

The cc-pV5Z-F12 basis set: reaching the basis set limit in explicitly correlated calculations

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Supporting Information

(1) cc-pV5Z-F12 basis sets

Note: [6s] contractions taken from standard cc-pV6Z basis set

p,H,5.0009,2.1439,0.9191,0.3940,0.1689

d,H,1.3104,0.5777,0.2547

f,H,0.6427,0.3330

g,H,0.5575

Note: [7s] contractions taken from standard aug-cc-pV6Z basis set

p,He,14.1317,5.4828,2.1272,0.8253,0.3202

d,He,4.3691,1.5154,0.5256

f,He,0.8373,0.4064

g,He,0.6712

Note: for B-Ne, [8s7p] contractions taken from standard aug-cc-pV6Z basis set plus uncontract the 7th most diffuse p-type function

d,B,4.3748,1.8133,0.7516,0.3115,0.1291
f,B,1.4530,0.7020,0.3391,0.1638
g,B,0.7275,0.3806,0.1991
h,B,0.4849,0.2407

d,C,7.4466,2.9061,1.1341,0.4426,0.1727
f,C,2.7869,1.2123,0.5274,0.2294
g,C,1.2535,0.5824,0.2706
h,C,0.6203,0.3007

d,N,10.6384,4.1361,1.6081,0.6252,0.2431
f,N,4.5264,1.8949,0.7933,0.3321
g,N,2.1107,0.8976,0.3817
h,N,0.9543,0.4524

d,O,11.6823,4.5148,1.7448,0.6743,0.2606
f,O,6.2191,2.5090,1.0122,0.4084
g,O,3.5330,1.3658,0.5280
h,O,2.1942,0.6648

d,F,15.9912,6.1203,2.3424,0.8965,0.3431
f,F,8.3547,3.2426,1.2585,0.4885
g,F,5.4453,1.8851,0.6526
h,F,3.7955,0.7816

d,Ne,20.2445,7.6340,2.8787,1.0855,0.4093
f,Ne,10.9600,4.1223,1.5505,0.5832
g,Ne,7.2314,2.4381,0.8220
h,Ne,5.2653,0.9830

(2) cc-pVnZ-F12rev2 basis sets for H

Note: s-type contractions taken from cc-pVnZ-F12 throughout

!cc-pVDZ-F12rev2 (2p)
p,H,0.5983,0.2232

! cc-pVTZ-F12rev2 (3p2d)
p,H,0.9312,0.3983,0.1704
d,H,0.6127,0.2653

! cc-pVQZ-F12rev2 (4p3d2f)
p,H,1.8317,0.8025,0.3516,0.1540
d,H,0.8859,0.4521,0.2307
f,H,0.6114,0.3135

! cc-pV5Z-F12rev2 (5p4d3f2g)
p,H,2.0171,1.0383,0.5344,0.2751,0.1416
d,H,2.2760,1.0833,0.5157,0.2455
f,H,1.1854,0.6176,0.3218
g,H,1.8204,0.5131