Supplementary material (ESI) for PCCP

Chemical shifts for β testosterone, given in ppm with respect to the shielding of the reference. tetramethylsilane at 168.50 ppm.

Carbon number	Expt.	Calc.
1	35.25	32.57
2	35.25	32.98
3	200.15	203.41
4	124.65	127.21
5	173.75	187.87
6	33.45	33.20
7	33.45	34.09
8	35.25	33.16
9	54.65	56.02
10	39.35	40.28
11	20.95	18.60
12	35.25	34.39
13	43.55	41.68
14	51.55	51.25
15	23.95	20.46
16	28.75	26.54
17	80.65	86.25
18	12.55	7.14
19	16.85	12.24

Supplementary material (ESI) for PCCP

Computed shielding tensor parameters for molecule V of α testosterone. Data for the components and for the anisotropy are given in ppm.

Carbon number	σ_{XX}	σ_{YY}	σ_{ZZ}	ζ	η
1	117.14	128.03	157.41	34.83	0.47
2	123.56	129.91	163.01	36.28	0.26
3	−107.91	−95.07	98.35	119.84	0.10
4	110.04	55.18	−36.88	−119.49	0.69
5	−133.22	−48.89	143.49	234.54	0.54
6	126.78	134.68	146.47	15.74	0.75
7	125.83	133.64	152.94	23.21	0.51
8	138.34	135.82	132.75	−4.33	0.88
9	126.39	123.35	93.60	−31.27	0.15
10	117.43	128.00	145.54	22.82	0.69
11	141.95	146.44	158.34	14.15	0.48
12	112.98	132.03	152.24	29.73	0.96
13	139.27	128.38	116.72	−17.11	0.95
14	102.97	114.39	138.03	29.35	0.58
15	163.24	148.51	130.24	−25.63	0.86
16	169.97	150.39	190.94	−50.24	0.58
17	50.22	79.38	119.45	54.65	0.80
18	173.58	162.65	149.82	−18.29	0.90
19	138.05	152.67	176.15	30.79	0.71

Supplementary material (ESI) for PCCP

Computed shielding tensor parameters for molecule U of α testosterone. Data for the components and for the anisotropy are given in ppm.

Carbon number	σ_{XX}	σ_{YY}	σ_{ZZ}	ζ	η
1	120.51	126.74	155.60	31.98	0.29
2	120.32	129.16	161.92	37.18	0.36
3	−108.21	−91.33	95.80	195.67	0.13
4	106.86	53.91	−37.51	−117.90	0.67
5	−132.64	−48.21	142.61	233.05	0.54
6	125.02	134.32	144.88	15.21	0.92
7	124.88	134.71	151.29	21.50	0.69
8	130.54	132.97	138.63	6.87	0.53
9	126.09	122.36	95.26	−28.96	0.19
10	117.76	127.38	142.48	19.92	0.72
11	156.45	150.47	143.48	−9.97	0.90
12	153.77	133.30	111.63	−31.90	0.96
13	118.29	126.87	139.73	17.15	0.75
14	101.33	114.57	139.50	31.55	0.63
15	164.69	146.85	128.93	−26.84	1.00
16	168.97	150.32	110.48	−49.17	0.57
17	51.91	83.67	123.58	55.79	0.85
18	151.91	160.92	172.80	16.39	0.82
19	138.82	151.72	174.12	28.85	0.67

Supplementary material (ESI) for PCCP

Computed shielding tensor parameters for β testosterone. Data for the components and for the anisotropy are given in ppm.

Carbon Number	σ_{XX}	σ_{YY}	σ_{ZZ}	ζ	η
1	121.15	128.90	157.71	32.69	0.36
2	120.25	126.04	160.27	37.12	0.23
3	–105.23	–94.39	94.91	194.73	0.08
4	107.74	52.38	–36.25	–116.31	0.71
5	–140.08	–60.51	142.50	242.80	0.49
6	125.54	133.00	147.34	18.07	0.62
7	121.38	130.52	151.32	25.37	0.54
8	132.38	133.19	140.44	7.65	0.16
9	125.99	118.20	93.22	–28.87	0.40
10	115.75	126.28	142.61	21.60	0.73
11	143.03	149.76	156.90	10.51	0.96
12	115.39	133.81	153.11	28.51	0.97
13	116.94	125.80	137.27	16.36	0.81
14	99.88	113.21	138.64	21.10	0.62
15	130.58	146.83	166.70	28.00	0.87
16	168.84	150.30	106.73	–52.85	0.53
17	49.10	79.10	118.54	54.44	0.83
18	154.91	159.33	169.84	12.72	0.52
19	138.11	152.70	177.96	32.55	0.67