Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Electronic supporting information for

Metal chemical shifts in model compounds of group-12 elements

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TABLE I Geometries of complexes used in the NMR calculations[a]

$M(CH_3)_2$	$r_{M–C}$	$r_{C–H}$	$\angle_{M–C–H}$	$\angle_{H–C–H}$
Zn[b]	1.936	1.099	111.0	107.88
Cd[b]	2.121	1.098	110.4	108.49
Hg[b]	2.114	1.097	110.3	108.68
Zn[c]	1.929	1.090		
Cd[c]	2.112	1.090		
Hg[d]	2.083	1.106		
$M(H_2O)_6^{2+}$	$r_{M–O}$	$r_{O–H}$	$\angle_{M–O–H}$	$\angle_{H–O–H}$
Zn	2.051	0.974	126.42	107.16
Cd	2.317	0.974	126.68	106.65
Hg	2.386	0.974	126.34	107.33

[a]DFT optimization with BP86 functional and aug-cc-pVTZ basis set. Bond lengths are measured in Ångströms and angles in degrees. [b]Optimized equilibrium geometry. [c]Experimental results: W. J. Hehre, L. Radom, P. von R. Schleyer, and J. A. Pople, *Ab Initio Molecular Orbital Theory*, John Wiley & Sons, 1986. [d]Experimental result: K. Kashiwabara, S. Konaka, T. Iijima, and M. Kimura, Bull. Chem. Soc. Jpn. **46**, 407 (1973).

TABLE II BPPT shielding constants of Zn^{2+} with increasing number of sets of tight functions added to the basis set[a]

	Number of sets of tight functions added to the Zn basis set										
	0	1	2	3	4	5	6	7	8	9	10
NR	2507.82	2507.83	2507.83	2507.83	2507.83	2507.83	2507.83	2507.83	2507.83	2507.83	2507.83
con	−107.86	−108.33	−109.00	−109.12	−109.37	−109.39	−109.48	−109.48	−109.52	−109.51	−109.53
d-KE	−88.81	−89.05	−89.39	−89.45	−89.58	−89.59	−89.63	−89.63	−89.65	−89.65	−89.66
p-OZ	−5.10	−5.10	−5.10	−5.10	−5.10	−5.10	−5.10	−5.10	−5.10	−5.10	−5.10
d/mv	149.55	150.19	151.18	151.32	151.70	151.73	151.88	151.88	151.95	151.94	151.97
d/Dar	−82.01	−82.49	−83.17	−83.29	−83.54	−83.56	−83.66	−83.66	−83.69	−83.69	−83.70
p/OZ-KE	21.21	21.22	21.23	21.23	21.23	21.23	21.23	21.23	21.23	21.23	21.23
FC/SZ-KE	338.05	340.01	342.80	343.31	344.31	344.41	344.79	344.79	344.94	344.93	344.99
FC-II(1)	−58.13	−58.47	−58.94	−59.03	−59.20	−59.22	−59.28	−59.28	−59.31	−59.31	−59.32
SD-II(1)	2.38	4.43	6.70	8.57	9.86	10.69	11.19	11.49	11.67	11.78	11.84
BPPT	169.29	172.42	176.31	178.43	180.32	181.20	181.94	182.25	182.52	182.62	182.72
Total[b]	2677.11	2680.25	2684.14	2686.26	2688.15	2689.03	2689.77	2690.07	2690.35	2690.45	2690.55

[a]DFT calculations with BHandHLYP hybrid functional. Results in ppm. Starting (0) basis set: FIVu/HIV. The BPPT-5 terms *p*-KE/OZ, *p*/mv, *p*/Dar, FC-I, and SD-I are omitted because they do not contribute to the shielding constants of the M^{2+} ions due to their spherical symmetry and the properties of the orbital Zeeman (OZ) interaction. [b]NR+BPPT.

TABLE III BPPT shielding constants of Cd^{2+} with increasing number of sets of tight functions added to the basis set[a]

	Number of sets of tight functions added to the Cd basis set										
	0	1	2	3	4	5	6	7	8	9	10
NR	4801.27	4801.27	4801.27	4801.27	4801.27	4801.27	4801.27	4801.27	4801.27	4801.27	4801.27
con	−457.61	−458.60	−460.00	−460.26	−460.76	−460.81	−461.00	−461.00	−461.08	−461.07	−461.10
d-KE	−384.86	−385.36	−386.07	−386.19	−386.45	−386.47	−386.57	−386.56	−386.60	−386.60	−386.61
p-OZ	−27.44	−27.45	−27.45	−27.45	−27.45	−27.45	−27.45	−27.45	−27.45	−27.45	−27.45
d/mv	650.12	651.44	653.50	653.79	654.59	654.64	654.96	654.96	655.10	655.09	655.15
d/Dar	−348.00	−349.00	−350.43	−350.68	−351.19	−351.24	−351.44	−351.44	−351.51	−351.51	−351.54
p/OZ-KE	103.07	103.10	103.11	103.11	103.11	103.11	103.11	103.11	103.11	103.11	103.11
FC/SZ-KE	1419.84	1423.90	1429.68	1430.72	1432.81	1433.00	1433.80	1433.79	1434.11	1434.07	1434.20
FC-II(1)	−242.65	−243.34	−244.32	−244.50	−244.85	−244.89	−245.02	−245.02	−245.07	−245.07	−245.09
SD-II(1)	15.91	25.46	34.05	40.13	44.17	46.63	48.12	48.99	49.51	49.80	49.98
BPPT	728.37	740.15	752.08	758.68	763.97	766.52	768.51	769.38	770.10	770.38	770.65
Total	5529.63	5541.42	5553.35	5559.95	5565.24	5567.79	5569.78	5570.65	5571.37	5571.65	5571.92

[a]See footnotes in Table II.

TABLE IV BPPT shielding constants of Hg^{2+} with increasing number of sets of tight functions added to the basis set[a]

	Number of sets of tight functions added to the Cd basis set												
	0	1	2	3	4	5	6	7	8	8+1g[b]	8+2g[c]	9	10
NR	9718.07	9718.08	9718.08	9718.08	9718.08	9718.08	9718.08	9718.08	9718.08	9718.08	9718.08	9718.08	9718.08
con	−2167.74	−2171.99	−2178.06	−2179.15	−2181.34	−2181.54	−2182.38	−2182.37	−2182.70	−2182.70	−2182.70	−2182.67	−2182.80
d-KE	−1866.58	−1868.73	−1871.78	−1872.32	−1873.42	−1873.52	−1873.94	−1873.93	−1874.10	−1874.10	−1874.10	−1874.08	−1874.15
p-OZ	−158.86	−158.88	−158.89	−158.89	−158.89	−158.89	−158.89	−158.89	−158.89	−158.89	−158.89	−158.89	−158.89
d/mv	3146.03	3151.73	3160.57	3161.83	3165.26	3165.47	3166.87	3166.86	3167.46	3167.46	3167.46	3167.43	3167.70
d/Dar	−1642.25	−1646.55	−1652.68	−1653.77	−1655.99	−1656.19	−1657.04	−1657.03	−1657.36	−1657.36	−1657.36	−1657.32	−1657.46
p/OZ-KE	572.98	573.10	573.16	573.16	573.17	573.16	573.17	573.16	573.17	573.17	573.17	573.17	573.17
FC/SZ-KE	6663.14	6680.52	6705.30	6709.74	6718.69	6719.51	6722.94	6722.90	6724.26	6724.26	6724.26	6724.10	6724.65
FC-II(1)	−1132.00	−1134.93	−1139.12	−1139.88	−1141.39	−1141.53	−1142.11	−1142.10	−1142.33	−1142.33	−1142.33	−1142.30	−1142.40
SD-II(1)	91.47	138.91	178.28	204.63	221.86	232.13	238.40	242.01	244.16	244.15	244.14	245.38	246.11
BPPT	3506.18	3563.19	3616.79	3645.36	3667.95	3678.61	3687.02	3690.62	3693.66	3693.65	3693.64	3694.82	3695.93
Total[d]	13224.26	13281.27	13334.87	13363.44	13386.02	13396.69	13405.10	13408.69	13411.74	13411.72	13411.72	13412.90	13414.01

[a]DFT calculations with BHandHLYP hybrid functional. Results in ppm. Starting (0) basis set: FIVu/HIV. [b]One g-type exponent added to the metal basis set. [c]Two g-type exponents added to the metal basis set. [d]NR+BPPT.

TABLE V BPPT shielding constants of Zn in $Zn(CH_3)_2$ with increasing number of sets of tight functions added to the basis set[a]

	Number of sets of tight functions added to the Zn basis set										
	0	1	2	3	4	5	6	7	8	9	10
NR	1473.83	1473.42	1473.21	1473.22	1473.21	1473.21	1473.21	1473.21	1473.21	1473.21	1473.21
con	−107.91	−108.38	−109.06	−109.18	−109.42	−109.44	−109.53	−109.53	−109.57	−109.57	−109.58
d-KE	−88.88	−89.12	−89.46	−89.52	−89.65	−89.66	−89.70	−89.70	−89.72	−89.72	−89.73
p-OZ	−5.11	−5.11	−5.11	−5.11	−5.11	−5.11	−5.11	−5.11	−5.11	−5.11	−5.11
d/mv	149.78	150.42	151.41	151.55	151.93	151.95	152.11	152.11	152.18	152.17	152.20
d/Dar	−82.14	−82.62	−83.30	−83.42	−83.67	−83.69	−83.79	−83.79	−83.82	−83.82	−83.83
p/OZ-KE	21.61	21.63	21.63	21.63	21.64	21.64	21.64	21.64	21.64	21.64	21.64
FC/SZ-KE	337.88	339.84	342.63	343.13	344.14	344.23	344.62	344.61	344.77	344.75	344.81
FC-II(1)	−58.19	−58.52	−59.00	−59.08	−59.26	−59.27	−59.34	−59.34	−59.36	−59.36	−59.37
SD-II(1)	2.42	4.46	6.74	8.60	9.90	10.72	11.23	11.53	11.71	11.81	11.87
p-KE/OZ	35.38	36.47	38.29	38.11	39.32	38.60	39.72	38.70	39.92	38.67	40.06
p/mv	−52.00	−53.66	−55.37	−55.52	−56.45	−56.07	−56.84	−56.21	−57.01	−56.22	−57.11
p/Dar	−10.25	−10.30	−10.37	−10.38	−10.40	−10.40	−10.41	−10.41	−10.42	−10.41	−10.42
FC-I(1)	8.35	8.39	8.44	8.45	8.47	8.47	8.48	8.48	8.48	8.48	8.48
SD-I(1)	−13.93	−14.43	−14.76	−14.92	−15.02	−15.07	−15.10	−15.12	−15.13	−15.13	−15.14
FC-I(2)	−1.46	−1.47	−1.48	−1.48	−1.48	−1.48	−1.48	−1.48	−1.48	−1.48	−1.48
SD-I(2)	0.14	0.11	0.11	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.10
BPPT	135.68	137.69	141.34	142.96	145.04	145.52	146.58	146.47	147.16	146.79	147.39
Total[b]	1609.51	1611.11	1614.55	1616.19	1618.25	1618.73	1619.80	1619.68	1620.37	1620.00	1620.60

[a]DFT calculations with BHandHLYP hybrid functional. Results in ppm. Starting (0) basis set: FIVu/HIV. [b]NR+BPPT.

TABLE VI BPPT shielding constants of Cd in $Cd(CH_3)_2$ with increasing number of sets of tight functions added to the basis set[a]

	Number of sets of tight functions added to the Cd basis set										
	0	1	2	3	4	5	6	7	8	9	10
NR	3117.13	3116.87	3116.72	3116.73	3116.72	3116.72	3116.72	3116.72	3116.72	3116.72	3116.72
con	−457.69	−458.67	−460.08	−460.33	−460.84	−460.89	−461.08	−461.08	−461.16	−461.15	−461.18
d-KE	−384.95	−385.45	−386.16	−386.28	−386.54	−386.56	−386.66	−386.66	−386.69	−386.69	−386.70
p-OZ	−27.45	−27.46	−27.46	−27.46	−27.46	−27.46	−27.46	−27.46	−27.46	−27.46	−27.46
d/mv	650.61	651.93	653.99	654.28	655.07	655.12	655.45	655.45	655.59	655.58	655.64
d/Dar	−348.28	−349.28	−350.70	−350.96	−351.47	−351.52	−351.72	−351.72	−351.79	−351.78	−351.82
p/OZ-KE	103.50	103.53	103.54	103.54	103.54	103.54	103.54	103.54	103.54	103.54	103.54
FC/SZ-KE	1419.65	1423.71	1429.49	1430.52	1432.61	1432.80	1433.60	1433.59	1433.91	1433.87	1434.00
FC-II(1)	−242.88	−243.57	−244.55	−244.73	−245.08	−245.12	−245.25	−245.25	−245.30	−245.30	−245.32
SD-II(1)	15.97	25.52	34.12	40.20	44.24	46.69	48.19	49.06	49.58	49.87	50.04
p-KE/OZ	168.07	171.83	177.94	177.38	181.42	179.04	182.77	179.39	183.44	179.28	183.92
p/mv	−218.56	−224.06	−229.71	−230.26	−233.34	−232.12	−234.66	−232.60	−235.23	−232.61	−235.59
p/Dar	−59.41	−59.54	−59.73	−59.76	−59.83	−59.83	−59.86	−59.86	−59.87	−59.87	−59.87
FC-I(1)	48.33	48.44	48.60	48.63	48.68	48.68	48.71	48.71	48.71	48.71	48.72
SD-I(1)	−72.36	−73.93	−75.03	−75.54	−75.88	−76.05	−76.17	−76.22	−76.26	−76.28	−76.29
FC-I(2)	−3.64	−3.65	−3.66	−3.66	−3.67	−3.67	−3.67	−3.67	−3.67	−3.67	−3.67
SD-I(2)	1.65	1.63	1.62	1.62	1.62	1.62	1.62	1.62	1.62	1.62	1.62
BPPT	592.56	600.98	612.20	617.18	623.06	624.29	627.36	626.85	628.95	627.67	629.59
Total	3709.69	3717.84	3728.92	3733.91	3739.78	3741.01	3744.07	3743.57	3745.66	3744.39	3746.30

[a]See footnotes in Table V.

TABLE VII BPPT shielding constants of Hg in $Hg(CH_3)_2$ with increasing number of sets of tight functions added to the basis set[a]

	Number of sets of tight functions added to the Hg basis set												
	0	1	2	3	4	5	6	7	8	8+1g[b]	8+2g[c]	9	10
NR	6537.95	6537.54	6537.32	6537.33	6537.31	6537.32	6537.32	6537.32	6537.32	6538.34	6537.53	6537.32	6537.32
con	−2167.88	−2172.13	−2178.21	−2179.29	−2181.48	−2181.68	−2182.52	−2182.51	−2182.85	−2182.85	−2182.85	−2182.81	−2182.94
d-KE	−1866.73	−1868.88	−1871.93	−1872.47	−1873.57	−1873.67	−1874.09	−1874.09	−1874.25	−1874.25	−1874.25	−1874.23	−1874.30
p-OZ	−158.87	−158.89	−158.90	−158.90	−158.90	−158.90	−158.90	−158.90	−158.90	−158.90	−158.90	−158.90	−158.90
d/mv	3147.23	3152.94	3161.78	3163.04	3166.47	3166.68	3168.08	3168.07	3168.67	3168.66	3168.67	3168.64	3168.91
d/Dar	−1642.94	−1647.23	−1653.36	−1654.46	−1656.67	−1656.88	−1657.72	−1657.71	−1658.05	−1658.05	−1658.05	−1658.01	−1658.15
p/OZ-KE	573.81	573.94	574.00	573.99	574.00	574.00	574.00	574.00	574.00	574.00	574.00	574.00	574.00
FC/SZ-KE	6662.92	6680.30	6705.08	6709.52	6718.47	6719.29	6722.72	6722.68	6724.04	6724.04	6724.04	6723.88	6724.43
FC-II(1)	−1132.67	−1135.61	−1139.81	−1140.56	−1142.07	−1142.21	−1142.79	−1142.78	−1143.01	−1143.01	−1143.01	−1142.99	−1143.08
SD-II(1)	91.64	139.09	178.46	204.81	222.04	232.32	238.59	242.20	244.35	244.34	244.34	245.57	246.30
p-KE/OZ	924.88	943.92	973.74	971.43	990.91	979.69	997.55	981.50	1000.81	1000.31	1000.49	980.99	1003.14
p/mv	−1287.95	−1315.47	−1343.23	−1346.28	−1361.27	−1355.56	−1367.78	−1358.02	−1370.61	−1373.60	−1376.59	−1358.11	−1372.34
p/Dar	−252.52	−253.05	−253.77	−253.90	−254.15	−254.18	−254.28	−254.27	−254.31	−251.79	−250.16	−254.31	−254.32
FC-I(1)	202.37	202.79	203.38	203.49	203.69	203.71	203.79	203.79	203.82	203.44	203.30	203.81	203.83
SD-I(1)	−386.51	−394.31	−399.71	−402.24	−403.91	−404.76	−405.31	−405.59	−405.77	−405.39	−405.28	−405.86	−405.92
FC-I(2)	−8.73	−8.75	−8.78	−8.78	−8.79	−8.79	−8.79	−8.79	−8.79	−8.75	−8.75	−8.79	−8.79
SD-I(2)	5.06	4.95	4.90	4.91	4.90	4.91	4.91	4.91	4.91	4.90	4.89	4.91	4.91
BPPT	2703.12	2743.60	2793.66	2814.33	2839.67	2843.97	2857.45	2854.48	2864.04	2863.11	2861.88	2857.79	2866.76
Total	9241.07	9281.14	9330.98	9351.66	9376.98	9381.28	9394.76	9391.79	9401.36	9401.45	9399.42	9395.10	9404.07

[a]See footnotes in Table V. [b]One g-type function added to the metal basis set. [c]Two g-type functions added to the metal basis set.

TABLE VIII Electron correlation dependence of the nonrelativistic shielding parameters in $M(CH_3)_2$ and M^{2+} (M = Zn, Cd, Hg)[a]

	HF	MP2	CCSD	CCSD(T)	BHandHLYP	B3LYP	BLYP
σ_{Zn}	1607.09	1495.38	1528.23	1511.91	1473.21	1378.22	1307.60
σ_{Cd}	3281.06	3169.62	3205.25	3192.18	3116.72	3017.51	2958.95
σ_{Hg}	6848.95	6652.30	6749.42	[b]	6537.32	6365.20	6263.83
σ^{2+}_{Zn}	2508.08	2507.08	2507.45	2507.36	2507.83	2507.35	2507.20
σ^{2+}_{Cd}	4801.22	4800.62	4800.69	4800.65	4801.27	4800.95	4800.94
σ^{2+}_{Hg}	9718.27	9717.64	9717.84	[b]	9718.08	9717.60	9717.47
$\Delta\sigma_{Zn}$	1341.84	1501.15	1453.53	1475.63	1531.45	1662.03	1757.03
$\Delta\sigma_{Cd}$	2252.24	2414.78	2361.27	2378.79	2487.79	2625.05	2702.77
$\Delta\sigma_{Hg}$	4215.69	4505.71	4359.19	[b]	4657.41	4892.80	5024.78
δ^{c}_{Zn}	903.26	1014.24	981.68	997.96	1037.22	1131.97	1202.62
δ^{c}_{Cd}	1527.50	1638.86	1603.14	1616.23	1692.67	1792.04	1850.87
δ^{c}_{Hg}	2897.48	3095.42	2997.55	[b]	3211.97	3385.29	3487.54

[a]FIVu2(M)/HIV(C, H) basis set. [b]Not calculated. [c]Chemical shift of $M(CH_3)_2$ with respect to NR shielding of M^{2+} ion computed at the same level.

TABLE IX BPPT results for Zn nuclear shielding constants[a]

	Zn^{2+}	$Zn(CH_3)_2$				$Zn(H_2O)_6^{2+}$			
σ	HF	BLYP	B3LYP	BH&HLYP	HF	BLYP	B3LYP	BH&HLYP	HF
NR	2508.08	1307.59	1378.21	1473.21	1607.08	1667.30	1730.97	1810.41	1915.96
con	−109.46	−109.63	−109.57	−109.57	−109.51	−109.60	−109.53	−109.53	−109.48
d-KE	−89.60	−89.78	−89.73	−89.72	−89.67	−89.83	−89.78	−89.78	−89.73
p-OZ	−5.08	−5.13	−5.12	−5.11	−5.10	−5.19	−5.18	−5.17	−5.16
d/mv	151.84	152.30	152.20	152.18	152.05	152.20	152.09	152.06	151.92
d/Dar	−83.67	−83.86	−83.82	−83.82	−83.79	−83.79	−83.75	−83.75	−83.71
p/OZ-KE	21.18	21.76	21.71	21.64	21.53	21.70	21.65	21.58	21.47
FC/SZ-KE	344.96	344.92	344.72	344.77	344.59	344.83	344.67	344.77	344.74
FC-II(1)	−59.36	−59.38	−59.35	−59.36	−59.34	−59.30	−59.28	−59.31	−59.33
SD-II(1)	11.65	11.73	11.72	11.71	11.69	11.70	11.69	11.68	11.66
p-KE/OZ	0.00	43.28	42.06	39.92	36.01	17.94	16.65	14.97	12.65
p/mv	0.00	−58.78	−58.26	−57.01	−53.33	−48.24	−44.75	−40.45	−34.91
p/Dar	0.00	−16.95	−14.13	−10.42	−6.00	5.08	5.24	5.36	5.39
FC-I(1)	0.00	3.34	5.97	8.48	12.26	3.45	3.27	2.72	2.03
SD-I(1)	0.00	−17.00	−16.35	−15.13	−12.84	−2.93	−2.58	−2.08	−1.34
FC-I(2)	0.00	−1.95	−1.81	−1.48	−0.91	−2.93	−2.67	−2.29	−1.86
SD-I(2)	0.00	0.01	0.08	0.10	0.06	−0.85	−0.77	−0.71	−0.66
BPPT-5(1)[a]	0.00	−46.11	−40.71	−34.15	−23.90	−24.69	−22.18	−19.49	−16.18
BPPT-5(1&2)[b]	0.00	−48.05	−42.45	−35.53	−24.74	−28.47	−25.63	−22.50	−18.70
SR[c]	−114.81	−146.78	−144.66	−141.92	−137.81	−139.72	−137.38	−134.72	−131.55
SO[d]	297.25	281.67	284.97	289.08	295.51	293.98	294.32	294.77	295.24
BPPT[e]	182.45	134.89	140.30	147.16	157.71	154.26	156.94	160.05	163.70
Total[f]	2690.53	1442.48	1518.51	1620.37	1764.79	1821.55	1887.91	1970.46	2079.65

[a]Sum of terms [*p*-KE/OZ, *p*/mv, *p*/Dar, FC-I(1), and SD-I(1)], which have been found the most important for heavy-atom δ and $\Delta\sigma$. They do not contribute to the shielding constants of the M^{2+} ions due to their spherical symmetry and the properties of the orbital Zeeman (OZ) interaction. [b]In addition to footnote *a* including also 2-electron SO effects FC-I(2) and SD-I(2). [c]Sum of all electron-spin-independent BPPT terms. [d]Sum of all electron-spin-dependent BPPT terms including also 2-electron SO terms. [e]SR+SO. [f]NR+BPPT. Shieldings of M^{2+} ions calculated at HF level with FIVu8 basis set. Results in ppm.

TABLE X BPPT results for Cd nuclear shielding constants[a]

	Cd^{2+}	$Cd(CH_3)_2$				$Cd(H_2O)_6^{2+}$			
σ	HF	BLYP	B3LYP	BH&HLYP	HF	BLYP	B3LYP	BH&HLYP	HF
NR	4801.22	2958.94	3017.51	3116.72	3281.05	3781.74	3847.91	3936.28	4061.76
con	−460.95	−461.29	−461.14	−461.16	−461.02	−461.23	−461.08	−461.10	−460.96
d-KE	−386.49	−386.81	−386.69	−386.69	−386.57	−386.84	−386.71	−386.72	−386.60
p-OZ	−27.40	−27.50	−27.48	−27.46	−27.42	−27.56	−27.54	−27.52	−27.47
d/mv	654.84	655.90	655.64	655.59	655.27	655.67	655.39	655.31	654.99
d/Dar	−351.47	−351.87	−351.79	−351.79	−351.72	−351.72	−351.63	−351.63	−351.55
p/OZ-KE	102.76	103.93	103.78	103.54	103.16	103.87	103.72	103.47	103.07
FC/SZ-KE	1433.95	1434.36	1433.85	1433.91	1433.38	1434.13	1433.69	1433.87	1433.66
FC-II(1)	−245.13	−245.38	−245.31	−245.30	−245.21	−245.18	−245.11	−245.14	−245.14
SD-II(1)	49.46	49.63	49.60	49.58	49.52	49.58	49.55	49.52	49.46
p-KE/OZ	0.00	194.76	191.34	183.44	167.32	70.90	65.25	57.81	47.61
p/mv	0.00	−191.37	−212.97	−235.23	−249.81	−140.46	−136.21	−126.78	−110.76
p/Dar	0.00	−109.81	−88.02	−59.87	−26.84	0.50	6.02	10.48	13.66
FC-I(1)	0.00	13.76	30.28	48.71	78.83	7.12	8.09	7.94	7.41
SD-I(1)	0.00	−86.16	−82.60	−76.26	−65.23	−19.20	−16.61	−13.42	−9.34
FC-I(2)	0.00	−3.65	−3.83	−3.67	−2.97	−4.90	−4.65	−4.21	−3.70
SD-I(2)	0.00	2.24	1.99	1.62	1.06	−0.35	−0.42	−0.50	−0.59
BPPT-5(1)	0.00	−178.82	−161.97	−139.21	−95.73	−81.14	−73.46	−63.97	−51.43
BPPT-5(1&2)	0.00	−180.24	−163.80	−141.26	−97.65	−86.39	−78.53	−68.68	−55.72
SR	-468.72	−574.08	−577.33	−579.64	−577.64	−536.87	−532.80	−526.66	−518.02
SO	1238.28	1164.80	1183.99	1208.59	1249.38	1221.20	1224.54	1228.06	1231.76
BPPT	769.56	590.72	606.66	628.95	671.74	684.33	691.74	701.40	713.74
Total	5570.78	3549.67	3624.16	3745.66	3952.79	4466.06	4539.65	4637.69	4775.50

[a]See footnotes in Table IX

TABLE XI BPPT results for Hg nuclear shielding constants[a]

	Hg^{2+}	$Hg(CH_3)_2$				$Hg(H_2O)_6^{2+}$			
σ	HF	BLYP	B3LYP	BH&HLYP	HF	BLYP	B3LYP	BH&HLYP	HF
NR	9718.27	6263.82	6365.19	6537.32	6820.60	7913.06	8029.42	8185.21	8407.27
con	−2182.37	−2183.20	−2182.78	−2182.85	−2182.50	−2183.08	−2182.66	−2182.73	−2182.39
d-KE	−1873.79	−1874.57	−1874.22	−1874.25	−1873.94	−1874.54	−1874.19	−1874.23	−1873.91
p-OZ	−158.75	−159.03	−158.97	−158.90	−158.76	−159.09	−159.03	−158.95	−158.82
d/mv	3166.80	3169.46	3168.77	3168.67	3167.87	3168.96	3168.20	3168.05	3167.22
d/Dar	−1657.26	−1658.23	−1658.02	−1658.05	−1657.87	−1657.92	−1657.67	−1657.67	−1657.48
p/OZ-KE	571.76	575.48	574.92	574.00	572.52	575.18	574.61	573.68	572.17
FC/SZ-KE	6723.73	6725.13	6723.79	6724.04	6722.82	6724.61	6723.42	6723.89	6723.26
FC-II(1)	−1142.46	−1143.22	−1143.03	−1143.01	−1142.76	−1142.75	−1142.57	−1142.61	−1142.58
SD-II(1)	243.99	244.52	244.42	244.35	244.19	244.39	244.28	244.19	244.01
p-KE/OZ	0.00	1055.86	1039.74	1000.81	921.29	369.39	339.60	300.50	247.39
p/mv	0.00	−1169.22	−1267.19	−1370.61	−1438.87	−698.52	−680.54	−635.81	−556.30
p/Dar	0.00	−485.22	−385.94	−254.31	−97.94	−3.48	27.28	52.46	70.09
FC-I(1)	0.00	35.35	112.78	203.82	342.75	29.45	38.43	41.86	43.21
SD-I(1)	0.00	−452.93	−436.22	−405.77	−352.44	−99.32	−85.91	−69.52	−48.84
FC-I(2)	0.00	−8.56	−9.11	−8.79	−6.72	−13.54	−13.34	−12.63	−11.72
SD-I(2)	0.00	6.93	6.12	4.91	3.17	−0.87	−1.12	−1.37	−1.64
BPPT-5(1)	0.00	−1016.16	−936.83	−826.06	−625.22	−402.47	−361.14	−310.52	−244.45
BPPT-5(1&2)	0.00	−1017.79	−939.82	−829.95	−628.77	−416.88	−375.60	−324.51	−257.81
SR	−2133.62	−2728.67	−2743.69	−2755.49	−2748.21	−2463.09	−2444.40	−2414.71	−2372.02
SO	5825.26	5407.21	5498.74	5619.53	5811.01	5741.97	5763.18	5783.82	5805.69
BPPT	3691.64	2678.55	2755.06	2864.04	3062.80	3278.88	3318.78	3369.11	3433.67
Total	13409.91	8942.37	9120.25	9401.36	9883.40	11191.94	11348.20	11554.32	11840.94

[a]See footnotes in Table IX