Entropy from State Probabilities: Hydration Entropy of Cations

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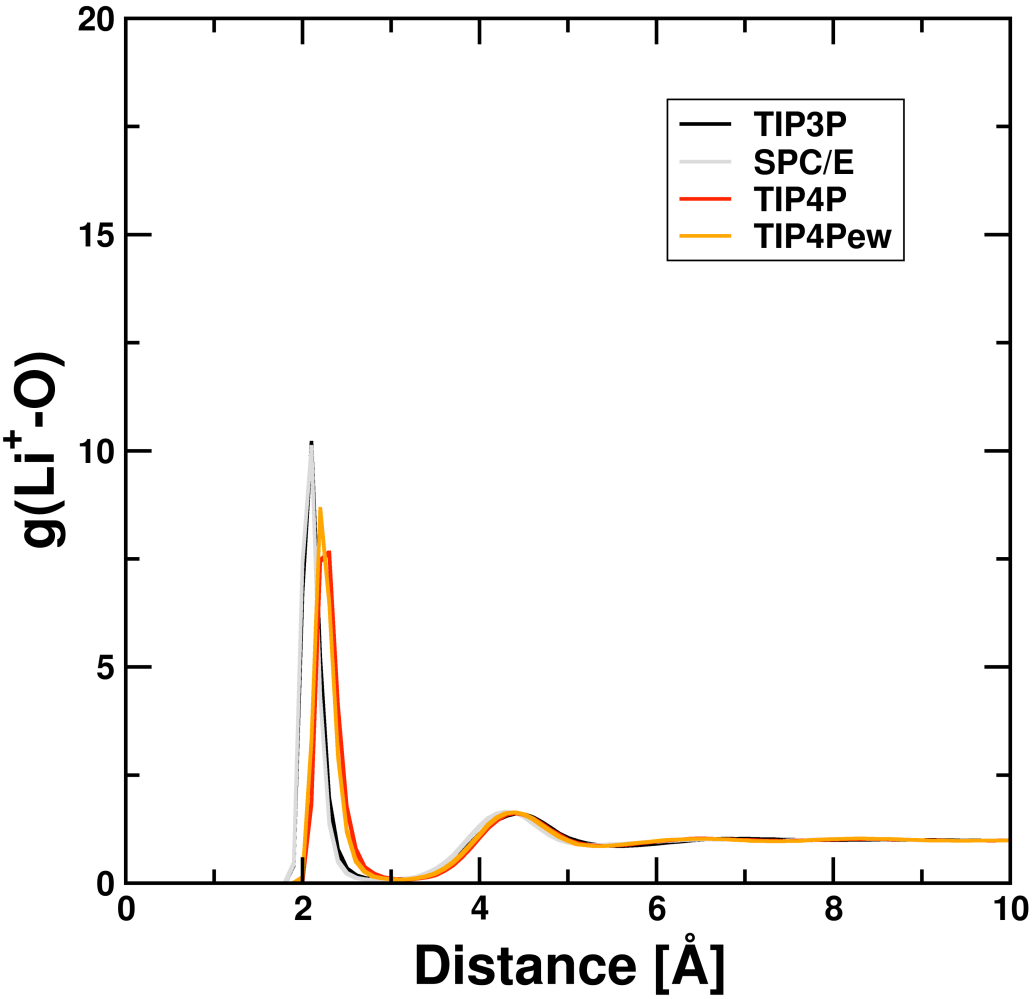
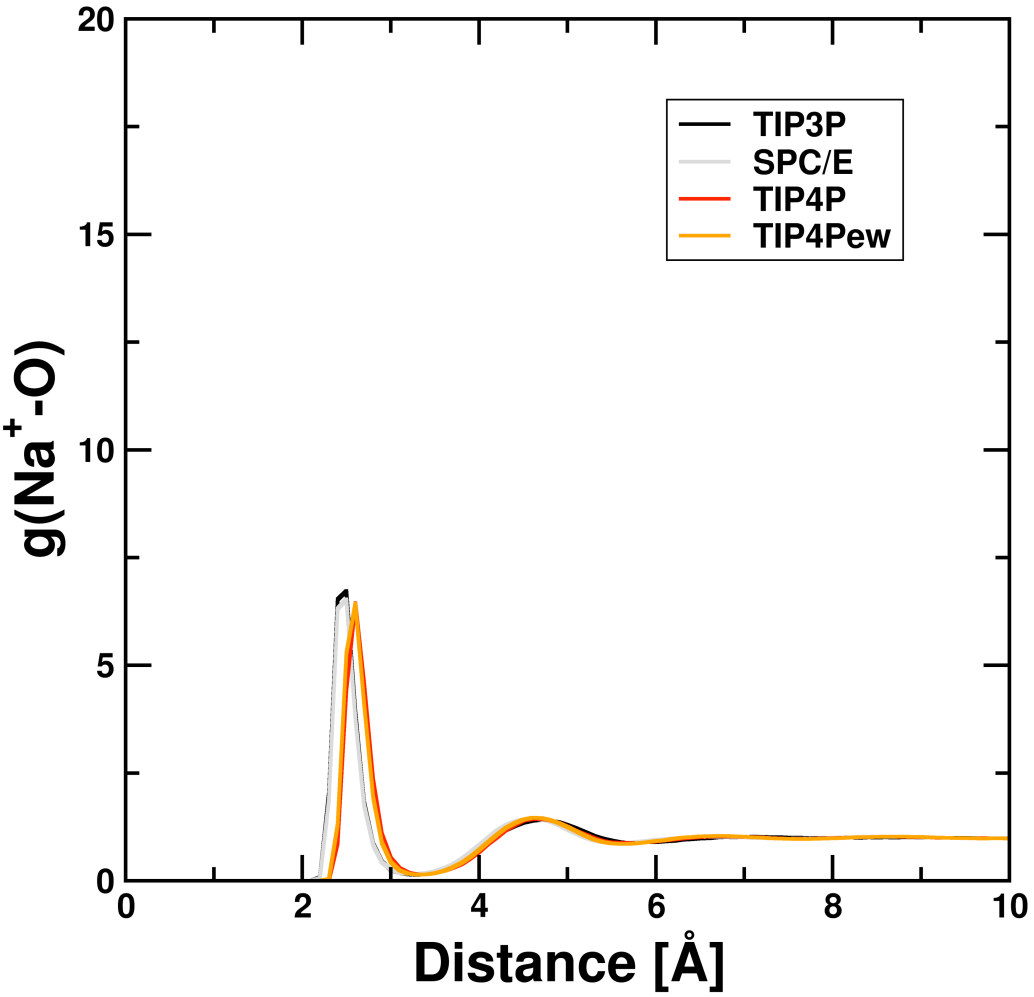
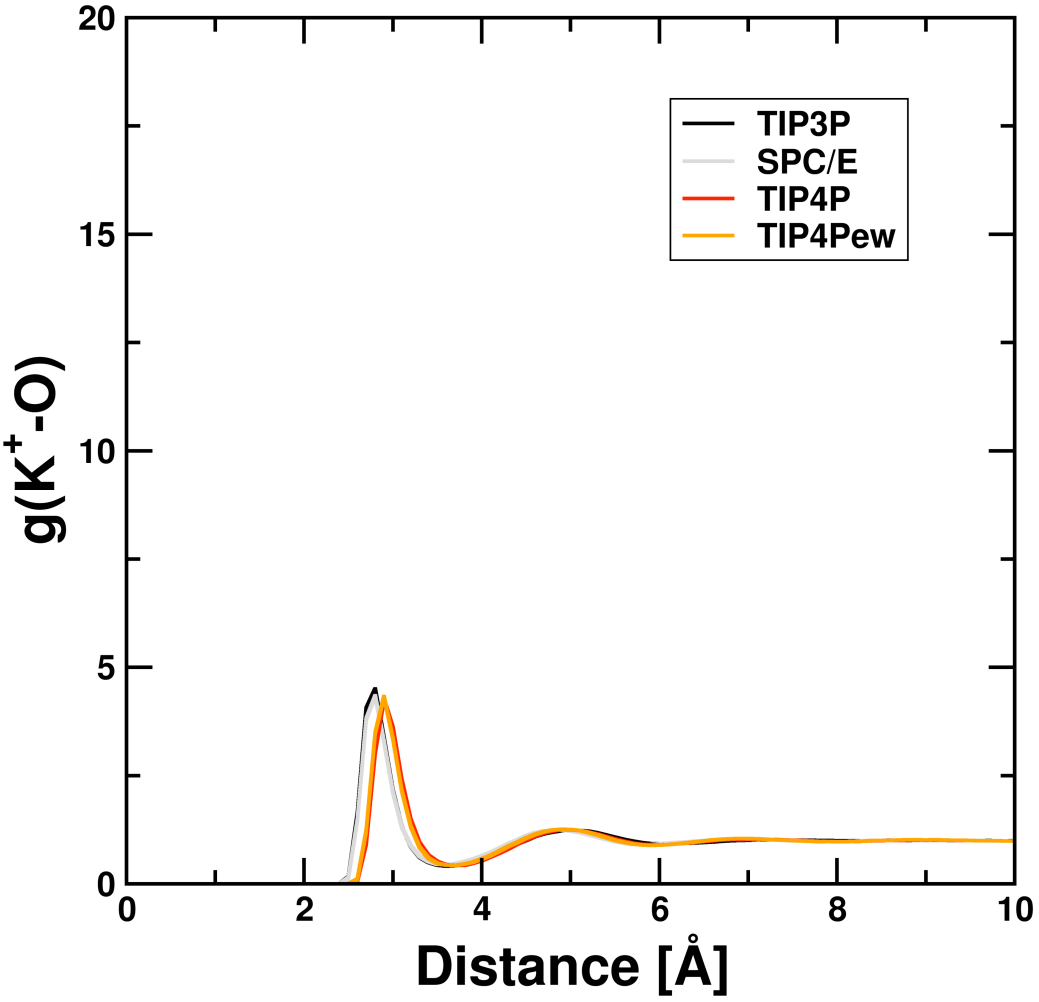
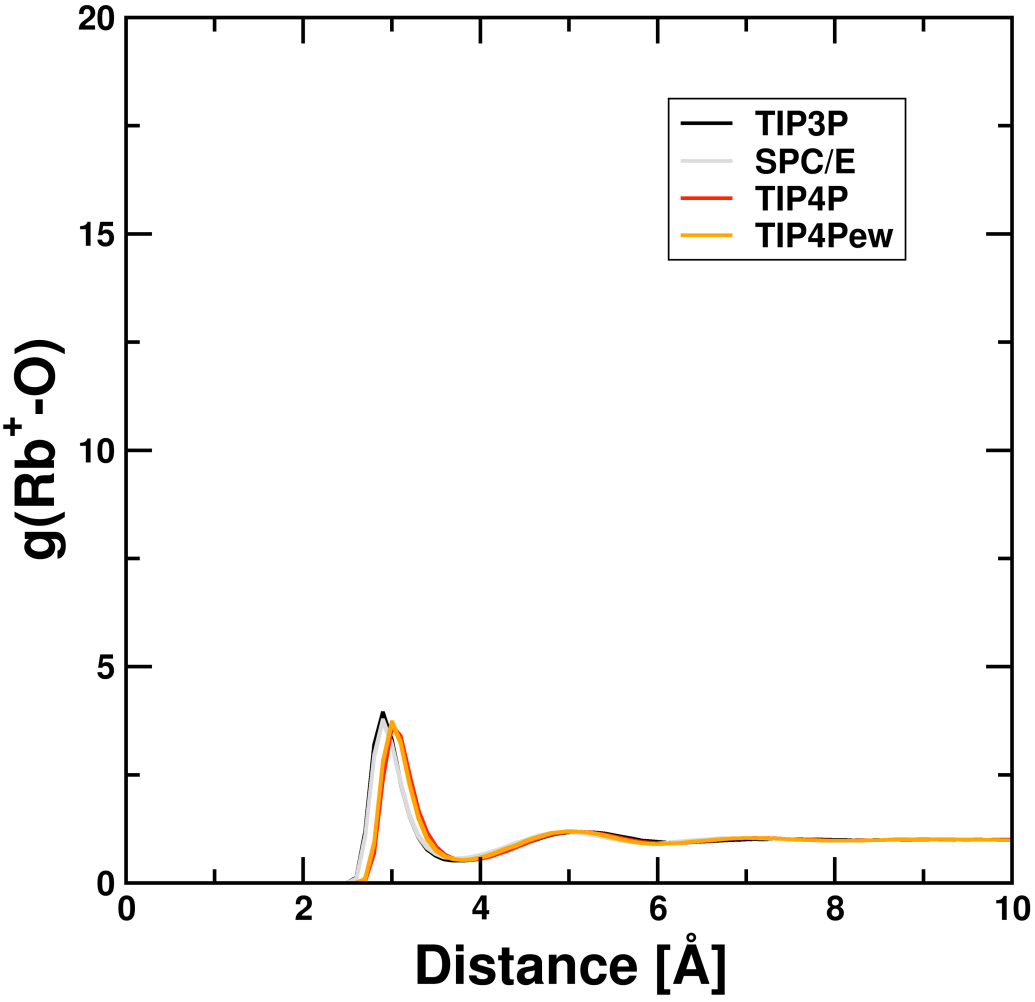
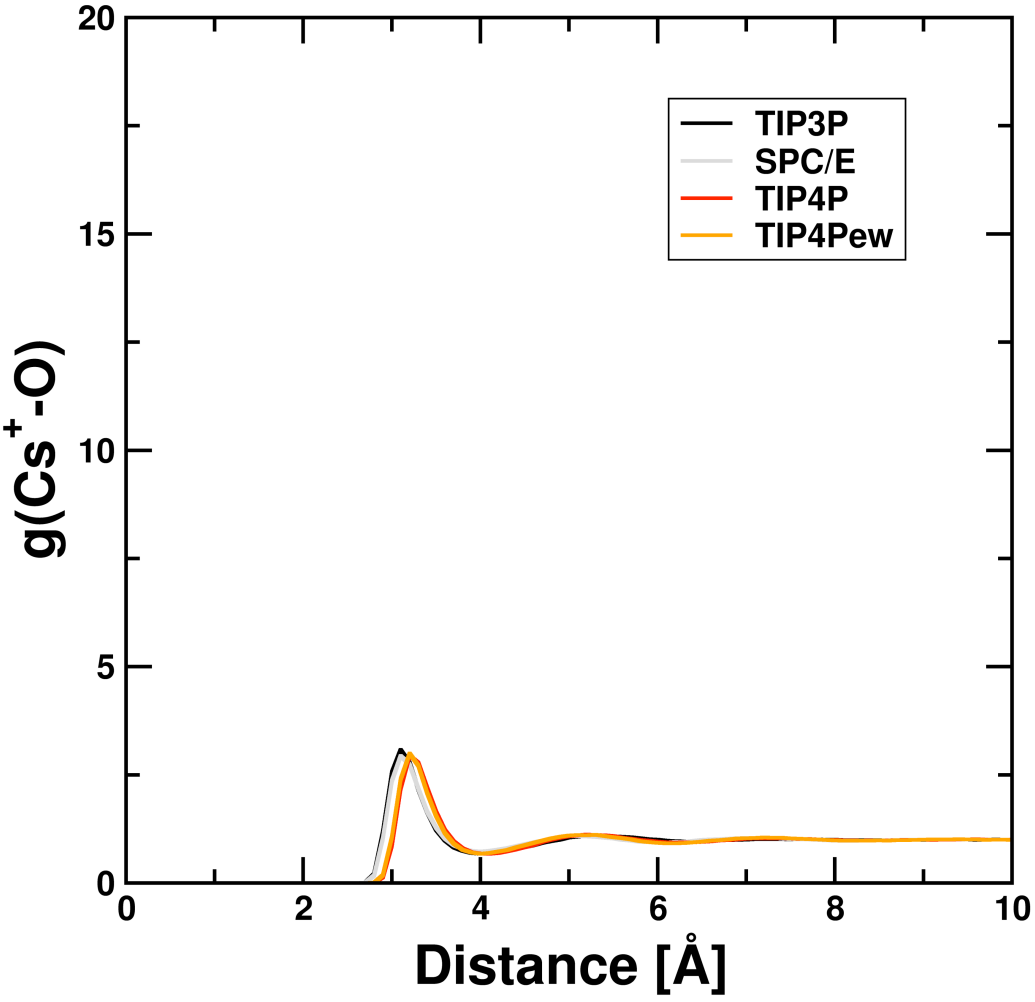
1. Radial Distribution Functions

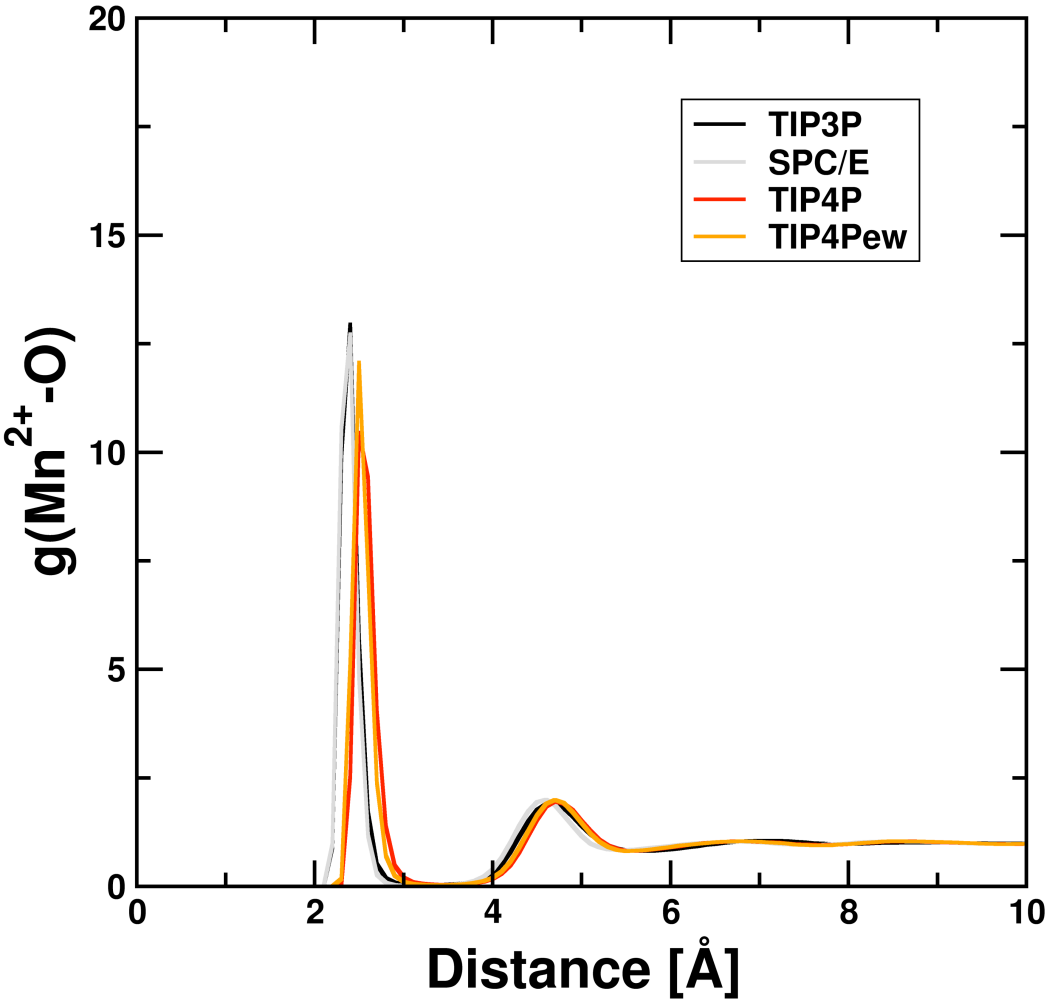


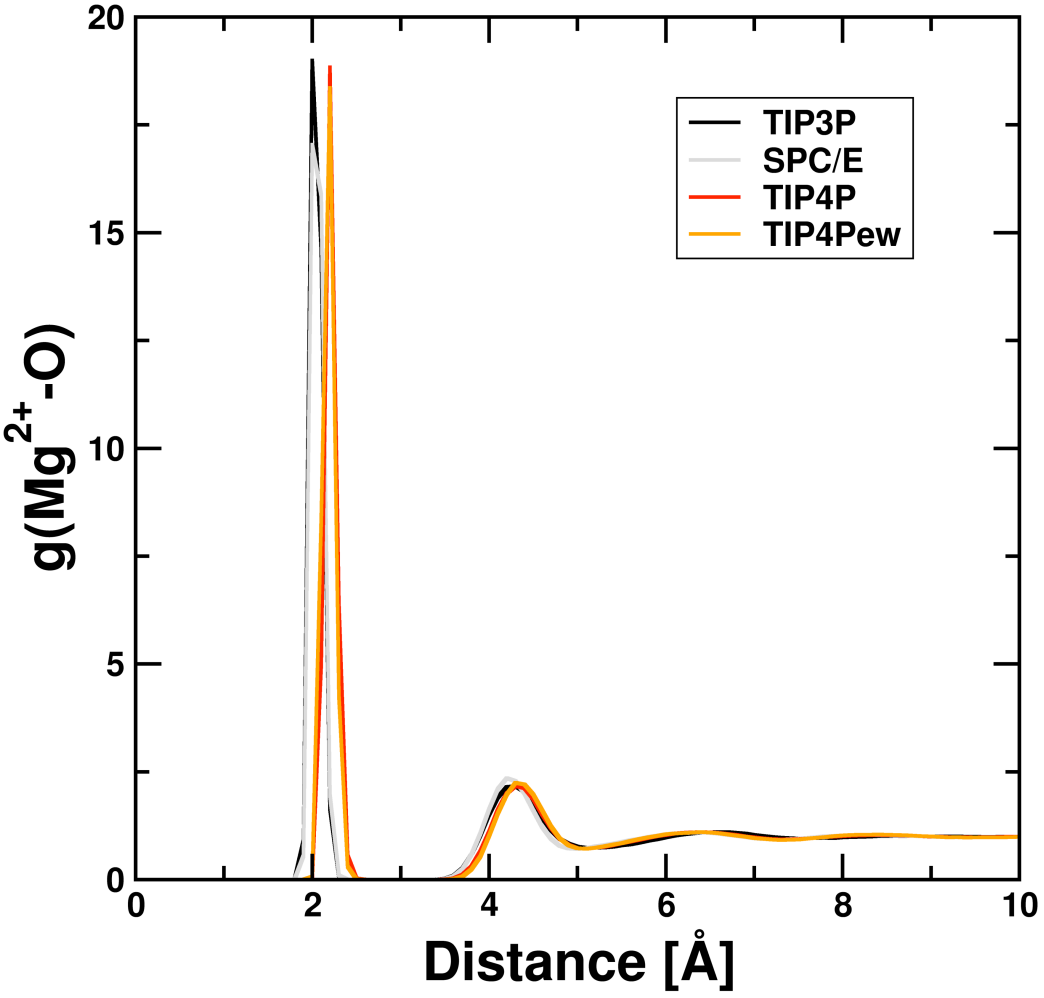

20
15
10
5
0
0
2
4
6
8
10
g(Na+-O)
Distance [Å]
TIP3P
SPC/E
TIP4P
TIP4Pew

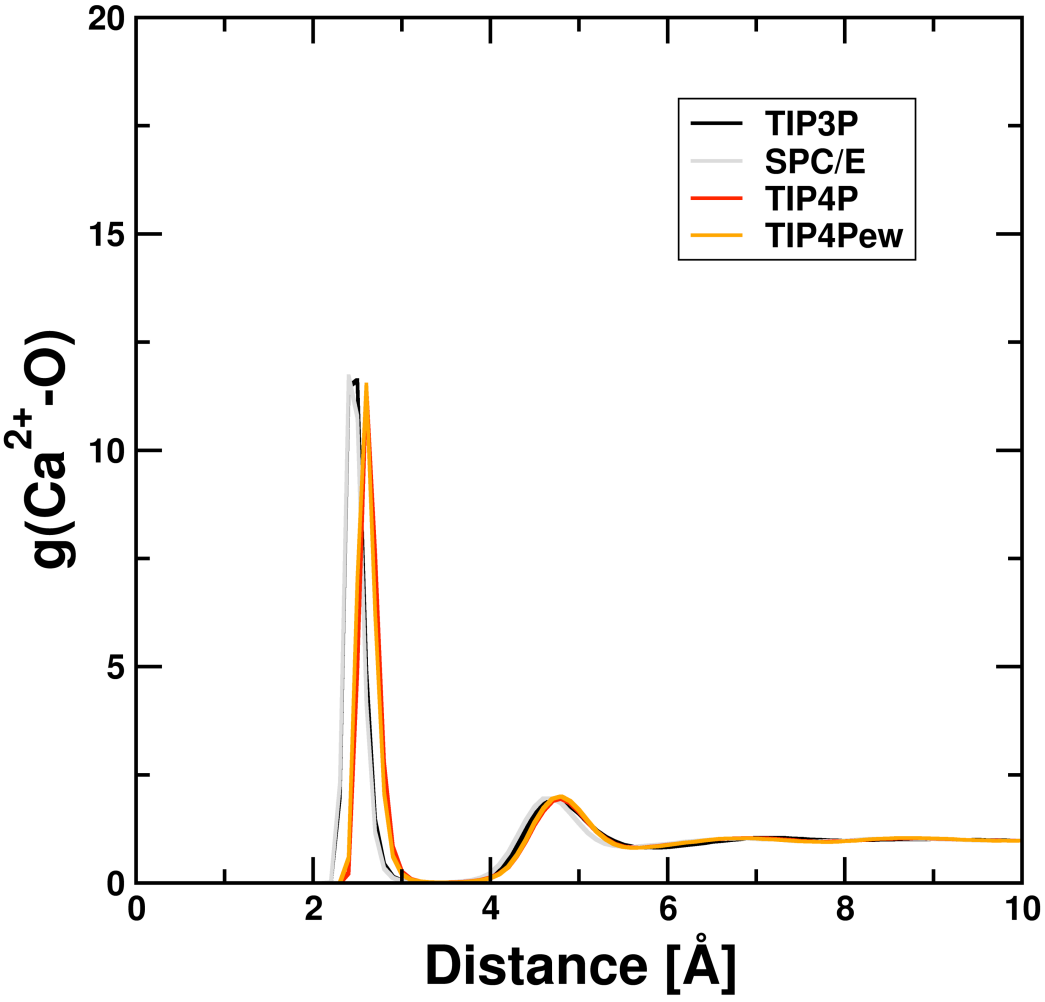

20
15
10
5
0
0
2
4
6
8
10
g(K+-O)
Distance [Å]
TIP3P
SPC/E
TIP4P
TIP4Pew


20
15
10
5
0
0
2
4
6
8
10
g(Rb+-O)
Distance [Å]
TIP3P
SPC/E
TIP4P
TIP4Pew


20
15
10
5
0
0
2
4
6
8
10
g(Cs+-O)
Distance [Å]
TIP3P
SPC/E
TIP4P
TIP4Pew

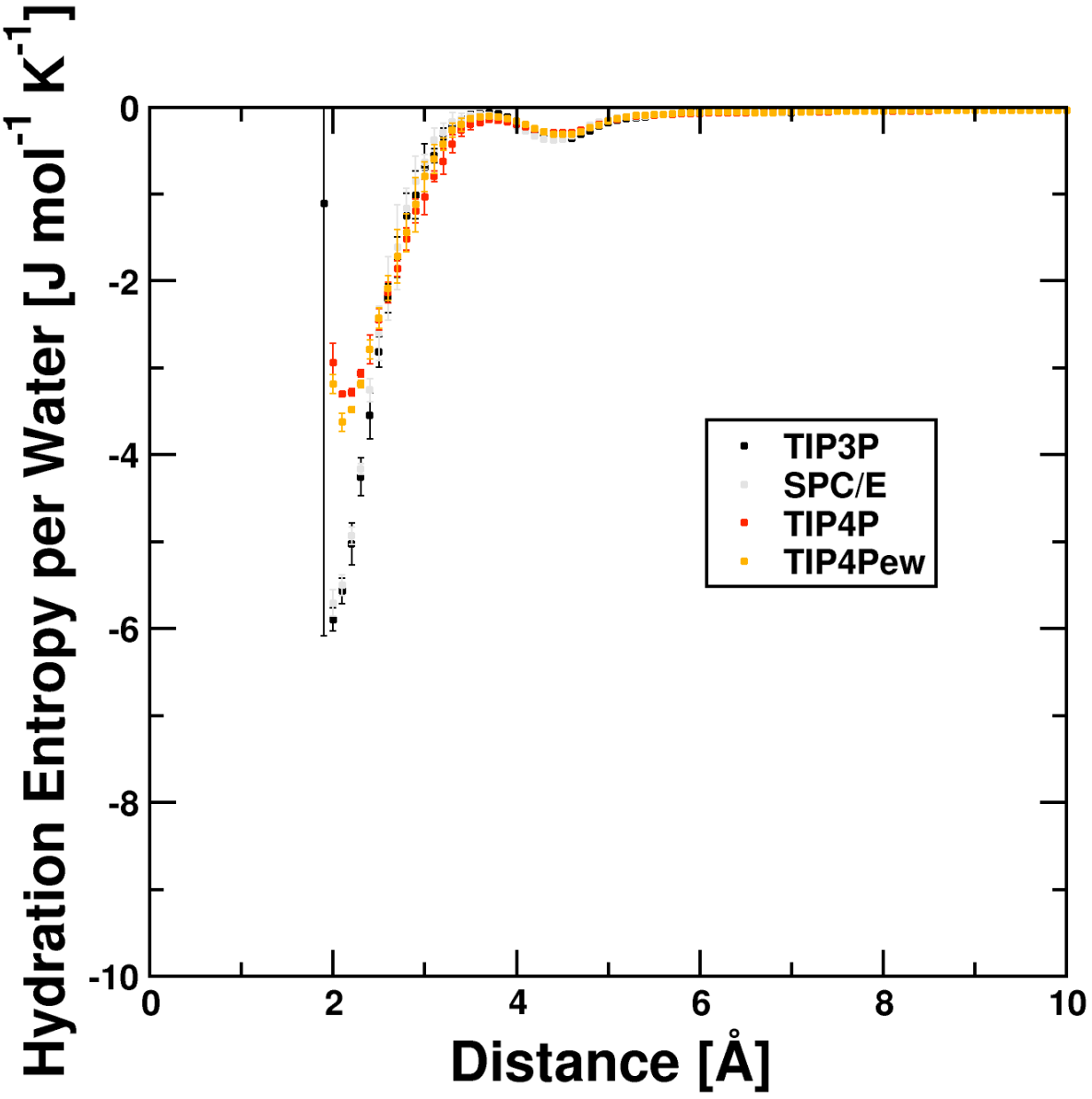

TIP3P
SPC/E
TIP4P
TIP4Pew
g(Mn2+-O)
Distance [Å]
0
5
10
15
20
0
2
4
6
8
10


20
15
10
5
0
0
2
4
6
8
10
g(Mg2+-O)
Distance [Å]
TIP3P
SPC/E
TIP4P
TIP4Pew

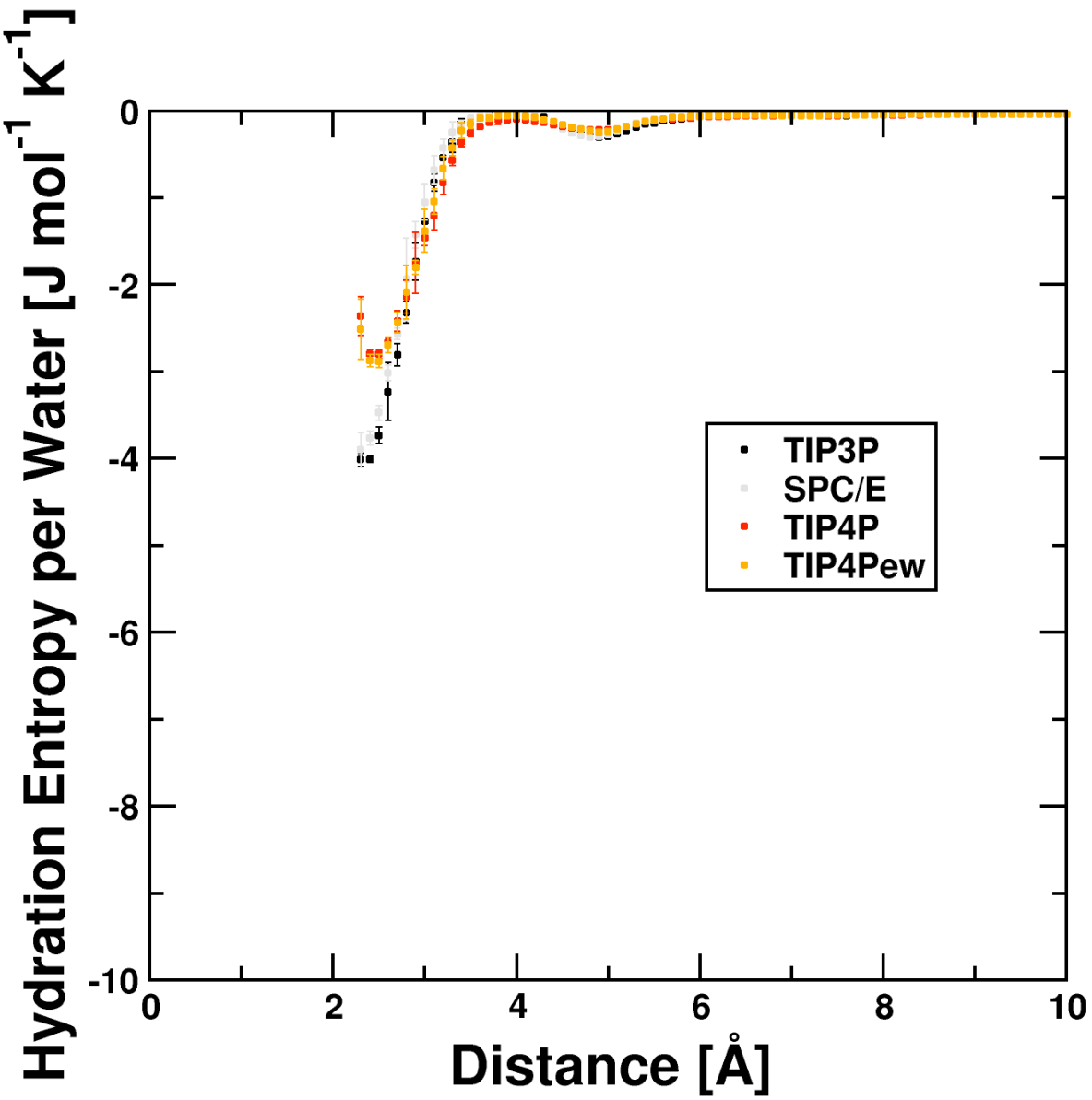

TIP3P
SPC/E
TIP4P
TIP4Pew
g(Ca2+-O)
Distance [Å]
0
5
10
15
20
0
2
4
6
8
10

2. Distance-Dependent Entropy

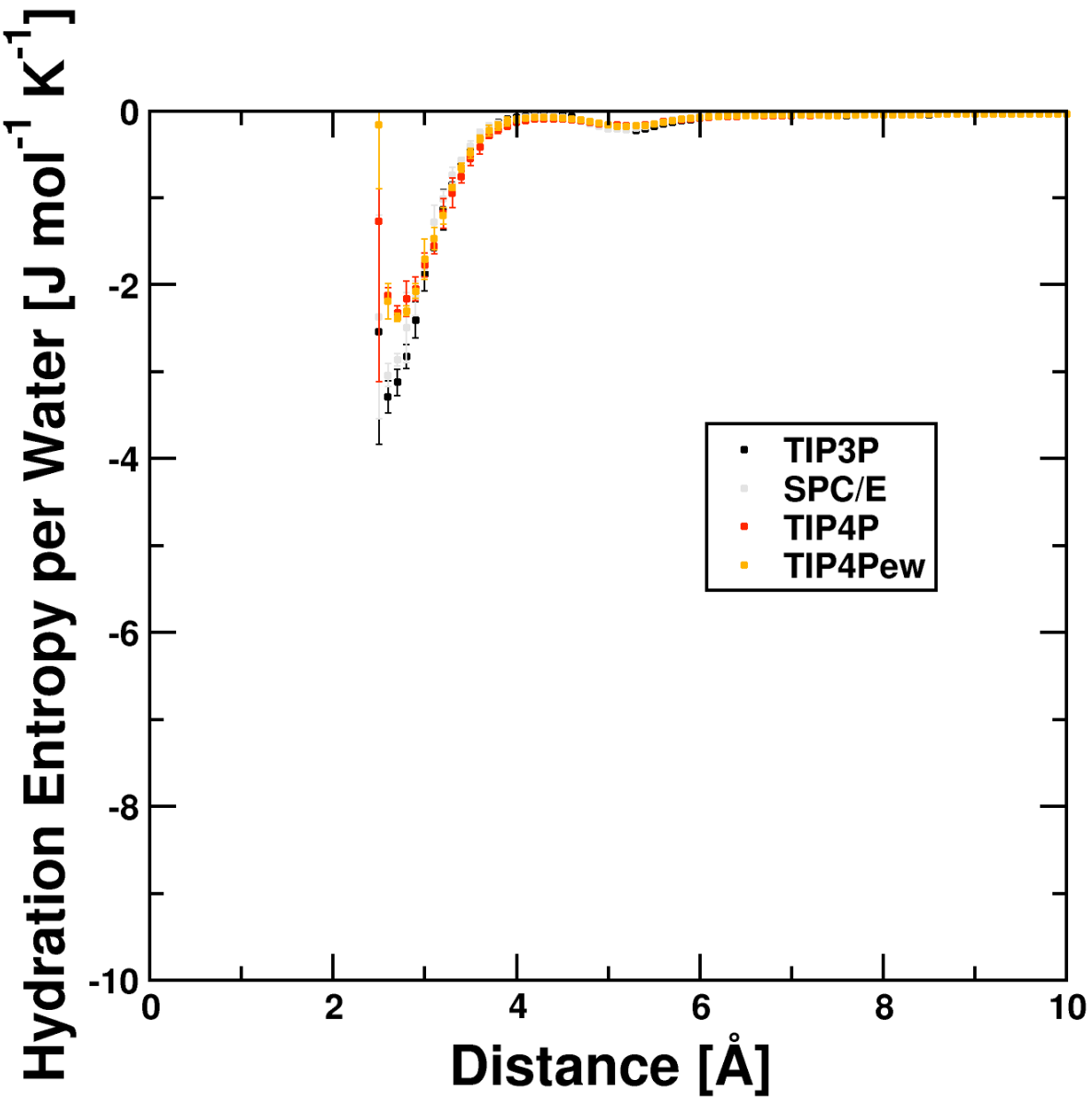
Li^+



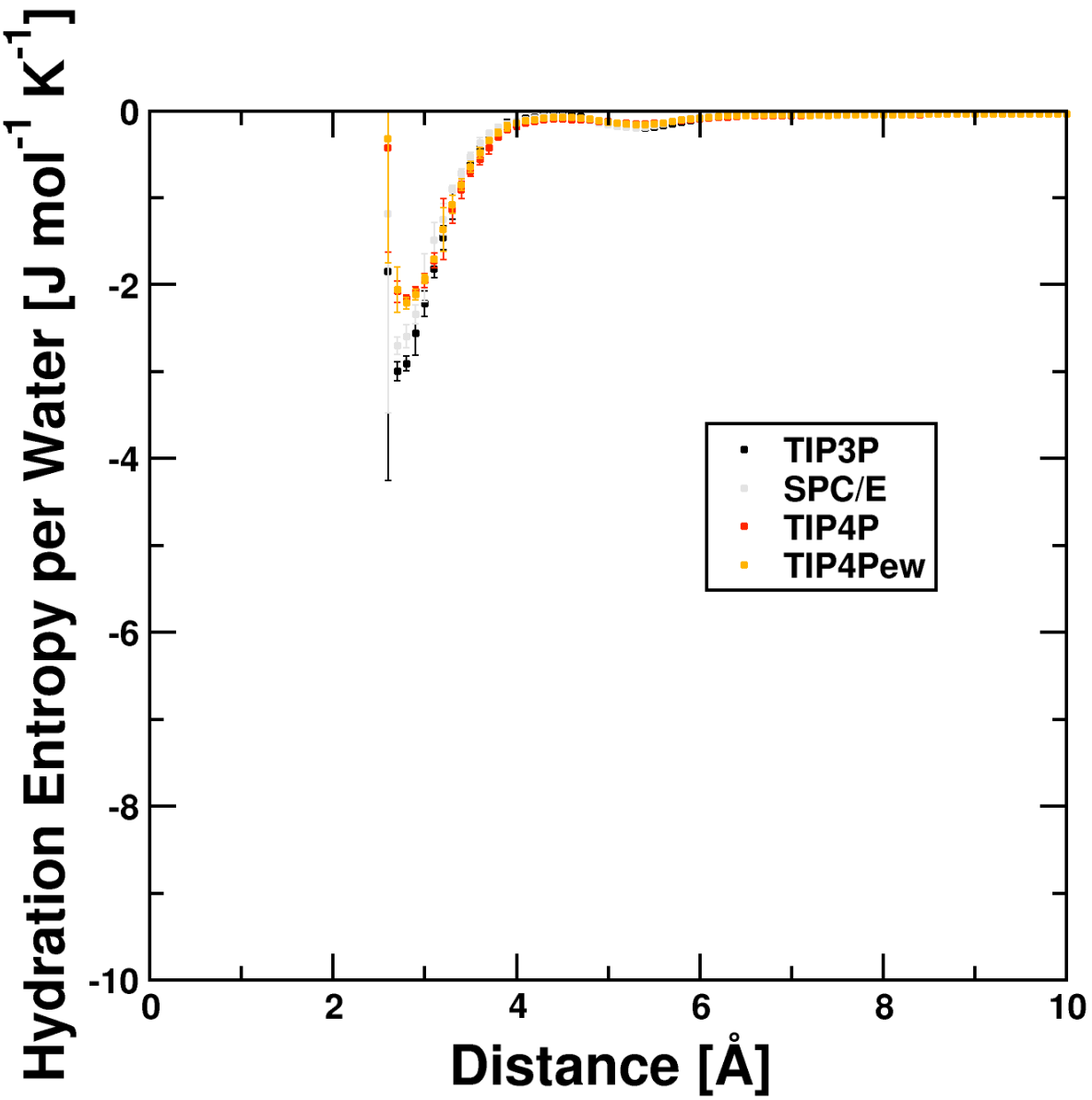
Na^+


Hydration Entropy per Water [J mol-1 K-1]
0
-2
-4
-6
-8
-10
0
2
4
6
8
10
Distance [Å]
TIP3P
SPC/E
TIP4P
TIP4Pew

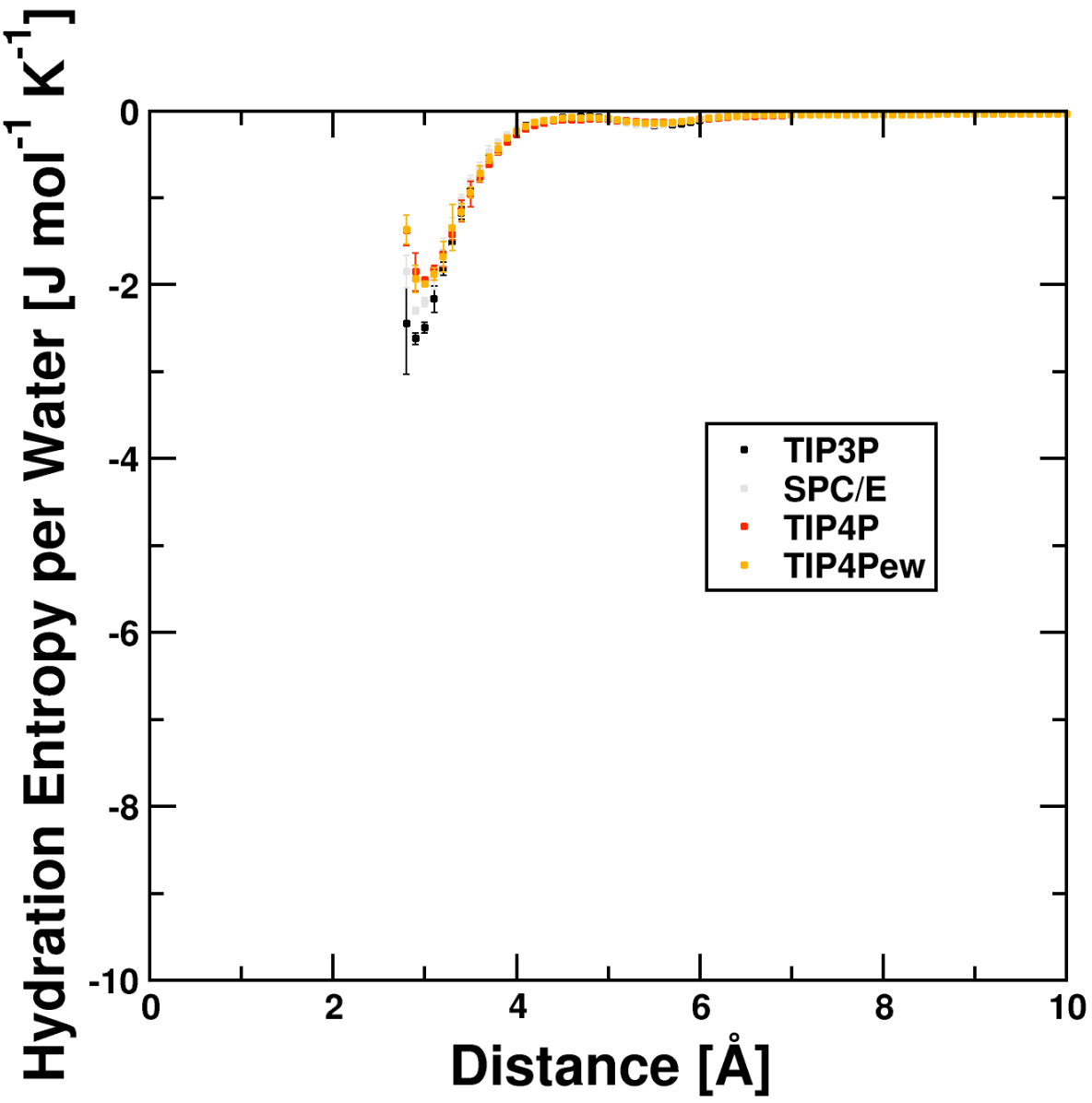
K^+


Hydration Entropy per Water [J mol-1 K-1]
0
-2
-4
-6
-8
-10
0
2
4
6
8
10
Distance [Å]
TIP3P
SPC/E
TIP4P
TIP4Pew

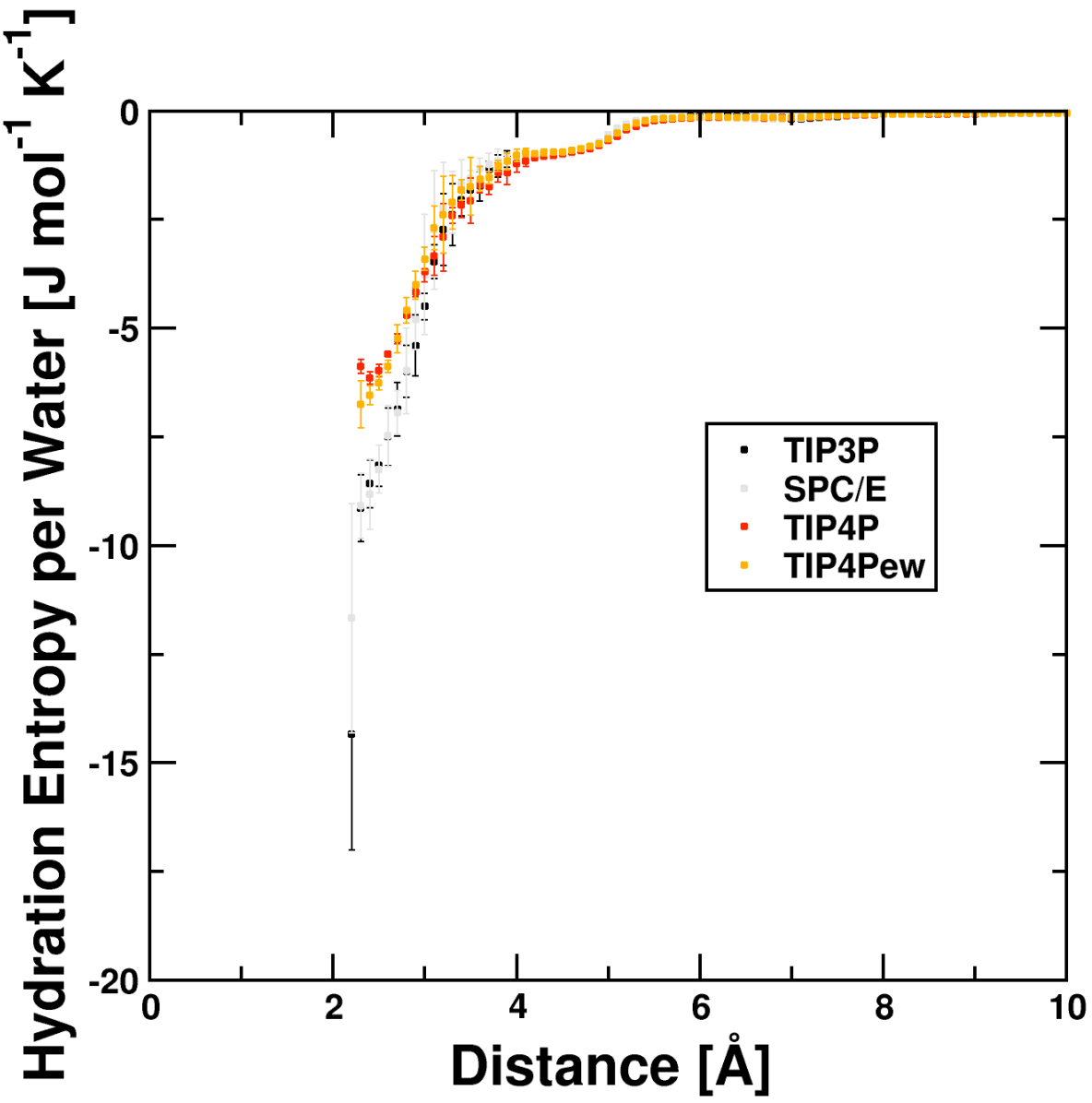
Rb^+


Hydration Entropy per Water [J mol-1 K-1]
0
-2
-4
-6
-8
-10
0
2
4
6
8
10
Distance [Å]
TIP3P
SPC/E
TIP4P
TIP4Pew

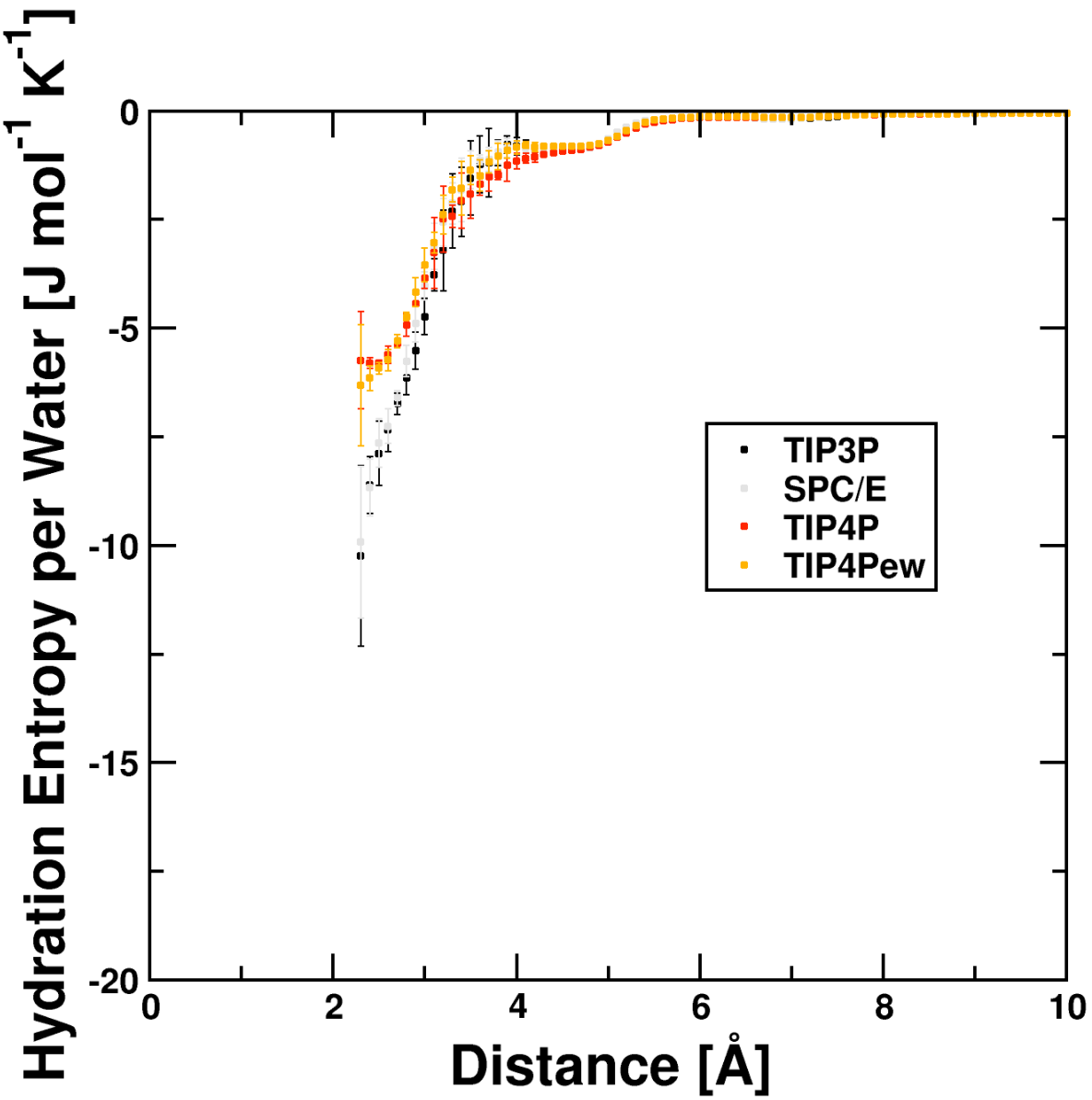
Cs^+


Hydration Entropy per Water [J mol-1 K-1]
0
-2
-4
-6
-8
-10
0
2
4
6
8
10
Distance [Å]
TIP3P
SPC/E
TIP4P
TIP4Pew

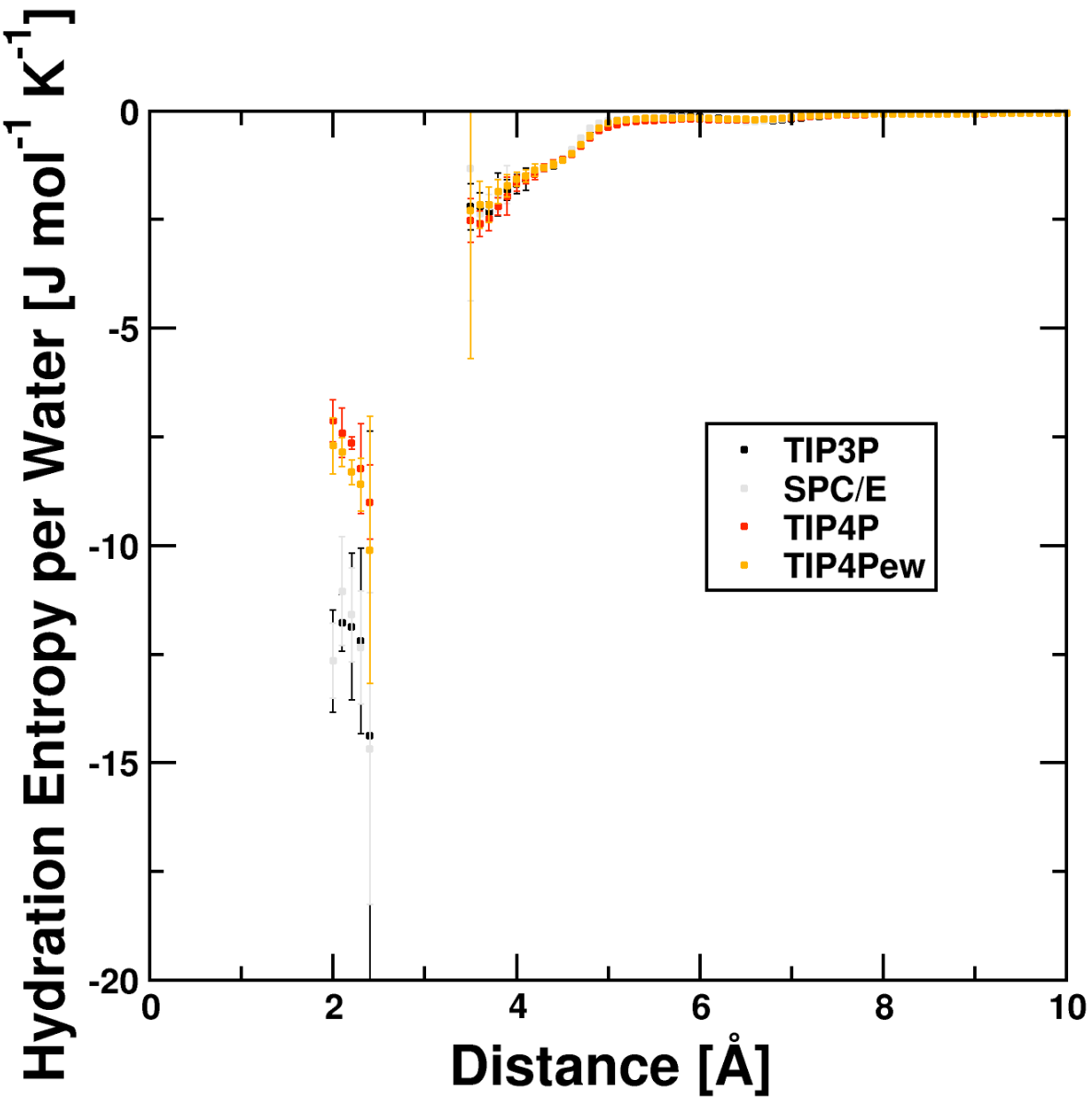
Mn^{2+}


Hydration Entropy per Water [J mol-1 K-1]
0
-5
-10
-15
-20
0
2
4
6
8
10
Distance [Å]
TIP3P
SPC/E
TIP4P
TIP4Pew

Ca^{2+}


Hydration Entropy per Water [J mol-1 K-1]
0
-5
-10
-15
-20
0
2
4
6
8
10
Distance [Å]
TIP3P
SPC/E
TIP4P
TIP4Pew

Mg^{2+}


Hydration Entropy per Water [J mol-1 K-1]
0
-5
-10
-15
-20
0
2
4
6
8
10
Distance [Å]
TIP3P
SPC/E
TIP4P
TIP4Pew