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Electronic Supplementary Information (ESI): Nuclear Magnetic Resonance Predictions for Graphenes: Concentric Finite Models and Extrapolation to Large Systems

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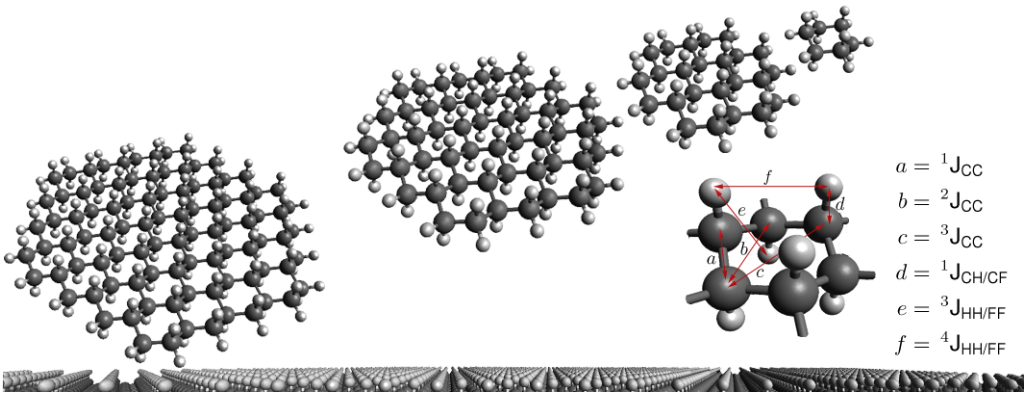

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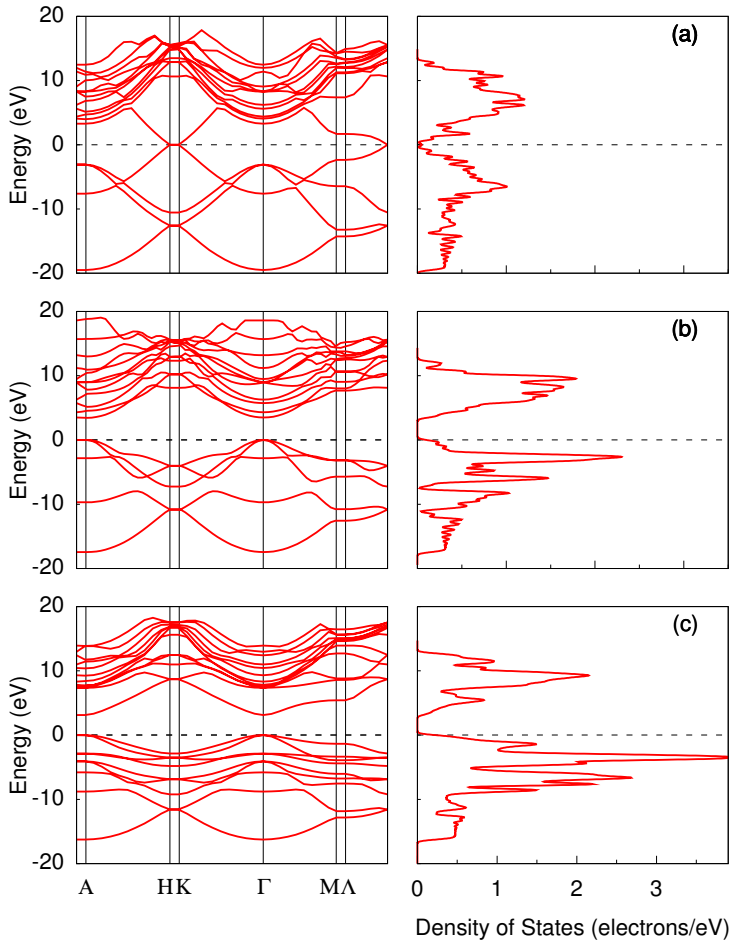

Figure S 1: Band structures for (a) graphene, (b) graphane, and (c) fluorographene (left) and densities of states (right).

1 Details of the co basis sets

The concept of completeness-optimised (co) basis was introduced by Manninen and Vaara.[1] The idea of the co method is to generate universal, element-independent (for adjacent elements in the periodic table) and high-quality Gaussian basis sets by using scheme where energetic criteria are abandoned and the optimisation is done systematically toward the basis set limit. The completeness profiles of Chong[2] are used, defined as

$$Y(\zeta) = \sum_m \langle g(\zeta)|\chi_m\rangle^2, \tag{1}$$

where $\{\chi_m\}$ is a set of orthonormalised basis set functions for a given angular momentum l and $g(\zeta)$ is an l-type test Gaussian orbital (GTO) with the exponent ζ. To analyse the completeness of $\{\chi_m\}$, $g(\zeta)$ is used, and the value of $Y(\zeta)$ equal to 1 would be obtained for all ζ for a complete set. A plot $[\log(\zeta), Y(\zeta)]$ can be used for portraying $Y(\zeta)$. In the plot, the profile of a basis set that is complete for a certain exponent range forms a plateau-like profile, as exemplified by Figure S2. Completeness-optimized basis sets are here generated by using the Kruununhaka code.[3] The code generates a primitive basis set for the desired exponent range $[\zeta_{\min}, \zeta_{\max}]$ for certain l and number of GTOs. The deviation from completeness[1]

$$\tau = \int_{\log(\zeta_{\min})}^{\log(\zeta_{\max})} [1 - Y(\zeta)] d\log(\zeta) \tag{2}$$

is optimized to be as small as deemed sufficient. Recently, the method has been used to produce accurate results for hyperfine properties with fewer basis functions than with traditional, energy-optimized basis sets.[1,4–8]

In this work uncontracted co basis sets were generated for the calculations of σ, $\Delta\sigma$, J, ΔJ, and $\chi_{^2\mathrm{H}}$ by the cluster method using a scheme similar to that in earlier studies.[4–8] First, an even-tempered reference basis set labelled as extreme was generated with exponent ranges slightly wider than those of the aug-cc-pCV5Z basis.[9] As monitored through the calculated properties of the trans-difluoroethane test molecule, even-tempered basis sets were then generated by expanding separately the exponent ranges for each l-value to both tight (high-exponent) and diffuse (low-exponent) directions until convergence was reached. The range that provided results of J and ΔJ within 0.3 Hz for ^{13}C and ^{19}F as well as 0.1 Hz for ^{1}H couplings was selected for the common set for both C and F, [co-NMR-b(C,F)] and of H [co-NMR-b(H)]. These sets were then made smaller by reducing the number of basis functions while maintaining the previously mentioned range, to provide results deviating from those of co-NMR-b maximally by 0.5 Hz for co-NMR-r(C,F) and by 0.2 Hz for co-NMR-r(H). It was possible to generate the basis sets for hydrogen using tighter criteria than for carbon and fluorine, due to the smaller exponent range. For H, d-type functions were needed to saturate the $\chi_{^2\mathrm{H}}$ value. The final exponents are given in Tables S1-S3.

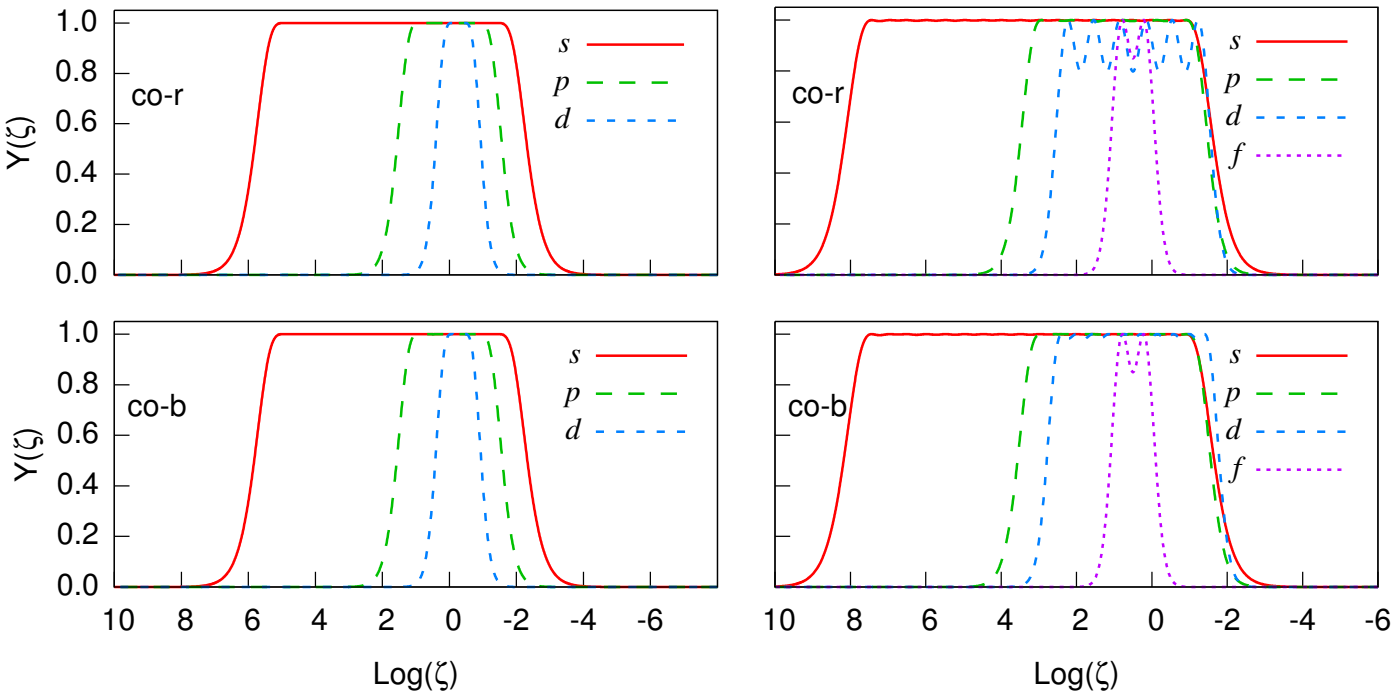

Figure S 2: Completeness profiles of the completeness-optimized basis sets, with hydrogen basis sets on the left and carbon/fluorine sets on the right.

Table S 1: Exponents of the completeness-optimized primitive Gaussian basis co-NMR-r.

Element	s-exponents	p-exponents	d-exponents	f-exponents
H	71244.05600000	5.44988090	2.00970130	-
	19207.48300000	1.00001530	0.56238213	
	4486.50470000	0.18349441	0.15734934	
	1037.62880000			
	234.96914000			
	55.09561900			
	12.83107900			
	2.94137300			
	0.70147158			
	0.16586887			
	0.04480405			
C, F	27299135.00000000	837.67380000	168.51725000	6.0209096
	8917212.60000000	359.95208000	34.76545400	1.6608939
	3247828.20000000	135.52469000	7.02515290	
	955334.01000000	49.33638100	1.41810730	
	297031.17000000	16.18444800	0.28702406	
	91306.53200000	5.70980650	0.05909971	
	29515.21700000	1.97345300		
	9793.24970000	0.73918977		
	3043.52100000	0.26082949		
	926.12601000	0.12166218		
	314.44885000			
	99.84893100			
	33.26893600			
	10.46833500			
	3.41728260			
	1.02880640			
	0.34674617			
	0.12434325			

Table S 2: Exponents of the completeness-optimized primitive Gaussian basis co-NMR-b.

Element	s-exponents	p-exponents	d-exponents	f-exponents
H	92484.42100000	8.17053536	0.33090037	-
	50926.98900000	4.44330808	0.55194379	
	21878.28300000	2.12132091	0.88633388	
	13197.08800000	0.98850335		
	4522.34760000	0.46067956		
	1967.02600000	0.21993046		
	617.03923000	0.1196066		
	308.39383000			
	133.08136000			
	57.30076400			
	26.54328100			
	9.36347380			
	4.40072060			
	1.7712436			
	0.81891716			
	0.22765488			
	0.17137059			
	0.05592994			
	0.03499544			
C, F	27299135.00000000	850.46897000	245.60620000	6.02090960
	8917212.60000000	455.86375000	100.97911000	1.66089390
	3247828.20000000	200.74579000	37.30825300	
	955334.01000000	78.62025700	13.97289100	
	297031.17000000	42.63055200	5.25456480	
	91306.53200000	13.22011000	1.95075200	
	29515.21700000	7.59306990	0.713894950	
	9793.24970000	2.98658410	0.26594312	
	3043.52100000	1.36010410		
	926.12601000	0.53153316		
	314.44885000	0.23081681		
	99.84893100	0.11166191		
	33.26893600			
	10.46833500			
	3.41728260			
	1.02880640			
	0.34674617			
	0.12434325			

Table S 3: Exponents of the even-tempered primitive Gaussian basis "extreme".

Element	s-exponents	p-exponents	d-exponents	f-exponents
H	92484.42100000	8.17053536	2.38996600	-
	50926.98900000	4.44330808	0.93501123	
	21878.28300000	2.12132091	0.33811504	
	13197.08800000	0.98850335	0.13231572	
	4522.34760000	0.46067956		
	1967.02600000	0.21993046		
	617.03923000	0.1196066		
	308.39383000			
	133.08136000			
	57.30076400			
	26.54328100			
	9.36347380			
	4.40072060			
	1.7712436			
	0.81891716			
	0.22765488			
	0.17137059			
	0.05592994			
	0.03499544			
C, F	80841578.000000000	2852.50290000	266.51672000	8.47600640
	42201234.00000000	1216.00980000	133.61175000	4.93458440
	25813548.00000000	479.01528000	64.10037400	2.54234660
	9836621.50000000	188.38915000	29.18013300	1.26600500
	3496178.00000000	71.775419000	13.04069700	0.61847205
	1239395.80000000	27.74814900	5.72673800	0.37259794
	411628.05000000	10.76791400	2.76202650	
	152285.33000000	4.402654500	1.27425560	
	64860.53500000	1.70498360	0.59281063	
	28824.31900000	0.61878512	0.30068352	
	7425,02070000	0.23670283	0.14316350	
	4759.64650000	0.08584428	0.06920693	
	1569.74040000	0.03883240	0.03550092	
	510.40041000			
	224.88594000			
	82.39272500			
	34.57586400			
	10.70872100			
	3.89784420			
	1.81189940			
	0.82483678			
	0.24670561			
	0.13481263			
	0.11932901			
	0.03824064			

Table S 4: Computed shielding and spin-spin coupling constants and corresponding anisotropies[a] in the locally dense basis-set method test for various sets in completely relaxed perhydrogenated coronene (HG2, relaxed). N denotes the number of basis functions. Shielding in ppm, coupling in Hz. PBE-functional was used.

		Shielding				Spin-spin coupling			
Basis set	N	σ_C	$\Delta\sigma_C$	σ_H	$\Delta\sigma_H$	$^1J_{CC}$	Δ^1J_{CC}	$^1J_{CH}$	Δ^1J_{CH}
co-NMR-r** [b]	1164	121.38	25.86	30.60	−1.13	33.34	35.88	127.63	−18.79
co-NMR-r* [c]	1488	120.88	25.85	30.65	−1.15	33.18	35.86	127.72	−18.98
co-NMR-r [d]	3108	120.72	25.34	30.67	−1.13	-	-	-	-

[a] Anisotropies defined in this table with respect to the direction of the largest component in the principal axis frame of each tensor.
[b] The innermost hexagon (C_6H_6) was calculated with the co-NMR-r basis set and the peripheral atoms with the def2-SVP basis set.[10]
[c] The innermost hexagon was calculated with the co-NMR-r basis set and the peripheral atoms with the def2-TZVP basis set.[10]
[d] The whole molecule was calculated with the co-NMR-r basis set.

Table S5: Computed shielding and spin-spin coupling constants and corresponding anisotropies[a] for trans-difluoroethane using DFT[b] and various basis sets. N denotes the number of basis functions. Shielding in ppm, coupling parameters in Hz. Shielding in ppm, coupling parameters in Hz.

		Shielding						Spin-spin coupling							
Basis set	N	σ_F	$\Delta\sigma_F$	σ_C	$\Delta\sigma_C$	σ_H	$\Delta\sigma_H$	$^3J_{FF}$	Δ^3J_{FF}	$^1J_{CF}$	Δ^1J_{CF}	$^1J_{CC}$	Δ^1J_{CC}	$^1J_{CH}$	Δ^1J_{CH}
cc-pCVDZ[c]	92	423.93	−23.15	111.23	88.19	26.76	4.26	−98.54	242.88	−250.83	105.41	19.01	30.49	112.55	−13.70
cc-pCVTZ	228	422.61	32.50	101.28	91.29	26.71	4.11	−65.28	408.76	−220.40	220.37	38.03	38.69	148.16	−26.03
cc-pCVQZ	456	421.77	34.76	99.85	92.29	26.60	4.17	−91.48	362.46	−247.49	175.15	29.43	35.98	144.76	−21.11
cc-pCV5Z	800	421.39	35.15	99.03	92.85	26.55	4.17	−85.40	383.48	−238.01	184.23	29.58	37.65	152.99	−18.45
aug-cc-pCVDZ[c]	144	423.87	32.99	110.29	90.00	26.60	4.21	−105.28	267.11	−249.77	106.59	19.93	29.97	118.10	−16.42
aug-cc-pCVTZ	328	422.21	34.42	101.20	92.21	26.62	4.15	−66.19	406.13	−219.38	214.03	33.49	38.08	146.82	−25.88
aug-cc-pCVQZ	620	421.41	34.65	99.75	92.62	26.57	4.16	−91.56	362.68	−248.17	174.56	29.32	35.95	148.52	−21.29
aug-cc-pCV5Z	1044	421.07	34.80	98.99	92.94	26.54	4.17	−85.38	383.27	−238.28	184.22	29.59	37.66	153.93	−18.63
pcJ-0[d]	72	394.65	38.99	111.49	84.18	27.81	4.19	−124.19	351.68	-335.97	117.94	20.85	29.70	138.21	7.88
pcJ-1	148	420.56	31.86	101.59	90.79	26.66	4.48	−86.37	347.42	−238.55	170.12	30.23	35.27	154.51	−19.72
pcJ-2	300	420.38	34.88	99.54	92.68	26.61	4.19	−90.88	371.33	−245.44	178.05	28.47	37.55	156.22	−17.44
pcJ-3	512	420.97	34.81	98.82	92.97	26.53	4.17	−88.34	382.36	−249.72	187.22	31.36	37.41	161.96	−19.91
pcJ-4	808	420.98	34.85	98.70	93.05	26.54	4.18	−88.05	384.06	−247.93	189.93	31.29	38.64	161.49	−18.41
extreme	924	420.97	34.86	98.68	93.05	26.54	4.17	−89.34	380.22	−249.12	186.04	31.17	37.95	161.44	−18.99
co-NMR-b	612	420.89	34.84	98.76	93.02	26.57	4.15	−89.24	379.70	−249.12	185.32	31.04	38.01	161.36	−18.89
co-NMR-r	508	420.89	34.62	98.99	92.80	26.59	4.16	−89.50	378.83	−249.57	185.50	30.93	38.43	161.52	−18.62

[a] Anisotropies defined in this table with respect to the direction of the largest component in the principal axis frame of each tensor.
[b] KT2-functional[11] was used.
[c] Ref.[9]
[d] Ref.[12]

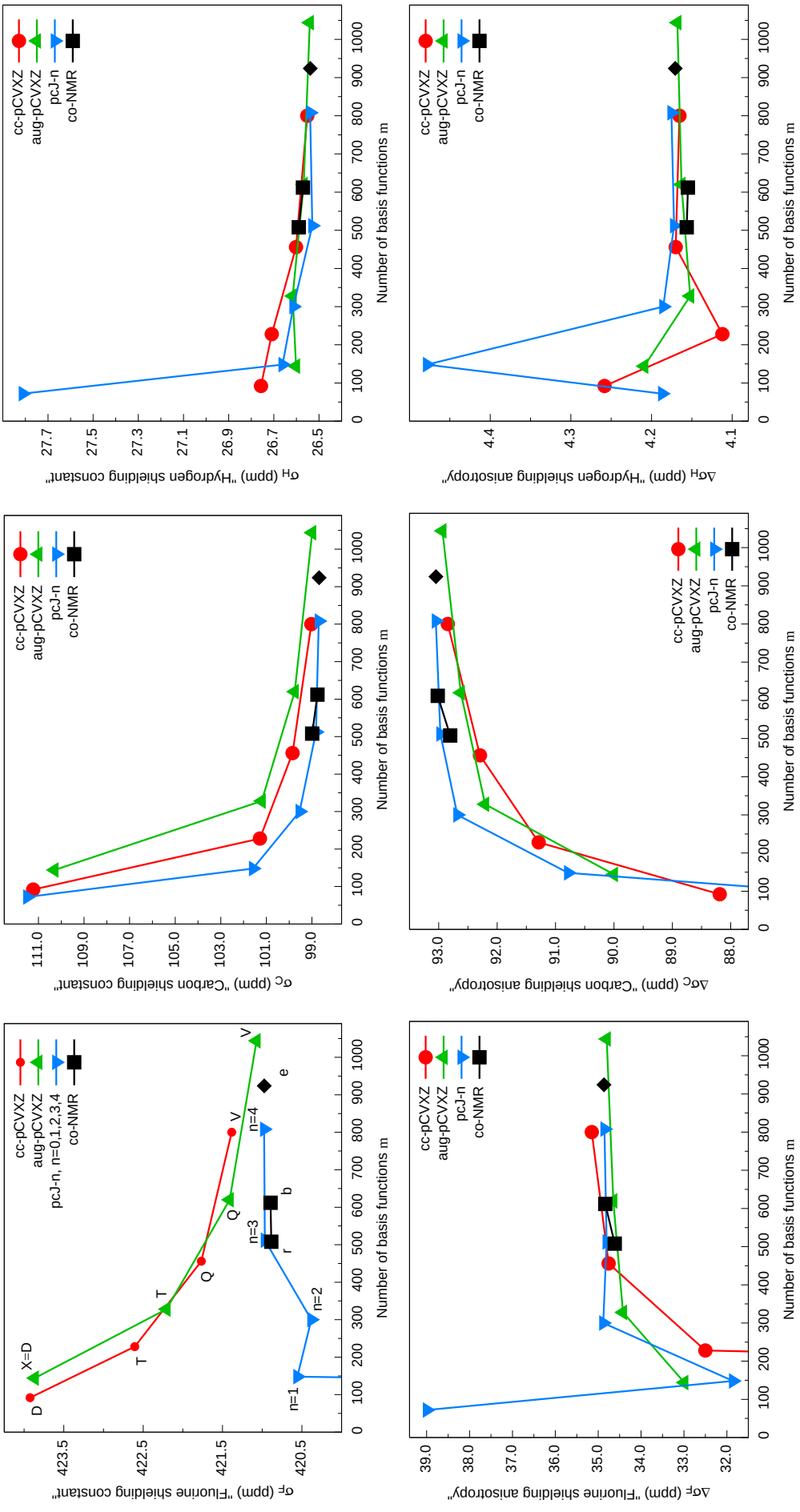

Figure S3: Nuclear shielding constants and anisotropies (defined here with respect to the direction of the largest component in the principal axis frame of each tensor) of trans-difluoroethane as a function of the number of basis functions N within various basis-set families. For co-NMR-basis sets, r indicates a reduced and b the best co-basis set. The label e indicates an extreme case where, for all the included angular momentum numbers l, all exponent ranges are spanned by the even-tempered method to ensure that the basis-set limit is reached.

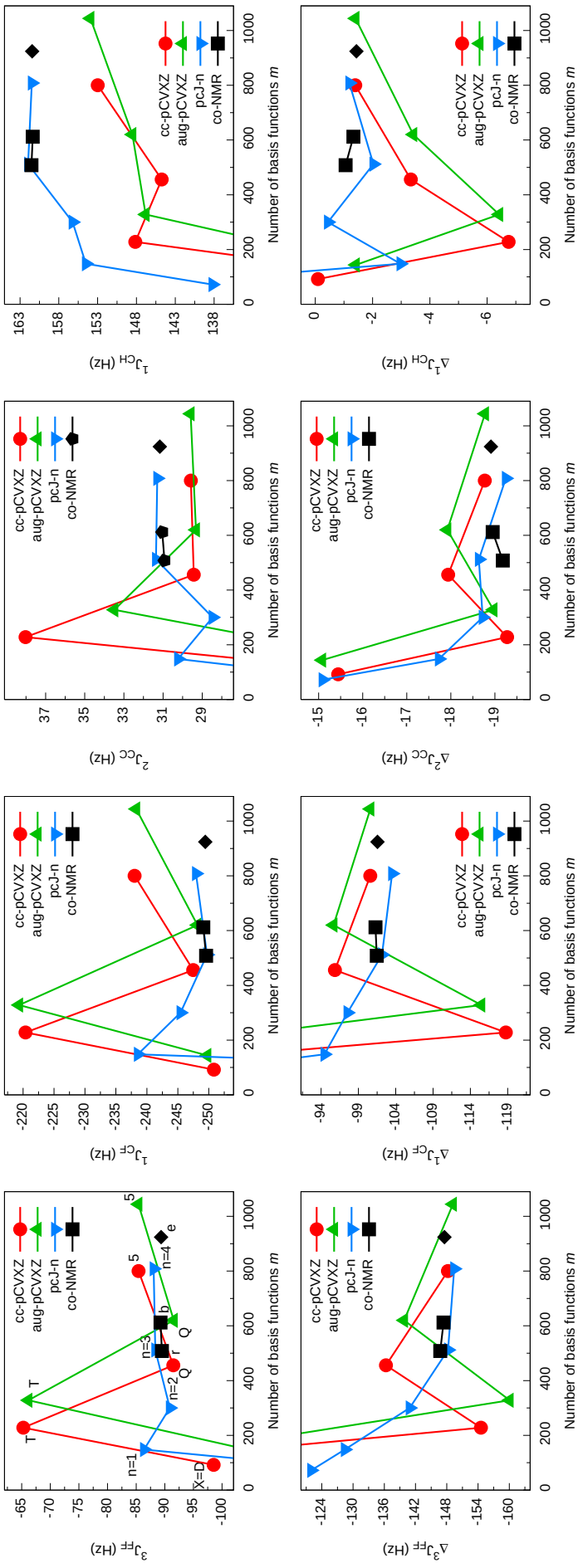

Figure S 4: As Figure S3, but for spin-spin coupling constants and corresponding anisotropies of trans-difluoroethane as a function of the number of basis functions within various basis-set families.

Table S 6: Nuclear shielding constants and anisotropies (ppm) of methane, fluoromethane, trans-difluoromethane, cyclohexane, and axially fluorinated cyclohexane with basis set co-NMR-r and various DFT functionals.

		Shielding						Chemical shift		
System[a]	Functional	σ_H	$\Delta\sigma_H$	σ_C	$\Delta\sigma_C$	σ_F	$\Delta\sigma_F$	δ_H[b]	δ_C[b]	δ_F[c]
CH_4[d]	BLYP	31.23	8.78	182.98	-	-	-	-	-	-
	B3LYP	31.17	9.12	185.49	-	-	-	-	-	-
	BHandHLYP	31.12	9.49	188.53	-	-	-	-	-	-
	KT2	31.17	9.24	192.06	-	-	-	-	-	-
	KT3	31.25	8.98	189.46	-	-	-	-	-	-
	PBE	31.11	9.17	187.17	-	-	-	-	-	-
	$PBE_{periodic}$	31.07	9.06	186.49	-	-	-	-	-	-
	PBE0	31.07	9.50	189.64	-	-	-	-	-	-
	CCSD[e]	30.32	10.13	198.28	-	-	-	-	-	-
	CCSD(T)[e]	30.29	10.14	198.71	-	-	-	-	-	-
	Exp.	30.61[f]	-	198.70[g]	-	-	-	-	-	-
CH_3F[h]	BLYP	26.90	5.13	95.53	116.44	449.29	−51.74	-	-	-
	B3LYP	27.02	4.77	101.47	112.01	458.20	−54.04	-	-	-
	BHandHLYP	27.19	4.32	109.24	105.87	468.76	−57.40	-	-	-
	KT2	26.87	4.93	108.86	111.16	454.21	−49.61	-	-	-
	KT3	27.06	4.84	107.90	109.04	446.72	−38.23	-	-	-
	PBE	26.76	5.08	100.30	115.98	453.32	−56.30	-	-	-
	$PBE_{periodic}$	26.44	5.40	98.23	117.54	454.42	−57.68	-	-	-
	PBE0	26.96	4.63	107.30	110.04	462.86	−57.26	-	-	-
	CCSD	26.38	4.29	119.73	105.75	479.62	−64.56	-	-	-
	CCSD(T)	26.28	4.27	118.97	107.28	478.27	−65.37	-	-	-
	Exp.	26.62[i]	4.89/4.64[i]	116.83[i]	117.2/113.8[i]	470.98[j]	-	-	-	-
$C_2H_4F_2$ [d]	BLYP	26.66	4.04	84.55	96.97	415.91	34.60	4.57	98.43	33.38
	B3LYP	26.75	4.06	91.13	95.13	426.55	36.28	4.42	94.36	31.65
	BHandHLYP	26.90	4.21	99.83	91.79	439.77	38.15	4.23	88.70	28.99
	KT2	26.59	4.16	98.99	92.80	420.89	34.62	4.58	93.07	33.32
	KT3	26.80	4.13	98.21	90.65	415.96	28.85	4.46	91.25	30.76
	PBE	26.49	4.12	89.87	97.09	418.80	36.51	4.62	97.30	34.52
	PBE0	26.66	4.19	97.68	94.39	431.10	37.53	4.41	91.96	31.76
	CCSD	26.08	4.46	110.26	92.27	449.60	43.08	4.24	88.02	30.02
	CCSD(T)	25.98	4.42	109.16	93.25	446.97	43.71	4.31	89.55	31.30
C_6H_{12}[k]	BLYP	30.04	3.75	140.01	2.18	-	-	1.18	42.97	-
	B3LYP	30.12	4.31	145.91	2.56	-	-	1.04	39.58	-
	BHandHLYP	30.27	4.96	153.09	2.64	-	-	0.86	35.44	-
	KT2	29.85	4.10	151.84	2.53	-	-	1.32	40.21	-
	KT3	30.02	4.09	150.56	2.90	-	-	1.23	38.90	-
	PBE	29.86	4.19	145.81	3.07	-	-	1.25	41.36	-
	PBE0	30.01	4.79	152.59	3.17	-	-	1.05	37.16	-
$C_6F_6H_6$[k]	BLYP	26.19	1.24	77.90	75.80	368.88	−7.04	5.04	105.08	80.41
	B3LYP	26.28	0.88	84.94	75.22	382.13	−9.77	4.89	100.55	76.07
	BHandHLYP	26.43	0.48	94.34	73.43	398.98	−14.75	4.69	94.18	69.78
	KT2	26.08	1.08	93.22	74.19	372.99	−5.55	5.09	98.84	81.22
	KT3	26.31	1.06	92.83	72.24	372.04	−26.95	4.94	96.63	74.68
	PBE	25.99	1.14	83.70	76.78	370.88	−9.67	5.12	103.47	82.44
	PBE0	26.17	0.71	92.05	75.65	386.91	−11.94	4.90	97.60	75.95

[a]Structures are optimized using the PBE functional and def2-TZVP basis. The following geometries were obtained (the units for the bond lengths and angles are Ångströms and degrees, respectively). CH_4: CH = 1.096, HCH = 109.5; CH_3F: CF = 1.395, CH = 1.100, HCF = 108.98; $C_2H_4F_2$: CC = 1.520, CF = 1.400, CH = 1.101, FCC = 108.3, CCH = 111.0, FCH = 108.5; C_6H_{12}: CC = 1.534, CH = 1.105 (ax), 1.102 (eq); $C_6F_6H_6$: CC = 1.533, CF = 1.399, CH = 1.103. [b]Chemical shift calculated with respect to CH_4 at the corresponding levels. [c]Chemical shift calculated with respect to CH_3F at the corresponding levels. [d]Anisotropies defined in this table with respect to the direction of the largest component in the principal axis frame of each tensor, unless otherwise noted. [e]Ab initio results used to benchmark the various DFT levels. [f]Ref. [13] [g]Ref. [14] [h]Anisotropies with respect to the direction of the CF-bond. [i]Ref. [15] [j]Ref. [16]
[k]Anisotropies defined as $\Delta T = T_{zz} - \frac{1}{2}(T_{xx} - T_{yy})$, where the z direction is normal to the plane of the molecule.

Table S7: Spin-spin coupling constants and anisotropies (Hz) for methane, fluoromethane, trans-difluoromethane, cyclohexane, and axially fluorinated cyclohexane with basis set co-NMR-r and different DFT functionals.

System	Functional	$^1J_{CH}$	Δ^1J_{CH}	$^1J_{CF}$	Δ^1J_{CF}	$^1J_{CC}$	Δ^1J_{CC}	$^3J_{HH}$	Δ^3J_{HH}	$^3J_{FF}$	Δ^3J_{FF}	$^3J_{CC}$	Δ^3J_{CC}
CH_4[a]	BLYP	135.86	−20.69	-	-	-	-	-	-	-	-	-	-
	B3LYP	135.39	−22.22	-	-	-	-	-	-	-	-	-	-
	BHandHLYP	144.51	−24.34	-	-	-	-	-	-	-	-	-	-
	KT2	132.59	−16.77	-	-	-	-	-	-	-	-	-	-
	KT3	138.88	−20.46	-	-	-	-	-	-	-	-	-	-
	PBE	133.58	−23.68	-	-	-	-	-	-	-	-	-	-
	PBE0	138.35	−25.16	-	-	-	-	-	-	-	-	-	-
	SOPPA(CCSD)	125.07	−24.39	-	-	-	-	-	-	-	-	-	-
	Exp.	120.87[b]	-	-	-	-	-	-	-	-	-	-	-
CH_3F[c]	BLYP	157.78	2.81	−260.04	216.25	-	-	-	-	-	-	-	-
	B3LYP	158.32	3.21	−234.13	230.04	-	-	-	-	-	-	-	-
	BHandHLYP	170.24	3.00	−197.26	264.75	-	-	-	-	-	-	-	-
	KT2	156.54	1.62	−251.50	209.03	-	-	-	-	-	-	-	-
	KT3	164.12	1.52	−256.31	230.47	-	-	-	-	-	-	-	-
	PBE	155.85	3.78	−256.50	230.21	-	-	-	-	-	-	-	-
	PBE0	162.71	3.92	−227.05	256.81	-	-	-	-	-	-	-	-
	SOPPA(CCSD)	148.63	3.63	−164.34	203.99	-	-	-	-	-	-	-	-
	Exp.	147.25[d]	-	−163.0[d]	350[d]	-	-	-	-	-	-	-	-
$C_2H_4F_2$[a]	BLYP	162.14	−21.15	−258.01	192.23	41.26	40.71	13.70	2.84	−85.42	355.33	-	-
	B3LYP	162.83	−22.26	−231.80	209.16	45.60	41.38	13.49	2.82	−67.04	335.89	-	-
	BHandHLYP	174.96	−23.95	−195.10	246.24	55.85	44.00	14.36	2.91	−39.71	330.92	-	-
	KT2	161.52	−18.62	−249.57	185.50	30.93	38.43	16.30	3.10	−89.50	378.83	-	-
	KT3	169.05	−21.86	−254.72	207.00	36.66	38.97	16.23	3.14	−80.58	353.63	-	-
	PBE	160.78	−24.22	−254.54	208.32	42.46	40.32	13.86	2.96	−80.51	366.85	-	-
	PBE0	167.90	−25.30	−224.40	238.19	49.86	42.19	14.36	3.05	−56.47	346.57	-	-
	SOPPA(CCSD)	153.12	−24.16	−165.85	187.74	49.13	38.99	11.69	2.62	−34.12	266.93	-	-
	Exp.	-	-	-	-	-	-	6.2[e]	-	−30[e]	-	-	-
C_6H_{12}[f]	BLYP	130.58	−16.49	-	-	30.29	−12.25	14.78	−1.02	-	-	2.28	−0.14
	B3LYP	130.91	−17.89	-	-	33.68	−12.35	14.65	−1.16	-	-	2.24	−1.16
	BHandHLYP	140.52	−19.52	-	-	42.04	−13.01	15.76	−1.50	-	-	2.33	−0.18
	KT2	128.47	−13.15	-	-	21.84	−11.37	17.34	−1.56	-	-	2.01	−0.12
	KT3	134.91	−16.51	-	-	26.75	−11.56	17.56	−1.50	-	-	2.11	−0.13
	PBE	130.10	−19.75	-	-	31.98	−12.11	14.95	−1.56	-	-	2.46	−0.16
	PBE0	135.72	−20.89	-	-	37.87	−12.54	15.65	−1.88	-	-	2.53	−0.18
	Exp.	122.4[g]	-	-	-	33.10[h]	-	13.12[i]	-	-	-	2.05[h]	-
$C_6F_6H_6$[f]	BLYP	-	-	−271.83	178.77	40.80	−20.00	-	-	−60.18	85.61	3.17	−0.66
	B3LYP	-	-	−244.38	197.76	45.51	−20.65	-	-	−45.85	95.64	3.27	−0.68
	BHandHLYP	-	-	−206.52	236.62	55.88	−22.42	-	-	−24.43	111.43	3.49	−0.71
	KT2	-	-	−264.01	173.10	31.01	−19.12	-	-	−65.01	93.95	2.83	−0.60
	KT3	-	-	−270.02	193.44	36.41	−19.44	-	-	−57.07	87.50	2.90	−0.60
	PBE	-	-	−268.35	195.02	42.71	−20.05	-	-	−56.41	86.06	3.38	−0.70
	PBE0	-	-	−236.82	226.92	50.43	−21.41	-	-	−37.46	101.07	3.61	−0.73

[a]Anisotropies defined in this table with respect to the direction of the largest component in the principal axis frame of each tensor unless otherwise noted. [b]Ref.[17] [c]Anisotropies defined with respect to the direction of the CF-bond. [d]Ref.[18] [e]Ref.[19] [f]Anisotropies defined as $\Delta T = T_{zz} - \frac{1}{2}(T_{xx} - T_{yy})$, where the z direction is normal to the plane of the molecule. [g]Ref.[20] [h]Ref.[21] [i]Ref.[22]

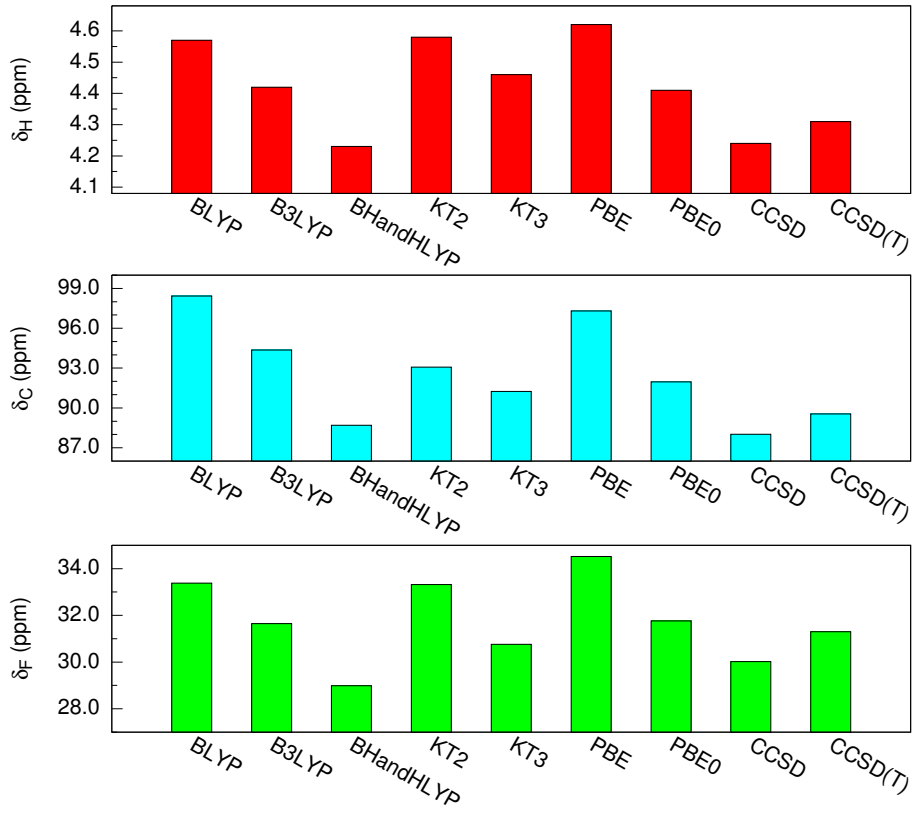

Figure S 5: Chemical shifts (ppm) in trans-difluoroethane with respect to methane (^{1}H,^{13}C) and fluoromethane (^{19}F), with different DFT functionals and coupled cluster methods.

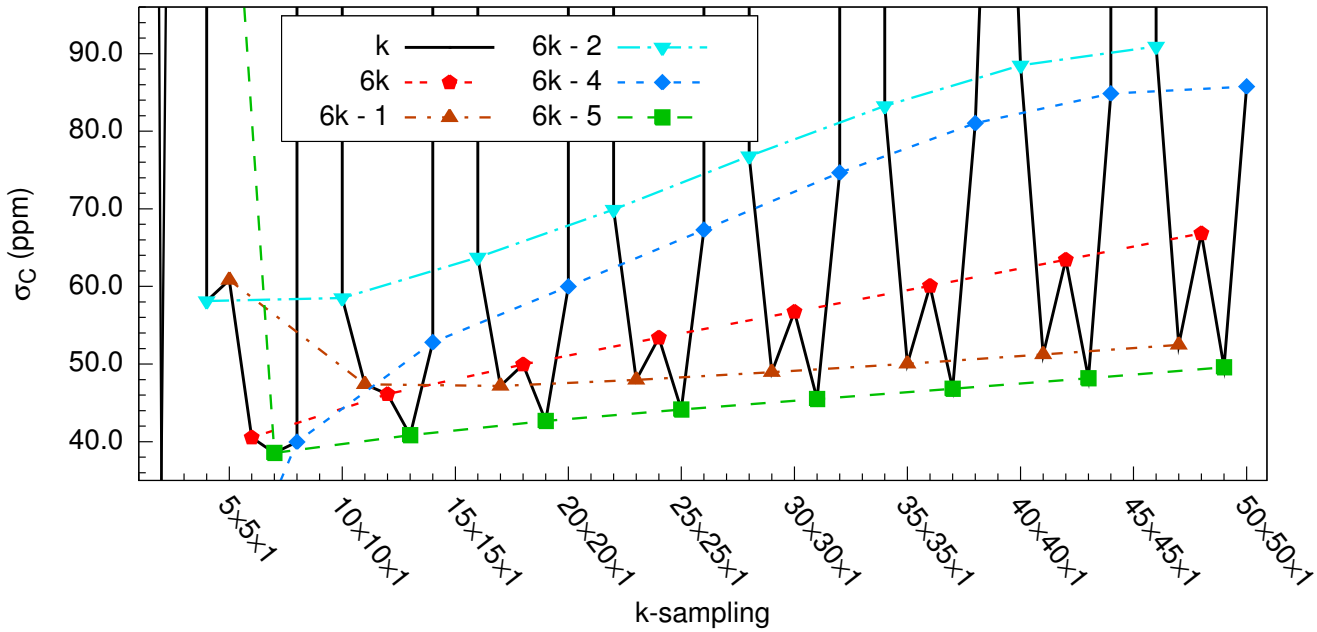

Figure S 6: The shielding constant of graphene as a function of k-sampling (solid line). The periodicity of the oscillation is six and different phases are highlighted with dashed lines. At values equal to 6k−3, one of the k-vectors hits precisely the K-point (Dirac point).

Table S 8: Innermost ^{13}C nuclear shielding constants (σ_{C}), anisotropies (δ_{C}),[a] and chemical shifts (δ_{C}) for finite cluster models of increasing size for graphene (Gn), with relaxed and fixed (to the periodic structure) geometries with the PBE functional (unless otherwise noted) and co-r basis set.

	G1		G2		G3		G4			G5	
Property	Relaxed	Fixed	Relaxed	Fixed	Relaxed	Fixed	Relaxed	Fixed	Fixed[b]	Relaxed	Fixed
σ_{C}	42.69	37.29	49.97	52.27	54.35	54.34	55.20	55.11	56.25	55.17	54.99
$\Delta\sigma_{\mathrm{C}}$	187.75	192.35	211.36	208.86	206.70	207.10	206.76	206.87	220.29	205.95	205.89
δ_{C}	144.49	149.88	137.20	134.90	132.83	132.83	131.97	132.07	132.28	132.01	132.18

[a]Anisotropies defined as $\Delta T = T_{zz} - \frac{1}{2}(T_{xx} - T_{yy})$, where the z direction is normal to the plane of the molecule.
[b]Calculated with the BHandHLYP functional.

Table S 9: As Table S 8 but for finite graphane models (HGn). Periodic results and ^{2}H quadrupole coupling are also reported (in kHz).

	HG1		HG2		HG3			HG4		HG∞
Property	Relaxed	Fixed	Relaxed	Fixed	Relaxed	Fixed	Fixed[b]	Relaxed	Fixed	Periodic[c]
σ_{H}	29.86	29.79	30.60	30.64	30.50	30.56	31.17	30.53	30.59	30.70
$\Delta\sigma_{\mathrm{H}}$	4.19	4.21	−0.67	−0.59	−3.06	−2.98	−2.52	−4.62	−4.57	−5.50
σ_{C}	145.81	143.94	121.38	122.04	123.13	123.68	133.28	123.22	123.73	121.89
δ_{H}	1.25	1.32	0.51	0.47	0.61	0.55	−0.05	0.58	0.52	0.41
δ_{C}	41.36	43.23	65.79	65.13	64.04	63.49	55.25	63.95	64.60	65.28
χ^{2}H	174.3	169.4	166.6	167.8	167.0	167.8	-	167.0	167.8	172.2

[a]Anisotropies defined as $\Delta T = T_{zz} - \frac{1}{2}(T_{xx} - T_{yy})$, where the z direction is normal to the plane of the molecule.
[b]Calculated with the BHandHLYP functional.
[c]The result at the numerical limit of the periodic method with respect to the cut-off energy and k-sampling.

Table S 10: Innermost ^{13}C and ^{19}F nuclear shielding constants ($\sigma_{\mathrm{C/F}}$), anisotropies ($\Delta\sigma_{\mathrm{C/F}}$),[a] and chemical shifts ($\delta_{\mathrm{C/F}}$) for finite cluster models of increasing size for fluorographene (FGn), with relaxed and fixed (to the periodic structure) geometries, as well as periodic results, with the PBE functional (unless otherwise noted) and co-r basis set.

	FG1		FG2		FG3			FG4		FG∞
Property	Relaxed	Fixed	Relaxed	Fixed	Relaxed	Fixed	Fixed[b]	Relaxed	Fixed	Periodic[c]
σ_{F}	370.88	384.48	353.78	348.09	350.59	343.85	372.59	348.60	342.76	340.22
$\Delta\sigma_{\mathrm{F}}$	−9.67	−31.32	−44.92	−45.31	−51.46	−44.25	−35.92	−54.57	−45.82	−44.44
σ_{C}	83.70	79.54	78.62	75.21	76.70	75.26	88.47	75.84	75.21	72.58
$\Delta\sigma_{\mathrm{C}}$	76.78	75.10	62.38	56.55	51.88	50.72	48.59	47.72	48.09	47.58
δ_{F}	82.44	68.84	99.54	105.23	102.73	109.47	96.17	104.72	110.56	114.20
δ_{C}	103.47	107.63	108.55	111.96	110.47	111.91	98.70	111.33	112.04	113.91

[a]Anisotopies defined as $\Delta T = T_{zz} - \frac{1}{2}(T_{xx} - T_{yy})$, where the z direction is normal to the plane of the molecule.
[b]Calculated with the BHandHLYP functional.
[c]The result at the numerical limit of the periodic method with respect to the cut-off energy and k-sampling.

Table S 11: Innermost spin-spin coupling constants J and anisotropies[a] ΔJ for increasing size n of finite cluster models for graphene (Gn), with relaxed and fixed (to the periodic structure) geometries, with the PBE functional and co-r basis set. The different physical contributions to J and ΔJ are also indicated.

		G1		G2		G3		G4		G5	
Property	Term[b]	Relaxed	Fixed	Relaxed	Fixed	Relaxed	Fixed	Relaxed	Fixed	Relaxed	Fixed
$^1J_{CC}$	Total	58.00	56.63	57.59	58.54	58.80	58.64	58.52	58.67	58.75	58.71
	DSO	0.22	0.20	0.40	0.40	0.43	0.43	0.44	0.44	0.45	0.45
	PSO	−6.91	−7.02	−5.51	−5.56	−5.66	−5.61	−5.48	−5.50	−5.56	−5.54
	SD	1.39	1.58	0.76	0.80	0.82	0.82	0.76	0.77	0.78	0.78
	FC	63.30	61.86	61.93	62.90	63.21	63.00	62.80	62.96	63.08	63.02
Δ^1J_{CC}	Total	5.82	7.65	−1.99	−1.57	−1.31	−1.37	−2.08	−1.92	−1.78	−1.75
	DSO	−2.05	-1.94	−1.80	−1.81	−1.80	−1.79	−1.78	−1.78	−1.78	−1.78
	PSO	10.49	10.68	7.95	8.02	8.07	8.03	7.82	7.84	7.90	7.88
	SD	1.50	1.77	0.09	0.17	0.23	0.21	0.09	0.12	0.15	0.15
	SD/FC	−4.12	−2.86	−8.23	−7.95	−7.82	−7.82	−8.20	−8.10	−8.20	−8.01
$^2J_{CC}$	Total	−3.45	−4.25	0.22	0.20	0.14	0.11	0.32	0.29	0.27	0.24
	DSO	−0.02	−0.02	0.11	0.11	0.13	0.13	0.14	0.14	0.15	0.15
	PSO	0.09	0.08	−0.04	−0.05	−0.06	−0.07	−0.07	−0.07	−0.07	−0.07
	SD	−0.84	−0.97	−0.22	−0.25	−0.28	−0.28	−0.22	−0.24	−0.25	−0.25
	FC	−2.68	−3.34	0.37	0.39	0.35	0.33	0.47	0.45	0.44	0.41
Δ^2J_{CC}	Total	−9.75	−11.05	−4.38	−4.61	−4.89	−4.87	−4.31	−4.43	−4.52	−4.57
	DSO	−0.48	−0.45	−0.36	−0.36	−0.35	−0.34	−0.34	−0.34	−0.33	−0.33
	PSO	0.10	0.13	0.11	0.13	0.10	0.11	0.10	0.10	0.09	0.09
	SD	−1.13	−1.34	−0.24	−0.28	−0.33	−0.34	−0.25	−0.27	−0.28	−0.29
	SD/FC	−8.25	−9.39	−3.89	−4.10	−4.31	−4.29	−3.82	−3.92	−3.82	−4.04
$^3J_{CC}$	Total	12.48	12.49	5.91	6.09	6.38	6.31	5.95	6.00	6.13	6.12
	DSO	−0.01	−0.01	0.10	0.10	0.13	0.13	0.13	0.13	0.14	0.14
	PSO	0.53	0.52	0.02	0.03	0.04	0.03	0.00	0.00	0.01	0.00
	SD	2.06	2.24	0.56	0.61	0.78	0.75	0.59	0.62	0.67	0.67
	FC	9.90	9.75	5.23	5.35	5.44	5.40	5.23	5.25	5.31	5.30
Δ^3J_{CC}	Total	9.24	10.89	2.39	2.66	3.39	3.33	2.50	2.64	2.87	2.89
	DSO	−0.31	−0.29	−0.21	−0.21	−0.20	−0.20	−0.19	−0.19	−0.19	−0.19
	PSO	−0.83	−0.81	−0.32	−0.33	−0.39	−0.38	−0.35	−0.35	−0.37	−0.36
	SD	2.99	3.26	0.86	0.94	1.18	1.15	0.91	0.95	1.03	1.02
	SD/FC	7.40	8.73	2.06	2.27	2.79	2.75	2.12	2.23	2.12	2.42

[a] Anisotropies defined as $\Delta T = T_{zz} - \frac{1}{2}(T_{xx} - T_{yy})$, where the z direction is normal to the plane of the molecule.
[b] The different physical contributions to J and ΔJ.

Table S 12: Innermost spin-spin coupling constants J and anisotropies[a] ΔJ for increasing size n of finite cluster models for graphane (HGn), with relaxed and fixed (to the periodic structure) geometries with the PBE functional and co-r basis set. The different physical contributions to J and ΔJ are also indicated.

		HG1		HG2		HG3		HG4
Property	Term[b]	Relaxed	Fixed	Relaxed	Fixed	Relaxed	Fixed	Relaxed[c]
$^1J_{CH}$	Total	130.10	125.22	127.63	127.11	127.91	127.21	127.88
	DSO	0.90	0.91	1.61	1.63	1.73	1.75	1.77
	PSO	0.95	0.97	0.42	0.44	0.34	0.34	0.30
	SD	0.08	0.04	−0.01	−0.01	−0.01	−0.01	−0.01
	FC	128.16	123.30	125.60	125.07	125.85	125.13	125.81
Δ^1J_{CH}	Total	−19.75	−17.91	−18.79	-18.62	−18.69	−18.56	−18.66
	DSO	19.48	19.35	19.67	19.74	19.77	19.83	19.80
	PSO	−15.82	−15.72	−16.09	−16.06	−16.14	−16.13	−16.16
	SD	-0.32	−0.42	−0.44	−0.45	−0.44	−0.45	−0.44
	SD/FC	−23.09	−21.14	−21.92	−21.85	−21.88	−21.81	−21.86
$^1J_{CC}$	Total	31.98	31.76	33.34	33.44	33.44	33.56	33.45
	DSO	0.22	0.22	0.39	0.40	0.42	0.43	0.43
	PSO	−0.44	−0.48	−0.90	−0.89	−0.93	−0.93	−0.94
	SD	1.22	1.21	1.19	1.19	1.19	1.19	1.19
	FC	30.99	31.76	32.66	32.75	32.75	32.88	32.76
Δ^1J_{CC}	Total	−12.11	−11.27	−11.43	−11.25	−11.33	−11.22	−11.30
	DSO	−1.15	−1.16	−1.04	−1.05	−1.02	−1.02	−1.01
	PSO	0.75	0.84	0.62	0.65	0.57	0.59	0.56
	SD	−0.68	−0.67	−0.67	−0.67	−0.66	−0.66	−0.66
	SD/FC	−11.03	−10.29	−10.34	−10.19	−10.21	−10.12	−10.19
$^2J_{CC}$	Total	−2.30	−2.42	−1.35	−1.30	−1.28	−1.27	−1.27
	DSO	0.03	0.03	0.14	0.14	0.17	0.17	0.18
	PSO	−0.18	−0.21	−0.30	−0.30	−0.32	-0.33	−0.33
	SD	−0.06	−0.06	−0.06	−0.06	−0.06	−0.06	*−0.06*
	FC	−2.09	−2.17	−1.13	−1.08	−1.06	−1.05	*−1.06*
Δ^2J_{CC}	Total	0.68	0.73	0.55	0.58	0.57	0.59	0.57
	DSO	−0.44	−0.44	−0.36	−0.37	−0.34	-0.35	−0.34
	PSO	0.56	0.60	0.44	0.45	0.43	0.44	0.42
	SD	0.04	0.04	0.05	0.05	0.05	0.05	*0.05*
	SD/FC	0.51	0.53	0.42	0.44	0.43	0.45	*0.43*
$^3J_{CC}$	Total	2.46	1.89	1.35	1.33	1.35	1.22	1.22
	DSO	0.01	0.01	0.11	0.11	0.13	0.17	0.14
	PSO	−0.08	−0.08	−0.14	−0.14	−0.16	0.16	−0.17
	SD	−0.01	−0.01	−0.01	−0.01	−0.01	−0.01	*−0.01*
	FC	2.54	1.97	1.39	1.38	1.26	1.26	*1.26*
Δ^3J_{CC}	Total	−0.16	−0.07	−0.09	−0.09	−0.09	−0.09	−0.09
	DSO	−0.25	−0.25	−0.18	−0.19	−0.17	−0.16	−0.16
	PSO	0.12	0.14	0.05	0.05	0.03	0.03	0.03
	SD	0.06	0.06	0.07	0.07	0.07	0.07	*0.07*
	SD/FC	−0.09	−0.03	−0.02	−0.02	−0.03	−0.03	*−0.03*
$^3J_{HH}$	Total	14.95	14.77	11.69	11.76	11.87	11.95	11.90
	DSO	−2.63	2.61	−1.61	−1.63	−1.25	−1.26	−1.11
	PSO	2.62	−1.64	1.84	1.85	1.56	1.57	1.45
	SD	0.02	0.03	0.05	0.05	0.05	0.05	*0.05*
	FC	14.94	14.75	11.42	11.48	11.51	11.59	*11.51*
Δ^3J_{HH}	Total	−1.56	−1.75	−1.41	−1.39	−1.33	−1.33	−1.30
	DSO	6.20	6.48	7.86	7.96	8.21	8.28	8.33
	PSO	−5.68	−5.92	−6.92	−7.01	−7.20	−7.26	−7.30
	SD	−0.03	−0.02	0.01	0.00	0.01	0.00	*0.01*
	SD/FC	−2.06	−2.28	−2.36	−2.35	−2.35	−2.36	*−2.35*
$^4J_{HH}$	Total	−0.43	−0.49	−0.02	−0.03	0.06	0.06	0.09
	DSO	1.32	1.64	2.86	2.93	3.25	3.30	3.40
	PSO	−1.33	−1.64	−2.52	−2.59	−2.83	−2.87	−2.95
	SD	0.03	0.03	0.02	0.02	0.02	0.02	*0.02*
	FC	−0.46	−0.51	−0.38	−0.39	−0.39	−0.39	*−0.39*
Δ^4J_{HH}	Total	0.65	0.95	0.96	1.01	1.04	1.06	1.06
	DSO	−2.70	−2.76	−2.26	−2.30	−2.06	−2.08	−1.96
	PSO	2.20	2.20	1.83	1.85	1.66	1.68	1.59
	SD	0.01	0.00	−0.01	−0.01	−0.01	−0.01	*−0.01*
	SD/FC	1.14	1.52	1.41	1.47	1.44	1.48	*1.44*

[a] Anisotropies defined as $\Delta T = T_{zz} - \frac{1}{2}(T_{xx} - T_{yy})$, where the z direction is normal to the plane of the molecule.
[b] The different physical contributions to J and ΔJ.
[c] "Fixed" results are not needed for this model due to the apparent convergence obtained in the smaller models. In the "Relaxed" column, the numbers in *italics* are adopted from the relaxed HG3 model.

Table S13: Innermost spin-spin coupling constants J and anisotropies[a] ΔJ for increasing size n of finite cluster models for fluorographene (FGn), with relaxed and fixed (to the periodic structure) geometries, with the PBE functional and co-r basis set. The different physical contributions to J and ΔJ are also indicated.

		FG1		FG2		FG3	
Property	Term[b]	Relaxed	Fixed	Relaxed	Fixed	Relaxed	Fixed
$^1J_{CF}$	Total	−268.36	−298.59	−301.61	−322.94	−323.39	−325.06
	DSO	1.07	1.10	1.98	2.05	2.23	2.25
	PSO	29.38	21.83	22.22	17.45	16.40	16.44
	SD	25.52	22.05	23.86	22.09	21.65	22.06
	FC	−324.33	−343.57	−349.67	−364.53	−363.67	−365.81
Δ^1J_{CF}	Total	195.02	233.45	229.29	245.88	248.79	248.16
	DSO	21.68	23.71	24.00	24.19	24.63	24.32
	PSO	−65.61	−61.78	−61.44	−55.31	−54.25	−54.00
	SD	38.77	38.72	40.49	39.27	38.79	39.39
	SD/FC	200.18	232.79	226.24	237.73	239.61	238.45
$^1J_{CC}$	Total	42.71	39.08	44.25	43.17	43.39	43.63
	DSO	0.41	0.40	0.66	0.67	0.72	0.72
	PSO	−1.11	−0.82	−1.16	−1.15	−1.20	−1.20
	SD	1.36	1.56	1.41	1.42	1.40	1.40
	FC	42.04	37.93	43.34	42.23	42.46	42.71
Δ^1J_{CC}	Total	−20.05	−18.89	−18.61	−18.40	−18.36	−18.30
	DSO	−1.55	−1.26	−1.20	−1.16	−1.13	−1.12
	PSO	0.76	0.94	0.35	0.34	0.29	0.29
	SD	−0.80	−0.79	−0.68	−0.66	−0.65	−0.64
	SD/FC	−18.46	−17.78	−17.08	−16.93	−16.86	−16.83
$^2J_{CC}$	Total	−0.20	−1.56	−0.12	−0.42	−0.29	−0.36
	DSO	0.12	0.12	0.30	0.31	0.35	0.35
	PSO	−0.11	−0.14	−0.29	−0.30	−0.33	−0.34
	SD	−0.02	−0.06	−0.08	−0.09	−0.09	−0.09
	FC	−0.20	−1.49	−0.05	−0.34	−0.21	−0.28
Δ^2J_{CC}	Total	0.07	0.49	0.17	0.28	0.26	0.28
	DSO	−0.49	−0.54	−0.45	−0.46	−0.43	−0.43
	PSO	0.40	0.49	0.36	0.38	0.34	0.34
	SD	0.09	0.03	0.05	0.04	0.05	0.05
	SD/FC	0.07	0.51	0.21	0.32	0.30	0.32
$^3J_{CC}$	Total	3.38	3.27	1.85	1.97	1.91	1.92
	DSO	0.09	0.09	0.24	0.24	0.29	0.29
	PSO	−0.24	−0.18	−0.26	−0.26	−0.29	−0.28
	SD	0.00	−0.01	−0.02	−0.02	−0.02	−0.02
	FC	3.53	3.38	1.88	1.99	1.93	1.93
Δ^3J_{CC}	Total	−0.70	−0.27	−0.22	−0.18	−0.17	−0.16
	DSO	−0.32	−0.35	−0.27	−0.27	−0.24	−0.24
	PSO	−0.02	0.18	0.12	0.15	0.12	0.13
	SD	0.08	0.07	0.07	0.07	0.07	0.07
	SD/FC	−0.44	−0.17	−0.15	−0.12	−0.12	−0.12
$^3J_{FF}$	Total	−56.41	−42.48	−18.87	−12.41	−12.29	−10.05
	DSO	−1.03	−1.02	0.16	0.27	0.77	0.82
	PSO	−44.08	−28.82	−10.75	−4.58	−4.47	−2.64
	SD	20.94	21.36	29.64	30.34	30.33	31.54
	FC	−32.25	−34.00	−37.91	−38.45	−38.93	−39.77
Δ^3J_{FF}	Total	86.06	71.42	14.45	8.89	3.16	4.02
	DSO	7.16	8.23	9.65	9.86	10.31	10.33
	PSO	14.35	2.41	−34.79	−39.45	−42.69	−42.82
	SD	16.90	20.98	26.56	27.02	26.39	27.70
	SD/FC	47.66	39.79	13.03	11.47	9.15	8.82
$^4J_{FF}$	Total	−2.03	46.16	19.83	32.40	28.05	31.09
	DSO	0.76	1.39	3.06	3.36	3.85	3.95
	PSO	−13.16	−27.29	−23.03	−26.14	−25.15	−26.78
	SD	1.20	0.76	1.03	0.98	1.00	0.92
	FC	9.16	71.31	38.77	54.21	48.35	53.00
Δ^4J_{FF}	Total	−32.93	−98.83	−64.47	−78.54	−72.65	−77.17
	DSO	−6.74	−10.11	−8.68	−9.35	−8.84	−9.02
	PSO	−5.23	−22.63	−7.49	−9.93	−9.13	−9.37
	SD	−1.33	−0.41	−1.63	−1.79	−1.76	−1.88
	SD/FC	−19.63	−65.68	−46.67	−57.47	−52.92	−56.90

[a] Anisotropies defined as $\Delta T = T_{zz} - \frac{1}{2}(T_{xx} - T_{yy})$, where the z direction is normal to the plane of the molecule.
[b] The different physical contributions to J and ΔJ.

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Appendix: geometries

A Graphene

NMR-properties are calculated for the first six tabulated carbon atoms.

G_periodic

```
LATTICE
       2.135670607256650       -1.233030000000000        0.000000000000000
       0.000000000000000        2.466060000000000        0.000000000000000
       0.000000000000000        0.000000000000000       18.000000000000000
POSITIONS
  C   0.3333333333333330   0.6666666666666670   0.5000000000000000
  C  -0.3333333333333330  -0.6666666666666670   0.5000000000000000
```

G1_relaxed

```
12

C     1.3973639     0.0000000     0.0000000
C     0.6986820     1.2101527     0.0000000
C    -0.6986820     1.2101527     0.0000000
C    -1.3973639     0.0000000     0.0000000
C    -0.6986820    -1.2101527     0.0000000
C     0.6986820    -1.2101527     0.0000000
H     2.4890204     0.0000000     0.0000000
H     1.2445102     2.1555549     0.0000000
H    -1.2445102     2.1555549     0.0000000
H    -2.4890204     0.0000000     0.0000000
H    -1.2445102    -2.1555549     0.0000000
H     1.2445102    -2.1555549     0.0000000
```

G1_fixed

```
12

C   -1.2330268    -0.7118884     0.0000000
C    1.2330268    -0.7118884     0.0000000
C   -1.2330268     0.7118884     0.0000000
C    1.2330268     0.7118884     0.0000000
C    0.0000000    -1.4237768     0.0000000
C    0.0000000     1.4237768     0.0000000
H   -2.1777787    -1.2573411     0.0000000
H   -2.1777787     1.2573411     0.0000000
H    2.1777787    -1.2573411     0.0000000
H    2.1777787     1.2573411     0.0000000
H    0.0000000    -2.5146822     0.0000000
H    0.0000000     2.5146822     0.0000000
```

G2_relaxed

```
36

8C    13.4894657    6.1506747    7.5000105
9C    12.7817860    7.3893358    7.5000104
11C    14.9160153    6.1442103    7.5000107
16C    15.6348910    7.3764064    7.5000109
17C    14.9272113    8.6150676    7.5000108
14C    13.5006618    8.6215319    7.5000106
1C    11.3489513    4.9572095    7.4999953
2C    10.6666486    6.1514431    7.4999960
3C    13.5039426    3.6999633    7.4999957
4C    12.7714028    4.9198596    7.5000021
5C    14.8793305    3.6937307    7.4999956
6C    11.3568361    7.3957937    7.5000022
7C    10.6779540    8.6463486    7.4999962
10C    15.6228950    4.9069373    7.5000024
12C    17.0456263    4.9313922    7.4999960
13C    11.3710508    9.8343501    7.4999952
15C    12.7937820    9.8588050    7.5000023
18C    17.7387230    6.1193937    7.4999958
19C    17.0598408    7.3699486    7.5000027
20C    13.5373466   11.0720114    7.4999958
21C    15.6452743    9.8458826    7.5000024
22C    14.9127345   11.0657788    7.4999956
23C    17.7500285    8.6142991    7.4999960
24C    17.0677259    9.8085327    7.4999960
25H    10.8012293    4.0118615    7.4999894
26H     9.5741303    6.1596799    7.4999933
27H    12.9505315    2.7579450    7.4999920
28H    15.4241808    2.7467343    7.4999905
29H     9.5854052    8.6480111    7.4999944
30H    17.5847555    3.9811180    7.4999923
31H    10.8319214   10.7846243    7.4999882
32H    18.8312718    6.1177312    7.4999909
33H    12.9924964   12.0190079    7.4999921
34H    15.4661452   12.0077973    7.4999906
35H    18.8425468    8.6060621    7.4999914
36H    17.6154475   10.7538809    7.4999920
```

G2_fixed

```
36

C8 15.661585 7.398182 9.000000
C9 14.949695 8.631212 9.000000
C14 15.661585 9.864242 9.000000
C17 17.085366 9.864242 9.000000
C16 17.797256 8.631212 9.000000
C11 17.085366 7.398182 9.000000
C1 13.525914 6.165152 9.000000
C2 12.814024 7.398182 9.000000
C3 15.661585 4.932122 9.000000
C4 14.949695 6.165152 9.000000
C5 17.085366 4.932122 9.000000
C6 13.525914 8.631212 9.000000
C7 12.814024 9.864242 9.000000
C10 17.797256 6.165152 9.000000
C12 19.221036 6.165152 9.000000
C13 13.525914 11.097272 9.000000
C15 14.949695 11.097272 9.000000
C18 19.932926 7.398183 9.000000
C19 19.221036 8.631212 9.000000
C20 15.661585 12.330302 9.000000
C21 17.797256 11.097272 9.000000
C22 17.085366 12.330302 9.000000
C23 19.932926 9.864243 9.000000
C24 19.221036 11.097272 9.000000
H 12.955914 5.177883 9.000000
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H 15.091585 3.944853 9.000000
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H 15.091585 13.317571 9.000000
H 17.655366 13.317571 9.000000
H 21.072926 9.864243 9.000000
H 19.791036 12.084541 9.000000
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G3_relaxed

```
72

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33C    15.6297737    7.3764293    7.4997956
34C    14.9246336    8.6106503    7.4997949
31C    13.5031989    8.6170918    7.4997959
1C     9.1999150    3.7339620    7.5000748
2C     8.5215301    4.9213420    7.5000781
3C    11.3501900    2.4838133    7.5000356
4C    10.6332151    3.6899198    7.4999968
5C    13.4966832    1.2271874    7.5000739
6C    12.7529794    2.4532305    7.4999968
7C    14.8641800    1.2209902    7.5000788
8C     9.2114658    6.1784339    7.4999969
9C     8.5365529    7.4085740    7.5000372
10C    11.3505664    4.9300447    7.4998979
11C    10.6440729    6.1666330    7.4998973
12C    13.4795013    3.6880049    7.4998979
13C    12.7727424    4.9221619    7.4998473
14C    15.6189657    2.4402415    7.4999972
15C    14.9036633    3.6815509    7.4998969
16C    17.0219744    2.4581089    7.5000370
17C     9.2225850    8.6325474    7.4999974
18C     8.5440710    9.8958413    7.5000787
19C    11.3595052    7.3957812    7.4998464
20C    10.6552406    8.6313631    7.4998973
23C    15.6215769    4.9092513    7.4998457
25C    17.7498488    3.6576681    7.4999963
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27C    19.1834890    3.6887170    7.5000792
28C     9.2331887   11.0770249    7.5000736
29C    11.3729118    9.8614974    7.4998981
30C    10.6668288   11.1080739    7.4999968
32C    12.7951004    9.8564909    7.4998477
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37C    19.8726065    4.8699005    7.5000726
38C    19.1940922    6.1331942    7.4999971
39C    11.3947031   12.3076333    7.5000354
40C    13.5130139   11.0841915    7.4998982
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42C    15.6439343    9.8435804    7.4998458
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44C    17.7726039    8.5991089    7.4998981
45C    17.0661101    9.8356974    7.4998970
46C    19.8801241    7.3571676    7.5000354
47C    19.2052111    8.5873078    7.4999968
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49C    15.6636973   12.3125119    7.4999967
50C    14.9199938   13.5385553    7.5000801
51C    17.7834614   11.0758222    7.4999968
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53C    19.8951465    9.8443997    7.5000735
```

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56H 7.4290408 4.9302051 7.5001440
57H 10.7991173 1.5392786 7.5000849
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59H 15.4095220 0.2743033 7.5001487
60H 7.4430277 7.4135275 7.5000891
61H 17.5644626 1.5086180 7.5000887
62H 7.4515454 9.8968791 7.5001486
63H 19.7220927 2.7381707 7.5001540
64H 8.6945848 12.0275711 7.5001188
65H 20.9651320 4.8688632 7.5001130
66H 10.8522151 13.2571243 7.5000844
67H 20.9736493 7.3522134 7.5000844
68H 13.0071548 14.4914392 7.5001125
69H 15.4738962 14.4802576 7.5001564
70H 17.6175586 13.2264641 7.5000901
71H 20.9876358 9.8355370 7.5001173
72H 19.7639599 11.9774047 7.5001511

G3_fixed

72

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2C 8.5215301 4.9213420 7.5000781
3C 11.3501900 2.4838133 7.5000356
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6C 12.7529794 2.4532305 7.4999968
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19C 11.3595052 7.3957812 7.4998464
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41C 12.7977117 12.3255009 7.4999970
42C 15.6439343 9.8435804 7.4998458
43C 14.9371755 11.0777375 7.4998968
44C 17.7726039 8.5991089 7.4998981
45C 17.0661101 9.8356974 7.4998970
46C 19.8801241 7.3571676 7.5000354
47C 19.2052111 8.5873078 7.4999968
48C 13.5524971 13.5447526 7.5000729
49C 15.6636973 12.3125119 7.4999967
50C 14.9199938 13.5385553 7.5000801
51C 17.7834614 11.0758222 7.4999968
52C 17.0664867 12.2819290 7.5000374
53C 19.8951465 9.8443997 7.5000735
54C 19.2167615 11.0317798 7.5000792
55H 8.6527164 2.7883372 7.5001245
56H 7.4290408 4.9302051 7.5001440
57H 10.7991173 1.5392786 7.5000849
58H 12.9427810 0.2854851 7.5001194
59H 15.4095220 0.2743033 7.5001487
60H 7.4430277 7.4135275 7.5000891
61H 17.5644626 1.5086180 7.5000887
62H 7.4515454 9.8968791 7.5001486
63H 19.7220927 2.7381707 7.5001540
64H 8.6945848 12.0275711 7.5001188
65H 20.9651320 4.8688632 7.5001130
66H 10.8522151 13.2571243 7.5000844
67H 20.9736493 7.3522134 7.5000844
68H 13.0071548 14.4914392 7.5001125
69H 15.4738962 14.4802576 7.5001564
70H 17.6175586 13.2264641 7.5000901
71H 20.9876358 9.8355370 7.5001173
72H 19.7639599 11.9774047 7.5001511

G4_relaxed

120

59C 15.6318071 7.3764204 7.4999979
60C 14.9256585 8.6124060 7.4999979
43C 13.4910186 6.1533362 7.4999979
44C 12.7848700 7.3893218 7.4999979
57C 13.5021907 8.6188561 7.4999979
46C 14.9144863 6.1468860 7.4999979
1C 19.9251670 12.3028667 7.4999979
2C 22.0397347 11.0716173 7.4999979
3C 21.3630386 12.2560391 7.4999979
4C 7.0536385 2.5097031 7.4999979
5C 6.3769423 3.6941248 7.4999979
6C 9.2011778 1.2628586 7.4999979
7C 8.4915100 2.4628755 7.4999979
8C 11.3449216 0.0121795 7.4999979
9C 10.6160608 1.2254585 7.4999979
10C 13.4871910 -1.2436904 7.4999979
11C 12.7388129 -0.0150356 7.4999979
12C 14.8512780 -1.2498718 7.4999979
13C 7.0667991 4.9565697 7.4999979
14C 6.3934191 6.1773221 7.4999979
15C 9.2092554 3.7092367 7.4999979
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C 14.949695 1.233032 9.000000
C 4.983231 8.631211 9.000000
C 4.271341 9.864241 9.000000
C 7.118902 7.398181 9.000000
C 6.407012 8.631211 9.000000
C 9.254573 6.165152 9.000000
C 8.542683 7.398181 9.000000
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C 10.678353 6.165152 9.000000
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C 17.085366 2.466062 9.000000
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C 17.797256 3.699092 9.000000
C 17.085366 4.932122 9.000000
C 19.221036 3.699092 9.000000
C 4.983231 13.563331 9.000000

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C 4.271341 14.796361 9.000000
C 7.118902 12.330301 9.000000
C 6.407012 13.563331 9.000000
C 9.254573 11.097272 9.000000
C 8.542683 12.330301 9.000000
C 11.390243 9.864242 9.000000
C 10.678353 11.097272 9.000000
C 13.525914 8.631212 9.000000
C 12.814024 9.864242 9.000000
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C 17.797256 6.165152 9.000000
C 17.085366 7.398182 9.000000
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C 19.221036 6.165152 9.000000
C 21.356707 4.932123 9.000000
C 4.983231 16.029391 9.000000
C 4.271341 17.262421 9.000000
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C 6.407012 16.029391 9.000000
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C 8.542683 14.796361 9.000000
C 11.390243 12.330302 9.000000
C 10.678353 13.563332 9.000000
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C 17.797256 8.631212 9.000000
C 17.085366 9.864242 9.000000
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C 19.221036 8.631212 9.000000
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C 21.356707 7.398183 9.000000
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C 10.678353 16.029392 9.000000
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C 21.356707 14.796363 9.000000
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H 10.820243 23.181811 9.000000
H 12.955914 24.414841 9.000000
H 15.519695 24.414841 9.000000
H 17.655366 23.181811 9.000000
H 19.791036 21.948781 9.000000
H 21.926707 20.715752 9.000000
```

B Graphane

NMR-properties are calculated for the first twelve tabulated atoms.

HG_periodic

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LATTICE
       2.195694827992952      -1.267685000000001       0.000000000000000
       0.000000000000000       2.535370000000000       0.000000000000000
       0.000000000000000       0.000000000000000      18.000000000000000
POSITIONS
  H   0.6666666666666666   0.3333333333333333   0.4256305694580078
  H   0.3333333333333333   0.6666666666666666  -0.4256305694580078
  C   0.6666666666666666   0.3333333333333333   0.4872972071170806
  C   0.3333333333333333   0.6666666666666666  -0.4872972071170806
```

HG1_relaxed

```
18

C    -1.2675878   -0.7318421   -0.2290111
C     0.0000000    1.4636843   -0.2290111
C     1.2675878   -0.7318421   -0.2290111
C    -1.2675878    0.7318421    0.2290111
C     1.2675878    0.7318421    0.2290111
C     0.0000000   -1.4636843    0.2290111
H    -1.3255014   -0.7652786   -1.3320510
H     1.3255014   -0.7652786   -1.3320510
H     1.3255014    0.7652786    1.3320510
H    -1.3255014    0.7652786    1.3320510
H     0.0000000   -1.5305572    1.3320510
H     0.0000000    1.5305572   -1.3320510
H     0.0000000    2.4998024    0.1457067
H     2.1648924   -1.2499012    0.1457067
H     2.1648924    1.2499012   -0.1457067
H     0.0000000   -2.4998024   -0.1457067
H    -2.1648924   -1.2499012    0.1457067
H    -2.1648924    1.2499012   -0.1457067
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HG1_fixed

```
18

C   -1.2678494   -0.7319932   -0.2286604
C    1.2678494   -0.7319932   -0.2286604
C   -1.2678494    0.7319932    0.2286604
C    1.2678494    0.7319932    0.2286604
C    0.0000000    1.4639864   -0.2286604
C    0.0000000   -1.4639864    0.2286604
H   -1.2678496   -0.7319933   -1.3385401
H    1.2678496   -0.7319933   -1.3385401
H    1.2678496    0.7319933    1.3385401
H   -1.2678496    0.7319933    1.3385401
H   0.0000000   -1.4639866    1.3385401
H   0.0000000    1.4639866   -1.3385401
H   2.1748056   -1.2556246    0.1082841
H   2.1748056    1.2556246   -0.1082841
H  -2.1748056   -1.2556246    0.1082841
H  -2.1748056    1.2556246   -0.1082841
H    0.0000000   -2.5112492   -0.1082841
H    0.0000000    2.5112492    0.1082841
```

HG2_relaxed

60

C23	-1.2738984	0.7354856	0.2271655
C35	0.0000000	1.4709711	-0.2271655
C40	1.2738984	0.7354856	0.2271655
C39	1.2738984	-0.7354856	-0.2271655
C27	0.0000000	-1.4709711	0.2271655
C22	-1.2738984	-0.7354856	-0.2271655
H25	-1.2797498	0.7388639	1.3382688
H37	0.0000000	1.4777278	-1.3382688
H42	1.2797498	0.7388639	1.3382688
H41	1.2797498	-0.7388639	-1.3382688
H29	0.0000000	-1.4777278	1.3382688
H24	-1.2797498	-0.7388639	-1.3382688
C5	-2.5464156	1.4701737	-0.2373478
C19	-2.5372998	2.9317838	0.2224104
C33	-1.2703493	3.6632580	-0.2224104
C36	0.0000000	2.9403475	0.2373478
C7	1.2703493	3.6632580	-0.2224104
C9	2.5372998	2.9317838	0.2224104
C8	2.5464156	1.4701737	-0.2373478
C11	3.8076492	0.7314742	0.2224104
C6	3.8076492	-0.7314742	-0.2224104
C43	2.5464156	-1.4701737	0.2373478
C32	2.5372998	-2.9317838	-0.2224104
C30	1.2703493	-3.6632580	0.2224104
C26	0.0000000	-2.9403475	-0.2373478
C17	-1.2703493	-3.6632580	0.2224104
C13	-2.5372998	-2.9317838	-0.2224104
C14	-2.5464156	-1.4701737	0.2373478
C1	-3.8076492	-0.7314742	-0.2224104
C2	-3.8076492	0.7314742	0.2224104
H4	-3.8673974	0.7804831	1.3254043
H20	-2.5380362	1.4653359	-1.3467318
H21	-2.6096169	2.9590229	1.3254043
H55	-1.2577805	3.7395060	-1.3254043
H38	0.0000000	2.9306718	1.3467318
H57	1.2577805	3.7395060	-1.3254043
H58	2.6096169	2.9590229	1.3254043
H47	2.5380362	1.4653359	-1.3467318
H60	3.8673974	0.7804831	1.3254043
H59	3.8673974	-0.7804831	-1.3254043
H45	2.5380362	-1.4653359	1.3467318
H56	2.6096169	-2.9590229	-1.3254043
H54	1.2577805	-3.7395060	1.3254043
H28	0.0000000	-2.9306718	-1.3467318
H52	-1.2577805	-3.7395060	1.3254043
H15	-2.6096169	-2.9590229	-1.3254043
H16	-2.5380362	-1.4653359	1.3467318
H3	-3.8673974	-0.7804831	-1.3254043
H50	-4.7031591	1.2502002	-0.1591508
H53	-3.4342847	3.4479551	-0.1591508
H34	-1.2688744	4.6981553	0.1591508
H46	1.2688744	4.6981553	0.1591508
H10	3.4342847	3.4479551	-0.1591508
H12	4.7031591	1.2502002	-0.1591508
H48	4.7031591	-1.2502002	0.1591508
H44	3.4342847	-3.4479551	0.1591508
H31	1.2688744	-4.6981553	-0.1591508
H18	-1.2688744	-4.6981553	-0.1591508
H51	-3.4342847	-3.4479551	0.1591508
H49	-4.7031591	-1.2502002	0.1591508

HG2_fixed

60

C28	-1.5013592	-0.0108223	0.2625263
C37	-0.7693654	1.2570273	-0.1947936
C40	0.6946212	1.2570273	0.2625263
C1	1.4266139	-0.0108223	-0.1947936
C30	0.6946212	-1.2786720	0.2625263
C27	-0.7693654	-1.2786720	-0.1947936
H29	-1.5013592	-0.0108223	1.3724060
H41	-0.7693654	1.2570273	-1.3046733
H43	0.6946212	1.2570273	1.3724060
H42	1.4266139	-0.0108223	-1.3046733
H33	0.6946212	-1.2786720	1.3724060
H31	-0.7693654	-1.2786720	-1.3046733
C23	-2.9653458	-0.0108223	-0.1947936
C24	-3.6973396	1.2570273	0.2625263
C35	-2.9653458	2.5248770	-0.1947936
C38	-1.5013592	2.5248770	0.2625263
C44	-0.7693654	3.7927266	-0.1947936
C45	0.6946212	3.7927266	0.2625263
C5	1.4266139	2.5248770	-0.1947936
C7	2.8906005	2.5248770	0.2625263
C6	3.6225943	1.2570273	-0.1947936
C3	2.8906005	-0.0108223	0.2625263
C2	3.6225943	-1.2786720	-0.1947936
C21	2.8906005	-2.5465216	0.2625263
C20	1.4266139	-2.5465216	-0.1947936
C17	0.6946212	-3.8143713	0.2625263
C14	-0.7693654	-3.8143713	-0.1947936
C15	-1.5013592	-2.5465216	0.2625263
C10	-2.9653458	-2.5465216	-0.1947936
C11	-3.6973396	-1.2786720	0.2625263
H26	-2.9653458	-0.0108223	-1.3046733
H25	-3.6973396	1.2570273	1.3724060
H36	-2.9653458	2.5248770	-1.3046733
H39	-1.5013592	2.5248770	1.3724060
H46	-0.7693654	3.7927266	-1.3046733
H48	0.6946212	3.7927266	1.3724060
H47	1.4266139	2.5248770	-1.3046733
H8	2.8906005	2.5248770	1.3724060
H9	3.6225943	1.2570273	-1.3046733
H4	2.8906005	-0.0108223	1.3724060
H34	3.6225943	-1.2786720	-1.3046733
H22	2.8906005	-2.5465216	1.3724060
H32	1.4266139	-2.5465216	-1.3046733
H19	0.6946212	-3.8143713	1.3724060
H18	-0.7693654	-3.8143713	-1.3046733
H16	-1.5013592	-2.5465216	1.3724060
H13	-2.9653458	-2.5465216	-1.3046733
H12	-3.6973396	-1.2786720	1.3724060
H54	-4.7448607	1.2484168	-0.0762271
H53	-3.4813078	3.4365577	0.1440352
H52	-1.3007625	4.6954371	0.1441582
H51	1.2259509	4.6954574	-0.0764618
H50	3.4066297	3.4364635	-0.0764124
H49	4.6700824	1.2481961	0.1440756
H60	4.6700716	-1.2699067	0.1441265
H59	3.4068295	-3.4579949	-0.0764139
H58	1.2259790	-4.7170974	-0.0764332
H57	-1.3007445	-4.7170651	0.1442011
H56	-3.4815127	-3.4580297	0.1441379
H55	-4.7448414	-1.2701299	-0.0763110

HG3_relaxed

126

C18	-1.2721656	0.7344851	0.2285228
C38	0.0000000	1.4689703	-0.2285228
C43	1.2721656	0.7344851	0.2285228
C42	1.2721656	-0.7344851	-0.2285228
C22	0.0000000	-1.4689703	0.2285228
C17	-1.2721656	-0.7344851	-0.2285228
H20	-1.2740597	0.7355787	1.3393011
H40	0.0000000	1.4711574	-1.3393011
H45	1.2740597	0.7355787	1.3393011
H44	1.2740597	-0.7355787	-1.3393011
H24	0.0000000	-1.4711574	1.3393011
H19	-1.2740597	-0.7355787	-1.3393011
C16	-2.5429272	1.4681597	-0.2336078
C35	-2.5453619	2.9372211	0.2230128
C37	-1.2710272	3.6729586	-0.2230128
C39	0.0000000	2.9363194	0.2336078
C60	1.2710272	3.6729586	-0.2230128
C65	2.5453619	2.9372211	0.2230128
C64	2.5429272	1.4681597	-0.2336078
C69	3.8163891	0.7357375	0.2230128
C68	3.8163891	-0.7357375	-0.2230128
C47	2.5429272	-1.4681597	0.2336078
C46	2.5453619	-2.9372211	-0.2230128
C26	1.2710272	-3.6729586	0.2230128
C21	0.0000000	-2.9363194	-0.2336078
C10	-1.2710272	-3.6729586	0.2230128
C6	-2.5453619	-2.9372211	-0.2230128
C7	-2.5429272	-1.4681597	0.2336078
C5	-3.8163891	-0.7357375	-0.2230128
C103	-3.8163891	0.7357375	0.2230128
C1	-6.3496979	-0.7330124	-0.2172371
C2	-6.3496979	0.7330124	0.2172371
C4	-5.0872512	1.4666501	-0.2477821
C14	-5.0736124	2.9292515	0.2013395
C31	-3.8137818	3.6723637	-0.2477821
C32	-3.8096563	5.1324935	0.2172371
C54	-2.5400416	5.8655059	-0.2172371
C56	-1.2734694	5.1390138	0.2477821
C59	0.0000000	5.8585029	-0.2013395
C61	1.2734694	5.1390138	0.2477821
C77	2.5400416	5.8655059	-0.2172371
C80	3.8096563	5.1324935	0.2172371
C79	3.8137818	3.6723637	-0.2477821
C84	5.0736124	2.9292515	0.2013395
C83	5.0872512	1.4666501	-0.2477821
C88	6.3496979	0.7330124	0.2172371
C87	6.3496979	-0.7330124	-0.2172371
C73	5.0872512	-1.4666501	0.2477821
C72	5.0736124	-2.9292515	-0.2013395
C51	3.8137818	-3.6723637	0.2477821
C50	3.8096563	-5.1324935	-0.2172371
C29	2.5400416	-5.8655059	0.2172371
C25	1.2734694	-5.1390138	-0.2477821
C12	0.0000000	-5.8585029	0.2013395
C9	-1.2734694	-5.1390138	-0.2477821
C96	-2.5400416	-5.8655059	0.2172371
C92	-3.8096563	-5.1324935	-0.2172371
C93	-3.8137818	-3.6723637	0.2477821
C91	-5.0736124	-2.9292515	-0.2013395
C98	-5.0872512	-1.4666501	0.2477821
H105	-3.8236879	0.7457788	1.3340565
H107	-2.5398197	1.4663656	-1.3443900
H36	-2.5577074	2.9385215	1.3340565
H57	-1.2659806	3.6843003	-1.3340565

H41	0.0000000	2.9327311	1.3443900
H62	1.2659806	3.6843003	-1.3340565
H67	2.5577074	2.9385215	1.3340565
H66	2.5398197	1.4663656	-1.3443900
H71	3.8236879	0.7457788	1.3340565
H70	3.8236879	-0.7457788	-1.3340565
H49	2.5398197	-1.4663656	1.3443900
H48	2.5577074	-2.9385215	-1.3340565
H28	1.2659806	-3.6843003	1.3340565
H23	0.0000000	-2.9327311	-1.3443900
H11	-1.2659806	-3.6843003	1.3340565
H106	-2.5577074	-2.9385215	-1.3340565
H8	-2.5398197	-1.4663656	1.3443900
H104	-3.8236879	-0.7457788	-1.3340565
H15	-5.1412732	2.9683155	1.3052882
H33	-3.7975741	3.6725910	-1.3569285
H34	-3.8891033	5.1560856	1.3198059
H118	-2.5207494	5.9461050	-1.3198059
H58	-1.2817700	5.1250911	1.3569285
H120	0.0000000	5.9366309	-1.3052882
H63	1.2817700	5.1250911	1.3569285
H122	2.5207494	5.9461050	-1.3198059
H123	3.8891033	5.1560856	1.3198059
H81	3.7975741	3.6725910	-1.3569285
H124	5.1412732	2.9683155	1.3052882
H85	5.0793441	1.4525002	-1.3569285
H126	6.4098527	0.7900195	1.3198059
H125	6.4098527	-0.7900195	-1.3198059
H75	5.0793441	-1.4525002	1.3569285
H121	5.1412732	-2.9683155	-1.3052882
H53	3.7975741	-3.6725910	1.3569285
H119	3.8891033	-5.1560856	-1.3198059
H117	2.5207494	-5.9461050	1.3198059
H27	1.2817700	-5.1250911	-1.3569285
H115	0.0000000	-5.9366309	1.3052882
H101	-1.2817700	-5.1250911	-1.3569285
H113	-2.5207494	-5.9461050	1.3198059
H94	-3.8891033	-5.1560856	-1.3198059
H95	-3.7975741	-3.6725910	1.3569285
H99	-5.1412732	-2.9683155	-1.3052882
H100	-5.0793441	-1.4525002	1.3569285
H3	-6.4098527	-0.7900195	-1.3198059
H109	-6.4098527	0.7900195	1.3198059
H102	-5.0793441	1.4525002	-1.3569285
H110	-7.2445449	1.2496973	-0.1685618
H114	-5.9708191	3.4472540	-0.1806739
H116	-4.7045421	5.6491113	-0.1685618
H55	-2.5400028	6.8988086	0.1685618
H76	0.0000000	6.8945080	0.180673
H78	2.5400028	6.8988086	0.1685618
H82	4.7045421	5.6491113	-0.1685618
H86	5.9708191	3.4472540	-0.1806739
H90	7.2445449	1.2496973	-0.1685618
H89	7.2445449	-1.2496973	0.1685618
H74	5.9708191	-3.4472540	0.1806739
H52	4.7045421	-5.6491113	0.1685618
H30	2.5400028	-6.8988086	-0.1685618
H13	0.0000000	-6.8945080	-0.1806739
H97	-2.5400028	-6.8988086	-0.1685618
H112	-4.7045421	-5.6491113	0.1685618
H111	-5.9708191	-3.4472540	0.1806739
H108	-7.2445449	-1.2496973	0.1685618

HG3_fixed

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C74	9.5159133	6.3392482	7.7286578
C88	10.2479071	7.6070979	7.2713380
C91	11.7118937	7.6070979	7.7286578
C1	12.4438865	6.3392482	7.2713380
C76	11.7118937	5.0713986	7.7286578
C73	10.2479071	5.0713986	7.2713380
H75	9.5159133	6.3392482	8.8385375
H92	10.2479071	7.6070979	6.1614583
H93	12.4438865	6.3392482	6.1614583
H94	11.7118937	7.6070979	8.8385375
H79	11.7118937	5.0713986	8.8385375
H77	10.2479071	5.0713986	6.1614583
C69	8.0519267	6.3392482	7.2713380
C70	7.3199329	7.6070979	7.7286578
C84	8.0519267	8.8749475	7.2713380
C89	9.5159133	8.8749475	7.7286578
C97	10.2479071	10.1427972	7.2713380
C100	11.7118937	10.1427972	7.7286578
C8	12.4438865	8.8749475	7.2713380
C10	13.9078731	8.8749475	7.7286578
C9	14.6398669	7.6070979	7.2713380
C3	13.9078731	6.3392482	7.7286578
C2	14.6398669	5.0713986	7.2713380
C60	13.9078731	3.8035489	7.7286578
C58	12.4438865	3.8035489	7.2713380
C54	11.7118937	2.5356993	7.7286578
C51	10.2479071	2.5356993	7.2713380
C52	9.5159133	3.8035489	7.7286578
C47	8.0519267	3.8035489	7.2713380
C48	7.3199329	5.0713986	7.7286578
C44	5.1239536	6.3392482	7.7286578
C65	5.8559464	7.6070979	7.2713380
C66	5.1239536	8.8749475	7.7286578
C82	5.8559464	10.1427972	7.2713380
C85	7.3199329	10.1427972	7.7286578
C95	8.0519267	11.4106468	7.2713380
C98	9.5159133	11.4106468	7.7286578
C104	10.2479071	12.6784964	7.2713380
C105	11.7118937	12.6784964	7.7286578
C17	12.4438865	11.4106468	7.2713380
C18	14.6398669	10.1427972	7.2713380
C19	13.9078731	11.4106468	7.7286578
C21	16.8358463	8.8749475	7.2713380
C22	16.1038535	10.1427972	7.7286578
C12	16.8358463	6.3392482	7.2713380
C13	16.1038535	7.6070979	7.7286578
C5	16.8358463	3.8035489	7.2713380
C6	16.1038535	5.0713986	7.7286578
C62	16.1038535	2.5356993	7.7286578
C59	14.6398669	2.5356993	7.2713380
C41	13.9078731	1.2678496	7.7286578
C40	12.4438865	1.2678496	7.2713380
C37	11.7118937	0.0000000	7.7286578
C34	10.2479071	0.0000000	7.2713380
C35	9.5159133	1.2678496	7.7286578
C30	8.0519267	1.2678496	7.2713380
C31	7.3199329	2.5356993	7.7286578
C26	5.8559464	2.5356993	7.2713380
C27	5.1239536	3.8035489	7.7286578
C43	5.8559464	5.0713986	7.2713380
H49	7.3199329	5.0713986	8.8385375
H72	8.0519267	6.3392482	6.1614583
H71	7.3199329	7.6070979	8.8385375
H87	8.0519267	8.8749475	6.1614583
H90	9.5159133	8.8749475	8.8385375
H101	10.2479071	10.1427972	6.1614583
H103	11.7118937	10.1427972	8.8385375
H102	12.4438865	8.8749475	6.1614583
H11	13.9078731	8.8749475	8.8385375
H15	14.6398669	7.6070979	6.1614583
H4	13.9078731	6.3392482	8.8385375
H80	14.6398669	5.0713986	6.1614583
H61	13.9078731	3.8035489	8.8385375
H78	12.4438865	3.8035489	6.1614583
H57	11.7118937	2.5356993	8.8385375
H55	10.2479071	2.5356993	6.1614583
H53	9.5159133	3.8035489	8.8385375
H50	8.0519267	3.8035489	6.1614583
H7	16.1038535	5.0713986	8.8385375
H14	16.1038535	7.6070979	8.8385375
H16	16.8358463	6.3392482	6.1614583
H20	13.9078731	11.4106468	8.8385375
H23	16.1038535	10.1427972	8.8385375
H24	14.6398669	10.1427972	6.1614583
H25	16.8358463	8.8749475	6.1614583
H28	5.1239536	3.8035489	8.8385375
H29	5.8559464	2.5356993	6.1614583
H32	7.3199329	2.5356993	8.8385375
H33	8.0519267	1.2678496	6.1614583
H36	9.5159133	1.2678496	8.8385375
H38	10.2479071	0.0000000	6.1614583
H39	11.7118937	0.0000000	8.8385375
H42	13.9078731	1.2678496	8.8385375
H45	5.1239536	6.3392482	8.8385375
H46	5.8559464	5.0713986	6.1614583
H56	12.4438865	1.2678496	6.1614583
H63	16.1038535	2.5356993	8.8385375
H64	14.6398669	2.5356993	6.1614583
H67	5.1239536	8.8749475	8.8385375
H68	5.8559464	7.6070979	6.1614583
H81	16.8358463	3.8035489	6.1614583
H83	5.8559464	10.1427972	6.1614583
H86	7.3199329	10.1427972	8.8385375
H96	8.0519267	11.4106468	6.1614583
H99	9.5159133	11.4106468	8.8385375
H106	10.2479071	12.6784964	6.1614583
H107	12.4438865	11.4106468	6.1614583
H108	11.7118937	12.6784964	8.8385375
H109	17.8834609	8.8659947	7.6100524
H110	16.6199099	11.0545008	7.3899029
H111	14.4312999	12.3172554	7.3860482
H112	12.2434265	13.5812483	7.3898736
H113	9.7163820	13.5812603	7.6100976
H114	7.5284695	12.3172338	7.6139568
H115	5.3398718	11.0544822	7.6101218
H116	4.0763697	8.8660331	7.3899080
H117	4.0770991	6.3392462	7.3860424
H118	4.0763780	3.8124744	7.3898816
H119	5.3398729	1.6240113	7.6101060
H120	7.5284747	0.3612492	7.6139312
H121	9.7163802	-0.9027472	7.6101388
H122	12.2433962	-0.9027265	7.3897926
H123	14.4313287	0.3612481	7.3860697
H124	16.6199163	1.6240011	7.3899062
H125	17.8834253	3.8124839	7.6101027
H126	17.8827004	6.3392459	7.6139544

HG4_relaxed

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C20	-1.2715111	-0.7341073	-0.2287993
C177	-1.2715111	0.7341073	0.2287993
C36	0.0000000	1.4682146	-0.2287993
C38	1.2715111	0.7341073	0.2287993
C37	1.2715111	-0.7341073	-0.2287993
C22	0.0000000	-1.4682146	0.2287993
H179	-1.2727240	-0.7348075	-1.3395879
H178	-1.2727240	0.7348075	1.3395879
H187	0.0000000	1.4696150	-1.3395879
H39	1.2727240	0.7348075	1.3395879
H48	1.2727240	-0.7348075	-1.3395879
H23	0.0000000	-1.4696150	1.3395879
C158	-3.8143918	-0.7349357	-0.2254588
C159	-3.8143918	0.7349357	0.2254588
C173	-2.5421141	1.4676903	-0.2321485
C174	-2.5436689	2.9358924	0.2254588
C181	-1.2707229	3.6708281	-0.2254588
C185	0.0000000	2.9353805	0.2321485
C58	1.2707229	3.6708281	-0.2254588
C60	2.5436689	2.9358924	0.2254588
C59	2.5421141	1.4676903	-0.2321485
C63	3.8143918	0.7349357	0.2254588
C62	3.8143918	-0.7349357	-0.2254588
C41	2.5421141	-1.4676903	0.2321485
C40	2.5436689	-2.9358924	-0.2254588
C25	1.2707229	-3.6708281	0.2254588
C21	0.0000000	-2.9353805	-0.2321485
C148	-1.2707229	-3.6708281	0.2254588
C146	-2.5436689	-2.9358924	-0.2254588
C162	-2.5421141	-1.4676903	0.2321485
C129	-6.3581772	0.7368951	0.2184598
C154	-5.0840905	1.4655797	-0.2421580
C155	-5.0859488	2.9363739	0.2055599
C169	-3.8112745	3.6701617	-0.2421580
C170	-3.8172584	5.1378954	0.2184598
C54	-2.5409187	5.8747905	-0.2184598
C182	-1.2728160	5.1357414	0.2421580
C76	0.0000000	5.8727478	-0.2055599
C189	1.2728160	5.1357414	0.2421580
C80	2.5409187	5.8747905	-0.2184598
C82	3.8172584	5.1378954	0.2184598
C81	3.8112745	3.6701617	-0.2421580
C85	5.0859488	2.9363739	0.2055599
C84	5.0840905	1.4655797	-0.2421580
C88	6.3581772	0.7368951	0.2184598
C87	6.3581772	-0.7368951	-0.2184598
C66	5.0840905	-1.4655797	0.2421580
C65	5.0859488	-2.9363739	-0.2055599
C44	3.8112745	-3.6701617	0.2421580
C43	3.8172584	-5.1378954	-0.2184598
C28	2.5409187	-5.8747905	0.2184598
C24	1.2728160	-5.1357414	-0.2421580
C150	0.0000000	-5.8727478	0.2055599
C147	-1.2728160	-5.1357414	-0.2421580
C125	-2.5409187	-5.8747905	0.2184598
C124	-3.8172584	-5.1378954	-0.2184598
C136	-3.8112745	-3.6701617	0.2421580
C132	-5.0859488	-2.9363739	-0.2055599
C133	-5.0840905	-1.4655797	0.2421580
C128	-6.3581772	-0.7368951	-0.2184598
C1	-8.8914062	-0.7343740	-0.2126293
C2	-8.8914062	0.7343740	0.2126293
C19	-7.6288655	1.4649067	-0.2569747
C121	-7.6140052	2.9301091	0.1829306
C142	-6.3527451	3.6677591	-0.2715572
C143	-6.3445515	5.1288674	0.1829306
C32	-5.0830792	5.8743380	-0.2569747
C33	-5.0816896	7.3329966	0.2126293
C52	-3.8097165	8.0673706	-0.2126293
C55	-2.5457863	7.3392447	0.2569747
C74	-1.2694537	8.0589765	-0.1829306
C77	0.0000000	7.3355182	0.2715572
C96	1.2694537	8.0589765	-0.1829306
C98	2.5457863	7.3392447	0.2569747
C101	3.8097165	8.0673706	-0.2126293
C103	5.0816896	7.3329966	0.2126293
C102	5.0830792	5.8743380	-0.2569747
C106	6.3445515	5.1288674	0.1829306
C105	6.3527451	3.6677591	-0.2715572
C109	7.6140052	2.9301091	0.1829306
C108	7.6288655	1.4649067	-0.2569747
C111	8.8914062	0.7343740	0.2126293
C100	8.8914062	-0.7343740	-0.2126293
C90	7.6288655	-1.4649067	0.2569747
C79	7.6140052	-2.9301091	-0.1829306
C68	6.3527451	-3.6677591	0.2715572
C57	6.3445515	-5.1288674	-0.1829306
C46	5.0830792	-5.8743380	0.2569747
C35	5.0816896	-7.3329966	-0.2126293
C30	3.8097165	-8.0673706	0.2126293
C27	2.5457863	-7.3392447	-0.2569747
C140	1.2694537	-8.0589765	0.1829306
C139	0.0000000	-7.3355182	-0.2715572
C119	-1.2694537	-8.0589765	0.1829306
C118	-2.5457863	-7.3392447	-0.2569747
C6	-3.8097165	-8.0673706	0.2126293
C5	-5.0816896	-7.3329966	-0.2126293
C16	-5.0830792	-5.8743380	0.2569747
C12	-6.3445515	-5.1288674	-0.1829306
C13	-6.3527451	-3.6677591	0.2715572
C8	-7.6140052	-2.9301091	-0.1829306
C9	-7.6288655	-1.4649067	0.2569747
H161	-3.8180938	-0.7407427	-1.3362206
H160	-3.8180938	0.7407427	1.3362206
H176	-2.5401846	1.4665763	-1.3429399
H175	-2.5505489	2.9361948	1.3362206
H184	-1.2675449	3.6769375	-1.3362206
H186	0.0000000	2.9331526	1.3429399
H191	1.2675449	3.6769375	-1.3362206
H61	2.5505489	2.9361948	1.3362206
H70	2.5401846	1.4665763	-1.3429399
H64	3.8180938	0.7407427	1.3362206
H71	3.8180938	-0.7407427	-1.3362206
H42	2.5401846	-1.4665763	1.3429399
H49	2.5505489	-2.9361948	-1.3362206
H26	1.2675449	-3.6769375	1.3362206
H166	0.0000000	-2.9331526	-1.3429399
H149	-1.2675449	-3.6769375	1.3362206
H164	-2.5505489	-2.9361948	-1.3362206
H163	-2.5401846	-1.4665763	1.3429399
H130	-6.3656947	0.7538129	1.3294192
H157	-5.0801929	1.4568438	-1.3529084
H156	-5.1000710	2.9445274	1.3165480
H172	-3.8017602	3.6711542	-1.3529084
H171	-3.8356685	5.1359469	1.3294192
H180	-2.5300263	5.8897598	-1.3294192
H183	-1.2784327	5.1279980	1.3529084
H188	0.0000000	5.8890548	-1.3165480
H190	1.2784327	5.1279980	1.3529084
H192	2.5300263	5.8897598	-1.3294192
H83	3.8356685	5.1359469	1.3294192
H92	3.8017602	3.6711542	-1.3529084
H86	5.1000710	2.9445274	1.3165480
H93	5.0801929	1.4568438	-1.3529084
H89	6.3656947	0.7538129	1.3294192
H94	6.3656947	-0.7538129	-1.3294192
H67	5.0801929	-1.4568438	1.3529084
H72	5.1000710	-2.9445274	-1.3165480
H45	3.8017602	-3.6711542	1.3529084
H50	3.8356685	-5.1359469	-1.3294192
H29	2.5300263	-5.8897598	1.3294192
H167	1.2784327	-5.1279980	-1.3529084
H151	0.0000000	-5.8890548	1.3165480
H152	-1.2784327	-5.1279980	-1.3529084
H126	-2.5300263	-5.8897598	1.3294192
H138	-3.8356685	-5.1359469	-1.3294192
H137	-3.8017602	-3.6711542	1.3529084
H135	-5.1000710	-2.9445274	-1.3165480
H134	-5.0801929	-1.4568438	1.3529084
H131	-6.3656947	-0.7538129	-1.3294192
H10	-7.6209777	-1.4438236	1.3660228
H3	-8.9516016	-0.7983339	-1.3148127
H4	-8.9516016	0.7983339	1.3148127
H122	-7.6209777	1.4438236	-1.3660228
H123	-7.6816521	2.9765067	1.2865678
H144	-6.3371382	3.6587484	-1.3805294
H145	-6.4185565	5.1642525	1.2865678
H165	-5.0608768	5.8780485	-1.3660228
H34	-5.1671782	7.3531475	1.3148127
H205	-3.7844234	8.1514814	-1.3148127
H56	-2.5601009	7.3218721	1.3660228
H207	-1.2630957	8.1407592	-1.2865678
H78	0.0000000	7.3174969	1.3805294
H209	1.2630957	8.1407592	-1.2865678
H99	2.5601009	7.3218721	1.3660228
H211	3.7844234	8.1514814	-1.3148127
H212	5.1671782	7.3531475	1.3148127
H113	5.0608768	5.8780485	-1.3660228
H213	6.4185565	5.1642525	1.2865678
H114	6.3371382	3.6587484	-1.3805294
H214	7.6816521	2.9765067	1.2865678
H115	7.6209777	1.4438236	-1.3660228
H216	8.9516016	0.7983339	1.3148127
H215	8.9516016	-0.7983339	-1.3148127
H91	7.6209777	-1.4438236	1.3660228
H210	7.6816521	-2.9765067	-1.2865678
H69	6.3371382	-3.6587484	1.3805294
H208	6.4185565	-5.1642525	-1.2865678
H47	5.0608768	-5.8780485	1.3660228
H206	5.1671782	-7.3531475	-1.3148127
H204	3.7844234	-8.1514814	1.3148127
H168	2.5601009	-7.3218721	-1.3660228
H202	1.2630957	-8.1407592	1.2865678
H153	0.0000000	-7.3174969	-1.3805294
H200	-1.2630957	-8.1407592	1.2865678
H127	-2.5601009	-7.3218721	-1.3660228
H198	-3.7844234	-8.1514814	1.3148127
H18	-5.1671782	-7.3531475	-1.3148127
H17	-5.0608768	-5.8780485	1.3660228
H15	-6.4185565	-5.1642525	-1.2865678
H14	-6.3371382	-3.6587484	1.3805294
H11	-7.6816521	-2.9765067	-1.2865678
H193	-9.7861667	-1.2487372	0.1764704
H194	-9.7861667	1.2487372	-0.1764704
H199	-8.5103052	3.4469857	-0.2026741
H201	-7.2403298	5.6466476	-0.2026741
H203	-5.9745215	7.8507003	-0.1764704

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H53    -3.8116452    9.0994375    0.1764704
H75    -1.2699754    9.0936334    0.2026741
H97     1.2699754    9.0936334    0.2026741
H117    3.8116452    9.0994375    0.1764704
H104    5.9745215    7.8507003   -0.1764704
H107    7.2403298    5.6466476   -0.2026741
H110    8.5103052    3.4469857   -0.2026741
H112    9.7861667    1.2487372   -0.1764704
H116    9.7861667   -1.2487372    0.1764704
H95     8.5103052   -3.4469857    0.2026741
H73     7.2403298   -5.6466476    0.2026741
H51     5.9745215   -7.8507003    0.1764704
H31     3.8116452   -9.0994375   -0.1764704
H141    1.2699754   -9.0936334   -0.2026741
H120   -1.2699754   -9.0936334   -0.2026741
H7     -3.8116452   -9.0994375   -0.1764704
H197   -5.9745215   -7.8507003    0.1764704
H196   -7.2403298   -5.6466476    0.2026741
H195   -8.5103052   -3.4469857    0.2026741


HG4_fixed

216

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23C 10.2479041 7.6070959 7.2713360
18C 11.7118907 7.6070959 7.7286548
17C 12.4438835 6.3392462 7.2713360
22C 11.7118907 5.0713966 7.7286548
25C 10.2479041 5.0713966 7.2713350
161H 9.5159113 6.3392462 8.8385345
174H 10.2479041 7.6070959 6.1614563
176H 11.7118907 7.6070959 8.8385345
175H 12.4438835 6.3392462 6.1614563
164H 11.7118907 5.0713966 8.8385345
162H 10.2479041 5.0713966 6.1614563
1C 11.7004983 15.2030970 7.7391461
2C 12.4438825 13.9463421 7.2713360
3C 11.7118907 12.6784924 7.7286558
4C 10.2479041 12.6784924 7.2713360
5C 9.5159103 13.9463421 7.7286558
6C 10.2479041 15.2141917 7.2713360
7C 12.4438825 11.4106438 7.2713360
8C 13.9078691 11.4106438 7.7286558
9C 14.6398629 12.6784924 7.2713360
10C 13.9078691 13.9463421 7.7286558
11C 14.6398629 10.1427942 7.2713360
12C 13.9078691 8.8749455 7.7286558
13C 12.4438835 8.8749455 7.2713360
14C 11.7118907 10.1427942 7.7286558
15C 14.6398629 7.6070959 7.2713360
16C 13.9078691 6.3392462 7.7286548
19C 14.6398629 5.0713976 7.2713350
20C 13.9078701 3.8035479 7.7286548
21C 12.4438835 3.8035479 7.2713350
26C 16.1038495 7.6070959 7.7286548
27C 16.8358423 6.3392472 7.2713360
28C 16.1038495 5.0713976 7.7286548
29C 14.6398639 2.5356993 7.2713350
30C 16.1038495 2.5356993 7.7286548
31C 16.8358423 3.8035489 7.2713350
32C 18.2998279 6.3392472 7.7286548
33C 19.0318217 5.0713986 7.2713350
34C 18.2998289 3.8035489 7.7286548
35C 16.8358423 1.2678496 7.2713350
36C 18.2998289 1.2678496 7.7286538
37C 19.0318217 2.5356993 7.2713340
38C 10.2479041 10.1427942 7.2713360
39C 9.5159103 8.8749445 7.7286548
40C 16.8358413 8.8749455 7.2713360
41C 16.1038485 10.1427952 7.7286558
42C 19.0318217 7.6070969 7.2713350
43C 18.2998279 8.8749455 7.7286548
44C 9.5159103 11.4106438 7.7286558
45C 16.8358413 11.4106438 7.2713360
46C 16.1038485 12.6784934 7.7286558
47C 19.0318217 10.1427952 7.2713350
48C 18.2998279 11.4106438 7.7286548
49C 13.9078701 1.2678496 7.7286548
50C 12.4438845 1.2678496 7.2713350
51C 11.7118917 2.5356983 7.7286548
52C 14.6398639 0.0000010 7.2713350
53C 13.9078711 -1.2678486 7.7286538
54C 12.4438845 -1.2678496 7.2713350
55C 11.7118917 0.0000000 7.7286548
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57C 9.5159123 -1.2678506 7.7286548
58C 10.2479061 -2.5356993 7.2713340
59C 11.7118927 -2.5356993 7.7286538
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74C 3.6599670 6.3392442 7.2713370
75C 2.9279732 5.0713956 7.7286558
76C 8.0519257 3.8035469 7.2713360
77C 7.3199319 5.0713956 7.7286558
78C 10.2479051 2.5356973 7.2713350
79C 9.5159113 3.8035469 7.7286548
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82C 5.1239536 8.8749435 7.7286568
83C 3.6599670 8.8749435 7.2713370
84C 2.9279732 7.6070939 7.7286568
85C 8.0519247 6.3392452 7.2713360
86C 7.3199309 7.6070939 7.7286558
87C 5.8559464 10.1427922 7.2713370
88C 5.1239536 11.4106418 7.7286578
89C 3.6599670 11.4106418 7.2713380
90C 2.9279732 10.1427932 7.7286578
91C 8.0519247 8.8749435 7.2713360
92C 7.3199309 10.1427932 7.7286558
93C 8.0519237 11.4106418 7.2713370
94C 7.3199309 12.6784914 7.7286568
95C 5.8559444 12.6784914 7.2713370
96C 8.0519247 13.9463421 7.2713360
97H 13.9078691 6.3392462 8.8385345
98H 16.1038495 5.0713976 8.8385345
99H 18.2998289 3.8035489 8.8385335
100H 13.9078691 8.8749445 8.8385345
101H 16.1038495 7.6070959 8.8385345
102H 18.2998279 6.3392472 8.8385345
103H 14.6398629 7.6070959 6.1614563
104H 16.8358423 6.3392472 6.1614563
105H 19.0318217 5.0713986 6.1614553
106H 13.9078691 11.4106438 8.8385345
107H 16.1038485 10.1427952 8.8385345
108H 18.2998279 8.8749455 8.8385345
109H 14.6398629 10.1427952 6.1614563
110H 16.8358413 8.8749455 6.1614563
111H 19.0318217 7.6070969 6.1614563
112H 13.9078691 13.9463421 8.8385345
113H 16.1038485 12.6784934 8.8385345
114H 18.2998279 11.4106438 8.8385345
115H 14.6398629 12.6784924 6.1614563
116H 16.8358413 11.4106438 6.1614563
117H 19.0318207 10.1427952 6.1614553
118H 2.9279742 2.5356963 8.8385345
119H 3.6599670 1.2678476 6.1614563
120H 5.1239536 1.2678476 8.8385345
121H 5.8559464 -0.0000010 6.1614563
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123H 8.0519257 -1.2678506 6.1614553
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125H 10.2479061 -2.5356993 6.1614553
126H 11.7118927 -2.5356993 8.8385335
127H 13.9078711 -1.2678496 8.8385335
128H 2.9279732 5.0713956 8.8385355
129H 3.6599670 3.8035459 6.1614573
130H 5.1239536 3.8035459 8.8385345
131H 5.8559454 2.5356973 6.1614563
132H 7.3199319 2.5356973 8.8385345
133H 8.0519257 1.2678486 6.1614563
134H 9.5159123 1.2678476 8.8385345
135H 10.2479051 0.0000000 6.1614553
136H 12.4438845 -1.2678486 6.1614553
137H 11.7118917 -0.0000010 8.8385335
138H 13.9078701 1.2678496 8.8385335
139H 16.1038505 0.0000000 8.8385335
140H 14.6398639 0.0000010 6.1614553
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142H 5.1239536 6.3392442 8.8385355
143H 5.8559454 5.0713956 6.1614573
144H 7.3199319 5.0713956 8.8385345
145H 8.0519247 3.8035469 6.1614563
146H 9.5159113 3.8035469 8.8385345
147H 10.2479051 2.5356983 6.1614563
148H 12.4438845 1.2678496 6.1614553
149H 11.7118917 2.5356983 8.8385345
150H 13.9078701 3.8035479 8.8385345
151H 16.1038505 2.5356993 8.8385335
152H 18.2998289 1.2678496 8.8385335
153H 14.6398639 2.5356993 6.1614553
154H 16.8358423 1.2678506 6.1614553
155H 2.9279742 10.1427922 8.8385365
156H 3.6599670 8.8749435 6.1614583
157H 5.1239536 8.8749425 8.8385365
158H 5.8559454 7.6070939 6.1614573
159H 7.3199309 7.6070939 8.8385355
160H 8.0519247 6.3392452 6.1614573
163H 12.4438835 3.8035479 6.1614563
165H 14.6398629 5.0713976 6.1614563
166H 16.8358423 3.8035489 6.1614553
167H 19.0318217 2.5356993 6.1614553
168H 3.6599670 11.4106418 6.1614583
169H 5.1239536 11.4106418 8.8385365
170H 5.8559454 10.1427932 6.1614583
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171H 7.3199309 10.1427922 8.8385355
172H 8.0519247 8.8749435 6.1614573
173H 9.5159113 8.8749455 8.8385345
177H 5.8559434 12.6784904 6.1614583
178H 7.3199309 12.6784914 8.8385355
179H 8.0519237 11.4106418 6.1614573
180H 9.5159113 11.4106438 8.8385355
181H 10.2479041 10.1427942 6.1614563
182H 12.4438835 8.8749455 6.1614563
183H 11.7118907 10.1427942 8.8385345
184H 8.0519237 13.9463421 6.1614573
185H 9.5159103 13.9463421 8.8385345
186H 10.2479041 12.6784924 6.1614563
187H 12.4438825 11.4106438 6.1614563
188H 11.7118907 12.6784924 8.8385345
189H 10.2479041 15.2141917 6.1614563
190H 12.4438825 13.9463421 6.1614563
191H 11.7118907 15.2141917 8.8385345
192H 3.1438885 0.3560432 7.6101811
93H 5.3323598 -0.9066145 7.6138658
194H 7.5286087 -2.1745676 7.6137227
195H 9.7163533 -3.4385231 7.6114990
196H 1.8811003 5.0712934 7.3860388
197H 1.8811512 7.6072851 7.3860168
198H 1.8804102 10.1338229 7.3899542
199H 3.1439818 12.3224738 7.6099412
200H 5.3324226 13.5851019 7.6139412
201H 7.5287207 14.8530924 7.6132528
202H 9.7163901 16.1168678 7.6103083
203H 12.2336182 16.1069447 7.4009935
204H 14.4311520 14.8532632 7.3860789
205H 16.6274946 13.5850739 7.3856710
206H 20.0794225 10.1338387 7.6102263
207H 18.8158591 12.3224328 7.3901547
208H 20.0787147 7.6072635 7.6142101
209H 20.0787112 5.0712958 7.6134638
210H 20.0794879 2.5447859 7.6103793
211H 18.8158489 0.3561517 7.3896983
212H 16.6274556 -0.9064621 7.3868039
213H 14.4313029 -2.1745021 7.3859919
214H 12.2436213 -3.4385562 7.3897280
215H 1.8803135 2.5447070 7.3902929
216H 2.9279732 7.6070939 8.8385365
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C Fluorographene

NMR-properties are calculated for the first twelve tabulated atoms.

FG_periodic

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LATTICE
       2.254041557522120       -1.301371500000001        0.000000000000000
       0.000000000000000        2.602743000000000        0.000000000000000
       0.000000000000000        0.000000000000000       18.000000000000000
POSITIONS
  C   0.6666666666666666   0.3333333333333333   0.5134990215301514
  C   0.3333333333333333   0.6666666666666666  -0.5134990215301514
  F   0.6666666666666666   0.3333333333333333   0.5903729796409607
  F   0.3333333333333333   0.6666666666666666  -0.5903729796409607
```

FG1_relaxed

```
18

C    -1.2953264    0.7478570   -0.1674514
C    -1.2953264   -0.7478570    0.1674514
F    -1.5325292   -0.8848061    1.5389982
C     0.0000000    1.4957141    0.1674514
F     0.0000000    1.7696123    1.5389982
C     1.2953264    0.7478570   -0.1674514
C     0.0000000   -1.4957141   -0.1674514
C     1.2953264   -0.7478570    0.1674514
F     0.0000000   -1.7696123   -1.5389982
F     1.5325292   -0.8848061    1.5389982
F     1.5325292    0.8848061   -1.5389982
F    -1.5325292    0.8848061   -1.5389982
H    -2.1222496    1.2252814    0.3839715
H     0.0000000    2.4505628   -0.3839715
H    -2.1222496   -1.2252814   -0.3839715
H     2.1222496    1.2252814    0.3839715
H     0.0000000   -2.4505628    0.3839715
H     2.1222496   -1.2252814   -0.3839715
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FG1_fixed

```
18

C   -1.3016519    0.7515091   -0.2423672
C   -1.3016519   -0.7515091    0.2423672
C    1.3016519    0.7515091   -0.2423672
C    1.3016519   -0.7515091    0.2423672
C    0.0000000   -1.5030181   -0.2423672
C    0.0000000    1.5030181    0.2423672
F   -1.3016426   -0.7515037    1.6255428
F    1.3016426   -0.7515037    1.6255428
F   -1.3016426    0.7515037   -1.6255428
F   -1.3016426    0.7515037   -1.6255428
F    0.0000000   -1.5030075   -1.6255428
F    0.0000000    1.5030075    1.6255428
H   -2.1968118    1.2683299    0.1395195
H   -2.1968118   -1.2683299   -0.1395195
H    2.1968118    1.2683299    0.1395195
H    2.1968118   -1.2683299   -0.1395195
H    0.0000000   -2.5366597    0.1395195
H    0.0000000    2.5366597   -0.1395195
```

FG2_relaxed

```
60

C22    -1.3001911   -0.7506657   -0.2293519
C23    -1.3001911    0.7506657    0.2293519
C35     0.0000000    1.5013314   -0.2293519
C40     1.3001911    0.7506657    0.2293519
C39     1.3001911   -0.7506657   -0.2293519
C27     0.0000000   -1.5013314    0.2293519
F25    -1.3434036    0.7756145    1.6144571
F37     0.0000000    1.5512289   -1.6144571
F42     1.3434036    0.7756145    1.6144571
F41     1.3434036   -0.7756145   -1.6144571
F29     0.0000000   -1.5512289    1.6144571
F24    -1.3434036   -0.7756145   -1.6144571
C1     -3.8874191   -0.7487636   -0.1843210
C2     -3.8874191    0.7487636    0.1843210
C5     -2.5925532    1.4968113   -0.2286864
C19    -2.5921579    2.9922219    0.1843210
C33    -1.2952613    3.7409855   -0.1843210
C36     0.0000000    2.9936225    0.2286864
C7      1.2952613    3.7409855   -0.1843210
C9      2.5921579    2.9922219    0.1843210
C8      2.5925532    1.4968113   -0.2286864
C11     3.8874191    0.7487636    0.1843210
C6      3.8874191   -0.7487636   -0.1843210
C43     2.5925532   -1.4968113    0.2286864
C32     2.5921579   -2.9922219   -0.1843210
C30     1.2952613   -3.7409855    0.1843210
C26     0.0000000   -2.9936225   -0.2286864
C17    -1.2952613   -3.7409855    0.1843210
C13    -2.5921579   -2.9922219   -0.1843210
C14    -2.5925532   -1.4968113    0.2286864
F4     -4.1687160    0.8687710    1.5348789
F20    -2.6531722    1.5318097   -1.6236838
F21    -2.8367358    3.1758285    1.5348789
F34    -1.3319802    4.0445995   -1.5348789
F38     0.0000000    3.0636194    1.6236838
F46     1.3319802    4.0445995   -1.5348789
F10     2.8367358    3.1758285    1.5348789
F47     2.6531722    1.5318097   -1.6236838
F12     4.1687160    0.8687710    1.5348789
F48     4.1687160   -0.8687710   -1.5348789
F45     2.6531722   -1.5318097    1.6236838
F44     2.8367358   -3.1758285   -1.5348789
F31     1.3319802   -4.0445995    1.5348789
F28     0.0000000   -3.0636194   -1.6236838
F18    -1.3319802   -4.0445995    1.5348789
F15    -2.8367358   -3.1758285   -1.5348789
F16    -2.6531722   -1.5318097    1.6236838
F3     -4.1687160   -0.8687710   -1.5348789
H50    -4.7062860    1.2180661   -0.3890569
H53    -3.4080192    3.4667302   -0.3890569
H55    -1.2982668    4.6847963    0.3890569
H57     1.2982668    4.6847963    0.3890569
H58     3.4080192    3.4667302   -0.3890569
H60     4.7062860    1.2180661   -0.3890569
H59     4.7062860   -1.2180661    0.3890569
H56     3.4080192   -3.4667302    0.3890569
H54     1.2982668   -4.6847963   -0.3890569
H52    -1.2982668   -4.6847963   -0.3890569
H51    -3.4080192   -3.4667302    0.3890569
H49    -4.7062860   -1.2180661    0.3890569
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FG2_fixed

```
60

C22   -1.3016411   -0.7515029   -0.2422157
C23   -1.3016411    0.7515029    0.2422157
C35    0.0000000    1.5030057   -0.2422157
C40    1.3016411    0.7515029    0.2422157
C39    1.3016411   -0.7515029   -0.2422157
C27    0.0000000   -1.5030057    0.2422157
F25   -1.3016809    0.7515258    1.6253923
F37    0.0000000    1.5030516   -1.6253923
F42    1.3016809    0.7515258    1.6253923
F41    1.3016809   -0.7515258   -1.6253923
F29    0.0000000   -1.5030516    1.6253923
F24   -1.3016809   -0.7515258   -1.6253923
C1    -3.9049285   -0.7515379   -0.2420401
C2    -3.9049285    0.7515379    0.2420401
```

```
C5    -2.6033053    1.5030190   -0.2423166
C19   -2.6033152    3.0059983    0.2420401
C33   -1.3016133    3.7575362   -0.2420401
C36    0.0000000    3.0060381    0.2423166
C7     1.3016133    3.7575362   -0.2420401
C9     2.6033152    3.0059983    0.2420401
C8     2.6033053    1.5030190   -0.2423166
C11    3.9049285    0.7515379    0.2420401
C6     3.9049285   -0.7515379   -0.2420401
C43    2.6033053   -1.5030190    0.2423166
C32    2.6033152   -3.0059983   -0.2420401
C30    1.3016133   -3.7575362    0.2420401
C26    0.0000000   -3.0060381   -0.2423166
C17   -1.3016133   -3.7575362    0.2420401
C13   -2.6033152   -3.0059983   -0.2420401
C14   -2.6033053   -1.5030190    0.2423166
Fb4   -3.9049280    0.7516306    1.6252168
F20   -2.6032355    1.5029787   -1.6258445
F21   -2.6033952    3.0059515    1.6252168
F34   -1.3015327    3.7575821   -1.6252168
F38    0.0000000    3.0059574    1.6258445
F46    1.3015327    3.7575821   -1.6252168
F10    2.6033952    3.0059515    1.6252168
F47    2.6032355    1.5029787   -1.6258445
F12    3.9049280    0.7516306    1.6252168
F48    3.9049280   -0.7516306   -1.6252168
F45    2.6032355   -1.5029787    1.6258445
F44    2.6033952   -3.0059515   -1.6252168
F31    1.3015327   -3.7575821    1.6252168
F28    0.0000000   -3.0059574   -1.6258445
F18   -1.3015327   -3.7575821    1.6252168
F15   -2.6033952   -3.0059515   -1.6252168
F16   -2.6032355   -1.5029787    1.6258445
F3    -3.9049280   -0.7516306   -1.6252168
H50   -4.7959236    1.2704462   -0.1486976
H53   -3.4982005    3.5181686   -0.1486976
H55   -1.2977231    4.7886148    0.1486976
H57    1.2977231    4.7886148    0.1486976
H58    3.4982005    3.5181686   -0.1486976
H60    4.7959236    1.2704462   -0.1486976
H59    4.7959236   -1.2704462    0.1486976
H56    3.4982005   -3.5181686    0.1486976
H54    1.2977231   -4.7886148   -0.1486976
H52   -1.2977231   -4.7886148   -0.1486976
H51   -3.4982005   -3.5181686    0.1486976
H49   -4.7959236   -1.2704462    0.1486976
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FG3_relaxed

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126

C19    -1.3012171    0.7512580    0.2414397
C39     0.0000000    1.5025160   -0.2414397
C44     1.3012171    0.7512580    0.2414397
C43     1.3012171   -0.7512580   -0.2414397
C23     0.0000000   -1.5025160    0.2414397
C18    -1.3012171   -0.7512580   -0.2414397
F21    -1.3134109    0.7582981    1.6184250
F41     0.0000000    1.5165963   -1.6184250
F46     1.3134109    0.7582981    1.6184250
F45     1.3134109   -0.7582981   -1.6184250
F25     0.0000000   -1.5165963    1.6184250
F20    -1.3134109   -0.7582981   -1.6184250
C104   -3.9020161    0.7532175    0.2278147
C17    -2.5991602    1.5006258   -0.2443901
C36    -2.6033136    3.0026363    0.2278147
C38    -1.2987026    3.7558539   -0.2278147
C40     0.0000000    3.0012517    0.2443901
C61     1.2987026    3.7558539   -0.2278147
C66     2.6033136    3.0026363    0.2278147
C65     2.5991602    1.5006258   -0.2443901
C70     3.9020161    0.7532175    0.2278147
C69     3.9020161   -0.7532175   -0.2278147
C48     2.5991602   -1.5006258    0.2443901
C47     2.6033136   -3.0026363   -0.2278147
C27     1.2987026   -3.7558539    0.2278147
C22     0.0000000   -3.0012517   -0.2443901
C11    -1.2987026   -3.7558539    0.2278147
C7     -2.6033136   -3.0026363   -0.2278147
C8     -2.5991602   -1.5006258    0.2443901
C6     -3.9020161   -0.7532175   -0.2278147
C1     -6.4877745   -0.7502091   -0.1846867
C2     -6.4877745    0.7502091    0.1846867
C5     -5.1924669    1.4969282   -0.2454322
C15    -5.1937412    2.9986079    0.1721533
C32    -3.8926113    3.7483442   -0.2454322
C33    -3.8935873    5.2434730    0.1846867
C55    -2.5941871    5.9936820   -0.1846867
C57    -1.2998556    5.2452724    0.2454322
C60     0.0000000    5.9972158   -0.1721533
C62     1.2998556    5.2452724    0.2454322
C78     2.5941871    5.9936820   -0.1846867
C81     3.8935873    5.2434730    0.1846867
C80     3.8926113    3.7483442   -0.2454322
C85     5.1937412    2.9986079    0.1721533
C84     5.1924669    1.4969282   -0.2454322
C89     6.4877745    0.7502091    0.1846867
C88     6.4877745   -0.7502091   -0.1846867
C74     5.1924669   -1.4969282    0.2454322
C73     5.1937412   -2.9986079   -0.1721533
C52     3.8926113   -3.7483442    0.2454322
C51     3.8935873   -5.2434730   -0.1846867
C30     2.5941871   -5.9936820    0.1846867
C26     1.2998556   -5.2452724   -0.2454322
C13     0.0000000   -5.9972158    0.1721533
C10    -1.2998556   -5.2452724   -0.2454322
C97    -2.5941871   -5.9936820    0.1846867
C93    -3.8935873   -5.2434730   -0.1846867
C94    -3.8926113   -3.7483442    0.2454322
C92    -5.1937412   -2.9986079   -0.1721533
C99    -5.1924669   -1.4969282    0.2454322
F106   -3.9628756    0.7835581    1.6089322
F108   -2.6137126    1.5090277   -1.6233048
F37    -2.6600190    3.0401719    1.6089322
F58    -1.3028566    3.8237300   -1.6089322
F42     0.0000000    3.0180553    1.6233048
F63     1.3028566    3.8237300   -1.6089322
F68     2.6600190    3.0401719    1.6089322
F67     2.6137126    1.5090277   -1.6233048
F72     3.9628756    0.7835581    1.6089322
F71     3.9628756   -0.7835581   -1.6089322
F50     2.6137126   -1.5090277    1.6233048
F49     2.6600190   -3.0401719   -1.6089322
F29     1.3028566   -3.8237300    1.6089322
F24     0.0000000   -3.0180553   -1.6233048
F12    -1.3028566   -3.8237300    1.6089322
F107   -2.6600190   -3.0401719   -1.6089322
F9     -2.6137126   -1.5090277    1.6233048
F105   -3.9628756   -0.7835581   -1.6089322
F4     -6.7723923    0.8707240    1.5326001
F103   -5.2718205    1.5015654   -1.6364148
F16    -5.4507588    3.1469971    1.5158274
F34    -3.9363040    3.8147478   -1.6364148
F35    -4.1402653    5.4297017    1.5326001
F56    -2.6321270    6.3004258   -1.5326001
F59    -1.3355165    5.3163132    1.6364148
F77     0.0000000    6.2939941   -1.5158274
F64     1.3355165    5.3163132    1.6364148
F79     2.6321270    6.3004258   -1.5326001
F83     4.1402653    5.4297017    1.5326001
F82     3.9363040    3.8147478   -1.6364148
F87     5.4507588    3.1469971    1.5158274
F86     5.2718205    1.5015654   -1.6364148
F91     6.7723923    0.8707240    1.5326001
F90     6.7723923   -0.8707240   -1.5326001
F76     5.2718205   -1.5015654    1.6364148
F75     5.4507588   -3.1469971   -1.5158274
F54     3.9363040   -3.8147478    1.6364148
F53     4.1402653   -5.4297017   -1.5326001
F31     2.6321270   -6.3004258    1.5326001
F28     1.3355165   -5.3163132   -1.6364148
F14     0.0000000   -6.2939941    1.5158274
F102   -1.3355165   -5.3163132   -1.6364148
F98    -2.6321270   -6.3004258    1.5326001
F95    -4.1402653   -5.4297017   -1.5326001
F96    -3.9363040   -3.8147478    1.6364148
F100   -5.4507588   -3.1469971   -1.5158274
F101   -5.2718205   -1.5015654    1.6364148
F3     -6.7723923   -0.8707240   -1.5326001
H110   -7.3073425    1.2156620   -0.3908804
H114   -6.0124158    3.4712699   -0.4013647
H116   -4.7064655    5.7205132   -0.3908804
H118   -2.6008771    6.9361753    0.3908804
H120    0.0000000    6.9425398    0.4013647
H122    2.6008771    6.9361753    0.3908804
H123    4.7064655    5.7205132   -0.3908804
H124    6.0124158    3.4712699   -0.4013647
H126    7.3073425    1.2156620   -0.3908804
H125    7.3073425   -1.2156620    0.3908804
H121    6.0124158   -3.4712699    0.4013647
H119    4.7064655   -5.7205132    0.3908804
H117    2.6008771   -6.9361753   -0.3908804
H115    0.0000000   -6.9425398   -0.4013647
H113   -2.6008771   -6.9361753   -0.3908804
H112   -4.7064655   -5.7205132    0.3908804
H111   -6.0124158   -3.4712699    0.4013647
H109   -7.3073425   -1.2156620    0.3908804
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FG3_fixed

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126

C16    -1.3016546   -0.7515106   -0.2423040
C15    -1.3016546    0.7515106    0.2423040
C28     0.0000000    1.5030213   -0.2423040
C30     1.3016546    0.7515106    0.2423040
C29     1.3016546   -0.7515106   -0.2423040
C17     0.0000000   -1.5030213    0.2423040
F67    -1.3016717    0.7515205    1.6255539
F77     0.0000000    1.5030410   -1.6255539
F80     1.3016717    0.7515205    1.6255539
F79     1.3016717   -0.7515205   -1.6255539
F69     0.0000000   -1.5030410    1.6255539
F66    -1.3016717   -0.7515205   -1.6255539
C14    -2.6032978   -1.5030147    0.2424922
C6     -3.9049408   -0.7515259   -0.2422341
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C1	-3.9049408	0.7515259	0.2422341
C7	-2.6032978	1.5030147	-0.2424922
C8	-2.6033109	3.0060149	0.2422341
C26	-1.3016298	3.7575409	-0.2422341
C27	0.0000000	3.0060294	0.2424922
C41	1.3016298	3.7575409	-0.2422341
C43	2.6033109	3.0060149	0.2422341
C42	2.6032978	1.5030147	-0.2424922
C45	3.9049408	0.7515259	0.2422341
C44	3.9049408	-0.7515259	-0.2422341
C32	2.6032978	-1.5030147	0.2424922
C31	2.6033109	-3.0060149	-0.2422341
C23	1.3016298	-3.7575409	0.2422341
C18	0.0000000	-3.0060294	-0.2424922
C19	-1.3016298	-3.7575409	0.2422341
C13	-2.6033109	-3.0060149	-0.2422341
C4	-6.5082335	-0.7515301	-0.2421642
C3	-6.5082335	0.7515301	0.2421642
C2	-5.2065868	1.5030273	-0.2425621
C10	-5.2066086	3.0060369	0.2421196
C9	-3.9049532	3.7575228	-0.2425621
C38	-3.9049609	5.2605305	0.2421642
C37	-2.6032726	6.0120605	-0.2421642
C36	-1.3016336	5.2605501	0.2425621
C39	0.0000000	6.0120737	-0.2421196
C40	1.3016336	5.2605501	0.2425621
C50	2.6032726	6.0120605	-0.2421642
C49	3.9049609	5.2605305	0.2421642
C48	3.9049532	3.7575228	-0.2425621
C52	5.2066086	3.0060369	0.2421196
C51	5.2065868	1.5030273	-0.2425621
C54	6.5082335	0.7515301	0.2421642
C53	6.5082335	-0.7515301	-0.2421642
C47	5.2065868	-1.5030273	0.2425621
C46	5.2066086	-3.0060369	-0.2421196
C33	3.9049532	-3.7575228	0.2425621
C34	3.9049609	-5.2605305	-0.2421642
C35	2.6032726	-6.0120605	0.2421642
C24	1.3016336	-5.2605501	-0.2425621
C25	0.0000000	-6.0120737	0.2421196
C22	-1.3016336	-5.2605501	-0.2425621
C21	-2.6032726	-6.0120605	0.2421642
C20	-3.9049609	-5.2605305	-0.2421642
C12	-3.9049532	-3.7575228	0.2425621
C11	-5.2066086	-3.0060369	-0.2421196
C5	-5.2065868	-1.5030273	0.2425621
F108	-3.9049440	0.7515517	1.6256238
F65	-2.6032922	1.5030114	-1.6255228
F75	-2.6033348	3.0060048	1.6256238
F76	-1.3016091	3.7575565	-1.6256238
F78	0.0000000	3.0060229	1.6255228
F88	1.3016091	3.7575565	-1.6256238
F91	2.6033348	3.0060048	1.6256238
F90	2.6032922	1.5030114	-1.6255228
F93	3.9049440	0.7515517	1.6256238
F92	3.9049440	-0.7515517	-1.6256238
F82	2.6032922	-1.5030114	1.6255228
F81	2.6033348	-3.0060048	-1.6256238
F71	1.3016091	-3.7575565	1.6256238
F68	0.0000000	-3.0060229	-1.6255228
F62	-1.3016091	-3.7575565	1.6256238
F59	-2.6033348	-3.0060048	-1.6256238
F60	-2.6032922	-1.5030114	1.6255228
F58	-3.9049440	-0.7515517	-1.6256238
F56	-6.5082375	0.7515471	1.6256937
F57	-5.2065873	1.5030015	-1.6257373
F64	-5.2066394	3.0060546	1.6257498
F73	-3.9049312	3.7575361	-1.6257373
F74	-3.9049776	5.2605255	1.6256937
F85	-2.6032599	6.0120726	-1.6256937
F86	-1.3016562	5.2605377	1.6257373
F87	0.0000000	6.0121093	-1.6257498
F89	1.3016562	5.2605377	1.6257373
F96	2.6032599	6.0120726	-1.6256937
F98	3.9049776	5.2605255	1.6256937
F97	3.9049312	3.7575361	-1.6257373
F100	5.2066394	3.0060546	1.6257498
F99	5.2065873	1.5030015	-1.6257373
F102	6.5082375	0.7515471	1.6256937
F101	6.5082375	-0.7515471	-1.6256937
F95	5.2065873	-1.5030015	1.6257373
F94	5.2066394	-3.0060546	-1.6257498
F84	3.9049312	-3.7575361	1.6257373
F83	3.9049776	-5.2605255	-1.6256937
F72	2.6032599	-6.0120726	1.6256937
F70	1.3016562	-5.2605377	-1.6257373
F63	0.0000000	-6.0121093	1.6257498
F61	-1.3016562	-5.2605377	-1.6257373
F106	-2.6032599	-6.0120726	1.6256937
F104	-3.9049776	-5.2605255	-1.6256937
F105	-3.9049312	-3.7575361	1.6257373
F103	-5.2066394	-3.0060546	-1.6257498
F107	-5.2065873	-1.5030015	1.6257373
F55	-6.5082375	-0.7515471	-1.6256937
H110	-7.3991883	1.2697849	-0.1492684
H114	-6.0991872	3.5213674	-0.1520803
H116	-4.7992601	5.7729925	-0.1492684
H118	-2.5999281	7.0427775	0.1492684
H120	0.0000000	7.0427348	0.1520803
H122	2.5999281	7.0427775	0.1492684
H123	4.7992601	5.7729925	-0.1492684
H124	6.0991872	3.5213674	-0.1520803
H126	7.3991883	1.2697849	-0.1492684
H125	7.3991883	-1.2697849	0.1492684
H121	6.0991872	-3.5213674	0.1520803
H119	4.7992601	-5.7729925	0.1492684
H117	2.5999281	-7.0427775	-0.1492684
H115	0.0000000	-7.0427348	-0.1520803
H113	-2.5999281	-7.0427775	-0.1492684
H112	-4.7992601	-5.7729925	0.1492684
H111	-6.0991872	-3.5213674	0.1520803
H109	-7.3991883	-1.2697849	0.1492684

FG4_relaxed

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Ca6	-1.3017281	-0.7515531	-0.2445876
Ca174	-1.3017281	0.7515531	0.2445876
Ca21	0.0000000	1.5031062	-0.2445876
Ca23	1.3017281	0.7515531	0.2445876
Ca22	1.3017281	-0.7515531	-0.2445876
Ca8	0.0000000	-1.5031062	0.2445876
F175	-1.3057790	-0.7538919	-1.6192527
F176	-1.3057790	0.7538919	1.6192527
F186	0.0000000	1.5077838	-1.6192527
F25	1.3057790	0.7538919	1.6192527
F24	1.3057790	-0.7538919	-1.6192527
F9	0.0000000	-1.5077838	1.6192527
C155	-2.6019638	-1.5022445	0.2476374
C150	-3.9046761	-0.7528639	-0.2390614
C151	-3.9046761	0.7528639	0.2390614
C170	-2.6019638	1.5022445	-0.2476374
C171	-2.6043373	3.0051168	0.2390614
C181	-1.3003388	3.7579807	-0.2390614
C185	0.0000000	3.0044890	0.2476374
C43	1.3003388	3.7579807	-0.2390614
C45	2.6043373	3.0051168	0.2390614
C44	2.6019638	1.5022445	-0.2476374
C49	3.9046761	0.7528639	0.2390614
C48	3.9046761	-0.7528639	-0.2390614
C27	2.6019638	-1.5022445	0.2476374
C26	2.6043373	-3.0051168	-0.2390614
C11	1.3003388	-3.7579807	0.2390614
C7	0.0000000	-3.0044890	-0.2476374
C159	-1.3003388	-3.7579807	0.2390614
C154	-2.6043373	-3.0051168	-0.2390614
C129	-5.2022103	-1.4995137	0.2549867
C124	-6.5052835	-0.7548623	-0.2246660
C125	-6.5052835	0.7548623	0.2246660
C146	-5.2022103	1.4995137	-0.2549867
C147	-5.2068490	3.0061757	0.2102678
C166	-3.8997221	3.7554895	-0.2549867
C167	-3.9063717	5.2563096	0.2246660
C40	-2.5989118	6.0111719	-0.2246660
C182	-1.3024882	5.2550031	0.2549867
C62	0.0000000	6.0123514	-0.2102678
C189	1.3024882	5.2550031	0.2549867
C65	2.5989118	6.0111719	-0.2246660
C67	3.9063717	5.2563096	0.2246660
C66	3.8997221	3.7554895	-0.2549867
C71	5.2068490	3.0061757	0.2102678
C70	5.2022103	1.4995137	-0.2549867
C75	6.5052835	0.7548623	0.2246660
C74	6.5052835	-0.7548623	-0.2246660
C53	5.2022103	-1.4995137	0.2549867
C52	5.2068490	-3.0061757	-0.2102678
C31	3.8997221	-3.7554895	0.2549867
C30	3.9063717	-5.2563096	-0.2246660
C14	2.5989118	-6.0111719	0.2246660
C10	1.3024882	-5.2550031	-0.2549867
C162	0.0000000	-6.0123514	0.2102678
C158	-1.3024882	-5.2550031	-0.2549867
C136	-2.5989118	-6.0111719	0.2246660
C132	-3.9063717	-5.2563096	-0.2246660
C133	-3.8997221	-3.7554895	0.2549867
C128	-5.2068490	-3.0061757	-0.2102678
C108	-7.7956648	-1.4968646	0.2521870
C1	-9.0906933	-0.7510704	-0.1829792
C2	-9.0906933	0.7510704	0.1829792
C5	-7.7956648	1.4968646	-0.2521870
C121	-7.7967025	3.0014774	0.1625326
C142	-6.4949743	3.7498752	-0.2717386
C143	-6.4977069	5.2514038	0.1625326
C18	-5.1941552	6.0028115	-0.2521870
C19	-5.1957927	7.4972361	0.1829792
C38	-3.8949006	8.2483066	-0.1829792
C41	-2.6015096	7.4996761	0.2521870
C60	-1.2989956	8.2528811	-0.1625326
C63	0.0000000	7.4997503	0.2717386
C82	1.2989956	8.2528811	-0.1625326
C84	2.6015096	7.4996761	0.2521870
C86	3.8949006	8.2483066	-0.1829792
C88	5.1957927	7.4972361	0.1829792
C87	5.1941552	6.0028115	-0.2521870
C92	6.4977069	5.2514038	0.1625326
C91	6.4949743	3.7498752	-0.2717386
C96	7.7967025	3.0014774	0.1625326

C95	7.7956648	1.4968646	-0.2521870
C100	9.0906933	0.7510704	0.1829792
C99	9.0906933	-0.7510704	-0.1829792
C79	7.7956648	-1.4968646	0.2521870
C78	7.7967025	-3.0014774	-0.1625326
C57	6.4949743	-3.7498752	0.2717386
C56	6.4977069	-5.2514038	-0.1625326
C35	5.1941552	-6.0028115	0.2521870
C34	5.1957927	-7.4972361	-0.1829792
C16	3.8949006	-8.2483066	0.1829792
C13	2.6015096	-7.4996761	-0.2521870
C140	1.2989956	-8.2528811	0.1625326
C139	0.0000000	-7.4997503	-0.2717386
C119	-1.2989956	-8.2528811	0.1625326
C118	-2.6015096	-7.4996761	-0.2521870
C105	-3.8949006	-8.2483066	0.1829792
C104	-5.1957927	-7.4972361	-0.1829792
C115	-5.1941552	-6.0028115	0.2521870
C111	-6.4977069	-5.2514038	-0.1625326
C112	-6.4949743	-3.7498752	0.2717386
C107	-7.7967025	-3.0014774	-0.1625326
F157	-2.6043032	-1.5035952	1.6228199
F152	-3.9225927	-0.7649829	-1.6149319
F153	-3.9225927	0.7649829	1.6149319
F172	-2.6043032	1.5035952	-1.6228199
F173	-2.6237909	3.0145735	1.6149319
F183	-1.2988017	3.7795563	-1.6149319
F187	0.0000000	3.0071903	1.6228199
F190	1.2988017	3.7795563	-1.6149319
F47	2.6237909	3.0145735	1.6149319
F46	2.6043032	1.5035952	-1.6228199
F51	3.9225927	0.7649829	1.6149319
F50	3.9225927	-0.7649829	-1.6149319
F29	2.6043032	-1.5035952	1.6228199
F28	2.6237909	-3.0145735	-1.6149319
F12	1.2988017	-3.7795563	1.6149319
F177	0.0000000	-3.0071903	-1.6228199
F161	-1.2988017	-3.7795563	1.6149319
F156	-2.6237909	-3.0145735	-1.6149319
F131	-5.2195869	-1.4934857	1.6328557
F126	-6.5669158	-0.7911802	-1.6049732
F127	-6.5669158	0.7911802	1.6049732
F148	-5.2195869	1.4934857	-1.6328557
F149	-5.2709202	3.0431672	1.5893460
F168	-3.9031900	3.7735520	-1.6328557
F169	-3.9686400	5.2915258	1.6049732
F180	-2.5982758	6.0827060	-1.6049732
F184	-1.3163969	5.2670377	1.6328557
F188	0.0000000	6.0863344	-1.5893460
F191	1.3163969	5.2670377	1.6328557
F192	2.5982758	6.0827060	-1.6049732
F69	3.9686400	5.2915258	1.6049732
F68	3.9031900	3.7735520	-1.6328557
F73	5.2709202	3.0431672	1.5893460
F72	5.2195869	1.4934857	-1.6328557
F77	6.5669158	0.7911802	1.6049732
F76	6.5669158	-0.7911802	-1.6049732
F55	5.2195869	-1.4934857	1.6328557
F54	5.2709202	-3.0431672	-1.5893460
F33	3.9031900	-3.7735520	1.6328557
F32	3.9686400	-5.2915258	-1.6049732
F15	2.5982758	-6.0827060	1.6049732
F178	1.3163969	-5.2670377	-1.6328557
F164	0.0000000	-6.0863344	1.5893460
F160	-1.3163969	-5.2670377	-1.6328557
F138	-2.5982758	-6.0827060	1.6049732
F134	-3.9686400	-5.2915258	-1.6049732
F135	-3.9031900	-3.7735520	1.6328557
F130	-5.2709202	-3.0431672	-1.5893460
F110	-7.8784080	-1.4920621	1.6423248
F3	-9.3751948	-0.8751866	-1.5301960
F4	-9.3751948	0.8751866	1.5301960
F122	-7.8784080	1.4920621	-1.6423248
F123	-8.0523017	3.1470324	1.5054319
F144	-6.5555981	3.7848763	-1.6603281
F145	-6.7515609	5.3999816	1.5054319
F165	-5.2313677	6.0768704	-1.6423248
F20	-5.4455313	7.6815635	1.5301960
F39	-3.9296635	8.5567502	-1.5301960
F42	-2.6470403	7.5689325	1.6423248
F61	-1.3007408	8.5470140	-1.5054319
F64	0.0000000	7.5697526	1.6603281
F83	1.3007408	8.5470140	-1.5054319
F85	2.6470403	7.5689325	1.6423248
F103	3.9296635	8.5567502	-1.5301960
F90	5.4455313	7.6815635	1.5301960
F89	5.2313677	6.0768704	-1.6423248
F94	6.7515609	5.3999816	1.5054319
F93	6.5555981	3.7848763	-1.6603281
F98	8.0523017	3.1470324	1.5054319
F97	7.8784080	1.4920621	-1.6423248
F102	9.3751948	0.8751866	1.5301960
F101	9.3751948	-0.8751866	-1.5301960
F81	7.8784080	-1.4920621	1.6423248
F80	8.0523017	-3.1470324	-1.5054319
F59	6.5555981	-3.7848763	1.6603281
F58	6.7515609	-5.3999816	-1.5054319
F37	5.2313677	-6.0768704	1.6423248
F36	5.4455313	-7.6815635	-1.5301960
F17	3.9296635	-8.5567502	1.5301960
F179	2.6470403	-7.5689325	-1.6423248
F141	1.3007408	-8.5470140	1.5054319
F163	0.0000000	-7.5697526	-1.6603281
F120	-1.3007408	-8.5470140	1.5054319
F137	-2.6470403	-7.5689325	-1.6423248
F106	-3.9296635	-8.5567502	1.5301960
F116	-5.4455313	-7.6815635	-1.5301960
F117	-5.2313677	-6.0768704	1.6423248
F113	-6.7515609	-5.3999816	-1.5054319
F114	-6.5555981	-3.7848763	1.6603281
F109	-8.0523017	-3.1470324	-1.5054319
H193	-9.9107454	-1.2140760	0.3938460
H194	-9.9107454	1.2140760	-0.3938460
H199	-8.6174874	3.4721605	-0.4096544
H201	-7.3157229	5.7268828	-0.4096544
H203	-6.0067933	7.9759193	-0.3938460
H205	-3.9039521	9.1899953	0.3938460
H207	-1.3017645	9.1990432	0.4096544
H209	1.3017645	9.1990432	0.4096544
H211	3.9039521	9.1899953	0.3938460
H212	6.0067933	7.9759193	-0.3938460
H213	7.3157229	5.7268828	-0.4096544
H214	8.6174874	3.4721605	-0.4096544
H216	9.9107454	1.2140760	-0.3938460
H215	9.9107454	-1.2140760	0.3938460
H210	8.6174874	-3.4721605	0.4096544
H208	7.3157229	-5.7268828	0.4096544
H206	6.0067933	-7.9759193	0.3938460
H204	3.9039521	-9.1899953	-0.3938460
H202	1.3017645	-9.1990432	-0.4096544
H200	-1.3017645	-9.1990432	-0.4096544
H198	-3.9039521	-9.1899953	-0.3938460
H197	-6.0067933	-7.9759193	0.3938460
H196	-7.3157229	-5.7268828	0.4096544
H195	-8.6174874	-3.4721605	0.4096544

FG4_fixed

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C6	8.2666007	3.9048809	7.2576260
C174	7.5150929	5.2065495	7.7423708
C21	8.2666007	6.5082042	7.2576410
C23	9.7696203	6.5081822	7.7423708
C22	10.5211280	5.2065135	7.2576260
C8	9.7696203	3.9048589	7.7423548
F175	8.2665837	3.9049089	5.8744494
F176	7.5151089	5.2065215	9.1255464
F186	8.2665837	6.5082322	5.8744654
F25	9.7696363	6.5081542	9.1255464
F24	10.5211120	5.2065415	5.8744494
F9	9.7696363	3.9048309	9.1255304
C155	7.5150929	2.6032263	7.7423548
C150	6.0120733	2.6032473	7.2576260
C151	5.2605645	3.9049169	7.7423708
C170	6.0120733	5.2065715	7.2576410
C171	5.2605645	6.5082402	7.7423858
C181	6.0120733	7.8098948	7.2576560
C185	7.5150929	7.8098728	7.7423858
C43	8.2666007	9.1115274	7.2576560
C45	9.7696203	9.1115054	7.7423858
C44	10.5211280	7.8098368	7.2576410
C49	12.0241476	7.8098158	7.7423708
C48	12.7756554	6.5081462	7.2576260
C27	12.0241476	5.2064915	7.7423548
C26	12.7756554	3.9048229	7.2576100
C11	12.0241476	2.6031683	7.7423398
C7	10.5211280	2.6031903	7.2576100
C159	9.7696203	1.3015356	7.7423398
C154	8.2666007	1.3015566	7.2576100
C129	5.2605645	1.3015936	7.7423548
C124	3.7575449	1.3016146	7.2576260
C125	3.0060372	2.6032843	7.7423708
C146	3.7575449	3.9049379	7.2576410
C147	3.0060372	5.2066075	7.7423858
C166	3.7575449	6.5082612	7.2576560
C167	3.0060372	7.8099308	7.7424008
C40	3.7575449	9.1115854	7.2576720
C182	5.2605645	9.1115634	7.7424008
C62	6.0120733	10.4132181	7.2576720
C189	7.5150929	10.4131961	7.7424008
C65	8.2666007	11.7148507	7.2576720
C67	9.7696203	11.7148297	7.7424008
C66	10.5211280	10.4131601	7.2576560
C71	12.0241476	10.4131391	7.7423858
C70	12.7756554	9.1114694	7.2576410
C75	14.2786750	9.1114484	7.7423708
C74	15.0301828	7.8097788	7.2576260
C53	14.2786750	6.5081252	7.7423548
C52	15.0301828	5.2064555	7.2576100
C31	14.2786750	3.9048009	7.7423398
C30	15.0301828	2.6031323	7.2575950
C14	14.2786750	1.3014776	7.7423238
C10	12.7756554	1.3014996	7.2575950
C162	12.0241476	-0.0001550	7.7423238
C158	10.5211280	-0.0001330	7.2575950
C136	9.7696203	-1.3017876	7.7423238

C132	8.2666007	-1.3017666	7.2575950
C133	7.5150929	-0.0000970	7.7423398
C128	6.0120733	-0.0000760	7.2576100
C108	3.0060372	-0.0000400	7.7423548
C1	1.5030176	-0.0000180	7.2576260
C2	0.7515098	1.3016506	7.7423708
C5	1.5030176	2.6033053	7.2576410
C121	0.7515098	3.9049739	7.7423858
C142	1.5030176	5.2066285	7.2576560
C143	0.7515098	6.5082982	7.7424008
C18	1.5030176	7.8099518	7.2576720
C19	0.7515098	9.1116214	7.7424168
C38	1.5030176	10.4132761	7.2576870
C41	3.0060372	10.4132541	7.7424168
C60	3.7575449	11.7149087	7.2576870
C63	5.2605645	11.7148867	7.7424168
C82	6.0120733	13.0165413	7.2576870
C84	7.5150929	13.0165203	7.7424168
C86	8.2666007	14.3181740	7.2576870
C88	9.7696203	14.3181530	7.7424168
C87	10.5211280	13.0164833	7.2576720
C92	12.0241476	13.0164623	7.7424008
C91	12.7756554	11.7147927	7.2576560
C96	14.2786750	11.7147717	7.7423858
C95	15.0301828	10.4131021	7.2576410
C100	16.5332024	10.4130811	7.7423708
C99	17.2847111	9.1114124	7.2576260
C79	16.5332024	7.8097578	7.7423548
C78	17.2847111	6.5080882	7.2576100
C57	16.5332024	5.2064345	7.7423398
C56	17.2847111	3.9047649	7.2575950
C35	16.5332024	2.6031113	7.7423238
C34	17.2847111	1.3014416	7.2575790
C16	16.5332024	-0.0002130	7.7423088
C13	15.0301828	-0.0001910	7.2575790
C140	14.2786750	-1.3018456	7.7423088
C139	12.7756554	-1.3018236	7.2575790
C119	12.0241476	-2.6034783	7.7423088
C118	10.5211280	-2.6034573	7.2575790
C105	9.7696203	-3.9051109	7.7423088
C104	8.2666007	-3.9050899	7.2575790
C115	7.5150929	-2.6034203	7.7423238
C111	6.0120733	-2.6033993	7.2575950
C112	5.2605645	-1.3017306	7.7423398
C107	3.7575449	-1.3017086	7.2576100
F157	7.5151089	2.6031983	9.1255304
F152	6.0120563	2.6032763	5.8744494
F153	5.2605815	3.9048889	9.1255464
F172	6.0120563	5.2065995	5.8744654
F173	5.2605815	6.5082122	9.1255614
F183	6.0120563	7.8099228	5.8744804
F187	7.5151089	7.8098448	9.1255614
F190	8.2665837	9.1115554	5.8744804
F47	9.7696363	9.1114774	9.1255614
F46	10.5211120	7.8098648	5.8744654
F51	12.0241636	7.8097868	9.1255464
F50	12.7756394	6.5081742	5.8744494
F29	12.0241636	5.2064635	9.1255304
F28	12.7756394	3.9048509	5.8744344
F12	12.0241636	2.6031403	9.1255154
F177	10.5211120	2.6032183	5.8744344
F161	9.7696363	1.3015076	9.1255154
F156	8.2665837	1.3015856	5.8744344
F131	5.2605815	1.3015646	9.1255304
F126	3.7575289	1.3016426	5.8744494
F127	3.0060542	2.6032553	9.1255464
F148	3.7575289	3.9049659	5.8744654
F149	3.0060542	5.2065795	9.1255614
F168	3.7575289	6.5082902	5.8744804
F169	3.0060542	7.8099028	9.1255764
F180	3.7575289	9.1116134	5.8744964
F184	5.2605815	9.1115354	9.1255764
F188	6.0120563	10.4132461	5.8744964
F191	7.5151089	10.4131681	9.1255764
F192	8.2665837	11.7148787	5.8744964
F69	9.7696363	11.7148007	9.1255764
F68	10.5211120	10.4131881	5.8744804
F73	12.0241636	10.4131101	9.1255614
F72	12.7756394	9.1114974	5.8744654
F77	14.2786920	9.1114204	9.1255464
F76	15.0301668	7.8098078	5.8744494
F55	14.2786920	6.5080962	9.1255304
F54	15.0301668	5.2064835	5.8744344
F33	14.2786920	3.9047729	9.1255154
F32	15.0301668	2.6031603	5.8744194
F15	14.2786920	1.3014496	9.1254994
F178	12.7756394	1.3015276	5.8744194
F164	12.0241636	-0.0001830	9.1254994
F160	10.5211120	-0.0001050	5.8744194
F138	9.7696363	-1.3018156	9.1254994
F134	8.2665837	-1.3017386	5.8744194
F135	7.5151089	-0.0001250	9.1255154
F130	6.0120563	-0.0000480	5.8744344
F110	3.0060542	-0.0000680	9.1255304
F3	1.5030016	0.0000100	5.8744494
F4	0.7515258	1.3016226	9.1255464
F122	1.5030016	2.6033333	5.8744654
F123	0.7515258	3.9049459	9.1255614
F144	1.5030016	5.2066565	5.8744804
F145	0.7515258	6.5082692	9.1255764
F165	1.5030016	7.8099808	5.8744964
F20	0.7515258	9.1115934	9.1255924
F39	1.5030016	10.4133041	5.8745114
F42	3.0060542	10.4132261	9.1255924
F61	3.7575289	11.7149367	5.8745114
F64	5.2605815	11.7148587	9.1255924
F83	6.0120563	13.0165693	5.8745114
F85	7.5151089	13.0164913	9.1255924
F103	8.2665837	14.3182020	5.8745114
F90	9.7696363	14.3181250	9.1255924
F89	10.5211120	13.0165123	5.8744964
F94	12.0241636	13.0164343	9.1255764
F93	12.7756394	11.7148217	5.8744804
F98	14.2786920	11.7147437	9.1255614
F97	15.0301668	10.4131311	5.8744654
F102	16.5332194	10.4130531	9.1255464
F101	17.2846941	9.1114404	5.8744494
F81	16.5332194	7.8097298	9.1255304
F80	17.2846941	6.5081172	5.8744344
F59	16.5332194	5.2064055	9.1255154
F58	17.2846941	3.9047929	5.8744194
F37	16.5332194	2.6030823	9.1254994
F36	17.2846941	1.3014696	5.8744034
F17	16.5332194	-0.0002410	9.1254844
F179	15.0301668	-0.0001630	5.8744034
F141	14.2786920	-1.3018736	9.1254844
F163	12.7756394	-1.3017956	5.8744034
F120	12.0241636	-2.6035063	9.1254844
F137	10.5211120	-2.6034283	5.8744034
F106	9.7696363	-3.9051399	9.1254844
F116	8.2665837	-3.9050619	5.8744034
F117	7.5151089	-2.6034493	9.1254994
F113	6.0120563	-2.6033713	5.8744194
F114	5.2605815	-1.3017586	9.1255154
F109	3.7575289	-1.3016806	5.8744344
H193	0.9906796	-0.8942725	7.6491487
H194	-0.2791110	1.3050728	7.3512111
H199	-0.2790735	3.9048203	7.3475012
H201	-0.2790608	6.5083140	7.3473516
H203	-0.2790694	9.1081535	7.3509942
H205	0.9906958	11.3075027	7.6492566
H207	3.2421465	12.6073039	7.6522320
H209	5.4967673	13.9089840	7.6525032
H211	7.7482558	15.2089094	7.6496989
H212	10.2879692	15.2089039	7.3502453
H213	12.5393521	13.9089663	7.3480492
H214	14.7939399	12.6072450	7.3472287
H216	17.0454843	11.3073645	7.3501784
H215	18.3153026	9.1079656	7.6501638
H210	18.3152420	6.5082064	7.6522133
H208	18.3152425	3.9047841	7.6530612
H206	18.3152894	1.3049328	7.6494018
H204	17.0455416	-0.8944078	7.3503933
H202	14.7940620	-2.1942482	7.3472767
H200	12.5394150	-3.4959576	7.3472752
H198	10.2879405	-4.7958649	7.3508983
H197	7.7483249	-4.7958835	7.6490991
H196	5.4968520	-3.4959498	7.6526953
H195	3.2421813	-2.1941917	7.6519670