

Erratum: “Relativistic calculation of nuclear magnetic shielding tensor using the regular approximation to the normalized elimination of the small component. II. Consideration of perturbations in the metric operator” [J. Chem. Phys. 126, 174102 (2007)]

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We found errors in our computer programs for our NESC (normalized elimination of the small component) calculations of ZORA, SORA, SORA+ J_{LL} , ZORA-Met, SORA-Met, and SORA+ J_{LL} -Met.¹ The results shown in Table I were not correct and should be read as presented below. The corrected results of ZORA-Met, SORA-Met, and SORA+ J_{LL} -Met yield considerably small $\Delta\sigma$ values compared with the Dirac-Hartree-Fock (DHF) results which are considered as the benchmark.

TABLE I. Calculated nuclear magnetic shielding tensor components (in ppm) in HX (X=F, Cl, Br, I) systems.

Molecule	Nucleus	Property	ZORA ^a	SORA ^a	SORA+ J_{LL} ^a	ZORA-Met ^a	SORA-Met ^a	SORA+ J_{LL} -Met ^a	DHF ^b	
HF	F	σ_{\perp} (para)	-92.4	-92.5	-93.1	-93.9	-94.0	-94.6		
		σ_{\perp} (dia)	481.9	481.9	481.8	482.1	482.1	482.1		
		σ_{\perp} (total)	389.4	389.4	388.7	388.2	388.1	387.4	384.9	
		σ_{\parallel} (para)	7.5	7.4	6.9	4.7	4.6	4.1		
		σ_{\parallel} (dia)	481.0	481.0	481.0	481.2	481.2	481.2		
		σ_{\parallel} (total)	488.5	488.4	487.9	485.9	485.8	485.3	485.6	
		σ^{iso} (total)	422.5	422.4	421.8	420.7	420.7	420.0	418.4	
		$\Delta\sigma$ (total)	99.0	99.0	99.2	97.7	97.7	97.8	100.7	
		H	σ_{\perp} (para)	18.89	18.89	18.85	18.89	18.89	18.85	
	σ_{\perp} (dia)		1.34	1.34	1.35	1.34	1.34	1.35		
	σ_{\perp} (total)		20.23	20.23	20.20	20.24	20.24	20.20	20.10	
	σ_{\parallel} (para)		0.00	0.00	0.00	-0.01	-0.01	0.00		
	σ_{\parallel} (dia)		44.05	44.05	44.07	44.05	44.05	44.07		
	σ_{\parallel} (total)		44.05	44.05	44.08	44.05	44.05	44.07	43.90	
	σ^{iso} (total)		28.17	28.17	28.16	28.17	28.17	28.16	28.03	
	$\Delta\sigma$ (total)		23.82	23.82	23.88	23.81	23.81	23.88	23.80	
	HCl		Cl	σ_{\perp} (para)	-237.4	-237.4	-240.2	-247.5	-247.7	-250.5
		σ_{\perp} (dia)		1146.7	1146.6	1146.5	1148.4	1148.4	1148.2	
σ_{\perp} (total)		909.3		909.2	906.2	900.9	900.7	897.7	888.5	
σ_{\parallel} (para)		52.1		52.1	49.8	32.0	31.9	29.5		
σ_{\parallel} (dia)		1143.9		1143.9	1143.7	1145.7	1145.6	1145.4		
σ_{\parallel} (total)		1196.0		1196.0	1193.5	1177.7	1177.5	1175.0	1176.7	
σ^{iso} (total)		1004.9		1004.8	1002.0	993.1	993.0	990.1	984.5	
$\Delta\sigma$ (total)		286.7		286.7	287.2	276.8	276.8	277.3	288.2	
H		σ_{\perp} (para)		22.49	22.49	22.32	22.49	22.49	22.32	
		σ_{\perp} (dia)	1.89	1.89	1.90	1.89	1.89	1.90		
		σ_{\perp} (total)	24.38	24.38	24.22	24.38	24.38	24.22	24.07	
		σ_{\parallel} (para)	-0.01	-0.01	0.00	-0.01	-0.01	0.00		
		σ_{\parallel} (dia)	45.38	45.38	45.42	45.38	45.38	45.42		
		σ_{\parallel} (total)	45.37	45.37	45.42	45.36	45.37	45.42	45.39	
		σ^{iso} (total)	31.37	31.38	31.29	31.37	31.38	31.29	31.18	
		$\Delta\sigma$ (total)	20.99	20.99	21.20	20.99	20.99	21.20	21.32	
		HBr	Br	σ_{\perp} (para)	-192.0	-176.1	-195.4	-279.0	-267.0	-286.1
σ_{\perp} (dia)				3086.4	3084.3	3082.9	3104.1	3102.5	3101.0	
σ_{\perp} (total)	2894.4			2908.2	2887.5	2825.1	2835.4	2814.9	2738.1	
σ_{\parallel} (para)	458.8			474.7	458.5	276.8	286.9	271.6		
σ_{\parallel} (dia)	3083.4			3081.3	3079.8	3101.1	3099.4	3098.0		

TABLE I. (Continued.)

Molecule	Nucleus	Property	ZORA ^a	SORA ^a	SORA+ J_{LL} ^a	ZORA-Met ^a	SORA-Met ^a	SORA+ J_{LL} -Met ^a	DHF ^b
		$\sigma_{\parallel}(\text{total})$	3542.1	3555.9	3538.3	3377.9	3386.3	3369.6	3402.1
		$\sigma^{\text{iso}}(\text{total})$	3110.3	3124.1	3104.5	3009.4	3019.1	2999.8	2959.4
		$\Delta\sigma(\text{total})$	647.8	647.8	650.8	552.8	550.9	554.7	664.0
	H	$\sigma_{\perp}(\text{para})$	30.12	30.12	29.53	30.12	30.12	29.53	
		$\sigma_{\perp}(\text{dia})$	-0.02	-0.02	0.00	-0.02	-0.02	0.00	
		$\sigma_{\perp}(\text{total})$	30.11	30.10	29.53	30.10	30.10	29.53	29.82
		$\sigma_{\parallel}(\text{para})$	-0.45	-0.45	-0.37	-0.46	-0.46	-0.38	
		$\sigma_{\parallel}(\text{dia})$	48.53	48.52	48.65	48.53	48.53	48.65	
		$\sigma_{\parallel}(\text{total})$	48.08	48.07	48.28	48.08	48.07	48.28	47.93
		$\sigma^{\text{iso}}(\text{total})$	36.10	36.09	35.78	36.09	36.09	35.78	35.86
		$\Delta\sigma(\text{total})$	17.97	17.97	18.75	17.98	17.97	18.74	18.11
HI	I	$\sigma_{\perp}(\text{para})$	578.8	879.8	816.8	298.4	537.5	474.7	
		$\sigma_{\perp}(\text{dia})$	5362.2	5345.4	5340.2	5428.8	5415.4	5410.1	
		$\sigma_{\perp}(\text{total})$	5941.0	6225.2	6157.0	5727.2	5952.9	5884.8	5571.9
		$\sigma_{\parallel}(\text{para})$	1615.7	1917.1	1872.8	972.3	1197.1	1153.3	
		$\sigma_{\parallel}(\text{dia})$	5358.9	5342.1	5336.9	5425.5	5412.1	5406.8	
		$\sigma_{\parallel}(\text{total})$	6974.6	7259.1	7209.6	6397.8	6609.2	6560.1	6597.1
		$\sigma^{\text{iso}}(\text{total})$	6285.6	6569.9	6507.9	5950.7	6171.7	6109.9	5913.7
		$\Delta\sigma(\text{total})$	1033.6	1033.9	1052.6	670.6	656.2	675.3	1025.2
	H	$\sigma_{\perp}(\text{para})$	50.94	50.95	49.44	50.94	50.95	49.45	
		$\sigma_{\perp}(\text{dia})$	-1.78	-1.82	-1.79	-1.78	-1.82	-1.79	
		$\sigma_{\perp}(\text{total})$	49.16	49.14	47.65	49.16	49.14	47.65	46.92
		$\sigma_{\parallel}(\text{para})$	-4.32	-4.32	-3.88	-4.32	-4.33	-3.89	
		$\sigma_{\parallel}(\text{dia})$	50.34	50.32	50.54	50.34	50.32	50.55	
		$\sigma_{\parallel}(\text{total})$	46.03	46.00	46.66	46.02	45.99	46.66	47.31
		$\sigma^{\text{iso}}(\text{total})$	48.12	48.09	47.32	48.12	48.09	47.32	47.05
		$\Delta\sigma(\text{total})$	-3.14	-3.14	-0.99	-3.14	-3.15	-0.99	0.39

^aCorrected values.^bDirac-Hartree-Fock results taken from Ref. 2.¹H. Maeda, Y. Ootani, and H. Fukui, *J. Chem. Phys.* **126**, 174102 (2007).²P. Manninen, K. Ruud, P. Lanto, and J. Vaara, *J. Chem. Phys.* **122**, 114107 (2005); *ibid.* **124**, 149901(E) (2006).