Supporting Information for the article in Journal of Chemical Theory and Computation:

^{1}H chemical shifts in paramagnetic Co(II) pyrazolylborate complexes: A first-principles study

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Table S1. Optimized geometry of system 1 in the .xyz format.

Atoms	*X*	*Y*	*Z*
B	0.248216952	2.742829284	-1.661246123
B	-0.249688074	-2.742030394	1.662565536
Co	0.000362663	0.00085606	0.00170871
C	-1.387569986	-0.247248543	-2.914001842
C	1.443284858	-2.493408289	-1.532859893
C	1.668104017	-3.862098312	-1.337107517
C	1.066601481	-4.137129777	-0.122809102
C	-3.097315368	-0.840321785	0.45522298
C	-3.830635421	-1.860369899	1.071522534
C	-2.868087336	-2.700575537	1.603219049
C	1.398817467	0.242406947	2.912639271
C	1.613438158	-0.55023483	4.045453709
C	1.02690895	-1.763484581	3.730390439
C	-1.595908351	0.541782065	-4.050505631
C	-1.014732713	1.757377732	-3.734390704
C	-1.450877398	2.493472075	1.530795957
C	-1.683782395	3.860126535	1.330180519
C	-1.080463463	4.135158337	0.116767696
C	3.097609138	0.846544137	-0.449034529
C	3.829883991	1.868466173	-1.063500023
C	2.866455563	2.707015449	-1.596191007
H	0.346354193	3.758773595	-2.290266881
H	4.899081881	1.98066388	-1.114110803
H	2.959652225	3.621379154	-2.157922461
H	1.740919975	-1.86002511	-2.353068746
H	2.189866788	-4.547587042	-1.982204278
H	0.984735691	-5.056376191	0.432655686
H	-3.444696484	0.026914854	-0.082838109
H	-4.899966994	-1.970418545	1.123841277
H	-2.962231895	-3.614448944	2.16560696
H	1.688580149	1.263439514	2.723433016
H	2.118019078	-0.281584369	4.957334053
H	-0.348445966	-3.758225076	2.291085314
H	0.943715008	-2.675126871	4.298079818
H	-1.675988654	-1.268549947	-2.724194999
H	-2.093307587	0.269486809	-4.965266333
H	-0.929649047	2.667687958	-4.303938733
H	-1.747018391	1.860708592	2.352046049
H	-2.211568626	4.544331527	1.971755123
H	-1.002726212	5.053172612	-0.441317529
H	3.445878758	-0.020271662	0.089167879
N	-0.504164252	1.674860162	-2.492285965
N	-1.790609099	-1.051148448	0.602935668
N	0.507343495	-1.676326793	2.492317854
N	0.734373861	-0.442759591	1.983648084
N	-0.731691965	0.442140065	-1.982059825
N	-0.533484367	2.9971734	-0.352648749
N	-0.759072523	1.984281817	0.514338952
N	1.653991976	2.200747935	-1.305946104
N	1.790709149	1.054900997	-0.598647105
N	0.528252765	-2.997132917	0.351751191
N	0.757576468	-1.982991276	-0.512873242
N	-1.655052132	-2.196822937	1.310772909

Table S2. Optimized geometry of system 2 in the .xyz format.

Atoms	*X*	*Y*	*Z*
Co	0.000098562	0.000014800	0.000014700
N	0.854285563	-1.930000000	-0.670000000
N	0.945358628	-2.080000000	-2.020000000
N	-1.496499462	-0.255000000	-1.600000000
N	-0.996336983	-0.666000000	-2.800000000
N	1.287376138	0.953000000	-1.520000000
N	1.328447164	0.317000000	-2.720000000
C	1.318826729	-3.050000000	-0.115000000
C	1.712045005	-3.950000000	-1.120000000
C	1.457433202	-3.290000000	-2.310000000
C	1.410125870	-3.250000000	1.360000000
C	-2.815721693	-0.097800000	-1.760000000
C	-3.171354521	-0.409000000	-3.090000000
C	-1.988242682	-0.763000000	-3.700000000
C	-3.724400586	0.319000000	-0.651000000
C	2.091292347	2.020000000	-1.610000000
C	2.664473008	2.070000000	-2.890000000
C	2.151778037	0.972000000	-3.560000000
C	2.282660618	2.990000000	-0.495000000
B	0.506900462	-0.963000000	-2.990000000
H	2.121987760	-4.930000000	-0.998000000
H	1.601544839	-3.590000000	-3.330000000
H	-4.154780187	-0.376000000	-3.520000000
H	-1.781490568	-1.070000000	-4.710000000
H	3.354368979	2.800000000	-3.270000000
H	2.313729317	0.612000000	-4.560000000
H	1.136669233	-4.270000000	1.630000000
H	2.430484308	-3.080000000	1.720000000
H	0.757122755	-2.560000000	1.900000000
H	-3.176566495	0.818000000	0.144000000
H	-4.496135159	0.995000000	-1.020000000
H	-4.232289427	-0.545000000	-0.215000000
H	1.968859082	2.570000000	0.456000000
H	3.331162356	3.290000000	-0.419000000
H	1.701820032	3.900000000	-0.665000000
H	0.696944960	-1.320000000	-4.120000000
N	-0.854098024	1.930000000	0.670000000
N	-0.945170238	2.080000000	2.020000000
C	-1.457586447	3.290000000	2.310000000
C	-1.712394265	3.950000000	1.120000000
C	-1.318913252	3.050000000	0.115000000
C	-1.410225007	3.250000000	-1.360000000
H	-1.137717321	4.270000000	-1.630000000
H	-2.430369676	3.080000000	-1.720000000
H	-0.756495280	2.560000000	-1.900000000
H	-2.122608157	4.930000000	0.998000000
H	-1.601776384	3.590000000	3.330000000
B	-0.506752743	0.963000000	2.990000000
N	0.996480375	0.666000000	2.800000000
N	1.496630661	0.255000000	1.600000000
N	-1.287217546	-0.953000000	1.520000000
N	-1.328343770	-0.317000000	2.720000000
C	-2.151929646	-0.971000000	3.560000000
C	-2.664685918	-2.070000000	2.890000000
C	-2.091263333	-2.020000000	1.610000000
C	-2.282508777	-2.990000000	0.495000000
H	-1.967477107	-2.570000000	-0.456000000
H	-3.331206159	-3.280000000	0.419000000
H	-1.702645915	-3.900000000	0.666000000
H	-3.354756054	-2.800000000	3.270000000
H	-2.314010223	-0.611000000	4.560000000
H	-0.696804685	1.320000000	4.120000000
C	2.815845072	0.097700000	1.760000000
C	3.171486652	0.409000000	3.090000000
C	1.988390172	0.763000000	3.700000000
H	1.781650328	1.070000000	4.710000000
H	4.154902541	0.375000000	3.520000000
C	3.724467355	-0.319000000	0.651000000
H	3.176652938	-0.818000000	-0.143000000
H	4.496489530	-0.994000000	1.020000000
H	4.231983115	0.545000000	0.215000000

Table S3. Optimized geometry of system 3 in the .xyz format (will be continued on the next page).

Atoms	*X*	*Y*	*Z*
Co	-0.000129223	-0.001333126	-0.001970839
S	0.078310074	3.809976356	4.400986017
S	-1.853940831	-5.370819798	0.132609748
S	-0.730127783	-1.57121898	3.763762464
N	2.213742961	0.139411037	2.061692729
N	1.073288754	0.839747376	1.826295313
N	1.609167497	-2.206880727	1.311026927
N	0.356288749	-2.090546194	0.798743262
N	-2.906911821	0.694963511	0.239443691
N	-1.930858756	0.230612817	1.06570758
C	1.027317738	1.804853189	2.776364408
C	2.159414272	1.699809129	3.609092054
C	2.8733546	0.636842461	3.120540541
C	-0.007088647	2.816650268	2.967396147
C	-1.096203447	3.185538545	2.221627294
C	-1.845101734	4.247633638	2.787303503
C	-1.328309599	4.688748068	3.970118412
C	-0.217655465	-3.307508786	0.925858809
C	0.688423594	-4.194605264	1.53923974
C	1.825032677	-3.455437737	1.757750367
C	-1.551165575	-3.689324815	0.475309625
C	-2.694974583	-2.961604317	0.275167045
C	-3.800490979	-3.74564652	-0.140736693
C	-3.495499489	-5.07040667	-0.258256103
C	-2.494398988	0.112486319	2.288523148
C	-3.846599839	0.496572495	2.223140042
C	-4.055810836	0.862169283	0.914646521
C	-1.855072909	-0.275223348	3.544494352
C	-2.16464226	0.288299201	4.761521866
C	-1.493063772	-0.311119046	5.852715269
C	-0.682241129	-1.337196034	5.459721477
B	2.652713005	-1.075839862	1.241814346
H	3.681965615	-1.486402411	1.698931502
H	2.415678851	2.326469576	4.445084482
H	3.801667111	0.198598	3.444538993
H	-1.350235909	2.71250055	1.291199648
H	-2.729913868	4.666135841	2.32842972
H	-1.689884209	5.480151699	4.606805302
H	0.515047081	-5.224180042	1.799519854
H	2.770884243	-3.724817932	2.196248351
H	-2.745319788	-1.899243683	0.435171829
H	-4.781526895	-3.338728137	-0.342526253
H	-4.138902953	-5.881911362	-0.558049721
H	-4.560264109	0.481046485	3.027623904
H	-4.937606053	1.222989766	0.412996179
H	-2.836213744	1.129694587	4.855850485
H	-1.599496641	0.011497506	6.87879224
H	-0.050060354	-1.961573932	6.070859616
N	-1.077031303	-0.840917168	-1.824433585
N	-0.360504248	2.090161203	-0.80053507
N	1.930628624	-0.237525034	-1.063901495
B	-2.657234142	1.074955692	-1.236528591
N	2.906778671	-0.694416265	-0.233479335
N	-2.216815547	-0.139015855	-2.058343682
C	-1.033408445	-1.806150174	-2.774504626
N	-1.615711204	2.207899253	-1.306991122
C	0.21249968	3.307882453	-0.926470555
C	2.497464894	-0.118220345	-2.285008357
H	-3.688214579	1.483535419	-1.69144479
C	4.058623306	-0.85647482	-0.904681751
C	-2.87874723	-0.636463999	-3.115799536
C	-2.16641111	-1.699889322	-3.605690427
C	0.004112513	-2.813736127	-2.970817179
C	-1.833232402	3.456990518	-1.751210217
C	-0.695715288	4.195848494	-1.535170527
C	1.54765912	3.688306352	-0.480202109
C	3.851430955	-0.495548392	-2.214734013
C	1.860738756	0.26786852	-3.542674361
H	4.940412953	-1.212862782	-0.399832692
H	-3.80743622	-0.19779462	-3.438115332

(Table S3 continued.)

Atoms	X	Y	Z
H	-2.424487847	-2.326799645	-4.4409409
S	-0.070308104	-3.790278022	-4.41640618
C	1.090604523	-3.187539421	-2.22364463
H	-2.781107864	3.727162291	-2.184796797
H	-0.523677426	5.22608733	-1.793806834
S	1.858548766	5.371474849	-0.153075807
C	2.687547893	2.956817216	-0.271657988
H	4.567850916	-0.477213357	-3.016716441
S	0.723739767	1.553435213	-3.762453857
C	2.181944113	-0.287540795	-4.760452037
C	1.336607711	-4.669773032	-3.988122339
C	1.845774711	-4.240734441	-2.797539465
H	1.338524409	-2.723923802	-1.286860597
C	3.498007234	5.066403986	0.243168786
C	3.796377962	3.739060716	0.138622064
H	2.732406248	1.892745279	-0.421233893
C	0.686900589	1.325850609	-5.459553664
C	1.509979076	0.309605721	-5.8525937
H	2.862220813	-1.121903291	-4.854894896
H	1.70401059	-5.45272513	-4.631878234
H	2.729504429	-4.661794703	-2.338896602
H	4.14508141	5.877449385	0.536204288
H	4.775010068	3.329130777	0.345804445
H	0.051628964	1.946385247	-6.071402624
H	1.624838662	-0.007644961	-6.879427939

Table S4. ^{1}H shielding constant (in ppm) of the diamagnetic reference molecule TMS at DFT(PBE and PBE0) level with SVP, TZVP, and QZVPP basis sets.

Basis	DFT(PBE)	DFT(PBE0)
SVP	31.5	31.6
TZVP	31.7	31.8
QZVPP	31.5	31.5

Table S5. g, D (in units of cm^{-1}), and E/D values at DFT, CASSCF, and NEVPT2 levels for system 1.

	DFT (PBE)[a]		CASSCF/DFT (PBE)[b]		NEVPT2/DFT (PBE)[c]	
Quantities	SVP	TZVP	SVP	TZVP*	SVP	TZVP*
D[d]	-6.459	-7.009	-112.384	-111.864	-112.990	-112.282
E/D	0.212	0.215	0.162	0.181	0.128	0.140
g_{iso}	2.074	2.076	2.103	2.102	2.116	2.119

[a] D, E/D, and g_{iso} values calculated at the DFT(PBE) level at the experimental geometry.
[b] D, E/D, and g_{iso} values calculated at the CASSCF/PBE level at the experimental geometry. The locally dense TZVP* basis was used in the calculation denoted as CASSCF/TZVP*.
[c] D, E/D, and g_{iso} values calculated at the NEVPT2/PBE level at the experimental geometry. The locally dense TZVP* basis was used in the calculation denoted as NEVPT2/TZVP*.
[d] D and E values are calculated from the principal values $D_{ii}(i = 1, 2, 3)$ of the traceless ZFS tensor as

$$D = D_{33} - 1/2(D_{11} + D_{22}) \tag{1}$$

and

$$E = 1/2(D_{11} - D_{22}) \tag{2}$$

with the eigenvalues numbered in such a way that the following relation is satisfied:

$$0 \leq E/D \leq 1/3. \tag{3}$$

The sign of D can be positive or negative depending on the assignment [1].

Table S6. Proton chemical shifts for system 1. Comparison between experimental and calculated chemical shifts at both experimental and optimized geometry.

Wavefunction for $\boldsymbol{g}$, $\boldsymbol{D}$/DFT functional for $\boldsymbol{A}$	Basis $\boldsymbol{g}$, $\boldsymbol{D}$/$\boldsymbol{A}$	Nucleus							
		3-H	Exp.[a]	4-H	Exp.	5-H	Exp.[a]	B-H	Exp.
Experimental geometry									
CASSCF/PBE	SVP/SVP	96.6	94.2	41.4	42.0	-74.2	-111.0	133.4	122.0
	TZVP*/TZVP	110.4		50.8		-82.9		130.5	
NEVPT2/PBE	SVP/SVP	96.9		41.6		-74.1		133.5	
	TZVP*/TZVP	110.8		51.2		-82.5		130.4	
CASSCF/PBE0	SVP/SVP	83.9		25.9		-93.9		139.6	
	TZVP*/TZVP	93.2		32.1		-100.2		137.0	
NEVPT2/PBE0	SVP/SVP	84.2		26.1		-93.8		139.7	
	TZVP*/TZVP	93.5		32.5		-100.0		136.9	
Optimized geometry									
CASSCF/PBE	SVP/SVP	98.8	94.2	49.9	42.0	-60.7	-111.0	123.5	122.0
	TZVP*/TZVP	111.4		60.3		-68.5		119.7	
NEVPT2/PBE	SVP/SVP	99.8		49.8		-62.7		125.5	
	TZVP*/TZVP	112.5		60.2		-70.3		121.6	
CASSCF/PBE0	SVP/SVP	86.2		31.6		-84.5		129.4	
	TZVP*/TZVP	94.6		38.4		-90.1		126.5	
	QZVPP*/QZVPP	94.9		40.1		-89.0		124.7	
NEVPT2/PBE0	SVP/SVP	87.2		31.4		-86.6		131.4	
	TZVP*/TZVP	95.5		38.3		-92.2		128.5	
	QZVPP*/QZVPP	95.8		40.0		-90.9		126.6	
CASSCF/PBE50	SVP/SVP	81.5		19.9		-96.5		133.9	
	TZVP*/TZVP	82.4		19.8		-98.7		136.0	
NEVPT2/PBE50	SVP/SVP	87.6		24.8		-101.1		131.8	
	TZVP*/TZVP	88.4		24.7		-103.2		133.8	

[a] The original signal assignment has been interchanged between these nuclei as a result of comparison with the present calculations.

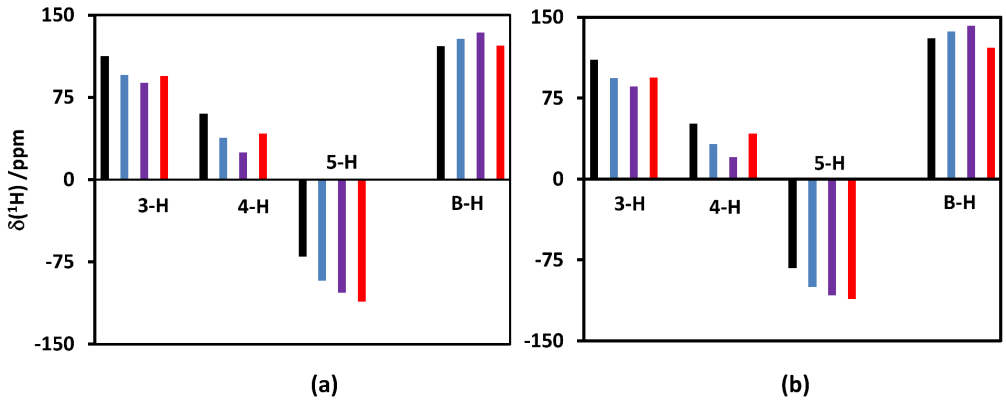


Figure S1. Comparison between calculated ^{1}H chemical shift with different functionals: PBE (black color), PBE0 (blue), and PBE50 (purple), with experimental data (red), for system 1. (a) Optimized structure; (b) x-ray structure. In these cases, the g- and $\boldsymbol{D}$ tensors were calculated at the NEVPT2 level with the TZVP* basis set and the $\boldsymbol{A}$ tensor was calculated at the DFT(PBE0) level with the TZVP basis set.

Table S7. Proton chemical shifts for system 2. Comparison between experimental and calculated chemical shifts at both experimental and optimized geometry.

		Nucleus							
Wavefunction for $\boldsymbol{g}$, $\boldsymbol{D}$/DFT functional for $\boldsymbol{A}$	Basis $\boldsymbol{g}$, $\boldsymbol{D}$/$\boldsymbol{A}$	3-H	Exp.	4-H	Exp.	5-H	Exp.	B-H	Exp.
Experimental geometry									
CASSCF/PBE	SVP/SVP	-91.1	-100.1	44.2	49.5	88.9	2.2	138.2	90.0
	TZVP*/TZVP	-86.5		54.5		99.1		134.5	
NEVPT2/PBE	SVP/SVP	-92.7		44.2		90.0		140.6	
	TZVP*/TZVP	-88.0		54.6		100.3		136.8	
CASSCF/PBE0	SVP/SVP	-97.8		27.6		78.6		144.7	
	TZVP*/TZVP	-95.0		34.7		87.5		140.9	
NEVPT2/PBE0	SVP/SVP	-99.4		27.5		79.6		147.2	
	TZVP*/TZVP	-96.6		34.7		88.5		143.2	
Optimized geometry									
CASSCF/PBE	SVP/SVP	-78.0	-100.1	49.9	49.5	87.2	2.2	121.5	90.9
	TZVP*/TZVP	-73.4		61.5		95.9		116.8	
NEVPT2/PBE	SVP/SVP	-80.9		49.5		89.3		126.4	
	TZVP*/TZVP	-76.5		61.2		98.2		122.0	
CASSCF/PBE0	SVP/SVP	-83.8		31.9		78.0		128.1	
	TZVP*/TZVP	-82.3		39.3		83.6		123.6	
NEVPT2/PBE0	SVP/SVP	-86.8		31.5		80.0		133.1	
	TZVP*/TZVP	-85.5		38.9		85.9		128.9	
CASSCF/PBE50	TZVP*/TZVP	-87.5		26.1		79.0		128.2	
NEVPT2/PBE50	TZVP*/TZVP	-90.9		25.7		81.2		133.6	

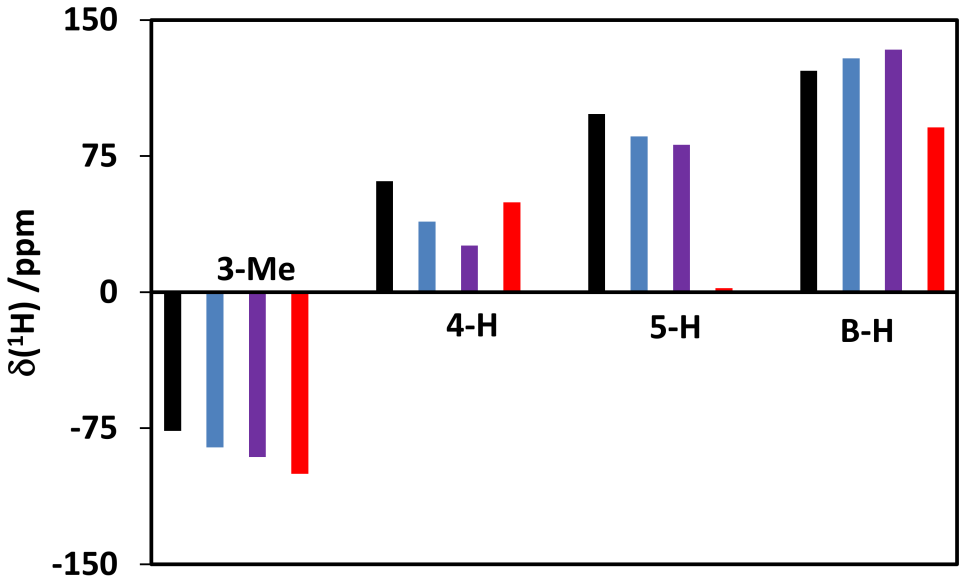


Figure S2. Comparison between calculated ^{1}H chemical shift with different functionals: PBE (black color), PBE0 (blue), and PBE50 (purple), with experimental data (red), for system 2 at the optimized structure. The g- and $\boldsymbol{D}$ tensors were calculated at the NEVPT2 level with the TZVP* basis set and the $\boldsymbol{A}$ tensor was calculated at the DFT(PBE0) level with the TZVP basis set.

Table S8. Proton chemical shifts for system 3. Comparison between experimental and calculated chemical shifts at both experimental and optimized geometry.

		Nucleus											
Wavefunction for $\boldsymbol{g}$, $\boldsymbol{D}$/DFT functional for $\boldsymbol{A}$	Basis $\boldsymbol{g}$, $\boldsymbol{D}$/$\boldsymbol{A}$	3-H′	Exp.[a]	4-H′	Exp.	5-H′	Exp.[a]	4-H	Exp.[a]	5-H	Exp.[a]	B-H	Exp.
Experimental geometry													
CASSCF/PBE	SVP/SVP	-9.4	-0.7	-5.8	0.2	-45.0	-25.1	69.9	65.4	47.0	47.5	108.5	83.3
	TZVP*/TZVP	-7.2		-4.2		-44.0		72.8		60.7		99.7	
NEVPT2/PBE	SVP/SVP	-10.3		-6.5		-45.3		73.4		45.9		117.6	
CASSCF/PBE0	SVP/SVP	-2.3		-7.1		-43.6		64.4		28.8		115.5	
	TZVP*/TZVP	-4.6		-5.7		-44.1		66.4		38.5		105.6	
NEVPT2/PBE0	SVP/SVP	-3.1		-7.8		-43.7		68.0		27.9		124.8	
Optimized geometry													
CASSCF/PBE	SVP/SVP	-3.3	-0.7	0.8	0.2	-25.3	-25.1	70.9	65.4	58.5	47.5	96.2	83.3
	TZVP*/TZVP	-2.7		1.2		-25.5		73.9		72.9		89.3	
NEVPT2/PBE	SVP/SVP	-4.0		0.2		-26.6		74.0		58.1		103.2	
	TZVP*/TZVP	-3.4		0.7		-26.6		77.4		72.4		97.2	
CASSCF/PBE0	SVP/SVP	0.8		0.3		-20.2		80.7		38.2		112.3	
	TZVP*/TZVP	-0.8		0.6		-22.3		69.5		48.2		95.8	
NEVPT2/PBE0	SVP/SVP	0.2		-0.3		-21.5		83.6		37.8		119.7	
	TZVP*/TZVP	-1.6		0.0		-23.4		72.8		47.7		103.9	

[a] The original signal assignment has been interchanged among these nuclei as a result of comparison with the present calculations.

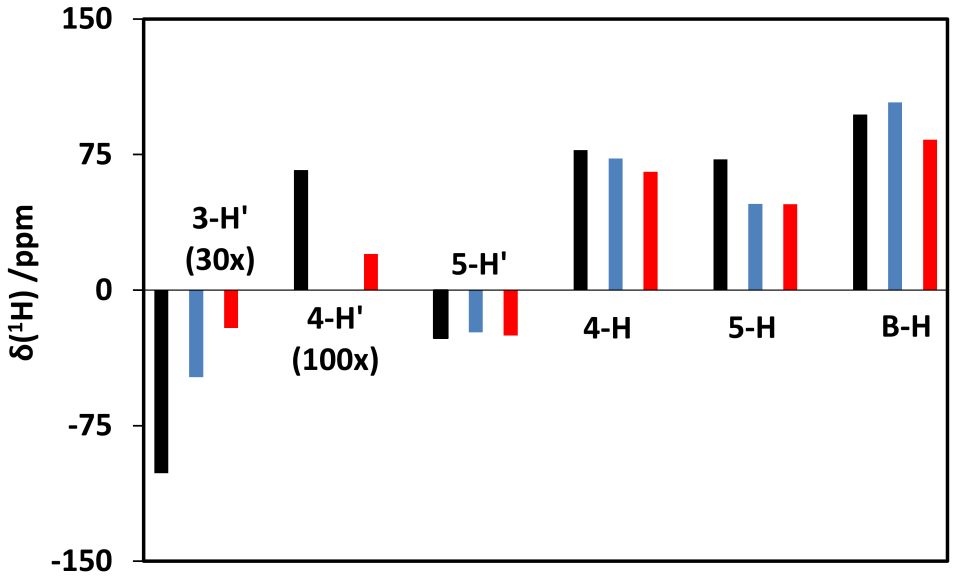


Figure S3. Comparison between calculated ^{1}H chemical shift with different functionals: PBE (black color) and PBE0 (blue), with experimental data (red), for system 3 at the optimized structure. The g- and $\boldsymbol{D}$ tensors were calculated at the NEVPT2 level with the TZVP* basis set and the $\boldsymbol{A}$ tensor was calculated at the DFT(PBE0) level with the TZVP basis set.

Table S9. Physical contributions to the total proton chemical shift for system 1 at the optimized geometry at the NEVPT2(TZVP*)/PBE0(TZVP) level.[a]

Term	3-H	4-H	5-H	B-H
orb	8.8	6.8	6.8	6.8
1st	26.0	36.2	31.3	-11.6
2nd	21.0	-4.3	-50.7	50.9
3rd	1.3	0.0	-2.9	2.7
4th	1.4	-0.2	-3.6	3.3
5th	0.0	0.0	0.0	0.0
6th	1.4	2.0	1.7	-0.6
7th	1.2	-0.2	-2.8	2.8
8th	3.2	4.5	3.9	-1.4
9th	31.2	-6.3	-75.9	75.7
Total	95.5	38.3	-92.2	128.5

[a] See Figure 1 for the labeling of the nuclei and Table 1 for the numbering of the physical terms.

Table S10. Physical contributions to the total proton chemical shift for system 2 at the optimized geometry at the NEVPT2(TZVP*)/PBE0(TZVP) level.[a]

Term	3-Me	4-H	5-H	B-H
orb	0.8	6.8	8.8	6.8
1st	-2.9	36.1	18.4	-11.8
2nd	-30.2	-3.2	20.4	49.4
3rd	-1.4	0.1	1.1	1.9
4th	-1.9	-0.2	1.3	3.0
5th	0.0	0.0	0.0	0.0
6th	0.0	0.3	0.1	-0.1
7th	-0.2	0.0	0.2	0.4
8th	-0.4	4.6	2.3	-1.5
9th	-49.3	-5.4	33.4	80.7
Total	-85.5	38.9	85.9	128.9

[a] See Figure 1 for the labeling of the nuclei and Table 1 for the numbering of the physical terms.

Table S11. Physical contributions to the total proton chemical shift for system 3 at the optimized geometry at the CASSCF(TZVP*)/PBE0(TZVP) level.[a]

Term	3-H′	4-H′	5-H′	4-H	5-H	B-H
orb	7.8	6.8	5.8	8.8	6.8	6.8
1st	0.0	-0.6	1.6	14.1	37.7	-12.9
2nd	-3.4	-2.3	-13.7	18.3	-1.3	43.4
3rd	-0.1	-0.1	-0.9	0.9	0.0	1.5
4th	-0.2	-0.1	-0.7	1.1	-0.1	2.7
5th	0.0	0.0	0.0	0.0	0.0	0.0
6th	0.0	-0.1	0.1	1.3	3.5	-1.2
7th	-0.3	-0.2	-1.3	1.7	-0.1	4.0
8th	0.0	-0.1	0.1	1.3	3.4	-1.2
9th	-5.3	-3.3	-14.5	25.5	-2.1	60.7
Total	-1.6	0.0	-23.4	72.8	47.7	103.9

[a] See Figure 1 for the labeling of the nuclei and Table 1 for the numbering of the physical terms.

References

[1] Boča, R. *Coord. Chem. Rev.* **2004**, *248*, 757.