Supporting Information for

Exploring New ^{129}Xe Chemical Shift Ranges in HXeY Compounds: Hydrogen More Relativistic than Xenon

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Computational methods in more detail.

Basis sets. The AIV set is based on the HIV (IGLO-IV) Huzinaga/Kutzelnigg basis sets [1, 2] for C, N, O, F, S, Cl, and H, and on the Fægri-IV (FIV) basis sets, which use primitive exponents from ref.[3] for Br, I, and Xe, contracted and polarized in the same manner as the HIV sets. The AIVd3 basis sets are based on the AIV basis sets modified in the following manner: a) three diffuse *s*, *p*, *d* sets of exponents were added by dividing the most diffuse existing exponent for each *l*-value by the factor of three and, b) the *f* functions present in the original AIV basis set were split so that the ratio between two consecutive coefficients was three. Additional details can be found in the earlier methodological study, ref. [4]

BPPT calculations. The basis set denoted as AIVut(6/2) was used, where the AIVu6 basis sets with six sets of tight basis functions for occupied atomic shells were added upon the uncontracted AIV basis set for 3rd row and heavier atoms (S, Cl, Br, I, and Xe). The HIVu2 basis with two sets of tight functions were used for the lighter, first- and second-row atoms (H, C, N, O, and F).[5] The BPPT calculations used common gauge origin (CGO) at the Xe atom. The error induced was estimated in HXeI by placing CGO at I, resulting in changes of about 3 and 1 ppm in the Xe and H1 shifts, respectively. While most of the BPPT calculations were done with DFT, an *ab initio* multiconfiguration self-consistent field (MCSCF) calculation for HXeI was carried out with the AIII basis set using the (26 12 12 4/18 8 8 2/8 4 4 2/1 0 0 0/8 4 4 4) active space with 36 active electrons in the (HF/inactive/RAS1/RAS2/RAS3) notation in the C_{2v} point group (symmetry species in the order A_1, B_1, B_2, and A_2). In the RAS1 subspace, excitations of 0 to 4 electrons from the valence occupied orbitals (in the HF determinant) and up to 2 electrons to virtual orbitals in the RAS3 subspace were allowed. The relative basis set corrections from AIII to AIVut6 basis was estimated at the DFT(BHandHLYP) level to BPPT-5 (BPPT-5+SOS of shielding anisotropy) contribution and added to the MCSCF results. Basis set corrections are: δ(Xe) = +6.7, δ(H1) = -1.8, $\Delta\sigma$(Xe) = +21.5, and $\Delta\sigma$(H1) = -2.7 ppm.

Shielding anisotropy in linear molecules. The anisotropic parameters of the shielding tensors are only treated in the case of linear molecules, for which only the shielding anisotropy (-CSA) is of significance. This is because there exist no general implementation of the purely anisotropic relativistic spin-Zeeman SO correction [6] that can only be computed rigorously for the special case of a linear molecule from the component of the SD-I(1) tensor [4] parallel to the symmetry axis.

Table S1. Calculated nuclear magnetic shieldings in reference molecules. In ppm.

Species	Nucleus	MP2/AIV	MP2/AIVd3	CCSD(T)/AIV	BPPT/BHandHLYP/AIVut(6/2)
Xe	Xe	5642.2	5642.0	5642.2	1103.6
CH_4	C	199.3	199.4	197.5	1.1
CH_4	H	31.1	31.1	31.2	0.0
NH_3	N	274.1	273.8	268.4	1.8
CH_3F	F	483.5	483.9	476.9	4.1

Table S2. Calculated harmonic vibrational frequencies (in cm^{-1}) for the series of novel Xe compounds.

Species	Level	ω1	ω2	ω3	ω4	ω5	ω6	ω7	ω8	ω9	ω10	ω11
HXeF	CCSD(T)/aug-cc-pVTZ	1970	449									
	CCSD(T)/aug-cc-pVQZ	1967	455									
HXeCl	CCSD(T)/aug-cc-pVTZ	1763	169									
HXeBr	CCSD(T)/aug-cc-pVTZ	1623	189									
HXeI	CCSD(T)/aug-cc-pVTZ	1351	151									
HXeH	CCSD(T)/aug-cc-pVTZ	1216	1139									
	CCSD(T)/aug-cc-pVQZ	1228	1135									
HXeCCH	CCSD(T)/aug-cc-pVTZ	3422	1990	1583	649	630	305					
HXeCCXeH	CCSD(T)/aug-cc-pVTZ	1992	1529	1450	632	629	414	122	110	51		
HXeCCCCH	CCSD(T)/aug-cc-pVTZ	3449	2203	2032	1625	928	638	591	465	224	222	53
HXeCCCN	CCSD(T)/aug-cc-pVTZ	2280	2081	1703	913	636	503	226	212	61		
HXeCN	CCSD(T)/aug-cc-pVTZ	2141	1713	635	283	141						
HXeNC	CCSD(T)/aug-cc-pVTZ	2064	1957	612	305	88						
HXeOH	CCSD(T)/aug-cc-pVTZ	3791	1705	820	619	577	433					
HXeOXeH	CCSD(T)/aug-cc-pVTZ	1620	1508	649	610	608	603	499	312	59		
HXeSH	CCSD(T)/aug-cc-pVTZ	2683	1272	625	508	449	246					
ClXeCN	CCSD(T)/aug-cc-pVTZ	2165	333	294	282	86						
ClXeNC	CCSD(T)/aug-cc-pVTZ	2047	358	301	204	75						

Table S3. Calculated contributions to the chemical shifts, δ, in novel Xe molecules. In ppm. Shielding values of the reference molecules are given in Table S1.

Compound	Atom	NR shift[a]	Basis corr.[b]	Rel. corr.[c]	Total
HXeH	H1	9.7	0.2	-5.6	4.3
	Xe2	693.8	-1.8	9.8	701.9
HXeF	H1	3.9	0.3	-15.9	-11.8
	Xe2	979.4	11.3	-1.3	989.5
	F3	329.4	1.8	-17.4	313.8
HXeCl	H1	7.2	0.2	-12.7	-5.4
	Xe2	672.9	13.2	-17.9	668.3
	Cl3	391.6	-35.2	-32.7	323.7
HXeBr	H1	8.5	0.2	-27.2	-18.5
	Xe2	573.4	7.1	-58.5	522.0
	Br3	1904.5	-20.5	-85.2	1798.8
HXeI	H1	10.6	0.2	-141.7	-130.9
	Xe2	396.2	8.8	-624.7	-219.7
	I3	3401.8	-12.0	-354.0	3035.9
HXeCN	H1	6.5	0.3	-12.3	-5.5
	Xe2	884.4	10.2	24.0	918.6
	C3	140.0	-0.2	-4.9	135.0
	N4	270.8	1.3	5.0	277.1
HXeNC	H1	4.4	0.3	-14.8	-10.1
	Xe2	961.1	13.1	19.7	993.8
	N3	256.4	-0.1	-5.5	250.7
	C4	160.3	0.7	1.5	162.4
HXeCCH	H1	7.1	0.3	-10.8	-3.4
	Xe2	811.6	5.5	14.3	831.4
	C3	116.7	-0.4	-6.7	109.7
	C4	67.3	0.3	3.7	71.2
	H5	0.5	-0.1	0.5	1.0
HXeCCCN	H1	6.6	0.3	-11.4	-4.5
	Xe2	845.3	9.0	18.2	872.6
	C3	121.1	0.8	-3.8	118.1
	C4	63.2	0.6	4.0	67.8
	C5	112.2	0.2	1.8	114.3
	N6	257.1	0.4	-0.2	257.4
HXeCCCCH	H1	6.9	0.3	-11.1	-3.9
	Xe2	824.9	7.2	14.3	846.3
	C3	114.3	0.5	-5.0	109.9
	C4	70.3	0.6	3.4	74.4
	C5	74.6	0.2	1.7	76.6
	C6	61.8	0.3	-0.3	61.8
	H7	0.7	0.0	0.2	0.9

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Table S3. Continues…

Compound	Atom	NR shift[a]	Basis corr.[b]	Rel. corr.[c]	Total
HXeCCXeH	H1	7.5	0.2	-10.2	-2.5
	Xe2	810.2	2.3	13.3	825.9
	C3	102.8	0.3	-6.0	97.2
HXeOXeH	H1	6.7	0.2	-16.8	-9.9
	Xe2	935.8	-1.1	-36.1	898.6
	O3	100.3	7.2	-2.9	104.7
HXeOH	H1	6.0	0.2	-15.3	-9.0
	Xe2	879.9	5.2	-19.4	865.6
	O3	-169.4	-0.5	-11.5	-181.4
	H4	2.3	0.0	-0.6	1.6
HXeSH	H1	2.6	0.2	-13.2	-10.5
	Xe2	498.1	-1.0	-48.5	448.6
	S3	376.9	-19.7	-19.5	337.7
	H4	10.5	-0.1	-1.7	8.7
ClXeCN	Cl1	398.4	-6.9	6.8	398.3
	Xe2	1116.5	27.7	22.1	1166.2
	C3	114.0	-0.6	-38.2	75.2
	N4	278.0	0.5	-1.2	277.2
ClXeNC	Cl1	326.5	-3.8	54.6	377.3
	Xe2	1583.0	49.3	6.7	1639.0
	N3	187.2	-0.8	-14.0	172.4
	C4	165.6	0.2	-3.7	162.1

[a] Nonrelativistic calculation at the CCSD(T)/AIV level. [b] Basis-set correction calculated as the difference MP2/AIVd3 – MP2/AIV. [c] Perturbational relativistic (BPPT) correction at the BHandHLYP/AIVut(6/2) level.

Table S4. Relativistic BPPT corrections to chemical shift, δ, in novel Xe molecules. In ppm.

			BPPT		REL-*p*			SO-I	
Compound	Atom	BPPT[a]	REL-*p*[b]	SO-I[c]	*p*-KE/OZ	*p*/mv	*p*/Dar	FC-I(1)	SD-I(1)
HXeH	H1	-5.6	-0.1	-5.4	0.0	-1.2	1.0	-5.2	-0.2
	Xe2	9.8	29.0	-19.0	-72.1	119.0	-17.9	5.1	-24.1
HXeF	H1	-15.9	0.1	-16.0	0.0	-0.3	0.4	-15.5	-0.5
	Xe2	-1.3	91.5	-92.7	-129.9	288.9	-67.5	-52.4	-40.3
	F3	-17.1	-26.5	9.6	-0.8	-90.4	64.7	6.2	3.3
HXeCl	H1	-12.7	0.1	-12.9	-0.1	-0.4	0.5	-12.5	-0.4
	Xe2	-17.9	46.3	-64.3	-77.8	184.1	-60.0	-24.2	-40.2
	Cl3	-30.3	-42.0	11.7	-4.0	-157.9	120.0	4.0	7.8
HXeBr	H1	-27.2	0.1	-27.4	-0.3	0.1	0.3	-27.0	-0.4
	Xe2	-58.5	31.7	-90.5	-63.0	133.4	-38.6	-58.2	-32.3
	Br3	-62.7	-51.9	-10.9	-37.8	-257.0	242.8	10.7	-21.6
HXeI	H1	-141.7	0.2	-142.0	-0.6	0.9	0.0	-140.9	-1.1
	Xe2	-624.0	9.4	-633.9	-36.5	39.7	6.2	-586.5	-47.3
	I3	-262.8	34.3	-297.6	-118.3	-181.1	333.7	32.4	-330.1
HXeCN	H1	-12.3	0.0	-12.4	0.0	-0.5	0.5	-12.0	-0.4
	Xe2	24.0	73.5	-49.4	-115.0	219.3	-30.9	-21.5	-27.9
	C3	-4.9	-0.6	-4.0	-0.3	-2.9	2.6	-4.0	0.0
	N4	5.0	5.6	-0.9	-0.2	17.8	-12.0	-2.1	1.1
HXeNC	H1	-14.8	0.0	-14.9	0.0	-0.3	0.3	-14.5	-0.5
	Xe2	19.7	97.8	-78.1	-132.7	282.8	-52.3	-45.2	-32.9
	N3	-5.5	-6.0	0.7	-0.5	-20.9	15.4	0.5	0.2
	C4	1.5	2.6	-1.4	0.0	8.9	-6.2	-2.0	0.6
HXeCCH	H1	-10.8	0.0	-10.8	0.0	-0.7	0.7	-10.5	-0.3
	Xe2	14.2	52.6	-38.2	-95.9	175.9	-27.5	-8.6	-29.6
	C3	-6.7	-1.1	-5.4	-0.2	-6.8	5.9	-5.0	-0.4
	C4	3.7	2.7	1.0	-0.1	8.6	-5.9	-0.2	1.2
	H5	0.5	0.1	0.5	0.1	0.0	-0.1	0.4	0.1
HXeCCCN	H1	-11.4	-10.6	0.4	0.0	0.5	-11.1	-0.4	0.7
	Xe2	18.2	63.3	-44.9	-105.4	199.3	-30.6	-15.4	-29.6
	C3	-3.8	-0.3	-3.2	-0.3	-5.3	5.2	-2.7	-0.5
	C4	4.0	2.5	1.5	-0.2	7.5	-4.8	0.5	1.0
	C5	1.8	0.0	1.8	-0.2	0.1	0.1	1.6	0.2
	N6	-0.1	-1.5	0.5	0.0	-2.7	1.2	-0.7	1.1

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Table S4. Continues…

			BPPT		REL-p			SO-I	
Compound	Atom	BPPT[a]	REL-p[b]	SO-I[c]	p-KE/OZ	p/mv	p/Dar	FC-I(1)	SD-I(1)
HXeCCCCH	H1	-11.1	0.0	-11.2	0.0	-0.7	0.6	-10.8	-0.4
	Xe2	14.2	56.4	-42.1	-99.1	185.4	-29.8	-11.6	-30.5
	C3	-5.0	-0.7	-3.9	-0.2	-6.6	6.1	-3.4	-0.5
	C4	3.4	2.6	0.8	-0.2	8.1	-5.3	-0.3	1.1
	C5	1.7	0.2	1.6	-0.1	0.2	0.0	1.8	-0.1
	C6	-0.3	-0.5	0.1	0.0	-1.2	0.7	-0.6	0.7
	H7	0.2	0.0	0.2	0.2	-0.2	0.0	0.2	0.0
HXeCCXeH	H1	-10.2	0.0	-10.3	-0.5	-0.2	0.8	-10.0	-0.3
	Xe2	13.3	51.3	-37.8	-95.1	177.6	-31.3	-7.8	-30.1
	C3	-6.0	1.7	-7.9	-2.5	7.1	-2.8	-8.7	0.8
HXeOXeH	H1	-16.8	0.2	-17.1	-0.7	0.1	0.8	-16.7	-0.4
	Xe2	-36.0	57.6	-93.8	-110.4	245.6	-77.6	-46.6	-47.2
	O3	-2.9	-21.0	18.0	-3.8	-127.2	110.1	15.8	2.2
ClXeCN	Cl1	9.2	-16.5	25.8	-4.3	-141.0	128.8	-1.3	27.1
	Xe2	22.0	100.0	-77.8	-166.5	353.2	-86.7	2.3	-80.1
	C3	-38.2	0.6	-38.7	-0.3	2.6	-1.7	-39.0	0.3
	N4	-1.2	1.3	-3.0	-0.3	10.4	-8.8	-5.1	2.1
ClXeNC	Cl1	56.8	5.1	51.9	-3.3	-112.8	121.2	-3.0	54.8
	Xe2	6.8	154.0	-147.3	-258.1	522.0	-109.9	3.6	-150.8
	N3	-14.0	-2.4	-11.3	-0.4	-8.5	6.4	-12.5	1.1
	C4	-3.7	0.2	-4.1	-0.1	6.0	-5.7	-4.0	-0.1
HXeOH	H1	-15.3	0.1	-15.4	0.0	-0.5	0.6	-15.0	-0.4
	Xe2	-19.4	64.6	-84.0	-109.0	234.1	-60.5	-41.0	-43.1
	O3	-11.4	-19.4	8.1	0.4	-73.4	53.5	5.7	2.5
	H4	-0.6	-0.2	-0.4	0.1	-0.9	0.7	-0.3	-0.1
HXeSH	H1	-13.2	0.0	-13.6	0.0	-0.8	0.8	-13.3	-0.3
	Xe2	-48.5	14.6	-64.7	-49.1	122.8	-59.1	-18.3	-46.3
	S3	-18.8	-25.5	7.0	-3.9	-128.3	106.7	3.5	3.5
	H4	-1.7	-0.1	-1.5	0.0	-0.8	0.7	-1.2	-0.3

[a] The total relativistic contributions as a sum of all 14 isotropic BPPT contributions. [b] Sum of scalar relativistic paramagnetic terms (p-KE/OZ + p/mv + p/Dar). [c] Sum of third-order spin-orbit contributions [FC-I(1)+SD-I(1)]. Only one-electron terms included. The sum of the REL-p and SO-I terms constitutes the sc. BPPT-5 approximation.

Table S5. Calculated contributions to the anisotropy of the nuclear shielding tensors in novel Xe compounds, $\Delta\sigma = -\mathrm{CSA}$,[a] in ppm.

Compound	Atom	NR[b]	Basis corr.[c]	Rel. corr.[d]	Total
HXeF	Xe2	1465.8	16.6	-274.4	1208.0
HXeCl	Xe2	1010.0	19.4	-302.2	727.2
HXeBr	Xe2	862.8	10.4	-338.9	534.3
HXeI	Xe2	600.4	12.8	-1129.0	-515.8
				-355.5[e]	257.7
HXeH	Xe2	1036.9	-2.9	-210.0	824.0
HXeCCH	Xe2	1216.1	8.0	-238.7	985.4
HXeCCXeH	Xe2	1215.4	3.2	-241.5	977.1
HXeCCCCH	Xe2	1236.2	86.9	-241.2	1081.9
HXeCCCN	Xe2	1266.2	13.2	-233.7	1045.7
HXeCN	Xe2	1323.6	14.9	-226.9	1111.6
HXeNC	Xe2	1438.1	19.2	-245.2	1212.1
ClXeCN	Xe2	1676.1	40.9	-445.2	1271.8
ClXeNC	Xe2	2372.8	73.2	-667.6	1778.4
HXeF	H1	33.7	0.0	-24.5	9.2
HXeCl	H1	36.9	-0.2	-19.9	16.8
HXeBr	H1	37.8	0.0	-41.6	-3.8
HXeI	H1	38.7	-0.1	-213.4	-174.8
				-53.2[e]	-14.6
HXeH	H1	30.5	0.0	-9.0	21.5
HXeCCH	H1	34.3	0.0	-17.0	17.3
HXeCCXeH	H1	34.4	0.0	-16.0	18.4
HXeCCCCH	H1	34.7	-2.5	-17.5	14.7
HXeCCCN	H1	34.8	0.1	-17.9	17.0
HXeCN	H1	34.5	0.1	-19.3	15.3
HXeNC	H1	34.0	0.1	-23.0	11.1
HXeCCH	C3	312.2	-0.5	-8.3	303.4
HXeCCH	C4	228.7	0.4	4.6	233.7
HXeCCXeH	C3	296.8	0.2	-7.9	289.1
HXeCCCCH	C3	310.2	28.7	-5.7	333.2
HXeCCCCH	C4	244.8	15.1	4.2	264.1
HXeCCCCH	C5	247.9	8.6	2.6	259.1
HXeCCCCH	C6	218.6	10.9	-0.1	229.4
HXeCCCN	C3	318.8	0.9	-4.5	315.2
HXeCCCN	C4	233.5	0.7	5.3	239.5
HXeCCCN	C5	303.6	0.2	2.9	306.7

Table continues in the next page.

Table S5. Continues…

Compound	Atom	NR[b]	Basis corr.[c]	Rel. corr.[d]	Total
HXeCN	C3	345.8	-0.5	-6.2	339.1
HXeNC	C4	362.3	0.9	1.6	364.8
ClXeCN	C3	311.6	-1.3	-54.9	255.4
ClXeNC	C4	370.1	0.0	-10.5	359.6
HXeCCCN	N6	497.4	1.0	0.6	499.0
HXeCN	N4	519.6	2.2	6.5	528.3
HXeNC	N3	514.2	0.1	-4.7	509.6
ClXeCN	N4	530.4	1.0	-54.9	476.5
ClXeNC	N3	415.0	-1.0	-6.9	407.1
HXeCCH	H5	17.9	0.0	0.7	18.6
HXeCCCCH	H7	17.1	0.1	0.3	17.5

[a] Defined as $\Delta\sigma = \sigma_{||} - \sigma_{\perp}$, where $\sigma_{||}$ and $\sigma_{\perp}$ are the shielding tensor components parallel with and perpendicular to the symmetry axis of the linear molecule, respectively. [b] Nonrelativistic calculation at the CCSD(T)/AIV level. [c] Basis-set correction calculated as the difference MP2/AIVd3 – MP2/AIV. [d] Perturbational relativistic (BPPT) correction at the BHandHLYP/AIVut(6/2) level.[e] Approximate relativistic BPPT-5 + SOS correction at the MCSCF level.

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Table S6: Nonrelativistic (NR) and 14 relativistic BPPT contributions to the ^{129}Xe chemical shift in novel Xe compounds.[a] In ppm.

Molecule	DFT func.	NR	BPPT	TOTAL	REL-*p*	SO-I	*p*-KE/OZ	*p*/mv	*p*/Dar	FC-I(1)	SD-I(1)	*con*	*d*-KE	*p*-OZ	*d*/mv	*d*/Dar	*p*/OZ-KE	FC/SZ-KE	FC-II(1)	SD-II(1)
HXeH	B3LYP	873.88	31.75	905.62	33.81	-1.81	-92.81	124.08	2.54	14.94	-16.75	0.02	0.01	-0.01	0.06	-0.02	-0.20	0.00	-0.05	-0.07
	BHandHLYP	752.56	9.80	762.37	29.03	-18.96	-72.09	118.99	-17.86	5.15	-24.11	0.03	0.01	-0.01	0.07	-0.02	-0.20	-0.01	-0.05	-0.08
HXeF	B3LYP	1115.59	7.99	1123.58	86.77	-78.72	-135.66	277.79	-55.36	-44.28	-34.43	0.02	0.03	0.01	0.03	0.01	-0.12	0.16	-0.13	-0.09
	BHandHLYP	1066.71	-1.26	1065.46	91.51	-92.70	-129.88	288.89	-67.50	-52.43	-40.27	0.02	0.03	0.01	0.03	0.01	-0.12	0.20	-0.15	-0.11
HXeCl	B3LYP	793.15	-8.91	784.24	40.25	-49.23	-84.15	173.67	-49.27	-15.90	-33.33	0.02	0.10	0.05	0.04	0.00	-0.18	0.28	-0.15	-0.08
	BHandHLYP	742.07	-17.89	724.18	46.32	-64.32	-77.79	184.10	-60.00	-24.17	-40.15	0.02	0.10	0.05	0.05	0.00	-0.18	0.38	-0.20	-0.10
HXeBr	B3LYP	686.23	-19.03	667.20	24.27	-43.55	-69.29	123.41	-29.85	-31.06	-12.49	0.02	0.47	0.30	0.01	0.03	-0.60	0.34	-0.25	-0.07
	BHandHLYP	638.60	-58.45	580.15	31.75	-90.49	-63.05	133.36	-38.57	-58.19	-32.30	0.02	0.47	0.30	0.01	0.03	-0.61	0.51	-0.35	-0.09
HXeI	B3LYP	516.35	-187.08	329.27	-0.44	-187.13	-44.31	32.28	11.60	-228.26	41.13	0.02	1.16	0.76	-0.04	0.07	-1.39	0.43	-0.46	-0.05
	BHandHLYP	462.44	-624.03	-161.59	9.38	-633.88	-36.49	39.66	6.20	-586.53	-47.35	0.02	1.16	0.76	-0.04	0.07	-1.41	0.94	-0.94	-0.09
HXeCN	B3LYP	1063.44	41.22	1104.66	73.49	-32.12	-127.91	215.61	-14.21	-11.46	-20.67	0.03	0.03	0.00	0.06	-0.01	-0.23	0.15	-0.07	-0.09
	BHandHLYP	976.92	23.96	1000.88	73.45	-49.39	-115.00	219.31	-30.85	-21.51	-27.87	0.03	0.03	0.00	0.06	-0.01	-0.24	0.20	-0.08	-0.10
HXeNC	B3LYP	1121.11	33.93	1155.04	96.98	-62.97	-141.88	275.46	-36.60	-37.47	-25.50	0.02	0.03	0.01	0.05	0.00	-0.18	0.20	-0.12	-0.10
	BHandHLYP	1051.49	19.66	1071.15	97.83	-78.09	-132.65	282.77	-52.29	-45.16	-32.93	0.02	0.03	0.00	0.05	0.00	-0.18	0.25	-0.14	-0.11
HXeCCH	B3LYP	987.28	31.27	1018.55	53.49	-22.00	-110.66	175.07	-10.91	0.97	-22.97	0.03	0.03	0.00	0.06	-0.02	-0.25	0.09	-0.08	-0.09
	BHandHLYP	893.60	14.24	907.84	52.64	-38.21	-95.85	175.94	-27.46	-8.60	-29.60	0.03	0.03	0.00	0.07	-0.02	-0.25	0.13	-0.09	-0.09
HXeCCCN	B3LYP	1011.66	32.59	1044.26	62.21	-29.45	-117.50	195.68	-15.97	-5.81	-23.64	0.03	0.03	0.01	0.06	-0.01	-0.27	0.14	-0.06	-0.09
	BHandHLYP	931.46	18.23	949.68	63.28	-44.94	-105.44	199.29	-30.56	-15.39	-29.55	0.03	0.03	0.01	0.06	-0.01	-0.27	0.18	-0.06	-0.08
HXeCCCCH	B3LYP	994.65	29.68	1024.33	55.95	-26.08	-112.65	182.95	-14.35	-1.85	-24.23	0.03	0.03	0.01	0.07	-0.02	-0.26	0.11	-0.07	-0.09
	BHandHLYP	907.37	14.25	921.61	56.44	-42.05	-99.15	185.38	-29.80	-11.58	-30.47	0.03	0.03	0.01	0.07	-0.02	-0.26	0.16	-0.07	-0.09
HXeCCXeH	B3LYP	992.21	31.71	1023.92	53.51	-21.72	-111.77	179.07	-13.79	1.51	-23.24	0.03	0.64	0.41	0.05	-0.02	-1.03	0.07	-0.13	-0.09
	BHandHLYP	888.94	13.31	902.25	51.27	-37.83	-95.08	177.62	-31.27	-7.76	-30.08	0.03	0.64	0.41	0.06	-0.02	-1.05	0.09	-0.17	-0.11
HXeOXeH	B3LYP	1086.55	-10.75	1075.80	61.98	-72.83	-126.37	247.81	-59.45	-36.23	-36.59	0.02	0.98	0.64	0.03	0.00	-1.45	0.08	-0.15	-0.06
	BHandHLYP	985.50	-36.03	949.47	57.60	-93.76	-110.39	245.61	-77.62	-46.61	-47.15	0.02	0.98	0.64	0.04	-0.01	-1.42	0.13	-0.20	-0.07
HXeOH	B3LYP	1034.65	-4.04	1030.61	61.79	-65.75	-118.37	226.00	-45.84	-30.09	-35.66	0.02	0.03	0.00	0.03	0.00	-0.12	0.13	-0.09	-0.09
	BHandHLYP	969.97	-19.42	950.55	64.64	-84.02	-108.96	234.07	-60.47	-40.96	-43.06	0.02	0.03	0.00	0.04	0.00	-0.12	0.21	-0.13	-0.10
HXeSH	B3LYP	659.64	-19.51	640.14	14.48	-34.00	-63.43	121.69	-43.78	3.01	-37.01	0.02	0.08	0.04	0.05	-0.02	-0.22	0.28	-0.15	-0.07
	BHandHLYP	570.50	-48.55	521.95	14.57	-64.66	-49.06	122.75	-59.12	-18.32	-46.34	0.02	0.08	0.04	0.06	-0.02	-0.22	3.07	-1.34	-0.16
ClXeCN	B3LYP	1374.43	23.90	1398.33	89.77	-65.77	-174.00	331.74	-67.97	5.31	-71.08	0.03	0.12	0.06	0.06	-0.02	-0.18	0.14	-0.16	-0.15
	BHandHLYP	1322.12	22.02	1344.14	99.97	-77.81	-166.50	353.19	-86.72	2.34	-80.15	0.03	0.12	0.06	0.07	-0.02	-0.19	0.18	-0.21	-0.18
ClXeNC	B3LYP	1894.87	9.69	1904.56	135.44	-125.87	-257.30	478.68	-85.93	5.47	-131.34	0.03	0.13	0.07	0.07	-0.03	0.09	0.10	-0.13	-0.20
	BHandHLYP	1894.50	6.85	1901.34	154.03	-147.28	-258.14	522.03	-109.86	3.57	-150.84	0.03	0.13	0.07	0.07	-0.03	0.10	0.10	-0.14	-0.23

[a] The specification of the BPPT terms can be found from the original papers.[7-10] The AIVut(6/2) basis set was used.

Figure S1. Nonrelativistic calculations of the ^{129}Xe chemical shift in studied Xe compounds. A comparison of different DFT functionals with CCSD(T), using the AIV basis set. Depicted are the deviations from the benchmark CCSD(T)/AIV results.

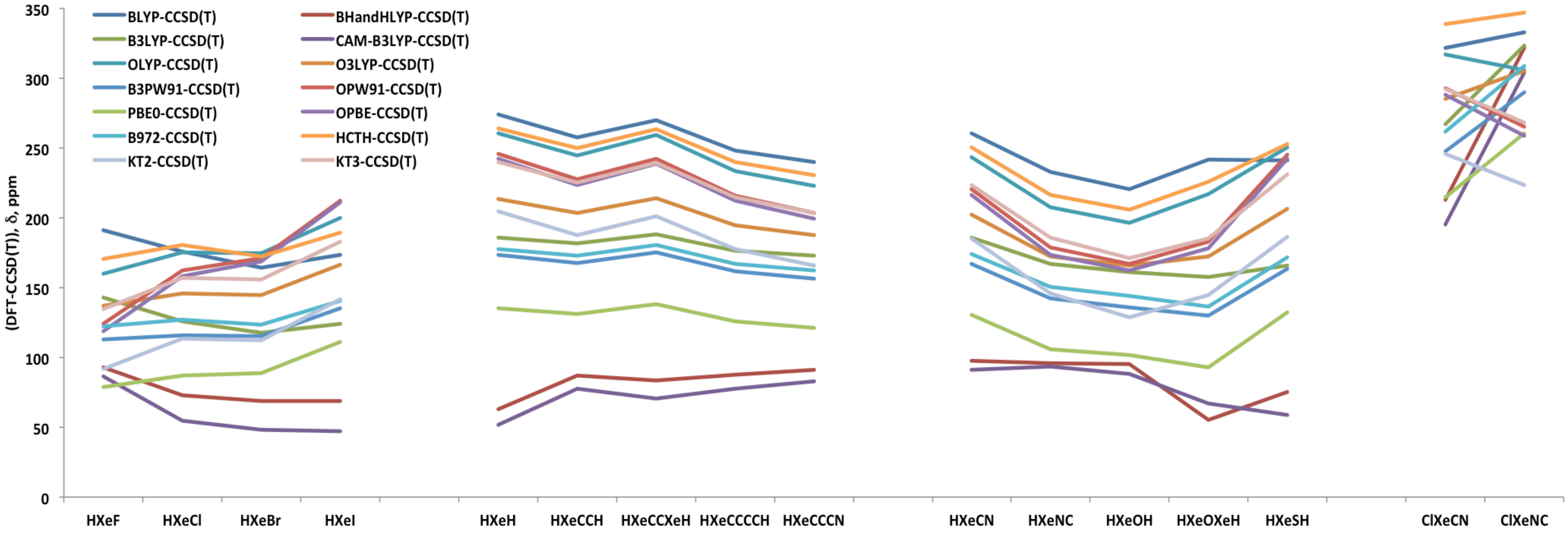

Table S7: Nonrelativistic (NR) and 14 relativistic BPPT contributions to the δ(H1) in novel Xe compounds.[a] In ppm.

Molecule	DFT func.	NR	BPPT	TOTAL	REL-*p*	SO-I	*p*-KE/OZ	*p*/mv	*p*/Dar	FC-I(1)	SD-I(1)	*con*	*d*-KE	*p*-OZ	*d*/mv	*d*/Dar	*p*/OZ-KE	FC/SZ-KE	FC-II(1)	SD-II(1)
HXeH	B3LYP	8.89	-4.90	3.99	-0.20	-4.65	0.00	-1.30	1.10	-4.49	-0.16	0.00	0.00	0.00	-0.10	0.06	0.00	0.01	-0.01	0.00
	BHandHLYP	8.62	-5.60	3.02	-0.15	-5.38	0.00	-1.16	1.01	-5.20	-0.18	0.00	0.00	0.00	-0.18	0.12	0.00	0.01	-0.01	0.00
HXeF	B3LYP	4.16	-14.32	-10.16	0.11	-14.41	-0.02	-0.41	0.54	-13.99	-0.42	0.00	0.01	0.00	-0.66	0.63	-0.01	0.04	-0.02	0.00
	BHandHLYP	3.77	-15.88	-12.11	0.09	-16.00	-0.02	-0.30	0.40	-15.53	-0.47	0.00	0.01	0.00	-0.68	0.69	-0.01	0.05	-0.03	0.00
HXeCl	B3LYP	7.47	-11.41	-3.94	0.07	-11.48	-0.05	-0.58	0.71	-11.17	-0.32	0.00	0.03	0.02	-0.56	0.54	-0.05	0.05	-0.02	0.00
	BHandHLYP	6.85	-12.75	-5.89	0.09	-12.88	-0.05	-0.36	0.50	-12.51	-0.37	0.00	0.03	0.02	-0.61	0.62	-0.05	0.06	-0.03	0.00
HXeBr	B3LYP	8.71	-24.07	-15.36	0.12	-24.18	-0.27	-0.12	0.51	-23.88	-0.31	0.00	0.18	0.12	-0.65	0.61	-0.27	0.05	-0.04	0.00
	BHandHLYP	8.07	-27.20	-19.13	0.14	-27.38	-0.27	0.11	0.30	-26.98	-0.40	0.00	0.18	0.12	-0.71	0.70	-0.27	0.08	-0.06	0.00
HXeI	B3LYP	10.43	-82.20	-71.77	0.16	-82.41	-0.65	0.64	0.16	-81.93	-0.48	0.00	0.46	0.30	-0.76	0.71	-0.65	0.07	-0.08	0.00
	BHandHLYP	9.82	-141.67	-131.84	0.20	-141.95	-0.65	0.89	-0.05	-140.88	-1.07	0.00	0.46	0.30	-0.85	0.83	-0.65	0.17	-0.17	0.00
HXeCN	B3LYP	6.38	-10.90	-4.52	-0.03	-10.90	-0.01	-0.72	0.70	-10.56	-0.34	0.00	0.01	0.00	-0.44	0.45	-0.01	0.03	-0.01	0.00
	BHandHLYP	6.03	-12.32	-6.29	0.00	-12.39	-0.01	-0.50	0.51	-12.00	-0.38	0.00	0.01	0.00	-0.50	0.54	-0.01	0.04	-0.01	0.00
HXeNC	B3LYP	4.64	-13.64	-9.00	0.03	-13.73	-0.01	-0.48	0.53	-13.31	-0.42	0.00	0.01	0.00	-0.55	0.58	-0.01	0.03	-0.02	0.00
	BHandHLYP	4.30	-14.80	-10.49	0.04	-14.94	-0.01	-0.29	0.34	-14.47	-0.46	0.00	0.01	0.00	-0.58	0.66	-0.01	0.04	-0.02	0.00
HXeCCH	B3LYP	6.84	-9.26	-2.42	-0.08	-9.20	-0.01	-0.95	0.88	-8.90	-0.29	0.00	0.00	0.00	-0.35	0.34	-0.01	0.04	-0.01	0.00
	BHandHLYP	6.45	-10.82	-4.37	-0.04	-10.83	-0.01	-0.73	0.70	-10.49	-0.34	0.00	0.00	0.00	-0.41	0.42	-0.01	0.05	-0.01	0.00
HXeCCCN	B3LYP	6.46	-9.94	-3.49	-0.05	-9.94	-0.02	-0.75	0.72	-9.61	-0.33	0.00	0.01	0.01	-0.43	0.44	-0.02	0.03	-0.01	0.00
	BHandHLYP	6.10	-11.42	-5.31	-0.01	-11.48	-0.02	-0.52	0.53	-11.11	-0.37	0.00	0.01	0.01	-0.48	0.52	-0.02	0.05	-0.01	0.00
HXeCCCCH	B3LYP	6.66	-9.54	-2.88	-0.07	-9.50	-0.02	-0.88	0.83	-9.19	-0.31	0.00	0.01	0.01	-0.38	0.38	-0.01	0.04	-0.01	0.00
	BHandHLYP	6.28	-11.14	-4.85	-0.03	-11.17	-0.02	-0.66	0.64	-10.82	-0.35	0.00	0.01	0.01	-0.44	0.46	-0.01	0.05	-0.01	0.00
HXeCCXeH	B3LYP	7.11	-8.68	-1.57	-0.02	-8.72	-0.52	-0.46	0.96	-8.44	-0.27	0.00	0.36	0.24	-0.33	0.29	-0.52	0.03	-0.02	0.00
	BHandHLYP	6.69	-10.19	-3.50	0.03	-10.28	-0.52	-0.24	0.78	-9.97	-0.31	0.00	0.36	0.24	-0.40	0.36	-0.52	0.05	-0.04	0.00
HXeOXeH	B3LYP	6.61	-14.08	-7.46	0.20	-14.28	-0.66	-0.03	0.89	-13.93	-0.35	0.00	0.47	0.31	-0.55	0.42	-0.66	0.04	-0.02	0.00
	BHandHLYP	6.13	-16.85	-10.71	0.22	-17.10	-0.66	0.13	0.76	-16.68	-0.42	0.00	0.47	0.31	-0.61	0.48	-0.66	0.07	-0.02	0.00
HXeOH	B3LYP	6.03	-13.11	-7.09	0.09	-13.15	-0.01	-0.65	0.76	-12.79	-0.36	0.00	0.01	0.00	-0.58	0.50	-0.01	0.04	-0.02	0.00
	BHandHLYP	5.50	-15.30	-9.80	0.10	-15.38	-0.01	-0.49	0.60	-14.97	-0.41	0.00	0.00	0.00	-0.63	0.57	-0.01	0.07	-0.03	0.00
HXeSH	B3LYP	9.96	-8.82	1.15	-0.05	-8.73	-0.04	-1.01	1.00	-8.50	-0.23	0.00	0.03	0.02	-0.37	0.31	-0.04	0.07	-0.03	0.00
	BHandHLYP	9.47	-13.24	-3.77	0.00	-13.62	-0.04	-0.80	0.85	-13.32	-0.30	0.00	0.03	0.02	-0.45	0.39	-0.04	0.76	-0.33	0.00

[a] The specification of the BPPT terms can be found from the original papers.[7-10] The AIVut(6/2) basis set was used.

Table S8: Nonrelativistic (NR) and 14 relativistic BPPT contributions to the C3 chemical shift $\delta(^{13}C)$ in novel Xe compounds.[a] In ppm.

Molecule	DFT func.	NR	BPPT	TOTAL	REL-*p*	SO-I	*p*-KE/OZ	*p*/mv	*p*/Dar	FC-I(1)	SD-I(1)	*con*	*d*-KE	*p*-OZ	*d*/mv	*d*/Dar	*p*/OZ-KE	FC/SZ-KE	FC-II(1)	SD-II(1)
HXeCN	B3LYP	154.58	-6.61	147.98	-1.02	-5.40	-0.27	-3.54	2.78	-5.48	0.08	0.00	0.07	0.05	0.06	-0.08	-0.19	-0.02	-0.08	0.00
	BHandHLYP	159.78	-4.85	154.92	-0.59	-4.03	-0.27	-2.92	2.60	-4.03	0.00	0.00	0.07	0.05	0.05	-0.08	-0.19	-0.04	-0.09	0.00
HXeCCH	B3LYP	137.17	-7.92	129.24	-1.25	-6.46	-0.21	-7.30	6.25	-6.35	-0.11	0.00	0.05	0.03	0.00	-0.03	-0.16	-0.05	-0.06	0.00
	BHandHLYP	136.66	-6.71	129.94	-1.07	-5.36	-0.21	-6.77	5.91	-5.00	-0.36	0.00	0.05	0.03	-0.01	-0.03	-0.17	-0.10	-0.06	0.00
HXeCCCN	B3LYP	145.26	-5.09	140.17	-0.61	-4.25	-0.26	-6.07	5.72	-4.04	-0.21	0.00	0.08	0.05	0.04	-0.07	-0.23	-0.04	-0.07	0.00
	BHandHLYP	146.08	-3.82	142.26	-0.34	-3.18	-0.27	-5.32	5.24	-2.73	-0.45	0.00	0.08	0.05	0.04	-0.07	-0.23	-0.07	-0.09	0.00
HXeCCCCH	B3LYP	136.96	-6.43	130.53	-0.95	-5.24	-0.25	-7.27	6.56	-5.05	-0.20	0.00	0.07	0.05	0.02	-0.05	-0.21	-0.05	-0.07	0.00
	BHandHLYP	136.97	-4.99	131.98	-0.74	-3.93	-0.25	-6.59	6.09	-3.43	-0.50	0.00	0.07	0.05	0.01	-0.05	-0.21	-0.10	-0.09	0.00
HXeCCXeH	B3LYP	117.60	-7.09	110.51	1.34	-8.67	-2.54	6.45	-2.57	-9.65	0.98	0.00	1.71	1.14	-0.06	0.01	-2.45	-0.05	-0.09	0.02
	BHandHLYP	121.04	-5.97	115.08	1.70	-7.87	-2.54	7.06	-2.83	-8.72	0.85	0.00	1.71	1.14	-0.07	0.02	-2.45	-0.11	-0.05	0.03
ClXeCN	B3LYP	123.95	-37.10	86.85	0.59	-37.58	-0.26	2.53	-1.69	-38.18	0.60	0.00	0.08	0.05	-0.17	0.13	-0.19	0.08	-0.11	0.00
	BHandHLYP	129.92	-38.19	91.74	0.61	-38.69	-0.26	2.56	-1.69	-39.00	0.31	0.00	0.08	0.05	-0.20	0.16	-0.18	0.13	-0.15	0.00

[a] The specification of the BPPT terms can be found from the original papers.[7-10] The AIVut(6/2) basis set was used.

Table S9: Nonrelativistic (NR) and 14 relativistic BPPT contributions to other δ (^{13}C) in the ligand Y in novel Xe compounds.[a] In ppm.

Molecule	DFT func.	NR	BPPT	TOTAL	REL-*p*	SO-I	*p*-KE/OZ	*p*/mv	*p*/Dar	FC-I(1)	SD-I(1)	*con*	*d*-KE	*p*-OZ	*d*/mv	*d*/Dar	*p*/OZ-KE	FC/SZ-KE	FC-II(1)	SD-II(1)
C4																				
HXeCCH	B3LYP	73.31	3.48	76.79	2.56	0.94	-0.05	8.56	-5.95	-0.15	1.08	0.00	-0.01	-0.01	-0.03	-0.01	0.04	0.01	0.00	0.00
	BHandHLYP	76.80	3.67	80.47	2.68	1.02	-0.06	8.63	-5.90	-0.17	1.19	0.00	-0.01	-0.01	-0.04	-0.01	0.03	0.00	0.00	0.00
HXeCCCCH	B3LYP	76.66	3.38	80.04	2.53	0.88	-0.17	8.11	-5.40	-0.09	0.97	0.00	0.06	0.04	-0.02	-0.02	-0.12	0.04	-0.02	0.00
	BHandHLYP	78.31	3.45	81.76	2.65	0.84	-0.18	8.14	-5.32	-0.27	1.11	0.00	0.06	0.04	-0.02	-0.03	-0.13	0.03	-0.01	0.00
HXeCCCN	B3LYP	68.22	3.98	72.20	2.46	1.57	-0.19	7.57	-4.92	0.68	0.89	0.00	0.07	0.05	0.00	-0.04	-0.15	0.03	-0.02	0.00
	BHandHLYP	70.42	4.00	74.43	2.54	1.52	-0.19	7.49	-4.75	0.52	1.00	0.00	0.07	0.05	-0.01	-0.05	-0.15	0.03	0.00	0.00
HXeNC	B3LYP	174.23	1.19	175.42	2.80	-1.84	-0.03	10.07	-7.24	-2.27	0.43	0.00	-0.08	-0.06	0.02	-0.01	0.31	-0.03	0.09	-0.01
	BHandHLYP	186.79	1.46	188.25	2.63	-1.40	-0.04	8.86	-6.19	-1.97	0.57	0.00	-0.08	-0.06	0.02	-0.02	0.31	-0.03	0.09	-0.01
ClXeNC	B3LYP	183.75	-2.65	181.10	-0.21	-2.69	-0.07	5.92	-6.06	-2.87	0.19	0.00	-0.06	-0.05	-0.08	0.08	0.31	-0.04	0.09	-0.01
	BHandHLYP	196.09	-3.68	192.41	0.20	-4.12	-0.07	6.00	-5.72	-3.98	-0.14	0.00	-0.06	-0.05	-0.08	0.08	0.31	-0.04	0.09	-0.01
C5																				
HXeCCCCH	B3LYP	82.40	1.33	83.73	0.11	1.27	-0.10	0.24	-0.02	1.33	-0.07	0.00	0.01	0.01	-0.03	0.02	-0.07	0.04	-0.04	0.00
	BHandHLYP	82.07	1.73	83.80	0.15	1.64	-0.10	0.25	0.00	1.78	-0.14	0.00	0.01	0.01	-0.03	0.02	-0.06	0.04	-0.06	0.00
HXeCCCN	B3LYP	121.22	1.64	122.86	0.03	1.61	-0.20	0.11	0.12	1.40	0.22	0.00	0.05	0.03	-0.01	0.01	-0.08	0.06	-0.06	0.00
	BHandHLYP	124.06	1.84	125.90	0.05	1.81	-0.20	0.12	0.13	1.63	0.18	0.00	0.05	0.03	-0.01	0.01	-0.08	0.07	-0.09	-0.01
C6																				
HXeCCCCH	B3LYP	68.43	0.08	68.52	-0.48	0.46	0.03	-1.27	0.76	-0.20	0.66	0.00	-0.06	-0.04	0.00	-0.02	0.17	0.02	0.02	0.00
	BHandHLYP	69.32	-0.26	69.06	-0.48	0.11	0.03	-1.18	0.67	-0.60	0.71	0.00	-0.06	-0.04	0.00	-0.03	0.17	0.02	0.04	0.01

[a] The specification of the BPPT terms can be found from the original papers.[7-10] The AIVut(6/2) basis set was used.

Table S10: Nonrelativistic (NR) and 14 relativistic BPPT contributions to chemical shifts δ(^{1}H), δ(^{15}N), and δ(^{19}F) in the ligand Y in novel Xe compounds.[a] In ppm.

Molecule	DFT func.	NR	BPPT	TOTAL	REL-*p*	SO-I	*p*-KE/OZ	*p*/mv	*p*/Dar	FC-I(1)	SD-I(1)	*con*	*d*-KE	*p*-OZ	*d*/mv	*d*/Dar	*p*/OZ-KE	FC/SZ-KE	FC-II(1)	SD-II(1)
H in Y																				
HXeCCH	B3LYP	0.40	0.49	0.88	0.07	0.42	0.12	0.05	-0.09	0.35	0.07	0.00	-0.07	-0.05	0.02	-0.02	0.11	0.00	0.00	0.00
	BHandHLYP	0.41	0.54	0.95	0.07	0.48	0.12	0.04	-0.09	0.39	0.09	0.00	-0.07	-0.05	0.02	-0.03	0.11	0.00	0.00	0.00
HXeCCCCH	B3LYP	0.49	0.16	0.64	-0.01	0.14	0.22	-0.24	0.01	0.11	0.03	0.00	-0.13	-0.09	0.07	-0.04	0.22	0.00	0.00	0.00
	BHandHLYP	0.56	0.23	0.79	-0.01	0.22	0.22	-0.25	0.02	0.17	0.05	0.00	-0.14	-0.09	0.07	-0.05	0.22	0.00	0.00	0.00
HXeOH	B3LYP	2.58	-0.57	2.02	-0.16	-0.37	0.05	-1.00	0.79	-0.27	-0.10	0.00	-0.03	-0.02	-0.09	0.05	0.05	0.01	0.00	0.00
	BHandHLYP	1.74	-0.64	1.10	-0.18	-0.41	0.05	-0.91	0.68	-0.29	-0.12	0.00	-0.03	-0.02	-0.10	0.05	0.05	0.01	0.00	0.00
HXeSH	B3LYP	2.63	-1.29	1.34	-0.08	-1.19	0.00	-0.86	0.77	-1.08	-0.11	0.00	0.00	0.00	-0.12	0.09	0.00	0.01	0.00	0.00
	BHandHLYP	1.85	-1.66	0.19	-0.12	-1.53	0.00	-0.80	0.68	-1.22	-0.31	0.00	0.00	0.00	-0.11	0.09	0.00	0.03	-0.01	0.00
N																				
HXeCN	B3LYP	293.79	4.61	298.40	5.50	-1.27	-0.24	18.19	-12.45	-2.24	0.97	0.01	-0.10	-0.08	-0.01	0.03	0.44	-0.02	0.10	0.00
	BHandHLYP	306.06	5.04	311.10	5.59	-0.92	-0.25	17.81	-11.97	-2.07	1.14	0.01	-0.10	-0.08	-0.01	0.03	0.44	-0.02	0.11	0.00
HXeNC	B3LYP	275.26	-8.28	266.98	-6.93	-1.09	-0.49	-21.53	15.09	-1.39	0.30	0.00	0.06	0.04	0.06	-0.10	-0.23	-0.02	-0.07	0.00
	BHandHLYP	284.10	-5.51	278.59	-5.96	0.74	-0.50	-20.86	15.40	0.53	0.21	0.00	0.06	0.04	0.06	-0.11	-0.23	-0.04	-0.07	0.00
HXeCCCN	B3LYP	216.76	0.11	216.87	-1.52	0.78	-0.01	-3.10	1.58	-0.33	1.12	0.01	-0.23	-0.18	-0.03	0.12	0.98	-0.02	0.20	0.01
	BHandHLYP	219.10	-0.14	218.96	-1.51	0.48	0.01	-2.75	1.23	-0.66	1.14	0.01	-0.24	-0.19	-0.03	0.11	0.99	-0.02	0.23	0.02
ClXeCN	B3LYP	306.19	-1.82	304.37	0.87	-3.08	-0.28	9.83	-8.68	-4.94	1.86	0.01	-0.08	-0.07	-0.14	0.16	0.44	-0.02	0.10	0.00
	BHandHLYP	318.68	-1.22	317.45	1.34	-2.97	-0.29	10.38	-8.76	-5.08	2.11	0.01	-0.09	-0.08	-0.15	0.17	0.45	-0.02	0.11	0.00
ClXeNC	B3LYP	193.85	-23.20	170.65	-2.55	-20.41	-0.39	-7.32	5.16	-22.70	2.29	0.00	0.07	0.05	-0.11	0.06	-0.25	0.01	-0.08	0.01
	BHandHLYP	204.72	-13.99	190.72	-2.43	-11.32	-0.40	-8.47	6.44	-12.47	1.15	0.00	0.07	0.05	-0.13	0.08	-0.23	0.01	-0.09	0.01
F																				
HXeF	B3LYP	378.44	-16.20	362.24	-25.38	9.33	-0.85	-94.04	69.52	5.30	4.03	0.00	-0.06	-0.04	-0.05	0.01	-0.03	-0.02	0.04	0.01
	BHandHLYP	345.02	-17.10	327.92	-26.50	9.56	-0.76	-90.43	64.69	6.24	3.31	0.00	-0.06	-0.05	-0.07	0.01	-0.01	-0.04	0.05	0.01

[a] The specification of the BPPT terms can be found from the original papers.[7-10] The AIVut(6/2) basis set was used.

Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Table S11: Nonrelativistic (NR) and 15 relativistic BPPT contributions to the shielding anisotropy $\Delta\sigma$ (^{129}Xe) in novel linear Xe compounds.[a] In ppm.

Molecule	DFT func.	NR	BPPT	TOTAL	REL-*p*	SO-I	SOS	*p*-KE/OZ	*p*/mv	*p*/Dar	FC-I(1)	SD-I(1)	*dip*	*d*-KE	*p*-OZ	*d*/mv	*d*/Dar	*p*/OZ-KE	SD/SZ-KE	FC-II(1)	SD-II(1)
HXeH	B3LYP	1312.77	-168.91	1143.86	50.72	214.06	-433.54	-139.21	186.12	3.82	22.41	191.65	0.01	-0.01	-0.02	-0.41	0.31	-0.31	0.03	0.27	-0.02
	BHandHLYP	1130.94	-209.98	920.96	43.55	196.51	-449.90	-108.14	178.48	-26.79	7.72	188.79	0.01	-0.01	-0.02	-0.40	0.31	-0.31	0.03	0.27	-0.02
HXeF	B3LYP	1678.41	-259.40	1419.01	130.16	153.52	-543.19	-203.49	416.69	-83.04	-66.42	219.94	0.01	0.02	0.00	-0.43	0.33	-0.20	0.03	0.33	0.02
	BHandHLYP	1605.03	-274.37	1330.66	137.27	133.67	-545.46	-194.81	433.34	-101.25	-78.65	212.32	0.02	0.02	0.00	-0.41	0.31	-0.20	0.10	0.31	-0.01
HXeCl	B3LYP	1196.07	-282.52	913.55	60.37	195.32	-538.33	-126.22	260.50	-73.91	-23.85	219.17	0.01	0.12	0.07	-0.30	0.23	-0.30	0.04	0.23	0.01
	BHandHLYP	1119.45	-302.23	817.22	69.48	178.90	-550.76	-116.68	276.15	-90.00	-36.25	215.15	0.01	0.12	0.06	-0.28	0.22	-0.30	0.13	0.20	-0.02
HXeBr	B3LYP	1036.94	-264.67	772.26	36.41	170.80	-472.26	-103.93	185.11	-44.78	-46.59	217.39	0.01	0.68	0.44	-0.34	0.23	-0.93	0.04	0.25	0.00
	BHandHLYP	965.49	-338.94	626.55	47.62	115.46	-502.40	-94.57	200.04	-57.85	-87.29	202.75	0.01	0.68	0.44	-0.32	0.22	-0.95	0.16	0.21	-0.07
HXeI	B3LYP	783.86	-440.19	343.66	-0.65	-121.15	-319.08	-66.46	48.41	17.40	-342.39	221.23	0.01	1.71	1.13	-0.49	0.26	-2.12	0.05	0.16	-0.02
	BHandHLYP	703.02	-1129.01	-425.98	14.07	-758.08	-385.47	-54.73	59.50	9.30	-879.79	121.71	0.01	1.71	1.13	-0.50	0.27	-2.15	0.29	-0.06	-0.22
HXeCN	B3LYP	1599.63	-194.69	1404.94	110.23	208.53	-513.43	-191.86	323.42	-21.32	-17.18	225.71	0.01	0.01	-0.01	-0.39	0.31	-0.37	0.04	0.35	0.02
	BHandHLYP	1469.91	-226.86	1243.05	110.18	188.92	-526.00	-172.50	328.96	-46.28	-32.27	221.19	0.01	0.01	-0.01	-0.37	0.30	-0.38	0.10	0.37	0.01
HXeNC	B3LYP	1599.63	-219.44	1380.19	145.47	176.04	-540.97	-212.82	413.19	-54.89	-56.20	232.24	0.01	0.01	0.00	-0.34	0.28	-0.29	0.05	0.29	0.02
	BHandHLYP	1469.91	-245.25	1224.66	146.75	157.77	-549.83	-198.98	424.16	-78.43	-67.75	225.52	0.01	0.01	-0.01	-0.32	0.26	-0.29	0.10	0.28	0.01
HXeCCH	B3LYP	1486.43	-206.97	1279.47	80.24	221.13	-508.27	-166.00	262.61	-16.37	1.45	219.68	0.01	0.01	-0.01	-0.46	0.35	-0.39	0.03	0.37	0.01
	BHandHLYP	1346.02	-238.68	1107.35	78.95	203.01	-520.63	-143.78	263.92	-41.18	-12.90	215.91	0.01	0.01	-0.01	-0.44	0.34	-0.40	0.09	0.39	0.00
HXeCCCN	B3LYP	1522.84	-207.49	1315.34	93.32	212.43	-513.22	-176.25	293.53	-23.96	-8.72	221.15	0.01	0.02	0.00	-0.42	0.33	-0.42	0.04	0.39	0.02
	BHandHLYP	1402.62	-233.73	1168.89	94.92	193.88	-522.59	-158.17	298.94	-45.85	-23.08	216.97	0.01	0.02	0.00	-0.40	0.32	-0.42	0.10	0.42	0.02
HXeCCCCH	B3LYP	1497.79	-212.63	1285.16	83.92	218.27	-514.80	-168.98	274.43	-21.52	-2.78	221.05	0.01	0.02	0.00	-0.44	0.34	-0.41	0.03	0.40	0.02
	BHandHLYP	1366.96	-241.16	1125.80	84.65	199.72	-525.59	-148.72	278.07	-44.69	-17.38	217.09	0.01	0.02	0.00	-0.43	0.33	-0.41	0.10	0.43	0.01
HXeCCXeH	B3LYP	1495.24	-207.48	1287.76	80.27	222.75	-510.67	-167.65	268.61	-20.69	2.27	220.48	0.01	0.92	0.60	-0.50	0.35	-1.56	0.03	0.31	0.00
	BHandHLYP	1340.48	-241.51	1098.96	76.90	205.04	-523.59	-142.62	266.43	-46.91	-11.63	216.68	0.01	0.92	0.60	-0.49	0.35	-1.58	0.08	0.26	-0.03
ClXeCN	B3LYP	2072.40	-420.68	1651.73	134.66	358.11	-913.54	-261.00	497.61	-101.95	7.97	350.14	0.02	0.15	0.08	-0.42	0.32	-0.31	-0.08	0.28	0.07
	BHandHLYP	1993.99	-445.19	1548.80	149.95	361.73	-956.87	-249.75	529.78	-130.08	3.51	358.22	0.02	0.14	0.08	-0.42	0.32	-0.33	-0.09	0.21	0.07
ClXeNC	B3LYP	2853.91	-623.54	2230.37	203.17	449.66	-1276.92	-385.95	718.02	-128.90	8.21	441.45	0.02	0.15	0.08	-0.46	0.33	0.09	-0.07	0.37	0.06
	BHandHLYP	2853.41	-667.61	2185.80	231.05	457.37	-1356.57	-387.21	783.05	-164.79	5.35	452.02	0.02	0.15	0.08	-0.46	0.33	0.10	-0.11	0.36	0.08

[a] The specification of the BPPT terms can be found from the original papers.[7-10] The SOS contribution is explained in Ref. 6. The AIVut(6/2) basis set was used.

Table S12: Nonrelativistic (NR) and 15 relativistic BPPT contributions to the H1 shielding anisotropy $\Delta\sigma$ (^{1}H) in novel linear Xe compounds.[a] In ppm.

Molecule	DFT func.	NR	BPPT	TOTAL	REL-*p*	SO-I	SOS	*p*-KE/OZ	*p*/mv	*p*/Dar	FC-I(1)	SD-I(1)	*dip*	*d*-KE	*p*-OZ	*d*/mv	*d*/Dar	*p*/OZ-KE	SD/SZ-KE	FC-II(1)	SD-II(1)
HXeH	B3LYP	28.95	-7.94	21.02	-0.30	-7.05	0.08	0.00	-1.94	1.64	-6.77	-0.28	0.00	0.00	0.00	-0.66	0.00	0.00	0.00	0.01	0.00
	BHandHLYP	28.60	-8.99	19.61	-0.22	-8.15	0.09	0.00	-1.73	1.51	-7.84	-0.32	0.00	0.00	0.00	-0.79	0.09	0.00	0.00	0.01	0.00
HXeF	B3LYP	33.68	-22.13	11.55	0.16	-21.89	0.48	-0.02	-0.61	0.80	-21.02	-0.87	0.00	0.00	0.00	-1.52	0.66	-0.02	0.00	0.00	0.00
	BHandHLYP	32.81	-24.54	8.27	0.13	-24.25	0.43	-0.02	-0.44	0.59	-23.33	-0.92	0.00	0.00	0.00	-1.55	0.71	-0.02	0.00	0.00	0.00
HXeCl	B3LYP	36.98	-17.83	19.14	0.73	-17.44	0.37	0.54	-0.87	1.05	-16.78	-0.66	0.00	0.04	0.03	-0.08	-0.08	-1.40	0.00	0.00	0.00
	BHandHLYP	35.65	-19.91	15.75	0.83	-19.51	0.33	0.62	-0.54	0.75	-18.79	-0.72	0.00	0.04	0.03	-0.08	-0.08	-1.46	0.00	0.00	0.00
HXeBr	B3LYP	37.70	-36.87	0.83	0.18	-36.42	0.23	-0.40	-0.17	0.76	-35.85	-0.58	0.00	0.26	0.17	-1.44	0.57	-0.40	0.00	-0.01	0.00
	BHandHLYP	36.28	-41.63	-5.34	0.21	-41.21	0.22	-0.40	0.17	0.45	-40.50	-0.72	0.00	0.26	0.17	-1.51	0.65	-0.40	0.00	-0.02	0.00
HXeI	B3LYP	38.05	-124.13	-86.07	0.25	-123.67	0.06	-0.97	0.97	0.24	-122.92	-0.75	0.00	0.68	0.45	-1.47	0.59	-0.97	0.00	-0.03	0.00
	BHandHLYP	36.66	-213.41	-176.75	0.30	-213.00	0.09	-0.97	1.34	-0.08	-211.35	-1.65	0.00	0.68	0.45	-1.57	0.69	-0.97	0.01	-0.07	-0.01
HXeCN	B3LYP	33.77	-17.07	16.69	-0.05	-16.53	0.29	-0.02	-1.08	1.04	-15.87	-0.66	0.00	0.00	0.00	-1.26	0.46	-0.01	0.00	0.02	0.00
	BHandHLYP	32.87	-19.25	13.62	0.00	-18.75	0.27	-0.02	-0.73	0.75	-18.04	-0.71	0.00	0.00	0.00	-1.34	0.55	-0.01	0.00	0.02	0.00
HXeNC	B3LYP	33.77	-21.19	12.58	0.05	-20.84	0.42	-0.02	-0.72	0.79	-19.99	-0.85	0.00	0.00	0.00	-1.43	0.60	-0.01	0.00	0.01	0.00
	BHandHLYP	32.87	-22.98	9.89	0.06	-22.63	0.39	-0.02	-0.43	0.51	-21.74	-0.89	0.00	0.00	0.00	-1.47	0.67	-0.01	0.00	0.01	0.00
HXeCCH	B3LYP	33.36	-14.58	18.78	-0.12	-13.96	0.27	-0.01	-1.42	1.31	-13.39	-0.58	0.00	0.00	0.00	-1.13	0.35	-0.01	0.00	0.02	0.00
	BHandHLYP	32.59	-16.97	15.62	-0.06	-16.40	0.25	-0.01	-1.09	1.05	-15.77	-0.63	0.00	0.00	0.00	-1.23	0.44	-0.01	0.00	0.03	0.00
HXeCCCN	B3LYP	33.99	-15.64	18.35	-0.07	-15.08	0.29	-0.03	-1.11	1.07	-14.44	-0.64	0.00	0.01	0.01	-1.24	0.45	-0.02	0.00	0.03	0.00
	BHandHLYP	33.16	-17.90	15.26	-0.02	-17.39	0.27	-0.03	-0.78	0.79	-16.70	-0.69	0.00	0.01	0.01	-1.32	0.54	-0.02	0.00	0.03	0.00
HXeCCCCH	B3LYP	33.75	-15.01	18.74	-0.10	-14.42	0.28	-0.02	-1.31	1.23	-13.82	-0.61	0.00	0.01	0.01	-1.17	0.39	-0.02	0.00	0.03	0.00
	BHandHLYP	32.94	-17.46	15.48	-0.05	-16.93	0.27	-0.02	-0.98	0.95	-16.26	-0.66	0.00	0.01	0.00	-1.26	0.48	-0.02	0.00	0.04	0.00
HXeCCXeH	B3LYP	33.35	-13.66	19.69	-0.03	-13.23	0.26	-0.78	-0.68	1.42	-12.70	-0.54	0.00	0.54	0.36	-1.07	0.27	-0.77	0.00	0.01	0.00
	BHandHLYP	32.62	-15.98	16.64	0.04	-15.58	0.24	-0.78	-0.35	1.17	-14.98	-0.59	0.00	0.54	0.36	-1.18	0.37	-0.77	0.00	-0.01	0.00

[a] The specification of the BPPT terms can be found from the original papers.[7-10] The SOS contribution is explained in Ref. 6. The AIVut(6/2) basis set was used.

Table S13: Nonrelativistic (NR) and 15 relativistic BPPT contributions to the C3 shielding anisotropy $\Delta\sigma$ (^{13}C) in novel linear Xe compounds.[a] In ppm.

Molecule	DFT func.	NR	BPPT	TOTAL	REL-*p*	SO-I	SOS	*p*-KE/OZ	*p*/mv	*p*/Dar	FC-I(1)	SD-I(1)	*dip*	*d*-KE	*p*-OZ	*d*/mv	*d*/Dar	*p*/OZ-KE	SD/SZ-KE	FC-II(1)	SD-II(1)
HXeCN	B3LYP	381.31	-8.56	372.74	-1.45	-9.44	2.87	-0.54	-5.17	4.25	-8.18	-1.25	0.00	0.10	0.07	-0.35	0.03	-0.32	0.01	-0.10	0.00
	BHandHLYP	384.58	-6.21	378.37	-0.82	-7.08	2.27	-0.54	-4.26	3.97	-6.00	-1.08	0.00	0.11	0.07	-0.37	0.04	-0.32	0.02	-0.12	0.00
HXeCCH	B3LYP	356.54	-9.74	346.80	-1.79	-11.81	4.44	-0.44	-10.81	9.46	-9.49	-2.32	0.00	0.07	0.05	-0.44	0.08	-0.26	0.01	-0.08	0.01
	BHandHLYP	351.36	-8.28	343.08	-1.53	-9.76	3.64	-0.44	-10.03	8.94	-7.46	-2.30	0.00	0.07	0.05	-0.47	0.10	-0.26	0.01	-0.11	0.00
HXeCCCCH	B3LYP	357.73	-7.34	350.40	-1.35	-10.14	4.76	-0.50	-10.77	9.92	-7.53	-2.61	0.00	0.10	0.07	-0.43	0.06	-0.33	0.01	-0.09	0.00
	BHandHLYP	353.29	-5.65	347.63	-1.04	-7.66	3.73	-0.50	-9.76	9.22	-5.10	-2.56	0.00	0.11	0.07	-0.46	0.08	-0.34	0.01	-0.15	0.00
HXeCCCN	B3LYP	368.52	-6.04	362.48	-0.84	-7.95	3.34	-0.53	-8.97	8.66	-6.02	-1.93	0.00	0.11	0.08	-0.39	0.04	-0.36	0.01	-0.08	0.00
	BHandHLYP	365.23	-4.48	360.74	-0.44	-5.97	2.59	-0.52	-7.86	7.94	-4.05	-1.92	0.00	0.12	0.08	-0.42	0.05	-0.37	0.01	-0.13	0.00
HXeCCXeH	B3LYP	332.78	-9.27	323.51	2.09	-14.38	2.96	-3.94	9.81	-3.79	-14.43	0.05	0.00	2.56	1.71	-0.62	0.18	-3.69	0.01	-0.12	0.03
	BHandHLYP	333.55	-7.87	325.68	2.62	-12.84	2.28	-3.93	10.72	-4.16	-13.04	0.19	0.00	2.56	1.71	-0.65	0.20	-3.69	0.02	-0.10	0.04
ClXeCN	B3LYP	340.11	-52.64	287.47	0.96	-59.60	6.67	-0.52	3.93	-2.46	-57.23	-2.37	0.00	0.12	0.08	-0.64	0.21	-0.31	0.00	-0.14	0.01
	BHandHLYP	344.29	-54.92	289.37	0.98	-60.71	5.55	-0.52	3.96	-2.46	-58.46	-2.25	0.00	0.12	0.08	-0.68	0.25	-0.30	0.00	-0.21	0.01

[a] The specification of the BPPT terms can be found from the original papers.[7-10] The SOS contribution is explained in Ref. 6. The AIVut(6/2) basis set was used.

Table S14: Nonrelativistic (NR) and 15 relativistic BPPT contributions to the other $\Delta\sigma(^{13}C)$ in the ligand Y in novel linear Xe compounds.[a] In ppm.

Molecule	DFT func.	NR	BPPT	TOTAL	REL-*p*	SO-I	SOS	*p*-KE/OZ	*p*/mv	*p*/Dar	FC-I(1)	SD-I(1)	*dip*	*d*-KE	*p*-OZ	*d*/mv	*d*/Dar	*p*/OZ-KE	SD/SZ-KE	FC-II(1)	SD-II(1)
C4																					
HXeCCH	B3LYP	251.62	4.12	255.74	3.92	2.72	-2.42	-0.21	12.98	-8.85	-0.18	2.90	0.00	-0.02	-0.01	-0.09	-0.01	0.04	0.00	0.00	0.00
	BHandHLYP	252.44	4.57	257.01	4.09	2.70	-2.13	-0.21	13.07	-8.77	-0.21	2.91	0.00	-0.02	-0.01	-0.11	0.00	0.03	0.01	0.00	0.00
HXeCCCCH	B3LYP	268.11	3.96	272.07	3.88	2.61	-2.35	-0.40	12.30	-8.03	-0.09	2.70	0.00	0.09	0.06	-0.10	-0.01	-0.20	0.00	-0.01	0.00
	BHandHLYP	266.29	4.22	270.51	4.04	2.40	-2.07	-0.39	12.34	-7.90	-0.36	2.76	0.00	0.09	0.07	-0.12	-0.01	-0.20	0.01	0.01	0.00
HXeCCCN	B3LYP	254.82	5.07	259.89	3.77	3.43	-1.94	-0.41	11.49	-7.30	1.06	2.37	0.00	0.11	0.08	-0.09	-0.03	-0.24	0.00	-0.01	0.00
	BHandHLYP	253.89	5.25	259.14	3.88	3.22	-1.68	-0.41	11.35	-7.06	0.83	2.40	0.00	0.11	0.08	-0.11	-0.02	-0.24	0.00	0.01	0.00
HXeNC	B3LYP	381.31	0.87	382.18	4.28	-1.60	-2.12	-0.18	15.24	-10.78	-3.37	1.77	0.00	-0.12	-0.09	-0.08	0.05	0.42	0.01	0.12	0.00
	BHandHLYP	384.58	1.57	386.15	4.02	-1.24	-1.51	-0.19	13.41	-9.21	-2.92	1.67	0.00	-0.12	-0.09	-0.08	0.05	0.41	0.02	0.13	0.00
ClXeNC	B3LYP	410.91	-9.42	401.48	-0.24	1.67	-11.19	-0.23	9.02	-9.02	-4.27	5.94	0.00	-0.10	-0.07	-0.11	0.08	0.41	0.00	0.12	0.00
	BHandHLYP	424.37	-10.53	413.84	0.37	-0.91	-10.34	-0.24	9.12	-8.51	-5.92	5.01	0.00	-0.10	-0.08	-0.11	0.08	0.42	0.01	0.12	0.00
C5																					
HXeCCCCH	B3LYP	273.38	2.03	275.41	0.24	2.05	-0.10	-0.29	0.49	0.04	2.04	0.02	0.00	0.02	0.01	-0.08	0.05	-0.11	0.00	-0.05	0.00
	BHandHLYP	268.41	2.64	271.05	0.30	2.58	-0.03	-0.28	0.50	0.08	2.72	-0.13	0.00	0.02	0.01	-0.09	0.05	-0.11	0.00	-0.09	0.00
HXeCCCN	B3LYP	330.96	2.61	333.56	0.12	2.42	0.21	-0.44	0.30	0.25	2.13	0.28	0.00	0.08	0.05	-0.04	0.02	-0.16	0.01	-0.08	0.00
	BHandHLYP	330.47	2.91	333.38	0.14	2.69	0.25	-0.43	0.30	0.27	2.48	0.21	0.00	0.07	0.05	-0.05	0.02	-0.15	0.01	-0.12	-0.01
C6																					
HXeCCCCH	B3LYP	242.49	0.41	242.89	-0.64	0.65	0.28	-0.08	-1.77	1.21	-0.27	0.92	0.00	-0.09	-0.06	0.02	-0.04	0.24	0.00	0.04	0.00
	BHandHLYP	239.31	-0.13	239.18	-0.65	0.15	0.23	-0.08	-1.65	1.08	-0.86	1.00	0.00	-0.09	-0.06	0.02	-0.04	0.24	0.01	0.07	0.00

[a] The specification of the BPPT terms can be found from the original papers.[7-10] The SOS contribution is explained in Ref. 6. The AIVut(6/2) basis set was used.

Table S15: Nonrelativistic (NR) and 15 relativistic BPPT contributions to the shielding anisotropies Δσ (^{1}H), Δσ (^{15}N), and Δσ (^{19}F) in the ligand Y in novel linear Xe compounds.[a] In ppm.

Molecule	DFT func.	NR	BPPT	TOTAL	REL-*p*	SO-I	SOS	*p*-KE/OZ	*p*/mv	*p*/Dar	FC-I(1)	SD-I(1)	*dip*	*d*-KE	*p*-OZ	*d*/mv	*d*/Dar	*p*/OZ-KE	SD/SZ-KE	FC-II(1)	SD-II(1)
H in Y																					
HXeCCH	B3LYP	17.48	0.67	18.15	0.11	0.61	-0.03	0.18	0.08	-0.15	0.49	0.12	0.00	-0.11	-0.07	0.00	-0.03	0.17	0.00	0.01	0.00
	BHandHLYP	17.66	0.75	18.41	0.11	0.70	-0.03	0.18	0.06	-0.14	0.55	0.14	0.00	-0.11	-0.07	0.00	-0.02	0.17	0.00	0.00	0.00
HXeCCCCH	B3LYP	16.65	0.20	16.85	-0.01	0.19	-0.01	0.33	-0.36	0.01	0.13	0.05	0.00	-0.20	-0.14	0.09	-0.05	0.32	0.00	0.01	0.00
	BHandHLYP	16.83	0.31	17.14	-0.01	0.30	-0.01	0.33	-0.36	0.02	0.23	0.08	0.00	-0.20	-0.14	0.09	-0.05	0.32	0.00	0.00	0.00
N																					
HXeCN	B3LYP	571.40	5.44	576.84	8.46	-0.35	-3.18	-0.55	27.75	-18.74	-3.47	3.12	0.00	-0.15	-0.12	-0.11	0.10	0.63	0.00	0.16	0.02
	BHandHLYP	587.70	6.49	594.19	8.58	-0.19	-2.43	-0.56	27.15	-18.00	-3.19	2.99	0.00	-0.16	-0.12	-0.12	0.10	0.64	0.00	0.18	0.02
HXeNC	B3LYP	571.40	-8.27	563.12	-10.19	-5.95	8.54	-0.92	-31.83	22.56	-2.20	-3.75	0.00	0.09	0.06	-0.42	0.04	-0.36	0.00	-0.08	0.01
	BHandHLYP	587.70	-4.71	582.99	-8.75	-2.56	7.28	-0.94	-30.86	23.05	0.70	-3.26	0.00	0.09	0.06	-0.45	0.04	-0.35	0.00	-0.08	0.01
HXeCCCN	B3LYP	557.31	0.98	558.29	-2.08	0.48	1.31	-0.20	-4.19	2.31	-0.62	1.09	0.00	-0.35	-0.27	-0.03	0.17	1.44	-0.01	0.30	0.02
	BHandHLYP	556.33	0.59	556.92	-2.07	0.09	1.23	-0.17	-3.69	1.80	-1.08	1.17	0.00	-0.36	-0.27	-0.03	0.17	1.47	-0.02	0.34	0.04
ClXeCN	B3LYP	590.11	-8.34	581.76	1.51	1.05	-11.42	-0.61	15.21	-13.09	-7.53	8.57	0.00	-0.13	-0.11	-0.17	0.15	0.63	-0.02	0.15	0.02
	BHandHLYP	606.48	-7.01	599.47	2.21	0.81	-10.56	-0.61	16.00	-13.18	-7.71	8.52	0.00	-0.14	-0.11	-0.19	0.16	0.65	-0.03	0.17	0.02
ClXeNC	B3LYP	442.37	-19.87	422.50	-3.62	-45.87	30.42	-0.77	-10.52	7.68	-34.16	-11.71	0.00	0.10	0.07	-0.72	0.25	-0.38	-0.03	-0.12	0.02
	BHandHLYP	456.81	-6.86	449.95	-3.45	-31.41	28.82	-0.79	-12.27	9.61	-18.80	-12.61	0.00	0.10	0.07	-0.77	0.29	-0.35	-0.02	-0.14	0.02
F																					
HXeF	B3LYP	617.15	-7.61	609.54	-37.43	-3.60	33.93	-1.38	-139.10	103.05	7.55	-11.16	0.00	-0.07	-0.06	-0.78	0.34	-0.07	0.04	0.08	0.02
	BHandHLYP	552.11	-11.08	541.04	-39.18	-1.06	29.65	-1.20	-133.86	95.88	9.03	-10.09	0.00	-0.07	-0.06	-0.83	0.35	-0.03	0.06	0.09	0.01

[a] The specification of the BPPT terms can be found from the original papers.[7-10] The SOS contribution is explained in Ref. 6.

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