

# Ionic PAA surrounded by Na<sup>+</sup> counter-ions

The dielectric and ion-accessibility coefficients are defined by a cubic-spline surface

```
-----
PRINT STATEMENTS
print force 1 (ion_solv) end
  Printing net forces (kJ/mol/A).
  Legend:
    tot -- Total force
    qf -- Fixed charge force
    db -- Dielectric boundary force
    ib -- Ionic boundary force
tot -1.418237503120E+02 -4.493048401068E+00 6.281203481312E+01
qf 3.460384482352E+01 -1.431963100446E+02 4.064059698634E+01
ib 0.000000000000E+00 0.000000000000E+00 0.000000000000E+00
db -1.764275951355E+02 1.387032616435E+02 2.217143782678E+01
```

**Total force = -1.418\*10<sup>2</sup>**

The dielectric and ion-accessibility coefficients are defined by a 7th order polynomial. This surface definition provides higher order continuity necessary for stable force calculations with atomic multipole force fields (up to quadrupole).

```
PRINT STATEMENTS
print force 1 (ion_solv) end
  Printing net forces (kJ/mol/A).
  Legend:
    tot -- Total force
    qf -- Fixed charge force
    db -- Dielectric boundary force
    ib -- Ionic boundary force
tot -1.271042794022E+02 1.253599446364E+02 1.173177405963E+02
qf 8.473310119365E+01 -1.415045494871E+02 5.063626130568E+01
ib 0.000000000000E+00 0.000000000000E+00 0.000000000000E+00
db -2.118373805958E+02 2.668644941235E+02 6.668147929063E+01
```

**Total force = -1.271\*10<sup>2</sup>**

## PAA undissociated

The dielectric and ion-accessibility coefficients are defined by a cubic-spline surface

```
-----
PRINT STATEMENTS
print force 1 (ion_solv) end
Printing net forces (kJ/mol/A).
Legend:
  tot -- Total force
  qf  -- Fixed charge force
  db  -- Dielectric boundary force
  ib  -- Ionic boundary force
tot -5.952088293553E+01 -1.164198843114E+01 7.725733186374E+01
qf  -3.859991952023E+01 -8.855839731306E+00 4.156450630717E+01
ib  0.000000000000E+00 0.000000000000E+00 0.000000000000E+00
db  -2.092096341530E+01 -2.786148699834E+00 3.569282555657E+01
-----
```

**Total force =  $-5.952 \times 10^1$**

The dielectric and ion-accessibility coefficients are defined by a 7th order polynomial. This surface definition provides higher order continuity necessary for stable force calculations with atomic multipole force fields (up to quadrupole).

```
PRINT STATEMENTS
print force 1 (ion_solv) end
Printing net forces (kJ/mol/A).
Legend:
  tot -- Total force
  qf  -- Fixed charge force
  db  -- Dielectric boundary force
  ib  -- Ionic boundary force
tot -7.741132166411E+01 -2.385207783321E+00 1.298072929864E+02
qf  -4.226975952602E+01 -9.241012257106E+00 5.155317072592E+01
ib  0.000000000000E+00 0.000000000000E+00 0.000000000000E+00
db  -3.514156213808E+01 6.855804473785E+00 7.825412226045E+01
```

**Total force =  $-7.741 \times 10^1$**