Table 1 The absolute isotropic shielding values (in ppm) of nuclei in H_2X (X = Se, Te, Po) subsystems in H_2X-H_2O systems (σ_{iso}^{super}), absolute property shifts, $\Delta\sigma_{iso}$, (in ppm) and relative property shifts, $\delta\sigma_{iso}$, (in percent in parenthesis), calculated in isolated H_2X molecules ("me") and in H_2X molecules with the presence of H_2O accounted for by FDE with unrelaxed and relaxed densities ("FDE(0)" and "FDE(4)", respectively) with various FDE approximations: 0, v, $v+w_u$, $v+w_u+w_c$ (explanation in text).

Species	Hamiltonian	Atom	σ_{iso}^{super}	$\Delta\sigma_{iso}^{FDE(4)}$ $\left(\delta\sigma_{iso}^{FDE(4)}\right)$				$\Delta\sigma_{iso}^{FDE(0)}$ $\left(\delta\sigma_{iso}^{FDE(0)}\right)$				$\Delta\sigma_{iso}^{me}$ $(\delta\sigma_{iso}^{me})$
				0	v	v+w_u	v+w_u+w_c	0	v	v+w_u	v+w_u+w_c	
H_2Se-H_2O	DC	Se	2378.03	-100.75 (-4.24)	-12.54 (-0.53)	-12.55 (-0.53)	-12.33 (-0.52)	-90.16 (-3.79)	-8.66 (-0.36)	-8.72 (-0.37)	-8.49 (-0.36)	38.25 (1.61)
		H_b	30.88	-0.39 (-1.27)	-0.83 (-2.68)	-0.67 (-2.16)	-0.62 (-2.01)	-0.55 (-1.79)	-0.95 (-3.08)	-0.79 (-2.57)	-0.75 (-2.42)	-2.09 (-6.77)
		H	33.42	0.24 (0.71)	0.02 (0.06)	0.03 (0.08)	0.03 (0.08)	0.25 (0.76)	0.06 (0.17)	0.06 (0.19)	0.06 (0.19)	0.43 (1.29)
H_2Te-H_2O	DC	Te	4667.85	-142.39 (-3.05)	-4.62 (-0.10)	-9.16 (-0.20)	-8.88 (-0.19)	-130.69 (-2.80)	-0.60 (-0.01)	-5.04 (-0.11)	-4.77 (-0.10)	67.48 (1.45)
		H_b	35.62	-0.29 (-0.80)	-0.68 (-1.90)	-0.44 (-1.23)	-0.42 (-1.18)	-0.38 (-1.07)	-0.75 (-2.11)	-0.51 (-1.44)	-0.49 (-1.39)	-1.70 (-4.77)
		H	37.85	-0.02 (-0.05)	0.01 (0.02)	0.02 (0.06)	0.02 (0.07)	0.01 (0.02)	0.04 (0.09)	0.05 (0.14)	0.05 (0.14)	0.54 (1.41)
H_2Po-H_2O	DC	Po	13985.80	-224.54 (-1.61)	18.28 (0.13)	-3.52 (-0.03)	-3.13 (-0.02)	-214.79 (-1.54)	21.32 (0.15)	0.19 (0.00)	0.58 (0.00)	137.84 (0.99)
		H_b	40.80	0.50 (1.23)	0.07 (0.16)	-0.09 (-0.23)	-0.09 (-0.23)	0.47 (1.15)	0.05 (0.11)	-0.11 (-0.27)	-0.11 (-0.26)	-0.57 (-1.40)
		H	42.29	-0.22 (-0.52)	-0.03 (-0.08)	0.00 (-0.01)	0.00 (-0.01)	-0.19 (-0.45)	-0.01 (-0.02)	0.02 (0.05)	0.02 (0.05)	0.89 (2.09)

Table 2 The absolute anisotropic shielding values (in ppm) of nuclei in H_2X (X = Se, Te, Po) subsystems in H_2X-H_2O systems (σ_{aniso}^{super}), absolute property shifts, $\Delta\sigma_{aniso}$, (in ppm) and relative property shifts, $\delta\sigma_{aniso}$, (in percent in parenthesis), calculated in isolated H_2X molecules ("me") and in H_2X molecules with the presence of H_2O accounted for by FDE with unrelaxed and relaxed densities ("FDE(0)" and "FDE(4)", respectively) with various FDE approximations: 0, v, $v+w_u$, $v+w_u+w_c$ (explanation in text).

Species	Hamiltonian	Atom	σ_{aniso}^{super}	$\Delta\sigma_{aniso}^{FDE(4)}$ $\left(\delta\sigma_{aniso}^{FDE(4)}\right)$				$\Delta\sigma_{aniso}^{FDE(0)}$ $\left(\delta\sigma_{aniso}^{FDE(0)}\right)$				$\Delta\sigma_{aniso}^{me}$ $(\delta\sigma_{aniso}^{me})$
				0	v	v+w_u	v+w_u+w_c	0	v	v+w_u	v+w_u+w_c	
H_2Se-H_2O	DC	Se	609.27	21.80 (3.58)	-0.13 (-0.02)	-0.43 (-0.07)	-0.19 (-0.03)	20.61 (3.38)	-0.07 (-0.01)	-0.38 (-0.06)	-0.13 (-0.02)	0.17 (0.03)
		H_b	22.19	5.05 (22.78)	6.00 (27.04)	5.76 (25.98)	5.70 (25.67)	5.26 (23.69)	6.12 (27.60)	5.89 (26.55)	5.82 (26.24)	7.29 (32.86)
		H	15.13	-1.17 (-7.72)	-0.22 (-1.47)	-0.22 (-1.44)	-0.21 (-1.42)	-1.07 (-7.07)	-0.20 (-1.33)	-0.20 (-1.31)	-0.19 (-1.29)	0.09 (0.59)
H_2Te-H_2O	DC	Te	1189.67	29.78 (2.50)	0.56 (0.05)	-1.22 (-0.10)	-1.21 (-0.10)	28.16 (2.37)	0.41 (0.03)	-1.29 (-0.11)	-1.28 (-0.11)	3.60 (0.30)
		H_b	14.59	0.50 (3.42)	0.02 (0.12)	0.24 (1.62)	0.28 (1.89)	0.43 (2.93)	-0.06 (-0.39)	0.17 (1.16)	0.21 (1.43)	-1.31 (-8.99)
		H	15.24	0.54 (3.57)	0.09 (0.62)	0.08 (0.53)	0.08 (0.53)	0.49 (3.23)	0.06 (0.38)	0.04 (0.29)	0.05 (0.30)	-0.64 (-4.21)
H_2Po-H_2O	DC	Po	5556.67	61.88 (1.11)	-15.12 (-0.27)	-18.36 (-0.33)	-18.61 (-0.33)	48.66 (0.88)	-26.12 (-0.47)	-29.42 (-0.53)	-29.81 (-0.54)	-463.51 (-8.34)
		H_b	105.25	0.98 (0.93)	-1.28 (-1.21)	-1.67 (-1.59)	-1.67 (-1.59)	0.78 (0.75)	-1.41 (-1.34)	-1.79 (-1.70)	-1.79 (-1.70)	-6.01 (-5.71)
		H	107.80	1.93 (1.79)	0.16 (0.15)	0.08 (0.08)	0.09 (0.08)	1.78 (1.65)	0.06 (0.06)	-0.02 (-0.02)	-0.02 (-0.02)	-4.03 (-3.74)

Table 3 The absolute isotropic, σ_{iso}, and anisotropic, σ_{aniso}, shielding values (in ppm) of nuclei in H_2X subsystems in H_2X-H2O (X = Se, Te, Po) systems, absolute property shifts, $\Delta\sigma_{iso}$ and $\Delta\sigma_{aniso}$, (in ppm) and relative property shifts, $\delta\sigma_{iso}$ and $\delta\sigma_{aniso}$, (in percent in parenthesis), calculated in isolated H_2X molecules ("me") and in H_2X molecules with the presence of H_2O accounted for by FDE with unrelaxed and relaxed densities ("FDE(0)" and "FDE(4)", respectively).

Species	Hamiltonian	Atom	$\sigma_{\mathrm{iso}}^{super}$	$\Delta(\sigma_{\mathrm{iso}})$ ($\delta(\sigma_{\mathrm{iso}})$)			$\sigma_{\mathrm{aniso}}^{super}$	$\Delta(\sigma_{\mathrm{aniso}})$ ($\delta(\sigma_{\mathrm{aniso}})$)		
				FDE(4)	FDE(0)	me		FDE(4)	FDE(0)	me
H_2Se-H_2O	ZORA-SO	Se	2261.59	-11.30 (-0.50)	-8.84 (-0.39)	34.89 (1.54)	628.15	4.43 (0.71)	4.50 (0.72)	4.89 (0.78)
		H_b	30.10	-0.77 (-2.57)	-0.86 (-2.85)	-2.07 (-6.89)	23.95	5.83 (24.33)	5.91 (24.67)	7.22 (30.14)
		H	32.55	-0.03 (-0.10)	-0.01 (-0.02)	0.35 (1.09)	16.97	-0.24 (-1.39)	-0.22 (-1.31)	0.11 (0.64)
H_2Te-H_2O	ZORA-SO	Te	4251.23	-9.61 (-0.23)	-6.42 (-0.15)	64.66 (1.52)	1219.57	0.55 (0.05)	0.51 (0.04)	0.80 (0.07)
		H_b	33.43	-0.46 (-1.38)	-0.52 (-1.54)	-1.59 (-4.76)	18.09	3.87 (21.41)	3.92 (21.69)	4.90 (27.11)
		H	35.47	0.00 (-0.01)	0.02 (0.05)	0.45 (1.27)	13.09	-0.33 (-2.52)	-0.32 (-2.44)	-0.09 (-0.72)
H_2Po-H_2O	ZORA-SO	Po	11168.82	-20.93 (-0.19)	-18.28 (-0.16)	101.35 (0.91)	3138.04	-45.36 (-1.45)	-50.82 (-1.62)	-304.56 (-9.71)
		H_b	37.46	-0.21 (-0.55)	-0.22 (-0.59)	-0.82 (-2.20)	62.41	-1.32 (-2.11)	-1.37 (-2.20)	-4.11 (-6.58)
		H	38.99	0.00 (0.00)	0.02 (0.04)	0.67 (1.71)	64.80	0.25 (0.39)	0.21 (0.32)	-2.05 (-3.17)

Table 4 Reduced indirect spin-spin couplings: isotropic (K_{iso}^{super}) and anisotropic (K_{aniso}^{super}) values (in SI) in H_2X subsystems in H2X-H2O (X = Se, Te, Po) systems with DC and ZORA-SO Hamiltonians, together with absolute (ΔK) and relative (δK, in percent in parenthesis) property shifts calculated in isolated H_2X molecules ("me") and in H_2X molecules with the presence of H_2O accounted for by FDE with unrelaxed and relaxed densities ("FDE(0)" and "FDE(4)", respectively).

Species	Hamiltonian	Nuclei		K_{iso}^{super}	K_{iso}			K_{aniso}^{super}	K_{aniso}		
					FDE(4)	FDE(0)	me		FDE(4)	FDE(0)	me
H_2Se-H_2O	ZORA-SO	H_b	Se	-12.63	1.08 (-8.56)	1.50 (-11.90)	6.58 (-52.12)	130.61	-2.01 (-1.54)	-1.87 (-1.43)	1.15 (0.88)
		H	Se	-16.41	0.87 (-5.28)	0.92 (-5.59)	1.88 (-11.47)	127.57	-0.24 (-0.19)	-0.31 (-0.25)	-1.03 (-0.81)
		H_b	H	-1.11	-0.03 (2.80)	-0.03 (3.01)	-0.07 (5.94)	-0.83	0.01 (-0.73)	0.01 (-0.79)	0.01 (-1.75)
	DC	H_b	Se	-11.22	1.52 (-13.52)	2.17 (-19.35)	7.25 (-64.63)	113.79	-1.23 (-1.08)	-1.14 (-1.00)	1.25 (1.10)
		H	Se	-16.04	0.07 (-0.42)	0.16 (-0.98)	1.51 (-9.43)	110.68	-0.33 (-0.30)	-0.42 (-0.38)	-1.01 (-0.91)
		H_b	H	-0.77	0.00 (-0.40)	0.00 (-0.10)	-0.02 (3.11)	0.89	0.00 (-0.43)	0.00 (-0.51)	-0.01 (-1.27)
H_2Te-H_2O	ZORA-SO	H_b	Te	-55.69	1.84 (-3.31)	2.26 (-4.05)	9.82 (-17.62)	226.45	-1.00 (-0.44)	-0.57 (-0.25)	8.95 (3.95)
		H	Te	-64.05	-0.02 (0.03)	0.06 (-0.09)	1.44 (-2.24)	214.87	-0.52 (-0.24)	-0.64 (-0.30)	-2.61 (-1.22)
		H_b	H	-0.94	-0.02 (2.47)	-0.03 (2.72)	-0.06 (6.50)	-0.34	0.00 (0.30)	0.00 (0.15)	0.00 (-1.04)
	DC	H_b	Te	-53.11	1.69 (-3.18)	2.24 (-4.22)	9.08 (-17.10)	208.54	-0.42 (-0.20)	-0.01 (-0.01)	8.07 (3.87)
		H	Te	-59.98	0.16 (-0.27)	0.27 (-0.45)	2.18 (-3.64)	198.09	-0.44 (-0.22)	-0.57 (-0.29)	-2.37 (-1.20)
		H_b	H	-0.75	0.00 (-0.01)	0.00 (0.23)	-0.03 (3.74)	0.42	0.00 (-0.21)	0.00 (-0.21)	0.00 (0.41)
H_2Po-H_2O	ZORA-SO	H_b	Po	-439.33	1.02 (-0.23)	0.98 (-0.22)	-0.87 (0.20)	343.71	1.40 (0.41)	2.15 (0.63)	666.43 (193.89)
		H	Po	-435.42	0.40 (-0.09)	0.48 (-0.11)	4.12 (-0.95)	-315.34	0.98 (-0.31)	1.12 (-0.35)	7.19 (-2.28)
		H_b	H	-0.80	-0.02 (2.81)	-0.02 (2.93)	-0.07 (8.42)	0.78	0.00 (0.28)	0.00 (0.47)	0.08 (10.45)
	DC	H_b	Po	-442.55	1.37 (-0.31)	1.41 (-0.32)	-1.25 (0.28)	429.17	3.10 (0.72)	4.18 (0.97)	41.96 (9.78)
		H	Po	-437.24	0.45 (-0.10)	0.57 (-0.13)	5.04 (-1.15)	388.29	-0.18 (-0.05)	-0.15 (-0.04)	2.24 (0.58)
		H_b	H	-0.61	0.00 (-0.31)	0.00 (-0.15)	-0.04 (6.02)	0.69	0.00 (-0.19)	0.00 (0.07)	1.32 (191.46)

Table 5 Absolute SO-ZORA isotropic and anisotropic shielding values (σ_{iso}^{super} and σ_{aniso}^{super}, in ppm) of nuclei in H_2X (X = Se, Te, Po) subsystems in H_2X–H_2O, and absolute shifts ($\Delta\sigma$, in ppm) for the isolated ("ME") and embedded ("FDE(4)") H_2X molecules in the presence of H_2O calculated with three different basis sets in the ADF software.

Atom	Basis set	σ_{iso}^{super}	$\Delta\sigma_{iso}^{FDE(4)}$	$\Delta\sigma_{iso}^{ME}$	σ_{aniso}^{super}	$\Delta\sigma_{aniso}^{FDE(4)}$	$\Delta\sigma_{aniso}^{ME}$
	TZP	2265.90	–9.87	35.75	621.50	1.89	3.04
Se	TZ2P	2261.59	–11.30	34.89	628.15	4.43	4.89
	QZ4P	2280.66	–12.04	38.90	615.07	–0.34	–0.19
	TZP	30.24	–0.78	–2.09	24.08	5.83	7.22
H_b	TZ2P	30.10	–0.77	–2.07	23.95	5.83	7.22
	QZ4P	30.09	–0.74	–2.06	23.77	5.76	7.13
	TZP	32.72	–0.02	0.37	17.07	–0.25	0.08
H	TZ2P	32.55	–0.03	0.35	16.97	–0.24	0.11
	QZ4P	32.57	–0.01	0.40	16.84	–0.29	0.07
	TZP	4256.56	–10.53	67.59	1215.68	0.77	1.76
Te	TZ2P	4251.23	–9.61	64.66	1219.57	0.55	0.80
	QZ4P	4270.26	–11.39	68.87	1239.64	–1.70	1.16
	TZP	33.33	–0.41	–1.61	18.75	3.93	5.17
H_b	TZ2P	33.43	–0.46	–1.59	18.09	3.87	4.90
	QZ4P	33.47	–0.45	–1.65	17.85	3.84	4.89
	TZP	35.41	0.01	0.47	13.55	–0.32	–0.03
H	TZ2P	35.47	0.00	0.45	13.09	–0.33	–0.09
	QZ4P	35.60	–0.01	0.48	12.87	–0.35	–0.09
	TZP	11160.06	–18.50	109.87	3216.05	–37.81	–311.11
Po	TZ2P	11168.82	–20.93	101.35	3138.04	–45.36	–304.56
	QZ4P	11800.79	–9.72	132.69	4513.02	–12.75	–365.17
	TZP	37.38	–0.14	–0.80	60.83	–0.97	–4.16
H_b	TZ2P	37.46	–0.21	–0.82	62.41	–1.32	–4.11
	QZ4P	37.11	–0.20	–0.84	65.70	–1.43	–4.46
	TZP	38.88	0.01	0.68	63.36	0.31	–1.98
H	TZ2P	38.99	0.00	0.67	64.80	0.25	–2.05
	QZ4P	38.74	0.00	0.76	68.14	0.13	–2.38

Table 6 SO-ZORA isotropic and anisotropic reduced indirect spin-spin couplings (K_{iso}^{super} and K_{aniso}^{super}, in SI) for the H_2X subsystem in H_2X–H_2O, and absolute shifts (ΔK, in SI) for the isolated ("ME") and embedded ("FDE(4)") H_2X molecules in the presence of H_2O calculated with three different basis sets in the ADF software..

Nuclei		Basis set	K_{iso}^{super}	$\Delta K_{iso}^{FDE(4)}$	ΔK_{iso}^{ME}	K_{aniso}^{super}	$\Delta K_{aniso}^{FDE(4)}$	ΔK_{aniso}^{ME}
		TZP	–11.35	1.18	6.84	127.51	–1.95	0.96
H_b	Se	TZ2P	–12.63	1.08	6.58	130.61	–2.01	1.15
		QZ4P	–15.38	2.40	8.45	132.31	–1.72	1.62
		TZP	–15.54	0.71	1.72	124.67	–0.35	–1.02
H	Se	TZ2P	–16.41	0.87	1.88	127.57	–0.24	–1.03
		QZ4P	–21.18	0.08	1.64	128.66	–0.31	–1.07
		TZP	–0.89	–0.01	–0.05	0.50	0.00	0.00
H_b	H	TZ2P	–1.11	–0.03	–0.07	0.51	0.01	–0.01
		QZ4P	–1.00	0.03	–0.01	0.89	0.00	–0.01
		TZP	–52.34	0.29	8.84	219.59	–0.70	8.58
H_b	Te	TZ2P	–55.69	1.84	9.82	226.45	–1.00	8.95
		QZ4P	–63.84	2.20	11.03	236.34	–0.37	9.40
		TZP	–59.63	0.23	1.53	208.62	–0.46	–2.37
H	Te	TZ2P	–64.05	–0.02	1.44	214.87	–0.53	–2.61
		QZ4P	–72.53	0.11	2.32	224.22	–0.50	–2.71
		TZP	–0.95	–0.01	–0.05	0.40	0.00	–0.01
H_b	H	TZ2P	–0.94	–0.02	–0.06	0.20	0.00	0.00
		QZ4P	–0.99	0.01	–0.03	0.34	0.01	0.01
		TZP	–425.78	–1.41	–2.34	337.14	0.24	33.59
H_b	Po	TZ2P	–439.33	1.02	–0.87	343.72	1.40	34.68
		QZ4P	–501.00	0.84	–2.12	454.11	3.39	47.78
		TZP	–420.47	0.78	4.07	303.25	–0.48	0.81
H	Po	TZ2P	–435.41	0.40	4.12	308.77	–0.49	0.87
		QZ4P	–493.97	0.43	6.12	407.17	–0.30	2.29
		TZP	–0.78	–0.01	–0.06	0.74	0.00	0.08
H_b	H	TZ2P	–0.80	–0.02	–0.07	0.78	0.00	0.08
		QZ4P	–0.83	–0.01	–0.05	0.85	0.01	0.09

Table 7 Isotropic ξ_{iso} magnetizability values (in SI units) calculated for H_2X-H_2O (X = Se, Te, Po) systems, for H_2X and H_2O subsystems (and their sums) treated as isolated species ("me") and with environmental effects acounted for by FDE with unrelaxed and relaxed densities ("FDE(0)" and "FDE(4)", respectively) with various FDE approximations: 0, v, $v+w_u$, $v+w_u+w_c$ (explanations in text). The absolute property shifts, $\Delta\xi_{iso}$, (in SI units), and the relative property shifts, $\delta\xi_{iso}$, (in percent in parenthesis), are calculated as differences between the value for supermolecule and the sum of magnetizability values for each subsystem.

Species	Hamiltonian	system	ξ_{iso}^{super}	$\xi_{iso}^{FDE(4)}$				$\xi_{iso}^{FDE(0)}$				ξ_{iso}^{me}
				0	v	v+w11	v+w11+w12	0	v	v+w11	v+w11+w12	
H_2Se-H_2O	DC	SeH_2	–	-183.07	-608.99	-606.54	-606.54	-254.81	-608.60	-606.14	-606.21	-602.19
		H_2O	–	781.33	-233.79	-233.78	-233.76	168.35	-233.95	-233.95	-233.39	-234.19
		sum	-836.26	598.26	-842.77	-840.32	-840.30	-86.46	-842.55	-840.08	-839.60	-836.31
		$\Delta\xi_{iso}$ ($\delta\xi_{iso}$)	0.0	-1434.52 (171.54)	6.51 (-0.78)	4.06 (-0.49)	4.04 (-0.48)	-749.80 (89.66)	6.29 (-0.75)	3.82 (-0.46)	3.34 (-0.40)	0.05 (-0.01)
H_2Te-H_2O	DC	TeH_2	–	-630.07	-858.94	-848.68	-848.74	-656.71	-858.64	-848.32	-848.38	-842.57
		H_2O	–	235.10	-233.74	-233.74	-233.60	-105.38	-233.85	-233.85	-234.28	-233.83
		sum	-1080.67	-394.97	-1092.69	-1082.42	-1082.33	-762.08	-1092.49	-1082.17	-1082.66	-1076.39
		$\Delta\xi_{iso}$ ($\delta\xi_{iso}$)	0.0	-685.71 (63.45)	12.01 (-1.11)	1.74 (-0.16)	1.66 (-0.15)	-318.59 (29.48)	11.82 (-1.09)	1.49 (-0.14)	1.99 (-0.18)	-4.28 (0.40)
H_2Po-H_2O	DC	PoH_2	–	-895.55	-1030.19	-949.80	-949.71	-903.29	-1030.07	-949.56	-949.45	-940.09
		H_2O	–	-169.52	-234.11	-234.10	-233.18	-230.95	-234.16	-234.15	-233.32	-234.02
		sum	-1184.04	-1065.08	-1264.30	-1183.91	-1182.89	-1134.24	-1264.22	-1183.71	-1182.78	-1174.11
		$\Delta\xi_{iso}$ ($\delta\xi_{iso}$)	0.0	-118.96 (10.05)	80.26 (-6.78)	-0.13 (0.01)	-1.15 (0.10)	-49.80 (4.21)	80.19 (-6.77)	-0.33 (0.03)	-1.26 (0.11)	-9.92 (0.84)

Table 8 First anisotropic ξ_{aniso1} magnetizability values (in SI units) calculated for H_2X-H_2O (X = Se, Te, Po) systems, for H_2X and H_2O subsystems (and their sums) treated as isolated species ("me") and with environmental effects acounted for by FDE with unrelaxed and relaxed densities ("FDE(0)" and "FDE(4)", respectively) with various FDE approximations: 0, v, $v+w_u$, $v+w_u+w_c$ (explanations in text). The absolute property shifts, $\Delta\xi_{aniso1}$, (in SI units), and the relative property shifts, $\delta\xi_{aniso1}$, (in percent in parenthesis), are calculated as differences between the value for supermolecule and the sum of magnetizability values for each subsystem.

Species	Hamiltonian	system	ξ_{aniso1}^{super}	$\xi_{aniso1}^{FDE(4)}$				$\xi_{aniso1}^{FDE(0)}$				ξ_{aniso1}^{me}
				0	v	v+w11	v+w11+w12	0	v	v+w11	v+w11+w12	
H_2Se-H_2O	DC	SeH_2	–	-358.80	-47.12	-45.88	-45.88	-305.13	-47.14	-45.91	-45.92	-45.97
		H_2O	–	-1396.29	-5.76	-5.76	-5.78	-553.52	-5.98	-5.98	-4.75	-6.51
		sum	-57.94	-1755.08	-52.88	-51.64	-51.66	-858.65	-53.12	-51.89	-50.67	-52.48
		$\Delta\xi_{aniso1}$ ($\delta\xi_{aniso1}$)	0.0	1697.14 (-2928.93)	-5.07 (8.75)	-6.31 (10.89)	-6.28 (10.85)	800.70(-1381.86)	-4.82 (8.31)	-6.05 (10.45)	-7.27 (12.55)	-5.47 (9.43)
H_2Te-H_2O	DC	TeH_2	–	-227.24	-86.32	-80.29	-80.32	-208.78	-86.34	-80.32	-80.34	-80.30
		H_2O	–	-650.52	-5.53	-5.53	-5.70	-180.04	-5.70	-5.70	-3.87	-6.06
		sum	-81.63	-877.77	-91.85	-85.82	-86.02	-388.82	-92.04	-86.01	-84.21	-86.36
		$\Delta\xi_{aniso1}$ ($\delta\xi_{aniso1}$)	0.0	796.14 (-975.36)	10.23 (-12.53)	4.19 (-5.13)	4.39 (-5.38)	307.20 (-376.35)	10.42 (-12.76)	4.39 (-5.38)	2.59 (-3.17)	4.73 (-5.80)
H_2Po-H_2O	DC	PoH_2	–	-290.25	-261.88	-91.58	-91.56	-289.59	-262.47	-91.58	-91.56	-91.79
		H_2O	–	-93.62	-6.45	-6.45	-7.47	-9.75	-6.55	-6.55	-7.45	-6.73
		sum	-89.81	-383.87	-268.34	-98.03	-99.02	-299.34	-269.02	-98.13	-99.01	-98.52
		$\Delta\xi_{aniso1}$ ($\delta\xi_{aniso1}$)	0.0	294.06 (-327.43)	178.53 (-198.78)	8.22 (-9.15)	9.21 (-10.26)	209.53 (-233.30)	179.21 (-199.54)	8.32 (-9.27)	9.20 (-10.25)	8.71 (-9.69)

Table 9 Second anisotropic ξ_{aniso2} magnetizability values (in SI units) calculated for H_2X-H_2O (X = Se, Te, Po) systems, for H_2X and H_2O subsystems (and their sums) treated as isolated species ("me") and with environmental effects acounted for by FDE with unrelaxed and relaxed densities ("FDE(0)" and "FDE(4)", respectively) with various FDE approximations: 0, v, $v+w_u$, $v+w_u+w_c$ (explanations in text). The absolute property shifts, $\Delta\xi_{aniso2}$, (in SI units), and the relative property shifts, $\delta\xi_{aniso2}$, (in percent in parenthesis), are calculated as differences between the value for supermolecule and the sum of magnetizability values for each subsystem.

Species	Hamiltonian	system	ξ_{aniso2}^{super}	$\xi_{aniso2}^{FDE(4)}$				$\xi_{aniso2}^{FDE(0)}$				ξ_{aniso2}^{me}
				0	v	v+w11	v+w11+w12	0	v	v+w11	v+w11+w12	
H_2Se-H_2O	DC	SeH_2	–	450.95	32.72	30.04	30.04	383.92	32.78	30.08	30.15	29.74
		H_2O	–	2514.94	3.84	3.84	3.89	997.13	3.81	3.81	2.46	3.64
		sum	36.04	2965.89	36.56	33.88	33.93	1381.05	36.58	33.88	32.61	33.38
		$\Delta\xi_{aniso2}$ ($\delta\xi_{aniso2}$)	0.0	-2929.85 (-8130.31)	-0.53 (-1.46)	2.15 (5.97)	2.10 (5.83)	-1345.02 (-3732.40)	-0.55 (-1.52)	2.15 (5.97)	3.43 (9.52)	2.66 (7.37)
H_2Te-H_2O	DC	TeH_2	–	252.91	67.03	54.45	54.51	232.07	67.13	54.49	54.55	54.62
		H_2O	–	1249.07	3.86	3.87	4.21	342.43	3.84	3.84	3.02	3.71
		sum	58.43	1501.98	70.89	58.32	58.73	574.50	70.97	58.33	57.57	58.33
		$\Delta\xi_{aniso2}$ ($\delta\xi_{aniso2}$)	0.0	-1443.55 (-2470.65)	-12.47 (-21.34)	0.11 (0.18)	-0.30 (-0.51)	-516.08 (-883.27)	-12.54 (21.46)	0.10 (0.17)	0.86 (1.46)	0.10 (0.17)
H_2Po-H_2O	DC	PoH_2	–	321.83	202.88	93.68	93.51	315.74	203.10	93.76	93.59	96.80
		H_2O	–	164.30	4.19	4.20	6.40	11.07	4.17	4.18	6.15	4.11
		sum	95.81	486.13	207.07	97.87	99.91	326.81	207.27	97.94	99.74	100.90
		$\Delta\xi_{aniso2}$ ($\delta\xi_{aniso2}$)	0.0	-390.33 (-407.40)	-11.26 (-116.13)	-2.07 (-2.16)	-4.10 (-4.28)	-231.00 (-241.11)	-111.46 (-116.34)	-2.13 (-2.22)	-3.93 (-4.10	-5.09 (-5.31)