415431,2.0469980702 \backslash C,-2.2859070897,2.5660602556,0.9002083914$ $\backslash \mathrm{H},-0.5763557969,3.3689494012,0.0084788632 \backslash \mathrm{C},-1.4244037542,3.776435694$ $3,2.7858493423 \backslash \mathrm{H}, 0.5847826688,3.8797679558,1.860672161 \backslash \mathrm{H}, 0.1692007271$, $2.3127076314,2.5835587201 \backslash \mathrm{H},-1.6251720966,4.7885604711,2.4184319548 \backslash \mathrm{H}$, $-1.2600959896,3.8228853517,3.8640286017 \backslash C,-2.556451624,2.8285554454,2$. $3832830126 \backslash \mathrm{H},-3.5514543684,3.2478820608,2.542918998 \backslash \mathrm{H},-2.483319026,1.8$ $935992714,2.9499174471 \backslash \mathrm{H},-2.7719644469,3.3066491086,0.2611423323 \backslash \mathrm{H},-2$. $5881088857,1.5686277154,0.5754296091 \backslash$ VVersion=EM64L-G09RevC. 01 \State=1 $-A \backslash H F=-8925.7400575 \backslash R M S D=4.017 e-09 \backslash R M S F=3.568 e-06 \backslash$ Dipole=$=0.6388454,4$.

2876107,3.0953515\Quadrupole=3.761819,2.6854786,-6.4472976,-1.9628887, $-2.7217304,16.0183344 \backslash \mathrm{PG}=\mathrm{C} 01 \quad[\mathrm{X}(\mathrm{C} 22 \mathrm{H} 28 \mathrm{Br} 3 \mathrm{~N} 104)] \backslash \backslash @$

## Frequency Calculation - CPCM with UFF, Water

## Piperidine

Sum of electronic and zero-point Energies= -251.639632
Sum of electronic and thermal Energies=
Sum of electronic and thermal Enthalpies=
Sum of electronic and thermal Free Energies=

$$
\begin{aligned}
& -251.634061 \\
& -251.633116 \\
& -251.668278
\end{aligned}
$$

$1 \backslash 1 \backslash A S N \_A L T I X-A L T I X 8 \backslash F r e q \backslash R M 062 X \backslash 6-31+G(d, p) \backslash C 5 H 11 N 1 \backslash A U B C R A \backslash 02-J u l-20$ $12 \backslash 0 \backslash \backslash \#$ freq=noraman M062X/6-31+g(d,p) scrf=(cpcm, solvent=water) <br>Titl e Card Required $\backslash \backslash 0,1 \backslash \mathrm{~N}, 0.000623,-1.466335,-0.185433 \backslash \mathrm{C}, 1.212418,-0.7528$ $83,0.22935 \backslash \mathrm{C},-1.211791,-0.753903,0.229309 \backslash \mathrm{H}, 0.000679,-1.550831,-1.2007$ $28 \backslash$ С, $1.256538,0.707188,-0.23241 \backslash \mathrm{H}, 2.082637,-1.304091,-0.140985 \backslash \mathrm{H}, 1.251$ 152,-0.78611,1.327369\C,-0.000603,1.452209,0.224693\н, 1.317675,0.73232 $3,-1.329423 \backslash \mathrm{H}, 2.159862,1.193477,0.153475 \backslash$ С, $-1.257142,0.706179,-0.23237$ $1 \backslash \mathrm{H},-0.000627,1.517582,1.322065 \backslash \mathrm{H},-0.001025,2.479279,-0.155578 \backslash \mathrm{H},-1.31$ $8318,0.731319,-1.32938 \backslash \mathrm{H},-2.160852,1.191726,0.153553 \backslash \mathrm{H},-2.081527,-1.30$ 5835,-0.141086\H,-1.250539,-0.787229,1.327323<br>Version=IA64L-G09RevC. 0 $1 \backslash$ State $=1-A \backslash H F=-251.7994894 \backslash$ RMSD=8.215e-09 $\backslash$ RMSF=1.829e-05 $\backslash$ ZeroPoint $=0$. $1598578 \backslash$ Thermal $=0.1654287 \backslash$ Dipole $=-0.0002516,0.6500467,-0.3154736 \backslash$ Dipol eDeriv $=-0.8167186,0.0001049,0.0000075,0.000105,-1.0229079,-0.0208938,0$ $.0000087,-0.0077165,-0.341602,0.5220623,0.2061453,0.0735215,0.1039562$, $0.4698052,-0.0212456,0.1961239,0.0198998,0.3743889,0.5223098,-0.206113$ $5,-0.0735104,-0.1039126,0.469518,-0.0213026,-0.1961558,0.0197229,0.374$ $3845,0.1062143,-0.0001156,-0.0000299,-0.0001208,0.404009,0.1157183,0.0$ $000165,-0.0412334,-0.0036926,0.0540329,0.0029971,0.004852,-0.0337191,-$ $0.0703886,0.019955,-0.019211,0.0360451,0.1914218,-0.1640035,0.0943936$, $0.0398665,0.1145197,-0.0638641,-0.0388915,0.0940386,-0.0465938,0.04973$ $81,0.0443351,-0.025535,0.0326512,-0.0434457,0.0131604,0.006031,-0.0630$ $263,0.0213323,-0.2418745,0.0640913,-0.000012,0.0000039,-0.0000264,0.12$ $07778,-0.0040733,-0.0000128,0.0284729,0.2063999,0.0443121,0.0237024,-0$ $.0100455,0.0248312,0.0190162,-0.0162318,0.0538859,0.0160717,-0.2471293$ ,-0.1922353,-0.1061337,-0.0581396,-0.1136457,-0.0279851,-0.0293989,-0. $0937741,-0.0508747,0.0454375,0.0539763,-0.0029209,-0.0049034,0.0337697$ , - 0.0703244, 0.0199233,0.019184,0.0360441,0.1914303,0.0011578,-0.000014 $5,0.0000003,-0.0000137,0.0610235,0.0075489,0.000028,-0.0663626,-0.2505$ $978,0.0280389,0.0000993,-0.0000197,0.0001062,-0.2421786,0.0613719,-0.0$ $000416,0.0952297,0.0455601,0.0443597,-0.0236705,0.0100556,-0.0247974,0$ $.0189818,-0.016211,-0.0539046,0.0160456,-0.2471496,-0.1924093,0.105986$ $7,0.0581758,0.113537,-0.0278274,-0.0293628,0.0938248,-0.0507991,0.0454$ $355,-0.1638129,-0.0944841,-0.039854,-0.1146194,-0.0640307,-0.0389339,-$ $0.0940124,-0.0466843,0.04973,0.044289,0.0255705,-0.0326319,0.0434758,0$ $.013215,0.0059969,0.063028,0.0214004,-0.2418806 \backslash \operatorname{Polar}=86.5446545,0.000$ $103,84.0279021,-0.0004509,0.5141551,81.4873246 \backslash \mathrm{PG}=\mathrm{CO} 1 \quad[\mathrm{X}(\mathrm{C} 5 \mathrm{H} 11 \mathrm{~N} 1)] \backslash \mathrm{NIm}$ $\mathrm{ag}=0 \backslash \backslash$

## Pyrrolidine

Sum of electronic and zero-point Energies=
-212. 364618
Sum of electronic and thermal Energies=
-212. 359601
Sum of electronic and thermal Enthalpies=
-212. 358657
Sum of electronic and thermal Free Energies=
$-212.393562$
$1 \backslash 1 \backslash G I N C-D M C 55 \backslash$ Freq $\backslash$ RM0 $62 X \backslash 6-31+G(d, p) \backslash C 4 H 9 N 1 \backslash A U B C R A \backslash 02-J u l-2012 \backslash 0 \backslash \backslash \#$ freq=noraman M062X/6-31+g(d,p) scrf=(cpcm, solvent=water) <br>Title Card R equired $\backslash 0,1 \backslash \mathrm{~N}, 0.000166,-1.264293,0.209992 \backslash \mathrm{C},-1.153475,-0.451221,-0.19$ $9144 \backslash \mathrm{C}, 1.153731,-0.450896,-0.198721 \backslash \mathrm{H},-0.000003,-1.328802,1.226859 \backslash \mathrm{C}$, $0.775067,1.023152,0.071997 \backslash \mathrm{H},-2.056149,-0.772546,0.325847 \backslash \mathrm{H},-1.312801$, $-0.608079,-1.272704 \backslash \mathrm{H},-1.160627,1.341339,1.044875 \backslash \mathrm{H},-1.193475,1.693867$ $,-0.682877 \backslash \mathrm{C}, 0.774625,1.023526,0.071512 \backslash \mathrm{H}, 1.160734,1.342921,1.043811 \backslash \mathrm{H}$ , 1. 192232, 1.693766, -0. $68447 \backslash \mathrm{H}, 2.056195,-0.77162,0.326959 \backslash \mathrm{H}, 1.313845,-0$ $.60816,-1.272107 \backslash \backslash V e r s i o n=E M 64 L-G 09 R e v C .01 \backslash$ State=1-A $\backslash H F=-212.4951649 \backslash R$ $M S D=5.854 e-09 \backslash \mathrm{RMSF}=2.408 \mathrm{e}-05 \backslash$ ZeroPoint=0.1305465\Thermal=0.1355635\Dip ole $=-0.000248,0.7040448,0.3541634 \backslash$ DipoleDeriv=-0.6832058, 0.0001068, -0. $0000191,0.0000124,-1.0628908,0.1460859,-0.0000878,0.0368002,-0.3603002$ , 0. $3982043,-0.160399,0.0626241,-0.0417543,0.4824745,-0.0027338,0.17669$ $4,-0.0260317,0.379792,0.3982676,0.1603699,-0.0627157,0.0416938,0.48244$ $39,-0.0027331,-0.1766641,-0.0260276,0.3797164,0.1185441,-0.0000492,0.0$ $000564,-0.0000194,0.3741937,-0.1306325,0.000027,0.0218797,0.0079077,0$. $0125696,-0.0837772,-0.0157142,-0.0078714,-0.0825393,-0.0249753,-0.0555$ $066,-0.0371513,0.1713576,-0.1450481,-0.0629523,0.055492,-0.0763342,0.0$ $106364,0.0311766,0.1137424,0.0451647,0.0231483,0.0358055,0.0012276,-0$. $0135417,0.0080211,-0.0087462,-0.0450095,-0.0964727,-0.0365702,-0.21441$ $29,-0.0167145,0.0403905,0.0666253,0.022904,0.014963,-0.0497044,0.10507$ $07,-0.1044262,-0.1410424,-0.0024926,0.071073,-0.0588012,0.0948262,-0.0$ $723896,0.083542,-0.0932492,0.1297357,-0.042585,0.0125303,0.0838352,0.0$ $156945,0.008033,-0.0824812,-0.0248296,0.0554783,-0.0372164,0.1714475,-$ $0.0167705,-0.0406673,-0.0666683,-0.0230985,0.0147227,-0.0499225,-0.105$ $1056,-0.1046517,-0.1407493,-0.0023893,-0.0708686,0.0588272,-0.0946487$, $-0.0722981,0.0836131,0.0933004,0.1299154,-0.0430094,-0.1450103,0.06285$ $54,-0.055616,0.076151,0.0107331,0.0312007,-0.1139041,0.0451815,0.02300$ $74,0.0357098,-0.001145,0.0137568,-0.007915,-0.0088221,-0.0450775,0.096$ $6773,-0.0366021,-0.2142778 \backslash \operatorname{Polar}=69.636522,0.0022302,69.3316096,-0.002$ $1382,-0.2901781,64.1914217 \backslash \mathrm{PG}=\mathrm{C01}[\mathrm{X}(\mathrm{C} 4 \mathrm{H} 9 \mathrm{~N} 1)] \backslash \mathrm{NImag}=0 \backslash \backslash$

## 1,1,1-tribromo-2,2-bis (3,4-dimethoxyphenyl)ethane

Sum of electronic and zero-point Energies=
Sum of electronic and thermal Energies=
Sum of electronic and thermal Enthalpies=
Sum of electronic and thermal Free Energies=

$$
\begin{aligned}
& -8712.915556 \\
& -8712.889516 \\
& -8712.888572 \\
& -8712.975503
\end{aligned}
$$

$1 \backslash 1 \backslash A S N \_A L T I X-A L T I X 8 \backslash F r e q \backslash R M 062 X \backslash 6-31+G(d, p) \backslash C 18 H 19 B r 304 \backslash A U B C R A \backslash 02-J u$ l-2012\0 <br>\# freq=noraman M062X/6-31+g(d,p) scrf=(cpcm, solvent=water) <br> Title Card Required <br>0,1\C,1.278567,1.339261, 0.331245\C,1.277553,0.412 $802,-0.724166 \backslash \mathrm{C}, 2.33936,2.211031,0.509096 \backslash \mathrm{H}, 0.434633,1.378829,1.007557$ $\backslash C, 0.090322,-0.513528,-0.933813 \backslash C, 2.334191,0.411438,-1.622074 \backslash C, 0.1864$ $22,-1.79651,-0.074825 \backslash \mathrm{C},-1.233698,0.231917,-0.853414 \backslash \mathrm{H}, 0.158661,-0.901$ $778,-1.956363 \backslash \mathrm{Br}, 1.688699,-2.863705,-0.707371 \backslash \mathrm{Br},-1.423272,-2.865968$, $0.27584 \backslash \mathrm{Br}, 0.475883,-1.493615,1.825356 \backslash \mathrm{C},-1.751108,0.747943,-2.03262 \backslash \mathrm{C}$
,-1.898543, 0.50189,0.352716\C,-2.898388,1.552266,-2.023239\H,-1.253755 , 0.548571,-2.977961 \C,-3.553068,1.826242,-0.82919\H,-3.27333,1.948854, $-2.959181 \backslash C,-3.043542,1.284616,0.374573 \backslash 0,-4.669401,2.587585,-0.708453$ $\backslash 0,-3.73416,1.589985,1.502527 \backslash \mathrm{H},-1.530682,0.08613,1.280235 \backslash \mathrm{C},-3.224284$ ,1.088808,2.730597\н,-3.896074,1.456046,3.504718\H,-2.209724,1.461924, $2.915222 \backslash \mathrm{H},-3.219828,-0.007158,2.736165 \backslash \mathrm{C},-5.18313,3.176417,-1.894099 \backslash$ H, -6.055706, 3.752286,-1.590003\H,-5.482486,2.408457,-2.615604\H,-4.443 $218,3.842465,-2.351216 \backslash \mathrm{C}, 3.404766,1.302199,-1.465602 \backslash \mathrm{H}, 2.338999,-0.283$ $584,-2.456609 \backslash \mathrm{C}, 3.421133,2.198932,-0.404981 \backslash \mathrm{H}, 4.215846,1.284484,-2.183$ $508 \backslash 0,4.403021,3.102347,-0.164533 \backslash 0,2.421192,3.122283,1.512921 \backslash \mathrm{C}, 1.356$ $565,3.143591,2.45268 \backslash \mathrm{H}, 1.619274,3.903033,3.187658 \backslash \mathrm{H}, 1.251467,2.17045,2$ $.945998 \backslash \mathrm{H}, 0.410878,3.411814,1.96784 \backslash \mathrm{C}, 5.484236,3.149253,-1.083969 \backslash \mathrm{H}, 6$. $149155,3.933256,-0.725385 \backslash \mathrm{H}, 5.130287,3.397422,-2.090311 \backslash \mathrm{H}, 6.020436,2.1$ 9455,-1.107501 <br>Version=IA64L-G09RevC.01 \State=1-A $\backslash H F=-8713.2574761 \backslash$ RM $S D=1.850 \mathrm{e}-09 \backslash \mathrm{RMSF}=9.322 \mathrm{e}-05 \backslash$ ZeroPoint $=0.3419202 \backslash$ Thermal=0.3679598\Dipo $l e=0.0861778,0.7630064,-0.8174437 \backslash$ DipoleDeriv $=-0.1643361,-0.0827697,-0$ $.1639637,0.1703827,-0.1530341,-0.1434386,0.08264,0.1239772,-0.1999,-0$. $0495906,0.2140773,-0.0291046,0.0607193,-0.2342902,0.0982691,-0.0736312$ , 0.0712048,-0.0364612,-0.2179274,-0.2517071,0.0299278,-0.0690144,0.851 7615,1.0182934,0.1955102,1.0995324,1.2786985,0.1262243,0.0028447,0.102 7793,0.0136081,0.1639058,0.0028164,0.1097496,-0.027724,0.0899643,0.092 $6052,0.0219803,0.0830676,-0.0546318,0.4488745,-0.2114542,-0.0234016,-0$ $.1269946,-0.1117938,-0.0215925,0.0065951,-0.1555035,0.0551948,-0.10283$ $81,0.0258978,-0.0446845,0.0731536,-0.0817518,1.4837265,0.0612093,-0.01$ $29505,0.0778207,0.8835823,0.4478248,0.0226096,0.3637034,1.2722216,0.17$ 44556,-0.1730874,-0.0128336,-0.0586516,-0.2343221,0.033903,0.1319575,-$0.021923,0.0308583,0.0456985,0.0105214,0.0032147,-0.0003633,-0.0163494$ $, 0.0621311,0.0045194,-0.0700982,-0.0553944,-0.6385394,0.3063608,0.1807$ 957,0.3450526,-0.3710328,-0.1625137,0.1956106,-0.1355717,-0.2539433,-0 $.7480305,-0.3665397,-0.0856755,-0.413252,-0.4071706,-0.070496,-0.07810$ $35,-0.0517274,-0.1607348,-0.181377,0.0042842,-0.1222841,-0.0135893,-0$. 1875914,-0.1446377,-0.0887713,-0.160974,-0.8018766,-0.1995227,-0.06179 $24,0.0853412,0.0193312,-0.1913834,-0.1023184,-0.0755339,0.0134961,-0.0$ $06016,-0.2831885,0.002714,0.1733441,-0.0178006,-0.1878236,-0.1419467,-$ $0.1763462,0.0778476,-0.2084149,-0.1891614,0.007407,-0.1535447,-0.06682$ $91,-0.2093244,0.0800723,0.1315368,-0.1365713,0.0156615,0.0721859,0.069$ $909,0.1085588,0.0645118,0.1343424,-0.038395,0.0847254,-0.0263332,-0.01$ $84017,1.5806999,-0.9881276,0.0800942,-1.0508716,0.8003046,-0.0099294,0$ $.1700191,-0.025624,-0.2152112,0.112293,0.0664324,-0.05608,0.0739014,0$. $1427067,0.0607436,-0.065115,0.0689335,0.0155483,0.3635969,-0.0395517,-$ $0.8494575,-0.0068869,0.0672691,0.3456656,-1.0836554,0.4484151,1.624674$ $,-1.8554786,1.0233161,-0.3364832,1.0850212,-1.1155882,0.3033183,-0.255$ $4098,0.234465,-0.7144716,-0.7833267,0.180945,0.5397496,0.2012911,-0.46$ 81833,-0.0892193,0.6213808,-0.0979654,-2.2477165,0.2023956,-0.0258193, $-0.032663,-0.0147694,0.194672,0.0431788,-0.0213931,0.0269628,0.0485994$ $, 0.3640745,-0.0066027,0.3293226,0.0436874,0.4424628,-0.3146028,0.02485$ $81,-0.1230731,1.0873876,0.0111534,0.0508908,0.1179964,0.0560538,0.0749$ $299,-0.0546541,0.0683872,-0.0197159,-0.0717961,-0.1181667,-0.0733702,-$ $0.1544231,-0.1028995,0.0234795,0.0458032,0.0355677,0.0247362,-0.008550$ $9,0.0806081,-0.0076209,-0.0933731,-0.0188182,-0.1663004,0.1016443,0.00$ $06144,-0.064612,-0.0095176,0.5781402,-0.1433871,0.214457,-0.2116247,0$. 5897026,-0.2213515,0.5413696,-0.4232008,0.7862867,-0.0681622,0.1238461
, -0.002423, 0.1186096, 0.0232963, 0.0115432,0.0495846, -0.0282338, 0.051598 $6,0.0516345,-0.0097658,-0.0211095,-0.0604096,-0.0819404,-0.1248051,-0$. $1465103,0.0183212,-0.0744983,-0.0516896,-0.1397326,0.0837462,-0.036602$ , -0.0278681, 0.062882,-0.078377,0.1145585,-0.0227174,-0.1903462,0.06846 $76,0.0248944,-0.170503,-0.2367003,0.1511251,-0.2247667,-0.0647661,-0.0$ $872314,0.1143292,-0.0386387,-0.0147195,-0.0298821,0.0435327,-0.1341026$ , -0.0033502,-0.1129349,0.0477012,1.4483369,1.1314642,0.2090229,1.11449 $32,0.9242189,0.0046816,0.2113065,-0.0028806,-0.0660451,0.0217081,-0.04$ $47713,0.0972866,-0.0423978,0.1603063,-0.022223,0.1086157,-0.017471,0.0$ $915474,-2.0528797,-1.010271,0.2376066,-1.0977665,-1.1345628,0.0094431$, $0.1421986,-0.0676974,-0.5645099,-0.6530903,0.0904097,0.3459908,0.02414$ $59,-1.0905774,-0.9057952,0.2733318,-0.9270924,-1.7144028,0.6884646,-0$. $2428602,-0.5133305,-0.0374847,0.3676244,-0.0266346,-0.2722671,0.142014$ $4,0.8181694,0.0630529,-0.0501929,-0.0284748,-0.0178453,-0.0094311,-0.1$ $354322,0.0116758,-0.1048904,-0.0336013,0.0224269,0.0749875,0.0892423,-$ $0.0395801,-0.1043631,0.1670255,0.0331908,0.0209151,-0.003241,-0.130214$ $6,0.1043999,0.0478049,0.0319573,0.0684155,0.0500684,-0.1260612,0.03363$ $34,-0.0423362,1.0108867,0.206911,-0.274407,-0.0051879,0.368092,-0.0523$ $954,-0.5385709,-0.2390909,0.6010274,-0.0369856,-0.0980998,0.0072458,-0$ $.1360867,-0.017176,-0.0330323,-0.0356655,-0.0634325,0.0623104,-0.03766$ $57,0.0155952,-0.1066762,0.0437929,0.0694245,0.0264824,0.0720934,0.1066$ $117,-0.1392035,-0.0374252,0.0091398,0.0279912,0.174173,-0.0950531,-0.0$ $134351,0.0885613,0.0781167,0.0274845 \backslash \operatorname{Polar}=430.0845583,-4.4883545,359$. $0357236,-20.6121399,23.1805178,386.9965873 \backslash \mathrm{PG}=\mathrm{CO1} \quad[\mathrm{X}(\mathrm{C} 18 \mathrm{H} 19 \mathrm{Br} 304)] \backslash \mathrm{NIm}$ ag=0<br>

Piperidine $+1,1,1$-tribromo-2,2-bis(3,4-dimethoxyphenyl)ethane

## 1 2

A
3
A
Frequencies -- -1181.1757
19.1081

Sum of electronic and zero-point Energies= -8964.542910
Sum of electronic and thermal Energies=
Sum of electronic and thermal Enthalpies=
Sum of electronic and thermal Free Energies=
$-8964.509382$
$-8964.508438$
$-8964.611583$
$1 \backslash 1 \backslash G I N C-D M C 200 \backslash$ Freq $\backslash$ RM0 $62 X \backslash 6-31+G(d, p) \backslash C 23 H 30 B r 3 N 104 \backslash A U B C R A \backslash 09-J u l-20$ $12 \backslash 0 \backslash \$ freq=noraman $\mathrm{M} 062 \mathrm{X} / 6-31+\mathrm{g}(\mathrm{d}, \mathrm{p})$ scrf=(cpcm, solvent=water) <br>Titl e Card Required $\backslash \backslash 0,1 \backslash C,-0.044149,0.261994,0.044886 \backslash C,-0.141678,0.61007$ $2,-1.356018 \backslash C,-0.978889,-0.796729,0.569055 \backslash C, 1.375931,0.038513,0.51774$ $7 \backslash H,-0.461324,1.569953,0.613494 \backslash \mathrm{Br},-1.939689,0.876397,-2.035295 \backslash \mathrm{Br}, 0.6$ $87595,-0.848782,-2.708199 \backslash B r, 0.870317,2.202225,-1.842566 \backslash \mathrm{C},-1.173515,-$ $0.898359,1.945728 \backslash C,-1.611047,-1.748283,-0.250577 \backslash C,-2.006757,-1.87794$ $1,2.494987 \backslash \mathrm{H},-0.65217,-0.220232,2.614868 \backslash \mathrm{C},-2.660333,-2.789233,1.67308$ $1 \backslash H,-2.136543,-1.917498,3.570043 \backslash \mathrm{C},-2.444395,-2.723183,0.28019 \backslash 0,-3.49$ $6477,-3.771651,2.104843 \backslash 0,-3.089319,-3.66038,-0.46746 \backslash \mathrm{H},-1.423116,-1.7$ $50946,-1.314047 \backslash \mathrm{C},-2.906282,-3.605814,-1.874353 \backslash \mathrm{H},-3.513812,-4.41002,-$ $2.286835 \backslash \mathrm{H},-1.855458,-3.764975,-2.141809 \backslash \mathrm{H},-3.244332,-2.644291,-2.2773$ $73 \backslash C,-3.69159,-3.884212,3.505813 \backslash \mathrm{H},-4.37661,-4.718749,3.647781 \backslash \mathrm{H},-4.13$ $6406,-2.970983,3.915761 \backslash \mathrm{H},-2.745861,-4.092762,4.017856 \backslash \mathrm{C}, 1.904193,-1.2$ $63739,0.485834 \backslash C, 2.207324,1.057514,0.97877 \backslash C, 3.200431,-1.530044,0.8862$ $61 \backslash \mathrm{H}, 1.296807,-2.092402,0.130818 \backslash \mathrm{C}, 4.030141,-0.488881,1.349769 \backslash 0,3.675$
$628,-2.818812,0.853269 \backslash C, 3.519556,0.806864,1.392845 \backslash 0,5.282414,-0.8467$ $41,1.730382 \backslash \mathrm{H}, 4.127377,1.630494,1.747657 \backslash \mathrm{H}, 1.855963,2.08314,1.009734 \backslash \mathrm{C}$ , 6.136837, 0.181322, 2. $211469 \backslash \mathrm{H}, 7.079197,-0.304339,2.459741 \backslash \mathrm{H}, 5.716906,0$ $.65015,3.107572 \backslash \mathrm{H}, 6.305993,0.941738,1.441999 \backslash \mathrm{C}, 4.506372,-3.074968,-0.2$ $8084 \backslash \mathrm{H}, 4.828999,-4.113677,-0.206025 \backslash \mathrm{H}, 5.379237,-2.414806,-0.276619 \backslash \mathrm{H}, 3$ $.935142,-2.931074,-1.205211 \backslash N,-0.7377,2.689583,1.132848 \backslash \mathrm{C},-0.890955,2$. $538574,2.602172 \backslash \mathrm{C},-1.939587,3.287479,0.495454 \backslash \mathrm{H}, 0.059402,3.302032,0.93$ $9946 \backslash \mathrm{C},-1.226836,3.864422,3.274819 \backslash \mathrm{H}, 0.03514,2.103714,2.98939 \backslash \mathrm{H},-1.700$ $973,1.818198,2.757424 \backslash \mathrm{C},-2.485036,4.473935,2.653605 \backslash \mathrm{H},-0.381168,4.5552$ $29,3.162014 \backslash \mathrm{H},-1.361876,3.691072,4.34659 \backslash \mathrm{C},-2.314719,4.617412,1.140582$ $\backslash \mathrm{H},-3.344322,3.82367,2.864317 \backslash \mathrm{H},-2.698296,5.447244,3.104927 \backslash \mathrm{H},-1.52769$ $3,5.352459,0.926301 \backslash \mathrm{H},-3.234108,4.98587,0.675634 \backslash \mathrm{H},-1.721298,3.407535$, $-0.567698 \backslash \mathrm{H},-2.746799,2.553191,0.597934 \backslash \backslash V e r s i o n=E M 64 \mathrm{~L}-\mathrm{G} 09 \mathrm{RevC} .01 \backslash$ Stat $e=1-A \backslash H F=-8965.0410797 \backslash R M S D=8.691 e-09 \backslash R M S F=7.325 e-06 \backslash$ ZeroPoint=0.49816 $99 \backslash$ Thermal $=0.5316974 \backslash$ Dipole $=-0.3177517,4.417157,3.3078027 \backslash$ DipoleDeriv= $-0.5627226,0.1490508,0.3735067,0.310855,-1.4626984,-1.0169921,0.635906$ $1,-0.8369926,-2.020013,1.7097641,-0.2497644,-0.6569813,-0.3899863,1.90$ $5601,1.0835675,-0.7625507,0.7761372,3.3704968,0.2150231,0.4333293,-0.3$ $912276,0.2756099,0.3237286,0.0061801,-0.3350154,-0.1445098,0.1955877,0$ $.3004156,-0.194023,0.2141319,-0.0373662,-0.0958573,0.3106318,0.2005132$ $, 0.1534328,0.0158046,0.3117888,-0.6412544,-0.5356171,-0.9187297,2.3605$ $423,1.9822268,-0.3732815,1.0434399,0.7111568,-0.9888592,0.1538991,-0.2$ $2909,0.1675742,-0.1864759,-0.0052652,-0.2892099,0.0150618,-0.2491067,-$ $0.6673631,0.4113594,0.8136033,0.4677863,-1.1572024,-1.3286382,0.441699$ $6,-0.7154598,-1.7442662,-0.4089391,-0.375853,0.1451804,-0.3314385,-0.8$ $383575,0.0443379,0.1140604,0.1720815,-0.2263308,-0.2177179,0.0374872,0$ $.0018409,-0.0598157,-0.2841058,-0.0327667,0.2064205,0.2216738,-0.06072$ 81,-0.2967809,-0.1176638,-0.0555005,-0.0142612,-0.248754,-0.0872047,0. $0933862,0.0463699,-0.181849,-0.1762021,0.1066826,0.1336805,0.1109192,-$ $0.1024874,0.2381194,-0.1003627,-0.0860125,-0.0024438,0.1039353,-0.1087$ $769,-0.0491938,-0.1120721,0.0568343,-0.0976968,-0.0642625,-0.0612091,0$ $.0563041,0.85317,0.845415,-0.6375357,0.844301,0.9862796,-0.75994,-0.72$ $65311,-0.8032852,0.2539935,0.1548677,-0.0479662,0.0402429,-0.043114,0$. $1514215,0.0209011,0.0519622,0.030492,-0.062117,0.4356451,0.5006008,0.6$ $163142,0.561109,0.934647,0.8160159,0.825073,1.05099,0.6856871,-1.15426$ $42,-0.8382242,0.7538625,-0.8933109,-1.2951722,0.8094279,0.6853502,0.68$ $73673,-1.3715042,-0.7357328,-0.5058834,-0.4065322,-0.5656356,-1.134595$ $8,-0.6978135,-0.5160422,-0.7899869,-1.626789,0.2081935,0.0341762,-0.01$ $37379,0.010492,0.1839895,0.0034414,-0.0191646,-0.0223692,0.0303404,0.3$ $617306,-0.0871394,-0.112198,-0.0503976,0.3529996,-0.0425202,0.1266766$, $0.2437399,1.161271,0.0263935,-0.1065249,-0.0677455,-0.1023286,-0.03226$ $5,-0.0990804,-0.0324321,-0.0524328,0.0067375,-0.1414045,0.0791272,0.12$ $8023,0.0411732,0.0829545,0.0325929,-0.0449684,-0.0416562,-0.0454426,0$. $0584956,0.0918941,0.0131672,0.1005748,-0.090795,0.1546668,-0.0275453,-$ $0.034998,-0.0556796,0.4382365,-0.0005122,-0.1155551,-0.0261516,0.38496$ 59,-0.065395,-0.398952,-0.3823458,1.2001859,0.0020362,-0.1194733,0.062 $6143,-0.1258646,-0.0422082,0.0694277,0.0240744,0.019584,0.0319867,0.03$ $46477,0.067707,0.0200404,0.1315488,-0.085775,-0.1323344,0.0777199,0.05$ $26586,-0.0676386,-0.1078832,0.0804774,-0.1459908,0.0380877,0.0737669$, -$0.0130031,0.0364516,0.0812184,-0.0814966,-0.130354,0.0295255,-0.056624$ $4,0.0104051,0.01243,-0.1132793,-0.0178851,0.0510683,-0.1440155,-0.0003$ $864,0.1660212,0.110971,-0.0487124,0.1069435,0.0221051,0.0927101,0.0207$
$66,-0.1423655,0.1621747,-0.315052,-0.0774866,-0.8713223,1.3822944,0.12$ $40436,-0.0881999,0.175157,-0.0593873,0.1319091,-0.0615091,-0.0409,-0.0$ $798031,0.0338269,-0.0318254,-0.0453908,-0.0585136,0.1553433,1.9619966$, $-0.2750231,0.7137071,-0.3938694,-0.0359101,-0.1984167,0.5831693,-0.119$ $8323,0.3596117,-0.9974832,0.5661481,0.2228274,0.6679811,-1.477323,-0.1$ $994896,0.3217092,-0.3171981,-0.7403839,-0.3374635,-0.1192708,-0.083372$ $4,0.3389692,-0.05562,0.1719083,0.0290337,-0.0251169,-0.2398719,-2.4373$ $177,-0.102661,-0.8678673,0.0379931,-0.6523746,-0.0369304,-0.7514105,-0$ $.1097896,-0.6889825,0.0389914,-0.0692755,-0.0755781,-0.0731374,0.03832$ $51,-0.0588744,-0.0717481,-0.0552475,0.1663264,0.0946943,0.1040777,0.00$ $88486,0.0896913,-0.1005795,-0.011494,-0.0153777,0.0092195,0.1570973,0$. $8413355,0.260339,0.217481,0.6298515,0.6224011,0.2847543,0.2543187,0.12$ $4658,0.5408764,-0.1171731,0.0281,-0.0774316,0.090052,0.0346448,0.01651$ $65,-0.0648645,-0.0033875,0.0824833,-0.0095295,0.0473578,0.1153381,-0.1$ $181801,-0.0034315,-0.1109728,0.0062263,-0.0840305,-0.0993499,0.0406301$ , -0.0013407,-0.028196,-0.1636952,-0.0611491,0.0206227,0.0267279,0.1256 $511,-0.0800644,0.7074136,-0.2659855,-0.2541106,-0.0835337,0.3833681,0$. $1164063,-0.3773891,0.3646974,0.7644789,0.0443341,0.0848372,0.0345337,0$ $.1163899,-0.1552165,-0.0160796,0.0351419,0.0116798,0.0567788,-0.090132$ $4,-0.0437372,0.0561941,-0.1459226,0.0197333,0.0231935,0.0045321,-0.050$ $7955,0.0331789,-0.0453631,0.0299593,-0.1339968,0.0234987,0.0774564,0.0$ $428764,-0.0052975,-0.0590145,-0.1432946,-0.5138344,0.6498717,0.3266865$ , 0.757616,-1.7363608,-1.1640942,0.189153,-0.6760705,-0.9678466, 0.19721 $86,0.0338097,-0.0846002,0.0456603,0.116158,-0.1373263,-0.116569,0.2121$ $047,0.7877009,0.5739827,-0.3558402,-0.0001437,-0.0874995,0.3081001,-0$. $0665931,0.1904982,-0.2337006,0.0172823,0.1874735,-0.0501742,-0.0150315$ $,-0.090732,0.2808237,0.0602322,-0.0432273,0.0681781,0.1947992,0.120375$ $7,0.0730164,0.0116932,0.0527891,0.1198343,0.0101279,0.0090457,-0.05516$ $28,-0.0205387,-0.053914,0.10286,-0.0652277,0.0885481,0.0407195,0.06875$ $07,-0.025901,0.0317913,0.0189325,-0.041928,-0.1330627,0.0218366,-0.081$ $1188,0.0287797,0.0359861,-0.0107213,-0.043716,0.0137211,0.1581211,0.00$ $20154,-0.0457409,0.0690685,0.0731479,-0.036952,-0.0153783,-0.0075253,0$ $.0932218,-0.1236986,-0.1024578,0.001556,-0.099332,-0.0712491,-0.016710$ $7,0.056321,0.050002,0.0755735,0.0598309,0.0339198,0.0367513,0.0295637$, $0.0248879,0.0230953,0.0074283,-0.0045339,-0.2084076,0.0764062,0.142070$ $6,0.0282477,0.0636958,0.1039898,-0.0118293,-0.0151705,0.0010799,0.1036$ $261,-0.1170129,-0.0883631,0.0346719,-0.1588825,-0.0252698,0.0725887,0$. $0090224,0.0347628,0.0154198,0.0411086,0.073843,0.0245087,0.0927489,-0$. $1505376,-0.1162934,0.0325094,-0.1049517,-0.0181175,-0.0763212,-0.16121$ $52,0.0668636,-0.0878565,-0.0559895,0.0184777,0.044076,-0.0020424,0.014$ $3612,-0.095841,0.1280716,-0.0837117,0.0891908,-0.0060613,-0.0018301,-0$ $.0817386,0.02282,-0.0254566,0.0351599,0.0188637,0.0604585,-0.0012499,0$ $.0997245,0.0091345,0.0025103,0.0134406,-0.0901155,-0.0418775,-0.027885$ $9,-0.0024593,-0.0984238,-0.0614982,0.0152856,0.0231607,0.0705627,0.093$ $2373 \backslash$ Polar $=520.9732315,22.6758177,517.2235442,-1.1058239,31.577615,518$ $.2806493 \backslash \mathrm{PG}=\mathrm{C01}[\mathrm{X}(\mathrm{C} 23 \mathrm{H} 30 \mathrm{Br} 3 \mathrm{~N} 104)] \backslash \mathrm{NImag}=1 \backslash \backslash$

Pyrrolidine $+1,1,1$-tribromo-2,2-bis(3,4-dimethoxyphenyl)ethane
1
2
A
Frequencies -- -1102.0189
19.4156

Sum of electronic and zero-point Energies= Sum of electronic and thermal Energies= Sum of electronic and thermal Enthalpies= Sum of electronic and thermal Free Energies=

> -8925.271277
> -8925.238793
> -8925.237849
> -8925.338462
$1 \backslash 1 \backslash A S N \_A L T I X-A L T I X 7 \backslash F r e q \backslash R M 062 X \backslash 6-31+G(d, p) \backslash C 22 H 28 B r 3 N 1 O 4 \backslash A U B C R A \backslash 12-$ Jul-2012 $\overline{\text { Jo }} 0 \backslash \#$ freq=noraman $\mathrm{M0} 62 \mathrm{X} / 6-31+\mathrm{g}(\mathrm{d}, \mathrm{p})$ scrf=(cpcm, solvent=water) $\backslash \backslash$ Title Card Required <br>0, 1 \C, 0.028254, 0.363975, 0.185719\C, 0.059184,1.2 $11378,-0.982887 \backslash C,-1.099275,-0.621905,0.325361 \backslash C, 1.36518,-0.235066,0.5$ $45601 \backslash \mathrm{H},-0.33322,1.402547,1.163929 \backslash \mathrm{Br},-1.639004,2.067142,-1.398878 \backslash \mathrm{Br}$, $0.612492,0.245722,-2.817396 \backslash \mathrm{Br}, 1.387386,2.633134,-0.874458 \backslash \mathrm{C},-1.410869$ $,-1.089375,1.601217 \backslash C,-1.843469,-1.118562,-0.758285 \backslash C,-2.45888,-1.9910$ $22,1.809382 \backslash \mathrm{H},-0.831693,-0.750003,2.457036 \backslash \mathrm{C},-3.214421,-2.451722,0.736$ $393 \backslash \mathrm{H},-2.678246,-2.322211,2.817693 \backslash \mathrm{C},-2.889644,-2.010622,-0.564713 \backslash 0,-$ $4.258581,-3.318163,0.831018 \backslash 0,-3.651887,-2.518535,-1.571055 \backslash \mathrm{H},-1.58908$ $3,-0.81736,-1.764652 \backslash C,-3.349137,-2.093095,-2.891376 \backslash \mathrm{H},-4.067855,-2.59$ $2305,-3.539527 \backslash \mathrm{H},-2.331836,-2.385424,-3.175404 \backslash \mathrm{H},-3.456517,-1.006809,-$ $2.98965 \backslash \mathrm{C},-4.588795,-3.793383,2.126667 \backslash \mathrm{H},-5.428282,-4.47388,1.992074 \backslash \mathrm{H}$ $,-4.886126,-2.968875,2.783808 \backslash H,-3.746681,-4.332863,2.573594 \backslash C, 1.72525$ $3,-1.48169,0.009927 \backslash C, 2.274866,0.397214,1.389483 \backslash C, 2.950515,-2.059688$, $0.291667 \backslash \mathrm{H}, 1.043486,-2.01248,-0.650125 \backslash \mathrm{C}, 3.866771,-1.405836,1.140065 \backslash 0$ , 3. $267077,-3.289464,-0.234003 \backslash C, 3.514573,-0.174387,1.690737 \backslash 0,5.039772$ , -2.051577,1.363474 \H, 4.191769, 0.349815, 2.354352\H, 2.034808,1.366573,1 $.815669 \backslash \mathrm{C}, 5.983081,-1.416153,2.214622 \backslash \mathrm{H}, 6.842966,-2.082433,2.259533 \backslash \mathrm{H}$, $5.571303,-1.277881,3.219746 \backslash \mathrm{H}, 6.289194,-0.447525,1.805412 \backslash \mathrm{C}, 4.1224,-3$. $201751,-1.375245 \backslash \mathrm{H}, 4.336334,-4.224318,-1.687124 \backslash \mathrm{H}, 5.055282,-2.68985,-1$ $.118904 \backslash \mathrm{H}, 3.614658,-2.666392,-2.185551 \backslash \mathrm{~N},-0.737123,2.286692,1.960242 \backslash \mathrm{C}$ , - 0. 151398, 2.149691,3.329903\C, -2.236486, 2.233987, 2.080969\H, -0.44893, $3.17401,1.548638 \backslash \mathrm{C},-1.296823,2.500718,4.273849 \backslash \mathrm{H}, 0.726641,2.790544,3.4$ $22347 \backslash \mathrm{H}, 0.161324,1.108358,3.46259 \backslash \mathrm{H},-1.400362,3.588477,4.349742 \backslash \mathrm{H},-1.1$ $44566,2.094047,5.275378 \backslash C,-2.503666,1.899291,3.550051 \backslash H,-3.459087,2.30$ $4669,3.887966 \backslash \mathrm{H},-2.523158,0.812798,3.69048 \backslash \mathrm{H},-2.644649,3.209017,1.8055$ $62 \backslash \mathrm{H},-2.62252,1.482907,1.389206 \backslash \backslash$ Version=IA64L-G09RevC. $01 \backslash$ State=1-A $\backslash \mathrm{HF}$ $=-8925.7400575 \backslash \mathrm{RMSD}=5.001 \mathrm{e}-09 \backslash \mathrm{RMSF}=3.591 \mathrm{e}-06 \backslash$ ZeroPoint=0.4687809\Therm $\mathrm{al}=0.5012647 \backslash$ Dipole $=-0.2949229,2.7147044,4.573437 \backslash$ DipoleDeriv=-0.61039 $11,-0.0455232,0.403284,-0.004836,-0.8497568,-0.5884802,0.7029703,-0.36$ $75522,-2.5534856,1.6902104,-0.0104095,-0.5493648,-0.0590813,1.4865675$, $0.4018171,-0.8934421,0.0585055,3.8767437,0.3605299,0.5207486,-0.208389$ $7,0.3730583,0.2005467,0.0946688,-0.256522,-0.0579235,0.1887857,0.23361$ $25,-0.3223458,0.1507078,-0.1531848,-0.1757507,0.167144,0.2038784,0.010$ $1571,0.1195408,0.3439046,-0.4567964,-0.8630475,-0.7410826,1.0797992,2$. $1692591,-0.6360924,1.0143476,1.7769215,-0.8894138,0.3676355,-0.0820816$ , 0.3936891, -0.3313533, 0.0322119,-0.1378052, 0.0436528, -0. $2221811,-0.561$ $2876,0.0597587,0.6279484,0.2553849,-0.5738967,-0.9920258,0.5247428,-0$. $2845679,-2.4456317,-0.5836495,-0.4444491,-0.0209569,-0.4098757,-0.6541$ $567,-0.16376,-0.0118962,-0.0530518,-0.2295084,-0.2377194,0.0271657,-0$. $0406534,-0.1382315,-0.3147533,-0.0802528,0.2009247,0.1288365,-0.027252$
$6,-0.315339,-0.0740172,-0.0942159,-0.0365436,-0.2257516,-0.0800353,0.0$ $914711,0.0097999,-0.1952836,-0.1137115,0.060735,0.1984008,0.1334884,-0$ $.1894879,0.1494038,-0.0884922,-0.1243264,0.0365427,0.0770495,-0.092971$ $9,-0.0913439,-0.0877954,0.1283686,-0.0933253,-0.1044361,-0.0438175,-0$. $0081948,1.2957024,1.0379371,-0.3968194,1.0517855,0.9528325,-0.294007$, -$0.4912187,-0.3290293,-0.1590805,0.1254901,-0.0639792,0.0418769,-0.0561$ $451,0.1451955,0.0694554,0.0560027,0.0770375,-0.0253997,0.5319355,0.253$ $1352,0.8626357,0.2349642,0.251661,0.5317383,1.124051,0.7380676,1.28825$ $31,-1.6159948,-1.0827114,0.5827671,-1.0921062,-1.2962293,0.5621247,0.4$ $736393,0.4601875,-0.9113819,-0.8730422,-0.3321256,-0.6064387,-0.340663$ $1,-0.5944015,-0.2945857,-0.7357928,-0.3701795,-2.0325759,0.2180784,0.0$ $303149,0.0112107,0.0082396,0.173339,0.0528774,-0.0144852,0.0196562,0.0$ $444621,0.3426726,-0.042264,-0.2000731,-0.0800644,0.389504,-0.258766,0$. $0914243,-0.0258855,1.1486878,-0.005084,-0.0725848,-0.1145844,-0.081799$ $1,0.0517832,-0.0756662,-0.0694548,-0.0351876,-0.0428586,-0.1176067,0.0$ $762556,0.1517739,0.091798,0.048359,0.0413819,-0.0330191,0.0019876,-0.0$ $338124,0.0824168,0.0371629,0.0650964,0.0577966,-0.1538295,0.119537,-0$. $0082467,-0.0549457,-0.0257975,0.483677,0.0714738,-0.1764026,0.1266268$, $0.5538254,-0.227213,-0.5065642,-0.482539,0.9805169,-0.0531655,-0.13418$ $45,0.0300431,-0.1298651,-0.0045987,0.0328762,-0.0204888,-0.0103837,0.0$ $525161,0.0578341,0.0289479,0.0167695,0.0783483,-0.0895589,-0.1342094,0$ $.1265663,0.032984,-0.08663,-0.0703983,0.1413048,-0.1067336,0.0484102,0$ $.0066537,0.0471467,0.0695252,0.1112259,-0.0499762,-0.1088137,0.0496447$ $,-0.0226974,0.0258164,-0.0044283,-0.0473582,-0.0012863,0.1227933,-0.14$ $6945,-0.0076077,0.1283515,0.1604774,-0.0700858,0.040689,0.089308,0.072$ $8545,0.0926924,-0.0812413,0.0238902,-0.1098846,-0.1194354,-0.6345148,1$ $.1783851,0.6135607,-0.3369619,0.6998286,0.2614284,0.1109364,-0.0484,-0$ $.0733992,-0.0610663,0.1063505,-0.053267,-0.0811884,-0.0779139,0.104956$ $9,1.7622624,-0.752158,0.5103622,-0.8004725,0.3159767,-0.3531946,0.3809$ $706,-0.2734399,0.1986955,-0.8746959,0.3964863,0.37337,0.4560835,-1.305$ $12,-0.442982,0.4760778,-0.5679813,-1.0417724,-0.2929691,-0.0535243,-0$. $0798264,0.304842,-0.1704082,0.2158285,0.1622265,0.0031589,-0.1570662,-$ $2.3103813,0.4763068,-0.8396497,0.5695362,-0.7116902,0.1156817,-0.70066$ $21,0.0248416,-0.7514171,0.0327581,-0.0217577,-0.1085152,-0.0292255,0.1$ $087804,-0.0750424,-0.1028154,-0.0683903,0.1032246,0.1100651,0.0619506$, $0.021274,0.0617543,-0.0530333,-0.0810497,-0.0058076,-0.0611887,0.13699$ $21,0.9179337,0.0873669,0.3372731,0.4111063,0.3865755,0.2054555,0.49277$ $3,0.0247946,0.7082855,-0.092302,0.0752324,-0.0641801,0.1252339,0.01197$ $72,0.0094695,-0.0288566,-0.0175874,0.0799146,-0.0210845,0.008955,0.122$ $5932,-0.0986559,0.0655694,-0.0655905,-0.0408167,-0.0147397,-0.1559083$, $0.0146043,-0.0079115,-0.0265804,-0.1794373,-0.0955355,0.0099772,-0.027$ $07,0.1126521,-0.0259544,0.684792,-0.2037555,-0.3436827,0.0104052,0.295$ $7716,-0.0408635,-0.3514956,0.2075572,0.8869856,0.0596015,0.0462268,0.0$ $525434,0.0719183,-0.1413617,-0.0968745,0.0674002,-0.0680992,0.0235613$, $-0.109254,-0.0471058,0.0368912,-0.1218075,0.046952,0.0162581,-0.056619$ $4,-0.0513977,0.0202258,-0.0301185,0.0868323,-0.099685,0.033512,0.03743$ $92,0.1347015,0.0049174,0.0201918,-0.1208876,-0.7274324,0.3401426,0.579$ $3509,0.4858938,-0.7936872,-1.2624655,0.4605904,-0.6287382,-1.6833414,0$ $.1540752,0.0802812,0.2611557,-0.039399,0.2229345,-0.1695551,0.0746519$, $0.0266106,0.7429091,0.6349621,-0.1190223,-0.2684082,-0.0021362,0.20841$ $02,-0.0717328,-0.0441633,0.0101845,0.1514064,0.1689698,-0.0029988,-0.0$ $189359,-0.0102293,0.2686962,0.0416968,-0.048708,0.0424757,0.202321,0.0$
$188717,-0.0355454,0.0014316,-0.0230903,0.1735383,0.0401784,0.0206688,-$ $0.0504789,-0.0037622,-0.0746238,-0.0670748,-0.0427892,-0.1075255,0.040$ $6758,-0.0061892,0.0325991,0.0213485,0.0275988,0.0665133,0.0122117,-0.0$ $290492,0.0804639,-0.1220877,0.0767211,-0.0058841,-0.0047442,0.0479395$, $0.0283923,0.0227986,0.0188076,0.0127192,-0.1772671,-0.0604785,0.000611$ $4,0.0072793,0.0614038,0.0676128,0.0195961,-0.0247283,0.0168298,0.06073$ $55,0.0784018,-0.0184953,0.0181521,-0.1668742,0.0433636,-0.0287553,0.02$ $50853,0.0284317,0.1333939,-0.0568947,0.012053,-0.0064256,-0.0109636,-0$ $.1184969,0.0491723,0.0845029,0.0675586,0.0645334,-0.0338811,0.0558566$, $-0.0242317,0.0336703,0.0592867,0.0104618,-0.0387792,-0.0431008,-0.1517$ 35,0.051635,-0.0086729,0.0278962,0.0557324,-0.023842,0.0407506,0.05239 $37,0.0718993,-0.1074823,0.0695802,-0.012859,0.0369799,0.0361555,0.0364$ $201,-0.0330874,-0.0285792,-0.0555739,0.0515417,-0.0403501,-0.0991284,-$ $0.0511367,-0.0011931 \backslash$ Polar $=520.4734541,18.5648859,458.8122521,5.602822$ $6,20.1438022,526.8915064 \backslash \mathrm{PG}=\mathrm{C01}$ [X(C22H28Br3N1O4)]\NImag=1<br>

## Optimization -CPCM with UFF, Methanol

## Piperidine

$\mathrm{N}-\mathrm{N}=2.589124993200 \mathrm{D}+02 \mathrm{E}-\mathrm{N}=-1.100626028869 \mathrm{D}+03 \mathrm{KE}=2.495315284771 \mathrm{D}+02$ $1 \backslash 1 \backslash G I N C-D M C 61 \backslash F O p t \backslash R M 062 X \backslash 6-31+G(d, p) \backslash C 5 H 11 N 1 \backslash A U B C R A \backslash 16-M a y-2012 \backslash 0 \backslash \backslash \#$ opt=(noeigen,Z-Matrix) M062X/6-31+G(d,p) scrf=(cpcm, solvent=methanol) <br>Title Card Required<br>0,1\N,0.0024983286,-1.4681685972,-0.1846920964\} C, 1. $2133636736,-0.7529904982,0.2298294689 \backslash \mathrm{C},-1.2108421208,-0.757062790$ $9,0.2296184074 \backslash \mathrm{H}, 0.0027317843,-1.5531583679,-1.1999453412 \backslash \mathrm{C}, 1.25567861$ $97,0.7069098165,-0.2326378656 \backslash \mathrm{H}, 2.0843020331,-1.3032827338,-0.14017605$ $02 \backslash \mathrm{H}, 1.2520612916,-0.7856349303,1.3278674197 \backslash \mathrm{C},-0.0024309464,1.4505700$ $686,0.2240138552 \backslash \mathrm{H}, 1.3168619094,0.7315883959,-1.3296587243 \backslash \mathrm{H}, 2.1583625$ $055,1.1945241874,0.1530741755 \backslash C,-1.2579974376,0.7027367347,-0.23277516$ $95 \backslash \mathrm{H},-0.0026161392,1.5164773331,1.3213547352 \backslash \mathrm{H},-0.0041193217,2.4774540$ $43,-0.1567558958 \backslash \mathrm{H},-1.3191275467,0.7272659844,-1.3298005011 \backslash \mathrm{H},-2.16234$ $63492,1.1873331704,0.1528493267 \backslash \mathrm{H},-2.0798562828,-1.310268064,-0.140569$ $5709 \backslash \mathrm{H},-1.2496260014,-0.7899027518,1.3276458266 \backslash$ VVersion=EM64L-G09RevC $.01 \backslash$ State=1-A $\backslash H F=-251.7994004 \backslash R M S D=1.465 e-09 \backslash R M S F=9.366 e-06 \backslash D i p o l e=-0$. $0010431,0.6461008,-0.3136598 \backslash$ Quadrupole=1.7204295,-3.6420339,1.9216044 , 0.008801, -0.0023168,1.3555027 \PG=C01 [X(C5H11N1)] <br>@

## Pyrrolidine

$\mathrm{N}-\mathrm{N}=1.899272616667 \mathrm{D}+02 \mathrm{E}-\mathrm{N}=-8.719568081801 \mathrm{D}+02 \mathrm{KE}=2.105983408410 \mathrm{D}+02$ $1 \backslash 1 \backslash G I N C-D M C 177 \backslash F O p t \backslash R M 062 X \backslash 6-31+G(d, p) \backslash C 4 H 9 N 1 \backslash A U B C R A \backslash 26-J u n-2012 \backslash 0 \backslash \backslash \#$ opt=(noeigen, z-matrix) $\mathrm{M0} 62 \mathrm{X} / 6-31+\mathrm{g}(\mathrm{d}, \mathrm{p}) \quad$ scrf=(cpcm, solvent=methanol) $\backslash \backslash$ Title Card Required <br>0,1\N, 0.0007683908, -1.6587674264, -0.0792200084\} $C, 1.153874793,-0.7898557456,0.1932412908 \backslash C,-1.1532197844,-0.7909563526$ , $0.1930584973 \backslash \mathrm{H}, 0.0010048545,-1.8871074281,-1.0720867712 \backslash \mathrm{C}, 0.774554706$ , $0.6215439702,-0.3116199052 \backslash \mathrm{H}, 2.0566778721,-1.1910048757,-0.2733469161$ $\backslash H, 1.3135730984,-0.7717183292,1.2780277551 \backslash \mathrm{H}, 1.1601312978,0.7792840846$ , $-1.3229623912 \backslash \mathrm{H}, 1.1925395647,1.4052959901,0.3256195665 \backslash \mathrm{C},-0.775034305$ $2,0.6210905947,-0.3109951343 \backslash H,-1.1613560635,0.7794930096,-1.321905957$ $1 \backslash H,-1.1931942291,1.4039297533,0.3271349483 \backslash H,-2.0554127778,-1.1927298$ $312,-0.2741527697 \backslash \mathrm{H},-1.3134824169,-0.7735024131,1.2777707933 \backslash$ \Version $=$ EM64L-G09RevC. 01 \State=1-A $\backslash H F=-212.4950632 \backslash R M S D=2.408 e-09 \backslash R M S F=3.931 e-$ $05 \backslash$ Dipole $=-0.0002496,0.6332214,-0.4605322 \backslash$ Quadrupole=1.5280116,-3.2167

049,1.6886932,0.0017684,-0.0010492,2.2149287\PG=C01 [X(C4H9N1)] <br>@

## 1,1,1-tribromo-2,2-bis(3,4-dimethoxyphenyl)ethane

$\mathrm{N}-\mathrm{N}=4.180487611382 \mathrm{D}+03 \mathrm{E}-\mathrm{N}=-2.907692368949 \mathrm{D}+04 \mathrm{KE}=8.651771356390 \mathrm{D}+03$ $1 \backslash 1 \backslash G I N C-D M C 61 \backslash F O p t \backslash R M 062 X \backslash 6-31+G(d, p) \backslash C 18 H 19 B r 304 \backslash A U B C R A \backslash 17-M a y-2012 \backslash$ $0 \backslash \ \#$ opt=(noeigen, Z-Matrix) M062X/6-31+G(d,p) scrf=(cpcm, solvent=metha nol) <br>Title Card Required <br>0,1\C,1.2774071906,1.3030953621, 0.372045347 $8 \backslash C, 1.2893008043,0.4071429612,-0.709309872 \backslash C, 2.3389601029,2.1641017576$ , $0.59198277 \backslash \mathrm{H}, 0.4225508201,1.3279272333,1.0352268087 \backslash \mathrm{C}, 0.0993322835,-0$ $.5035296247,-0.9659276899 \backslash C, 2.3607805658,0.425308672,-1.5892629681 \backslash C, 0$ $.1679398528,-1.8078705772,-0.1374660367 \backslash \mathrm{C},-1.218827593,0.2526426115,-0$ $.8914250441 \backslash \mathrm{H}, 0.1842408676,-0.8659904227,-1.996664419 \backslash \mathrm{Br}, 1.6661068335$, $-2.8776566446,-0.7750924443 \backslash \mathrm{Br},-1.451698277,-2.8518559391,-0.385653138$ $5 \backslash \mathrm{Br}, 0.4346586037,-1.5534232414,1.7729710557 \backslash \mathrm{C},-1.7000499808,0.8181064$ $239,-2.063301193 \backslash C,-1.9105323393,0.4870151377,0.3070631874 \backslash C,-2.835698$ $2664,1.6387041045,-2.0521143338 \backslash H,-1.1818643651,0.6462942131,-3.002942$ $6179 \backslash \mathrm{C},-3.516037318,1.8786391676,-0.8649491849 \backslash \mathrm{H},-3.1813754291,2.07512$ $01056,-2.9816169044 \backslash C,-3.0449471614,1.2849436165,0.3298707483 \backslash 0,-4.622$ $8149818,2.6535500286,-0.7432218722 \backslash 0,-3.7597371284,1.5580083868,1.4511$ $865004 \backslash \mathrm{H},-1.571680122,0.032251042,1.2273387584 \backslash \mathrm{C},-3.2896831546,1.00143$ $791,2.6713067059 \backslash \mathrm{H},-3.9758074757,1.3491283838,3.441980203 \backslash \mathrm{H},-2.2747128$ $824,1.3506750278,2.896670779 \backslash \mathrm{H},-3.3019736044,-0.094040695,2.6340412229$ $\backslash C,-5.0944039789,3.2967990264,-1.9175920094 \backslash \mathrm{H},-5.9658100051,3.87498739$ $39,-1.6142769752 \backslash \mathrm{H},-5.3857546396,2.5630691071,-2.6769766642 \backslash \mathrm{H},-4.33186$ $93842,3.9677981828,-2.3278759725 \backslash C, 3.43285365,1.305674369,-1.389818918$ $2 \backslash H, 2.375817539,-0.2455006722,-2.4433039171 \backslash \mathrm{C}, 3.4356930312,2.172166816$ $4,-0.3041679025 \backslash \mathrm{H}, 4.2555901693,1.304349518,-2.0946247062 \backslash 0,4.417238278$ $3,3.063927951,-0.0227727221 \backslash 0,2.4073538227,3.046756324,1.622003197 \backslash C, 1$ $.3256900743,3.0477445918,2.542355191 \backslash \mathrm{H}, 1.5783777855,3.7851806392,3.303$ $0310822 \backslash \mathrm{H}, 1.206539609,2.0617777436,3.0064649991 \backslash \mathrm{H}, 0.3903923985,3.33463$ $02367,2.0478337594 \backslash C, 5.5124961711,3.1318637667,-0.9237905572 \backslash \mathrm{H}, 6.17527$ $25782,3.9020240359,-0.5327190907 \backslash \mathrm{H}, 5.1752365124,3.4105219687,-1.927925$ $7411 \backslash \mathrm{H}, 6.0449425427,2.1756939996,-0.9667074242 \backslash$ VVersion=EM64L-G09RevC. $01 \backslash$ State $=1-A \backslash H F=-8713.2570835 \backslash R M S D=2.599 e-09 \backslash R M S F=1.056 e-04 \backslash D i p o l e=0.1$ $090834,0.7859035,-0.7900474 \backslash$ Quadrupole=1.1521092,-11.8040286,10.651919 $3,-2.2027811,-4.3543243,-4.6276103 \backslash \mathrm{PG}=\mathrm{C01}[\mathrm{X}(\mathrm{C} 18 \mathrm{H} 19 \mathrm{Br} 304)] \backslash \backslash @$

## Piperidine + 1,1,1-tribromo-2,2-bis(3,4-dimethoxyphenyl)ethane

$\mathrm{N}-\mathrm{N}=5.572036852299 \mathrm{D}+03 \mathrm{E}-\mathrm{N}=-3.244619012401 \mathrm{D}+04 \mathrm{KE}=8.901074189484 \mathrm{D}+03$ $1 \backslash 1 \backslash A S N \_A L T I X-A L T I X 7 \backslash F T S \backslash R M 062 X \backslash 6-31+G(d, p) \backslash C 23 H 30 B r 3 N 104 \backslash A U B C R A \backslash 15-J$ un-2012 $\overline{0} \backslash \backslash \#$ opt $=(c a l c f c, t s, n o e i g e n, m a x c y c l e=600, m o d r e d u n d a n t) ~ M 062 X / 6$ $-31+g(d, p) \quad s c r f=(c p c m, s o l v e n t=m e t h a n o l) \backslash \backslash T i t l e ~ C a r d ~ R e q u i r e d \backslash \backslash 0,1 \backslash C, 0$. $0025334762,0.2793766056,0.013672108 \backslash C,-0.0714338973,0.562816588,-1.402$ $6921011 \backslash C,-0.9846144234,-0.706082648,0.5822905138 \backslash C, 1.407812977,0.0124$ $337294,0.5074039783 \backslash \mathrm{H},-0.3554221628,1.6360196511,0.5151600533 \backslash \mathrm{Br},-1.85$ $13429313,0.8817622747,-2.1070673859 \backslash \mathrm{Br}, 0.6927370404,-0.9983024953,-2.6$ $772300226 \backslash \mathrm{Br}, 1.0185591855,2.0790783974,-1.9594548103 \backslash \mathrm{C},-1.1899826125$, $0.7313542924,1.9609321807 \backslash C,-1.6586076898,-1.6647175853,-0.1946683724 \backslash$ $\mathrm{C},-2.0723040591,-1.6417221902,2.551131259 \backslash \mathrm{H},-0.6388290122,-0.047857789$ $7,2.6000799536 \backslash \mathrm{C},-2.7658423039,-2.5590858565,1.7697597675 \backslash \mathrm{H},-2.2083930$ $876,-1.6230308009,3.6259782772 \backslash C,-2.5407086383,-2.5712800563,0.3768083$ $906 \backslash 0,-3.6507200966,-3.4777724445,2.2426613999 \backslash 0,-3.2269255231,-3.5114$
$261467,-0.3290013232 \backslash \mathrm{H},-1.4659283352,-1.7282383421,-1.2553906077 \backslash \mathrm{C},-3$. $0342663838,-3.5348279217,-1.7353681151 \backslash \mathrm{H},-3.6780190839,-4.3280818209$, $2.1126392098 \backslash \mathrm{H},-1.9910420426,-3.7573441224,-1.9869310053 \backslash \mathrm{H},-3.32316286$ $58,-2.5790467882,-2.1873623602 \backslash C,-3.8565811707,-3.5133612219,3.6459276$ $104 \backslash \mathrm{H},-4.5818268524,-4.3060991799,3.8233361116 \backslash \mathrm{H},-4.2582613809,-2.5611$ $075195,4.0090754635 \backslash \mathrm{H},-2.9241292536,-3.7424408441,4.1734000083 \backslash \mathrm{C}, 1.873$ $2768384,-1.3134824815,0.5429384695 \backslash C, 2.2849163831,1.0120580782,0.92399$ $2379 \backslash C, 3.1533699663,-1.6212373202,0.964946342 \backslash H, 1.2285998404,-2.128700$ $2926,0.2244560599 \backslash C, 4.0298339875,-0.5992260792,1.3827359331 \backslash 0,3.566533$ $0839,-2.9310813219,0.9980788268 \backslash C, 3.5817036309,0.719882795,1.359011044$ $2 \backslash 0,5.2619621098,-0.9971477215,1.7886914292 \backslash \mathrm{H}, 4.2267422535,1.530062934$ $1,1.6772058496 \backslash \mathrm{H}, 1.983088632,2.053592753,0.9019735452 \backslash \mathrm{C}, 6.1622079372,0$ $.011274837,2.2250409555 \backslash \mathrm{H}, 7.0791347018,-0.5058725048,2.503226918 \backslash \mathrm{H}, 5.7$ $611212624,0.5428893916,3.0943787153 \backslash \mathrm{H}, 6.3711734706,0.7243187283,1.4207$ $241014 \backslash C, 4.3885818435,-3.281805694,-0.1167715513 \backslash \mathrm{H}, 4.6601008091,-4.330$ $0077677,0.0103659726 \backslash H, 5.2924619492,-2.6651246786,-0.1387230303 \backslash H, 3.82$ $89544602,-3.155610419,-1.0507834103 \backslash N,-0.579450142,2.7885862172,0.9757$ $747108 \backslash C,-0.7465347682,2.7166867542,2.4496531893 \backslash C,-1.74819665,3.41142$ $76493,0.3014795478 \backslash \mathrm{H}, 0.2473373384,3.3515592992,0.7585875065 \backslash \mathrm{C},-1.02147$ $41182,4.0882807488,3.0547654609 \backslash H, 0.1558750642,2.2574025527,2.86364956$ $99 \backslash \mathrm{H},-1.5907866409,2.0440073465,2.6337456795 \backslash \mathrm{C},-2.2459275693,4.7263004$ $088,2.3958503735 \backslash \mathrm{H},-0.1430239525,4.7315861849,2.9146753847 \backslash \mathrm{H},-1.169748$ $3992,3.97408732,4.1327016763 \backslash C,-2.0617517251,4.7875929544,0.8788822263$ $\backslash \mathrm{H},-3.136502067,4.1289437063,2.6317364618 \backslash \mathrm{H},-2.4142508654,5.7295106737$ , 2. $7980049582 \backslash \mathrm{H},-1.2392869475,5.4728847664,0.6347920517 \backslash \mathrm{H},-2.960102220$ $5,5.1766134721,0.3901869609 \backslash \mathrm{H},-1.5191245437,3.4686492248,-0.7646218456$ $\backslash H,-2.5901208254,2.722309305,0.4337057762 \backslash \backslash V e r s i o n=I A 64 L-G 09 R e v C .01 \backslash S t$ ate $=1-A \backslash H F=-8965.040424 \backslash R M S D=8.020 e-09 \backslash R M S F=7.350 e-06 \backslash$ Dipole= $=0.129034$ $2,4.564465,3.0754627 \backslash$ Quadrupole $=2.1706132,4.0201457,-6.1907588,-0.5354$ $105,-1.2334465,14.2789463 \backslash \mathrm{PG}=\mathrm{C01}[\mathrm{X}(\mathrm{C} 23 \mathrm{H} 30 \mathrm{Br} 3 \mathrm{~N} 104)] \backslash \backslash @$

## Pyrrolidine + 1,1,1-tribromo-2,2-bis(3,4-dimethoxyphenyl)ethane

$\mathrm{N}-\mathrm{N}=5.361474555267 \mathrm{D}+03 \mathrm{E}-\mathrm{N}=-3.193442667059 \mathrm{D}+04 \mathrm{KE}=8.862181910850 \mathrm{D}+03$ $1 \backslash 1 \backslash A S N \_A L T I X-A L T I X 7 \backslash F T S \backslash R M 062 X \backslash 6-31+G(d, p) \backslash C 22 H 28 B r 3 N 104 \backslash A U B C R A \backslash 09-J$ ul-2012 $\overline{0} \backslash \backslash \#$ opt=(calcfc,ts, noeigen, maxcycle=600) M062X/6-31+g(d,p) sc $r f=(c p c m, s o l v e n t=m e t h a n o l) \backslash \backslash T i t l e ~ C a r d$ Required $\backslash \backslash 0,1 \backslash C, 0.1783541222,0$. $3020239765,-0.1128346337 \backslash C, 0.1608863341,0.6058381899,-1.5237356657 \backslash C$, -$0.8602209445,-0.641034879,0.4295916665 \backslash C, 1.5543834404,0.0233731393,0.4$ $388080502 \backslash \mathrm{H},-0.299235867,1.6129327694,0.3683721286 \backslash \mathrm{Br},-1.5965428114,1$. $0638938285,-2.2251134909 \backslash \mathrm{Br}, 0.8398580204,-0.9629304324,-2.8218643384 \backslash \mathrm{~B}$ $r, 1.3547252958,2.0646538227,-2.0180685458 \backslash C,-1.1579013777,-0.581255768$ $8,1.7902119815 \backslash C,-1.5330803394,-1.5967113607,-0.3506645412 \backslash C,-2.126677$ $7785,-1.4129759521,2.3597694889 \backslash \mathrm{H},-0.6299725055,0.1241925899,2.4279507$ $053 \backslash C,-2.8143282759,-2.3324716912,1.574896449 \backslash \mathrm{H},-2.3383397895,-1.32876$ $98279,3.4193063412 \backslash C,-2.5004986398,-2.4253935524,0.2016329128 \backslash 0,-3.779$ $7608938,-3.1774896249,2.0262602959 \backslash 0,-3.1918645146,-3.3618253947,-0.50$ $2973262 \backslash \mathrm{H},-1.2832487556,-1.7048224691,-1.3966708879 \backslash \mathrm{C},-2.8971635298,-3$ $.4796258967,-1.8867729433 \backslash \mathrm{H},-3.5537930583,-4.2603734502,-2.2677650683 \backslash$ $\mathrm{H},-1.8516917987,-3.7686923821,-2.0432275326 \backslash \mathrm{H},-3.0975696469,-2.5397513$ $416,-2.4137638269 \backslash \mathrm{C},-4.0951883281,-3.1192251164,3.4082992688 \backslash \mathrm{H},-4.8679$ $827365,-3.8688829398,3.5718947802 \backslash \mathrm{H},-4.4788542818,-2.1304570837,3.6827$ $22053 \backslash \mathrm{H},-3.2187655343,-3.355360955,4.0216133064 \backslash \mathrm{C}, 2.0361476333,-1.2951$
$577335,0.4467468995 \backslash C, 2.3846098841,1.0218933468,0.9418669517 \backslash C, 3.30118$ $75004,-1.5967704971,0.9193590104 \backslash \mathrm{H}, 1.4196964602,-2.1064501126,0.067294$ $2151 \backslash C, 4.1359586551,-0.5761163089,1.4175747382 \backslash 0,3.7379575381,-2.89972$ $79941,0.9301014663 \backslash C, 3.6630649616,0.7353313021,1.4295331482 \backslash 0,5.356544$ $4299,-0.9676223243,1.864640885 \backslash H, 4.2756616139,1.5417001964,1.814588775$ $8 \backslash H, 2.0496127825,2.0547132064,0.9436777375 \backslash \mathrm{C}, 6.2197732684,0.0396294683$ , 2. $3722786019 \backslash \mathrm{H}, 7.1343831391,-0.4709315431,2.6692599358 \backslash \mathrm{H}, 5.7746499964$ , 0.5336639774, 3.2422431944 \H, 6.4476678377, 0.7844156653,1.602311316\C, 4 $.6077526015,-3.2024769457,-0.1622259096 \backslash \mathrm{H}, 4.9187415042,-4.240062525,-0$ $.0381133869 \backslash \mathrm{H}, 5.4854345083,-2.5485999262,-0.1483609756 \backslash \mathrm{H}, 4.073033702$, -$3.0875725835,-1.1119130425 \backslash N,-0.7983010571,2.6993870968,0.7435397117 \backslash C$ , - 0. $2343021015,3.1813581674,2.0426108469 \backslash \mathrm{C},-2.289318424,2.5624306992,0$ $.898250684 \backslash \mathrm{H},-0.5814423715,3.3666449855,0.0035385776 \backslash \mathrm{C},-1.4283013503,3$ $.7765278326,2.7817685942 \backslash \mathrm{H}, 0.5800050618,3.882625329,1.8546427769 \backslash \mathrm{H}, 0.1$ $679447773,2.3155229022,2.57948736 \backslash \mathrm{H},-1.6314250559,4.7878770868,2.41347$ $35274 \backslash \mathrm{H},-1.2630945293,3.8245594975,3.85974083 \backslash \mathrm{C},-2.5588079093,2.825897$ $244,2.3813009802 \backslash \mathrm{H},-3.554510928,3.2432973976,2.5415952082 \backslash \mathrm{H},-2.4831536$ $924,1.8915879201,2.9486607173 \backslash \mathrm{H},-2.7771089321,3.3015625682,0.258814775$ $6 \backslash \mathrm{H},-2.5896833096,1.5641314072,0.5745561574 \backslash \backslash V e r s i o n=1 A 64 \mathrm{~L}-\mathrm{G0} 9 \mathrm{RevC} .01 \backslash$ State $=1-A \backslash H F=-8925.7394146 \backslash R M S D=2.995 e-09 \backslash R M S F=3.615 e-06 \backslash D i p o l e=-0.648$ 6926,4.267031,3.0837384\Quadrupole=3.7267612,2.7727043,-6.4994654,-2.0 $071892,-2.7474489,15.9678491 \backslash P G=C 01 \quad[X(C 22 H 28 B r 3 N 104)] \backslash \backslash @$

## Frequency Calculation - CPCM with UFF, Methanol

## Piperidine

Sum of electronic and zero-point Energies=
-251.639539
Sum of electronic and thermal Energies=
Sum of electronic and thermal Enthalpies=
Sum of electronic and thermal Free Energies=

$$
\begin{aligned}
& -251.633968 \\
& -251.633024 \\
& -251.668186
\end{aligned}
$$

$1 \backslash 1 \backslash A S N \_A L T I X-A L T I X 8 \backslash F r e q \backslash R M 062 X \backslash 6-31+G(d, p) \backslash C 5 H 11 N 1 \backslash A U B C R A \backslash 16-M a y-20$ $12 \backslash 0 \backslash \ \mathrm{~N}^{-}$Geom=AllCheck Guess=TCheck SCRF=Check GenChk RM062X/6-31+G(d, p) Freq $\backslash$ Title Card Required $\backslash \backslash 0,1 \backslash \mathrm{~N}, 0.000628,-1.466335,-0.185433 \backslash \mathrm{C}, 1.2$ $1242,-0.752879,0.22935 \backslash C,-1.211789,-0.753907,0.229309 \backslash \mathrm{H}, 0.000684,-1.55$ $0831,-1.200728 \backslash C, 1.256536,0.707192,-0.23241 \backslash \mathrm{H}, 2.082641,-1.304085,-0.14$ $0985 \backslash \mathrm{H}, 1.251154,-0.786106,1.327369 \backslash \mathrm{C},-0.000607,1.452209,0.224693 \backslash \mathrm{H}, 1.3$ $17673,0.732327,-1.329423 \backslash H, 2.159858,1.193484,0.153475 \backslash \mathrm{C},-1.257144,0.70$ $6175,-0.232371 \backslash \mathrm{H},-0.000632,1.517582,1.322065 \backslash \mathrm{H},-0.001033,2.479279,-0.1$ $55578 \backslash \mathrm{H},-1.31832,0.731315,-1.32938 \backslash \mathrm{H},-2.160856,1.191719,0.153553 \backslash \mathrm{H},-2$. $081523,-1.305841,-0.141086 \backslash \mathrm{H},-1.250537,-0.787233,1.327323 \backslash$ VVersion=IA6 $4 L-G 09 R e v C .01 \backslash S t a t e=1-A \backslash H F=-251.7994004 \backslash R M S D=1.280 e-09 \backslash R M S F=9.342 e-06 \backslash$ ZeroPoint $=0.1598613 \backslash$ Thermal $=0.165432 \backslash$ Dipole $=-0.0002535,0.6462554,-0.31$ $33452 \backslash$ DipoleDeriv $=-0.81236,0.0001047,0.0000073,0.0001044,-1.0182566,-0$ $.0208204,0.000008,-0.0069818,-0.3384777,0.5196102,0.2044685,0.0730768$, $0.1035726,0.4676289,-0.0210169,0.1951468,0.0194187,0.3715074,0.5198559$ $,-0.204437,-0.0730656,-0.1035291,0.4673411,-0.0210743,-0.1951785,0.019$ $2413,0.3715031,0.1053827,-0.0001163,-0.0000305,-0.0001216,0.4023121,0$. $1153616,0.0000163,-0.0409626,-0.0042701,0.0538926,0.003188,0.0049292,-$ $0.0335023,-0.0702383,0.0199555,-0.0191714,0.0359486,0.1902598,-0.16325$ $6,0.0939251,0.03959,0.113801,-0.0634166,-0.0385816,0.0937628,-0.046403$ $4,0.0495576,0.0441728,-0.0254248,0.032533,-0.0433372,0.0131083,0.00563$
$71,-0.0627524,0.0211832,-0.240108,0.0636961,-0.0000127,0.0000037,-0.00$ $00263,0.1202667,-0.0041724,-0.0000128,0.0283326,0.2046876,0.0440332,0$. $0236334,-0.0101772,0.0247711,0.0188073,-0.0162676,0.0536353,0.0160141$, $-0.2456841,-0.1913499,-0.1056137,-0.0577146,-0.1131016,-0.0278566,-0.0$ $292054,-0.0934052,-0.0507073,0.0452237,0.0538375,-0.003111,-0.0049804$, $0.0335538,-0.0701741,0.0199238,0.0191444,0.0359477,0.1902683,0.0010292$ , - 0.0000147, 0.0000003, -0.0000139, 0.0607828, 0.0077691, 0.000028, -0.06601 $41,-0.2488145,0.0278378,0.0001002,-0.0000199,0.0001067,-0.2409593,0.06$ $09274,-0.0000416,0.0948692,0.0453934,0.0440806,-0.0236017,0.0101877,-0$ $.0247373,0.0187724,-0.0162464,-0.0536542,0.0159877,-0.2457041,-0.19152$ $5,0.1054667,0.0577509,0.1129922,-0.0276983,-0.0291692,0.0934562,-0.050$ $6315,0.0452215,-0.1630638,-0.0940149,-0.039577,-0.1138995,-0.0635831,-$ $0.0386238,-0.0937358,-0.0464939,0.0495497,0.0441261,0.0254603,-0.03251$ $36,0.0433672,0.0131632,0.0056036,0.062754,0.0212514,-0.2401137 \backslash$ Polar=8 $6.1252047,0.0001156,83.5854288,-0.0004616,0.5119543,80.9463897 \backslash \mathrm{PG}=\mathrm{C} 01$ $[\mathrm{X}(\mathrm{C} 5 \mathrm{H} 11 \mathrm{~N} 1)] \backslash \mathrm{NImag}=0 \backslash \backslash$

## Pyrrolidine

Sum of electronic and zero-point Energies=
$-212.364516$
Sum of electronic and thermal Energies=
-212. 359495
Sum of electronic and thermal Enthalpies=
Sum of electronic and thermal Free Energies=
-212. 358551
-212. 393514
$1 \backslash 1 \backslash G I N C-D M C 49 \backslash$ Freq $\backslash$ RM0 $62 X \backslash 6-31+G(d, p) \backslash C 4 H 9 N 1 \backslash A U B C R A \backslash 02-J u l-2012 \backslash 0 \backslash \backslash \#$ freq=noraman $M 062 \mathrm{X} / 6-31+g(d, p) \quad \operatorname{scrf}=(\mathrm{cpcm}$, solvent=methanol) <br>Title Car d Required $\backslash \backslash 0,1 \backslash N,-0.000074,-1.26427,0.209803 \backslash C,-1.15351,-0.451042,-0$. $19903 \backslash \mathrm{C}, 1.153585,-0.451139,-0.198618 \backslash \mathrm{H},-0.000307,-1.329774,1.226481 \backslash \mathrm{C}$, $-0.77481,1.023387,0.07201 \backslash \mathrm{H},-2.056191,-0.77221,0.326037 \backslash \mathrm{H},-1.313117,-0$ $.607865,-1.272588 \backslash \mathrm{H},-1.160542,1.34174,1.044752 \backslash \mathrm{H},-1.193056,1.69414,-0$. $683114 \backslash \mathrm{C}, 0.774779,1.023484,0.071503 \backslash \mathrm{H}, 1.160945,1.342743,1.04373 \backslash \mathrm{H}, 1.19$ $2678,1.693541,-0.684333 \backslash \mathrm{H}, 2.055899,-0.772071,0.327207 \backslash \mathrm{H}, 1.313939,-0.60$ 849,-1.271985<br>Version=EM64L-G09RevC. $01 \backslash$ State=1-A $\backslash \mathrm{HF}=-212.4950632 \backslash \mathrm{RMSD}$ $=5.683 \mathrm{e}-09 \backslash \mathrm{RMSF}=3.927 \mathrm{e}-05 \backslash$ ZeroPoint $=0.130547 \backslash$ Thermal=0.1355678\Dipole= $-0.0000503,0.6991087,0.3525721 \backslash$ DipoleDeriv=-0.6797575,0.0000519,-0.000 $0147,-0.0000564,-1.0587655,0.1452815,-0.0000703,0.0355224,-0.3573498,0$ $.3965125,-0.1590023,0.0622979,-0.0417854,0.4807035,-0.0028953,0.175902$ $,-0.0255307,0.3775255,0.3966481,0.1590399,-0.0623843,0.0417278,0.48057$ $34,-0.0028225,-0.1758666,-0.0254748,0.3774921,0.1176485,-0.0000102,0.0$ $000466,0.0000235,0.3728725,-0.1298987,0.0000254,0.0220052,0.0073036,0$. $0126375,-0.0836686,-0.0156355,-0.008054,-0.0822576,-0.0250124,-0.05516$ $1,-0.0371405,0.1706436,-0.1444227,-0.0626264,0.0552302,-0.0758025,0.01$ $06263,0.0309554,0.1134534,0.0449378,0.023009,0.0356398,0.0011547,-0.01$ $34848,0.0080208,-0.0087679,-0.0444688,-0.0961965,-0.0362492,-0.2131471$ $,-0.0167955,0.0402114,0.0662194,0.0227473,0.0148387,-0.0493197,0.10462$ $13,-0.1040432,-0.1404385,-0.0025272,0.0706466,-0.0583932,0.0943833,-0$. $0720932,0.0830583,-0.0929089,0.1293018,-0.0424996,0.0125361,0.0835821$, $0.0155857,0.0080674,-0.0823928,-0.0248364,0.0551949,-0.0371093,0.17051$ $3,-0.0168334,-0.0404215,-0.0662625,-0.0229106,0.0146775,-0.0495058,-0$. $1047011,-0.1042208,-0.1401807,-0.0024894,-0.070461,0.0584517,-0.094151$ $1,-0.071833,0.0830257,0.0929279,0.1293118,-0.0427207,-0.1443396,0.0625$ $961,-0.0553421,0.0757113,0.0106536,0.030995,-0.1136133,0.0450014,0.022$ $8525,0.035543,-0.0010927,0.0136857,-0.0079213,-0.0088355,-0.0445564,0$.
$0963926,-0.0363118,-0.213003 \backslash \operatorname{Polar}=69.307311,0.0002157,68.9770321,-0.0$ $018003,-0.2895032,63.8152159 \backslash \mathrm{PG}=\mathrm{C01} \quad[\mathrm{X}(\mathrm{C} 4 \mathrm{H} 9 \mathrm{~N} 1)] \backslash \mathrm{NImag}=0 \backslash \backslash$

## 1,1,1-tribromo-2,2-bis (3,4-dimethoxyphenyl)ethane

Sum of electronic and zero-point Energies= Sum of electronic and thermal Energies=
Sum of electronic and thermal Enthalpies=
Sum of electronic and thermal Free Energies=
$-8712.915160$
-8712.889161
$-8712.888216$
-8712.974537
$1 \backslash 1 \backslash G I N C-D M C 27 \backslash$ Freq $\backslash$ RM0 62X $\backslash 6-31+G(d, p) \backslash C 18 H 19 B r 304 \backslash A U B C R A \backslash 30-M a y-2012 \backslash$ $0 \backslash \ \#$ freq=noraman $M 062 \mathrm{X} / 6-31+G(d, p) \quad s c r f=(c p c m, s o l v e n t=m e t h a n o l) \ \backslash i t l$ e Card Required <br>0,1\C,1.276438,1.332704, 0.339914\C,1.278527,0.412869, $-0.721264 \backslash \mathrm{C}, 2.333401,2.207976,0.522472 \backslash \mathrm{H}, 0.43269,1.364684,1.016871 \backslash \mathrm{C}, 0$ $.093021,-0.514037,-0.93719 \backslash C, 2.334799,0.420968,-1.619562 \backslash C, 0.187855,-1$ $.798797,-0.081176 \backslash \mathrm{C},-1.230751,0.231684,-0.857061 \backslash \mathrm{H}, 0.163945,-0.898742$, $-1.960898 \backslash \mathrm{Br}, 1.685057,-2.869044,-0.720295 \backslash \mathrm{Br},-1.425843,-2.862667,-0.27$ $8373 \backslash \mathrm{Br}, 0.484342,-1.499169,1.81829 \backslash \mathrm{C},-1.736963,0.766355,-2.032857 \backslash \mathrm{C},-1$ $.904325,0.486622,0.347541 \backslash \mathrm{C},-2.879931,1.57671,-2.020568 \backslash \mathrm{H},-1.2331,0.57$ $8197,-2.977145 \backslash \mathrm{C},-3.542384,1.837057,-0.827603 \backslash \mathrm{H},-3.245321,1.98903,-2.9$ $53525 \backslash \mathrm{C},-3.04565,1.274586,0.371929 \backslash 0,-4.654193,2.604479,-0.704293 \backslash 0,-3$ $.74397,1.566266,1.498921 \backslash H,-1.545741,0.05569,1.271799 \backslash \mathrm{C},-3.248195,1.04$ $1467,2.722934 \backslash \mathrm{H},-3.924469,1.400145,3.497271 \backslash \mathrm{H},-2.2329,1.40482,2.923109$ $\backslash \mathrm{H},-3.250805,-0.054639,2.710291 \backslash \mathrm{C},-5.151547,3.216943,-1.884478 \backslash \mathrm{H},-6.02$ $3116,3.793898,-1.579287 \backslash \mathrm{H},-5.448744,2.463766,-2.62225 \backslash \mathrm{H},-4.402385,3.88$ $5429,-2.322558 \backslash C, 3.401753,1.315229,-1.4581 \backslash \mathrm{H}, 2.341745,-0.268664,-2.458$ $584 \backslash C, 3.414744,2.205843,-0.392223 \backslash H, 4.212465,1.305526,-2.176641 \backslash 0,4.39$ $2461,3.112516,-0.147551 \backslash 0,2.410845,3.114091,1.531262 \backslash \mathrm{C}, 1.344891,3.1259$ $55,2.46969 \backslash \mathrm{H}, 1.60342,3.882517,3.20933 \backslash \mathrm{H}, 1.242865,2.149609,2.957609 \backslash \mathrm{H}, 0$ $.398731,3.393221,1.984936 \backslash C, 5.471684,3.170114,-1.06842 \backslash \mathrm{H}, 6.133685,3.95$ $4804,-0.705967 \backslash H, 5.114935,3.423125,-2.07261 \backslash H, 6.012303,2.218068,-1.099$ $112 \backslash \backslash$ Version=EM64L-G09RevC. $01 \backslash$ State $=1-A \backslash H F=-8713.2570835 \backslash$ RMSD $=2.440 \mathrm{e}-0$ $9 \backslash \operatorname{RMSF}=1.056 e-04 \backslash$ ZeroPoint $=0.3419234 \backslash$ Thermal=0.3679229\Dipole=0.088349 $6,0.7689413,-0.8091029 \backslash$ DipoleDeriv=-0.1638894,-0.081367,-0.1626192,0.1 $685251,-0.1543708,-0.1436894,0.0820172,0.1228939,-0.1990052,-0.0468848$ , 0. $2117922,-0.0278987,0.0586709,-0.2359811,0.0974196,-0.0710112,0.0724$ $686,-0.0361103,-0.2159412,-0.2537471,0.0250077,-0.0729483,0.8334197,1$. $0084437,0.1908653,1.0902152,1.2793445,0.1240803,0.0015365,0.101933,0.0$ $134225,0.1656374,0.0025314,0.1088977,-0.027667,0.089244,0.0894089,0.02$ $23273,0.0841647,-0.0528187,0.4460181,-0.2055991,-0.0235284,-0.1240577$, $-0.1109521,-0.0210578,0.008923,-0.1542409,0.0569082,-0.1021923,0.02489$ $52,-0.0449038,0.0727035,-0.0790847,1.4719267,0.0613921,-0.0121423,0.07$ $69837,0.8766838,0.4428727,0.0231805,0.3602225,1.2578335,0.1756251,-0.1$ $735746,-0.0124562,-0.0588042,-0.2359007,0.0320446,0.1323839,-0.0243438$ $, 0.0284826,0.0446475,0.0112079,0.0032215,-0.0000824,-0.0158218,0.06229$ $21,0.0043268,-0.069176,-0.0549982,-0.629801,0.3042715,0.1805021,0.3415$ $499,-0.3685579,-0.1622599,0.195296,-0.1359215,-0.2523903,-0.7447126,-0$ $.3636102,-0.0844113,-0.4085016,-0.4031323,-0.0681293,-0.0761338,-0.050$ $1995,-0.1580141,-0.1812795,0.0047026,-0.1231017,-0.0149959,-0.1859293$, $-0.1433654,-0.0904557,-0.1598444,-0.7931375,-0.2008544,-0.0623186,0.08$ $11517,0.0199942,-0.1876513,-0.1059813,-0.0773874,0.012081,-0.0073633,-$ $0.2841127,0.0002364,0.1692636,-0.0142478,-0.1784378,-0.1424949,-0.1753$ $888,0.0753748,-0.2074108,-0.1878721,0.0111523,-0.1542611,-0.0697594,-0$
$.2070004,0.0774572,0.1272165,-0.1400229,0.0150929,0.0708543,0.0687458$, $0.1098898,0.0632199,0.1332668,-0.0359484,0.0859872,-0.0237369,-0.01726$ $31,1.5570358,-0.9866292,0.0818038,-1.0559381,0.8088397,-0.0052863,0.16$ 85793,-0.0173195,-0.2131714,0.1136293,0.0657997,-0.0531119, 0.0745117,0 $.1384735,0.0628327,-0.0623808,0.071009,0.0167685,0.3779965,-0.0305701$, $-0.8526812,0.0053117,0.0530201,0.3237923,-1.0862445,0.4248979,1.607826$ $5,-1.8297017,1.0241364,-0.3272477,1.0884199,-1.1312898,0.3082087,-0.24$ $65191,0.2383595,-0.7059938,-0.7850482,0.1723223,0.5504549,0.1934229,-0$ $.4633677,-0.0609337,0.6333075,-0.0690728,-2.2236849,0.2018014,-0.02575$ $24,-0.0313804,-0.014462,0.1893886,0.0449261,-0.020488,0.029386,0.04851$ $43,0.3613045,-0.0104165,0.317962,0.047002,0.4473307,-0.3252709,0.01782$ 81,-0.1331826,1.077,0.0097445,0.0492286,0.1189061,0.0555978,0.0749231, $-0.0524644,0.069555,-0.0170316,-0.0708467,-0.1165961,-0.0695228,-0.155$ $2052,-0.1017007,0.0227852,0.0466357,0.0317192,0.0242873,-0.0086758,0.0$ $808304,-0.0068561,-0.0918636,-0.0211637,-0.1655637,0.09895,0.0002627,-$ $0.0669972,-0.0095547,0.5679482,-0.1427491,0.2067517,-0.2181397,0.60006$ $17,-0.2264036,0.5333441,-0.4291495,0.7777712,-0.0669995,0.1244713,-0.0$ $016997,0.1180445,0.0218438,0.0120739,0.0502869,-0.0280811,0.0521022,0$. $0528196,-0.0107099,-0.020244,-0.0583546,-0.0791335,-0.1254142,-0.14576$ $23,0.0187802,-0.0779901,-0.0528433,-0.1418074,0.0814351,-0.0355426,-0$. $0291083,0.0615657,-0.0789592,0.1126434,-0.019859,-0.1894744,0.0678047$, $0.0239662,-0.169675,-0.2363776,0.1495084,-0.226264,-0.0667999,-0.08532$ , 0.1134858,-0.0385906,-0.0142454,-0.0300069,0.0437902,-0.1327546,-0.00 $3135,-0.1129493,0.0449711,1.4328791,1.1249274,0.2108671,1.1130307,0.92$ $87204,0.008708,0.2167418,0.0030465,-0.0661022,0.0222734,-0.0452769,0.0$ $963776,-0.042515,0.1591615,-0.0216734,0.108222,-0.016219,0.0901212,-2$. $035153,-1.0106884,0.2325292,-1.0997272,-1.1363431,0.0092374,0.137468,-$ $0.0678203,-0.5613084,-0.649999,0.0899423,0.347449,0.0227212,-1.0719752$ , -0.8931171,0.2739117,-0.9156524,-1.7096459,0.6864193,-0.2364234,-0.50 $97557,-0.0348489,0.3641876,-0.0298937,-0.2696893,0.1386703,0.8127244,0$ $.0629009,-0.0496631,-0.0283653,-0.017247,-0.0083172,-0.1350838,0.01199$ $61,-0.1042811,-0.0347795,0.0221672,0.0743925,0.0890525,-0.0388922,-0.1$ $046981,0.165753,0.0326162,0.0206665,-0.0014752,-0.1319288,0.102015,0.0$ $471684,0.0313151,0.0682291,0.050773,-0.1254468,0.0335527,-0.0419497,1$. $0060738,0.211577,-0.2712086,0.0010305,0.3692433,-0.0547998,-0.5369591$, $-0.243031,0.5970894,-0.0360296,-0.0979016,0.0069521,-0.1359667,-0.0176$ $153,-0.0327845,-0.0363414,-0.0637768,0.0617759,-0.0378232,0.0160679,-0$ $.1065441,0.0429293,0.0681055,0.0269231,0.0716279,0.1078908,-0.137796,-$ $0.0378502,0.0092025,0.0278743,0.1737265,-0.0943647,-0.0144967,0.089361$ , 0.0771841, 0.0272209 $\backslash$ Polar $=426.9283647,-4.2350683,357.1556725,-20.9714$ $762,21.9219911,383.5385581 \backslash \mathrm{PG}=\mathrm{C01} \quad[\mathrm{X}(\mathrm{C} 18 \mathrm{H} 19 \mathrm{Br} 304)] \backslash \mathrm{NImag}=0 \backslash \backslash$

## Piperidine $+1,1,1$-tribromo-2,2-bis(3,4-dimethoxyphenyl)ethane

## 1

2
A
Frequencies -- -1166.5767
Sum of electronic and zero-point Energies= -8964.542234 Sum of electronic and thermal Energies= Sum of electronic and thermal Enthalpies= Sum of electronic and thermal Free Energies=
$1 \backslash 1 \backslash A S N \_A L T I X-A L T I X 9 \backslash F r e q \backslash R M 062 X \backslash 6-31+G(d, p) \backslash C 23 H 30 B r 3 N 104 \backslash A U B C R A \backslash 23-$ Jun-2012 $\overline{\text { Jo }}$ <br>\# freq=noraman $M 062 \mathrm{X} / 6-31+\mathrm{g}(\mathrm{d}, \mathrm{p})$ scrf=(cpcm, solvent=methan ol) $\backslash \backslash$ Title Card Required $\backslash \backslash 0,1 \backslash \mathrm{C},-0.043696,0.261299,0.045087 \backslash \mathrm{C},-0.14110$ 7,0.60989,-1.355232\C,-0.979212,-0.796496,0.569298\C,1.376109,0.037433 $, 0.518243 \backslash \mathrm{H},-0.461556,1.573276,0.614482 \backslash \mathrm{Br},-1.939079,0.878187,-2.03439$ $3 \backslash \mathrm{Br}, 0.686587,-0.848998,-2.70877 \backslash \mathrm{Br}, 0.872216,2.20155,-1.841973 \backslash \mathrm{C},-1.17$ 3253,-0.898916,1.946007\C,-1.612858,-1.746831,-0.250622\C,-2.007444,-1 $.877881,2.494959 \backslash \mathrm{H},-0.650335,-0.222159,2.615338 \backslash \mathrm{C},-2.66259,-2.787751,1$ $.672758 \backslash \mathrm{H},-2.136539,-1.918288,3.570072 \backslash \mathrm{C},-2.447143,-2.721073,0.279817 \backslash$ $0,-3.499785,-3.769396,2.10416 \backslash 0,-3.093359,-3.657023,-0.468071 \backslash \mathrm{H},-1.425$ $025,-1.749158,-1.314109 \backslash \mathrm{C},-2.909918,-3.602409,-1.874805 \backslash \mathrm{H},-3.518279,-4$ $.405874,-2.287533 \backslash \mathrm{H},-1.859203,-3.76264,-2.142084 \backslash \mathrm{H},-3.246761,-2.640424$ ,-2.277793\C,-3.693655,-3.883337,3.504957\H,-4.379456,-4.717297,3.6466 $51 \backslash \mathrm{H},-4.137132,-2.970111,3.916488 \backslash \mathrm{H},-2.747682,-4.093494,4.015975 \backslash \mathrm{C}, 1.9$ $03765,-1.265075,0.486203 \backslash C, 2.208115,1.055927,0.979265 \backslash \mathrm{C}, 3.199933,-1.53$ $2082,0.886323 \backslash \mathrm{H}, 1.295938,-2.093374,0.131115 \backslash \mathrm{C}, 4.030255,-0.491342,1.349$ $649 \backslash 0,3.674573,-2.820917,0.85293 \backslash C, 3.520318,0.804618,1.393065 \backslash 0,5.2826$ $45,-0.849795,1.729531$ \ $\mathrm{H}, 4.128741,1.627922,1.747616 \backslash \mathrm{H}, 1.857404,2.08181$, $1.01001 \backslash \mathrm{C}, 6.137495,0.177607,2.21061 \backslash \mathrm{H}, 7.079742,-0.308485,2.458542 \backslash \mathrm{H}, 5$. $718064,0.646426,3.107002 \backslash \mathrm{H}, 6.306853,0.938263,1.441362 \backslash \mathrm{C}, 4.504203,-3.07$ $7295,-0.281816 \backslash \mathrm{H}, 4.825708,-4.116411,-0.207752 \backslash \mathrm{H}, 5.377846,-2.418122,-0$. $277778 \backslash \mathrm{H}, 3.932557,-2.932212,-1.205753 \backslash \mathrm{~N},-0.736319,2.690001,1.132357 \backslash \mathrm{C}$, $-0.88924,2.538216,2.601704 \backslash$ С, $-1.937924,3.288989,0.495228 \backslash \mathrm{H}, 0.061447,3$. $301491,0.939129 \backslash \mathrm{C},-1.224137,3.863974,3.274929$ \H, $0.036756,2.102519,2.98$ 8199 \H, $-1.699519,1.818067,2.756562 \backslash \mathrm{C},-2.48199,4.474711,2.654179 \backslash \mathrm{H},-0.3$ $77998,4.554285,3.162407 \backslash \mathrm{H},-1.35912,3.690263,4.346645 \backslash \mathrm{C},-2.311808,4.618$ 833,1.141189\н,-3.341716,3.824979,2.8647\H,-2.694496,5.447929,3.106042 \H, -1.524316, $5.353469,0.927134 \backslash \mathrm{H},-3.230975,4.988278,0.676609 \backslash \mathrm{H},-1.7194$ $66,3.409112,-0.567866 \backslash \mathrm{H},-2.745477,2.555088,0.597462 \backslash \backslash$ Version=IA64L-G09 RevC.01 \State=1-A $\backslash H F=-8965.040424 \backslash$ RMSD $=9.046 e-09 \backslash$ RMSF $=7.354 \mathrm{e}-06 \backslash$ ZeroPo int $=0.4981898 \backslash$ Thermal $=0.5317166 \backslash$ Dipole $=-0.3218302,4.3972246,3.2970067 \backslash$ DipoleDeriv=-0.5608583,0.1461946,0.3699432,0.3063452,-1.4496057,-1.004 $3705,0.6288561,-0.8270582,-2.0048699,1.6923693,-0.2451868,-0.6499063,-$ $0.3866943,1.8842894,1.0722091,-0.7539885,0.765024,3.3404277,0.2147689$, $0.432432,-0.3892998,0.2745961,0.3210763,0.0060953,-0.3330672,-0.143856$ $4,0.1938153,0.2996946,-0.1927182,0.2140196,-0.0360471,-0.0933235,0.307$ $2536,0.2008771,0.1518222,0.0176344,0.3089772,-0.6351992,-0.5289877,-0$. $911661,2.3436651,1.9618686,-0.3703386,1.0356715,0.7033778,-0.9808061,0$ $.1545926,-0.2270249,0.1671017,-0.186017,-0.0048207,-0.286507,0.0147311$ $,-0.2461035,-0.661501,0.4042923,0.8050774,0.4620894,-1.1447436,-1.3164$ $611,0.436553,-0.7056359,-1.7306815,-0.4065194,-0.3738111,0.144175,-0.3$ 29281,-0.8328365,0.044606,0.1132603,0.1709542,-0.2255885,-0.2155204,0. $0383528,0.0022344,-0.0607399,-0.2850679,-0.0324003,0.2065103,0.222559$, $-0.0628039,-0.2966211,-0.1213348,-0.0534119,-0.0141024,-0.2465824,-0.0$ 87928,0.0933228,0.046811,-0.181812,-0.175418,0.1047009,0.1347072,0.112 $019,-0.0988842,0.2346928,-0.1007906,-0.0874796,0.000072,0.1024363,-0.1$ 088729,-0.0493414,-0.1116913, 0.0563158,-0.0965224,-0.0643295,-0.061223 $3,0.054895,0.8506354,0.8425535,-0.6367227,0.8412443,0.9813871,-0.75608$ $54,-0.7240328,-0.7990612,0.2520736,0.153451,-0.0475679,0.0393772,-0.04$ $25605,0.1503717,0.0203225,0.0517842,0.0306113,-0.0627572,0.4371709,0.5$ 018096,0.6112997,0.5589429,0.9268594,0.8096324,0.8218692,1.0426439,0.6 $836516,-1.1507952,-0.8362886,0.7512732,-0.8906159,-1.2883662,0.8063783$
, 0. $6844108,0.686464,-1.3637792,-0.7331297,-0.5045053,-0.4049442,-0.564$ $1628,-1.1265052,-0.691773,-0.5156652,-0.7849055,-1.6139295,0.2064448,0$ $.0347253,-0.0133933,0.0106967,0.1820484,0.0035345,-0.0193605,-0.022311$ $9,0.0298437,0.3589469,-0.0846754,-0.1101667,-0.0485648,0.351633,-0.041$ $1705,0.1277627,0.2429712,1.1527481,0.0258476,-0.1065481,-0.0680442,-0$. $1023531,-0.032281,-0.0990528,-0.0323576,-0.0521266,0.0069198,-0.139913$ , 0.078632, 0.1268923, 0.0411422,0.0828917,0.0326944,-0.0449318, -0.041348 $1,-0.0450894,0.0586492,0.0913662,0.0135601,0.0999328,-0.0904659,0.1536$ $823,-0.0273486,-0.0348073,-0.0553862,0.4364077,0.0000557,-0.1148391,-0$ $.0251048,0.3845107,-0.0660531,-0.4001513,-0.3839248,1.1945751,0.001537$ $4,-0.1192845,0.0627182,-0.1256323,-0.0421553,0.0695284,0.0239059,0.019$ $5124,0.0322783,0.0344627,0.0672992,0.0197338,0.131154,-0.0856864,-0.13$ $23978,0.0778016,0.0522406,-0.0679621,-0.1071563,0.0808519,-0.1455371,0$ $.038092,0.0730551,-0.0129037,0.0365623,0.0810413,-0.0811785,-0.1301134$ , 0.0313767, -0.0569583, 0.0112255, 0.0103113, -0.1119404, -0.0180242, 0.0514 531,-0.1430557,-0.0014894,0.1649287,0.1087747,-0.0497484,0.1057216,0.0 $219984,0.0926221,0.0201447,-0.1412191,0.1624538,-0.3146774,-0.0778035$, $-0.8691608,1.3747974,0.1247743,-0.0882081,0.1733921,-0.0589855,0.13132$ $3,-0.0606101,-0.0402643,-0.0791973,0.0341037,-0.0315585,-0.0447192,-0$. $0582183,0.153353,1.9537306,-0.2738822,0.7083833,-0.39345,-0.0368461,-0$ $.1981277,0.5797102,-0.1191264,0.3556593,-0.9928352,0.5635389,0.2213282$ , 0.6674991, -1.4682579,-0.1985557,0.3207867,-0.3160032,-0.7342436,-0.33 $44916,-0.1181713,-0.0821519,0.3374959,-0.055631,0.1709771,0.0287981,-0$ $.0258312,-0.2378717,-2.4286888,-0.1007698,-0.8628052,0.0377585,-0.6471$ $269,-0.036846,-0.7484197,-0.1087367,-0.6840688,0.0383278,-0.0688486,-0$ $.0749624,-0.0735033,0.0371601,-0.058898,-0.071219,-0.0548051,0.1647272$ , 0.093155, 0.1030109, 0.0085947,0.0902837, -0.101899, -0.0114834, -0.015381 $8,0.0091354,0.155628,0.8401543,0.2579393,0.2171887,0.6287022,0.6178794$ , 0. $2834406,0.2545106,0.1233104,0.5384835,-0.1172055,0.0280241,-0.07717$ $21,0.0903066,0.0347929,0.0167524,-0.0645014,-0.0033048,0.0821127,-0.00$ $91944,0.0472894,0.1150595,-0.1179427,-0.0037473,-0.1107443,0.0059096,-$ $0.0835879,-0.0993399,0.0404855,-0.0010901,-0.027943,-0.163408,-0.06124$ $84,0.020563,0.026893,0.1251001,-0.0797673,0.7044463,-0.2663132,-0.2522$ $9,-0.08409,0.3828587,0.115569,-0.3758884,0.3629201,0.7574923,0.044087$, $0.0842269,0.0342939,0.1163249,-0.1550426,-0.0164188,0.0346859,0.011636$ $4,0.0569125,-0.0903927,-0.0430135,0.055869,-0.1456413,0.0197374,0.0232$ $987,0.0045862,-0.0501232,0.033108,-0.0449657,0.029691,-0.1329338,0.023$ $0253,0.0768716,0.0430002,-0.0052497,-0.0583408,-0.1414762,-0.5077407,0$ $.6462103,0.3240492,0.7543273,-1.7281589,-1.1569064,0.1887877,-0.674127$ $5,-0.9585736,0.1948383,0.0331808,-0.0842398,0.0443358,0.1171214,-0.134$ $0116,-0.1157326,0.211683,0.7800221,0.5677443,-0.3552716,0.0008243,-0.0$ $896203,0.3077475,-0.0638468,0.1885292,-0.2307596,0.0168705,0.1866605,-$ $0.0506412,-0.0158577,-0.0900712,0.2803324,0.0600648,-0.043036,0.068618$ $2,0.1938934,0.1197453,0.0720247,0.0116872,0.0522849,0.1181054,0.010322$ $4,0.0087097,-0.0540987,-0.0190957,-0.0524684,0.1021164,-0.0638924,0.08$ $75252,0.0403889,0.0680249,-0.0256191,0.0316667,0.0194714,-0.0409579,-0$ $.1315715,0.0210733,-0.0798267,0.0299284,0.0355274,-0.0109991,-0.043448$ $5,0.0138663,0.1566742,0.0017838,-0.0453175,0.0682117,0.0723816,-0.0364$ $327,-0.0150979,-0.0073853,0.0922706,-0.1228731,-0.1013679,0.0016048,-0$ $.0982866,-0.0704573,-0.0167706,0.0560439,0.0498077,0.0750816,0.0595565$ $, 0.0337629,0.0364404,0.0293087,0.0251235,0.0235626,0.0073204,-0.004618$ $6,-0.2060463,0.0766002,0.1408468,0.027145,0.0633784,0.1033671,-0.01259$
$01,-0.015114,0.0005287,0.1026628,-0.1155525,-0.0874702,0.0340317,-0.15$ $75882,-0.0244874,0.0721791,0.0085116,0.0345744,0.0155206,0.0412371,0.0$ $730452,0.0241958,0.092287,-0.1497163,-0.1158863,0.0324152,-0.1044972$, -$0.017821,-0.0758568,-0.1602072,0.066394,-0.0868265,-0.0549388,0.018166$ $3,0.043856,-0.0023547,0.0141608,-0.0945785,0.127408,-0.0828073,0.08817$ $73,-0.0056803,-0.0016938,-0.0809731,0.0227871,-0.0248238,0.0350464,0.0$ $18858,0.0595856,-0.0013299,0.0991129,0.0087452,0.0023713,0.0131995,-0$. $0879824,-0.040423,-0.0272222,-0.0025163,-0.0969114,-0.0601882,0.015187$ , 0.0225282, 0.0700903, 0.0927035 \Polar=517.5480418, 22.4870405,513.351598 $8,-1.0506678,31.0321576,513.842784 \backslash \mathrm{PG}=\mathrm{C01} \quad[\mathrm{X}(\mathrm{C} 23 \mathrm{H} 30 \mathrm{Br} 3 \mathrm{~N} 104)] \backslash \mathrm{NImag}=1 \backslash \backslash$

Pyrrolidine $+1,1,1$-tribromo-2,2-bis(3,4-dimethoxyphenyl)ethane

| 1 | 2 | 3 |
| :--- | :--- | :--- |
| A | A | A |

Frequencies -- -1083.6209
19.5317 24.9863

Sum of electronic and zero-point Energies= Sum of electronic and thermal Energies= Sum of electronic and thermal Enthalpies= Sum of electronic and thermal Free Energies=
$-8925.270609$
$-8925.238129$
$-8925.237185$
$-8925.337777$
$1 \backslash 1 \backslash G I N C-D M C 134 \backslash$ Freq $\backslash$ RM0 62X $\backslash 6-31+G(d, p) \backslash C 22 H 28 B r 3 N 104 \backslash A U B C R A \backslash 12-J u l-20$ $12 \backslash 0 \backslash \$ freq=noraman $M 062 X / 6-31+g(d, p)$ scrf=(cpcm,solvent=methanol) <br>T itle Card Required $\backslash \backslash 0,1 \backslash C, 0.028638,0.362901,0.186098 \backslash C, 0.059612,1.2115$ $82,-0.980964 \backslash C,-1.098832,-0.622861,0.325048 \backslash C, 1.365529,-0.235783,0.546$ $254 \backslash \mathrm{H},-0.33562,1.403911,1.166785 \backslash \mathrm{Br},-1.638645,2.067928,-1.396772 \backslash \mathrm{Br}, 0$. $613215,0.24837,-2.817515 \backslash \mathrm{Br}, 1.387587,2.633616,-0.871136 \backslash \mathrm{C},-1.410029,-1$ $.092309,1.600293 \backslash C,-1.843656,-1.117619,-0.759069 \backslash C,-2.458335,-1.99388$, $1.807428 \backslash \mathrm{H},-0.830025,-0.754849,2.456326 \backslash \mathrm{C},-3.214551,-2.452525,0.734048$ $\backslash H,-2.677205,-2.326955,2.815231 \backslash C,-2.89008,-2.009565,-0.566521 \backslash 0,-4.25$ $8977,-3.3187,0.82765 \backslash 0,-3.652715,-2.515758,-1.573257 \backslash \mathrm{H},-1.589138,-0.81$ $5158,-1.765037 \backslash \mathrm{C},-3.349385,-2.089488,-2.893072 \backslash \mathrm{H},-4.068159,-2.587916,-$ $3.541777 \backslash \mathrm{H},-2.332107,-2.382,-3.177031 \backslash \mathrm{H},-3.456207,-1.003064,-2.990635 \backslash$ $\mathrm{C},-4.588301,-3.796615,2.122279 \backslash \mathrm{H},-5.428015,-4.476682,1.986816 \backslash \mathrm{H},-4.885$ $074,-2.97354,2.781554 \backslash \mathrm{H},-3.74599,-4.337263,2.567524 \backslash \mathrm{C}, 1.726004,-1.4819$ $15,0.009694 \backslash C, 2.27504,0.396128,1.390567 \backslash C, 2.951469,-2.059705,0.290862 \backslash$ $\mathrm{H}, 1.044457,-2.01233,-0.65087 \backslash \mathrm{C}, 3.867577,-1.40609,1.139584 \backslash 0,3.268505$, -$3.288807,-0.235805 \backslash C, 3.515,-0.175238,1.691273 \backslash 0,5.04103,-2.051436,1.36$ $2096 \backslash \mathrm{H}, 4.192181,0.348771,2.35506 \backslash \mathrm{H}, 2.034753,1.365234,1.817226 \backslash \mathrm{C}, 5.9841$ $26,-1.416353,2.213364 \backslash H, 6.844354,-2.082261,2.257582 \backslash \mathrm{H}, 5.572619,-1.2790$ $17,3.218772 \backslash \mathrm{H}, 6.289778,-0.44721,1.804917 \backslash \mathrm{C}, 4.12348,-3.199731,-1.37706 \backslash$ $H, 4.337563,-4.221972,-1.689939 \backslash H, 5.056356,-2.687912,-1.120431 \backslash H, 3.6154$ $69,-2.663688,-2.186761 \backslash N,-0.739974,2.285392,1.960315 \backslash \mathrm{C},-0.154049,2.148$ $782,3.329989 \backslash C,-2.239396,2.230296,2.080826 \backslash \mathrm{H},-0.452761,3.172823,1.5482$ $02 \backslash \mathrm{C},-1.300207,2.497446,4.273901 \backslash \mathrm{H}, 0.722992,2.790978,3.422656 \backslash \mathrm{H}, 0.1603$ $1,1.107869,3.461853 \backslash \mathrm{H},-1.405629,3.584994,4.350399 \backslash \mathrm{H},-1.147333,2.090588$ , 5. $27526 \backslash \mathrm{C},-2.50593,1.894251,3.549673 \backslash \mathrm{H},-3.462108,2.297617,3.887845 \backslash \mathrm{H}$, $-2.523431,0.807623,3.689276 \backslash \mathrm{H},-2.648868,3.204931,1.805957 \backslash \mathrm{H},-2.62391,1$ $.479092,1.38841 \backslash$ Version=EM64L-G09RevC. $01 \backslash$ State=1-A $\backslash H F=-8925.7394146 \backslash R$ $M S D=5.022 e-09 \backslash \operatorname{RMSF}=3.611 e-06 \backslash$ ZeroPoint $=0.4688053 \backslash$ Thermal=0. $5012852 \backslash \mathrm{Dip}$ ole $=-0.306092,2.6945792,4.5588692 \backslash$ DipoleDeriv=-0.6093216, -0.0464148, 0. $401562,-0.0072973,-0.8444708,-0.5772425,0.698849,-0.3567605,-2.5330311$
,1.6750955,-0.0082076,-0.5452718,-0.0572702,1.4731772,0.393543,-0.8889 $905,0.0474468,3.8425906,0.35935,0.5183669,-0.2072748,0.3722418,0.19929$ $3,0.093191,-0.2550823,-0.0581645,0.1880838,0.2329306,-0.3203647,0.1501$ $187,-0.1522957,-0.1740576,0.1647691,0.2042365,0.0091584,0.1196309,0.34$ $41859,-0.4549016,-0.8595757,-0.7376355,1.0690598,2.1475893,-0.6334557$, $1.0046484,1.7604029,-0.8830612,0.3659089,-0.0810409,0.3908086,-0.32920$ $59,0.0311937,-0.1360379,0.0433109,-0.2205825,-0.5579813,0.057081,0.622$ $5142,0.2526956,-0.5667884,-0.9800189,0.5213581,-0.2753531,-2.4260375,-$ $0.5793252,-0.441748,-0.020491,-0.4065679,-0.6497477,-0.1626339,-0.0123$ $786,-0.0533159,-0.2282163,-0.2363725,0.0270838,-0.0392896,-0.1385732,-$ $0.3140268,-0.0807712,0.200261,0.1277432,-0.02835,-0.3138777,-0.0744991$ , -0.094968, -0.0373413, -0.223986, -0.0798775, 0.090498, 0.009727, -0. 193814 $7,-0.1126698,0.0603781,0.1978329,0.1327333,-0.1879427,0.1476131,-0.088$ $4963,-0.1250538,0.0373451,0.0760585,-0.0928153,-0.0914748,-0.0870434,0$ $.1271635,-0.0916623,-0.1044164,-0.043925,-0.0092147,1.2903648,1.034765$ $7,-0.3948488,1.0479243,0.9491404,-0.2917758,-0.4880804,-0.3262755,-0.1$ $596159,0.1243371,-0.0634137,0.0410913,-0.0555179,0.1439998,0.0692166,0$ $.0559419,0.0772548,-0.0261516,0.5304734,0.2516097,0.8588553,0.2328496$, $0.248877,0.5275037,1.1194767,0.7334907,1.2806467,-1.6094697,-1.0801113$ , 0. $5789006,-1.089243,-1.2918988,0.5594329,0.4721309,0.459337,-0.903681$ , -0. $8689122,-0.3305787,-0.6037781,-0.338192,-0.5894848,-0.2913127,-0.7$ $341566,-0.36794,-2.0179879,0.2163303,0.0306593,0.0115305,0.0086554,0.1$ $712925,0.0526087,-0.0145164,0.0193428,0.0441042,0.3403325,-0.0407488$, -$0.1969515,-0.0786102,0.3867863,-0.2565653,0.0932089,-0.0249977,1.14078$ $58,-0.0054073,-0.0724151,-0.1148243,-0.0817228,0.0516097,-0.0756635,-0$ $.0693949,-0.0350274,-0.0427027,-0.116315,0.0756873,0.1506579,0.0912454$ , 0.0483302, 0.0417687, -0.0329732, 0.0021849, -0.0333452, 0.082297, 0.036834 $8,0.0652107,0.0573702,-0.1529639,0.1185331,-0.0080439,-0.0547633,-0.02$ $55882,0.4822232,0.0722964,-0.1751634,0.12858,0.553861,-0.2268319,-0.50$ $67475,-0.4830221,0.9739179,-0.0533841,-0.1339853,0.0300711,-0.1295024$, $-0.004878,0.0328574,-0.0207486,-0.0105753,0.0527982,0.0575002,0.028873$ $4,0.0164424,0.0781093,-0.0891027,-0.1340361,0.1265159,0.0328159,-0.087$ $1557,-0.0697787,0.1413363,-0.1061914,0.0479782,0.0061354,0.0467867,0.0$ $694817,0.1109434,-0.0496469,-0.1087242,0.0503609,-0.0226154,0.0267607$, $-0.0055645,-0.047665,-0.0016942,0.1214611,-0.1457244,-0.0084013,0.1276$ $796,0.1585383,-0.0703115,0.040451,0.088856,0.0720828,0.0916696,-0.0814$ $249,0.0251022,-0.1108763,-0.11996,-0.634469,1.1709272,0.6109888,-0.337$ $561,0.6957129,0.2609031,0.1106437,-0.0477629,-0.0723392,-0.0607137,0.1$ $058124,-0.052466,-0.0802831,-0.0770663,0.103509,1.7558719,-0.7475322,0$ $.5070817,-0.7970395,0.3127442,-0.3510608,0.3785674,-0.2714061,0.195912$ $6,-0.8711544,0.3955726,0.3717635,0.4565195,-1.2961791,-0.4404444,0.475$ $9828,-0.5653986,-1.0344602,-0.2905862,-0.0529436,-0.0792293,0.3035593$, $-0.1687399,0.2143631,0.1621288,0.0031014,-0.1551311,-2.302504,0.474775$ $2,-0.8346977,0.566939,-0.7061135,0.1147225,-0.6980863,0.0251251,-0.746$ $2876,0.0321219,-0.0216334,-0.1077226,-0.0298093,0.1074806,-0.0751175,-$ $0.1024128,-0.068055,0.1016908,0.1083619,0.0613092,0.0209301,0.0621846$, $-0.0540865,-0.0809973,-0.0054053,-0.0611616,0.1352297,0.9158566,0.0854$ $539,0.3357891,0.4098069,0.3840584,0.2041195,0.4925345,0.0234793,0.7047$ $666,-0.0924843,0.075011,-0.0638962,0.1252853,0.0121214,0.0097389,-0.02$ $83457,-0.0174801,0.079735,-0.0206919,0.008764,0.1222472,-0.0984429,0.0$ $650368,-0.0653349,-0.0409726,-0.0144457,-0.1556968,0.014657,-0.007686$, $-0.0262826,-0.1791061,-0.0955811,0.0097551,-0.0270397,0.1119783,-0.025$
$8703,0.6820411,-0.2039689,-0.3421839,0.0100752,0.2952354,-0.0398179,-0$ $.3503617,0.2075357,0.8797696,0.0591559,0.0460636,0.0522014,0.0722943,-$ $0.1409244,-0.0970506,0.0670633,-0.0679766,0.0235751,-0.1090358,-0.0465$ $218,0.0367454,-0.1215926,0.0464088,0.0162195,-0.0565077,-0.050924,0.02$ $03429,-0.0300182,0.0860504,-0.0989537,0.0328396,0.0370844,0.1338055,0$. $0047973,0.0200889,-0.1192352,-0.7222464,0.3392632,0.5789689,0.4841574$, $-0.7859522,-1.2522936,0.4602525,-0.6252636,-1.6699472,0.1529787,0.0800$ $846,0.2578062,-0.0384759,0.2202888,-0.1662492,0.0735526,0.0276546,0.73$ $68456,0.6297247,-0.1184742,-0.26668,-0.0032184,0.2063567,-0.0719396,-0$ $.0451842,0.0095769,0.1506128,0.1678273,-0.0036821,-0.0196714,-0.010095$ $2,0.26784,0.0409497,-0.0489183,0.0429038,0.2021421,0.0186103,-0.035686$ $4,0.0014988,-0.0234055,0.1729688,0.0396061,0.0206079,-0.0497664,-0.002$ $387,-0.0734193,-0.0666837,-0.0422532,-0.1069301,0.0406866,-0.0060119,0$ $.0324275,0.0214596,0.0278636,0.0663091,0.0116328,-0.0288339,0.0795154$, $-0.119798,0.075289,-0.0058726,-0.0048778,0.0480976,0.0281617,0.023003$, $0.0189002,0.0131016,-0.1760322,-0.0604733,0.0005814,0.0074903,0.061097$ , 0.0673129, 0.0193794, -0.0249438, 0.0166892, 0.0606223, 0.0784545, -0.01817 $3,0.0177295,-0.1648746,0.0442254,-0.0287848,0.0249665,0.028074,0.13167$ 55,-0.055103, 0.0119429,-0.006026, -0.0113197,-0.1175345,0.0486534,0.084 $083,0.0667515,0.0644045,-0.0338035,0.0552828,-0.023935,0.0337522,0.058$ $7973,0.0108183,-0.0387672,-0.0422457,-0.149537,0.0508013,-0.0089135,0$. $0276771,0.0559565,-0.0232978,0.0400227,0.0517631,0.0710799,-0.1063892$, $0.0688229,-0.0128956,0.0368613,0.0363917,0.0367358,-0.0323391,-0.02789$ $68,-0.0541568,0.0525226,-0.0388793,-0.0976167,-0.0499525,-0.0010184 \backslash \mathrm{Po}$ lar $=517.1931203,18.4229737,455.3423559,5.4775668,19.806714,522.3877614$ $\backslash \mathrm{PG}=\mathrm{C01}[\mathrm{X}(\mathrm{C} 22 \mathrm{H} 28 \mathrm{Br} 3 \mathrm{~N} 104)] \backslash \mathrm{NImag}=1 \backslash \backslash$

## Gaussian 09 Reference

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