Comparison of the mesomorphic behaviour of 1:1 and 1:2 mixtures of charged Gay-Berne GB(4.4,20.0,1,1) and Lennard-Jones particles

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Supporting Information

In the following pages we report the radial distribution functions of the systems investigated. Stoichiometry, density, packing fraction, charge and temperature are indicated in each panel.
GB:LJ = 1:1, $\rho^* = 0.261$, $\eta^* = 0.371$

$q^* = 0.0/0.0$

\begin{align*}
T^* &= 0.80 \\
T^* &= 1.10 \\
T^* &= 1.20 \\
T^* &= 1.50
\end{align*}
GB:LJ = 1:1, $\rho^* = 0.261$, $\eta^* = 0.371$

$q^* = +0.50/−0.50$

![GB:LJ plots](attachment:gb_lj_plot.png)
GB:LJ = 1:1, $\rho^* = 0.261, \eta^* = 0.371$

$q^* = +2.0/ -2.0$

$T^* = 0.50$

$T^* = 0.60$

$T^* = 0.65$
**GB:LJ = 1:1, \( \rho^* = 0.303, \eta^* = 0.428 \)**

\[ q^* = 0.0 / 0.0 \]

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**T* = 0.70**

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**T* = 1.50**

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**T* = 1.80**

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**T* = 2.00**
GB: LJ = 1:1, $\rho^* = 0.303$, $\eta^* = 0.428$

$q^* = 0.5/−0.5$

### $T^* = 0.70$

### $T^* = 1.00$

### $T^* = 1.20$

### $T^* = 1.30$
**GB:LJ = 1:1, \( \rho^* = 0.303, \eta^* = 0.428 \)**

\( q^* = 2.0/ -2.0 \)

![Graphs showing \( g(r) \) for different temperatures.](image)
GB:LJ = 1:1, ρ* = 0.363, η* = 0.514
q* = 0.0/−0.0
GB:LJ = 1:1, $\rho^* = 0.363$, $\eta^* = 0.514$

$q^* = 0.5/ -0.5$

\begin{center}
\begin{tabular}{cc}
\multicolumn{1}{c}{$T^* = 1.00$} & \multicolumn{1}{c}{$T^* = 3.00$} \\
\includegraphics[width=0.4\textwidth]{g1.png} & \includegraphics[width=0.4\textwidth]{g3.png} \\
\multicolumn{1}{c}{$T^* = 4.00$} & \multicolumn{1}{c}{$T^* = 5.00$} \\
\includegraphics[width=0.4\textwidth]{g4.png} & \includegraphics[width=0.4\textwidth]{g5.png}
\end{tabular}
\end{center}
**GB: LJ = 1:1, ρ* = 0.363, η* = 0.514**

q* = 2.0/−2.0

![Graphs showing g(r) for different temperatures](image-url)
GB: LJ = 1:2, \( \rho^* = 0.332, \eta^* = 0.371 \)

\( q^* = 0.0/ -0.0 \)
GB:LJ = 1:2, ρ* = 0.332, η* = 0.371

q* = 0.5/−0.25

T* = 0.60

T* = 0.70

T* = 0.90
**GB:LJ = 1:2**, $\rho^* = 0.332$, $\eta^* = 0.371$

$q^* = \frac{1.0}{-0.5}$
**GB:LJ = 1:2, \( \rho^* = 0.383, \eta^* = 0.428 \)**

\( q^* = 0.0/−0.0 \)

![Graphs showing g(r) for different temperatures (T* = 1.00, 1.20, 1.70, 2.20).](image-url)
**GB:LJ = 1:2**, \( \rho^* = 0.383, \eta^* = 0.428 \)

\( q^* = 0.50/ -0.25 \)

T* = 0.70

T* = 0.90

T* = 1.00

T* = 1.20
GB:LJ = 1:2, \( \rho^* = 0.383, \eta^* = 0.428 \)

\( q^* = 1.00/ -0.50 \)
**GB:LJ = 1:2, ρ* = 0.383, η* = 0.428**

q* = 2.00/−1.00

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**T* = 0.40**

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**T* = 0.60**

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**T* = 0.80**

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**T* = 1.00**
GB:LJ = 1:2, $\rho^* = 0.460$, $\eta^* = 0.514$

$q^* = 0.0/ -0.0$

$T^* = 2.00$

$T^* = 2.50$

$T^* = 4.00$

$T^* = 4.50$
GB:LJ = 1:2, \( \rho^* = 0.460, \eta^* = 0.514 \)

\( q^* = 0.50/ -0.25 \)
GB:LJ = 1:2, \( \rho^* = 0.460 \), \( \eta^* = 0.514 \)

\[ q^* = 1.00 \text{/} -0.50 \]
**GB:LJ = 1:2**, $\rho^* = 0.460$, $\eta^* = 0.514$

$q^* = 2.00/ -1.00$

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![Graph](image1)

$T^* = 0.40$

![Graph](image2)

$T^* = 0.80$