Supporting information for
Pairwise additivity in the nuclear magnetic resonance interactions of atomic xenon

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Atomic coordinates (in Å) of xenon clusters Xe_n ($n = 2 - 12$).[a]

n	Atom number	x	y	z
2	1	0.0000000000000000	0.0000000000000000	2.1813500000000000
	2	0.0000000000000000	0.0000000000000000	-2.1813500000000000
3	1	1.7067990866484800	0.4301002933603940	-1.8017304647473800
	2	-2.0152973775612500	1.4964571188079400	0.2087500252235240
	3	0.3084982909127710	-1.9265574121683300	1.5929804395238500
4	1	-1.4055765760193000	0.1709826193103080	2.2655093814598800
	2	0.9739699451344120	2.4072748233361300	-0.6275531554172890
	3	-1.5868552554260500	-0.8597881380812930	-1.9697903598471400
	4	2.0184618859222700	-1.7184693045651500	0.3318341341932210
5	1	-1.0123827656385500	2.8618520080369900	1.8372784281401600
	2	1.0123813905156600	-2.8618533664469700	-1.8372788486836800
	3	-1.6110112740047000	-1.4196641721432300	1.3236469755527100
	4	-0.7556300460532800	1.1051789634464600	-2.1378588931906400
	5	2.3666426951808800	0.3144865671067540	0.8142123381814460
6	1	2.8878366672163200	1.0290505186847700	-0.1821223134153450
	2	-2.8878368401755300	-1.0290508855915000	0.1821201216917730
	3	0.7685126221408810	-1.7285116552650400	2.4193691232454100
	4	-0.7685146401278970	1.7285123082346400	-2.4193681022030600
	5	-0.7081648280747600	2.3205622959173900	1.8828703000317500
	6	0.7081670190209870	-2.3205625819802700	-1.8828691289618600
7	1	-3.7015989340488600	0.0618193329747526	-0.3267966147808660
	2	-0.9829326455734090	3.3419932741947700	-1.2951276543309600
	3	-1.3047751558655600	-3.3037857306214400	1.0931738055483900
	4	3.0941083031624800	2.0036436650060300	-0.4736415538529350
	5	2.8952029319855400	-2.1036715590984200	1.0023929039780700
	6	-0.1718437812773930	0.7594581044586500	2.0901455821315100
	7	0.1718392808398610	-0.7594570865256770	-2.0901464690818900

[a] For Xe_2, R_e is taken from R. A. Aziz and M. J. Slaman, Mol. Phys. **57**, 825 (1986), and for the other clusters, the Lennard-Jones geometries of M. Hoare and P. Pal, Adv. Phys. **20**, 161 (1971), are used.

(Table continued.)

n	Atom number	x	y	z
8	1	1.0614601989969600	4.4579284143243300	-1.2902286103381400
	2	-1.8379684650414500	-2.4189745158343500	2.9788680393762100
	3	-3.7571162175575800	-0.9301150248621570	-0.6600023392245450
	4	2.4134298940082100	-1.4101541556909300	2.7574074609640900
	5	3.1231543936206400	0.6405450339526510	-1.0257868071392100
	6	-0.6935395833857340	0.9375327918316070	-3.1395398566352300
	7	0.2486680720378160	-2.5836917390391000	-0.8119880438636470
	8	-0.5580882922901840	1.3069291957066300	1.1912701572491500
9	1	-3.3032464469116200	0.2917420212292050	2.9363166481559500
	2	-1.5012323282812300	-0.5559555470316730	-4.1298578706142000
	3	0.4283245833309530	2.5141718671095300	3.6213146661812900
	4	2.2303322616599500	1.6664667317860100	-3.4448457251250600
	5	-2.5857391850902600	-2.5076106054233300	-0.3585862678048900
	6	3.3851798035081300	1.0485301193706100	0.7374961337128960
	7	0.5281717715832810	-1.6774074948142400	2.5649652972043600
	8	1.5814053005890600	-2.1728715614296100	-1.5650688277850800
	9	-0.7631957607769360	1.3929344692035000	-0.3617340539252680
10	1	-0.4379504512439080	4.4866399264090400	-0.7572900287911340
	2	1.7705190297462000	-0.5507446244996850	4.1781777533970000
	3	-4.1853994807368000	-1.8378381556393300	-0.0029522050951005
	4	3.0016532564339200	2.5285670123973200	1.2376344177707300
	5	-0.6087067185492540	-3.5645492249102700	1.9643770805406100
	6	-2.7363860431743700	1.2885578935768000	-2.7905415850355600
	7	2.9126978009047300	-1.7034716198314200	0.1877376687055550
	8	-0.5641808727601500	-2.4548365086482900	-2.2530750386737600
	9	1.6234624921309100	1.2371956987822400	-2.6934338325913100
	10	-0.7757090127512610	0.5704796019748930	0.9293657697729340
11	1	4.0974198452024100	-0.8195641073781940	2.2079352841182200
	2	0.7477625520986630	2.4445223503969600	-3.9750010706719800
	3	1.1631844793606500	2.3066172065229700	3.3997359850012900
	4	1.8939225168093900	-3.8199003002971300	-0.2304492794789040
	5	-0.7749047165040770	4.1951962313027000	-0.1776794580860790
	6	-0.0441679546781038	-1.9313132303877300	-3.8078601789861100
	7	0.0975355907323604	-1.9628236790501800	3.3322118688052000

(Table continued.)

n	Atom number	x	y	z
12	1	0.9927647482226990	-2.9528046662657200	3.1326353879060400
	2	2.0534546840629600	3.8470788203399700	0.7080656513199400
	3	-2.3311800135051900	3.3711363811666400	1.6489692801908500
	4	4.1077771274180500	-0.0613509481604760	1.6249612291887000
	5	-2.9867257038062400	-0.8314395295439380	3.1474170852783700
	6	-0.8665463497811500	3.0689239149799100	-2.4857249901447100
	7	2.3768345203401000	-3.1018054140268900	-1.0380229122243500
	8	-1.9015271454121100	-3.5662099094352100	-0.1199109440973480
	9	3.0164942946378700	0.9989423646137430	-2.5001957387272100
	10	-3.9060594752317700	0.2475074224521470	-1.0146480481799300
	11	-0.6351100414477480	-1.1666006060608000	-3.5496814989366300
	12	0.0798233545025344	0.1466221699406260	0.4461354980376030

Comparison of the the anisotropy ($\Delta\sigma$, in ppm) and asymmetry parameter (η_σ) of the ^{129}Xe shielding tensor in Xe_n ($n = 2 - 12$) as calculated quantum-chemically (QC) and from the different pairwise additive models, PAA(bin) and PAA(eff).

		Anisotropy $\Delta\sigma$			Asymmetry parameter η		
n	G_s	PAA(bin)	PAA(eff)	QC	PAA(bin)	PAA(eff)	QC
2	C_{2v}	46.82	30.50	46.51	0.0000	0.0000	0.0000
3	C_{2v}	58.53	38.12	50.05	0.6000	0.6000	0.3837
4	C_{3v}	70.24	45.74	53.86	0.0000	0.0000	0.0000
5	C_{3v}	71.30	46.59	54.96	0.0000	0.0000	0.0000
	C_{2v}	58.05	37.69	39.29	1.0440	1.0569	0.9545
6	C_{4v}	49.78	32.39	44.18	0.0000	0.0000	0.0000
7	C_{2v}	62.03	40.85	44.04	0.8235	0.8003	0.6523
	C_{5v}	11.97	6.36	10.31	0.0001	0.0002	0.0001
8	$C_1(1)$	73.65	48.43	57.98	0.0108	0.0147	0.0097
	$C_1(2)$	63.17	41.71	45.20	0.7786	0.7478	0.5933
	$C_s(1)$	62.89	41.54	44.89	0.8094	0.7826	0.6331
	$C_s(2)$	39.37	25.83	22.08	1.7615	1.7569	1.9361
	$C_1(3)$	12.27	6.60	10.57	0.1476	0.2105	0.2038
	$C_1(4)$	47.18	31.81	33.49	-0.2670	-0.1861	0.0987
9	C_1	65.35	43.43	47.35	0.6863	0.6397	0.4866
	$C_s(1)$	44.19	29.68	26.95	1.4424	1.3728	1.3522
	$C_s(2)$	12.76	7.04	10.69	1.0097	1.4065	1.0984
	C_{2v}	60.28	40.88	38.40	0.6764	0.7630	0.7237
10	$C_s(1)$	69.39	46.59	51.03	0.4992	0.4250	0.2904
	$C_s(2)$	51.40	35.28	33.36	1.0725	0.9624	0.8475
	$C_s(3)$	16.14	9.69	11.92	0.7857	1.0170	0.9366
	C_{3v}	42.20	30.15	24.77	3.0000	3.0000	3.0000
11	$C_s(1)$	71.37	48.16	52.04	0.4502	0.3685	0.2450
	C_1	57.20	39.77	37.48	0.8522	0.7383	0.6203
	$C_s(2)$	24.46	16.11	15.48	0.7276	0.8710	1.0028
	$C_s(3)$	21.85	14.14	14.32	0.3321	0.3918	0.4538
	C_{2v}	67.58	46.30	38.65	1.6413	1.7641	1.4895
12	$C_s(1)$	64.13	45.19	41.29	0.6291	0.5182	0.4151
	$C_s(2)$	40.47	28.78	23.64	0.0363	0.0497	0.0472
	$C_{5v}(1)$	35.72	25.04	20.84	0.0000	0.0000	0.0000
	$C_{5v}(2)$	37.89	26.97	14.66	2.9998	2.9998	2.9991
rms error		16.15	6.32		0.16	0.13	

As the previous table but for the nuclear quadrupole coupling tensor components χ_{33} and χ_{22} (in kHz).[a]

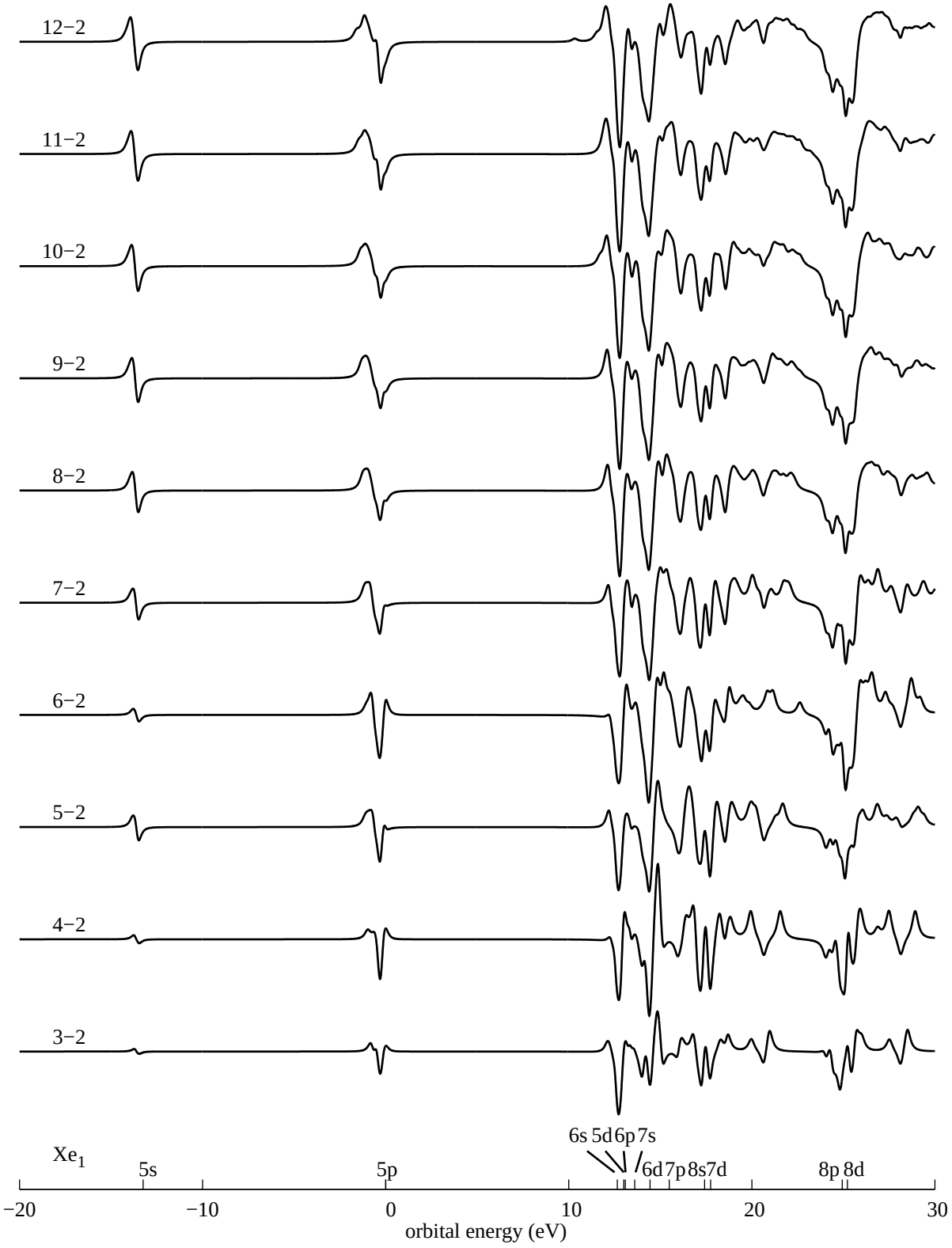
		Largest component χ_{33}			Second-largest component χ_{22}		
n	G_s	PAA(bin)	PAA(eff)	QC	PAA(bin)	PAA(eff)	QC
2	C_{2v}	2259	1688	2257	-1129	-844	-1128
3	C_{2v}	2823	2111	2551	-2259	-1688	-2187
4	C_{3v}	3388	2533	2735	-1694	-1266	-1368
5	C_{3v}	3441	2591	2761	-1721	-1296	-1381
	C_{2v}	-2866	-2153	-2412	2796	2079	1968
6	C_{4v}	2388	1800	1635	-1194	-900	-818
7	C_{2v}	-2723	-2034	-2220	3002	2293	2114
	C_{5v}	526	259	-440	-263	-130	232
8	$C_1(1)$	3562	2714	2858	-1804	-1382	-1481
	$C_1(2)$	-2702	-2013	-2185	3060	2348	2175
	$C_s(1)$	-2740	-2051	-2233	3047	2339	2146
	$C_s(2)$	-2626	-1985	-2014	1900	1445	1134
	$C_1(3)$	541	280	-455	-224	-95	286
	$C_1(4)$	2313	1828	2336	-892	-822	-1525
9	C_1	3174	2460	2279	-2644	-1956	-2119
	$C_s(1)$	-2600	-1956	-1983	2154	1702	1250
	$C_s(2)$	53	151	570	566	324	-467
	C_{2v}	-2544	-2186	-2962	2962	2361	2808
10	$C_s(1)$	3386	2665	2490	-2480	-1795	-1939
	$C_s(2)$	-2561	-1912	-1930	2532	2065	1635
	$C_s(3)$	-39	70	497	744	494	-293
	C_{3v}	-4248	-3648	-4296	2124	1824	2149
11	$C_s(1)$	3490	2767	2612	-2465	-1776	-1932
	C_1	-2550	-1917	-1940	2834	2353	1937
	$C_s(2)$	-1061	-916	-564	-119	8	450
	$C_s(3)$	-334	-213	191	-709	-569	-177
	C_{2v}	-4493	-3868	-4129	3335	2695	2725
12	$C_s(1)$	3195	2699	2294	-2519	-1906	-1928
	$C_s(2)$	2023	1736	982	-1056	-922	-556
	$C_{5v}(1)$	1772	1493	659	-886	-747	-340
	$C_{5v}(2)$	-3799	-3232	-3053	1900	1616	1527
rms error		670	416		635	370	

[a] As $\boldsymbol{\chi}$ is a traceless tensor, the smallest (in absolute value) component can be obtained as $\chi_{11} = -(\chi_{22} + \chi_{33})$.

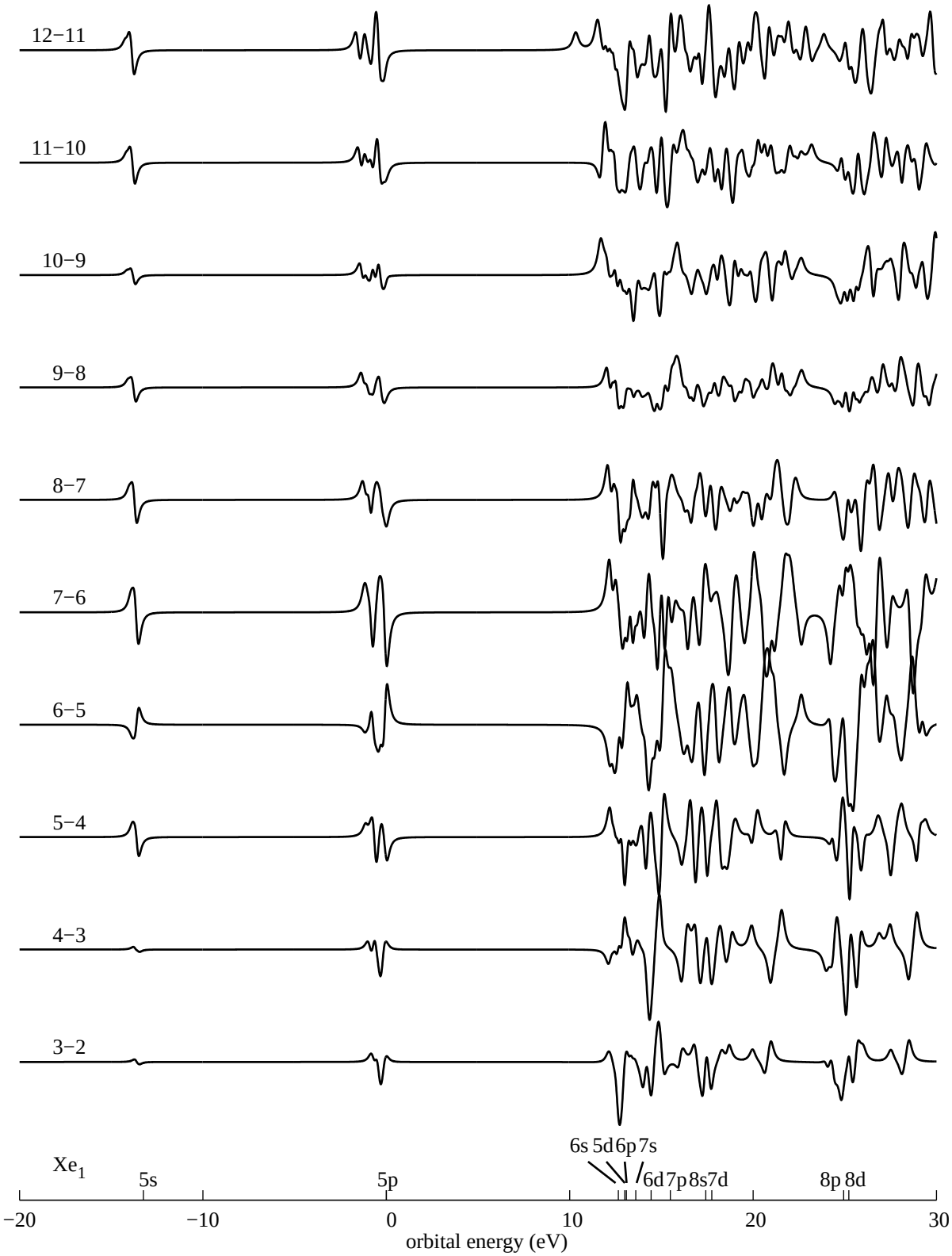
As previous tables but for the total (in Hz) and electronic (in kHz a.u.) spin-rotation constants.[a]

		Total spin-rotation constant C			Electronic spin-rotation constant C^e		
n	G_s	PAA(bin)	PAA(eff)	QC	PAA(bin)	PAA(eff)	QC
2	C_{2v}	21.84	14.40	20.27	451.3	418.8	444.5
3	C_{2v}	32.76	21.64	28.74	902.6	837.6	875.2
4	C_{3v}	32.76	21.64	25.83	1353.9	1256.4	1293.1
5	C_{3v}	21.04	14.14	16.67	1583.8	1487.1	1518.8
	C_{2v}	30.53	20.17	22.99	1806.8	1676.6	1711.1
6	C_{4v}	22.73	15.21	17.89	2076.2	1945.6	1992.2
7	C_{2v}	16.46	11.18	12.27	2263.3	2135.6	2158.8
	C_{5v}	25.36	16.80	17.70	2723.2	2525.9	2546.1
8	$C_1(1)$	10.17	6.77	7.56	2224.1	2114.7	2138.2
	$C_1(2)$	12.74	8.39	9.27	2454.2	2313.9	2339.3
	$C_s(1)$	13.11	9.00	9.62	2486.1	2358.7	2376.1
	$C_s(2)$	15.91	10.75	11.49	2719.1	2558.2	2578.7
	$C_1(3)$	19.54	13.07	13.56	2953.8	2757.0	2771.3
	$C_1(4)$	22.25	14.78	15.33	3191.3	2958.7	2975.9
9	C_1	10.87	7.22	7.76	2671.4	2531.8	2550.3
	$C_s(1)$	13.11	8.95	9.35	2936.8	2779.0	2792.2
	$C_s(2)$	16.27	10.98	11.23	3184.7	2988.7	2997.3
	C_{2v}	21.37	14.26	14.39	3675.3	3405.0	3408.2
10	$C_s(1)$	9.19	6.15	6.43	2877.8	2739.7	2750.7
	$C_s(2)$	10.78	7.14	7.46	3107.5	2941.0	2952.7
	$C_s(3)$	13.71	9.34	9.37	3411.8	3217.1	3218.2
	C_{3v}	21.23	14.29	14.06	4205.3	3889.8	3876.5
11	$C_s(1)$	8.06	5.37	5.50	3081.0	2940.0	2946.1
	C_1	9.25	6.16	6.26	3306.9	3143.2	3146.9
	$C_s(2)$	11.64	7.74	7.75	3589.0	3383.8	3383.0
	$C_s(3)$	11.75	8.07	7.91	3634.0	3441.3	3433.7
	C_{2v}	21.49	14.61	14.01	4766.7	4401.0	4366.0
12	$C_s(1)$	8.13	5.44	5.39	3504.1	3345.1	3341.8
	$C_s(2)$	10.04	6.70	6.49	3778.2	3580.7	3567.4
	$C_{5v}(1)$	10.25	7.07	6.72	3831.0	3643.7	3625.1
	$C_{5v}(2)$	23.74	16.43	15.10	5449.3	5014.1	4932.9
rms error		4.99	2.06		196.24	25.81	

[a] The electronic spin-rotation constants are presented without the appropriate $\boldsymbol{I}^{-1}$ factor.



Normalized difference in the density of states (DOS) in the valence region of Lennard-Jones clusters Xe_n and xenon dimer Xe_2, $\frac{2}{n}\times$DOS(Xe_n)-DOS(Xe_2), ($n = 3 - 12$) estimated using Lorentzian broadening (width = 0.2 eV) of Hartree-Fock orbital energies. The ticks for Xe_1 as in Fig. 6 of the article.



As the previous figure but for the normalized difference in the density of states (DOS) of successive Lennard-Jones clusters, $\frac{n-1}{n}\times$DOS(Xe$_n$)–DOS(Xe$_{n-1}$).