

Supporting material

Structure and dynamics of the $[\text{Zn}(\text{NH}_3)(\text{H}_2\text{O})_5]^{2+}$ complex in aqueous solution obtained by an ab initio QM/MM molecular dynamics study

Original basis set for Zn

```
$basis
*
zn LANL2DZ ECP
*
  2 s
    0.799700000      -0.648611200
    0.175200000      1.31382910
  1 s
    0.556000000E-01  1.00000000
  1 p
    0.120200000      1.00000000
  1 p
    0.351000000E-01  1.00000000
  4 d
    68.8500000      0.258532000E-01
    18.3200000      0.165119500
    5.92200000      0.446821200
    1.92700000      0.583108000
  1 d
    0.552800000      1.00000000
*
$ecp
*
zn LANL2DZ ECP
*
  ncore = 18   lmax = 3
f
  -18.00000000  1   386.73796600
  -124.35274030 2   72.85873590
  -30.66018220  2   15.90661700
  -10.63589890  2    4.35023400
  -0.76836230  2    1.28421990
s-f
  3.00000000  0   19.08678580
  22.52342250  1    5.02310800
  48.44659420  2    1.27017440
  -44.55601190 2    1.06712870
  12.99839580  2    0.92641900
p-f
  5.00000000  0   43.49277500
  20.74355890  1   20.86926690
  90.30271580  2   21.71183780
  74.66103160  2    6.36169150
  9.88944240  2    1.22911950
d-f
  -4.84903590  2   13.58518000
  3.69133790  2    9.83730500
  -0.50373190  2    0.83731130
*
$end
```

Basis Sets Modified for Zn(II) ion

\$basis

*

zn LANL2DZ ECP

*

2	s		
		0.799700000	-0.648611200
		0.175200000	1.31382910
1	p		
		0.120200000	1.00000000
4	d		
		68.8500000	0.258532000E-01
		18.3200000	0.165119500
		5.92200000	0.446821200
		1.92700000	0.583108000
1	d		
		0.552800000	1.00000000

*

\$ecp

*

zn LANL2DZ ECP

*

ncore = 18 lmax = 3

f

-18.00000000	1	386.73796600
-124.35274030	2	72.85873590
-30.66018220	2	15.90661700
-10.63589890	2	4.35023400
-0.76836230	2	1.28421990

s-f

3.00000000	0	19.08678580
22.52342250	1	5.02310800
48.44659420	2	1.27017440
-44.55601190	2	1.06712870
12.99839580	2	0.92641900

p-f

5.00000000	0	43.49277500
20.74355890	1	20.86926690
90.30271580	2	21.71183780
74.66103160	2	6.36169150
9.88944240	2	1.22911950

d-f

-4.84903590	2	13.58518000
3.69133790	2	9.83730500
-0.50373190	2	0.83731130

*

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