

Quantum chemical investigation of hyperfine coupling constants  
on first coordination sphere water molecule of Gd(III)  
aquacomplexes.

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- Supporting information -

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## Geometry of Gd aquacomplex

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Gd	0.	0.	0.
O	-1.26113	2.04195	0.
O	-1.26113	0.	2.04195
O	-1.26113	0.	-2.04195
O	-1.26113	-2.04195	0.
O	1.26113	1.44387	1.44387
O	1.26113	-1.44387	1.44387
O	1.26113	1.44387	-1.44387
O	1.26113	-1.44387	-1.44387
H	-0.92205	2.96355	0.
H	-2.23701	2.15141	0.
H	-0.92205	0.	2.96355
H	-2.23701	0.	2.15141
H	-0.92205	0.	-2.96355
H	-2.23701	0.	-2.15141
H	-0.92205	-2.96355	0.
H	-2.23701	-2.15141	0.
H	2.23701	1.52128	1.52128
H	0.92205	2.09554	2.09554
H	2.23701	-1.52128	1.52128
H	0.92205	-2.09554	2.09554
H	2.23701	1.52128	-1.52128
H	0.92205	2.09554	-2.09554
H	2.23701	-1.52128	-1.52128
H	0.92205	-2.09554	-2.09554

## GTO basis sets

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Gd 0

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S 1 1.00 0.000000000000
 3.7001721D+10 0.1000000000D+01
S 1 1.00 0.000000000000
 4.4233374D+09 0.1000000000D+01
S 1 1.00 0.000000000000
 736627460. 0.1000000000D+01
S 1 1.00 0.000000000000
 157466940. 0.1000000000D+01
S 1 1.00 0.000000000000
 39988049. 0.1000000000D+01
S 1 1.00 0.000000000000
 11295642. 0.1000000000D+01
S 1 1.00 0.000000000000
 3442911.2 0.1000000000D+01
S 1 1.00 0.000000000000
 1134401.6 0.1000000000D+01
S 1 1.00 0.000000000000
 396957.84 0.1000000000D+01
S 1 1.00 0.000000000000
 146564.47 0.1000000000D+01
S 1 1.00 0.000000000000
 56594.524 0.1000000000D+01
S 1 1.00 0.000000000000
 22562.053 0.1000000000D+01
S 1 1.00 0.000000000000
 9206.7332 0.1000000000D+01
S 1 1.00 0.000000000000
 3830.1031 0.1000000000D+01
S 1 1.00 0.000000000000
 1630.5186 0.1000000000D+01
S 1 1.00 0.000000000000
 716.1974 0.1000000000D+01
S 1 1.00 0.000000000000
 325.13703 0.1000000000D+01
S 1 1.00 0.000000000000
 141.13836 0.1000000000D+01
S 1 1.00 0.000000000000
 65.402596 0.1000000000D+01
S 1 1.00 0.000000000000
 26.424389 0.1000000000D+01
S 1 1.00 0.000000000000
 13.671169 0.1000000000D+01
S 1 1.00 0.000000000000
 5.3756862 0.1000000000D+01
S 1 1.00 0.000000000000
 2.6791504 0.1000000000D+01
S 1 1.00 0.000000000000
 0.76814741 0.1000000000D+01
S 1 1.00 0.000000000000
 0.35394983 0.1000000000D+01
S 1 1.00 0.000000000000
 0.062875056 0.1000000000D+01
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S 1 1.00 0.000000000000
0.025554319 0.1000000000D+01
S 1 1.00 0.000000000000
0.010874178 1.0

P 1 1.00 0.000000000000
52152768. 0.1000000000D+01
P 1 1.00 0.000000000000
7440218.2 0.1000000000D+01
P 1 1.00 0.000000000000
1535484.4 0.1000000000D+01
P 1 1.00 0.000000000000
390559.57 0.1000000000D+01
P 1 1.00 0.000000000000
115469.69 0.1000000000D+01
P 1 1.00 0.000000000000
38541.383 0.1000000000D+01
P 1 1.00 0.000000000000
14246.672 0.1000000000D+01
P 1 1.00 0.000000000000
5740.2012 0.1000000000D+01
P 1 1.00 0.000000000000
2485.2794 0.1000000000D+01
P 1 1.00 0.000000000000
1142.7899 0.1000000000D+01
P 1 1.00 0.000000000000
552.63076 0.1000000000D+01
P 1 1.00 0.000000000000
278.5198 0.1000000000D+01
P 1 1.00 0.000000000000
145.30926 0.1000000000D+01
P 1 1.00 0.000000000000
77.642981 0.1000000000D+01
P 1 1.00 0.000000000000
41.886077 0.1000000000D+01
P 1 1.00 0.000000000000
22.880971 0.1000000000D+01
P 1 1.00 0.000000000000
12.554862 0.1000000000D+01
P 1 1.00 0.000000000000
6.6694959 0.1000000000D+01
P 1 1.00 0.000000000000
3.4809842 0.1000000000D+01
P 1 1.00 0.000000000000
1.7661486 0.1000000000D+01
P 1 1.00 0.000000000000
0.81730209 0.1000000000D+01
P 1 1.00 0.000000000000
0.37081054 0.1000000000D+01
P 1 1.00 0.000000000000
0.15135526 0.1000000000D+01
P 1 1.00 0.000000000000
0.064406494 0.1000000000D+01

D 1 1.00 0.000000000000
19762.544 0.1000000000D+01
D 1 1.00 0.000000000000

```

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4952.9396 0.1000000000D+01
D 1 1.00 0.000000000000
1693.2815 0.1000000000D+01
D 1 1.00 0.000000000000
698.38712 0.1000000000D+01
D 1 1.00 0.000000000000
305.48376 0.1000000000D+01
D 1 1.00 0.000000000000
140.53492 0.1000000000D+01
D 1 1.00 0.000000000000
67.860905 0.1000000000D+01
D 1 1.00 0.000000000000
33.708372 0.1000000000D+01
D 1 1.00 0.000000000000
17.12325 0.1000000000D+01
D 1 1.00 0.000000000000
8.6140811 0.1000000000D+01
D 1 1.00 0.000000000000
4.1984878 0.1000000000D+01
D 1 1.00 0.000000000000
1.9508518 0.1000000000D+01
D 1 1.00 0.000000000000
0.78058449 0.1000000000D+01
D 1 1.00 0.000000000000
0.28167361 0.1000000000D+01
D 1 1.00 0.000000000000
0.090559037 0.1000000000D+01
D 1 1.00 0.000000000000
0.030186346 1.0

F 1 1.00 0.000000000000
383.57372 0.1000000000D+01
F 1 1.00 0.000000000000
131.6883 0.1000000000D+01
F 1 1.00 0.000000000000
56.216693 0.1000000000D+01
F 1 1.00 0.000000000000
26.307294 0.1000000000D+01
F 1 1.00 0.000000000000
12.948024 0.1000000000D+01
F 1 1.00 0.000000000000
6.4445078 0.1000000000D+01
F 1 1.00 0.000000000000
3.1334851 0.1000000000D+01
F 1 1.00 0.000000000000
1.4695379 0.1000000000D+01
F 1 1.00 0.000000000000
0.65277113 0.1000000000D+01
F 1 1.00 0.000000000000
0.26165607 0.1000000000D+01
F 1 1.00 0.000000000000
0.08721869 1.0
*****

O 0
S 1 1.00 0.000000000000
1.0923490D+05 0.1000000000D+01

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S	1	1.00	0.000000000000
		1.5421330D+04	0.1000000000D+01
S	1	1.00	0.000000000000
		3.2728280D+03	0.1000000000D+01
S	1	1.00	0.000000000000
		8.7010720D+02	0.1000000000D+01
S	1	1.00	0.000000000000
		2.6827060D+02	0.1000000000D+01
S	1	1.00	0.000000000000
		9.1492820D+01	0.1000000000D+01
S	1	1.00	0.000000000000
		3.3617400D+01	0.1000000000D+01
S	1	1.00	0.000000000000
		1.3046480D+01	0.1000000000D+01
S	1	1.00	0.000000000000
		5.2035230D+00	0.1000000000D+01
S	1	1.00	0.000000000000
		1.4774290D+00	0.1000000000D+01
S	1	1.00	0.000000000000
		5.7775210D-01	0.1000000000D+01
S	1	1.00	0.000000000000
		2.1267430D-01	0.1000000000D+01
P	1	1.00	0.000000000000
		3.6640670D+02	0.1000000000D+01
P	1	1.00	0.000000000000
		6.6279560D+01	0.1000000000D+01
P	1	1.00	0.000000000000
		1.8745580D+01	0.1000000000D+01
P	1	1.00	0.000000000000
		6.4268600D+00	0.1000000000D+01
P	1	1.00	0.000000000000
		2.4445130D+00	0.1000000000D+01
P	1	1.00	0.000000000000
		9.5771700D-01	0.1000000000D+01
P	1	1.00	0.000000000000
		3.6884010D-01	0.1000000000D+01
P	1	1.00	0.000000000000
		1.3644960D-01	0.1000000000D+01
D	1	1.00	0.000000000000
		1.4000000000	1.0000000000
D	1	1.00	0.000000000000
		0.3500000000	1.0000000000

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H 0

S	1	1.00	0.000000000000
		8.2932759D+01	1.00000000
S	1	1.00	0.000000000000
		1.2452437D+01	1.00000000
S	1	1.00	0.000000000000
		2.8330596D+00	1.00000000
S	1	1.00	0.000000000000
		8.0001038D-01	1.00000000
S	1	1.00	0.000000000000
		2.5859498D-01	1.00000000
S	1	1.00	0.000000000000

8.9969184D-02      1.0000000

P 1 1.00      0.000000000000  
1.3000000000      1.0000000000  
P 1 1.00      0.000000000000  
0.3300000000      1.0000000000

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