Supplementary Material for "Non-perturbative Calculation of Magnetic Properties within Current-Density Functional Theory"

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The individual data points used to calculate the errors and error distributions for shielding constants and magnetizabilities presented in the main manuscript are presented below.

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MAGNETIZABILITIES

TABLE I. Molecular magnetizabilities (10^{-30} J T^{-2}) calculated using DFT functionals in the aug-cc-pCVTZ basis set. Errors are given relative to CCSD(T) benchmark data from Ref. **?** .

Molecule	LDA	KT3	PBE
AlF	−396.3	−394.3	−397.2
C_3H_4	−465.0	−453.9	−460.1
FCCH	−438.9	−437.5	−438.0
C_2H_4	−331.6	−333.1	−331.4
H_2C_2O	−427.7	−417.2	−422.0
CH_3F	−315.5	−305.5	−311.4
CH_4	−329.1	−311.5	−320.0
CO	−206.8	−206.2	−205.7
FCN	−365.8	−365.5	−365.4
HCN	−265.3	−267.2	−264.7
HCP	−477.9	−484.2	−479.6
HF	−181.3	−176.6	−180.3
LiH	−135.4	−137.3	−134.5
LiF	−196.5	−193.8	−196.3
NH_3	−298.0	−286.7	−292.9
N_2	−201.1	−201.1	−199.8
N_2O	−334.8	−328.6	−332.4
PN	−286.4	−292.4	−285.9
H_4C_2O	−529.2	−516.0	−523.3
HFCO	−297.4	−297.9	−297.3
CH_2O	−99.0	−120.0	−107.6
OCS	−577.2	−572.2	−575.4
OF_2	−220.4	−223.8	−221.8
HOF	−229.1	−225.2	−227.6
H_2O	−241.0	−233.8	−238.5
H_2S	−466.1	−450.6	−458.6
SO_2	−296.8	−294.1	−295.2
ME	4.98	8.07	5.22
MAE	9.16	8.83	5.59
SD	10.82	7.77	6.36

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TABLE II. Molecular magnetizabilities (10^{-30} J T^{-2}) calculated using DFT functionals with VRG(LHC) current correction in the aug-cc-pCVTZ basis set. Errors are given relative to CCSD(T) benchmark data from Ref. **?** .

Molecule	LDA(LHC)	KT3(LHC)	PBE(LHC)
AlF	−394.6	−392.7	−395.6
C_3H_4	−453.0	−441.1	−447.8
FCCH	−433.9	−432.3	−432.9
C_2H_4	−326.5	−328.2	−326.4
H_2C_2O	−420.9	−410.3	−415.0
CH_4	−328.8	−311.1	−319.6
CO	−205.2	−204.6	−204.1
FCN	−362.1	−361.9	−361.8
HF	−181.3	−176.6	−180.3
LiH	−117.9	−127.1	−119.7
LiF	−183.5	−177.8	−181.6
NH_3	−297.7	−286.3	−292.5
N_2	−199.6	−199.7	−198.3
N_2O	−325.8	−319.9	−323.3
PN	−282.8	−289.0	−282.3
HFCO	−292.7	−293.2	−292.6
HOF	−224.3	−220.3	−222.6
H_2O	−240.9	−233.6	−238.4
H_2S	−465.7	−450.1	−458.2
ME	11.82	16.10	14.15
MAE	16.23	16.12	15.99
SD	26.66	25.08	25.96

TABLE III. Molecular magnetizabilities (10^{-30} J T^{-2}) calculated using DFT functionals with VRG(TP) current correction in the aug-cc-pCVTZ basis set. Errors are given relative to CCSD(T) benchmark data from Ref. **?** .

Molecule	LDA(TP)	KT3(TP)	PBE(TP)
AlF	−395.8	−393.9	−396.8
C_3H_4	−462.3	−451.1	−457.4
FCCH	−437.8	−436.4	−436.9
C_2H_4	−330.4	−331.9	−330.1
H_2C_2O	−426.2	−415.6	−420.4
CH_3F	−314.0	−303.9	−309.8
CH_4	−329.1	−311.4	−319.9
CO	−206.3	−205.7	−205.2
FCN	−364.9	−364.7	−364.6
HCN	−264.9	−266.8	−264.2
HCP	−477.4	−483.7	−479.1
HF	−181.3	−176.6	−180.3
LiH	−133.1	−135.7	−132.5
LiF	−194.8	−191.7	−194.3
NH_3	−297.9	−286.6	−292.8
N_2	−200.6	−200.6	−199.2
N_2O	−333.0	−326.8	−330.5
PN	−285.3	−291.3	−284.7
H_4C_2O	−527.0	−513.8	−521.0
HFCO	−296.2	−296.7	−296.1
CH_2O	−95.8	−117.1	−104.6
OCS	−575.8	−570.9	−574.0
OF_2	−218.7	−222.2	−220.2
HOF	−228.0	−224.1	−226.5
H_2O	−241.0	−233.7	−238.5
H_2S	−466.0	−450.5	−458.5
SO_2	−295.5	−292.7	−293.9
ME	6.11	9.18	7.85
MAE	9.89	9.82	9.61
SD	11.30	8.19	9.44

HYPER-MAGNETIZABILITIES

TABLE IV. Hypermagnetizability tensor elements (SI a.u.) calculated using DFT functionals in the aug-cc-pCVTZ basis set. The corresponding Hartree–Fock results are included for comparison.

	HF			KT3			PBE		
	xxxx	yyyy	zzzz	xxxx	yyyy	zzzz	xxxx	yyyy	zzzz
AlF	94.9	94.9	91.0	90.9	90.9	95.5	84.7	84.7	95.7
C_3H_4	−3.8	−250.0	222.0	45.0	−300.0	233.0	25.3	−297.0	223.0
FCCH	−9.6	−9.6	40.3	−19.0	−19.0	45.8	−21.6	−21.6	45.8
C_2H_4	−60.1	−41.1	−4.6	−50.4	−70.9	−45.0	−69.9	−91.7	−43.5
H_2C_2O	−1.3	−94.4	228.0	−6.8	−115.0	252.0	−10.6	−113.0	259.0
CH_3F	−6.7	−6.7	102.0	−29.0	−29.0	129.0	−31.0	−31.0	132.0
CH_4	91.0	91.1	100.0	104.0	104.0	115.0	105.0	105.0	116.0
CO	−6.4	−6.4	17.5	15.8	15.8	21.2	9.9	9.9	21.8
FCN	−10.1	−10.1	23.4	−12.6	−12.6	26.6	−16.0	−16.0	26.7
HCN	−9.0	−9.0	25.9	−5.5	−5.5	28.3	−14.2	−14.2	28.3
HCP	−8.4	−8.4	82.6	−16.4	−16.4	81.0	−42.9	−42.9	81.5
HF	7.9	7.9	5.7	11.8	11.8	8.8	11.9	11.9	9.2
LiH	75.1	75.1	67.9	160.0	160.0	94.9	157.0	157.0	97.4
LiF	4.9	4.9	12.7	41.7	41.7	26.7	35.3	35.3	26.8
NH_3	38.9	38.9	50.7	49.2	49.2	60.3	49.3	49.3	61.0
N_2	−16.7	−16.7	15.8	6.4	6.4	17.8	−1.7	−1.7	18.2
N_2O	−69.6	−69.6	19.1	−81.6	−81.6	21.8	−85.3	−85.3	22.2
PN	−230.0	−230.0	56.2	−294.0	−294.0	57.0	−381.0	−381.0	57.4
H_4C_2O	250.0	53.5	102.0	268.0	18.9	117.0	266.0	15.6	122.0
HFCO	16.4	−20.5	−65.2	22.4	−18.9	−49.3	27.1	−26.2	−66.1
CH_2O	−73.7	−68.6	−619.0	−141.0	−64.8	−704.0	−147.0	−78.7	−931.0
OCS	−53.7	−53.7	55.5	−64.9	−64.9	58.4	−69.9	−69.9	59.6
OF_2	24.9	30.3	33.6	−30.0	30.3	27.3	−40.4	28.6	22.3
HOF	29.9	26.6	15.9	6.1	−12.7	24.4	5.1	−18.7	24.9
H_2O	22.3	14.8	13.5	30.6	21.5	21.7	30.7	21.8	21.8
H_2S	197.0	81.7	117.0	206.0	90.0	124.0	209.0	90.4	125.0
SO_2	45.7	−442.0	−84.4	72.9	−274.0	−82.6	79.9	−322.0	−91.8

TABLE V. Hyper-magnetizability data (SI a.u.) calculated using VRG(TP) current corrected functionals in the aug-cc-pCVTZ basis set. Hartree–Fock results are included for comparison.

	HF			KT3			PBE		
	xxxx	yyyy	zzzz	xxxx	yyyy	zzzz	xxxx	yyyy	zzzz
AlF	94.9	94.9	91.0	90.7	90.7	95.5	84.5	84.5	95.7
C_3H_4	−3.8	−250.0	222.0	43.9	−353.0	226.0	23.8	−345.0	217.0
FCCH	−9.6	−9.6	40.3	−26.7	−26.7	45.8	−29.1	−29.1	45.8
C_2H_4	−60.1	−41.1	−4.6	−51.9	−72.1	−59.3	−71.5	−93.0	−58.4
H_2C_2O	−1.3	−94.4	228.0	−1.2	−135.0	253.0	−16.1	−133.0	260.0
CH_3F	−6.7	−6.7	102.0	−40.2	−40.2	131.0	−42.4	−42.5	134.0
CH_4	91.0	91.1	100.0	104.0	105.0	115.0	105.0	106.0	116.0
CO	−6.4	−6.4	17.5	15.0	15.0	21.2	8.9	8.9	21.8
FCN	−10.1	−10.1	23.4	−15.6	−15.6	26.6	−19.1	−19.1	26.7
HCN	−9.0	−9.0	25.9	−6.3	−6.3	28.3	−15.1	−15.1	28.3
HCP	−8.4	−8.4	82.6	−18.1	−18.1	81.0	−44.9	−44.9	81.5
HF	7.9	7.9	5.7	11.8	11.8	8.8	11.9	11.9	9.2
LiH	75.1	75.1	67.9	160.0	160.0	94.9	151.0	151.0	97.4
LiF	4.9	4.9	12.7	22.6	22.6	26.7	17.7	17.7	26.8
NH_3	38.9	38.9	50.7	49.2	49.2	60.5	49.3	49.4	61.3
N_2	−16.7	−16.7	15.8	5.6	5.6	17.8	−2.7	−2.7	18.2
N_2O	−69.6	−69.6	19.1	−99.6	−99.6	21.8	−104.0	−104.0	22.2
PN	−230.0	−230.0	56.2	−302.0	−302.0	57.0	−390.0	−390.0	57.4
H_4C_2O	250.0	53.5	102.0	270.0	−3.7	110.0	267.0	−7.7	115.0
HFCO	16.4	−20.5	−65.2	19.4	−20.3	−50.8	24.2	−27.6	−67.9
CH_2O	−73.7	−68.6	−619.0	−185.0	−67.2	−733.0	−193.0	−81.4	−967.0
OCS	−53.7	−53.7	55.5	−75.8	−75.8	58.4	−81.4	−81.4	59.6
OF_2	24.9	30.3	33.6	−32.2	28.0	25.3	−42.6	25.9	20.0
HOF	29.9	26.6	15.9	0.8	−19.1	24.4	−0.3	−25.6	25.0
H_2O	22.3	14.8	13.5	30.7	21.5	21.6	30.8	21.8	21.7
H_2S	197.0	81.7	117.0	207.0	90.1	124.0	210.0	90.4	125.0
SO_2	45.7	−442.0	−84.4	72.5	−280.1	−84.2	79.1	−330.0	−94.0

SHIELDING CONSTANTS

TABLE VI. Absolute shielding constants (ppm) calculated without VRG current correction in the aug-cc-pCVTZ basis set. Errors are given relative to CCSD(T) benchmark data from Ref. **?** .

Molecule	Nucleus	LDA	KT3	PBE
HF	H	29.43	30.21	30.06
	F	416.64	411.75	412.63
CO	C	−19.71	5.56	−12.62
	O	−86.11	−54.86	−77.23
N_2	N	−89.15	−60.52	−81.35
H_2O	O	334.90	327.39	329.49
	H	30.98	31.64	31.47
HCN	H	28.97	29.06	29.21
	C	66.24	86.26	72.57
	N	−54.26	−16.47	−42.04
HOF	O	−137.17	−94.80	−122.55
	H	18.58	20.21	19.47
	F	163.94	158.72	154.64
NH_3	N	267.71	263.35	263.34
	H	31.57	32.08	31.93
CH_2O	O	−488.94	−368.25	−443.38
	C	−38.52	−2.93	−24.73
	H	20.17	21.54	20.84
CH_4	C	194.14	193.55	191.44
	H	31.24	31.68	31.53
C_2H_4	C	42.95	64.76	49.99
	H	25.12	26.12	25.68
AlF	Al	531.79	566.52	542.22
	F	142.92	175.20	154.24
CH_3F	C	105.09	114.05	107.06
	F	474.21	456.23	462.43
	H	26.64	27.44	27.14
C_3H_4	C	178.52	181.80	178.03
(cyclopropene)	C	58.82	77.80	64.58
	H	23.74	24.53	24.23
	H	30.25	30.79	30.62
FCCH	C	166.80	181.97	171.59
	C	79.04	95.66	84.40
	H	30.64	31.00	31.00
	F	393.09	393.17	390.19
FCN	F	344.95	337.71	340.31
	C	65.65	83.48	70.97
	N	92.87	122.58	102.51
H2S	S	726.85	725.04	716.39
	H	30.43	31.03	30.87
HCP	H	29.40	29.44	29.61
	C	7.75	32.76	15.83
	P	287.67	393.07	327.81
HFCO	O	−137.50	−89.70	−121.90
	C	18.15	37.11	23.80
	F	85.39	116.44	95.92
	H	22.94	23.59	23.33
H_2C_2O	C	187.25	190.74	186.68
(ketene)	C	−19.77	−2.66	−15.42
	O	−21.10	−0.20	−17.35
	H	29.00	29.60	29.44
LiF	Li	85.61	90.05	86.85
	F	342.63	359.46	345.21
LiH	H	25.74	26.73	26.29
	Li	86.57	92.30	88.35
N_2O	N	89.40	102.63	93.45
	N	0.05	15.03	4.48
	O	180.97	176.95	178.14
OCS	O	72.22	84.27	73.76
	C	20.92	37.42	25.46
	S	754.20	780.01	762.40
OF_2	O	−660.44	−540.93	−618.16
	F	−91.50	−64.83	−84.70
H_4C_2O	O	338.72	337.20	334.11
(oxirane)	C	137.79	145.45	139.26
	H	28.65	29.41	29.13
PN	N	−419.91	−365.17	−406.76
	P	−83.93	43.40	−42.02
SO_2	S	−298.27	−182.15	−257.46
	O	−317.64	−283.26	−307.04
	ME	−29.98	−10.49	−24.33
	MAE	29.99	13.20	24.39
	SD	40.85	23.20	32.46

TABLE VII. Absolute shielding constants (ppm) calculated with the VRG(LHC) current correction in the aug-cc-pCVTZ basis set. Errors are given relative to CCSD(T) benchmark data from Ref. **?** . For some molecules the SCF cycles could not be converged with the LHC correction, results for these molecules have been omitted.

Molecule	Nucleus	LDA(LHC)	KT3(LHC)	PBE(LHC)
HF	H	29.45	30.23	30.08
	F	416.31	411.34	412.26
CO	C	−24.01	1.75	−16.77
	O	−93.06	−61.26	−84.02
N_2	N	−94.66	−65.56	−86.72
H_2O	O	335.07	327.51	329.65
	H	30.98	31.64	31.48
HOF	O	−146.61	−102.92	−131.55
	H	18.32	19.98	19.22
	F	164.27	158.03	154.42
NH_3	N	268.64	264.42	264.34
	H	31.56	32.08	31.93
CH_4	C	194.27	193.71	191.58
	H	31.24	31.68	31.53
C_2H_4	C	40.59	62.71	47.74
	H	25.06	26.06	25.61
AlF	Al	527.78	562.74	538.25
	F	137.13	169.64	148.52
C_3H_4	C	178.85	182.14	178.37
(cyclopropene)	C	56.43	75.56	62.23
	H	23.62	24.40	24.11
	H	30.16	30.69	30.52
FCCH	C	166.29	181.63	171.15
	C	76.90	93.56	82.27
	H	30.68	31.03	31.03
	F	392.69	392.65	389.69
FCN	F	344.44	337.02	339.71
	C	63.59	81.58	68.96
	N	90.90	120.94	100.67
H_2S	S	726.29	724.46	715.80
	H	30.43	31.03	30.87
HFCO	O	−145.71	−97.35	−129.97
	C	16.10	35.23	21.81
	F	78.79	109.98	89.30
	H	22.85	23.50	23.23
H_2C_2O	C	187.40	190.90	186.82
(ketene)	C	−23.00	−5.79	−18.63
	O	−26.91	−5.93	−23.20
	H	29.00	29.59	29.44
LiF	Li	82.61	85.97	83.35
	F	285.89	298.37	283.26
LiH	H	25.39	26.50	25.97
	Li	81.98	89.75	84.46
N_2O	N	87.72	101.02	91.79
	N	−3.50	11.69	0.98
	O	180.58	176.40	177.68
PN	N	−432.48	−376.44	−419.01
	P	−99.35	29.93	−56.84
	ME	−24.47	−10.46	−21.09
	MAE	24.53	10.92	21.26
	SD	31.53	17.44	26.06

TABLE VIII. Absolute shielding constants (ppm) calculated using VRG(TP) current correction in the aug-cc-pCVTZ basis set. Errors are given relative to CCSD(T) benchmark data from Ref. **?** .

Molecule	Nucleus	LDA(TP)	KT3(TP)	PBE(TP)
HF	H	29.44	30.22	30.07
	F	416.48	411.56	412.45
CO	C	−21.18	4.27	−14.03
	O	−88.64	−57.18	−79.70
N_2	N	−91.18	−62.38	−83.33
H_2O	O	334.83	327.30	329.42
	H	30.98	31.64	31.47
HCN	H	28.98	29.07	29.21
	C	65.47	85.59	71.83
	N	−56.07	−18.09	−43.79
HOF	O	−140.59	−97.69	−125.78
	H	18.50	20.14	19.40
	F	163.83	158.28	154.34
NH_3	N	267.82	263.47	263.45
	H	31.57	32.08	31.93
CH_2O	O	−496.55	−374.49	−450.48
	C	−39.73	−3.89	−25.82
	H	20.10	21.48	20.77
CH_4	C	194.09	193.51	191.39
	H	31.24	31.68	31.53
C_2H_4	C	42.14	64.05	49.21
	H	25.11	26.10	25.66
AlF	Al	530.59	565.41	541.04
	F	141.12	173.50	152.48
CH_3F	C	104.66	113.64	106.64
	F	473.95	455.78	462.06
	H	26.62	27.42	27.11
C_3H_4	C	178.51	181.80	178.02
(cyclopropene)	C	58.02	77.07	63.80
	H	23.71	24.50	24.20
	H	30.24	30.77	30.60
FCCH	C	166.54	181.77	171.35
	C	78.38	95.03	83.75
	H	30.65	31.00	31.01
	F	392.89	392.94	389.97
FCN	F	344.59	337.31	339.93
	C	64.97	82.86	70.31
	N	91.99	121.83	101.68
H_2S	S	726.43	724.60	715.95
	H	30.43	31.03	30.87
HCP	H	29.41	29.45	29.62
	C	6.76	31.88	14.88
	P	284.91	390.66	325.18
HFCO	O	−140.33	−92.28	−124.65
	C	17.40	36.42	23.07
	F	83.32	114.47	93.87
	H	22.91	23.57	23.30
H_2C_2O	C	187.16	190.66	186.58
(ketene)	C	−20.83	−3.68	−16.48
	O	−23.13	−2.16	−19.38
	H	29.00	29.59	29.44
LiF	Li	85.25	89.61	86.45
	F	336.04	353.04	338.31
LiH	H	25.69	26.69	26.24
	Li	86.01	91.88	87.83
N_2O	N	88.58	101.86	92.64
	N	−1.13	13.91	3.32
	O	180.38	176.33	177.54
OCS	O	70.90	82.98	72.44
	C	20.09	36.63	24.64
	S	753.55	779.38	761.76
OF_2	O	−667.86	−546.78	−624.98
	F	−93.70	−67.08	−86.97
H_4C_2O	O	338.75	337.19	334.10
(oxirane)	C	137.52	145.19	138.99
	H	28.63	29.39	29.11
PN	N	−424.25	−369.06	−410.98
	P	−89.26	38.77	−47.13
SO_2	S	−302.77	−186.25	−261.82
	O	−321.40	−286.81	−310.75
	ME	−31.17	−11.58	−25.49
	MAE	31.18	13.62	25.55
	SD	42.31	23.72	33.73

REFERENCES

O. B. Lutnæs, A. M. Teale, T. Helgaker, D. J. Tozer, K. Ruud, and J. Gauss, J. Chem. Phys. **131**, 144104 (2009).
A. M. Teale, O. B. Lutnæs, T. Helgaker, D. J. Tozer, and J. Gauss, J. Chem. Phys. **138**, 024111 (2013).