Supporting Information

DFT/NMR Approach for the Configuration Assignment of Groups of Stereoisomers by the Combination and Comparison of Experimental and Predicted Sets of Data

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Table of contents

Table S1. ^{13}C experimental related to exp_**1a** set of data and calculated NMR chemical shifts (MPW1PW91/6-31g(d,p) level of theory) related to calc_**1a**, calc_**1b**, calc_**1c**, calc_**1d** sets of data, with $^a|\Delta\delta|(^{13}C)$ and ^{b}MAE values. Chemical shift data here reported were produced using benzene as reference compound for sp^2 carbons (highlighted in yellow), and tetramethylsilane (TMS) for sp^3 carbons.

	δ_exp(^{13}C), ppm	δ_calc(^{13}C), ppm				|Δδ| (^{13}C), ppm^a			
Position	exp_**1a**	calc_**1a**	calc_**1b**	calc_**1c**	calc_**1d**	calc_**1a**	calc_**1b**	calc_**1c**	calc_**1d**
1	169.9	163.65	163.79	163.82	163.62	6.25	6.11	6.08	6.29
3	76.3	72.81	73.56	73.37	72.48	3.49	2.74	2.93	3.82
4	33.6	34.93	33.52	33.73	35.02	1.33	0.08	0.13	1.42
4a	141.8	143.10	143.24	143.31	143.05	1.30	1.44	1.51	1.25
5	106.7	105.75	105.80	105.76	105.75	0.95	0.90	0.94	0.95
6	163.1	160.89	160.91	160.89	160.92	2.21	2.19	2.21	2.18
7	102.0	101.15	101.10	101.10	101.15	0.85	0.90	0.90	0.85
8	164.3	165.73	165.74	165.75	165.76	1.43	1.44	1.45	1.46
8a	101.5	104.34	104.27	104.25	104.32	2.84	2.77	2.75	2.82
9	39.3	40.76	38.21	40.74	42.54	1.46	1.09	1.44	3.24
10	66.6	64.23	65.24	71.87	71.21	2.37	1.36	5.27	4.61
11	30.9	31.53	30.46	30.94	31.66	0.63	0.44	0.04	0.76
12	18.1	20.24	20.19	24.80	24.74	2.14	2.09	6.70	6.64
13	30.9	30.21	30.54	32.33	32.55	0.69	0.36	1.43	1.65
14	68.0	66.65	66.18	71.98	71.73	1.35	1.82	3.98	3.73
15	18.9	18.45	19.27	22.82	22.76	0.45	0.37	3.92	3.86
MAE^b						1.86	1.63	2.61	2.85

^{a} $|\Delta\delta|(^{13}C) = |\delta_{exp} - \delta_{calc}|$ (^{13}C), ppm: absolute differences for experimental versus calculated ^{13}C NMR chemical shifts

^{b} **MAE** $= \Sigma[|(\delta_{exp} - \delta_{calcd})|]/n$, summation through n of the absolute error values (difference of the absolute values between corresponding experimental and ^{13}C chemical shifts), normalized to the number of the chemical shifts

Table S2. [13]C experimental related to exp_**1b** set of data and calculated NMR chemical shifts (MPW1PW91/6-31g(d,p) level of theory) related to calc_**1a**, calc_**1b**, calc_**1c**, calc_**1d** sets of data, with [a]$|\Delta\delta|$(^{13}C) and [b]MAE values. Chemical shift data here reported were produced using benzene as reference compound for sp[2] carbons (highlighted in yellow), and tetramethylsilane (TMS) for sp[3] carbons.

Position	δ_{exp}(^{13}C), ppm	δ_{calc}(^{13}C), ppm				$|\Delta\delta|$ (^{13}C), ppm[a]			
	exp_**1b**	calc_**1a**	calc_**1b**	calc_**1c**	calc_**1d**	calc_**1a**	calc_**1b**	calc_**1c**	calc_**1d**
1	170.0	163.65	163.79	163.82	163.62	6.35	6.21	6.18	6.38
3	76.6	72.81	73.56	73.37	72.48	3.79	3.04	3.23	4.12
4	32.6	34.93	33.52	33.73	35.02	2.33	0.92	1.13	2.42
4a	141.6	143.10	143.24	143.31	143.05	1.50	1.64	1.71	1.45
5	106.7	105.75	105.80	105.76	105.75	0.95	0.90	0.94	0.95
6	163.0	160.89	160.91	160.89	160.92	2.11	2.09	2.11	2.08
7	102.0	101.15	101.10	101.10	101.15	0.85	0.90	0.90	0.85
8	164.4	165.73	165.74	165.75	165.76	1.33	1.34	1.35	1.36
8a	101.6	104.34	104.27	104.25	104.32	2.74	2.67	2.65	2.72
9	37.3	40.76	38.21	40.74	42.54	3.46	0.91	3.44	5.24
10	67.2	64.23	65.24	71.87	71.21	2.97	1.96	4.67	4.01
11	29.8	31.53	30.46	30.94	31.66	1.73	0.66	1.14	1.86
12	18.1	20.24	20.19	24.80	24.74	2.14	2.09	6.70	6.64
13	31.5	30.21	30.54	32.33	32.55	1.29	0.96	0.83	1.05
14	67.4	66.65	66.18	71.98	71.73	0.75	1.22	4.58	4.33
15	19.7	18.45	19.27	22.82	22.76	1.25	0.43	3.12	3.06
MAE[b]						2.22	1.75	2.79	3.03

[a] $|\Delta\delta|$(^{13}C) = $|\delta_{exp} - \delta_{calc}|$ (^{13}C), ppm: absolute differences for experimental versus calculated ^{13}C NMR chemical shifts

[b] **MAE** = $\Sigma[|(\delta_{exp} - \delta_{calcd})|]/n$, summation through n of the absolute error values (difference of the absolute values between corresponding experimental and ^{13}C chemical shifts), normalized to the number of the chemical shifts

Table S3. [13]C experimental related to exp_**1c** set of data and calculated NMR chemical shifts (MPW1PW91/6-31g(d,p) level of theory) related to calc_**1a**, calc_**1b**, calc_**1c**, calc_**1d** sets of data, with [a]|Δδ|(^{13}C) and [b]MAE values. Chemical shift data here reported were produced using benzene as reference compound for sp[2] carbons (highlighted in yellow), and tetramethylsilane (TMS) for sp[3] carbons.

Position	δ_{exp}(^{13}C), ppm	δ_{calc}(^{13}C), ppm				$|\Delta\delta|$ (^{13}C), ppm[a]			
	exp_1c	calc_1a	calc_1b	calc_1c	calc_1d	calc_1a	calc_1b	calc_1c	calc_1d
1	171.7	163.65	163.79	163.82	163.62	8.05	7.91	7.88	8.08
3	78.0	72.81	73.56	73.37	72.48	5.19	4.44	4.63	5.52
4	34.5	34.93	33.52	33.73	35.02	0.43	0.98	0.77	0.52
4a	143.6	143.10	143.24	143.31	143.05	0.50	0.36	0.29	0.55
5	108.1	105.75	105.80	105.76	105.75	2.35	2.30	2.34	2.35
6	165.8	160.89	160.91	160.89	160.92	4.91	4.89	4.91	4.88
7	102.3	101.15	101.10	101.10	101.15	1.15	1.20	1.20	1.15
8	166.4	165.73	165.74	165.75	165.76	0.67	0.66	0.65	0.64
8a	101.8	104.34	104.27	104.25	104.32	2.54	2.47	2.45	2.52
9	42.2	40.76	38.21	40.74	42.54	1.44	3.99	1.46	0.34
10	75.2	64.23	65.24	71.87	71.21	10.97	9.96	3.33	3.99
11	32.5	31.53	30.46	30.94	31.66	0.97	2.04	1.56	0.84
12	22.6	20.24	20.19	24.80	24.74	2.36	2.41	2.20	2.14
13	33.8	30.21	30.54	32.33	32.55	3.59	3.26	1.47	1.25
14	75.5	66.65	66.18	71.98	71.73	8.85	9.32	3.52	3.77
15	24.7	18.45	19.27	22.82	22.76	6.25	5.43	1.88	1.94
MAE[b]						3.76	3.85	2.53	2.53

[a] $|\Delta\delta|$(^{13}C) = $|\delta_{exp} - \delta_{calc}|$ (^{13}C), ppm: absolute differences for experimental versus calculated ^{13}C NMR chemical shifts
[b] MAE = $\Sigma[|(\delta_{exp} - \delta_{calcd})|]/n$, summation through n of the absolute error values (difference of the absolute values between corresponding experimental and ^{13}C chemical shifts), normalized to the number of the chemical shifts

Table S4. ^{13}C experimental related to exp_**1d** set of data and calculated NMR chemical shifts (MPW1PW91/6-31g(d,p) level of theory) related to calc_**1a**, calc_**1b**, calc_**1c**, calc_**1d** sets of data, with ^{a}|Δδ|(^{13}C) and ^{b}MAE values. Chemical shift data here reported were produced using benzene as reference compound for sp^2 carbons (highlighted in yellow), and tetramethylsilane (TMS) for sp^3 carbons.

Position	δ$_{exp}$(^{13}C), ppm	δ$_{calc}$(^{13}C), ppm				|Δδ| (^{13}C), ppm^a			
	exp_**1d**	calc_**1a**	calc_**1b**	calc_**1c**	calc_**1d**	calc_**1a**	calc_**1b**	calc_**1c**	calc_**1d**
1	171.7	163.65	163.79	163.82	163.62	8.05	7.91	7.88	8.08
3	77.6	72.81	73.56	73.37	72.48	4.79	4.04	4.23	5.12
4	34.6	34.93	33.52	33.73	35.02	0.33	1.08	0.87	0.42
4a	143.7	143.10	143.24	143.31	143.05	0.60	0.46	0.39	0.65
5	108.0	105.75	105.80	105.76	105.75	2.25	2.20	2.24	2.25
6	165.8	160.89	160.91	160.89	160.92	4.91	4.89	4.91	4.88
7	102.3	101.15	101.10	101.10	101.15	1.15	1.20	1.20	1.15
8	166.4	165.73	165.74	165.75	165.76	0.67	0.66	0.65	0.64
8a	101.7	104.34	104.27	104.25	104.32	2.64	2.57	2.55	2.62
9	43.0	40.76	38.21	40.74	42.54	2.24	4.79	2.26	0.46
10	74.8	64.23	65.24	71.87	71.21	10.57	9.56	2.93	3.59
11	33.1	31.53	30.46	30.94	31.66	1.57	2.64	2.16	1.44
12	22.5	20.24	20.19	24.80	24.74	2.26	2.31	2.30	2.24
13	34.5	30.21	30.54	32.33	32.55	4.29	3.96	2.17	1.95
14	75.3	66.65	66.18	71.98	71.73	8.65	9.12	3.32	3.57
15	24.8	18.45	19.27	22.82	22.76	6.35	5.53	1.98	2.04
MAE^b						3.83	3.93	2.63	2.57

^{a} **|Δδ|(^{13}C)** = |δ$_{exp}$ −δ$_{calc}$| (^{13}C), ppm: absolute differences for experimental versus calculated ^{13}C NMR chemical shifts
^{b} **MAE** = Σ[|(δ$_{exp}$ − δ$_{calcd}$)|]/n, summation through n of the absolute error values (difference of the absolute values between corresponding experimental and ^{13}C chemical shifts), normalized to the number of the chemical shifts

Table S5. [13]C experimental related to exp_**1a** set of data and calculated NMR chemical shifts (MPW1PW91/6-311+g(d,p) level of theory) related to calc_**1a**, calc_**1b**, calc_**1c**, calc_**1d** sets of data, with [a]|Δδ|(^{13}C) and [b]MAE values. Chemical shift data here reported were produced using benzene as reference compound for sp[2] carbons (highlighted in yellow), and tetramethylsilane (TMS) for sp[3] carbons.

Position	δ_{exp}(^{13}C), ppm	δ_{calc}(^{13}C), ppm				$|\Delta\delta|$ (^{13}C), ppm[a]			
	exp_1a	calc_1a	calc_1b	calc_1c	calc_1d	calc_1a	calc_1b	calc_1c	calc_1d
1	169.9	174.92	174.85	174.99	174.84	5.02	4.95	5.09	4.94
3	76.3	76.11	77.30	77.23	75.96	0.19	1.00	0.93	0.34
4	33.6	37.32	35.68	35.96	37.41	3.72	2.08	2.36	3.81
4a	141.8	143.90	144.02	144.05	143.74	2.10	2.22	2.25	1.94
5	106.7	104.22	103.73	103.70	104.59	2.48	2.97	3.00	2.11
6	163.1	163.20	163.66	163.57	163.48	0.10	0.56	0.47	0.38
7	102.0	98.44	98.67	98.64	98.83	3.56	3.33	3.36	3.17
8	164.3	167.21	167.47	167.47	167.13	2.91	3.17	3.17	2.83
8a	101.5	100.45	100.42	100.43	100.19	1.05	1.08	1.07	1.31
9	39.3	43.97	40.97	43.72	45.32	4.67	1.67	4.42	6.02
10	66.6	66.34	68.35	75.57	74.23	0.26	1.75	8.97	7.63
11	30.9	34.67	33.04	33.68	34.59	3.77	2.14	2.78	3.69
12	18.1	22.22	22.10	27.49	27.31	4.12	4.00	9.39	9.21
13	30.9	33.13	33.71	35.67	35.97	2.23	2.81	4.77	5.07
14	68.0	70.78	70.14	76.32	75.88	2.78	2.14	8.32	7.88
15	18.9	18.69	20.13	23.93	23.97	0.21	1.23	5.03	5.07
MAE[b]						2.45	2.32	4.09	4.09

[a] $|\Delta\delta|$(^{13}C) = $|\delta_{exp} - \delta_{calc}|$ (^{13}C), ppm: absolute differences for experimental versus calculated ^{13}C NMR chemical shifts

[b] **MAE** = $\Sigma[|(\delta_{exp} - \delta_{calcd})|]/n$, summation through n of the absolute error values (difference of the absolute values between corresponding experimental and ^{13}C chemical shifts), normalized to the number of the chemical shifts

Table S6. ^{13}C experimental related to exp_**1b** set of data and calculated NMR chemical shifts (MPW1PW91/6-311+g(d,p) level of theory) related to calc_**1a**, calc_**1b**, calc_**1c**, calc_**1d** sets of data, with [a]$|\Delta\delta|(^{13}C)$ and [b]MAE values. Chemical shift data here reported were produced using benzene as reference compound for sp^2 carbons (highlighted in yellow), and tetramethylsilane (TMS) for sp^3 carbons.

Position	$\delta_{exp}(^{13}C)$, ppm	$\delta_{calc}(^{13}C)$, ppm				$|\Delta\delta|\ (^{13}C)$, ppm[a]			
	exp_**1b**	calc_**1a**	calc_**1b**	calc_**1c**	calc_**1d**	calc_**1a**	calc_**1b**	calc_**1c**	calc_**1d**
1	170.0	174.92	174.85	174.99	174.84	4.92	4.85	4.99	4.84
3	76.6	76.11	77.30	77.23	75.96	0.49	0.70	0.63	0.64
4	32.6	37.32	35.68	35.96	37.41	4.72	3.08	3.36	4.81
4a	141.6	143.90	144.02	144.05	143.74	2.30	2.42	2.45	2.14
5	106.7	104.22	103.73	103.70	104.59	2.48	2.97	3.00	2.11
6	163.0	163.20	163.66	163.57	163.48	0.20	0.66	0.57	0.48
7	102.0	98.44	98.67	98.64	98.83	3.56	3.33	3.36	3.17
8	164.4	167.21	167.47	167.47	167.13	2.81	3.07	3.07	2.73
8a	101.6	100.45	100.42	100.43	100.19	1.15	1.18	1.17	1.41
9	37.3	43.97	40.97	43.72	45.32	6.67	3.67	6.42	8.02
10	67.2	66.34	68.35	75.57	74.23	0.86	1.15	8.37	7.03
11	29.8	34.67	33.04	33.68	34.59	4.87	3.24	3.88	4.79
12	18.1	22.22	22.10	27.49	27.31	4.12	4.00	9.39	9.21
13	31.5	33.13	33.71	35.67	35.97	1.63	2.21	4.17	4.47
14	67.4	70.78	70.14	76.32	75.88	3.38	2.74	8.92	8.48
15	19.7	18.69	20.13	23.93	23.97	1.01	0.43	4.23	4.27
MAE[b]						2.82	2.48	4.25	4.29

[a] $|\Delta\delta|(^{13}C) = |\delta_{exp} - \delta_{calc}|\ (^{13}C)$, ppm: absolute differences for experimental versus calculated ^{13}C NMR chemical shifts

[b] **MAE** = $\Sigma[|(\delta_{exp} - \delta_{calcd})|]/n$, summation through n of the absolute error values (difference of the absolute values between corresponding experimental and ^{13}C chemical shifts), normalized to the number of the chemical shifts

Table S7. [13]C experimental related to exp_**1c** set of data and calculated NMR chemical shifts (MPW1PW91/6-311+g(d,p) level of theory) related to calc_**1a**, calc_**1b**, calc_**1c**, calc_**1d** sets of data, with [a]$|\Delta\delta|$(^{13}C) and [b]MAE values. Chemical shift data here reported were produced using benzene as reference compound for sp[2] carbons (highlighted in yellow), and tetramethylsilane (TMS) for sp[3] carbons.

Position	δ_{exp}(^{13}C), ppm	δ_{calc}(^{13}C), ppm				$|\Delta\delta|$ (^{13}C), ppm[a]			
	exp_**1c**	calc_**1a**	calc_**1b**	calc_**1c**	calc_**1d**	calc_**1a**	calc_**1b**	calc_**1c**	calc_**1d**
1	171.7	174.92	174.85	174.99	174.84	3.22	3.15	3.29	3.14
3	78.0	76.11	77.30	77.23	75.96	1.89	0.70	0.77	2.04
4	34.5	37.32	35.68	35.96	37.41	2.82	1.18	1.46	2.91
4a	143.6	143.90	144.02	144.05	143.74	0.30	0.42	0.45	0.14
5	108.1	104.22	103.73	103.70	104.59	3.88	4.37	4.40	3.51
6	165.8	163.20	163.66	163.57	163.48	2.60	2.14	2.23	2.32
7	102.3	98.44	98.67	98.64	98.83	3.86	3.63	3.66	3.47
8	166.4	167.21	167.47	167.47	167.13	0.81	1.07	1.07	0.73
8a	101.8	100.45	100.42	100.43	100.19	1.35	1.38	1.37	1.61
9	42.2	43.97	40.97	43.72	45.32	1.77	1.23	1.52	3.12
10	75.2	66.34	68.35	75.57	74.23	8.86	6.85	0.37	0.97
11	32.5	34.67	33.04	33.68	34.59	2.17	0.54	1.18	2.09
12	22.6	22.22	22.10	27.49	27.31	0.38	0.50	4.89	4.71
13	33.8	33.13	33.71	35.67	35.97	0.67	0.09	1.87	2.17
14	75.5	70.78	70.14	76.32	75.88	4.72	5.36	0.82	0.38
15	24.7	18.69	20.13	23.93	23.97	6.01	4.57	0.77	0.73
MAE[b]						2.83	2.32	1.88	2.13

[a] $|\Delta\delta|$(^{13}C) = $|\delta_{exp} - \delta_{calc}|$ (^{13}C), ppm: absolute differences for experimental versus calculated ^{13}C NMR chemical shifts

[b] **MAE** = $\Sigma[|(\delta_{exp} - \delta_{calcd})|]/n$, summation through n of the absolute error values (difference of the absolute values between corresponding experimental and ^{13}C chemical shifts), normalized to the number of the chemical shifts

Table S8. [13]C experimental related to exp_1d set of data and calculated NMR chemical shifts (MPW1PW91/6-311+g(d,p) level of theory) related to calc_1a, calc_1b, calc_1c, calc_1d sets of data, with [a]|Δδ|(^{13}C) and [b]MAE values. Chemical shift data here reported were produced using benzene as reference compound for sp[2] carbons (highlighted in yellow), and tetramethylsilane (TMS) for sp[3] carbons.

	δ_{exp}(^{13}C), ppm	δ_{calc}(^{13}C), ppm				|Δδ| (^{13}C), ppm[a]			
Position	exp_1d	calc_1a	calc_1b	calc_1c	calc_1d	calc_1a	calc_1b	calc_1c	calc_1d
1	171.7	174.92	174.85	174.99	174.84	3.22	3.15	3.29	3.14
3	77.6	76.11	77.30	77.23	75.96	1.49	0.30	0.37	1.64
4	34.6	37.32	35.68	35.96	37.41	2.72	1.08	1.36	2.81
4a	143.7	143.90	144.02	144.05	143.74	0.20	0.32	0.35	0.04
5	108.0	104.22	103.73	103.70	104.59	3.78	4.27	4.30	3.41
6	165.8	163.20	163.66	163.57	163.48	2.60	2.14	2.23	2.32
7	102.3	98.44	98.67	98.64	98.83	3.86	3.63	3.66	3.47
8	166.4	167.21	167.47	167.47	167.13	0.81	1.07	1.07	0.73
8a	101.7	100.45	100.42	100.43	100.19	1.25	1.28	1.27	1.51
9	43.0	43.97	40.97	43.72	45.32	0.97	2.03	0.72	2.32
10	74.8	66.34	68.35	75.57	74.23	8.46	6.45	0.77	0.57
11	33.1	34.67	33.04	33.68	34.59	1.57	0.06	0.58	1.49
12	22.5	22.22	22.10	27.49	27.31	0.28	0.40	4.99	4.81
13	34.5	33.13	33.71	35.67	35.97	1.37	0.79	1.17	1.47
14	75.3	70.78	70.14	76.32	75.88	4.52	5.16	1.02	0.58
15	24.8	18.69	20.13	23.93	23.97	6.11	4.67	0.87	0.83
MAE[b]						2.70	2.30	1.75	1.95

[a] |Δδ|(^{13}C) = |δ_{exp} − δ_{calc}| (^{13}C), ppm: absolute differences for experimental versus calculated ^{13}C NMR chemical shifts

[b] **MAE** = Σ[|(δ_{exp} − δ_{calcd})|]/n, summation through n of the absolute error values (difference of the absolute values between corresponding experimental and ^{13}C chemical shifts), normalized to the number of the chemical shifts

Table S9. ^{13}C experimental related to exp_**1a** set of data and calculated NMR chemical shifts (B97-2/cc-pVTZ level of theory) related to calc_**1a**, calc_**1b**, calc_**1c**, calc_**1d** sets of data, with ^{a}|Δδ|(^{13}C) and ^{b}MAE values. Chemical shift data here reported were produced using benzene as reference compound for sp^2 carbons (highlighted in yellow), and tetramethylsilane (TMS) for sp^3 carbons.

Position	δ_exp(^{13}C), ppm	δ_calc(^{13}C), ppm				|Δδ| (^{13}C), ppm^a			
	exp_1a	calc_1a	calc_1b	calc_1c	calc_1d	calc_1a	calc_1b	calc_1c	calc_1d
1	169.9	163.65	163.79	163.82	163.62	6.25	6.11	6.08	6.29
3	76.3	72.81	73.56	73.37	72.48	3.49	2.74	2.93	3.82
4	33.6	34.93	33.52	33.73	35.02	1.33	0.08	0.13	1.42
4a	141.8	145.27	145.07	145.11	145.30	3.47	3.27	3.31	3.50
5	106.7	104.00	104.01	104.00	104.01	2.70	2.69	2.70	2.69
6	163.1	164.20	164.19	164.17	164.08	1.10	1.09	1.07	0.98
7	102.0	98.85	98.84	98.80	98.83	3.15	3.16	3.20	3.17
8	164.3	168.76	168.71	168.70	168.71	4.46	4.41	4.40	4.41
8a	101.5	101.38	101.20	101.15	101.45	0.12	0.30	0.35	0.05
9	39.3	40.76	38.21	40.74	42.54	1.46	1.09	1.44	3.24
10	66.6	64.23	65.24	71.87	71.21	2.37	1.36	5.27	4.61
11	30.9	31.53	30.46	30.94	31.66	0.63	0.44	0.04	0.76
12	18.1	20.24	20.19	24.80	24.74	2.14	2.09	6.70	6.64
13	30.9	30.21	30.54	32.33	32.55	0.69	0.36	1.43	1.65
14	68.0	66.65	66.18	71.98	71.73	1.35	1.82	3.98	3.73
15	18.9	18.45	19.27	22.82	22.76	0.45	0.37	3.92	3.86
MAE^b						2.20	1.96	2.93	3.18

^{a} |**Δδ**|(**^{13}C**) = |δ_exp −δ_calc| (^{13}C), ppm: absolute differences for experimental versus calculated ^{13}C NMR chemical shifts
^{b} **MAE** = Σ[|(δ_exp − δ_calcd)|]/n, summation through n of the absolute error values (difference of the absolute values between corresponding experimental and ^{13}C chemical shifts), normalized to the number of the chemical shifts

Table S10. [13]C experimental related to exp_**1b** set of data and calculated NMR chemical shifts (B97-2/cc-pVTZ level of theory) related to calc_**1a**, calc_**1b**, calc_**1c**, calc_**1d** sets of data, with [a]$|\Delta\delta|$(^{13}C) and [b]MAE values. Chemical shift data here reported were produced using benzene as reference compound for sp^2 carbons (highlighted in yellow), and tetramethylsilane (TMS) for sp^3 carbons.

	δ_{exp}(^{13}C), ppm	δ_{calc}(^{13}C), ppm				$|\Delta\delta|$ (^{13}C), ppm[a]			
Position	exp_**1b**	calc_**1a**	calc_**1b**	calc_**1c**	calc_**1d**	calc_**1a**	calc_**1b**	calc_**1c**	calc_**1d**
1	170.0	163.65	163.79	163.82	163.62	6.35	6.21	6.18	6.38
3	76.6	72.81	73.56	73.37	72.48	3.79	3.04	3.23	4.12
4	32.6	34.93	33.52	33.73	35.02	2.33	0.92	1.13	2.42
4a	141.6	145.27	145.07	145.11	145.30	3.67	3.47	3.51	3.70
5	106.7	104.00	104.01	104.00	104.01	2.70	2.69	2.70	2.69
6	163.0	164.20	164.19	164.17	164.08	1.20	1.19	1.17	1.08
7	102.0	98.85	98.84	98.80	98.83	3.15	3.16	3.20	3.17
8	164.4	168.76	168.71	168.70	168.71	4.36	4.31	4.30	4.31
8a	101.6	101.38	101.20	101.15	101.45	0.22	0.40	0.45	0.15
9	37.3	40.76	38.21	40.74	42.54	3.46	0.91	3.44	5.24
10	67.2	64.23	65.24	71.87	71.21	2.97	1.96	4.67	4.01
11	29.8	31.53	30.46	30.94	31.66	1.73	0.66	1.14	1.86
12	18.1	20.24	20.19	24.80	24.74	2.14	2.09	6.70	6.64
13	31.5	30.21	30.54	32.33	32.55	1.29	0.96	0.83	1.05
14	67.4	66.65	66.18	71.98	71.73	0.75	1.22	4.58	4.33
15	19.7	18.45	19.27	22.82	22.76	1.25	0.43	3.12	3.06
MAE[b]						2.58	2.10	3.15	3.39

[a] $|\Delta\delta|$([13]**C**) = $|\delta_{exp} - \delta_{calc}|$ (^{13}C), ppm: absolute differences for experimental versus calculated ^{13}C NMR chemical shifts

[b] **MAE** = $\Sigma[|(\delta_{exp} - \delta_{calcd})|]/n$, summation through n of the absolute error values (difference of the absolute values between corresponding experimental and ^{13}C chemical shifts), normalized to the number of the chemical shifts

Table S11. [13]C experimental related to exp_**1c** set of data and calculated NMR chemical shifts (B97-2/cc-pVTZ level of theory) related to calc_**1a**, calc_**1b**, calc_**1c**, calc_**1d** sets of data, with [a]|Δδ|(^{13}C) and [b]MAE values. Chemical shift data here reported were produced using benzene as reference compound for sp^2 carbons (highlighted in yellow), and tetramethylsilane (TMS) for sp^3 carbons.

Position	δ_{exp}(^{13}C), ppm	δ_{calc}(^{13}C), ppm				|Δδ| (^{13}C), ppm[a]			
	exp_1c	calc_1a	calc_1b	calc_1c	calc_1d	calc_1a	calc_1b	calc_1c	calc_1d
1	171.7	163.65	163.79	163.82	163.62	8.05	7.91	7.88	8.08
3	78.0	72.81	73.56	73.37	72.48	5.19	4.44	4.63	5.52
4	34.5	34.93	33.52	33.73	35.02	0.43	0.98	0.77	0.52
4a	143.6	145.27	145.07	145.11	145.30	1.67	1.47	1.51	1.70
5	108.1	104.00	104.01	104.00	104.01	4.10	4.09	4.10	4.09
6	165.8	164.20	164.19	164.17	164.08	1.60	1.61	1.63	1.72
7	102.3	98.85	98.84	98.80	98.83	3.45	3.46	3.50	3.47
8	166.4	168.76	168.71	168.70	168.71	2.36	2.31	2.30	2.31
8a	101.8	101.38	101.20	101.15	101.45	0.42	0.60	0.65	0.35
9	42.2	40.76	38.21	40.74	42.54	1.44	3.99	1.46	0.34
10	75.2	64.23	65.24	71.87	71.21	10.97	9.96	3.33	3.99
11	32.5	31.53	30.46	30.94	31.66	0.97	2.04	1.56	0.84
12	22.6	20.24	20.19	24.80	24.74	2.36	2.41	2.20	2.14
13	33.8	30.21	30.54	32.33	32.55	3.59	3.26	1.47	1.25
14	75.5	66.65	66.18	71.98	71.73	8.85	9.32	3.52	3.77
15	24.7	18.45	19.27	22.82	22.76	6.25	5.43	1.88	1.94
MAE[b]						3.86	3.96	2.65	2.63

[a] **|Δδ|(^{13}C)** = |δ_{exp} −δ_{calc}| (^{13}C), ppm: absolute differences for experimental versus calculated ^{13}C NMR chemical shifts

[b] **MAE** = Σ[|(δ_{exp} − δ_{calcd})|]/n, summation through n of the absolute error values (difference of the absolute values between corresponding experimental and ^{13}C chemical shifts), normalized to the number of the chemical shifts

Table S12. [13]C experimental related to exp_**1d** set of data and calculated NMR chemical shifts (B97-2/cc-pVTZ level of theory) related to calc_**1a**, calc_**1b**, calc_**1c**, calc_**1d** sets of data, with [a]$|\Delta\delta|$(^{13}C) and [b]MAE values. Chemical shift data here reported were produced using benzene as reference compound for sp[2] carbons (highlighted in yellow), and tetramethylsilane (TMS) for sp[3] carbons.

Position	δ_{exp}(^{13}C), ppm	δ_{calc}(^{13}C), ppm				$|\Delta\delta|$ (^{13}C), ppm[a]			
	exp_**1d**	calc_**1a**	calc_**1b**	calc_**1c**	calc_**1d**	calc_**1a**	calc_**1b**	calc_**1c**	calc_**1d**
1	171.7	163.65	163.79	163.82	163.62	8.05	7.91	7.88	8.08
3	77.6	72.81	73.56	73.37	72.48	4.79	4.04	4.23	5.12
4	34.6	34.93	33.52	33.73	35.02	0.33	1.08	0.87	0.42
4a	143.7	145.27	145.07	145.11	145.30	1.57	1.37	1.41	1.60
5	108.0	104.00	104.01	104.00	104.01	4.00	3.99	4.00	3.99
6	165.8	164.20	164.19	164.17	164.08	1.60	1.61	1.63	1.72
7	102.3	98.85	98.84	98.80	98.83	3.45	3.46	3.50	3.47
8	166.4	168.76	168.71	168.70	168.71	2.36	2.31	2.30	2.31
8a	101.7	101.38	101.20	101.15	101.45	0.32	0.50	0.55	0.25
9	43.0	40.76	38.21	40.74	42.54	2.24	4.79	2.26	0.46
10	74.8	64.23	65.24	71.87	71.21	10.57	9.56	2.93	3.59
11	33.1	31.53	30.46	30.94	31.66	1.57	2.64	2.16	1.44
12	22.5	20.24	20.19	24.80	24.74	2.26	2.31	2.30	2.24
13	34.5	30.21	30.54	32.33	32.55	4.29	3.96	2.17	1.95
14	75.3	66.65	66.18	71.98	71.73	8.65	9.12	3.32	3.57
15	24.8	18.45	19.27	22.82	22.76	6.35	5.53	1.98	2.04
MAE[b]						3.90	4.01	2.72	2.64

[a] $|\Delta\delta|$(^{13}C) = $|\delta_{exp} - \delta_{calc}|$ (^{13}C), ppm: absolute differences for experimental versus calculated ^{13}C NMR chemical shifts
[b] **MAE** = $\Sigma[|(\delta_{exp} - \delta_{calcd})|]/n$, summation through n of the absolute error values (difference of the absolute values between corresponding experimental and ^{13}C chemical shifts), normalized to the number of the chemical shifts

Table S13. Comparison of the results obtained by computing the $MAE_{\Delta\Delta\delta}$ values (bottom) and the AVER_MAE values (top), the latter defined as the average of the four possible MAE values obtained from the comparison of the calculated and experimental chemical shifts, for each of the 24 comparison alignments. The comparison of the predicting power between the two approaches has been evaluated considering the "% error from the best value" parameter, defined as (e.g. for the AVER_MAE data): $((AVER\_MAE/AVER\_MAE_{best\ value})-1)\times100)$.

MPW1PW91/6-31g(d,p)			MPW1PW91/6-311+g(d,p)			B97-2/cc-pVTZ		
comparison alignment[a]	AVER_MAE	% error from best AVER_MAE value	comparison alignment[a]	AVER_MAE	% error from best AVER_MAE value	comparison alignment[a]	AVER_MAE	% error from best AVER_MAE value
exp_**1a** exp_**1b** exp_**1c** exp_**1d**	2.177	0.000	exp_**1a** exp_**1b** exp_**1c** exp_**1d**	2.190	0.000	exp_**1a** exp_**1b** exp_**1c** exp_**1d**	2.397	0.000
exp_**1a** exp_**1b** exp_**1d** exp_**1c**	2.191	0.643	exp_**1a** exp_**1b** exp_**1d** exp_**1c**	2.202	0.548	exp_**1a** exp_**1b** exp_**1d** exp_**1c**	2.411	0.584
exp_**1b** exp_**1a** exp_**1c** exp_**1d**	2.239	2.848	exp_**1b** exp_**1a** exp_**1c** exp_**1d**	2.243	2.420	exp_**1b** exp_**1a** exp_**1c** exp_**1d**	2.459	2.587
exp_**1b** exp_**1a** exp_**1d** exp_**1c**	2.253	3.491	exp_**1b** exp_**1a** exp_**1d** exp_**1c**	2.255	2.968	exp_**1b** exp_**1a** exp_**1d** exp_**1c**	2.473	3.171
exp_**1c** exp_**1b** exp_**1a** exp_**1d**	2.671	22.692	exp_**1a** exp_**1c** exp_**1d** exp_**1b**	2.703	23.425	exp_**1c** exp_**1b** exp_**1a** exp_**1d**	2.883	20.275
exp_**1d** exp_**1b** exp_**1a** exp_**1c**	2.678	23.013	exp_**1a** exp_**1d** exp_**1c** exp_**1b**	2.730	24.658	exp_**1d** exp_**1b** exp_**1a** exp_**1c**	2.891	20.609
exp_**1c** exp_**1a** exp_**1b** exp_**1d**	2.689	23.519	exp_**1a** exp_**1c** exp_**1b** exp_**1d**	2.742	25.205	exp_**1c** exp_**1a** exp_**1b** exp_**1d**	2.901	21.026
exp_**1d** exp_**1a** exp_**1b** exp_**1c**	2.697	23.886	exp_**1b** exp_**1c** exp_**1d** exp_**1a**	2.746	25.388	exp_**1d** exp_**1a** exp_**1b** exp_**1c**	2.909	21.360
exp_**1d** exp_**1b** exp_**1c** exp_**1a**	2.739	25.815	exp_**1b** exp_**1d** exp_**1c** exp_**1a**	2.773	26.621	exp_**1d** exp_**1b** exp_**1c** exp_**1a**	2.957	23.363
exp_**1c** exp_**1b** exp_**1d** exp_**1a**	2.746	26.137	exp_**1a** exp_**1d** exp_**1b** exp_**1c**	2.781	26.986	exp_**1c** exp_**1b** exp_**1d** exp_**1a**	2.963	23.613
exp_**1d** exp_**1a** exp_**1c** exp_**1b**	2.758	26.688	exp_**1c** exp_**1b** exp_**1d** exp_**1a**	2.788	27.306	exp_**1d** exp_**1a** exp_**1c** exp_**1b**	2.975	24.113
exp_**1c** exp_**1a** exp_**1d** exp_**1b**	2.764	26.964	exp_**1d** exp_**1b** exp_**1c** exp_**1a**	2.788	27.306	exp_**1c** exp_**1a** exp_**1d** exp_**1b**	2.981	24.364
exp_**1a** exp_**1c** exp_**1b** exp_**1d**	2.768	27.147	exp_**1b** exp_**1c** exp_**1a** exp_**1d**	2.795	27.626	exp_**1a** exp_**1c** exp_**1b** exp_**1d**	2.985	24.531
exp_**1a** exp_**1d** exp_**1b** exp_**1c**	2.778	27.607	exp_**1c** exp_**1a** exp_**1d** exp_**1b**	2.797	27.717	exp_**1a** exp_**1d** exp_**1b** exp_**1c**	2.996	24.990
exp_**1b** exp_**1c** exp_**1a** exp_**1d**	2.812	29.169	exp_**1d** exp_**1a** exp_**1c** exp_**1b**	2.797	27.717	exp_**1b** exp_**1c** exp_**1a** exp_**1d**	3.029	26.366
exp_**1b** exp_**1d** exp_**1a** exp_**1c**	2.822	29.628	exp_**1b** exp_**1d** exp_**1a** exp_**1c**	2.834	29.406	exp_**1b** exp_**1d** exp_**1a** exp_**1c**	3.039	26.783
exp_**1a** exp_**1d** exp_**1c** exp_**1b**	2.839	30.409	exp_**1c** exp_**1a** exp_**1b** exp_**1d**	2.836	29.498	exp_**1a** exp_**1d** exp_**1c** exp_**1b**	3.062	27.743
exp_**1a** exp_**1c** exp_**1d** exp_**1b**	2.843	30.593	exp_**1c** exp_**1b** exp_**1a** exp_**1d**	2.836	29.498	exp_**1a** exp_**1c** exp_**1d** exp_**1b**	3.065	27.868
exp_**1b** exp_**1d** exp_**1c** exp_**1a**	2.883	32.430	exp_**1d** exp_**1a** exp_**1b** exp_**1c**	2.849	30.091	exp_**1b** exp_**1d** exp_**1c** exp_**1a**	3.105	29.537
exp_**1b** exp_**1c** exp_**1d** exp_**1a**	2.886	32.568	exp_**1d** exp_**1b** exp_**1a** exp_**1c**	2.849	30.091	exp_**1b** exp_**1c** exp_**1d** exp_**1a**	3.108	29.662
exp_**1d** exp_**1c** exp_**1a** exp_**1b**	3.330	52.963	exp_**1d** exp_**1c** exp_**1b** exp_**1a**	3.340	52.511	exp_**1d** exp_**1c** exp_**1a** exp_**1b**	3.544	47.851
exp_**1d** exp_**1c** exp_**1b** exp_**1a**	3.330	52.963	exp_**1d** exp_**1c** exp_**1a** exp_**1b**	3.350	52.968	exp_**1d** exp_**1c** exp_**1b** exp_**1a**	3.544	47.851
exp_**1c** exp_**1d** exp_**1a** exp_**1b**	3.333	53.101	exp_**1c** exp_**1d** exp_**1b** exp_**1a**	3.367	53.744	exp_**1c** exp_**1d** exp_**1a** exp_**1b**	3.548	48.018
exp_**1c** exp_**1d** exp_**1b** exp_**1a**	3.333	53.101	exp_**1c** exp_**1d** exp_**1a** exp_**1b**	3.376	54.155	exp_**1c** exp_**1d** exp_**1b** exp_**1a**	3.548	48.018

S18

MPW1PW91/6-31g(d,p)			MPW1PW91/6-311+g(d,p)			B97-2/cc-pVTZ		
comparison alignment[a]	$MAE_{\Delta\Delta\delta}$	% error from best $MAE_{\Delta\Delta\delta}$ value	comparison alignment[a]	$MAE_{\Delta\Delta\delta}$	% error from best $MAE_{\Delta\Delta\delta}$ value	comparison alignment[a]	$MAE_{\Delta\Delta\delta}$	% error from best $MAE_{\Delta\Delta\delta}$ value
exp_**1a** exp_**1b** exp_**1c** exp_**1d**	1.066	0.000	exp_**1a** exp_**1b** exp_**1c** exp_**1d**	1.089	0.000	exp_**1a** exp_**1b** exp_**1c** exp_**1d**	1.070	0.000
exp_**1a** exp_**1b** exp_**1d** exp_**1c**	1.120	5.066	exp_**1a** exp_**1b** exp_**1d** exp_**1c**	1.157	6.244	exp_**1a** exp_**1b** exp_**1d** exp_**1c**	1.124	5.047
exp_**1b** exp_**1a** exp_**1c** exp_**1d**	1.224	14.822	exp_**1b** exp_**1a** exp_**1c** exp_**1d**	1.291	18.549	exp_**1b** exp_**1a** exp_**1c** exp_**1d**	1.232	15.140
exp_**1b** exp_**1a** exp_**1d** exp_**1c**	1.298	21.764	exp_**1b** exp_**1a** exp_**1d** exp_**1c**	1.380	26.722	exp_**1b** exp_**1a** exp_**1d** exp_**1c**	1.308	22.243
exp_**1c** exp_**1b** exp_**1a** exp_**1d**	2.487	133.302	exp_**1c** exp_**1b** exp_**1a** exp_**1d**	2.617	140.312	exp_**1c** exp_**1b** exp_**1a** exp_**1d**	2.471	130.935
exp_**1d** exp_**1b** exp_**1a** exp_**1c**	2.515	135.929	exp_**1d** exp_**1b** exp_**1a** exp_**1c**	2.635	141.965	exp_**1d** exp_**1b** exp_**1a** exp_**1c**	2.496	133.271
exp_**1c** exp_**1a** exp_**1b** exp_**1d**	2.541	138.368	exp_**1c** exp_**1a** exp_**1b** exp_**1d**	2.674	145.546	exp_**1c** exp_**1a** exp_**1b** exp_**1d**	2.525	135.981
exp_**1d** exp_**1b** exp_**1c** exp_**1a**	2.581	142.120	exp_**1d** exp_**1b** exp_**1c** exp_**1a**	2.702	148.118	exp_**1d** exp_**1a** exp_**1b** exp_**1c**	2.568	140.000
exp_**1d** exp_**1a** exp_**1b** exp_**1c**	2.585	142.495	exp_**1a** exp_**1c** exp_**1b** exp_**1d**	2.706	148.485	exp_**1d** exp_**1b** exp_**1c** exp_**1a**	2.582	141.308
exp_**1c** exp_**1b** exp_**1d** exp_**1a**	2.601	143.996	exp_**1d** exp_**1a** exp_**1b** exp_**1c**	2.706	148.485	exp_**1c** exp_**1b** exp_**1d** exp_**1a**	2.603	143.271
exp_**1a** exp_**1c** exp_**1b** exp_**1d**	2.609	144.747	exp_**1c** exp_**1b** exp_**1d** exp_**1a**	2.725	150.230	exp_**1a** exp_**1c** exp_**1b** exp_**1d**	2.613	144.206
exp_**1a** exp_**1d** exp_**1b** exp_**1c**	2.647	148.311	exp_**1a** exp_**1d** exp_**1b** exp_**1c**	2.743	151.882	exp_**1a** exp_**1d** exp_**1b** exp_**1c**	2.650	147.664
exp_**1d** exp_**1a** exp_**1c** exp_**1b**	2.649	148.499	exp_**1a** exp_**1c** exp_**1d** exp_**1b**	2.746	152.158	exp_**1d** exp_**1a** exp_**1c** exp_**1b**	2.653	147.944
exp_**1b** exp_**1c** exp_**1d** exp_**1a**	2.656	149.156	exp_**1b** exp_**1c** exp_**1d** exp_**1a**	2.749	152.433	exp_**1c** exp_**1a** exp_**1d** exp_**1b**	2.678	150.280
exp_**1c** exp_**1a** exp_**1d** exp_**1b**	2.671	150.563	exp_**1a** exp_**1d** exp_**1c** exp_**1b**	2.773	154.637	exp_**1b** exp_**1c** exp_**1d** exp_**1a**	2.681	150.561
exp_**1a** exp_**1c** exp_**1d** exp_**1b**	2.674	150.844	exp_**1d** exp_**1a** exp_**1c** exp_**1b**	2.778	155.096	exp_**1b** exp_**1c** exp_**1a** exp_**1d**	2.688	151.215
exp_**1b** exp_**1c** exp_**1a** exp_**1d**	2.681	151.501	exp_**1b** exp_**1d** exp_**1c** exp_**1a**	2.784	155.647	exp_**1a** exp_**1c** exp_**1d** exp_**1b**	2.698	152.150
exp_**1b** exp_**1d** exp_**1c** exp_**1a**	2.691	152.439	exp_**1b** exp_**1c** exp_**1a** exp_**1d**	2.805	157.576	exp_**1b** exp_**1d** exp_**1c** exp_**1a**	2.715	153.738
exp_**1a** exp_**1d** exp_**1c** exp_**1b**	2.711	154.315	exp_**1c** exp_**1a** exp_**1d** exp_**1b**	2.812	158.219	exp_**1b** exp_**1d** exp_**1a** exp_**1c**	2.729	155.047
exp_**1b** exp_**1d** exp_**1a** exp_**1c**	2.721	155.253	exp_**1b** exp_**1d** exp_**1a** exp_**1c**	2.856	162.259	exp_**1a** exp_**1d** exp_**1c** exp_**1b**	2.734	155.514
exp_**1d** exp_**1c** exp_**1b** exp_**1a**	3.205	200.657	exp_**1d** exp_**1c** exp_**1b** exp_**1a**	3.410	213.131	exp_**1d** exp_**1c** exp_**1b** exp_**1a**	3.203	199.346
exp_**1c** exp_**1d** exp_**1b** exp_**1a**	3.236	203.565	exp_**1c** exp_**1d** exp_**1b** exp_**1a**	3.433	215.243	exp_**1c** exp_**1d** exp_**1b** exp_**1a**	3.235	202.336
exp_**1d** exp_**1c** exp_**1a** exp_**1b**	3.289	208.537	exp_**1d** exp_**1c** exp_**1a** exp_**1b**	3.496	221.028	exp_**1d** exp_**1c** exp_**1a** exp_**1b**	3.290	207.477
exp_**1c** exp_**1d** exp_**1a** exp_**1b**	3.324	211.820	exp_**1c** exp_**1d** exp_**1a** exp_**1b**	3.528	223.967	exp_**1c** exp_**1d** exp_**1a** exp_**1b**	3.328	211.028

[a]considering calc_**1a** calc_**1b** calc_**1c** and calc_**1d** starting fixed sequence related to the calculated sets of data

Table S14. [13]C experimental related to exp_**2a** set of data and calculated NMR chemical shifts (MPW1PW91/6-31g(d,p) level of theory) related to calc_**2a**, calc_**2b**, calc_**2c**, calc_**2d** sets of data, with [a]$|\Delta\delta|$(^{13}C) and [b]MAE values.

Position	δ_{exp}(^{13}C), ppm	δ_{calc}(^{13}C), ppm				$|\Delta\delta|$ (^{13}C), ppm[a]			
	exp_**2a**	calc_**2a**	calc_**2b**	calc_**2c**	calc_**2d**	calc_**2a**	calc_**2b**	calc_**2c**	calc_**2d**
1	69.2	73.07	70.28	71.09	75.87	3.87	1.08	1.89	6.67
2	40	33.70	41.02	43.23	41.97	6.30	1.02	3.23	1.97
3	62.8	62.50	65.76	58.40	61.16	0.30	2.96	4.40	1.64
5	60.9	63.02	71.07	62.53	67.53	2.12	10.17	1.63	6.63
6	78.4	74.87	76.99	81.77	72.30	3.53	1.41	3.37	6.10
7	71.8	68.76	71.10	70.07	71.28	3.04	0.70	1.73	0.52
7a	75.6	74.03	75.46	68.45	66.39	1.57	0.14	7.15	9.21
8	62.4	60.06	64.71	62.69	65.55	2.34	2.31	0.29	3.15
9	42.8	44.23	45.18	46.38	39.33	1.43	2.38	3.58	3.47
11	173.9	163.51	164.23	165.97	164.45	10.39	9.67	7.93	9.45
12	22.6	23.07	23.00	23.35	22.78	0.47	0.40	0.75	0.18
MAE[b]						3.21	2.93	3.27	4.45

[a] $|\Delta\delta|$(^{13}C) = $|\delta_{exp} - \delta_{calc}|$ (^{13}C), ppm: absolute differences for experimental versus calculated ^{13}C NMR chemical shifts
[b] **MAE** = $\Sigma[|(\delta_{exp} - \delta_{calcd})|]/n$, summation through n of the absolute error values (difference of the absolute values between corresponding experimental and ^{13}C chemical shifts), normalized to the number of the chemical shifts

Table S15. ^{13}C experimental related to exp_**2b** set of data and calculated NMR chemical shifts (MPW1PW91/6-31g(d,p) level of theory) related to calc_**2a**, calc_**2b**, calc_**2c**, calc_**2d** sets of data, with [a]$|\Delta\delta|(^{13}$C) and [b]MAE values.

Position	$\delta_{exp}(^{13}$C), ppm	$\delta_{calc}(^{13}$C), ppm				$|\Delta\delta|$ (^{13}C), ppm[a]			
	exp_**2b**	calc_**2a**	calc_**2b**	calc_**1c**	calc_**2d**	calc_**2a**	calc_**2b**	calc_**2c**	calc_**2d**
1	70.7	73.07	70.28	71.09	75.87	2.37	0.42	0.39	5.17
2	39	33.70	41.02	43.23	41.97	5.30	2.02	4.23	2.97
3	69.7	62.50	65.76	58.40	61.16	7.20	3.94	11.30	8.54
5	71.4	63.02	71.07	62.53	67.53	8.38	0.33	8.87	3.87
6	76.9	74.87	76.99	81.77	72.30	2.03	0.09	4.87	4.60
7	72.4	68.76	71.10	70.07	71.28	3.64	1.30	2.33	1.12
7a	76.5	74.03	75.46	68.45	66.39	2.47	1.04	8.05	10.11
8	65.9	60.06	64.71	62.69	65.55	5.84	1.19	3.21	0.35
9	42.3	44.23	45.18	46.38	39.33	1.93	2.88	4.08	2.97
11	173.9	163.51	164.23	165.97	164.45	10.39	9.67	7.93	9.45
12	22.6	23.07	23.00	23.35	22.78	0.47	0.40	0.75	0.18
MAE[b]						4.55	2.12	5.09	4.48

[a] $|\Delta\delta|(^{13}$C) = $|\delta_{exp} - \delta_{calc}|$ (^{13}C), ppm: absolute differences for experimental versus calculated ^{13}C NMR chemical shifts
[b] MAE = $\Sigma[|(\delta_{exp} - \delta_{calcd})|]/n$, summation through n of the absolute error values (difference of the absolute values between corresponding experimental and ^{13}C chemical shifts), normalized to the number of the chemical shifts

Table S16. ^{13}C experimental related to exp_**2c** set of data and calculated NMR chemical shifts (MPW1PW91/6-31g(d,p) level of theory) related to calc_**2a**, calc_**2b**, calc_**2c**, calc_**2d** sets of data, with $^a|\Delta\delta|(^{13}C)$ and ^{b}MAE values.

Position	$\delta_{exp}(^{13}C)$, ppm	$\delta_{calc}(^{13}C)$, ppm				$|\Delta\delta|$ (^{13}C), ppm^a			
	exp_2c	calc_2a	calc_2b	calc_2c	calc_2d	calc_2a	calc_2b	calc_2c	calc_2d
1	73.7	73.07	70.28	71.09	75.87	0.63	3.42	2.61	2.17
2	43.6	33.70	41.02	43.23	41.97	9.90	2.58	0.37	1.63
3	61.6	62.50	65.76	58.40	61.16	0.90	4.16	3.20	0.44
5	62.5	63.02	71.07	62.53	67.53	0.52	8.57	0.03	5.03
6	78.7	74.87	76.99	81.77	72.30	3.83	1.71	3.07	6.40
7	68.9	68.76	71.10	70.07	71.28	0.14	2.20	1.17	2.38
7a	73.9	74.03	75.46	68.45	66.39	0.13	1.56	5.45	7.51
8	63.3	60.06	64.71	62.69	65.55	3.24	1.41	0.61	2.25
9	40.8	44.23	45.18	46.38	39.33	3.43	4.38	5.58	1.47
11	173.7	163.51	164.23	165.97	164.45	10.19	9.47	7.73	9.25
12	22.6	23.07	23.00	23.35	22.78	0.47	0.40	0.75	0.18
MAE^b						3.03	3.62	2.78	3.52

^{a} $|\Delta\delta|(^{13}C) = |\delta_{exp} - \delta_{calc}|$ (^{13}C), ppm: absolute differences for experimental versus calculated ^{13}C NMR chemical shifts
^{b} $MAE = \Sigma[|(\delta_{exp} - \delta_{calcd})|]/n$, summation through n of the absolute error values (difference of the absolute values between corresponding experimental and ^{13}C chemical shifts), normalized to the number of the chemical shifts

Table S17. [13]C experimental related to exp_**2d** set of data and calculated NMR chemical shifts (MPW1PW91/6-31g(d,p) level of theory) related to calc_**2a**, calc_**2b**, calc_**2c**, calc_**2d** sets of data, with [a]|Δδ|(^{13}C) and [b]MAE values..

	δ_{exp}(^{13}C), ppm	δ_{calc}(^{13}C), ppm				|Δδ| (^{13}C), ppm[a]			
Position	exp_**2d**	calc_**2a**	calc_**2b**	calc_**2c**	calc_**2d**	calc_**2a**	calc_**2b**	calc_**2c**	calc_**2d**
1	76.6	73.07	70.28	71.09	75.87	3.53	6.32	5.51	0.73
2	39.8	33.70	41.02	43.23	41.97	6.10	1.22	3.43	2.17
3	66.2	62.50	65.76	58.40	61.16	3.70	0.44	7.80	5.04
5	71.5	63.02	71.07	62.53	67.53	8.48	0.43	8.97	3.97
6	74.1	74.87	76.99	81.77	72.30	0.77	2.89	7.67	1.80
7	73.9	68.76	71.10	70.07	71.28	5.14	2.80	3.83	2.62
7a	70.8	74.03	75.46	68.45	66.39	3.23	4.66	2.35	4.41
8	68.7	60.06	64.71	62.69	65.55	8.64	3.99	6.01	3.15
9	42.8	44.23	45.18	46.38	39.33	1.43	2.38	3.58	3.47
11	173.7	163.51	164.23	165.97	164.45	10.19	9.47	7.73	9.25
12	22.6	23.07	23.00	23.35	22.78	0.47	0.40	0.75	0.18
MAE[b]						4.70	3.18	5.24	3.34

[a] **|Δδ|(^{13}C)** = |δ_{exp} −δ_{calc}| (^{13}C), ppm: absolute differences for experimental versus calculated ^{13}C NMR chemical shifts
[b] **MAE** = $\Sigma[|(\delta_{exp} - \delta_{calcd})|]/n$, summation through n of the absolute error values (difference of the absolute values between corresponding experimental and ^{13}C chemical shifts), normalized to the number of the chemical shifts

Table S18. ^{13}C experimental related to exp_**2a** set of data and calculated NMR chemical shifts (MPW1PW91/6-311+g(d,p) level of theory) related to calc_**2a**, calc_**2b**, calc_**2c**, calc_**2d** sets of data, with $^a|\Delta\delta|(^{13}$C) and ^{b}MAE values.

Position	$\delta_{exp}(^{13}$C), ppm	$\delta_{calc}(^{13}$C), ppm				$|\Delta\delta|$ $(^{13}$C), ppm^a			
	exp_2a	calc_2a	calc_2b	calc_2c	calc_2d	calc_2a	calc_2b	calc_2c	calc_2d
1	69.2	76.05	72.57	75.11	79.20	6.85	3.37	5.91	10.00
2	40	35.23	42.70	45.60	42.85	4.77	2.70	5.60	2.85
3	62.8	65.72	65.60	62.44	65.47	2.92	2.80	0.36	2.67
5	60.9	66.48	71.60	66.56	71.66	5.58	10.70	5.66	10.76
6	78.4	78.14	78.24	86.17	76.19	0.26	0.16	7.77	2.21
7	71.8	71.51	72.59	74.34	75.86	0.29	0.79	2.54	4.06
7a	75.6	80.71	76.59	73.28	70.73	5.11	0.99	2.32	4.87
8	62.4	64.21	65.42	66.53	68.98	1.81	3.02	4.13	6.58
9	42.8	44.91	42.35	48.05	41.42	2.11	0.45	5.25	1.38
11	173.9	177.01	177.14	178.89	177.26	3.11	3.24	4.99	3.36
12	22.6	24.52	24.20	25.08	24.29	1.92	1.60	2.48	1.69
MAE^b						3.16	2.71	4.27	4.59

^{a} $|\Delta\delta|(^{13}$C) = $|\delta_{exp} - \delta_{calc}|$ $(^{13}$C), ppm: absolute differences for experimental versus calculated ^{13}C NMR chemical shifts
^{b} **MAE** = $\Sigma[|(\delta_{exp} - \delta_{calcd})|]/n$, summation through n of the absolute error values (difference of the absolute values between corresponding experimental and ^{13}C chemical shifts), normalized to the number of the chemical shifts

Table S19. [13]C experimental related to exp_**2b** set of data and calculated NMR chemical shifts (MPW1PW91/6-311+g(d,p) level of theory) related to calc_**2a**, calc_**2b**, calc_**2c**, calc_**2d** sets of data, with [a]$|\Delta\delta|$(^{13}C) and [b]MAE values.

Position	δ_{exp}(^{13}C), ppm	δ_{calc}(^{13}C), ppm				$|\Delta\delta|$ (^{13}C), ppm[a]			
	exp_**2b**	calc_**2a**	calc_**2b**	calc_**2c**	calc_**2d**	calc_**2a**	calc_**2b**	calc_**2c**	calc_**2d**
1	70.7	76.05	72.57	75.11	79.20	5.35	1.87	4.41	8.50
2	39	35.23	42.70	45.60	42.85	3.77	3.70	6.60	3.85
3	69.7	65.72	65.60	62.44	65.47	3.98	4.10	7.26	4.23
5	71.4	66.48	71.60	66.56	71.66	4.92	0.20	4.84	0.26
6	76.9	78.14	78.24	86.17	76.19	1.24	1.34	9.27	0.71
7	72.4	71.51	72.59	74.34	75.86	0.89	0.19	1.94	3.46
7a	76.5	80.71	76.59	73.28	70.73	4.21	0.09	3.22	5.77
8	65.9	64.21	65.42	66.53	68.98	1.69	0.48	0.63	3.08
9	42.3	44.91	42.35	48.05	41.42	2.61	0.05	5.75	0.88
11	173.9	177.01	177.14	178.89	177.26	3.11	3.24	4.99	3.36
12	22.6	24.52	24.20	25.08	24.29	1.92	1.60	2.48	1.69
MAE[b]						3.06	1.53	4.67	3.25

[a] $|\Delta\delta|$(^{13}C) = $|\delta_{exp} - \delta_{calc}|$ (^{13}C), ppm: absolute differences for experimental versus calculated ^{13}C NMR chemical shifts
[b] **MAE** = $\Sigma[|(\delta_{exp} - \delta_{calcd})|]/n$, summation through n of the absolute error values (difference of the absolute values between corresponding experimental and ^{13}C chemical shifts), normalized to the number of the chemical shifts

Table S20. ^{13}C experimental related to exp_**2c** set of data and calculated NMR chemical shifts (MPW1PW91/6-311+g(d,p) level of theory) related to calc_**2a**, calc_**2b**, calc_**2c**, calc_**2d** sets of data, with $^a|\Delta\delta|(^{13}C)$ and ^{b}MAE values.

Position	$\delta_{exp}(^{13}C)$, ppm	$\delta_{calc}(^{13}C)$, ppm				$|\Delta\delta|$ (^{13}C), ppm^a			
	exp_**2c**	calc_**2a**	calc_**2b**	calc_**2c**	calc_**2d**	calc_**2a**	calc_**2b**	calc_**2c**	calc_**2d**
1	73.7	76.05	72.57	75.11	79.20	2.35	1.13	1.41	5.50
2	43.6	35.23	42.70	45.60	42.85	8.37	0.90	2.00	0.75
3	61.6	65.72	65.60	62.44	65.47	4.12	4.00	0.84	3.87
5	62.5	66.48	71.60	66.56	71.66	3.98	9.10	4.06	9.16
6	78.7	78.14	78.24	86.17	76.19	0.56	0.46	7.47	2.51
7	68.9	71.51	72.59	74.34	75.86	2.61	3.69	5.44	6.96
7a	73.9	80.71	76.59	73.28	70.73	6.81	2.69	0.62	3.17
8	63.3	64.21	65.42	66.53	68.98	0.91	2.12	3.23	5.68
9	40.8	44.91	42.35	48.05	41.42	4.11	1.55	7.25	0.62
11	173.7	177.01	177.14	178.89	177.26	3.31	3.44	5.19	3.56
12	22.6	24.52	24.20	25.08	24.29	1.92	1.60	2.48	1.69
MAE^b						3.55	2.79	3.64	3.95

^{a} $|\Delta\delta|(^{13}C) = |\delta_{exp} - \delta_{calc}|$ (^{13}C), ppm: absolute differences for experimental versus calculated ^{13}C NMR chemical shifts
^{b} **MAE** = $\Sigma[|(\delta_{exp} - \delta_{calcd})|]/n$, summation through n of the absolute error values (difference of the absolute values between corresponding experimental and ^{13}C chemical shifts), normalized to the number of the chemical shifts

Table S21. [13]C experimental related to exp_**2d** set of data and calculated NMR chemical shifts (MPW1PW91/6-311+g(d,p) level of theory) related to calc_**2a**, calc_**2b**, calc_**2c**, calc_**2d** sets of data, with [a]$|\Delta\delta|$(^{13}C) and [b]MAE values.

Position	δ_{exp}(^{13}C), ppm	δ_{calc}(^{13}C), ppm				$|\Delta\delta|$ (^{13}C), ppm[a]			
	exp_**2d**	calc_**2a**	calc_**2b**	calc_**2c**	calc_**2d**	calc_**2a**	calc_**2b**	calc_**2c**	calc_**2d**
1	76.6	76.05	72.57	75.11	79.20	0.55	4.03	1.49	2.60
2	39.8	35.23	42.70	45.60	42.85	4.57	2.90	5.80	3.05
3	66.2	65.72	65.60	62.44	65.47	0.48	0.60	3.76	0.73
5	71.5	66.48	71.60	66.56	71.66	5.02	0.10	4.94	0.16
6	74.1	78.14	78.24	86.17	76.19	4.04	4.14	12.07	2.09
7	73.9	71.51	72.59	74.34	75.86	2.39	1.31	0.44	1.96
7a	70.8	80.71	76.59	73.28	70.73	9.91	5.79	2.48	0.07
8	68.7	64.21	65.42	66.53	68.98	4.49	3.28	2.17	0.28
9	42.8	44.91	42.35	48.05	41.42	2.11	0.45	5.25	1.38
11	173.7	177.01	177.14	178.89	177.26	3.31	3.44	5.19	3.56
12	22.6	24.52	24.20	25.08	24.29	1.92	1.60	2.48	1.69
MAE[b]						3.53	2.51	4.19	1.60

[a] $|\Delta\delta|$(^{13}C) = $|\delta_{exp} - \delta_{calc}|$ (^{13}C), ppm: absolute differences for experimental versus calculated ^{13}C NMR chemical shifts
[b] **MAE** = $\Sigma[|(\delta_{exp} - \delta_{calcd})|]/n$, summation through n of the absolute error values (difference of the absolute values between corresponding experimental and ^{13}C chemical shifts), normalized to the number of the chemical shifts

Table S22. ^{13}C experimental related to exp_**2a** set of data and calculated NMR chemical shifts (B97-2/cc-pVTZ level of theory) related to calc_**2a**, calc_**2b**, calc_**2c**, calc_**2d** sets of data, with ^{a}|Δδ|(^{13}C) and ^{b}MAE values.

Position	δ$_{exp}$(^{13}C), ppm	δ$_{calc}$(^{13}C), ppm				|Δδ| (^{13}C), ppm^a			
	exp_**2a**	calc_**2a**	calc_**2b**	calc_**2c**	calc_**2d**	calc_**2a**	calc_**2b**	calc_**2c**	calc_**2d**
1	69.2	77.10	73.18	75.81	78.99	7.90	3.98	6.61	9.79
2	40	35.66	43.07	45.53	41.93	4.34	3.07	5.53	1.93
3	62.8	66.73	67.70	62.97	67.15	3.93	4.90	0.17	4.35
5	60.9	67.55	72.90	67.07	72.76	6.65	12.00	6.17	11.86
6	78.4	79.39	80.47	86.37	78.04	0.99	2.07	7.97	0.37
7	71.8	72.86	73.56	75.09	76.47	1.06	1.76	3.29	4.67
7a	75.6	78.75	77.54	73.28	71.30	3.15	1.94	2.32	4.30
8	62.4	64.06	65.84	67.08	69.30	1.66	3.44	4.68	6.90
9	42.8	46.80	44.15	48.68	42.94	4.00	1.35	5.88	0.14
11	173.9	173.34	174.13	175.50	174.14	0.56	0.23	1.60	0.24
12	22.6	24.09	23.94	24.38	23.86	1.49	1.34	1.78	1.26
MAE^b						3.25	3.28	4.18	4.16

^{a} |**Δδ**|(**^{13}C**) = |δ$_{exp}$ −δ$_{calc}$| (^{13}C), ppm: absolute differences for experimental versus calculated ^{13}C NMR chemical shifts
^{b} **MAE** = Σ[|(δ$_{exp}$ − δ$_{calcd}$)|]/n, summation through n of the absolute error values (difference of the absolute values between corresponding experimental and ^{13}C chemical shifts), normalized to the number of the chemical shifts

Table S23. ^{13}C experimental related to exp_**2b** set of data and calculated NMR chemical shifts (B97-2/cc-pVTZ level of theory) related to calc_**2a**, calc_**2b**, calc_**2c**, calc_**2d** sets of data, with ^{a}|Δδ|(^{13}C) and ^{b}MAE values.

Position	δ_exp(^{13}C), ppm	δ_calc(^{13}C), ppm				|Δδ| (^{13}C), ppm^a			
	exp_**2b**	calc_**2a**	calc_**2b**	calc_**2c**	calc_**2d**	calc_**2a**	calc_**2b**	calc_**2c**	calc_**2d**
1	70.7	77.10	73.18	75.81	78.99	6.40	2.48	5.11	8.29
2	39	35.66	43.07	45.53	41.93	3.34	4.07	6.53	2.93
3	69.7	66.73	67.70	62.97	67.15	2.97	2.00	6.73	2.55
5	71.4	67.55	72.90	67.07	72.76	3.85	1.50	4.33	1.36
6	76.9	79.39	80.47	86.37	78.04	2.49	3.57	9.47	1.13
7	72.4	72.86	73.56	75.09	76.47	0.46	1.16	2.69	4.07
7a	76.5	78.75	77.54	73.28	71.30	2.25	1.04	3.22	5.20
8	65.9	64.06	65.84	67.08	69.30	1.84	0.06	1.18	3.40
9	42.3	46.80	44.15	48.68	42.94	4.50	1.85	6.38	0.64
11	173.9	173.34	174.13	175.50	174.14	0.56	0.23	1.60	0.24
12	22.6	24.09	23.94	24.38	23.86	1.49	1.34	1.78	1.26
MAE^b						2.74	1.75	4.46	2.82

^{a} **|Δδ|(^{13}C)** = |δ_exp −δ_calc| (^{13}C), ppm: absolute differences for experimental versus calculated ^{13}C NMR chemical shifts
^{b} **MAE** = Σ[|(δ_exp − δ_calcd)|]/n, summation through n of the absolute error values (difference of the absolute values between corresponding experimental and ^{13}C chemical shifts), normalized to the number of the chemical shifts

Table S24. ^{13}C experimental related to exp_**2c** set of data and calculated NMR chemical shifts (B97-2/cc-pVTZ level of theory) related to calc_**2a**, calc_**2b**, calc_**2c**, calc_**2d** sets of data, with ^{a}|Δδ|(^{13}C) and ^{b}MAE values.

Position	δ$_{exp}$(^{13}C), ppm	δ$_{calc}$(^{13}C), ppm				|Δδ| (^{13}C), ppm^a			
	exp_**2c**	calc_**2a**	calc_**2b**	calc_**2c**	calc_**2d**	calc_**2a**	calc_**2b**	calc_**2c**	calc_**2d**
1	73.7	77.10	73.18	75.81	78.99	3.40	0.52	2.11	5.29
2	43.6	35.66	43.07	45.53	41.93	7.94	0.53	1.93	1.67
3	61.6	66.73	67.70	62.97	67.15	5.13	6.10	1.37	5.55
5	62.5	67.55	72.90	67.07	72.76	5.05	10.40	4.57	10.26
6	78.7	79.39	80.47	86.37	78.04	0.69	1.77	7.67	0.67
7	68.9	72.86	73.56	75.09	76.47	3.96	4.66	6.19	7.57
7a	73.9	78.75	77.54	73.28	71.30	4.85	3.64	0.62	2.60
8	63.3	64.06	65.84	67.08	69.30	0.76	2.54	3.78	6.00
9	40.8	46.80	44.15	48.68	42.94	6.00	3.35	7.88	2.14
11	173.7	173.34	174.13	175.50	174.14	0.36	0.43	1.80	0.44
12	22.6	24.09	23.94	24.38	23.86	1.49	1.34	1.78	1.26
MAE^b						3.60	3.21	3.61	3.95

^{a} |Δδ|(^{13}C) = |δ$_{exp}$ −δ$_{calc}$| (^{13}C), ppm: absolute differences for experimental versus calculated ^{13}C NMR chemical shifts
^{b} **MAE** = Σ[|(δ$_{exp}$ − δ$_{calcd}$)|]/n, summation through n of the absolute error values (difference of the absolute values between corresponding experimental and ^{13}C chemical shifts), normalized to the number of the chemical shifts

Table S25. [13]C experimental related to exp_**2d** set of data and calculated NMR chemical shifts (B97-2/cc-pVTZ level of theory) related to calc_**2a**, calc_**2b**, calc_**2c**, calc_**2d** sets of data, with [a]$|\Delta\delta|$(^{13}C) and [b]MAE values.

Position	δ_{exp}(^{13}C), ppm	δ_{calc}(^{13}C), ppm				$|\Delta\delta|$ (^{13}C), ppm[a]			
	exp_**2d**	calc_**2a**	calc_**2b**	calc_**2c**	calc_**2d**	calc_**2a**	calc_**2b**	calc_**2c**	calc_**2d**
1	76.6	77.10	73.18	75.81	78.99	0.50	3.42	0.79	2.39
2	39.8	35.66	43.07	45.53	41.93	4.14	3.27	5.73	2.13
3	66.2	66.73	67.70	62.97	67.15	0.53	1.50	3.23	0.95
5	71.5	67.55	72.90	67.07	72.76	3.95	1.40	4.43	1.26
6	74.1	79.39	80.47	86.37	78.04	5.29	6.37	12.27	3.94
7	73.9	72.86	73.56	75.09	76.47	1.04	0.34	1.19	2.57
7a	70.8	78.75	77.54	73.28	71.30	7.95	6.74	2.48	0.50
8	68.7	64.06	65.84	67.08	69.30	4.64	2.86	1.62	0.59
9	42.8	46.80	44.15	48.68	42.94	4.00	1.35	5.88	0.14
11	173.7	173.34	174.13	175.50	174.14	0.36	0.43	1.80	0.44
12	22.6	24.09	23.94	24.38	23.86	1.49	1.34	1.78	1.26
MAE[b]						3.08	2.64	3.75	1.47

[a] $|\Delta\delta|$(^{13}C) = $|\delta_{exp} - \delta_{calc}|$ (^{13}C), ppm: absolute differences for experimental versus calculated ^{13}C NMR chemical shifts
[b] MAE = $\Sigma[|(\delta_{exp} - \delta_{calcd})|]/n$, summation through n of the absolute error values (difference of the absolute values between corresponding experimental and ^{13}C chemical shifts), normalized to the number of the chemical shifts

Table S26. Sampled and DFT geometry optimized conformers related to calc_**1a**, with energy values (Hartree) and related % contribution on the final Boltzmann distribution for the three employed functional/basis set combinations.

Conformer	MPW1PW91/6-31g(d,p)		MPW1PW91/6-311+g(d,p)		B97-2/cc-pVTZ	
	Energy (Hartree)	% contribution on the Boltzmann distribution	Energy (Hartree)	% contribution on the Boltzmann distribution	Energy (Hartree)	% contribution on the Boltzmann distribution
calc_**1a** conf_1	-997.7100047	52.18%	-997.9450900	64.59%	-997.9038062	63.05%
calc_**1a** conf_2	-997.7088563	15.46%	-997.9435817	13.07%	-997.9025508	16.68%
calc_**1a** conf_3	-997.7083563	9.10%	-997.9428143	5.80%	-997.9016043	6.12%
calc_**1a** conf_4	-997.7082807	8.40%	-997.9430366	7.34%	-997.9014365	5.12%
calc_**1a** conf_5	-997.7077996	5.05%	-997.9421001	2.72%	-997.9009142	2.95%
calc_**1a** conf_6	-997.7069035	1.95%	-997.9413632	1.25%	-997.8999644	1.08%
calc_**1a** conf_7	-997.7065498	1.34%	-997.9410529	0.90%	-997.8992952	0.53%
calc_**1a** conf_8	-997.7065316	1.32%	-997.9406889	0.61%	-997.8985534	0.24%
calc_**1a** conf_9	-997.7065042	1.28%	-997.9411241	0.97%	-997.9001548	1.32%
calc_**1a** conf_10	-997.7064842	1.25%	-997.9412112	1.06%	-997.9001646	1.33%
calc_**1a** conf_11	-997.7064661	1.23%	-997.9405997	0.56%	-997.8988813	0.34%
calc_**1a** conf_12	-997.7051654	0.31%	-997.9390339	0.11%	-997.8973415	0.07%
calc_**1a** conf_13	-997.7049233	0.24%	-997.9399940	0.29%	-997.8990698	0.42%
calc_**1a** conf_14	-997.7049203	0.24%	-997.9398862	0.26%	-997.8989558	0.37%
calc_**1a** conf_15	-997.7046194	0.17%	-997.9391947	0.13%	-997.8975500	0.08%
calc_**1a** conf_16	-997.7045258	0.16%	-997.9391402	0.12%	-997.8975233	0.08%
calc_**1a** conf_17	-997.7036931	0.07%	-997.9381556	0.04%	-997.8968189	0.04%
calc_**1a** conf_18	-997.7036183	0.06%	-997.9383642	0.05%	-997.8971150	0.05%
calc_**1a** conf_19	-997.7031591	0.04%	-997.9383256	0.05%	-997.8969003	0.04%
calc_**1a** conf_20	-997.7031085	0.04%	-997.9380534	0.04%	-997.8965821	0.03%
calc_**1a** conf_21	-997.7030426	0.03%	-997.9372161	0.02%	-997.8963949	0.02%
calc_**1a** conf_22	-997.7025020	0.02%	-997.9365943	0.01%	-997.8939768	0.00%
calc_**1a** conf_23	-997.7024711	0.02%	-997.9366162	0.01%	-997.8944996	0.00%
calc_**1a** conf_24	-997.7023113	0.02%	-997.9370736	0.01%	-997.8957753	0.01%
calc_**1a** conf_25	-997.7022650	0.01%	-997.9364762	0.01%	-997.8944422	0.00%
calc_**1a** conf_26	-997.7005001	0.00%	-997.9343100	0.00%	-997.8923604	0.00%
calc_**1a** conf_27	-997.6985464	0.00%	-997.9338218	0.00%	-997.8915728	0.00%

Table S27. Cartesian coordinates of the optimized geometries for the conformers related to calc_**1a**. The related energies and % contribution on the final Boltzmann distribution for the three employed functional/basis set combinations are reported in Table S26.

```
calc_1a conf_1

C   -5.7028004057    0.1252675446    3.626082063
C   -6.4765350458    0.0458975075    2.4749069827
C   -5.9161264461   -0.3304778576    1.2446825126
C   -4.5672593435   -0.6137808691    1.1774870237
C   -3.7564570587   -0.5214768629    2.3249839931
C   -4.3399762212   -0.1702163411    3.5661743008
O   -3.6301790667   -0.1097732216    4.6906907846
O   -7.8000267818    0.3187252075    2.4791182461
C   -3.8982038905   -1.0601586625   -0.091751582
C   -2.4570278509   -0.5851596574   -0.1154207915
O   -1.7651406027   -1.0334757411    1.0716722742
C   -2.3309739461   -0.8258908194    2.2686448041
O   -1.623267428    -0.9203752227    3.2667984604
C   -1.659698452    -1.1035592403   -1.2971019195
C   -0.2596633373   -0.5138051864   -1.3851381537
C    0.5562434291   -1.1018517604   -2.5319097751
C    1.8954012064   -0.3760565276   -2.6527678917
C    1.6634304127    1.1311419816   -2.7550557685
C    0.7721733727    1.6443923556   -1.6205334802
O   -0.4336902832    0.885803272    -1.5579142293
C    1.4763108474    1.7209574503   -0.2688444473
H   -6.1329634183    0.4003750881    4.5839867927
H   -6.5554810117   -0.391688831     0.3716011196
H   -2.7128839711   -0.4081852107    4.4581081802
H   -8.0702488338    0.5654031683    3.3734010062
H   -4.4270663075   -0.6727810017   -0.9675286616
H   -3.9203387134   -2.1565228384   -0.1584225392
H   -2.4264446933    0.5096940577   -0.1138933834
H   -2.2017007566   -0.8527090717   -2.216278581
H   -1.5941410674   -2.1957054886   -1.2346703076
H    0.2607737731   -0.7117972903   -0.4370119364
H   -0.0130008634   -0.9870004661   -3.4638427703
H    0.7059647587   -2.1752632973   -2.3685874878
H    2.4497493952   -0.7337318876   -3.5268620676
H    2.5156056302   -0.6059932697   -1.7774212686
H    2.6141370993    1.6759605439   -2.7559030134
H    1.1648736111    1.3502558141   -3.7068032053
H    0.4265655219    2.651829159    -1.8750847356
H    2.2795288812    2.4632800296   -0.3067642443
H    1.9204233957    0.7691177925    0.0336210453
H    0.7661144616    2.022335651     0.5055526512

calc_1a conf_2

C   -5.7663930421    0.0425980704    3.5039931249
C   -6.3760227421    0.1729049941    2.262499665
C   -5.6872983739   -0.1279925238    1.0773578359
C   -4.3746473175   -0.5473850328    1.1493681451
C   -3.7266766812   -0.6682866902    2.3934086755
C   -4.4424073472   -0.3923368026    3.5833629037
O   -3.8946002167   -0.5324891286    4.7881601984
O   -7.6553707707    0.5873854259    2.1304282026
C   -3.5782429005   -0.9216428035   -0.0687700996
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S33

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C   -2.1108554107   -0.6016212635    0.1511195908
O   -1.6350485467   -1.2496484873    1.3512147868
C   -2.3416007507   -1.1175033697    2.4831772868
O   -1.7937230186   -1.4010400261    3.5433609905
C   -1.2013581235   -1.0676329616   -0.9701158964
C    0.2396330712   -0.56877036     -0.8070907774
C    1.1978635872   -1.1306297478   -1.8588226554
C    1.0037643447   -0.4637356476   -3.2178951842
C    1.0835842081    1.0516393629    -3.0558734959
C    0.0978542072    1.5311198421    -1.9946788313
O    0.3014288138    0.8534005105    -0.7595607381
C    0.2278746289    3.0106002641    -1.6897378285
H   -6.2982495222    0.2578754135     4.4254609846
H   -6.2017930872   -0.0248833704     0.1289498455
H   -2.9859886126   -0.9028385363     4.6410963761
H   -8.0232135871    0.7654651881     3.0060065816
H   -3.9436120811   -0.3875378307    -0.9510021122
H   -3.6883911297   -1.9956368959    -0.2715554127
H   -1.9842862279    0.4775326266     0.2966436536
H   -1.2031122918   -2.163539855     -0.9908881527
H   -1.6271458038   -0.7322188322    -1.9220858985
H    0.5791609586   -0.8792648559     0.1849527158
H    1.0765928588   -2.2174282624    -1.9272798335
H    2.2222556387   -0.9436977602    -1.5161417766
H    0.0301026741   -0.7389012907    -3.6443069426
H    1.7607741354   -0.8178467012    -3.9255220353
H    0.877525738     1.5618145541    -4.0037006155
H    2.0965821642    1.3374894036    -2.7444218153
H   -0.9243562888    1.3332143356    -2.3600382062
H    1.2325498118    3.2313556417    -1.3179558363
H   -0.4917756626    3.3090636167    -0.9231767703
H    0.0486226964    3.6070497862    -2.5889406486
```

calc_**1a** conf_3

```
C   -5.8456043311    0.0791484077     3.2974420107
C   -6.0677400596    0.5095667        1.9950118303
C   -5.1263843087    0.2796207655     0.9803171559
C   -3.9513165547   -0.3762685795     1.2872317515
C   -3.6930150912   -0.8041970346     2.6036966006
C   -4.6641923556   -0.5942037404     3.611829829
O   -4.4908784037   -1.018059544      4.8621478626
O   -7.1961459501    1.1628874249     1.6383259593
C   -2.910482609    -0.6970488754     0.2539063637
C   -1.5306908686   -0.6757828807     0.8838374661
O   -1.4870346646   -1.5756107269     2.0156398475
C   -2.4580181302   -1.5040013726     2.9381040428
O   -2.2629445242   -2.04361677       4.0230665679
C   -0.3908539321   -1.1113700784    -0.0257523531
C    0.1128959472   -0.0359805289    -0.9772581621
C    1.3496886452   -0.4906695708    -1.7482044864
C    1.7596131016    0.5620249566    -2.7750895876
C    0.566666606     0.9091481457    -3.6627765473
C   -0.6602075121    1.2950749436    -2.8327548203
O   -0.9485885707    0.2842082134    -1.86641205
C   -0.5659603311    2.681812881     -2.2025196771
H   -6.5773432209    0.2391701538     4.0831268844
H   -5.3418056196    0.6193436049    -0.0260850432
H   -3.6347709068   -1.5195048539     4.8700788944
```

```
H   -7.763323996    1.2620574931    2.4142622216
H   -2.9323498654   0.0035500386   -0.582213112
H   -3.0943024179  -1.6979105098   -0.1597314802
H   -1.3263140321   0.3315746033    1.2721466075
H   -0.6894247371  -1.9956164973   -0.60014595
H    0.4421573665  -1.4105620167    0.6190497718
H    0.3790410698   0.8557403527   -0.384611778
H    1.1146868726  -1.4338243349   -2.2579352908
H    2.1662787292  -0.6930169118   -1.0463169665
H    2.5927907407   0.1987958229   -3.3855601681
H    2.1233499595   1.458960763    -2.2582215781
H    0.8134332073   1.7203887689   -4.3566467311
H    0.3077863617   0.0333717892   -4.269458568
H   -1.540957301    1.2827279322   -3.4829543923
H    0.3247873476   2.80656003     -1.5808019546
H   -1.4443709263   2.8709404241   -1.5794311863
H   -0.5311547344   3.4465706114   -2.9843397844

calc_1a conf_4

C   -5.9352955581  -0.9158737704    2.7619282609
C   -6.1582912927   0.4335186197    2.5192018545
C   -5.1038710293   1.2980296055    2.1855243393
C   -3.8241974638   0.7918551868    2.0874838464
C   -3.5737670635  -0.5759943881    2.3073783463
C   -4.6412967548  -1.4322883946    2.6693255483
O   -4.4571571866  -2.7254241434    2.9249014892
O   -7.3901713759   0.9834601784    2.5962178491
C   -2.6291742392   1.6535131446    1.7975672786
C   -1.5792920276   0.8800539618    1.0135505201
O   -1.2483273271  -0.3513748104    1.6964872419
C   -2.2288009703  -1.1273375434    2.1785860659
O   -1.944800474   -2.277701427     2.5007818183
C   -1.9735814295   0.5821534576   -0.4283278928
C   -0.8568774329  -0.0756711193   -1.2255887284
C   -1.2810039469  -0.4442906445   -2.6433280723
C   -0.0832290208  -0.9728862092   -3.4308584679
C    1.0695041791   0.0277853918   -3.3608116043
C    1.3923004576   0.4204397711   -1.9164479103
O    0.2121609834   0.8610554053   -1.2481453877
C    2.1306725272  -0.6602863485   -1.1317818053
H   -6.7435184221  -1.5871742331    3.0347300809
H   -5.3161199748   2.3475950821    2.017931765
H   -3.4797359563  -2.8857483829    2.8568365382
H   -8.0291794231   0.2990010557    2.8347197268
H   -2.188670367    1.9865381187    2.7461303657
H   -2.9142494464   2.5539668057    1.2458684508
H   -0.6360694474   1.4271871905    1.0049100428
H   -2.2331295985   1.5296368631   -0.9152532986
H   -2.8665810532  -0.0522156137   -0.4519183294
H   -0.5406320731  -0.9880422198   -0.6987610739
H   -1.6824521852   0.4518590768   -3.1343818006
H   -2.0855013875  -1.1877617457   -2.608561455
H   -0.3596682201  -1.1583905102   -4.4741582479
H    0.2278583587  -1.9402541358   -3.0170567439
H    1.9669542062  -0.3719533492   -3.8462634527
H    0.7852046547   0.9357375538   -3.9060456715
H    2.0255348619   1.313808727    -1.9300253879
H    1.6084752979  -1.6206482651   -1.1318781702
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S35

```
H   2.2563424178    -0.3460093152    -0.0923543845
H   3.1226342034    -0.8238686264    -1.5641135438

calc_1a conf_5

C  -5.7542268419     0.0617368229     3.3863784529
C  -5.764845985      0.9975475601     2.3591571451
C  -4.7754815531     0.9992220216     1.3641758127
C  -3.7665531984     0.0589696186     1.415948051
C  -3.7216601019    -0.8876075431     2.4571440923
C  -4.7421161113    -0.8977295226     3.4384972541
O  -4.7727558099    -1.7970061124     4.419722763
O  -6.7240666532     1.9444962435     2.2615584933
C  -2.6956170041    -0.0320527712     0.3672642591
C  -1.4049563596    -0.5402261475     0.9813145617
O  -1.6327534769    -1.7925397242     1.6661615743
C  -2.6656757346    -1.8910038136     2.5166887491
O  -2.6768969942    -2.8345712687     3.3010400675
C  -0.2766856313    -0.8203364262     0.0010283151
C   0.3729246609     0.4357173182    -0.5923103219
C   1.6893239825     0.1393874044    -1.3168908572
C   1.4504235774    -0.5155829347    -2.6743055436
C   0.4869872618     0.3432478041    -3.4885662973
C  -0.7926852151     0.6116209935    -2.702902918
O  -0.5043555035     1.1842194105    -1.4295538791
C  -1.7214314235     1.5836434942    -3.403632594
H  -6.5255668545     0.0453706068     4.1500436105
H  -4.8240877593     1.7387991354     0.5733875468
H  -4.0186316143    -2.4190927615     4.2511323852
H  -7.3436592184     1.8451834845     2.9963349844
H  -2.5104850731     0.9334251174    -0.1075949008
H  -3.0111948079    -0.7264855274    -0.4238544797
H  -1.0616827186     0.1786610194     1.7383198818
H   0.49297137      -1.3731973992     0.5505091577
H  -0.6403048084    -1.4959226605    -0.7804868545
H   0.5834340273     1.1213857622     0.2371498609
H   2.3313173216    -0.4808665845    -0.6823187557
H   2.2102808436     1.0918196803    -1.4697956886
H   1.0321446269    -1.52182467      -2.5440119092
H   2.3993939846    -0.641435282     -3.2058870579
H   0.2358160757    -0.1395241482    -4.4396898389
H   0.9588932355     1.3056428974    -3.7255557022
H  -1.3199692814    -0.3462243215    -2.5619342308
H  -1.2268085814     2.5506355108    -3.5326906602
H  -2.6317105713     1.740847292     -2.8192173496
H  -2.0040460821     1.2016504212    -4.3887571792

calc_1a conf_6

C  -5.9451858806    -1.0203796414     2.6503891195
C  -6.1709819289     0.247218393      2.1292870136
C  -5.1061667661     1.0770564893     1.7442130504
C  -3.8124637043     0.6173221685     1.8785857541
C  -3.5561700619    -0.670929283      2.3851872548
C  -4.6373292831    -1.4882187364     2.7939944327
O  -4.4532733506    -2.6996465481     3.3130572618
O  -7.4157468521     0.748460069      1.9712319423
C  -2.6128365535     1.4590935222     1.5522020373
C  -1.4655302207     0.5960044646     1.0491805354
```

```
O  -1.1819445976  -0.4611407444   1.9939709025
C  -2.1925446764  -1.1758477546   2.5096961673
O  -1.919887503   -2.2296346452   3.0770093742
C  -1.685778582   -0.0024321955  -0.3363158172
C  -0.4241439646  -0.6858193698  -0.8763124393
C  -0.6504798936  -1.4335378919  -2.1915069343
C  -0.7759250843  -0.4765698512  -3.3742139602
C   0.4263368016   0.4639511197  -3.3959221035
C   0.5859968062   1.167622737   -2.0514485492
O   0.6624234976   0.2291364178  -0.9846106358
C   1.8483655866   2.0037305369  -1.9681470203
H  -6.7628164249  -1.6619991308   2.9634678513
H  -5.3225476825   2.0656183896   1.3560015128
H  -3.4710765558  -2.8278434047   3.3794109842
H  -8.0618708381   0.0949454821   2.2698321229
H  -2.2876443126   1.9861937545   2.458403669
H  -2.8558602929   2.2241200046   0.8090654693
H  -0.5395184998   1.1736510414   1.0326917606
H  -2.5055645915  -0.7285887548  -0.2994665844
H  -2.0139011231   0.7972182566  -1.0096387642
H  -0.0892869272  -1.3992030452  -0.1175598323
H  -1.5325383531  -2.0775671646  -2.104587296
H   0.2110188522  -2.0907580377  -2.3580425512
H  -1.702387135    0.1075807934  -3.2971521491
H  -0.8435210353  -1.0387318669  -4.3115504983
H   0.3284626981   1.2122429349  -4.1907082102
H   1.3401986458  -0.1096035691  -3.5982367714
H  -0.2860942851   1.8267765414  -1.9016615175
H   1.9269687808   2.4842909685  -0.9895803263
H   1.8494661849   2.7792348503  -2.7395395584
H   2.7287791063   1.3699827      -2.107676697

calc_1a conf_7

C  -5.8757080863  -0.7794434174   2.3556051759
C  -5.7886106866   0.3726029519   1.5837378208
C  -4.5506811835   0.9704688489   1.3026466101
C  -3.3975974124   0.3946665824   1.7960914154
C  -3.4566902499  -0.785553789    2.5608584685
C  -4.7129978481  -1.3642931574   2.8603371919
O  -4.8293806289  -2.4579539883   3.611076637
O  -6.8842031035   0.9766676583   1.0713134601
C  -2.0404195157   1.004261287    1.5955721005
C  -0.9707420724  -0.0737686421   1.5159736053
O  -1.0506737215  -0.9524323428   2.6627016193
C  -2.2422850465  -1.4154184036   3.066310244
O  -2.2537042514  -2.3533284714   3.858453333
C  -0.9896373469  -0.917296879    0.2402698978
C  -0.3122580342  -0.2664196605  -0.9585234189
C  -0.2134740968  -1.2202622315  -2.1473155336
C   0.3581454215  -0.5026000716  -3.368165818
C  -0.4483647263   0.76354305    -3.6498897082
C  -0.5633677327   1.6462424108  -2.4057995466
O  -1.0609961702   0.8911521579  -1.301671406
C   0.7208071954   2.3943695966  -2.0588488614
H  -6.8315004004  -1.2380964173   2.5891618223
H  -4.5239300285   1.8742084114   0.7052997036
H  -3.9118437322  -2.6870707185   3.9121017877
H  -7.6702434497   0.477760841    1.3297644818
```

```
H   -1.8158055337    1.6636043035    2.4440949192
H   -2.0034892057    1.6019077973    0.6837921032
H    0.0170203874    0.382416331     1.6235747153
H   -2.0188977867   -1.1818631979   -0.0266215077
H   -0.457431907    -1.8490300966    0.459075394
H    0.7084046487    0.0306205012   -0.6624417841
H   -1.2191180859   -1.5958411302   -2.3754225067
H    0.4038921149   -2.0837202862   -1.8753210591
H    0.3436263134   -1.1627342713   -4.2416472646
H    1.4112832859   -0.2517206791   -3.1889713219
H   -0.0068218813    1.3379558942   -4.4718472063
H   -1.4601380975    0.4790766116   -3.9619777788
H   -1.3471044549    2.3914062712   -2.576748547
H    0.9706656621    3.0993222344   -2.8576080608
H    1.5789478414    1.7297869423   -1.9270539605
H    0.5853236063    2.9618071686   -1.1339372164
```

calc_**1a** conf_8

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C   -5.6686246361   -0.5212398905    1.8334752355
C   -5.3780463147    0.711425831     1.2628782252
C   -4.0669415304    1.2122333987    1.2375894653
C   -3.046416518     0.4583863671    1.7823732395
C   -3.3121214848   -0.8026019298    2.3490729737
C   -4.6422196996   -1.2849109258    2.3927768807
O   -4.9554467527   -2.4523015138    2.9500808184
O   -6.3345082305    1.4906740097    0.710874891
C   -1.6277885924    0.9458351137    1.8531953461
C   -0.6530535149   -0.2172467957    1.7619620106
O   -0.9695941019   -1.2220604782    2.7532974603
C   -2.2405534164   -1.6139960164    2.9173114833
O   -2.4464280408   -2.6429436861    3.5540918693
C   -0.5555386786   -0.8924485184    0.3943495811
C    0.2497859732   -0.0993448409   -0.6440775795
C    0.5868754926   -0.9244606973   -1.8900533802
C   -0.626876741    -1.093575602    -2.7997272418
C   -1.2159672681    0.2781679794   -3.1169856011
C   -1.5113751287    1.0508597506   -1.8356019828
O   -0.3523893594    1.1388113749   -1.0076914472
C   -1.9478186139    2.4781842345   -2.1023468706
H   -6.6822358638   -0.9080570291    1.8697318792
H   -3.8838706337    2.1869522222    0.8006384054
H   -4.1136790067   -2.8125259516    3.3337020405
H   -7.1899361423    1.0488410988    0.7929314312
H   -1.4746379816    1.4603072476    2.8106454017
H   -1.4023698816    1.6555143956    1.0547333932
H    0.3435038283    0.119879103     2.0598052303
H   -0.0430934154   -1.8476981787    0.552260087
H   -1.5577850808   -1.1338381375    0.0249311557
H    1.1902417465    0.2029095774   -0.1673583159
H    1.0011546183   -1.8940819864   -1.5934588376
H    1.3717393736   -0.3937736293   -2.4418608267
H   -1.3846454106   -1.7204781097   -2.3127579791
H   -0.3403100472   -1.6131500941   -3.7200424623
H   -2.1356261075    0.1858111283   -3.705556837
H   -0.5014296723    0.8571134984   -3.7164682568
H   -2.311897557     0.5299255848   -1.2865878536
H   -1.1591644766    3.0221901572   -2.6302560265
H   -2.1547695553    3.0044974362   -1.1666620814
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H  -2.8541415772   2.4942145023   -2.7142149241

calc_1a conf_9

C  -5.5189209604  -0.3032289356   4.0931611035
C  -6.236356258    0.4648880254   3.184524649
C  -5.787246225    0.6445511125   1.8668711805
C  -4.6033281606   0.0558899567   1.472872824
C  -3.8468932127  -0.7113198859   2.3796506112
C  -4.3257838933  -0.9095575292   3.697340797
O  -3.6738420991  -1.6593640234   4.5828497232
O  -7.3973171536   1.0708132904   3.5153361369
C  -4.0725521817   0.1693302407   0.0721350949
C  -2.5533143417   0.1369746153   0.0821301009
O  -2.0890397444  -1.0450161078   0.7671960292
C  -2.5971994277  -1.3415980781   1.9739255571
O  -1.9874695108  -2.1447250171   2.6724490059
C  -1.9492691065   0.1377308309  -1.3087274112
C  -0.4298554535   0.2846368383  -1.3771891703
C   0.3471603698  -1.0036419842  -1.1218627894
C   1.837439006   -0.7866036457  -1.3742036013
C   2.0481656026  -0.2078880142  -2.7711559066
C   1.190558729    1.0396677369  -2.9950111508
O  -0.1760161559   0.7772129101  -2.6874219252
C   1.7110259501   2.2787445909  -2.2707139766
H  -5.8685156851  -0.4588831109   5.1089176762
H  -6.3816976838   1.2416254475   1.185071767
H  -2.8957779224  -2.0461140572   4.1047838386
H  -7.6043655521   0.8788026708   4.4394609518
H  -4.4174946374   1.0927663224  -0.4016608499
H  -4.4442439422  -0.6654130202  -0.5371768276
H  -2.1818802165   1.0014026495   0.6495048082
H  -2.37175338     0.9924995361  -1.848353572
H  -2.2623220768  -0.7655642094  -1.8445577942
H  -0.1198305166   1.0397658389  -0.6342507699
H  -0.0333816112  -1.7729359544  -1.8065014081
H   0.1605993135  -1.355652439   -0.1045562136
H   2.3831225434  -1.7299936951  -1.2679834328
H   2.2460256535  -0.1083569183  -0.6139977487
H   3.1028862939   0.0315371917  -2.9480251265
H   1.7588914835  -0.9602232872  -3.5145663698
H   1.1705381485   1.2649927953  -4.0665694985
H   2.6866790329   2.5673674141  -2.673656318
H   1.8333316736   2.1210238415  -1.195607665
H   1.0192433084   3.1128560566  -2.4164323292

calc_1a conf_10

C  -5.6148711677  -0.5450433466   4.0095492508
C  -6.0276236825   0.6213304456   3.3775319666
C  -5.3923288604   1.0845579323   2.2145830732
C  -4.3295138475   0.3723088022   1.6986701364
C  -3.8785029497  -0.8024487925   2.3310510417
C  -4.5470856355  -1.2755269104   3.4861438046
O  -4.1919291187  -2.4023236238   4.0988381365
O  -7.0566277516   1.3636384702   3.8402114987
C  -3.6208909065   0.7802735498   0.4380977626
C  -2.1601283248   0.3655517782   0.4981347176
O  -2.0600231958  -1.0475350654   0.7716215447
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S39

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C  -2.7625326565  -1.5677812548   1.7912780106
O  -2.4371010631  -2.6747435163   2.2068994995
C  -1.4058282064   0.6377203045  -0.7915719757
C   0.1246904677   0.5081172008  -0.69760902
C   0.6671506363  -0.9217996626  -0.7431222294
C   0.5850442927  -1.5092453752  -2.1500186716
C   1.2413566996  -0.5590254374  -3.148225499
C   0.6524220146   0.8423493044  -3.0215916061
O   0.7531660002   1.3185789053  -1.6839512652
C   1.3598900026   1.8653887473  -3.8884451226
H  -6.111802447   -0.9173863722   4.8998351573
H  -5.7516512078   1.9928127987   1.7448163691
H  -3.467556004   -2.8032388204   3.5531756635
H  -7.4118986084   0.9525060544   4.6393030532
H  -3.6895825003   1.8611379017   0.2852496676
H  -4.0943252259   0.2996840859  -0.4286366909
H  -1.6750120829   0.8895474081   1.3332856646
H  -1.8241864745  -0.0029930852  -1.5751932886
H  -1.6129889006   1.6751425086  -1.0784136809
H   0.4313957742   0.9703798425   0.2482985947
H   0.1343566487  -1.546484613   -0.022630884
H   1.7194921464  -0.8846470959  -0.4367968007
H  -0.4628281913  -1.6771266263  -2.4312139024
H   1.0682133777  -2.4915173418  -2.1749851754
H   1.1179658682  -0.9177446101  -4.1766707388
H   2.3194293991  -0.5003477337  -2.9496615378
H  -0.4102075072   0.8016363233  -3.3154678091
H   2.4148830134   1.9319821641  -3.6069737386
H   0.9095022482   2.8530157727  -3.7601513129
H   1.2970679269   1.586298983   -4.9442436638
```

calc_**1a** conf_11

```
C  -5.7595852361  -0.2566692914   3.2475952216
C  -5.5908745571   1.1114469396   3.0736022628
C  -4.4913006865   1.6271483597   2.3702691899
C  -3.553022837    0.7562781753   1.8555170418
C  -3.6879286862  -0.6333766685   2.0379163465
C  -4.8196089806  -1.1427423241   2.7189952252
O  -5.0221510689  -2.4489137904   2.877794923
O  -6.4727917153   2.0113937456   3.5618025416
C  -2.37408164     1.2167815056   1.0472076124
C  -1.1950020905   0.2917658526   1.2937721885
O  -1.5607398608  -1.0729123854   0.9963299236
C  -2.7028493252  -1.5633871208   1.4983779357
O  -2.8669926044  -2.7795285215   1.4735168184
C   0.0689536681   0.6020150291   0.5011758366
C  -0.1288607863   1.0268353132  -0.9616368371
C   1.2018632585   1.19438877    -1.7036662895
C   1.806156309   -0.1539484345  -2.0910684605
C   0.7665589219  -0.9902173165  -2.8333985935
C  -0.5124910201  -1.1078938458  -2.0114873547
O  -1.0151136248   0.1882970529  -1.6821354501
C  -1.6311747614  -1.8183041364  -2.745493314
H  -6.6173258064  -0.6623948268   3.7747682258
H  -4.4044927303   2.699812803    2.2414300602
H  -4.2929706369  -2.9065928045   2.3849551193
H  -7.1832328362   1.5433136984   4.0198601672
H  -2.1014353509   2.2455001266   1.3024404518
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```
H   -2.6265029431    1.189653535    -0.0189418286
H   -0.945734837     0.3147529137    2.3629944359
H    0.5885875595    1.4233872307    1.0094178557
H    0.7258068877   -0.2699614303    0.5832767655
H   -0.6392720199    1.9967996851   -0.9537608889
H    1.8991861536    1.7810765469   -1.0944808639
H    1.0080571638    1.7707735703   -2.6157118962
H    2.1392674408   -0.694311373    -1.1957453185
H    2.6977018734   -0.0026895251   -2.7088769297
H    1.1545960345   -1.9916616894   -3.0511280816
H    0.5251153906   -0.5174359911   -3.7943718683
H   -0.2947232568   -1.6549413209   -1.0836172459
H   -1.3255477476   -2.8315096306   -3.0215772354
H   -1.8961821193   -1.2720527443   -3.6558877052
H   -2.5178608953   -1.8869756822   -2.1110299874

calc_**1a** conf_12

C   -5.9249304362   -0.5357044603    3.023367344
C   -5.9327495481    0.7211107323    2.4306493957
C   -4.8199116534    1.2010472088    1.723789544
C   -3.6903882079    0.41354019      1.6274774475
C   -3.6499721856   -0.8564930325    2.2357912533
C   -4.7908717957   -1.3421936793    2.9198448433
O   -4.8227724165   -2.5520860826    3.4748141676
O   -7.0064111377    1.5391225048    2.4989154397
C   -2.474580505    0.8384033223     0.8544784903
C   -1.2325511351   0.249924011      1.5003746162
O   -1.3486967947  -1.1874697711     1.6051785448
C   -2.4683131225  -1.704600019      2.1338572706
O   -2.4457970628  -2.8770326212     2.4959931539
C    0.1016520069   0.5494945386     0.8309028825
C    0.2839343806   0.2726486859    -0.6599519715
C    0.001258536   -1.153550631     -1.1232385523
C    0.2218246768  -1.2562354665    -2.6315355269
C   -0.6154792524  -0.1988249825    -3.3500342085
C   -0.369268446    1.2015502644    -2.7823927427
O   -0.5245151953   1.2078755754    -1.3638156141
C    0.961097925    1.8139998562    -3.2134375046
H   -6.7884120403   -0.9191529107    3.5578754103
H   -4.8696799845    2.181971384     1.2655128638
H   -3.9622950418   -2.9881662541    3.2432418765
H   -7.7037315731    1.1046086758    3.0073719725
H   -2.3866625442    1.927625901     0.8212833856
H   -2.5427407253    0.5055401743   -0.1858310882
H   -1.1710680638    0.6268835407    2.5304523962
H    0.3102612171    1.6137617911    0.9880838096
H    0.8687655009   -0.0081235633    1.3793843471
H    1.3444960411    0.4875469289   -0.8728798144
H   -1.0316525228   -1.4215499037   -0.8810244487
H    0.6437198836   -1.8535155311   -0.5788849544
H   -0.0441473751   -2.2556629481   -2.9910165308
H    1.2866785      -1.1187102763   -2.8600682318
H   -1.6774174334   -0.4403202005   -3.2211099434
H   -0.4149677847   -0.2001851171   -4.4273189818
H   -1.1673734363    1.8664882124   -3.1287134356
H    0.9616972095    1.9815810684   -4.2948161512
H    1.8194538072    1.1781347113   -2.9798959479
H    1.1055177357    2.7777181733   -2.717674806
```

calc_**1a** conf_13

```
C  -5.611353231   -0.0793545962   3.9153905794
C  -5.9299432686   0.8710752571    2.953470279
C  -5.2345006433   0.9374809586    1.7361023439
C  -4.2066931543   0.0479831564    1.4987327675
C  -3.8493955103  -0.9107421812    2.4654334342
C  -4.5789262209  -0.9877681595    3.6764709117
O  -4.3137727339  -1.9022419164    4.6062586559
O  -6.9207492054   1.771432269     3.1338144595
C  -3.4398822977   0.028223636     0.2064919027
C  -2.0101512748  -0.4206146265    0.4549246829
O  -1.9991627301  -1.6941746034    1.1361417298
C  -2.7678437108  -1.8580544688    2.2236516664
O  -2.5303376534  -2.8107407214    2.9587590151
C  -1.1742562366  -0.6348831158   -0.7967137274
C  -0.9110904541   0.6257629749   -1.6329207422
C  -0.0209103419   1.6716131779   -0.9545145074
C   1.4396638444   1.2270124628   -0.9149015302
C   1.8951454042   0.8417603103   -2.3203608315
C   0.9501577224  -0.1898649729   -2.9297268694
O  -0.3943966623   0.2801888975   -2.9102727948
C   1.2662711842  -0.5008528822   -4.3791675427
H  -6.1558084881  -0.14665752      4.8520228896
H  -5.5219121513   1.6850848515    1.0058256997
H  -3.6018840694  -2.4834557602    4.232678474
H  -7.3235113967   1.631424187     4.0009357646
H  -3.4493864981   1.01829302     -0.2574696809
H  -3.9142826318  -0.6650867741   -0.5010824661
H  -1.5226774146   0.2985654771    1.125769159
H  -0.2347450528  -1.0974254172   -0.4799933528
H  -1.6837647576  -1.3620378381   -1.4384284117
H  -1.8754737769   1.0885642596   -1.8688667377
H  -0.3914636532   1.8993462622    0.0513130998
H  -0.094120377    2.5985933685   -1.5352333722
H   1.5606314279   0.3706838576   -0.2392935934
H   2.0667534911   2.0286827242   -0.5110671041
H   2.9157374      0.4429193774   -2.3072004912
H   1.8998225605   1.7311085845   -2.9638727062
H   1.0221335779  -1.1202636186   -2.343475163
H   2.2781613072  -0.9050424815   -4.4743901588
H   1.1940314173   0.4071154324   -4.9850300289
H   0.5588862596  -1.2336528485   -4.775205702
```

calc_**1a** conf_14

```
C  -5.75895123     0.0108768015    3.6460255225
C  -5.9975405948   0.7447655917    2.4908218592
C  -5.1512827634   0.6439913943    1.375768987
C  -4.0548012028  -0.1917681642    1.4362625852
C  -3.7783053389  -0.9301542729    2.6020360153
C  -4.6572224267  -0.8439390408    3.7087738575
O  -4.4703316052  -1.5538051872    4.8186985801
O  -7.0507849942   1.5834282568    2.3773480379
C  -3.1234567599  -0.3862457057    0.2732751008
C  -1.717637622   -0.6754325483    0.7708724959
O  -1.7292450055  -1.7983249858    1.6780501859
C  -2.6259054977  -1.8209286524    2.6751253741
```

```
O   -2.440310754    -2.6049894733    3.5999725747
C   -0.7204408531   -1.0531644058   -0.3108948549
C   -0.4411565952    0.0251358657   -1.3524750777
C    0.1509273404    1.3098931558   -0.7768819728
C    0.5699649275    2.2575472498   -1.8998333464
C    1.4875298188    1.530099801    -2.8800212354
C    0.8613690936    0.2213570329   -3.367547993
O    0.4614301957   -0.5837021004   -2.2618267005
C   -0.2674245526    0.4162877736   -4.3763848595
H   -6.418927579     0.0713516657    4.5057349906
H   -5.3791565571    1.2228056754    0.4881074023
H   -3.6858343959   -2.1371540298    4.6487381247
H   -7.5579658288    1.5691449072    3.1996663336
H   -3.1186645595    0.5007743956   -0.3665294312
H   -3.4649516647   -1.2279145697   -0.344454451
H   -1.3565349701    0.1884648023    1.3430287045
H   -1.0808307205   -1.9486971531   -0.8278877031
H    0.2251901358   -1.3249521222    0.1691498975
H   -1.3770218536    0.2756710822   -1.8792787744
H    1.0247756501    1.0469950082   -0.1666337076
H   -0.5729345435    1.8004120931   -0.1155903112
H    1.0749353897    3.1377282286   -1.488504195
H   -0.3228313735    2.6288233922   -2.4189951272
H    1.7334772577    2.1675549941   -3.736618314
H    2.4303484691    1.2905631159   -2.3743212935
H    1.6379408379   -0.3806653597   -3.8503296707
H   -1.060021456     1.0733228871   -4.007571187
H   -0.7141336157   -0.5500538816   -4.6252035525
H    0.1247177973    0.8598964824   -5.2966728706

calc_1a conf_15

C   -5.7652652314   -0.7110813385    2.2179141988
C   -5.7252099573    0.6682988225    2.3767283573
C   -4.5050535319    1.3544500149    2.4873465157
C   -3.325432795     0.6423686406    2.4288773054
C   -3.3372117081   -0.7544447318    2.2507881848
C   -4.5742640201   -1.4375628701    2.1628248655
O   -4.6465667471   -2.7591116945    2.0261200264
O   -6.8471624612    1.4175854827    2.4374243364
C   -1.9800395477    1.2864001892    2.6008583669
C   -0.9181958711    0.5548084438    1.7892401171
O   -0.9285151425   -0.8521052207    2.1164748173
C   -2.0959235278   -1.5128822613    2.1637005884
O   -2.0581437464   -2.7396273404    2.1363576021
C   -1.0370493366    0.7677327722    0.2835453734
C    0.1188315004    0.1713770251   -0.540503847
C   -0.0213741532   -1.3131512053   -0.8849311985
C   -1.0786523263   -1.5418694808   -1.9627993486
C   -0.7924710736   -0.6479664135   -3.1663332244
C   -0.6488099901    0.8071876781   -2.7307721779
O    0.3425561071    0.9393560826   -1.7177794308
C   -0.2254390915    1.7267860552   -3.8591473435
H   -6.7051122506   -1.2491405312    2.1442943724
H   -4.5162445126    2.4298082603    2.622071466
H   -3.7134525349   -3.0951072258    2.0523026175
H   -7.6190666321    0.8425621558    2.3518293925
H   -1.6988547074    1.2492104528    3.6611291577
H   -2.0062109685    2.3412815425    2.3137030039
```

```
H    0.0737295959    0.8781588678    2.1165079572
H   -2.0126392424    0.4071043127   -0.0589522329
H   -1.0206514772    1.8502261258    0.1109706198
H    1.0404798662    0.3122825593    0.0366016618
H   -0.2369342914   -1.8928660816    0.0159612163
H    0.9486855894   -1.6543516239   -1.2658520133
H   -2.0804411493   -1.3220706938   -1.5704421957
H   -1.0919695702   -2.5963440006   -2.2571548426
H   -1.5861565211   -0.7300462673   -3.9179218433
H    0.1448235723   -0.9600561701   -3.6449808099
H   -1.6206634075    1.1509427483   -2.3372652134
H   -0.1274582597    2.7543523016   -3.4996139109
H   -0.9602513735    1.7082165921   -4.669265546
H    0.7427809258    1.4112880251   -4.2588569417
```

calc_**1a** conf_16

```
C   -5.8528468508   -0.8767026667    2.6097247782
C   -5.9175756005    0.5068038721    2.7156381648
C   -4.7606137072    1.2989111158    2.6406352896
C   -3.5392272393    0.6883093806    2.447353547
C   -3.4477874955   -0.7106210503    2.3168620327
C   -4.6184055071   -1.5002434241    2.4189134003
O   -4.5873018038   -2.8281153889    2.3374021005
O   -7.0856368706    1.159287899     2.9006034389
C   -2.2465632717    1.4518824365    2.4192222262
C   -1.2389881394    0.7825749785    1.4928742156
O   -1.0809386375   -0.6075431089    1.8529738937
C   -2.1656468156   -1.3630466663    2.0850066458
O   -2.0194521691   -2.5818506176    2.0967614087
C   -1.571453685     0.9383520104    0.014724098
C   -0.5264360684    0.3798994801   -0.9508007093
C   -0.635791394    -1.1206469858   -1.2075801887
C    0.3419274161   -1.5483362957   -2.3001397796
C    0.1347030379   -0.6924865678   -3.547425869
C    0.1827468848    0.8009710494   -3.2151883189
O   -0.7169651403    1.1126858911   -2.1550655405
C    1.5915334263    1.322444758    -2.9418168749
H   -6.7416128076   -1.495891786     2.6800041289
H   -4.8513764333    2.374290987     2.7402605484
H   -3.6320071958   -3.0808972748    2.2492354678
H   -7.8070127752    0.5171368687    2.9332859276
H   -1.8272298436    1.4821542161    3.4330360358
H   -2.4060264626    2.4880577757    2.1080204313
H   -0.2452991909    1.1994033456    1.6780102629
H   -1.6448932501    2.0125461366   -0.1885810116
H   -2.555059524     0.5087885995   -0.2061471744
H    0.4764145736    0.5967858181   -0.5441585879
H   -1.6627743876   -1.3383523094   -1.529871505
H   -0.4582715609   -1.6741658554   -0.2819352008
H    0.2053878333   -2.6080337673   -2.539543484
H    1.3712937336   -1.4462927338   -1.9334163267
H    0.8790679807   -0.9249377613   -4.3175154056
H   -0.8507198383   -0.9171547543   -3.9725899585
H   -0.2207127375    1.3632179267   -4.0639974818
H    1.5480128375    2.3742526296   -2.646086418
H    2.2027598561    1.2455896335   -3.8463414578
H    2.1037788231    0.7669722056   -2.1513467499
```

S44

calc_**1a** conf_17

```
C   -5.9467511321   -0.2222408025    2.9318451372
C   -6.095565431     0.0277006989    1.5731809724
C   -5.0324392026   -0.1595262301    0.6773458514
C   -3.8117626376   -0.5875085188    1.1594486027
C   -3.6288366603   -0.8274008321    2.5337928143
C   -4.7178654558   -0.6650673312    3.4235202661
O   -4.6123965558   -0.920974638     4.7256579702
O   -7.2644059365    0.4558153582    1.0459138802
C   -2.6379729261   -0.845974965     0.2568540567
C   -1.3415102975   -0.5633291333    0.9913867048
O   -1.290186581    -1.3116544889    2.2296214691
C   -2.3453096765   -1.2855250369    3.0533635708
O   -2.1860330973   -1.6655999609    4.2096215134
C   -0.0528007369   -0.9431933285    0.274302488
C    0.2331373776   -0.1958065441   -1.0341523584
C   -0.3074575899   -0.8699979747   -2.294310351
C   -0.0113900054   -0.0033050431   -3.5171754237
C   -0.5362545186    1.4138716106   -3.2914436356
C   -0.023916547     2.0060948022   -1.9761369363
O   -0.2860706319    1.1182134475   -0.8905684098
C    1.4388988078    2.4383601176   -2.0208699611
H   -6.7696214988   -0.0951375178    3.6283196561
H   -5.1911539695    0.0361927114   -0.3768111352
H   -3.6962707622   -1.2762889215    4.8657381879
H   -7.9153199912    0.5507759067    1.7536249152
H   -2.6893455107   -0.206099947    -0.62649017
H   -2.6520916288   -1.8906125597   -0.0827035802
H   -1.3077666676    0.4989957969    1.2508708014
H   -0.0525994886   -2.022596958     0.0845816068
H    0.7564846813   -0.7518990657    0.9853137818
H    1.3280739619   -0.1444795748   -1.1431657527
H   -1.3884849925   -1.0244472265   -2.2045630974
H    0.1515439016   -1.8598823909   -2.3980746941
H   -0.4642787925   -0.4356383266   -4.4154663583
H    1.0711216333    0.017342786    -3.6966243446
H   -0.2632474724    2.071824456    -4.1239382381
H   -1.6320059429    1.3857657332   -3.2515613272
H   -0.6235586143    2.8888120831   -1.7315959152
H    1.5633788354    3.261531834    -2.7310189182
H    2.1131651981    1.6344927533   -2.3287304339
H    1.7538665547    2.7873972213   -1.0339032055
```

calc_**1a** conf_18

```
C   -5.9614232783   -0.1246225212    3.0356710715
C   -6.2929897444   -0.320554015     1.7008087831
C   -5.331100221    -0.7249354769    0.7623518646
C   -4.0281378623   -0.9169068504    1.1749850493
C   -3.6618043994   -0.7052424847    2.5168999578
C   -4.6473591942   -0.32939477      3.4602722764
O   -4.3650009828   -0.161917846     4.7502039807
O   -7.5505314155   -0.1396578066    1.2392804281
C   -2.94310813    -1.3856299967     0.2474282861
C   -1.6091844758   -0.7878748842    0.6622088773
O   -1.3409661595   -1.1377710696    2.0417960674
C   -2.288618742    -0.9165756802    2.96263542
O   -1.9601988129   -0.9191906011    4.1450149802
```

```
C  -0.4004307954  -1.2770945746  -0.1287867228
C   0.0143686653  -0.3940386178  -1.3032624243
C  -1.0022079756  -0.256059154   -2.4339468916
C  -0.458018345    0.6864900286  -3.506291062
C  -0.0737131817   2.0200174222  -2.8664728969
C   0.8636279996   1.8275985511  -1.6712151531
O   0.3259945958   0.8763934415  -0.7546073799
C   2.3000208185   1.4923300598  -2.0630697088
H  -6.7045696185   0.1712357218   3.7695401818
H  -5.6323348896  -0.8799931054  -0.2672622541
H  -3.4115100325  -0.4138331234   4.8615698384
H  -8.1194564972   0.1364209751   1.9698408801
H  -3.1755536186  -1.1216533478  -0.7869165971
H  -2.8661932811  -2.4808953023   0.2894023527
H  -1.6537598933   0.3056729441   0.6142198289
H  -0.5624643005  -2.3024211256  -0.4811484884
H   0.4432226778  -1.3032624552   0.5663994399
H   0.9250588197  -0.8476249981  -1.7269692169
H  -1.9345977678   0.1622790682  -2.0355484724
H  -1.2330661746  -1.242565678   -2.8527209634
H  -1.2013859643   0.8451704091  -4.294474214
H   0.4138004187   0.2278559378  -3.9900464373
H   0.3933094799   2.6879232193  -3.5986397381
H  -0.9846403491   2.517720782   -2.5129081237
H   0.8857512001   2.7554649631  -1.0907534195
H   2.3719795188   0.6121610745  -2.7080764755
H   2.8954852467   1.3061489832  -1.1654423422
H   2.7467066621   2.3328319034  -2.6029705823

calc_1a conf_19

C  -5.841627879   -0.1987831443   2.5892284915
C  -5.4803007121   1.1341051437    2.4399827648
C  -4.136546218    1.5124685478    2.2912999889
C  -3.1608589211   0.5375042062    2.2834755146
C  -3.5014001654  -0.8220443399    2.4111130429
C  -4.8571119479  -1.1888869135    2.5866110139
O  -5.2336278406  -2.4548479614    2.7499036395
O  -6.3926305738   2.1302521537    2.4367233846
C  -1.6968605418   0.8581572079    2.1970774685
C  -0.9413424688  -0.2440449391    1.4660947051
O  -1.2152238757  -1.5241523115    2.0777567416
C  -2.4784481091  -1.8608813309    2.3819115081
O  -2.7114164595  -3.0383254174    2.6359631258
C  -1.2199050234  -0.343193173   -0.0323416953
C  -0.6455735938   0.8107908717   -0.8693054476
C   0.8823650686   0.8183908079   -0.9811976109
C   1.3853105513  -0.2842229982   -1.9103424458
C   0.6612436893  -0.1961012716   -3.2513494166
C  -0.8507551636  -0.1954902131   -3.0477702025
O  -1.2407575973   0.8470811437   -2.1584612561
C  -1.6236181647   0.0346784137   -4.3312428802
H  -6.8771601453  -0.4971148397    2.7194303712
H  -3.8938395997   2.5639636248    2.1909053046
H  -4.4006998274  -2.9935708001    2.7699469322
H  -7.2758987162   1.7526487623    2.5413895055
H  -1.2882863843   0.9478532191    3.2117130062
H  -1.533581913    1.8213498283    1.7060469507
H   0.1307253853  -0.1188153741    1.633518704
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S46

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H   -0.8160768681   -1.3034813844   -0.3667792679
H   -2.3012054357   -0.3711069765   -0.204909131
H   -0.9668133052    1.7556372295   -0.4170772547
H    1.3441380589    0.7377522273    0.0093531799
H    1.1813647169    1.7909159733   -1.3895567647
H    1.2125343282   -1.2705967551   -1.4613185225
H    2.4678792713   -0.1949091454   -2.0485769515
H    0.944152539    -1.028579554    -3.9054170715
H    0.9430419677    0.7328279467   -3.7638716208
H   -1.1479535193   -1.1682197112   -2.6234506016
H   -1.4013850899   -0.7496212985   -5.06050134
H   -1.355289726     1.0021926872   -4.7654991095
H   -2.6985597907    0.0344198581   -4.1344767536

calc_1a conf_20

C   -5.8224991423   -0.2662873471    2.5047814668
C   -5.4949338161    0.9962516178    2.0277402624
C   -4.1586447681    1.3714103267    1.8164549582
C   -3.1558697407    0.4612093921    2.0789298663
C   -3.4614021345   -0.8322648325    2.5419042062
C   -4.8105120217   -1.1893926705    2.7767974088
O   -5.1558275184   -2.3839539446    3.2505302608
O   -6.4350829205    1.9264230377    1.7506906334
C   -1.6986821384    0.7969840914    1.9461712391
C   -0.899046535    -0.4290493967    1.5256738066
O   -1.1492904679   -1.5216660971    2.4370311968
C   -2.4089861456   -1.8100399419    2.7975583763
O   -2.6165007842   -2.8889623658    3.3432091085
C   -1.1508990009   -0.9187084859    0.1026667852
C   -0.7433326412    0.0450974895   -1.0073980784
C    0.7394450608    0.411647889    -1.0048296368
C    1.0939698173    1.2252813358   -2.2490588125
C    0.6313578422    0.4886322283   -3.5043059
C   -0.8454562225    0.0977078276   -3.4110938421
O   -1.0943573553   -0.6240470209   -2.2080058045
C   -1.8060307103    1.270306718    -3.5905903138
H   -6.8525328035   -0.5579186355    2.6844377079
H   -3.942564549     2.3714873153    1.4588253466
H   -4.3089007885   -2.8708537067    3.4249174348
H   -7.3095093247    1.5581763331    1.9335934784
H   -1.3202697212    1.1447396399    2.9159398718
H   -1.5435323534    1.6127353962    1.2347159866
H    0.1659482541   -0.2328628131    1.6655160471
H   -2.212578397    -1.1526602768   -0.0267088279
H   -0.5989919023   -1.8541756481   -0.0356749457
H   -1.3346611758    0.9714777464   -0.9214045023
H    1.3263136173   -0.5158614974   -0.9864593742
H    0.991768669     0.975540097    -0.0990435827
H    2.1729254753    1.4071783284   -2.2915506409
H    0.617244381     2.2120917594   -2.1900006504
H    0.8010562566    1.0947328404   -4.4012132058
H    1.2214477555   -0.4283792148   -3.6168856542
H   -1.0649231149   -0.6344898889   -4.1948833576
H   -2.8348354499    0.9348406848   -3.4351672912
H   -1.7246412879    1.6691726279   -4.6063845523
H   -1.6081821973    2.0934490618   -2.8984264755

calc_1a conf_21
```

```
C  -5.8695402111  -0.1997215474   3.2145434085
C  -5.7512769287   1.0981961222   2.7334596497
C  -4.624316131    1.5049160121   2.0031784173
C  -3.6089986816   0.5987042017   1.7731338859
C  -3.6936004353  -0.7161210332   2.2676425543
C  -4.8501718641  -1.123091694    2.9749537106
O  -5.0031746974  -2.3659427309   3.4259758875
O  -6.7104841541   2.0291499821   2.935981009
C  -2.3898337737   0.9347353351   0.9632941518
C  -1.195708564    0.1584002931   1.4881190889
O  -1.4764433512  -1.2557101662   1.4927005816
C  -2.6248805554  -1.6826565651   2.0298517971
O  -2.7324507526  -2.8764241631   2.2954224361
C   0.1110205832   0.3631438099   0.7291486564
C   0.0327809098   0.4671819469  -0.7893327933
C   1.4224634663   0.6162165506  -1.4070093283
C   1.3392707303   0.5868255851  -2.9309827447
C   0.5866921829  -0.6642349093  -3.3785566251
C  -0.7708989636  -0.7843113665  -2.6818772397
O  -0.6219475384  -0.6935747897  -1.2662407266
C  -1.8198016378   0.1885371946  -3.2150065649
H  -6.7462441672  -0.5252615089   3.7657142498
H  -4.5755634027   2.5223197274   1.6325245261
H  -4.2127212531  -2.8759380653   3.1074233214
H  -7.4305324492   1.6356821218   3.4461799117
H  -2.1809744709   2.008602688    0.9952772856
H  -2.5570886729   0.6582031325  -0.0840056569
H  -1.0276926961   0.4404534016   2.5362736175
H   0.7778058909  -0.4618448178   1.0011885994
H   0.5744026239   1.2849531499   1.1000591965
H  -0.5566782549   1.3617840875  -1.0544287392
H   2.0484805968  -0.214361197   -1.0565087121
H   1.8860830084   1.5454905373  -1.0561172794
H   2.3422059517   0.6042818348  -3.3702663529
H   0.8284223735   1.4888539469  -3.290943878
H   0.4473119372  -0.6736373231  -4.4652931958
H   1.1821906475  -1.5481798153  -3.1218090481
H  -1.1523488533  -1.7993175981  -2.8305248082
H  -2.7571142532   0.0679301389  -2.6648596134
H  -2.0192872766  -0.0166402289  -4.2713186923
H  -1.5093569124   1.2344077197  -3.1369639438

calc_**1a** conf_22

C  -5.5704414552   0.1482927901   1.6128158626
C  -5.2346277469   1.4568986853   1.9354385566
C  -3.9179088812   1.8086117732   2.2671213414
C  -2.9402160523   0.8327441474   2.2592901192
C  -3.2492679948  -0.4946341883   1.9227814866
C  -4.5850650141  -0.8408920397   1.6091515287
O  -4.9426661917  -2.0866015221   1.3087841265
O  -6.151470946    2.4507859228   1.9531276032
C  -1.5258852258   1.1138962282   2.6742241541
C  -0.51519802     0.2040453574   1.9809940664
O  -0.9294348379  -1.1749283334   2.0204034031
C  -2.2146988672  -1.5199319438   1.8667758234
O  -2.4660248898  -2.712429649    1.7159818931
C  -0.0933132179   0.6159565013   0.568988925
```

S48

```
C  -1.1662708349   0.6794678882  -0.526469378
C  -0.6524172109   1.3483528703  -1.8061806564
C   0.2948651659   0.4350501047  -2.5803922745
C  -0.3832602883  -0.9117860597  -2.8181608311
C  -0.8867372102  -1.5111332504  -1.5080152556
O  -1.7322867935  -0.5908394782  -0.8186392726
C  -1.7063557114  -2.7698238796  -1.712409705
H  -6.5889037754  -0.1334757566   1.3643539404
H  -3.6960666695   2.8368147685   2.5289764521
H  -4.1219750337  -2.6380396599   1.393345295
H  -7.0133922323   2.0895110477   1.708534045
H  -1.4452525087   0.9573816509   3.7575059564
H  -1.261588008    2.1596690322   2.4900908903
H   0.3976933926   0.1999415295   2.5831935308
H   0.3574889134   1.6124954902   0.6608435271
H   0.7186752227  -0.0520780316   0.2649847045
H  -2.0112373653   1.2646510003  -0.1502120192
H  -0.1757761199   2.3050898807  -1.5641745129
H  -1.5209171799   1.5727699201  -2.4363303088
H   1.2274660681   0.2880625548  -2.0205239155
H   0.5762435235   0.9001038458  -3.5312607359
H   0.3015485462  -1.6177068708  -3.3015434532
H  -1.2406897739  -0.777836682   -3.4904634874
H  -0.0211543193  -1.7541231319  -0.872282649
H  -2.5910788986  -2.5492265914  -2.3172688224
H  -2.0309966668  -3.1707169254  -0.7504326576
H  -1.1124048912  -3.530388996   -2.2279472963

calc_**1a** conf_23

C  -5.8153531164  -0.905058447    2.271835407
C  -5.7580109645   0.1913598777   1.4209133233
C  -4.5375083458   0.813473724    1.1150567706
C  -3.3726950571   0.3155667941   1.6632929163
C  -3.400773544   -0.8073597564   2.5116457839
C  -4.6406550628  -1.4075330937   2.8358336117
O  -4.7306165157  -2.4444868288   3.6652766558
O  -6.8656122051   0.7182879519   0.8526274522
C  -2.03114255     0.9491122473   1.4443900304
C  -0.9296270483  -0.0979429928   1.4447062371
O  -0.9914677909  -0.8759742439   2.6646625858
C  -2.171784451   -1.3502187765   3.0847004765
O  -2.1684605867  -2.2215679076   3.9497110479
C  -0.900345281   -1.0814962783   0.2724181961
C  -0.6402327485  -0.4629872253  -1.1090983538
C  -1.9026010596  -0.1416323857  -1.9076795971
C  -1.5353830357   0.5447740784  -3.2225184865
C  -0.6371091524   1.7496360429  -2.9499621774
C   0.5743925899   1.3697101343  -2.0953209734
O   0.1570552967   0.696185716   -0.9086812024
C   1.6432379673   0.5862625462  -2.8518654454
H  -6.7576656412  -1.380298544    2.5259914266
H  -4.5361859046   1.6799675986   0.4637726244
H  -3.8106299829  -2.6135730542   3.998683564
H  -7.6389161775   0.2152647498   1.1400168451
H  -1.832016968    1.6540061766   2.2622372501
H  -1.9887678852   1.5222747457   0.5169721813
H   0.0375555522   0.3991039162   1.501179726
H  -0.1070564921  -1.7974858833   0.5071466294
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S49

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H  -1.8371066076  -1.6487812351   0.2384854844
H  -0.0670557174  -1.1989146247  -1.6945780843
H  -2.5661175205   0.5042574259  -1.321553159
H  -2.4525682217  -1.0711884266  -2.0937516259
H  -2.4376733702   0.85810904    -3.7578500639
H  -1.0212642268  -0.1700971175  -3.8776117069
H  -1.2137639821   2.5097089438  -2.4089849424
H  -0.3004112846   2.2092689438  -3.8858736645
H   1.0389352598   2.2860670838  -1.7168866618
H   2.0777165001   1.2106871917  -3.6384325372
H   1.2526366364  -0.3172581925  -3.3276237567
H   2.4430486956   0.2917700852  -2.1672837874
```

calc_**1a** conf_24

```
C  -5.9792167008  -0.7194278962   3.3468630007
C  -6.2107189118   0.5458894058   2.8218163626
C  -5.2654057462   1.1771502779   1.9988959048
C  -4.0777394905   0.5327889793   1.7188440648
C  -3.8088662167  -0.7413464428   2.2553796434
C  -4.7847328884  -1.3809654497   3.0585682217
O  -4.6042441564  -2.6023860332   3.5553536237
O  -7.3500835578   1.2284603928   3.067969247
C  -3.035216657    1.1261921761   0.8135518385
C  -1.6515227337   0.6622939547   1.2415051303
O  -1.5908844085  -0.7774579807   1.3137024253
C  -2.5620366301  -1.4382140346   1.963117594
O  -2.3560366002  -2.6084360836   2.2673321665
C  -0.4904056578   1.1257853984   0.3657541965
C  -0.1405464005   0.279276469   -0.8582578547
C  -1.2311319139   0.1385054395  -1.9152808192
C  -0.6826310819  -0.5721934792  -3.1527833546
C   0.5792810596   0.1287292629  -3.648596838
C   1.601850118    0.2991124949  -2.5223897787
O   1.0005658813   0.9357094086  -1.399152485
C   2.3175825164  -0.9932705527  -2.1383138841
H  -6.7126280318  -1.2206646646   3.9706272091
H  -5.4886016026   2.1593179216   1.5984918667
H  -3.7383515745  -2.9263661416   3.1960740619
H  -7.9192995463   0.7004886761   3.6432701656
H  -3.0696171183   2.2192822028   0.8493239916
H  -3.2349851712   0.8355239395  -0.2236290088
H  -1.484002271    1.033936584    2.2606762776
H  -0.6879179564   2.1529126433   0.0378647438
H   0.4180563466   1.1658946181   0.9738117743
H   0.1355783838  -0.7253669682  -0.5099168826
H  -1.5951403698   1.1372900217  -2.1909645294
H  -2.0732801226  -0.4274887808  -1.5048644088
H  -1.4389966855  -0.5973759911  -3.9443327778
H  -0.4634118431  -1.6176065744  -2.9026091294
H   0.3116726138   1.1247025784  -4.0214421738
H   1.0312604921  -0.4179533847  -4.4838958103
H   2.3626497218   1.0177855332  -2.844964136
H   2.9813542745  -0.8115435948  -1.2888165388
H   2.9233470176  -1.3504607146  -2.9769335079
H   1.62845362    -1.7965036111  -1.8636495924
```

calc_**1a** conf_25

```
C   -5.68044338     -0.4532429345    2.2736636696
C   -5.5480286316    0.8250336917     2.8004363497
C   -4.2894487515    1.4316522988     2.9319453106
C   -3.1648945766    0.7457578627     2.5189520017
C   -3.2736124414   -0.5424249857     1.9627671609
C   -4.5450752368   -1.1537121247     1.8607988164
O   -4.7013887219   -2.3857614718     1.3817377183
O   -6.6140155437    1.5454838309     3.2162236229
C   -1.7768167134    1.3018722149     2.6737671881
C   -0.8770814493    0.7967885583     1.5531056806
O   -0.9107328955   -0.6423394063     1.5068997218
C   -2.0916802617   -1.2759116064     1.5193195708
O   -2.1172333825   -2.4588192212     1.1988481451
C   -1.2185040546    1.4351204079     0.2041939693
C   -0.6320835718    0.7779589098    -1.0433813744
C    0.8439487523    0.3995185775    -0.9443236081
C    1.2815812196   -0.3350293802    -2.2099205203
C    0.3561347944   -1.5266985445    -2.4494028156
C   -1.114461144    -1.102782469     -2.4730154276
O   -1.4462484479   -0.3513382341    -1.3092400126
C   -1.5252332604   -0.3760788375    -3.7514327005
H   -6.6490838141   -0.9347132374     2.1827320235
H   -4.2262411451    2.4257621393     3.359349733
H   -3.788409127    -2.7310656307     1.2010749564
H   -7.4188516332    1.0297523803     3.075477754
H   -1.3618810256    0.9807437209     3.6375692481
H   -1.7901797284    2.3959973947     2.6785397155
H    0.166402709     1.0072991872     1.7980465973
H   -0.8737675126    2.4752131794     0.2540362624
H   -2.3044089825    1.4665195038     0.0682538038
H   -0.7414414707    1.5051589533    -1.8660143883
H    0.987953495    -0.2591026198    -0.0816817739
H    1.4460324215    1.3025668766    -0.7851329788
H    2.3188772977   -0.6736004484    -2.1168992169
H    1.2545275117    0.3503059603    -3.0670073075
H    0.6069683795   -2.0396541937    -3.384642764
H    0.4881399889   -2.2483700593    -1.6353844605
H   -1.7365251741   -1.998299395     -2.3806233893
H   -0.9136016609    0.5079218438    -3.9530556563
H   -2.5686650026   -0.0578526052    -3.678750321
H   -1.4295278282   -1.0456300873    -4.6118303045
```

calc_**1a** conf_26

```
C   -5.4276304476    0.0479316898     1.3697794818
C   -5.1186574388    1.3877192406     1.5706642129
C   -3.836734173     1.7834389604     1.9778173302
C   -2.8653372106    0.820193832      2.173917798
C   -3.1428572909   -0.5384098105     1.9534833261
C   -4.4476313557   -0.9258046545     1.5671525989
O   -4.7739218738   -2.2017414873     1.3635851577
O   -6.0306822251    2.3700500968     1.39250661
C   -1.5065523776    1.1574962024     2.7121951104
C   -0.4304203024    0.1652447773     2.2790476493
O   -0.8666378422   -1.1972518725     2.4331665221
C   -2.1180987688   -1.5635032746     2.1384528601
O   -2.3655365848   -2.7636532059     2.0797377522
C    0.1903519473    0.4040875044     0.9029286517
C   -0.668701723     0.3234613341    -0.3568689517
```

```
C   0.0817380405    0.9409672784   -1.539017758
C  -0.6310290238    0.6586535808   -2.8571716061
C  -0.8557121972   -0.8438976373   -2.9925937961
C  -1.6005906597   -1.406183706    -1.7806705811
O  -0.9340912045   -1.0543928721   -0.5668101247
C  -3.0824040557   -1.0472427905   -1.7574608351
H  -6.4206298284   -0.2685388338    1.0660058801
H  -3.6381409146    2.8356416757    2.1466178862
H  -3.965395224    -2.7320749958    1.5997408257
H  -6.8705941887    1.9762084159    1.1223701343
H  -1.5633648708    1.1511821171    3.8082635323
H  -1.2078392518    2.1695182971    2.4222467186
H   0.3940862413    0.2365572351    2.993883564
H   1.0063016247   -0.3158735601    0.7771360032
H   0.6496862475    1.400029717     0.9453361518
H  -1.6127026285    0.8727712995   -0.2151144622
H   1.0922932701    0.5122482237   -1.5722997774
H   0.1917224399    2.0190990489   -1.3735793489
H  -0.041618796     1.03658795     -3.6992729112
H  -1.5897854454    1.1916009322   -2.8836977229
H  -1.4106209874   -1.081752204    -3.9066739691
H   0.1174259754   -1.3442726165   -3.0653509564
H  -1.5222288219   -2.4976887377   -1.7994802641
H  -3.5588882705   -1.3732781557   -2.6876902737
H  -3.2551731624    0.0278555582   -1.6550632104
H  -3.5813966411   -1.5529845527   -0.9292192084


calc_**1a** conf_27

C  -5.5098594803   -0.2213091951    1.4827671242
C  -5.2544179095    1.1428858401    1.5453841515
C  -3.9865838125    1.630095684     1.8967073734
C  -2.9720468988    0.7338743277    2.1730889227
C  -3.2010056159   -0.6510653808    2.1061496358
C  -4.4917367573   -1.1311279824    1.7729539389
O  -4.7733609347   -2.4302604908    1.7224010454
O  -6.2052423695    2.0651909762    1.2799040183
C  -1.6139421406    1.1832581144    2.628412193
C  -0.5032775295    0.1904732567    2.2923994875
O  -0.8920830366   -1.166660292     2.5973721763
C  -2.1373153588   -1.6083756758    2.3911737085
O  -2.3335392286   -2.817793143     2.4663798909
C   0.126192383     0.2454001863    0.9006982848
C  -0.7419928577    0.0301155522   -0.3393271181
C  -1.3921126716    1.3002729008   -0.8824582952
C  -2.1000030648    1.0151244902   -2.2057176093
C  -1.1298520343    0.3554649064   -3.1830270386
C  -0.4424387225   -0.8600842533   -2.5557430568
O   0.1497132757   -0.5111518948   -1.3073943456
C  -1.3440595836   -2.0870699496   -2.4430353625
H  -6.4913869411   -0.6062302655    1.2245476197
H  -3.8306209602    2.701551305     1.9500138995
H  -3.9470563519   -2.9052023015    2.0027668109
H  -7.0309821083    1.6156083489    1.0568868385
H  -1.6459072843    1.3080201506    3.7183378877
H  -1.3625642968    2.1625687913    2.2103923558
H   0.3172147939    0.3668214476    2.9926506205
H   0.8914347268   -0.5365315276    0.880698236
H   0.6568997752    1.2017450837    0.8111891571
```

```
H  -1.5275683669  -0.7068844198  -0.1168451074
H  -0.6014826184   2.0458062265  -1.0410315994
H  -2.097233413    1.711751426   -0.1543818085
H  -2.497885376    1.9415040276  -2.6335152338
H  -2.9638027597   0.3633718597  -2.0247185378
H  -1.6393286161   0.0595954021  -4.1070410725
H  -0.3559364524   1.0815157561  -3.459540653
H   0.4173850785  -1.1355980961  -3.1753490988
H  -2.2754814009  -1.8867970061  -1.90610862
H  -0.8170255689  -2.8886172906  -1.9187990264
H  -1.6117075109  -2.4472568953  -3.4412417928
```

Table S28. Sampled and DFT geometry optimized conformers related to calc_**1b**, with energy values (Hartree) and related % contribution on the final Boltzmann distribution for the three employed functional/basis set combinations.

Conformer	MPW1PW91/6-31g(d,p)		MPW1PW91/6-311+g(d,p)		B97-2/cc-pVTZ	
	Energy (Hartree)	% contribution on the Boltzmann distribution	Energy (Hartree)	% contribution on the Boltzmann distribution	Energy (Hartree)	% contribution on the Boltzmann distribution
calc_**1b** conf_1	-997.7082456	19.24%	-997.9430329	22.99%	-997.9016822	22.15%
calc_**1b** conf_2	-997.7082366	19.06%	-997.9426204	14.85%	-997.9010254	11.05%
calc_**1b** conf_3	-997.7080968	16.44%	-997.9428186	18.32%	-997.9017245	23.16%
calc_**1b** conf_4	-997.7075007	8.74%	-997.9415396	4.73%	-997.9000598	3.97%
calc_**1b** conf_5	-997.7072530	6.73%	-997.9418359	6.47%	-997.9003408	5.35%
calc_**1b** conf_6	-997.7072304	6.57%	-997.9422580	10.12%	-997.9012476	13.98%
calc_**1b** conf_7	-997.7069103	4.68%	-997.9416668	5.41%	-997.8997560	2.88%
calc_**1b** conf_8	-997.7068459	4.37%	-997.9414214	4.17%	-997.8997007	2.72%
calc_**1b** conf_9	-997.7066271	3.47%	-997.9406073	1.76%	-997.8995792	2.39%
calc_**1b** conf_10	-997.7064987	3.03%	-997.9413636	3.92%	-997.9004836	6.22%
calc_**1b** conf_11	-997.7064751	2.95%	-997.9409618	2.56%	-997.8994905	2.17%
calc_**1b** conf_12	-997.7056865	1.28%	-997.9399959	0.92%	-997.8980080	0.45%
calc_**1b** conf_13	-997.7052806	0.83%	-997.9402889	1.26%	-997.8986986	0.94%
calc_**1b** conf_14	-997.7045734	0.39%	-997.9389238	0.30%	-997.8970238	0.16%
calc_**1b** conf_15	-997.7045361	0.38%	-997.9385410	0.20%	-997.8965329	0.09%
calc_**1b** conf_16	-997.7044740	0.35%	-997.9390994	0.36%	-997.8978334	0.38%
calc_**1b** conf_17	-997.7043919	0.32%	-997.9389223	0.30%	-997.8977294	0.34%
calc_**1b** conf_18	-997.7043755	0.32%	-997.9392081	0.40%	-997.8978188	0.37%
calc_**1b** conf_19	-997.7041880	0.26%	-997.9384613	0.18%	-997.8968367	0.13%
calc_**1b** conf_20	-997.7035032	0.13%	-997.9385881	0.21%	-997.8976405	0.31%
calc_**1b** conf_21	-997.7034597	0.12%	-997.9377278	0.08%	-997.8974459	0.25%
calc_**1b** conf_22	-997.7030853	0.08%	-997.9380240	0.11%	-997.8967727	0.12%
calc_**1b** conf_23	-997.7029295	0.07%	-997.9378796	0.10%	-997.8969067	0.14%
calc_**1b** conf_24	-997.7027131	0.05%	-997.9376709	0.08%	-997.8968085	0.13%
calc_**1b** conf_25	-997.7023620	0.04%	-997.9373878	0.06%	-997.8955501	0.03%
calc_**1b** conf_26	-997.7023246	0.04%	-997.9373578	0.06%	-997.8963432	0.08%
calc_**1b** conf_27	-997.7018829	0.02%	-997.9369733	0.04%	-997.8941580	0.01%

calc **1b** conf_28	-997.7011556	0.01%	-997.9360458	0.01%	-997.8944661	0.01%
calc **1b** conf_29	-997.7011477	0.01%	-997.9361415	0.02%	-997.8947181	0.01%
calc **1b** conf_30	-997.7009035	0.01%	-997.9359564	0.01%	-997.8943459	0.01%
calc **1b** conf_31	-997.6997696	0.00%	-997.9345213	0.00%	-997.8926399	0.00%
calc **1b** conf_32	-997.6993183	0.00%	-997.9344931	0.00%	-997.8923420	0.00%
calc **1b** conf_33	-997.6991047	0.00%	-997.9343415	0.00%	-997.8923284	0.00%

Table S29. Cartesian coordinates of the optimized geometries for the conformers related to calc_**1b**. The related energies and % contribution on the final Boltzmann distribution for the three employed functional/basis set combinations are reported in Table S28.

```
calc_1b conf_1

C   -7.4862612556   -1.2758579582   -0.3769165576
C   -7.1823774215   -0.017648539    -0.8819287549
C   -5.9783307725    0.6260274706   -0.5581920551
C   -5.0746634381   -0.0103853821    0.2681769084
C   -5.3490086987   -1.2939938063    0.7769069794
C   -6.5805616351   -1.9203705952    0.4668597494
O   -6.9105385857   -3.1142731991    0.954529194
O   -8.0251622235    0.650075487    -1.7003736322
C   -3.7833178698    0.6319165625    0.6909127599
C   -2.7218160544   -0.4281933726    0.919217264
O   -3.1928143206   -1.4347005492    1.8417599496
C   -4.4054086653   -1.9748342259    1.6558125642
O   -4.6700866987   -3.0154227878    2.2501277223
C   -1.4225460226    0.0834829537    1.5183882456
C   -0.7388889097    1.159627862     0.6676232164
C    0.6548360216    1.5307483884    1.1806494653
C    1.6915760892    0.4639133764    0.8333349458
C    1.6264955337    0.146996986    -0.6587818107
C    0.2034881525   -0.2196199188   -1.0673571878
O   -0.7063020315    0.8186817493   -0.7130068423
C    0.0472887211   -0.4287440908   -2.5603699455
H   -8.4224335713   -1.7731168843   -0.6106126284
H   -5.7820352982    1.6115268258   -0.9643004927
H   -6.1776260189   -3.376778165     1.5698711867
H   -8.8127342479    0.111410555    -1.8528019778
H   -3.4354523692    1.3299662559   -0.0748022623
H   -3.9372197348    1.2025810471    1.61724611
H   -2.5185117914   -0.930064206    -0.0334808083
H   -1.632298266     0.5028391382    2.5093942351
H   -0.767286442    -0.7779632292    1.6822045716
H   -1.3644240536    2.0582701397    0.6957271171
H    0.6160421142    1.7075955037    2.2613360667
H    0.94686071      2.4765912787    0.7096842994
H    1.5076734018   -0.4505885355    1.4113081966
H    2.6927797581    0.8080979956    1.11281811
H    2.3053318703   -0.6739540877   -0.9156105893
H    1.9388744515    1.024089345    -1.2401662897
H   -0.0809453327   -1.148161503    -0.5442932754
H    0.3145149308    0.4847481132   -3.099483949
H   -0.9873330576   -0.6805013823   -2.8072541843
H    0.694623032    -1.2400146159   -2.905155614

calc_1b conf_2

C   -7.6455820726   -0.8334521337    0.0468593176
C   -7.2103107966   -0.7227126526   -1.268180886
C   -5.8443633544   -0.73689791     -1.58788376
C   -4.9157119853   -0.8781456406   -0.5764537345
C   -5.3316786328   -1.0131976675    0.7625865814
C   -6.711907538    -0.9646585681    1.075545581
O   -7.1577995716   -1.0412482894    2.3278700503
O   -8.0729511872   -0.5905741736   -2.3002095653
C   -3.4360043722   -0.8570135486   -0.8301230265
```

S56

```
C  -2.73054578    -1.7413052392   0.1827118024
O  -3.0715669874   -1.3433688739   1.5288101463
C  -4.3626059732   -1.1561293366   1.8423578885
O  -4.6639401875   -1.1041170545   3.030855802
C  -1.2100897095   -1.7652104003   0.1188169023
C  -0.4933904122   -0.4558328407   0.4230096574
C   0.9980804176   -0.6782860138   0.6656548276
C   1.7246396529    0.655133998    0.8255951025
C   1.4135279072    1.5618216193  -0.3632874521
C  -0.0943719622    1.696557693   -0.5859798927
O  -0.6973955093    0.4069833315  -0.6905619732
C  -0.7899348884    2.5816168825   0.4448668029
H  -8.7002064216   -0.8062753764   0.302457433
H  -5.5448720097   -0.6341687288  -2.6244814294
H  -6.3544267544   -1.0664334379   2.9092559018
H  -8.9772287364   -0.5948242476  -1.9598208917
H  -3.2051242624   -1.2070399501  -1.8404301913
H  -3.0448374839    0.1626282792  -0.7571094336
H  -3.0948802959   -2.7700597565   0.0582349223
H  -0.8656966407   -2.5159180149   0.8383872353
H  -0.9077108546   -2.1080656491  -0.877225172
H  -0.9395448235   -0.0137016239   1.3255117
H   1.4137776358   -1.2257339138  -0.1907104725
H   1.1352048471   -1.3062202198   1.5531116471
H   2.8049147802    0.4958068277   0.9082521209
H   1.4106681273    1.1342296389   1.7612721964
H   1.8554518311    1.1277367699  -1.268065904
H   1.8593838673    2.5538636771  -0.2303103483
H  -0.2651447408    2.1370768542  -1.5738098336
H  -0.6314596004    2.2441342899   1.4724912774
H  -1.8671762878    2.6028602003   0.2588233021
H  -0.4121892339    3.6061412003   0.3723057683

calc_**1b** conf_3

C  -7.5365478045   -1.2026820033  -0.4196827823
C  -7.0519101815   -0.0779044448  -1.0755216093
C  -5.7919360579    0.4576302232  -0.76886179
C  -5.0154810511   -0.1546565342   0.1942009745
C  -5.474538399    -1.3068793135   0.8594677661
C  -6.7603835309   -1.819513578    0.5629174393
O  -7.2625784065   -2.8796201181   1.1919433745
O  -7.7642899893    0.558626108   -2.0317609464
C  -3.6723706015    0.3793544256   0.6054172497
C  -2.7675155235   -0.7598504465   1.0377162623
O  -3.4052070596   -1.54646078     2.0687023941
C  -4.6667313823   -1.957865255    1.8853625041
O  -5.0922337437   -2.8570677689   2.6040740256
C  -1.4355641256   -0.3322285762   1.6309232941
C  -0.5485354205    0.4433364038   0.6679084888
C   0.8201435022    0.7542942999   1.2668042028
C   1.7209052271    1.4111803678   0.2234106454
C   1.7737068609    0.5417231529  -1.0316626444
C   0.3716309679    0.2039696508  -1.5453757604
O  -0.426159303    -0.3522841291  -0.5015293993
C  -0.3253205061    1.3710264265  -2.2392459909
H  -8.5169553751   -1.6129850926  -0.6404707422
H  -5.4540860233    1.3430821539  -1.2948767526
H  -6.5979869287   -3.1337534091   1.8839737194
```

S57

```
H  -8.6059879029   0.1010466979  -2.157213588
H  -3.2069358258   0.9213449962  -0.2220618851
H  -3.7914860969   1.0877564104   1.4369262704
H  -2.5881720671  -1.4209906309   0.1840733357
H  -1.6183627359   0.2772408564   2.5234254585
H  -0.908357991   -1.2349051571   1.9569816664
H  -1.0380238982   1.3988612625   0.4152205776
H   1.2722850616  -0.1858183663   1.6071903731
H   0.7012640784   1.3973592186   2.1462039387
H   2.7291197948   1.5585013473   0.6242791908
H   1.336097969    2.4097350611  -0.0197422804
H   2.2861351517  -0.3974120653  -0.7921230422
H   2.3498212768   1.0297732115  -1.8256175929
H   0.4506881565  -0.6144811481  -2.2680892539
H   0.2279931942   1.6574555782  -3.1387797585
H  -0.4011425782   2.2580741182  -1.6041964049
H  -1.3349907316   1.0779868466  -2.5403109284
```

calc_**1b** conf_4

```
C  -7.6347482852  -0.9970501824  -0.0129540801
C  -7.1438201099  -0.4741826556  -1.203040416
C  -5.7686350624  -0.279259466   -1.4014178162
C  -4.8862644622  -0.6262554714  -0.3984858924
C  -5.3565567159  -1.1769206691   0.809608557
C  -6.7489873675  -1.3395164641   1.0095745647
O  -7.2508404475  -1.8134627616   2.1479983941
O  -7.9583598876  -0.1234705307  -2.222784462
C  -3.4050220516  -0.4079070735  -0.5145558867
C  -2.6663423138  -1.4840242999   0.2618810248
O  -3.1181668844  -1.5168923779   1.6330282554
C  -4.4370217333  -1.5418388808   1.8805832471
O  -4.8049489656  -1.863585326    3.0058148323
C  -1.1507118141  -1.3546756531   0.3196635081
C  -0.6244462848  -0.0871160661   1.0069327275
C   0.8500811546  -0.1893556516   1.4044078872
C   1.7714688989  -0.0628242283   0.1938574569
C   1.4333261868   1.2157669016   -0.5686991107
C  -0.0512758669   1.259663547    -0.9177038351
O  -0.8566613164   1.0953076839   0.243806843
C  -0.472498603    2.5756724202   -1.5422040298
H  -8.6985007069  -1.1352455015   0.1531701298
H  -5.4267298067   0.14391407     -2.3388503768
H  -6.4822424568  -1.9366491898   2.7627847612
H  -8.874541868   -0.3011603005   -1.9723797047
H  -3.0887857638  -0.4342691963   -1.5620754514
H  -3.1277438448   0.5773882986   -0.1247855207
H  -2.9143063219  -2.4615330987   -0.1734830727
H  -0.7759615339  -2.2236748203   0.8718112088
H  -0.7614836134  -1.4458146434   -0.6998706789
H  -1.2200561462   0.0615892831   1.9121537134
H   1.0260293404  -1.1256156179   1.9447295071
H   1.0671976057   0.628303041    2.1017358529
H   1.6535299439  -0.9311492559   -0.467790274
H   2.8191737007  -0.0570472484   0.5122633979
H   2.0268145043   1.2975775446   -1.4863939719
H   1.6698140321   2.0895301652   0.0521576325
H  -0.2626535205   0.445245908    -1.63130988
H   0.0873513804   2.7616399668   -2.4633223685
```

S58

```
H  -0.2850264254   3.3992652902   -0.8472230931
H  -1.5394465675   2.5666325107   -1.7796335802

calc_1b conf_5

C  -7.5032824587   -1.7218929886   -0.2114660432
C  -7.6332800334   -0.4115023576   -0.6545691829
C  -6.6242154968    0.5374322855   -0.4298474466
C  -5.4759030653    0.1557692196    0.233536374
C  -5.3106733912   -1.1705086829    0.6756977972
C  -6.3484678483   -2.1111375305    0.4687504384
O  -6.2635200411   -3.3664917525    0.9033288807
O  -8.7311638531    0.0172329262   -1.3154287866
C  -4.3673611717    1.1204805427    0.5460080788
C  -3.0294017432    0.4012574315    0.5656911701
O  -3.0857632046   -0.7190272708    1.4787209743
C  -4.1074135771   -1.5825338856    1.3880760249
O  -3.9868242099   -2.6774076215    1.9294922835
C  -1.8821217805    1.2916390758    1.0144046124
C  -0.4828123025    0.8096166822    0.6381780275
C  -0.0323843148   -0.4922015845    1.2944021212
C   1.3452815728   -0.886894359     0.7672386291
C   1.3119705441   -0.9488524955   -0.7591968621
C   0.7708003247    0.3473697606   -1.3672043874
O  -0.4793875664    0.700783796    -0.7787941313
C   1.7633705352    1.5064491404   -1.3290712342
H  -8.2865203703   -2.4569255031   -0.3681234081
H  -6.7680539041    1.5523257027   -0.7820666718
H  -5.4108651252   -3.430697112     1.4066980825
H  -9.350412216    -0.7181357567   -1.412612244
H  -4.3367737617    1.9270875971   -0.192128096
H  -4.5431574028    1.5849109634    1.5261929935
H  -2.8121681232    0.0013931198   -0.4306352156
H  -2.0231024745    2.2715417685    0.545099837
H  -1.9462590966    1.4358277052    2.0985236261
H   0.2175421311    1.6041645205    0.9450204753
H  -0.7568244298   -1.2819445912    1.0753297724
H  -0.0185571246   -0.3674705163    2.3829097265
H   1.6496602754   -1.8554832073    1.177113117
H   2.0953949836   -0.1590195599    1.1033487001
H   0.6548551603   -1.7716523287   -1.0648422885
H   2.3057547414   -1.1608909089   -1.1693688247
H   0.5159316898    0.1631109021   -2.4161657376
H   1.2939492964    2.4114953373   -1.7241118466
H   2.6354842579    1.2744011185   -1.9480880682
H   2.1246745746    1.7233804176   -0.3200412674

calc_1b conf_6

C  -7.7837670923   -1.6172330331    0.003169464
C  -7.9071750404   -0.3050508298   -0.436195352
C  -6.8293811186    0.5914364652   -0.3665504127
C  -5.6214552088    0.1540774911    0.136483536
C  -5.4633565537   -1.1767161885    0.5695764659
C  -6.5672317946   -2.0623232421    0.5228657157
O  -6.4881295942   -3.3172001412    0.9591152483
O  -9.0623639094    0.1762639573   -0.9447177244
C  -4.4310408819    1.0588510292    0.2819101822
C  -3.1486827449    0.2646012099    0.1053685781
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S59

```
O   -3.1196205753   -0.8492237214    1.0230279745
C   -4.1931015003   -1.6507461331    1.1058019363
O   -4.0546110821   -2.7444879993    1.6434921989
C   -1.8972134465    1.080313695     0.3624934955
C   -0.5850335926    0.3146151098    0.2310536164
C   -0.327031548    -0.2468149651   -1.1645509882
C    1.0779674519   -0.842152918    -1.2466341463
C    2.1085866106    0.1855412266   -0.7844707724
C    1.7510168876    0.7603776528    0.5887428484
O    0.4159598987    1.2581391547    0.5873034253
C    2.0056369276   -0.20173995      1.7459418449
H   -8.6178505529   -2.3109569266   -0.0326260589
H   -6.9694318365    1.6105974455   -0.7077801605
H   -5.5789248752   -3.4245297283    1.3409083139
H   -9.7270275842   -0.5251210372   -0.9430542937
H   -4.4645953875    1.870743239    -0.4504420439
H   -4.4324875305    1.5211634496    1.2780576296
H   -3.13121328     -0.1555531454   -0.9083670738
H   -1.8820096687    1.9230109587   -0.3387527975
H   -1.9437381809    1.5031096418    1.3717939433
H   -0.5937494532   -0.5158256983    0.9508892253
H   -0.4278325489    0.5667925458   -1.8955469772
H   -1.0759086121   -1.0080720904   -1.409754232
H    1.2972643007   -1.1660198145   -2.2695268356
H    1.1298325336   -1.7412727017   -0.6203560622
H    2.1349574025    1.0121998485   -1.5045476255
H    3.1139159495   -0.2497188867   -0.756406234
H    2.3564301333    1.6564539945    0.7615121046
H    1.6733311591    0.2507574782    2.684061376
H    3.0757966976   -0.4155499793    1.8280418024
H    1.4862692419   -1.1567364633    1.6286688655

calc_1b conf_7

C   -7.3937360349   -0.2741995704    0.6991464761
C   -7.0559208475    0.3183817752   -0.5108388602
C   -5.8219193931    0.0611354751   -1.1291729982
C   -4.9257388203   -0.7885332994   -0.5139011968
C   -5.233730378    -1.3835757689    0.7245987767
C   -6.4923713321   -1.1392896149    1.3233560848
O   -6.8527521841   -1.7056919731    2.4725810165
O   -7.891373982     1.1620138594   -1.1561120058
C   -3.6101749577   -1.1708326321   -1.1271664835
C   -2.5613353761   -1.391671596    -0.0478952845
O   -3.0344314008   -2.3627454639    0.9132245231
C   -4.2791117486   -2.2581237226    1.399471573
O   -4.564395526    -2.9154458768    2.396027907
C   -2.1184001209   -0.1366955316    0.6992057087
C   -1.4086407923    0.8858116266   -0.195397917
C   -0.8342417033    2.0684453021    0.58921169
C    0.4399948391    1.6872814864    1.3393935578
C    1.4248175586    1.0297569075    0.3758438393
C    0.7672465759   -0.1376141186   -0.3527627388
O   -0.4186479697    0.2848269389   -1.0222111669
C    1.6573782609   -0.7509115625   -1.4155025067
H   -8.3523642707   -0.0923695758    1.1748244154
H   -5.6023094846    0.5283989556   -2.0821940915
H   -6.1117316817   -2.3151488691    2.7270419863
H   -8.7041935185    1.258648001    -0.6426069492
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H  -3.73287376    -2.1062379263   -1.6878669915
H  -3.2621152377  -0.4213198047   -1.8420559614
H  -1.6856370257  -1.8689071797   -0.4890969269
H  -2.9877452298   0.3503225172    1.1554558658
H  -1.4734895091  -0.4581322862    1.5232926988
H  -2.1411501593   1.2758704226   -0.9101812028
H  -1.5944697848   2.4623867364    1.2727626065
H  -0.5994184707   2.8651985349   -0.1261668445
H   0.2093090092   0.9956530379    2.1594759178
H   0.8845864173   2.5749651165    1.801241354
H   2.3157451854   0.6747145115    0.9059018385
H   1.7586498127   1.7615509216   -0.3711781958
H   0.5116885126  -0.9119478089    0.3898458775
H   2.581717888   -1.1303815061   -0.9708810301
H   1.9142853897  -0.0022227046   -2.170491544
H   1.1470012505  -1.5783637341   -1.9152228178

calc_**1b** conf_8

C  -7.2849970551  -0.1201415231    0.3710432166
C  -6.7125644842   0.3182212859   -0.8161153761
C  -5.4354594878  -0.1099870577   -1.2114190385
C  -4.7343358129  -0.9751615749   -0.3964289338
C  -5.281858463   -1.4162362881    0.8231568855
C  -6.5817432519  -0.9999145932    1.1968531961
O  -7.164568614   -1.4165191755    2.3184065196
O  -7.3513464363   1.1683849596   -1.6506074601
C  -3.3908472857  -1.534814745    -0.7640229323
C  -2.5412040474  -1.754426208     0.4777895261
O  -3.2537481642  -2.5787595496    1.4284013154
C  -4.5364030091  -2.3097706387    1.7056690925
O  -5.0355828802  -2.8391244943    2.6944008746
C  -2.0762064811  -0.485050262     1.1879274501
C  -1.1725344545   0.399549007     0.3405030703
C  -0.6093872571   1.5788535902    1.1286649555
C   0.3869902495   2.3594156663    0.2744372153
C   1.4524426886   1.4099008503   -0.270060833
C   0.8282976689   0.21029312     -0.9875568148
O  -0.1313874249  -0.4325873425   -0.1500971647
C   0.2549403526   0.5461505321   -2.3616209183
H  -8.2784644484   0.1947140472    0.6748160149
H  -5.0305336187   0.2400794962   -2.1539573549
H  -6.5374059048  -2.0650299944    2.7332230967
H  -8.2159989341   1.3871421337   -1.2789312528
H  -3.5287241588  -2.501109004    -1.2658972562
H  -2.8635637381  -0.8871697041   -1.4688030627
H  -1.6646781383  -2.3482039331    0.2210252643
H  -2.9420825726   0.1036988848    1.5104958286
H  -1.5350514575  -0.7930342954    2.0887603466
H  -1.7550290815   0.8006014179   -0.5054319419
H  -0.1062797637   1.1917712856    2.0237822254
H  -1.4298844821   2.222052017     1.4660678186
H   0.8549684601   3.1565236349    0.8614003077
H  -0.1423565877   2.8530549674   -0.5504433283
H   2.0531261894   1.0332978685    0.5661955693
H   2.1363876127   1.9314131613   -0.9487654353
H   1.5989096784  -0.5549774884   -1.1257683979
H   1.0552565718   0.8710202711   -3.0334105141
H  -0.4898892997   1.3462386792   -2.3273050711
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H  -0.2152026767   -0.340359004    -2.7963767031

calc_1b conf_9

C  -7.5543445892   -1.5259585858    0.1698284815
C  -7.7575476651   -0.1942377181   -0.1699603358
C  -6.7045187844    0.7332936403   -0.1454956796
C  -5.4410396619    0.3088478876    0.2116743267
C  -5.2045634339   -1.0390161961    0.5430350222
C  -6.2808899406   -1.95865473      0.542556015
O  -6.1227525604   -3.2340476259    0.8886545293
O  -8.9701013076    0.276875577    -0.5348785022
C  -4.2682115369    1.2453978673    0.2915859801
C  -2.9814722379    0.5053450585   -0.0338272925
O  -2.8489513616   -0.6427803223    0.8298094499
C  -3.8774576801   -1.4943285844    0.9391436878
O  -3.6552667669   -2.613361138     1.3917896534
C  -1.7272783071    1.347150012     0.1524214972
C  -0.5409263733    0.8873969164   -0.7089135752
C   0.7405237715    1.6821038019   -0.4369471383
C   1.4250545976    1.2327220359    0.8532098255
C   1.5993520597   -0.284733749     0.8457464038
C   0.2597503692   -0.9675317573    0.592793216
O  -0.3080612161   -0.5054933522   -0.632820411
C   0.3536737183   -2.4741524824    0.4716077563
H  -8.367443123    -2.2450722653    0.167687592
H  -6.9061765015    1.7653715052   -0.4081741438
H  -5.1781264198   -3.3318801985    1.1750572802
H  -9.6100465626   -0.4469628265   -0.5189613907
H  -4.3948658877    2.084000352    -0.3996414698
H  -4.1942683861    1.6683693772    1.3028139348
H  -3.0303752278    0.1267281414   -1.062742621
H  -1.9557182443    2.3824477743   -0.1284196938
H  -1.4823246914    1.3629071192    1.2196317822
H  -0.8316635743    1.0449441912   -1.7550111533
H   0.5199071927    2.7558343076   -0.4148685576
H   1.4241209341    1.5128436061   -1.2770763757
H   0.8246074202    1.5254644137    1.7244857631
H   2.3911473513    1.7373651462    0.9610191396
H   2.0165745816   -0.6338148692    1.7971263315
H   2.3005947344   -0.577819055     0.053666588
H  -0.4235542437   -0.7258973591    1.4188859203
H   0.7963444838   -2.9042014246    1.3748210108
H   0.9735652589   -2.7491951669   -0.3871981804
H  -0.643270188    -2.900269324     0.3388853336

calc_1b conf_10

C  -7.823636073    -1.5479135926    0.0553008187
C  -7.7432769478   -0.4308121699   -0.7666366645
C  -6.5723804295    0.3402380919   -0.8360265882
C  -5.4778723093   -0.0287096411   -0.0814954463
C  -5.5258127262   -1.1681243563    0.7444777395
C  -6.7228950709   -1.9195878641    0.8289475794
O  -6.8399213785   -2.9790527936    1.6255974173
O  -8.7797986512   -0.0264843814   -1.5326213417
C  -4.2015823443    0.7636643637   -0.0680182628
C  -3.0166162517   -0.1585886682    0.1623734431
O  -3.2102809604   -0.9281040478    1.3666275982

S62
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C   -4.3777501942    -1.5652840255     1.5508270164
O   -4.4249820239    -2.4455792525     2.4030949394
C   -1.7001206808     0.5809034532     0.3183167295
C   -0.4852968711    -0.3242233836     0.5734440971
C   -0.0459790067    -1.1587476022    -0.6323326836
C    0.6569099336    -0.3070800267    -1.6879482639
C    1.7825775083     0.4927576981    -1.0374149981
C    1.2579754689     1.2856934365     0.156193156
O    0.6047297014     0.4307803024     1.0860349142
C    2.355978383      1.9902949045     0.9285076158
H   -8.7312256469    -2.1390879851     0.12628453
H   -6.5535086243     1.2120306504    -1.4797360252
H   -5.9891618812    -3.0457256565     2.1311696113
H   -9.5247554802    -0.6280030581    -1.4031195358
H   -4.0693030649     1.3066144006    -1.008507335
H   -4.2343198082     1.5112153226     0.7358116707
H   -2.9599487632    -0.8737268167    -0.6688281168
H   -1.558602537      1.1920134604    -0.5800917061
H   -1.7817577611     1.2684523006     1.1673979714
H   -0.7502619221    -0.9959289673     1.393674316
H   -0.9009192106    -1.6939698013    -1.0606356997
H    0.6512483354    -1.9232128354    -0.2706989998
H   -0.0559962172     0.3801040068    -2.1629672115
H    1.0472056653    -0.9442652849    -2.4885895677
H    2.2485249604     1.1746338351    -1.7580471815
H    2.5640618205    -0.191196874     -0.6820867296
H    0.5446634046     2.0413758419    -0.2140159261
H    3.0727838039     1.2599464541     1.3148601035
H    1.9355420278     2.5367681332     1.7764064304
H    2.888761823      2.6969224288     0.2854705861

calc_1b conf_11

C   -7.439084488     -1.3326947211    -0.4890109461
C   -6.9152216088    -0.2846415637    -1.2360741194
C   -5.6651722192     0.2747527047    -0.931321992
C   -4.9376208202    -0.2359279199     0.1246685752
C   -5.4368096009    -1.3114592137     0.8842956499
C   -6.7129934046    -1.8466145434     0.5864646073
O   -7.2521340528    -2.8326841199     1.3006366417
O   -7.579634367      0.250641593     -2.2846139103
C   -3.6115117339     0.3316257862     0.5409670703
C   -2.7353665774    -0.7653575221     1.1155009742
O   -3.4216566866    -1.4344669928     2.1997695683
C   -4.6811382194    -1.8530701537     2.0079667799
O   -5.1444344494    -2.6684032199     2.7998485645
C   -1.4173315065    -0.2965851949     1.7158760052
C   -0.307973275      0.0745162321     0.7362462036
C    0.1601832947    -1.0645272427    -0.1675317325
C    1.2515948425    -0.5651656363    -1.1122037814
C    0.751885683      0.6608347148    -1.8741801588
C    0.2139857283     1.7356162151    -0.9254830609
O   -0.7545880053     1.181891568     -0.0342009985
C    1.3050464616     2.4990803452    -0.1798428013
H   -8.4130397766    -1.7584301062    -0.7093157621
H   -5.2961721209     1.0998025268    -1.5294531211
H   -6.6227774129    -3.012649257      2.0463396545
H   -8.4203349277    -0.2122809517    -2.396352683
H   -3.0906586327     0.8083918955    -0.2908367453
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S63

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H  -3.7610173677   1.103360484    1.3081250191
H  -2.5569975316  -1.5246632955   0.3444006838
H  -1.6125641099   0.5611576893   2.3684682886
H  -1.0442790705  -1.1042804901   2.3547204714
H   0.5516537652   0.3854678427   1.3515341188
H  -0.6839484255  -1.4376650545  -0.7596525122
H   0.5217618423  -1.8972307047   0.4462642487
H   1.5438733522  -1.3532621027  -1.8138068084
H   2.1509602901  -0.315054608   -0.5354207362
H  -0.0607480821   0.3555281779  -2.5441929599
H   1.5435009162   1.0850471165  -2.5017156978
H  -0.3621710733   2.4621048598  -1.5075911984
H   0.852861801    3.1937014585   0.5329791156
H   1.9063383618   3.0772903192  -0.8879417067
H   1.9857332075   1.8423030853   0.3686711916
```

calc_**1b** conf_12

```
C  -7.5310598127  -0.5351012456   0.8408322238
C  -7.5241152324  -0.2835357338  -0.5253115062
C  -6.3797551043  -0.5176091787  -1.304217973
C  -5.2382006785  -0.9961668657  -0.6953445096
C  -5.2119336564  -1.2395149723   0.6912634198
C  -6.3802374198  -1.0258028545   1.4609425566
O  -6.423416867   -1.2755194586   2.7676185585
O  -8.6107129506   0.1898184873  -1.1741568546
C  -3.988688943   -1.3344265967  -1.4562494084
C  -2.7533147194  -1.0725734593  -0.6061374844
O  -2.8629317133  -1.7903501504   0.6456689698
C  -4.0030809567  -1.7256519789   1.3475045823
O  -3.9784939532  -2.0915533169   2.5193664032
C  -2.4788308144   0.4103718491  -0.3617785653
C  -1.0576375741   0.7415473477   0.0871511091
C  -0.6530224835   0.2038208346   1.4573068958
C   0.8097444241   0.5425102613   1.7357560782
C   1.681536143    0.0251872422   0.5931578527
C   1.1860801596   0.5242200743  -0.7663040877
O  -0.2025664439   0.2439481538  -0.9342208095
C   1.5040602975   1.9928396756  -1.034921623
H  -8.4170849375  -0.3709947736   1.4460647857
H  -6.4188305684  -0.3231610344  -2.369770679
H  -5.5407764633  -1.661758305    3.006466969
H  -9.3316394951   0.3083143534  -0.5417730774
H  -4.0106084975  -2.3981134018  -1.726364413
H  -3.9255923928  -0.7693149483  -2.3901844348
H  -1.8747983643  -1.5122975289  -1.0796193804
H  -2.6474132056   0.9352605401  -1.308709907
H  -3.1975073893   0.8158691444   0.3582417612
H  -0.9845741961   1.8412643339   0.1196410365
H  -0.7955027909  -0.8807181794   1.4814336481
H  -1.3090030477   0.628784697    2.225607117
H   1.1308491551   0.1008242454   2.6847514414
H   0.9279827485   1.6284994906   1.8442140958
H   1.6465841569  -1.0706052678   0.5900819511
H   2.7295199738   0.314115625    0.7315572214
H   1.6629882086  -0.0689935644  -1.5536529378
H   1.1236220535   2.6584367346  -0.2551961248
H   1.0661652488   2.3000859504  -1.9884985865
H   2.5871981024   2.1380437745  -1.0922163146
```

calc_**1b** conf_13

```
C  -7.3433489268  -0.2017467764   0.3802674666
C  -7.2896518442  -0.6203972949  -0.9429717088
C  -6.1778181075  -1.3169538628  -1.4426000899
C  -5.1159774582  -1.5798351353  -0.6024427861
C  -5.1359067019  -1.1493807273   0.7379332253
C  -6.2732455442  -0.4693162282   1.2361824011
O  -6.3624508529  -0.0695599945   2.5023087942
O  -8.2974785028  -0.3876765802  -1.8118112246
C  -3.9180478429  -2.3739300898  -1.0375353283
C  -2.6640730984  -1.9143547259  -0.3058702011
O  -2.8816214556  -1.9242974335   1.1226447181
C  -4.0087681313  -1.3993258826   1.6283455193
O  -4.0392485124  -1.1636496822   2.8323031122
C  -2.1605153179  -0.5501360516  -0.7582591677
C  -0.9686192439  -0.0109154528   0.0255456039
C   0.2613662208  -0.9138433491  -0.0028617454
C   1.4483964338  -0.2135002279   0.657455934
C   1.6637776503   1.16046555      0.0266410847
C   0.3736646465   1.9848754732    0.0247887742
O  -0.6871532301   1.2461214625   -0.5738449079
C  -0.0078548664   2.5343695103    1.3968007875
H  -8.2054132854   0.3256501821    0.7764654398
H  -6.1789536833  -1.6376909999   -2.4778610291
H  -5.5383947234  -0.3873499664    2.9544600653
H  -9.0010073321   0.0968094897   -1.3600842422
H  -4.0903836596  -3.4342358019   -0.8128109238
H  -3.7642205025  -2.2968115243   -2.1177473445
H  -1.8766365974  -2.6588967701   -0.4413335054
H  -1.872941459   -0.6249020734   -1.8139387582
H  -2.9675008185   0.1881960718   -0.7039532486
H  -1.2712042712   0.1328653739    1.0728959172
H   0.5032863798  -1.1486107126   -1.0484238519
H   0.0461882249  -1.857252521     0.5105336405
H   2.3539669619  -0.8217277089    0.5606942536
H   1.2578460111  -0.1129397832    1.7332064984
H   1.9864382126   1.0283248907   -1.0130684133
H   2.4575127041   1.711333846     0.5436940586
H   0.5029571638   2.8369097952   -0.6509498638
H  -0.9686519667   3.0523482433    1.3352605587
H   0.7468039127   3.250260625     1.7369935409
H  -0.0911165859   1.7557068431    2.1599469467
```

calc_**1b** conf_14

```
C  -7.206854015   -0.4289626081  -0.1455324212
C  -6.4776434722  -0.2733997271  -1.3180318836
C  -5.13650262    -0.6767859473  -1.401563571
C  -4.5297284834  -1.2305103049  -0.2927845122
C  -5.2394954231  -1.3789960639   0.9136255683
C  -6.599356836   -0.9916608476   0.978299206
O  -7.3283528529  -1.1441592339   2.0820895612
O  -7.0197933282   0.2650697507   -2.4334762208
C  -3.121690589   -1.7490186176  -0.3183075676
C  -2.4600445416  -1.5874881011   1.041972387
O  -3.2805839723  -2.1754397967   2.0791579088
C  -4.6007787693  -1.9420173552   2.097632444
```

S65

```
O  -5.2176334786   -2.2259537167    3.1205335422
C  -2.1367955724   -0.1484438142    1.4469519518
C  -0.9554137993    0.518804428     0.745332747
C   0.3866945206   -0.1901897089    0.9174618852
C   1.4750925001    0.5678511718    0.1584113017
C   1.0560745281    0.7533817193   -1.2990971051
C  -0.3345059196    1.3832064025   -1.4132658815
O  -1.2810201991    0.6552776523   -0.6308662095
C  -0.3641332243    2.8765910426   -1.100732123
H  -8.2490721639   -0.1326086029   -0.0789213182
H  -4.6028346519   -0.5473004778   -2.3356808016
H  -6.7420702758   -1.6006489588    2.7400956655
H  -7.9398172938    0.5007494727   -2.2558062502
H  -3.1387803004   -2.815741068    -0.5774798086
H  -2.522028376    -1.2272954354   -1.0654829304
H  -1.5526776478   -2.1929482232    1.0800564451
H  -3.0226547949    0.47811765      1.2981724528
H  -1.9242128536   -0.1559806368    2.5214992111
H  -0.8606760214    1.5203938157    1.1947274476
H   0.3193656918   -1.211561077     0.5237673901
H   0.6303702846   -0.2666166158    1.9832361057
H   2.4274868383    0.030310477     0.2122496995
H   1.6430384296    1.5423453074    0.6343085553
H   1.0302821624   -0.2278399118   -1.7880809711
H   1.7847052863    1.3643729835   -1.8433156398
H  -0.6971763465    1.2513343864   -2.4378169228
H  -1.3946001427    3.2405996125   -1.1265507561
H   0.2128569871    3.4262398359   -1.8506054857
H   0.0579607361    3.1169211424   -0.121183096

calc_**1b** conf_15

C  -6.7006951234   -0.4376701581    1.4258431391
C  -7.1225576766    0.1686940314    0.2496456506
C  -6.3710716772    0.0690698247   -0.9313620346
C  -5.1846154783   -0.6361536166   -0.9165830004
C  -4.724585437    -1.2429765007    0.2669794078
C  -5.5050924278   -1.1587491048    1.4437854584
O  -5.1383638696   -1.747217961     2.5800393383
O  -8.2721312077    0.876737216      0.1782540398
C  -4.3459004429   -0.8332678756   -2.1484472931
C  -2.8725989742   -0.9153578755   -1.7740526262
O  -2.6689032746   -1.9385768878   -0.7800983711
C  -3.4649631764   -1.9790785337    0.2968226865
O  -3.1152908565   -2.6710987443    1.2477454647
C  -2.2935571619    0.4316897369   -1.3352313138
C  -0.9869657746    0.3317477179   -0.5554818813
C  -0.1240214439    1.5862970913   -0.6569652745
C   1.0904444843    1.4605119834    0.2622947085
C   0.6450070844    1.1152506892    1.6832619072
C  -0.290566731    -0.0967508599    1.7056140835
O  -1.3668772358    0.1057355457     0.791900097
C   0.407509686    -1.4356267878    1.4876682657
H  -7.2839780832   -0.3764763552    2.3393264884
H  -6.7399308605    0.5458822886    -1.8321665987
H  -4.3050323892   -2.2465091994    2.3777840772
H  -8.6973894984    0.8777201145     1.0458417731
H  -4.6429686276   -1.7650596911    -2.6462110588
H  -4.5038530583   -0.0218119695    -2.8653899814
```

```
H   -2.2942679558   -1.2894532348   -2.6226278901
H   -2.1444076147    1.0280232494   -2.2432555455
H   -3.0079304453    0.9735027499   -0.7066153673
H   -0.4054661249   -0.5258238215   -0.9296393176
H   -0.7295645202    2.4529945605   -0.3614449498
H    0.187849468     1.7421719726   -1.6965432058
H    1.6704402877    2.3895975817    0.2630379757
H    1.7582702953    0.6799780227   -0.1241382591
H    0.1050402367    1.9719786682    2.1038494617
H    1.5103809153    0.9303269228    2.3296402049
H   -0.7911558825   -0.138237152     2.6780553597
H   -0.3416733077   -2.2275746326    1.4135680165
H    1.0663342191   -1.6537842773    2.3341262661
H    1.0210996612   -1.4546547281    0.5821700988
```

calc_**1b** conf_16

```
C   -7.8382842972   -1.1701313421    0.6091087475
C   -7.7515732828   -0.2478397339   -0.4262946672
C   -6.5104688699    0.2331645344   -0.8723027363
C   -5.3559454201   -0.2326554387   -0.2785015773
C   -5.4141541361   -1.1840217567    0.7586583554
C   -6.6737814385   -1.6361008514    1.2214178946
O   -6.7908051228   -2.4986958168    2.2278923904
O   -8.8470077968    0.2366183357   -1.0502572843
C   -3.9904359462    0.2606024733   -0.6652225051
C   -2.9805965248   -0.8619134088   -0.496240347
O   -3.0126837335   -1.3589943969    0.8599693045
C   -4.2012332839   -1.6810484316    1.3972224028
O   -4.2066416263   -2.3719574284    2.4105383693
C   -1.5359152815   -0.5251395291   -0.8372435455
C   -0.9333438832    0.7536497654   -0.2347413419
C   -0.6902013697    0.7242653327    1.2755421271
C    0.5020639234   -0.158330258     1.6368568945
C    1.7209195436    0.2632232215    0.8199132594
C    1.392433719     0.2837711481   -0.6696922771
O    0.2573532477    1.1033014696   -0.9316756244
C    2.5180465854    0.8413139245   -1.5185248658
H   -8.7954490894   -1.5331247892    0.9701307484
H   -6.4855670597    0.9630769756   -1.6730743193
H   -5.8728720707   -2.6612007513    2.5663540371
H   -9.636977603    -0.162504388    -0.6626199078
H   -3.9784077967    0.6165420522   -1.6997609414
H   -3.717729957     1.1101628103   -0.027096243
H   -3.2889577457   -1.6973788943   -1.1384678849
H   -0.9339711622   -1.4019805833   -0.5801950944
H   -1.476990456    -0.414886054    -1.9261956588
H   -1.6086593056    1.5846546248   -0.4645971834
H   -1.5912816455    0.3932284692    1.7979121869
H   -0.4798809102    1.75194989      1.595902827
H    0.2651962187   -1.2120807661    1.4438197879
H    0.7113587271   -0.0838036878    2.7089620477
H    2.5682133825   -0.4087439108    0.9987250717
H    2.0353476062    1.2718032826    1.1186605075
H    1.1823218649   -0.7484443413   -0.9947209557
H    2.7402743067    1.870504729    -1.2216356042
H    2.2359642821    0.8438116495   -2.5745047629
H    3.4243234078    0.2403318702   -1.4000216322
```

calc_**1b** conf_17

```
C  -7.8232385658  -0.8480250894   0.4809358693
C  -7.5623525504  -0.3159439241  -0.7756952117
C  -6.247765288   -0.153516783   -1.2400302105
C  -5.1969995726  -0.5446231915  -0.436126826
C  -5.433931573   -1.1060101763   0.8335167533
C  -6.7636579334  -1.2343311019   1.3031985871
O  -7.0445671425  -1.7150112399   2.5119038508
O  -8.5505392629   0.0765838852  -1.6087872162
C  -3.7602337155  -0.3659964441  -0.8382648204
C  -2.9205949429  -1.4834296299  -0.2417221651
O  -3.0872018561  -1.5204807491   1.192154765
C  -4.3316801255  -1.5163328606   1.6958332962
O  -4.480304547   -1.84656385     2.8677413592
C  -1.4319378369  -1.4315501089  -0.5432899126
C  -0.6698365109  -0.148331791   -0.2189496504
C  -0.4745476437   0.1225544329   1.2696470613
C   0.4446794265   1.3250887151   1.473124572
C   1.749678577    1.1182434459   0.7084091909
C   1.4901632836   0.7747784713  -0.7604867504
O   0.5829607263  -0.3185848342  -0.8706697694
C   1.0504747836   1.9706103561  -1.601723563
H  -8.8367427052  -0.9605656448   0.8528895747
H  -6.0854008659   0.2780337303  -2.2209289905
H  -6.173860268   -1.8712907283   2.9607614057
H  -9.4048981551  -0.0830515733  -1.1865260877
H  -3.6536776385  -0.3659046458  -1.9271081058
H  -3.4001072646   0.605611788    -0.4781837645
H  -3.3034083827  -2.4389411403  -0.6236651489
H  -0.946560323   -2.2686585382  -0.03046712
H  -1.311275061   -1.6125051519  -1.6172803116
H  -1.1951140853   0.7105535289  -0.6683119065
H  -0.0284440689  -0.769198493    1.7271993319
H  -1.441967693    0.2767448911   1.7546568958
H   0.6491555437   1.4725697076   2.5386778911
H  -0.059085875    2.2371481156   1.1275311587
H   2.2989814389   0.285375671    1.163053611
H   2.3927083135   2.0032007731   0.7741110264
H   2.4140649669   0.3824658892  -1.198284147
H   0.8149519729   1.6435534319  -2.6181400787
H   1.857161801    2.7080421551  -1.6568635558
H   0.1709506197   2.4766887011  -1.1938408876
```

calc_**1b** conf_18

```
C  -7.2759784011  -0.1403709592   0.0837977407
C  -6.9882963882  -0.5038105385  -1.2253820592
C  -5.8170393119  -1.2088484742  -1.5454700744
C  -4.9328525979  -1.5352129229  -0.5384503013
C  -5.1902789319  -1.1616205549   0.7942439239
C  -6.3869061906  -0.4735457122   1.1077675063
O  -6.7008180578  -0.1263066048   2.3532355008
O  -7.8145915599  -0.2070538598  -2.2521523075
C  -3.689384964   -2.3408917111  -0.781201196
C  -2.5821579092  -1.933198551    0.1819956132
O  -3.0534366452  -2.0016314381   1.545015818
C  -4.2495902015  -1.4791373164   1.8626630838
O  -4.4996891397  -1.3040462344   3.0503446645
```

```
C   -1.9939871388   -0.5553864783   -0.1066561735
C   -0.8663390314   -0.1435131209    0.8516882576
C    0.4665476167   -0.8572548862    0.6051829651
C    1.1754822403   -0.3273646672   -0.640359336
C    1.2768296274    1.1942656293   -0.5701435522
C   -0.0969645179    1.8097983093   -0.3235191452
O   -0.688452911     1.2664848221    0.850017388
C   -0.0477758302    3.3109323959   -0.1191846189
H   -8.1857855046    0.3930724056    0.3404863832
H   -5.6345838824   -1.4869761325   -2.5770058819
H   -5.9817169549   -0.4847990336    2.9348869432
H   -8.5808417444    0.2751872955   -1.9144053746
H   -3.915466665    -3.4041483591   -0.6295017839
H   -3.3427246407   -2.2322527324   -1.8128647689
H   -1.7904796631   -2.6861005178    0.1553347612
H   -1.6499405384   -0.5574596293   -1.1473361974
H   -2.7835523301    0.2004733248   -0.0354539916
H   -1.2046714968   -0.3648001631    1.8675973945
H    0.3143461428   -1.9408316361    0.5409700727
H    1.104866556    -0.6831856678    1.4789370186
H    0.6250476142   -0.6153773309   -1.5458435353
H    2.1691271991   -0.7791841897   -0.7294883617
H    1.7054420354    1.6022153999   -1.4927688969
H    1.9394583636    1.4850229762    0.2551554572
H   -0.7383316227    1.5911968989   -1.1940930986
H   -1.0511996573    3.7038541837    0.0623644253
H    0.3689613107    3.8070974999   -1.0005976965
H    0.5757257227    3.5537082814    0.7461934338

calc_**1b** conf_19

C   -7.2482792327    0.2393562729    0.0104781697
C   -7.1694203342   -0.276497516    -1.2768325133
C   -6.0864254508   -1.075499318    -1.6773323984
C   -5.0774012695   -1.3403708548   -0.7751251797
C   -5.1221815617   -0.8131381001    0.5293689645
C   -6.2325172916   -0.0317367661    0.9295557278
O   -6.3447903347    0.4615169536    2.160395718
O   -8.1246899935   -0.0443353064   -2.2034729158
C   -3.9105630944   -2.2296756589   -1.0932706553
C   -2.6632121518   -1.7552669726   -0.3608976212
O   -2.9301654102   -1.677438503     1.057191505
C   -4.0447848255   -1.0654054822    1.48020182
O   -4.1090213139   -0.7437153357    2.6640554543
C   -2.1046790053   -0.4224405636   -0.8714332602
C   -0.5747107362   -0.339018804    -0.7685132473
C   -0.0211865584    1.0323705863   -1.1660832957
C   -0.222737892     2.0654103012   -0.0588457705
C    0.3188273205    1.5190479059    1.2596660749
C   -0.3073997816    0.1635822468    1.5710555066
O   -0.0850979256   -0.7483154056    0.4952656622
C    0.2651064075   -0.4982420492    2.8069523437
H   -8.0900582949    0.8451474302    0.331017397
H   -6.068953385    -1.4719691132   -2.6859079064
H   -5.5616910888    0.1236949039    2.6683589784
H   -8.8140142619    0.5114684587   -1.8166421208
H   -4.1410796543   -3.2541490887   -0.7734407274
H   -3.719879708    -2.2665566637   -2.1695840781
H   -1.8851612588   -2.5187239544   -0.4224121892
```

```
H   -2.3717640174   -0.2986441633   -1.9276991478
H   -2.5917310555    0.4015673838   -0.340917426
H   -0.1693523092   -1.0910176677   -1.4571738886
H   -0.4798102325    1.3630599265   -2.1051608564
H    1.0529081582    0.9205017113   -1.3546279356
H   -1.2888754328    2.3013767804    0.0536711363
H    0.2739135223    3.0043303944   -0.3256483756
H    0.1171356199    2.2134382917    2.0830472348
H    1.4078717707    1.3968480331    1.1937327008
H   -1.3890327699    0.2967786608    1.7164661971
H    0.1151843148    0.1355378331    3.6855629954
H    1.3372902824   -0.677565527     2.6817571813
H   -0.2315697639   -1.4553112605    2.9812207417

calc_1b conf_20

C   -7.8777869465   -1.1221354418    0.1008990155
C   -7.5311375631   -0.0284378605   -0.6826386062
C   -6.2191242213    0.4697317504   -0.6989963658
C   -5.2546146553   -0.1499094676    0.0688892534
C   -5.5745553661   -1.2721050234    0.8558002123
C   -6.908416862    -1.7455824658    0.888299777
O   -7.2764192187   -2.7741222835    1.6482631761
O   -8.4311408297    0.6124293482   -1.459964248
C   -3.8363734219    0.3427730277    0.1350071313
C   -2.8896474883   -0.8234490816    0.3582744954
O   -3.281263287    -1.5630793319    1.5336891674
C   -4.5639273969   -1.9306882098    1.6750430147
O   -4.8278858511   -2.798028107     2.5009603328
C   -1.4320112666   -0.4528949342    0.5789117662
C   -0.7696867943    0.1870903852   -0.6588547194
C   -0.6602212671    1.7144468075   -0.5923538
C    0.4319762686    2.1579671536    0.3795625749
C    1.7411040584    1.443195353     0.0536370571
C    1.5227016728   -0.0651604912   -0.000621905
O    0.4987259299   -0.3884300481   -0.9342097234
C    2.754940662    -0.8321852583   -0.4368131121
H   -8.8940281189   -1.5024642951    0.1304110877
H   -5.9914320685    1.3322571751   -1.3146210821
H   -6.4751474086   -3.0372796759    2.1706136262
H   -9.2919222019    0.1827115781   -1.369791384
H   -3.571476567     0.8693508016   -0.7863191462
H   -3.7264671876    1.0579723983    0.9616482907
H   -2.9643889977   -1.5111278481   -0.495199497
H   -1.3646956706    0.1886850217    1.4644145394
H   -0.8999788814   -1.3796168136    0.8130978829
H   -1.3626908132   -0.0835977193   -1.5408615934
H   -1.6257349885    2.1535803812   -0.3177798731
H   -0.4140607311    2.0795838082   -1.596385539
H    0.1378013345    1.9265907233    1.411801549
H    0.5592186784    3.2445272198    0.3319399325
H    2.5117442883    1.6803666765    0.7958150435
H    2.1141959932    1.7750739381   -0.9237850536
H    1.2221316479   -0.4119238218    1.0027690946
H    3.5835082497   -0.656629463     0.2553284336
H    3.0626695823   -0.5149754195   -1.4375266042
H    2.5465177049   -1.9045104865   -0.4673542018

calc_1b conf_21
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```
C   -7.7176395556   -1.3738322877   -0.2508455708
C   -7.92125013     -0.0692632515    0.1813260185
C   -6.8535454606    0.7269038351    0.6236536274
C   -5.5762961779    0.2045737905    0.6166209681
C   -5.3395128381   -1.1082066694    0.1659966277
C   -6.4290841544   -1.9105841541   -0.2505205671
O   -6.2689574355   -3.1709331075   -0.6468915861
O   -9.1479464249    0.497061868     0.202832899
C   -4.3840769307    0.9771454328    1.1057272695
C   -3.1415345931    0.553704752     0.3417590993
O   -2.9580844039   -0.8705986958    0.4373914366
C   -3.9941211498   -1.6728904631    0.1592735597
O   -3.7625312224   -2.8550953444   -0.0758057217
C   -1.8676674151    1.2207029892    0.8313287498
C   -0.5917446352    0.715802936     0.1577187765
C    0.4868984445    1.788097144     0.0251460887
C    1.7587991191    1.177385634    -0.5613903512
C    2.1805956042   -0.0482904463    0.2497271184
C    1.0220050813   -1.0336921014    0.4330374429
O   -0.1191233694   -0.3573472559    0.9510543296
C    0.6909403857   -1.8504573963   -0.8136684339
H   -8.5410338129   -2.0000635937   -0.5797369774
H   -7.05479021     1.7363105605     0.9634116162
H   -5.3074512008   -3.3829693217   -0.5212817031
H   -9.7974735209   -0.1402481654   -0.1221297455
H   -4.5424386983    2.0537370884    0.9914649383
H   -4.2267267405    0.7843717398    2.1753527411
H   -3.282819852     0.7834960115   -0.7238609156
H   -1.9807232903    2.2969706959    0.6553686697
H   -1.7573113058    1.0739704098    1.9108849649
H   -0.8439057182    0.3524152516   -0.8519871008
H    0.6926258558    2.2028989118    1.0206251742
H    0.1235879177    2.6091837342   -0.6043720835
H    2.5682884725    1.91488825     -0.5802010304
H    1.5750071686    0.8943285271   -1.605816787
H    2.5093817349    0.2801619874    1.2429418622
H    3.0315349526   -0.5540039208   -0.2205625754
H    1.2820361479   -1.7369817515    1.2306392905
H    0.543624968    -1.2311142305   -1.7032812015
H   -0.2236357083   -2.4242249521   -0.6429264487
H    1.5061001016   -2.5473144405   -1.0320044689

calc_1b conf_22

C   -7.2796136087   -0.1422958164    0.0941220131
C   -6.9988772868   -0.4994604887   -1.2171398862
C   -5.8261175512   -1.1998185497   -1.5465276542
C   -4.9316988255   -1.5306509837   -0.5469704221
C   -5.1843915903   -1.1650554071    0.7858796444
C   -6.3838899131   -0.4791635514    1.1080641698
O   -6.6886233119   -0.1398552921    2.3579558784
O   -7.9027588351   -0.1487895478   -2.1586770302
C   -3.6871723789   -2.3302058082   -0.8051754962
C   -2.5763659103   -1.9290172181    0.1568820637
O   -3.042737709    -2.0113195051    1.5196486677
C   -4.2377620742   -1.4900318386    1.8474848221
O   -4.4803866482   -1.3242588473    3.037228647
C   -1.9916406572   -0.547894229    -0.1228704962
```

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C   -0.8797470423   -0.1278804772    0.850345774
C    0.4553777824   -0.8492468139    0.6411846014
C    1.1917473027   -0.3400614683   -0.5971703187
C    1.296042699     1.1822897316   -0.5476044626
C   -0.0805364941    1.8051732363   -0.3382233924
O   -0.6971640689    1.281237073     0.8309405469
C   -0.0311499609    3.309107217    -0.1558507074
H   -8.1927961533    0.3867904965    0.3349497651
H   -5.6280326987   -1.4830585428   -2.5772293497
H   -5.9678083659   -0.5001919879    2.9341027191
H   -7.6010066681   -0.4611964678   -3.0213614396
H   -3.908543909    -3.3958996561   -0.6638096629
H   -3.3447996803   -2.2093138834   -1.8372176964
H   -1.7835234417   -2.6802087929    0.1194370359
H   -1.6331369478   -0.5483556752   -1.1587638907
H   -2.7857175457    0.2041960886   -0.0622621561
H   -1.2382356068   -0.3332961892    1.8625602731
H    0.3015309368   -1.9332763738    0.591206633
H    1.0760466058   -0.6632038121    1.525125946
H    0.6598326512   -0.6406368579   -1.5096976832
H    2.1857936726   -0.7956503024   -0.6583150595
H    1.7449304626    1.575385775    -1.4670478198
H    1.9423557065    1.4833269605    0.2868749664
H   -0.7048049648    1.5752270946   -1.2183534781
H    0.4045904397    3.7906291201   -1.0362338021
H    0.5756359493    3.5635683922    0.717978726
H   -1.0368443601    3.7073631987   -0.0004709885

calc_1b conf_23

C   -7.7815940579   -1.0851508318   -0.202011421
C   -7.4216965693    0.1845503679   -0.6363166121
C   -6.157403109     0.7223111848   -0.348709766
C   -5.2522946878   -0.033645858     0.3675216161
C   -5.5840732026   -1.3310198453    0.8011544004
C   -6.8736135043   -1.8492858301    0.5332071224
O   -7.2563609368   -3.0506522965    0.959246899
O   -8.2634948618    0.9659814143   -1.3478420173
C   -3.8929605704    0.4759178506    0.7529304141
C   -2.8975545288   -0.6715568504    0.788359419
O   -3.3745719215   -1.6941177713    1.6923233544
C   -4.6358682165   -2.1340536856    1.5650725178
O   -4.9364407695   -3.1906466733    2.1108776134
C   -1.4992114814   -0.2989193719    1.2673494493
C   -0.4913055983   -0.0299833235    0.1541516023
C   -0.8249013264    1.1566124036   -0.7470816004
C    0.325624976     1.4372576463   -1.713111767
C    1.632761051     1.588931804    -0.9384605427
C    1.8726713623    0.3971491337   -0.0084901592
O    0.7387753317    0.1807939821    0.8270244262
C    2.3036382575   -0.8739529465   -0.7348472294
H   -8.7636063039   -1.5001215831   -0.4062645005
H   -5.9195056264    1.7221371555   -0.693058825
H   -6.509092451    -3.4039089841    1.5079377563
H   -9.0965910491    0.4953641649   -1.4827304465
H   -3.5537011617    1.2514482264    0.0616872152
H   -3.9344271997    0.9320608776    1.7512214752
H   -2.8449704006   -1.1341423277   -0.2071989361
H   -1.5373629818    0.5706236592    1.9332232392
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S72

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H  -1.1138016903   -1.1335039636    1.8590879436
H  -0.4237034013   -0.9350236343   -0.4732920436
H  -1.0026259109    2.0367928987   -0.1150710911
H  -1.7466810864    0.9584579255   -1.3064872767
H   0.1225341468    2.3411622762   -2.2968733241
H   0.4048126261    0.6149238467   -2.4353350547
H   1.581288648     2.4968824318   -0.32597971
H   2.4824586919    1.7072657683   -1.6200527538
H   2.6637854541    0.6594963787    0.7014108786
H   1.6039016131   -1.1741019709   -1.5197425814
H   2.3887542876   -1.6983451991   -0.0219676942
H   3.2804081592   -0.7239884502   -1.2048619898
```

calc_**1b** conf_24

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C  -7.7691823038   -0.9976330888   -0.1438127667
C  -7.2934963115    0.154991461    -0.7564894723
C  -5.9731718057    0.5903390234   -0.5645363018
C  -5.1302120918   -0.1506037579    0.2384073613
C  -5.5803738144   -1.3335164029    0.853257422
C  -6.9237945962   -1.7449702265    0.6778350888
O  -7.4156096031   -2.8291927817    1.2722460225
O  -8.0708210311    0.9151922218   -1.5586205153
C  -3.7162798025    0.2689456799    0.5270306757
C  -2.8392602743   -0.953069219     0.7361035539
O  -3.3985366932   -1.7991191533    1.7626332279
C  -4.6995180276   -2.1204404661    1.70844739
O  -5.0915066872   -3.0577971185    2.395501902
C  -1.4135503586   -0.6745999937    1.1823525505
C  -0.5639142117    0.0822916214    0.1576393106
C  -0.4575605049    1.5823994967    0.4268376817
C   0.5031444511    2.2391723685   -0.5612255457
C   1.8473513419    1.5148149708   -0.5271682221
C   1.6778982324    0.0055554004   -0.7178314503
O   0.7232738546   -0.5165355006    0.203581566
C   1.3682464133   -0.4001208211   -2.1566136222
H  -8.7939488298   -1.330911931    -0.2745460183
H  -5.6439208989    1.502124612    -1.0494076625
H  -6.6925507047   -3.1820985392    1.8530042053
H  -8.9502199488    0.518964043    -1.616730104
H  -3.3225546425    0.8720439145   -0.2959916548
H  -3.6877038012    0.8927893133    1.4307358231
H  -2.8229797137   -1.5404530575   -0.1921488392
H  -1.4332847284   -0.1430382322    2.140400741
H  -0.930625886    -1.6387070068    1.3619582805
H  -0.9965574749   -0.0654704079   -0.8479536232
H  -0.0833303627    1.7164084803    1.4498653466
H  -1.4470120614    2.0503867641    0.3820484795
H   0.6371627185    3.2988878256   -0.3198845318
H   0.075163715     2.2047319922   -1.5713696586
H   2.3175083801    1.6870195484    0.4481718703
H   2.528901726     1.9111101294   -1.288087286
H   2.6085776615   -0.4913303532   -0.4253501477
H   2.2155976563   -0.1573097629   -2.8050731265
H   0.488846104     0.1077913284   -2.5624986079
H   1.1938049158   -1.4780423743   -2.2097193424
```

calc_**1b** conf_25

S73

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C   -7.0248812447   0.0924539983   0.1328744829
C   -6.5544619945  -0.0420133986  -1.1670274884
C   -5.4078843811  -0.8009804393  -1.4520999699
C   -4.7325113858  -1.4131050131  -0.4160460382
C   -5.1755297017  -1.2748879524   0.9126636858
C   -6.3489892974  -0.5315683305   1.183782293
O   -6.8364689153  -0.4007400921   2.4148173589
O   -7.1720068598   0.5380407558  -2.2191841711
C   -3.5358036048  -2.2929720261  -0.6308652882
C   -2.5735946269  -2.18693452     0.5439291747
O   -3.2684211105  -2.4788622007   1.7760649798
C   -4.4556126964  -1.9026335516   2.0166350439
O   -4.8910514918  -1.9393693596   3.1629186822
C   -1.8423835598  -0.8546414944   0.694693066
C   -0.8732443996  -0.5549416118  -0.4678249559
C   -1.4199066472   0.4456620094  -1.4920117647
C   -1.4035535473   1.8720341551  -0.946748101
C   -0.0141389773   2.2105949264  -0.4139601027
C    0.439073467    1.1549974628   0.5885487776
O    0.4023289174  -0.1417284793   0.0018171888
C    1.8594561914   1.3611123197   1.0755872556
H   -7.9193975391   0.6644120408   0.3586431132
H   -5.0846474053  -0.8999103878  -2.4820076091
H   -6.2579583308  -0.9512626522   3.0041725754
H   -7.9448372785   1.025851944   -1.9052454818
H   -3.8668194573  -3.336070703   -0.7140944013
H   -3.0233920794  -2.0507640844  -1.5658452791
H   -1.831307399   -2.986606184    0.476330852
H   -2.574527399   -0.0517130623   0.8312833791
H   -1.2597415899  -0.9222121911   1.6180935819
H   -0.6544393461  -1.499131425   -0.9822703479
H   -2.4344347305   0.1647782612  -1.7951229258
H   -0.7868745329   0.3972654057  -2.3858965102
H   -2.1405206895   1.9770908661  -0.1399505174
H   -1.703210576    2.5761996457  -1.7298814749
H   -0.0055690902   3.198606942    0.0599708205
H    0.7072493374   2.2371116611  -1.2408074498
H   -0.2440996766   1.1810915235   1.4545673898
H    2.138455939    0.5767381943   1.7835774155
H    1.9603393235   2.3310562533   1.5708519333
H    2.5563183862   1.3249507938   0.2330668276

calc_1b conf_26

C   -7.7937331577  -1.1192862544  -0.0813807873
C   -7.3861538447  -0.0334146311  -0.8461220124
C   -6.0770237512   0.4665937447  -0.7629221914
C   -5.1772174836  -0.1436059408   0.0862984859
C   -5.5582811947  -1.2583042553   0.8567741973
C   -6.8899445916  -1.7332096753   0.7876140952
O   -7.3171040555  -2.7538313722   1.5270852902
O   -8.2212193992   0.5986259247  -1.6994804903
C   -3.7701588417   0.3491155401   0.2690660352
C   -2.842538704   -0.8176474088   0.5635649775
O   -3.3257293734  -1.5337532252   1.7225535458
C   -4.6156551375  -1.9034651549   1.7638172955
O   -4.9442017143  -2.7607048728   2.576968169
C   -1.3970401963  -0.4322308882   0.8676822675
C   -0.4318482544  -0.6400860246  -0.3093209259
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C   -0.6697890343    0.2540365136   -1.5282817942
C   -0.2348532351    1.6930023003   -1.2615173486
C    1.2102831441    1.7021976669   -0.7678027458
C    1.3783305949    0.7690724467    0.4282248116
O    0.9175719688   -0.5425177377    0.1206640474
C    2.8218777396    0.616996313     0.8647831547
H   -8.8090435495   -1.500273051    -0.1285136967
H   -5.8016341888    1.3240378217   -1.3660004313
H   -6.5608577654   -3.0090462584    2.1161184043
H   -9.087062092     0.1703838315   -1.6731562594
H   -3.4279283448    0.8943370523   -0.6146001615
H   -3.7281813904    1.0490421642    1.1145548365
H   -2.8760436116   -1.5250885777   -0.2770679504
H   -1.3628420734    0.5968058493    1.2409468337
H   -1.0459757876   -1.0751909303    1.6795064162
H   -0.5317901727   -1.6864219259   -0.620968928
H   -1.717095126     0.2022198483   -1.8464372848
H   -0.073628187    -0.1482453249   -2.3557482061
H   -0.8842221455    2.1556957378   -0.5064392352
H   -0.337414316     2.2960714048   -2.1697768615
H    1.5249111066    2.7146766157   -0.4906748533
H    1.8760435001    1.3616292681   -1.5713145851
H    0.7951071053    1.1741400945    1.2715226273
H    3.2415510487    1.5846378472    1.1546638277
H    3.4226026946    0.2056578411    0.048324642
H    2.8919318172   -0.0636523175    1.7167927887


calc_1b conf_27

C   -6.3517370232    0.3614967164   -0.3048366429
C   -5.8927031064   -0.1337591214   -1.5207216144
C   -4.8695173497   -1.0891183834   -1.5763590809
C   -4.3098361059   -1.5506576046   -0.4002419163
C   -4.7528664069   -1.0657312413    0.8415425823
C   -5.792752499    -0.1024322686    0.8862570698
O   -6.2661746774    0.3777876885     2.033825381
O   -6.4095205177    0.2751855971    -2.7012160124
C   -3.2973767055   -2.657453191    -0.4024323518
C   -2.4440343507   -2.7313700924    0.8631324842
O   -3.193488134    -2.4500970298    2.0636427257
C   -4.1976528046   -1.5667099379    2.0918562857
O   -4.6244199334   -1.2322082266    3.1943386102
C   -1.1435781147   -1.9299526181    0.8829260926
C   -1.1898299226   -0.4207131387    0.691208519
C    0.157236001     0.2027464548    1.0619861778
C    0.2095229362    1.6801008773    0.6829776549
C   -0.1828852166    1.8489093062   -0.7828740755
C   -1.5302388866    1.1851324293   -1.0740624453
O   -1.5040682578   -0.1859040199   -0.672485029
C   -2.7159658972    1.9463193738   -0.49035381
H   -7.149450065     1.0958617582   -0.2523258726
H   -4.5406243739   -1.4546200973   -2.5421167164
H   -5.7830919854   -0.1038670094    2.7561300813
H   -7.1070113079    0.9225132364   -2.533664111
H   -3.8416043988   -3.6043748032   -0.5101313986
H   -2.6384294404   -2.5653441712   -1.2687700152
H   -2.1503141906   -3.775140607     1.0032353692
H   -0.6669920192   -2.1381511717    1.8472456971
H   -0.4871779594   -2.3419918661    0.1065454369
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H   -1.969947378    0.0137133259    1.3357981119
H    0.9474476361   -0.3400960447    0.5260700624
H    0.3386768777    0.0665154568    2.1340178715
H    1.2125354684    2.0831977722    0.8584840847
H   -0.4701668632    2.2518440238    1.3265417184
H    0.5797379439    1.3782887976   -1.4149682973
H   -0.2250290606    2.9079574768   -1.0606857387
H   -1.6698643611    1.1270032803   -2.1583564604
H   -2.7770441793    2.9395767967   -0.9464389706
H   -2.6403346088    2.0866464266    0.5912860394
H   -3.6464287618    1.4148958498   -0.6980074966

calc_1b conf_28

C   -7.2243521279   -0.0402002481    0.3786108263
C   -6.6803662567    0.2492077953   -0.8660806888
C   -5.4538380881   -0.3012609133   -1.2712633655
C   -4.773252356    -1.1345717703   -0.407188702
C   -5.2916325941   -1.4263591773    0.8682212826
C   -6.5432915049   -0.8896986112    1.2531833313
O   -7.1006713386   -1.1643112188    2.429642552
O   -7.2994156698    1.062778068    -1.7495917159
C   -3.4870302485   -1.8156472374   -0.7753265076
C   -2.5978843323   -1.9828430057    0.448774183
O   -3.3193258031   -2.6713748539    1.4929000269
C   -4.5681971531   -2.2890437164    1.7972883025
O   -5.0539559234   -2.6951631132    2.8480072519
C   -2.0051461492   -0.6988868003    1.0218607573
C   -1.0106672521   -0.0009169461    0.0874986971
C   -1.5756869249    1.2419225186   -0.5966179901
C   -0.4941670305    1.9386803415   -1.4185596295
C    0.7173426691    2.2241462815   -0.5329505108
C    1.1906364337    0.9655470088    0.1996526187
O    0.1092357339    0.3442618738    0.8899533037
C    1.9432195304   -0.0184593546   -0.6927913659
H   -8.1798075855    0.3688287819    0.6918740245
H   -5.0722892011   -0.0676179118   -2.2586050791
H   -6.4999968636   -1.8149002133    2.8781187427
H   -8.1277320182    1.3779137071   -1.3644669256
H   -3.7102939823   -2.8099578058   -1.1829212029
H   -2.9542384281   -1.2676126583   -1.557350048
H   -1.7814199339   -2.669655211     0.2108636174
H   -2.8085328538   -0.0125032648    1.3106787544
H   -1.4659879484   -0.9678351253    1.9339340165
H   -0.6888703559   -0.7136139698   -0.6931230204
H   -1.9418744397    1.9209522981    0.1838453838
H   -2.438371625     0.9778553672   -1.2185512352
H   -0.8774137281    2.8702674305   -1.8479463899
H   -0.2068975098    1.3029745596   -2.2662374744
H    0.4377193209    2.9724413502    0.2179615237
H    1.5430506022    2.6460991285   -1.1166237882
H    1.8669169238    1.2643478542    1.0071045904
H    2.1908399051   -0.9198640965   -0.1258344437
H    2.8762315947    0.4326701517   -1.0442697942
H    1.371414513    -0.3175972931   -1.5756739089

calc_1b conf_29

C   -7.3973210916   -0.2033074186    0.266852206
```

```
C   -6.9081200586   -0.0110929031   -1.0188180354
C   -5.653276033    -0.5096062079   -1.4033203241
C   -4.8901482549   -1.1939875624   -0.4797431283
C   -5.3529246189   -1.3834877772    0.8351675698
C   -6.6311417869   -0.9005532699    1.203138046
O   -7.1354299047   -1.0865703948    2.4204659455
O   -7.6091946583    0.6548523747   -1.9626627812
C   -3.56375861     -1.8100101601   -0.8224030649
C   -2.6350050959   -1.7880041524    0.3851095244
O   -3.2836056151   -2.4237735357    1.5102362543
C   -4.545485818    -2.0924773644    1.8211251014
O   -4.9695053154   -2.4175778067    2.9255390274
C   -2.1361900956   -0.3986859596    0.7932410866
C   -0.7673561413   -0.0227901887    0.2310089758
C   -0.698220651     0.0954397133   -1.2896471701
C    0.6635087198    0.6366151109   -1.7246785541
C    0.9703514938    1.935027049    -0.9824649629
C    0.8207238551    1.7629196168    0.5306354334
O   -0.4568446706    1.2164348039    0.8464984153
C    1.9577988139    0.9773083871    1.178209113
H   -8.3728499869    0.166575355     0.5665384464
H   -5.3126196325   -0.3511376841   -2.4199931595
H   -6.4758462002   -1.6396285846    2.9141428205
H   -8.4479530032    0.9509637515   -1.5851609577
H   -3.7185171899   -2.8516749896   -1.1317079177
H   -3.1003050264   -1.290495922    -1.6643560926
H   -1.7787861315   -2.4428750404    0.2009482893
H   -2.8606486866    0.376075904     0.5195703278
H   -2.0435061401   -0.3783445546    1.8827240388
H   -0.042659296    -0.79070894      0.5521850201
H   -1.492740604     0.7750958197   -1.6248944571
H   -0.8804243378   -0.8814554657   -1.7528004043
H    0.6801042142    0.8038595638   -2.8067566165
H    1.4379639884   -0.1123823988   -1.5164004852
H    0.2657344165    2.7081863348   -1.3107987347
H    1.9778440445    2.2946986858   -1.2193374355
H    0.7942133011    2.7539075866    0.9952288195
H    1.7537783048    0.8393303319    2.2432763053
H    2.8987450951    1.526845971     1.0771098003
H    2.1036184076   -0.0095080782    0.7299937146

calc_1b conf_30

C   -7.0411492462   -0.1145011113   -0.1664352005
C   -6.4167610027   -0.2802402471   -1.3959659338
C   -5.1895822971   -0.9539223584   -1.5052178443
C   -4.5919984091   -1.4509892044   -0.3649859361
C   -5.1920931771   -1.2765484134    0.8951427659
C   -6.4423240248   -0.6203599406    0.9893642785
O   -7.0748529421   -0.4638681565    2.1494305812
O   -6.9533335495    0.1879603847   -2.5441263034
C   -3.3116352298   -2.2352043559   -0.3978919871
C   -2.5004408019   -1.9873385512    0.8679215674
O   -3.3120900874   -2.2757950989    2.0295226062
C   -4.5570150396   -1.7834400113    2.1064274681
O   -5.1135921483   -1.7948068347    3.1995220576
C   -1.9022115368   -0.5805017257    0.9867793948
C   -0.4278605822   -0.4888194388    0.5606083598
C   -0.1372092649   -0.7628969115   -0.916179125
```

```
C  -0.6075544687   0.3881830136  -1.8014967134
C   0.0024665243   1.6931199771  -1.2954131241
C  -0.2897473512   1.8892729189   0.1901691532
O   0.1294957115   0.7583288749   0.9483058168
C   0.4313557048   3.0837659382   0.782253491
H  -7.9971886036   0.3916367315  -0.0766318694
H  -4.7423490296  -1.0783133075  -2.4847425939
H  -6.526429235   -0.9306599463   2.8321143089
H  -7.7917562567   0.6263264636  -2.3475572173
H  -3.5438557613  -3.305586403   -0.4670219355
H  -2.7224636107  -1.977691243   -1.2813022908
H  -1.7016543055  -2.7305345497   0.9438818698
H  -2.524027849    0.1362867984   0.4411577466
H  -1.9321705889  -0.2906844405   2.0410457777
H   0.1233464269  -1.2200078966   1.1639609555
H  -0.5741199143  -1.7183038161  -1.2275129316
H   0.9487468865  -0.8700575221  -1.022976869
H  -1.7031465435   0.4615909566  -1.7868315947
H  -0.3225764119   0.2077757633  -2.8434103488
H  -0.37913105     2.5510450622  -1.8603521766
H   1.0909458868   1.667655801   -1.4354212651
H  -1.3751359022   2.0330201536   0.3162857024
H   0.1336970934   4.0049832622   0.2730576527
H   1.5134692778   2.9610710536   0.6791871196
H   0.1979327092   3.181048331    1.8453345866

calc_**1b** conf_31

C  -6.6856202094   0.1594411994   0.1400087909
C  -6.1398422171   0.1087644402  -1.1370691676
C  -4.9896785344  -0.6448504202  -1.4082455299
C  -4.3801705419  -1.3388091057  -0.3833963854
C  -4.9042927702  -1.2952823229   0.9206601832
C  -6.0791160164  -0.5461148808   1.1791514831
O  -6.6323861313  -0.4884833771   2.3891165685
O  -6.6901069062   0.7725290537  -2.1783493352
C  -3.2024662986  -2.2379932201  -0.6253253213
C  -2.3162878624  -2.4294136759   0.6040992739
O  -3.0897068544  -2.6217054399   1.8082505861
C  -4.261742429   -2.0074603293   2.0162221223
O  -4.745497339   -2.0829243507   3.1425416016
C  -1.231459612   -1.3814503562   0.8622995195
C  -1.6493494037   0.093774038    0.8573422172
C  -0.6560655066   1.0002335364   1.5904264035
C   0.6188360634   1.2136681832   0.7794250582
C   0.2491535748   1.7211552424  -0.6115784192
C  -0.7522346351   0.7840019793  -1.2802968835
O  -1.8968029422   0.5739932416  -0.4615656909
C  -1.2706086967   1.3221278922  -2.6000778803
H  -7.5827369225   0.7316055338   0.3547064119
H  -4.5974200671  -0.661724154   -2.4180094054
H  -6.0873470426  -1.0782588156   2.972473497
H  -7.4688358421   1.2541965884  -1.8700704086
H  -3.5851028378  -3.2207809265  -0.9293011408
H  -2.5964327814  -1.8602432738  -1.4517606514
H  -1.7983411226  -3.3865485667   0.5000112636
H  -0.7958390629  -1.6284049286   1.8367279165
H  -0.4366345787  -1.5449344488   0.1259965324
H  -2.6192361451   0.1844176255   1.3545782775
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S78

```
H   -0.4377237336   0.585720481    2.5804320617
H   -1.1407505737   1.9708049333   1.7486555498
H    1.180876039    0.2740871551   0.6958634365
H    1.2787324387   1.9245440566   1.287637515
H    1.136988068    1.8176749419  -1.2468472389
H   -0.204847347    2.7174483132  -0.5317782676
H   -0.2478793363  -0.1799000642  -1.466004176
H   -0.4464481588   1.4825171132  -3.3011828781
H   -1.7866170046   2.2732497707  -2.441948184
H   -1.9799587202   0.6233273376  -3.0508193056

calc_1b conf_32

C   -6.3302112195   0.5584526836   0.1159147467
C   -6.0924954503   0.087783833   -1.1695262366
C   -5.2183109711  -0.9852053395  -1.4022134738
C   -4.5779466756  -1.575031194   -0.3306470663
C   -4.7874613407  -1.1078362848   0.9786075738
C   -5.6887254523  -0.0383334229   1.2029782774
O   -5.9452598228   0.4292406909   2.4216370302
O   -6.688806931    0.6285547057  -2.2542435349
C   -3.6939645866  -2.7775506222  -0.4868801618
C   -2.5965122032  -2.8536347083   0.5725499089
O   -3.11155782    -2.5889373679   1.8957694455
C   -4.0800774087  -1.692300191    2.1113036686
O   -4.3248242663  -1.3889035218   3.2763445781
C   -1.3309575638  -2.0471551988   0.2887121701
C   -1.4225108883  -0.5351464113   0.0750172384
C   -1.3784853849   0.2831633697   1.3632034504
C   -1.3059668472   1.7751462769   1.0452940268
C   -0.1332027482   2.0488821341   0.1065564427
C   -0.1759177635   1.1407336249  -1.1249740094
O   -0.2943722328  -0.2258471823  -0.7386689623
C   -1.2374825832   1.5421594458  -2.1465764958
H   -7.0140768508   1.3800627242   0.3045469401
H   -5.0698392474  -1.3340215135  -2.4175701668
H   -5.4314656508  -0.1405149064   3.0524007152
H   -7.2686205015   1.3484845363  -1.9726835254
H   -4.3201322076  -3.6751200599  -0.4046251646
H   -3.2384919026  -2.8031846845  -1.4810583981
H   -2.2758253471  -3.8958107651   0.6472499576
H   -0.6093256839  -2.255428138    1.0863673823
H   -0.9035453815  -2.4646872348  -0.6302957192
H   -2.3425380197  -0.2932391378  -0.476513592
H   -2.2415968224   0.066317514    1.9982133786
H   -0.4851194201  -0.0191265948   1.9248843066
H   -1.1969424225   2.3563538803   1.9668822319
H   -2.2490170565   2.098862316    0.5868365782
H    0.8030636865   1.8541384373   0.6430266614
H   -0.113015445    3.0989217294  -0.2065003872
H    0.7980208166   1.1800237319  -1.6242642683
H   -1.0054356494   2.5281143316  -2.5610388574
H   -2.2425647376   1.592680066   -1.7186995975
H   -1.2544819965   0.8209384482  -2.9683170923

calc_1b conf_33

C   -6.7937413613   0.3057345874   0.4043563784
C   -6.6245548314   0.0369544605  -0.9481632322
```

S79

```
C   -5.6287255208   -0.8445633592   -1.3966242251
C   -4.7975086698   -1.44581634     -0.4733774227
C   -4.9351243588   -1.1778089907    0.9002079298
C   -5.9574302978   -0.302308718     1.3420957601
O   -6.1509998354   -0.0306646564    2.6298069861
O   -7.4062249973    0.5981302731   -1.8954933874
C   -3.7673266432   -2.4631531567   -0.8677770075
C   -2.5699484084   -2.5072160625    0.0788499925
O   -2.9770118036   -2.4795474305    1.4636689559
C   -4.0339598607   -1.7708046399    1.8791583824
O   -4.1898990697   -1.6455922431    3.0912154598
C   -1.4537160823   -1.4966012317   -0.1926806192
C   -1.7907978465    0.0055971031   -0.211847587
C   -1.7245259931    0.6922285481    1.1566294041
C   -0.2832841767    0.8918110827    1.6237243266
C    0.5293426358    1.5844128329    0.533280729
C    0.4012553191    0.8292984874   -0.7849992271
O   -0.9657089749    0.687035193    -1.1523306366
C    1.0790226171    1.5342642961   -1.943430653
H   -7.5684598646    0.9779916792    0.7594040901
H   -5.5369093182   -1.0391259098   -2.4588321058
H   -5.4907541646   -0.5761063538    3.1319890619
H   -8.0484564943    1.1834075406   -1.4727092282
H   -4.2463263576   -3.4505333659   -0.8669262313
H   -3.4140371372   -2.2876130497   -1.8881208122
H   -2.108590814    -3.4939188227   -0.0131517363
H   -0.6508383715   -1.7098629933    0.5208270945
H   -1.061802462    -1.7438839726   -1.1868359799
H   -2.7949949601    0.1342637308   -0.6241965078
H   -2.2910380452    0.1280210232    1.9025483618
H   -2.2056392382    1.672596383     1.0610239926
H    0.17611461     -0.0750405898    1.8669766663
H   -0.2697230563    1.476808101     2.5491581289
H    1.5856791388    1.6585939928    0.8164756459
H    0.157450192     2.6064085537    0.3842242401
H    0.8538517287   -0.1693256518   -0.6612231969
H    2.1487067098    1.6557301426   -1.7496018636
H    0.6362427583    2.5233906913   -2.0922718896
H    0.953393306     0.9618088357   -2.8660280374
```

Table S30. Sampled and DFT geometry optimized conformers related to calc_**1c**, with energy values (Hartree) and related % contribution on the final Boltzmann distribution for the three employed functional/basis set combinations.

Conformer	MPW1PW91/6-31g(d,p)		MPW1PW91/6-311+g(d,p)		B97-2/cc-pVTZ	
	Energy (Hartree)	% contribution on the Boltzmann distribution	Energy (Hartree)	% contribution on the Boltzmann distribution	Energy (Hartree)	% contribution on the Boltzmann distribution
calc_**1c** conf_1	-997.7128633	30.73%	-997.9473639	23.32%	-997.906243	18.46%
calc_**1c** conf_2	-997.7127837	28.25%	-997.9476911	32.98%	-997.906957	39.32%
calc_**1c** conf_3	-997.7119331	11.47%	-997.9466498	10.95%	-997.905516	8.54%
calc_**1c** conf_4	-997.7118445	10.45%	-997.9469827	15.57%	-997.906352	20.72%
calc_**1c** conf_5	-997.7115434	7.59%	-997.9463331	7.83%	-997.905056	5.25%
calc_**1c** conf_6	-997.7112678	5.67%	-997.9456922	3.97%	-997.904662	3.46%
calc_**1c** conf_7	-997.7103432	2.13%	-997.9447668	1.49%	-997.903149	0.70%
calc_**1c** conf_8	-997.7098307	1.24%	-997.9449555	1.82%	-997.903769	1.34%
calc_**1c** conf_9	-997.7093698	0.76%	-997.9438321	0.55%	-997.902300	0.28%
calc_**1c** conf_10	-997.7091792	0.62%	-997.9438379	0.56%	-997.903029	0.61%
calc_**1c** conf_11	-997.7090163	0.52%	-997.9432388	0.30%	-997.901909	0.19%
calc_**1c** conf_12	-997.7079788	0.17%	-997.9427438	0.17%	-997.902746	0.45%
calc_**1c** conf_13	-997.7075991	0.12%	-997.9426792	0.16%	-997.902091	0.23%
calc_**1c** conf_14	-997.7074178	0.10%	-997.9424855	0.13%	-997.902011	0.21%
calc_**1c** conf_15	-997.7073956	0.09%	-997.9422959	0.11%	-997.900200	0.03%
calc_**1c** conf_16	-997.7066684	0.04%	-997.9413475	0.04%	-997.901716	0.15%
calc_**1c** conf_17	-997.7059392	0.02%	-997.9409557	0.03%	-997.899743	0.02%
calc_**1c** conf_18	-997.7057660	0.02%	-997.9408909	0.02%	-997.899825	0.02%
calc_**1c** conf_19	-997.7038946	0.00%	-997.9392581	0.00%	-997.897492	0.00%
calc_**1c** conf_20	-997.7015944	0.00%	-997.9351053	0.00%	-997.892976	0.00%

Table S31. Cartesian coordinates of the optimized geometries for the conformers related to calc_**1c**. The related energies and % contribution on the final Boltzmann distribution for the three employed functional/basis set combinations are reported in Table S30.

calc_**1c** conf_1

```
C   -7.4302241253   -0.514733415    3.4644105364
C   -6.4045823942   -1.4037444659   3.7621244368
C   -5.344891342    -1.6203565001   2.8684921032
C   -5.3292943839   -0.9464897701   1.6639444379
C   -6.3679069808   -0.0557975357   1.3292320308
C   -7.4149551492    0.178310847     2.2533308167
O   -8.3968287604    1.0433702131    2.0074970962
O   -6.3704707534   -2.0967609776   4.921888837
C   -4.208091769    -1.0862066147   0.6748972863
C   -4.7440454681   -0.9158728226  -0.7352159142
O   -5.4467054963    0.340429772    -0.8612498573
C   -6.3613478112    0.6684084897    0.0639459614
O   -7.1455333817    1.574978675    -0.198808145
C   -3.7157810299   -0.9358480939  -1.8565630326
C   -2.6524992941    0.1539341574   -1.814197291
C   -1.9513557805    0.3217114276   -3.1604536542
C   -0.815460357    1.3363096926   -3.0501029768
C    0.1059557734    0.9757232826   -1.8870017594
C   -0.6996073842    0.7774445875   -0.6065355059
O   -1.7135103878   -0.2007490641   -0.8068610749
C    0.1434413278    0.3054895188    0.5610654268
H   -8.2440279357   -0.3300131561   4.1585979961
H   -4.5568253474   -2.3117403017   3.1436990574
H   -8.17936714     1.4735583236    1.1404721981
H   -7.1453758686   -1.8668628322   5.4513072441
H   -3.7223837507   -2.06210376     0.763965652
H   -3.4332690152   -0.3361397031   0.8634645624
H   -5.4802676883   -1.7079032765  -0.9271346627
H   -3.2156996052   -1.9108024963  -1.8598739206
H   -4.2642090351   -0.8494379674  -2.8005969296
H   -3.1265630107    1.1112464286   -1.5416800202
H   -1.5536564703   -0.6532157568  -3.4715349694
H   -2.6792788636    0.6351380168   -3.9170198118
H   -0.2531521676    1.3896168807   -3.9882161909
H   -1.2393867387    2.3351899013   -2.8805077448
H    0.6399166153    0.0423581671   -2.1067353012
H    0.8609567822    1.7547761581   -1.7316709274
H   -1.1845408026    1.7345593983   -0.3458179261
H    0.9309832167    1.0306784773    0.7846619531
H    0.6121291221   -0.6546212562    0.3258550204
H   -0.4722873486    0.1761673511    1.454924963
```

calc_**1c** conf_2

```
C   -7.3076771057   -1.1505263238   3.4048008439
C   -6.0496592961   -0.8786267753   3.9278987954
C   -5.0581247974   -0.2568543248   3.1540816957
C   -5.3362592072    0.0780493656    1.8443034401
C   -6.5958966076   -0.2046523021    1.2838783914
C   -7.5982292008   -0.803848414     2.0842841738
O   -8.8206065909   -1.0524837733    1.6198590911
```

```
O  -5.718006277   -1.1903120599   5.2005803353
C  -4.3413064866   0.7806443972   0.9640186634
C  -4.5458642125   0.3736724463  -0.4836671022
O  -5.9162363794   0.5985584128  -0.8829317759
C  -6.904753458    0.1524337127  -0.0965271871
O  -8.0337560377   0.079724985   -0.5720607751
C  -3.707991812    1.1423323941  -1.4920799762
C  -2.2076552486   0.9695144479  -1.3089287802
C  -1.4040978022   1.6445488398  -2.4174734509
C   0.0840510004   1.340512249   -2.2580269805
C   0.3028701574  -0.1654842436  -2.1274703302
C  -0.5842828943  -0.7441364999  -1.0291725496
O  -1.9485921583  -0.4239995879  -1.272999068
C  -0.5004844331  -2.2531795392  -0.9222426073
H  -8.0849754249  -1.6166325776   4.0021351429
H  -4.092839238   -0.0507070402   3.6019139443
H  -8.8489762356  -0.6840522207   0.6986628071
H  -6.4733932526  -1.6119427705   5.6309427108
H  -3.3208025301   0.5365972435   1.2709908138
H  -4.4621186328   1.8686573229   1.059416014
H  -4.344930061   -0.697202778   -0.587456399
H  -3.9903871531   0.7999611569   -2.4930881618
H  -3.9589587753   2.207428779    -1.4317236608
H  -1.8984881648   1.4101877232   -0.3434539922
H  -1.7607062901   1.2648667076   -3.3830699071
H  -1.5876963266   2.7248544091   -2.403151198
H   0.6513551406   1.7425784619   -3.1038353289
H   0.4648060527   1.8426809547   -1.3582372503
H   0.0510627212  -0.6632534342   -3.0724746244
H   1.3532702927  -0.3898529699   -1.9101535927
H  -0.287724436   -0.2914046167   -0.0658657785
H  -0.8041956989  -2.7168436024   -1.8652344217
H  -1.1617323202  -2.6188063541   -0.1325469754
H   0.5219891801  -2.5670018011   -0.693894989

calc_**1c** conf_3

C  -7.5538907057  -1.3447939653   3.0346003195
C  -6.6838997021  -0.8246443147   3.9848858879
C  -5.6177136657   0.0104724633   3.6173917067
C  -5.4236663114   0.3078310232   2.2839213619
C  -6.2784649592  -0.2224788186   1.2990730035
C  -7.369018542   -1.0384768598   1.6855623168
O  -8.2336556537  -1.5305253666   0.8010667442
O  -6.8196882025  -1.0885992785   5.3030903574
C  -4.3261512237   1.2187726979   1.8122581204
C  -3.8576469848   0.803220257    0.428347968
O  -4.9825864741   0.7569092596   -0.4789262043
C  -6.0862905324   0.0890431062   -0.1122105726
O  -6.8940854011  -0.2136271855   -0.9850645739
C  -2.8345698327   1.7567561119   -0.1678536396
C  -1.9925900915   1.1872670368   -1.3071864521
C  -2.7460983417   0.8629497289   -2.5944446142
C  -1.7906421164   0.2386946857   -3.6100027165
C  -1.0638722421  -0.9497186787   -2.9840322715
C  -0.4004205504  -0.5433136446   -1.6717121664
O  -1.351674101    0.0330832117   -0.7859559268
C   0.2346303459  -1.7056872056   -0.9354742082
H  -8.3900733957  -1.97824557     3.3136898803

S83
```

```
H   -4.9672204649    0.4044855297    4.3896395756
H   -7.9736061243   -1.1580776907   -0.0809409649
H   -7.5788678633   -1.6720370015    5.4332457373
H   -3.4805250119    1.1971248046    2.5056428482
H   -4.6899496206    2.2548841597    1.7761050305
H   -3.4318562344   -0.204924604     0.4735294366
H   -3.3448991549    2.6675163609   -0.4993166318
H   -2.1445374695    2.0415482124    0.6340661049
H   -1.2177408531    1.9376901668   -1.5479505596
H   -3.5646557174    0.1722240392   -2.3729166894
H   -3.2007855783    1.7768404803   -2.9927984186
H   -2.3337447082   -0.0700719288   -4.5091295245
H   -1.052703099     0.9876637657   -3.9295347718
H   -1.7785196191   -1.7562799249   -2.7763155094
H   -0.307991323    -1.3517128137   -3.6684222447
H    0.3708833202    0.216437064    -1.8915553746
H    1.0126806516   -2.1706882347   -1.5475459041
H   -0.5199249809   -2.4620572866   -0.7001470984
H    0.6840325348   -1.3664537929    0.0013206384


calc_**1c** conf_4

C   -7.9641493562   -0.9651084611    3.2559244832
C   -7.0736344323   -0.4394728669    4.18373287
C   -5.874416458     0.1678892698    3.7799100992
C   -5.5710228921    0.2306920565    2.4355637001
C   -6.4462816001   -0.3128007607    1.475379385
C   -7.6671063788   -0.8954173541    1.8939053868
O   -8.5515212589   -1.385872648     1.0286797363
O   -7.3137330936   -0.479338293     5.512405506
C   -4.3282969022    0.8974092314    1.9179418455
C   -3.8608269006    0.2107163124    0.6466548493
O   -4.9259147637    0.1838488562   -0.3267287227
C   -6.1391847488   -0.249043834     0.0514202856
O   -6.938906774    -0.5587123306   -0.8253819916
C   -2.6806887604    0.8993418456   -0.0096465872
C   -2.2137522154    0.2786035199   -1.321506283
C   -1.7543516454   -1.1724470206   -1.203785843
C   -1.1630140645   -1.6497129933   -2.5299898635
C   -0.0983819301   -0.6725083117   -3.0232576722
C   -0.649483738     0.7504943804   -3.0436549978
O   -1.1473186107    1.1049937585   -1.7613270575
C    0.3886158137    1.7903295502   -3.4146657526
H   -8.9007476995   -1.4215895258    3.5602768925
H   -5.2117249847    0.5773198358    4.5335336234
H   -8.1953862874   -1.1922432946    0.1234336935
H   -8.160628067    -0.9172368672    5.6695769256
H   -3.5300656876    0.87230259      2.6655176767
H   -4.5341956163    1.9537157265    1.6992930913
H   -3.6141105862   -0.8329651845    0.8796529891
H   -2.9338995613    1.9477730589   -0.2002936083
H   -1.8415460872    0.8943321989    0.6959361218
H   -3.0349097602    0.3295982731   -2.0538946501
H   -0.9981114511   -1.2391171484   -0.4102977562
H   -2.5951972362   -1.812857986    -0.9156161531
H   -0.7469558551   -2.6571879417   -2.4245281009
H   -1.965686263    -1.7182082009   -3.2762462122
H    0.7719779784   -0.696394303    -2.3549835891
H    0.2510024825   -0.9499834339   -4.0243629688
```

```
H  -1.4835313189   0.7919662976   -3.7665024124
H   0.785795247    1.5989746326   -4.4156435826
H   1.218137414    1.7691007337   -2.7016616682
H  -0.0508459499   2.790816632    -3.3987636879
```

calc_**1c** conf_5

```
C  -7.0696408206   0.2747556966    3.4375822878
C  -5.875547279   -0.3085734157    3.8414532968
C  -5.0075061315  -0.9084414127    2.9155945132
C  -5.3462082242  -0.9074966502    1.5778530777
C  -6.539774651   -0.3034984702    1.1393611496
C  -7.4197633049   0.2734338705    2.0855983637
O  -8.5792784229   0.8229310669    1.7324116569
O  -5.4908076868  -0.335402475     5.1369112358
C  -4.5114189802  -1.5769249601    0.5248218945
C  -4.6106038236  -0.8304986136   -0.7967566944
O  -5.9966289645  -0.6846631084   -1.1821068705
C  -6.8951065613  -0.2753497644   -0.2768382938
O  -7.991747915    0.0991227899   -0.6818047707
C  -3.9521510721   0.5466263345   -0.8229980464
C  -2.4386957597   0.5123487452   -0.6690345765
C  -1.8072300742   1.8923980041   -0.8317981166
C  -0.2839086201   1.7890729623   -0.7907861509
C   0.1999155757   0.7368120228   -1.7865287194
C  -0.5323637494  -0.5846581446   -1.5712721631
O  -1.939457523   -0.3905787146   -1.6420209128
C  -0.182359549   -1.6387541559   -2.6019432731
H  -7.7527378307   0.72649847      4.1500611918
H  -4.0929242249  -1.3681863603    3.2720122808
H  -8.6693433911   0.6774221073    0.7543458035
H  -6.163713228    0.0999785496    5.676642855
H  -4.8760199428  -2.6010066845    0.3736697758
H  -3.4659584102  -1.6584876384    0.8333820643
H  -4.1793412641  -1.4349438203   -1.5941068829
H  -4.1999979704   1.0083848655   -1.7846317069
H  -4.3741534759   1.1819390362   -0.0365732502
H  -2.1743539369   0.1316472037    0.334304015
H  -2.1273663656   2.3082132626   -1.7953015736
H  -2.1761128247   2.5627502486   -0.0473775374
H   0.1736848315   2.7612042558   -1.0016851207
H   0.0347956028   1.5056983733    0.2215152245
H   0.006614115    1.0753421772   -2.8123137047
H   1.2804375799   0.5790993328   -1.693476788
H  -0.2835337874  -0.9612504501   -0.5627416033
H  -0.4330833727  -1.2847502428   -3.6061140913
H  -0.741161144   -2.5591867329   -2.4143021049
H   0.8865525775  -1.8680275606   -2.5710077347
```

calc_**1c** conf_6

```
C  -7.2329173675  -1.3152185264    3.2402709552
C  -5.9002747923  -1.3486937135    3.6324195284
C  -4.8951857156  -0.7582878565    2.8514783919
C  -5.2376824998  -0.1431411063    1.6642766885
C  -6.578366568   -0.1135421971    1.2343825734
C  -7.5872422613  -0.685235689     2.0463391364
O  -8.8749120625  -0.6452494772    1.7098909812
O  -5.5054156137  -1.9425454874    4.7807168603
```

```
C   -4.2285938598    0.5452276391    0.7913226498
C   -4.6455542062    0.4363285269   -0.6631675422
O   -5.9834081019    0.957774813    -0.8398188993
C   -6.9539800861    0.5409468086   -0.0133983654
O   -8.1185201527    0.7422433311   -0.344260144
C   -3.7910972141    1.2186170662   -1.6495638894
C   -2.3852981085    0.6911459389   -1.9158330791
C   -2.3138463702   -0.7512686318   -2.4148210564
C   -0.8574581736   -1.150812013    -2.6457730938
C   -0.0280791585   -0.8639206549   -1.395100703
C   -0.2295575033    0.5761586892   -0.932247871
O   -1.6120026908    0.849181475    -0.7356066975
C    0.4745220145    0.892286513     0.3717438242
H   -8.0172251113   -1.7554867556    3.8480563898
H   -3.868859365    -0.7935276286    3.1979925184
H   -8.9287424293   -0.1088617254    0.8769075785
H   -6.2785984739   -2.3083569952    5.2301479914
H   -3.2282482629    0.1266925027    0.9146759756
H   -4.1613893399    1.6072341243    1.0626213804
H   -4.6846280214   -0.6222646674   -0.9481061657
H   -4.3311102862    1.2385395579   -2.6022685365
H   -3.7147735228    2.255455047    -1.3050878221
H   -1.9502852305    1.3367801558   -2.6994296313
H   -2.7578980055   -1.4196124924   -1.6676643748
H   -2.8992678108   -0.8559845277   -3.3353991038
H   -0.7863407758   -2.2075058262   -2.9233548809
H   -0.4533538136   -0.5761025659   -3.4900806703
H   -0.3332681201   -1.5350147039   -0.5818851337
H    1.0362236261   -1.0449186381   -1.5829530908
H    0.1440947358    1.252413294    -1.7215414719
H    1.5546393215    0.7562977116    0.2677789022
H    0.1187340698    0.2317969783    1.1682387164
H    0.2801673077    1.925431707     0.6701011812
```

calc_**1c** conf_7

```
C   -7.6031760476    0.3254319419    3.1524191012
C   -6.7553354562   -0.4346459666    3.9481054519
C   -5.6775393392   -1.1442812991    3.3952067186
C   -5.4523980012   -1.0736139838    2.0360940961
C   -6.2839446386   -0.2936865297    1.2098987569
C   -7.3837988631    0.394864811     1.7752074977
O   -8.2243960792    1.1153087895    1.0363939219
O   -6.9240659298   -0.5365147121    5.2848127254
C   -4.3636793982   -1.8462405571    1.3490946951
C   -3.8287780576   -1.0748510246    0.1504574904
O   -4.9203809288   -0.7275182799   -0.7334027315
C   -6.0405353616   -0.1948271637   -0.2249770129
O   -6.8216436133    0.3488591007   -1.0007681505
C   -3.0193779192    0.1640728307    0.5300048148
C   -2.1332973562    0.7230183814   -0.5801828581
C   -2.8610842652    1.3251304735   -1.7799338169
C   -1.8447757878    1.7814643679   -2.8244508456
C   -0.8999960618    0.6331143669   -3.1711814605
C   -0.2740269143    0.0530696889   -1.9066763823
O   -1.28023875     -0.3390503924   -0.9814413497
C    0.5820213956   -1.1699630845   -2.1669825565
H   -8.4473680543    0.8639026826    3.5715651353
H   -5.0477804989   -1.7380801432    4.0475282033
```

```
H   -7.9364778554    0.9988760344    0.0936470878
H   -7.6910626643   -0.0115188207    5.5490199284
H   -4.7703370086   -2.803458629     0.9980293204
H   -3.5467705464   -2.0806567319    2.0370674559
H   -3.1999421059   -1.7237924983   -0.4600832352
H   -3.6825085141    0.9498383953    0.9071456384
H   -2.3594158312   -0.1195479291    1.3574232223
H   -1.5108974337    1.5176602072   -0.1297067187
H   -3.5343442802    0.5785738454   -2.2110359282
H   -3.4841755005    2.1634857442   -1.4480322231
H   -2.3543583601    2.1472774163   -3.7217651044
H   -1.2616879708    2.6242898433   -2.427682133
H   -1.4548817541   -0.164293803    -3.6818282802
H   -0.1085501831    0.9674948268   -3.8517250517
H    0.3434441419    0.837073145    -1.4326067935
H    1.4064546879   -0.9261161116   -2.84297941
H   -0.0182196909   -1.9623308024   -2.6239650999
H    0.9993267959   -1.5518184302   -1.2317141191

calc_1c conf_8

C   -6.9856162526    0.1575908949    3.4788579687
C   -6.5784694713   -1.1438056255    3.7427891714
C   -6.0381251518   -1.9573549777    2.7341644408
C   -5.9007019441   -1.4470504485    1.4600888507
C   -6.2858634508   -0.1241465128    1.1702525038
C   -6.8529731106    0.6775862115    2.1898704217
O   -7.2677901036    1.9219310376    1.9656507354
O   -6.6847532568   -1.6949682455    4.9714729648
C   -5.394640773    -2.26848598      0.3093142576
C   -4.6464566894   -1.3988768532   -0.6924028407
O   -5.4614639182   -0.2757703277   -1.0941946833
C   -6.1208891947    0.4351522806   -0.1659722504
O   -6.5670693831    1.5297434135   -0.4954621586
C   -3.2916918106   -0.9205251665   -0.187022105
C   -2.5660988184    0.0529297556   -1.1093219318
C   -2.2934708712   -0.4862845472   -2.5109547063
C   -1.4335200509    0.5016789284   -3.2989192466
C   -0.1903479769    0.8855569129   -2.4997320882
C   -0.5791750036    1.3519347759   -1.0995655401
O   -1.3498695493    0.3547814401   -0.4440603228
C    0.6137414547    1.6396727064   -0.2103348142
H   -7.4169512699    0.7872538029    4.2506851743
H   -5.7446580568   -2.9720072726    2.9770661662
H   -7.1352853293    2.0904368491    0.9968633383
H   -7.0632054899   -1.0460544343    5.5792563046
H   -6.2467678069   -2.7394963376   -0.1970250979
H   -4.7427715048   -3.0753976167    0.6564026603
H   -4.5153618224   -1.9546758696   -1.6233349515
H   -3.3998051771   -0.4454541437    0.7938300412
H   -2.6523167342   -1.7996704413   -0.0416433313
H   -3.161601521     0.9758194891   -1.202604278
H   -1.7725160376   -1.4490814966   -2.4233732062
H   -3.2383369844   -0.6634345436   -3.0359856775
H   -1.1558422127    0.0792457223   -4.2703854041
H   -2.0241463308    1.4039528456   -3.5066055377
H    0.4762944178    0.0189404086   -2.4024214248
H    0.3728230496    1.6746264899   -3.011098709
H   -1.1942507063    2.2646297418   -1.1928927234
```

```
H   0.2823603799    1.9551894302    0.7821222654
H   1.2333070029    2.4318982586   -0.6402770912
H   1.2272774598    0.7409894448   -0.0970971448
```

calc_**1c** conf_9

```
C  -6.8689042652   -0.4293935992    3.4232670961
C  -5.704460115    -1.1844858334    3.4891072731
C  -4.9549224957   -1.4711825659    2.3380533991
C  -5.3808092852   -0.9845676491    1.1190199024
C  -6.5448239729   -0.1980769793    1.0283306106
C  -7.3063066681    0.0629695423    2.1924444877
O  -8.4347170771    0.7691379673    2.1586162041
O  -5.2388038432   -1.6839221784    4.6559546973
C  -4.6753220604   -1.3000684898   -0.1677056553
C  -4.806075021    -0.1478944244   -1.1523730394
O  -6.1954480017    0.2183516099   -1.3239497908
C  -6.9899397749    0.3425085882   -0.2509173838
O  -8.071073881     0.904374939    -0.4014931338
C  -4.0183645231    1.1110228699   -0.7874037503
C  -2.5127210817    1.0759939081   -1.0368255589
C  -2.1004167431    0.8491758819   -2.4906570696
C  -0.5768559525    0.8451432021   -2.6038215348
C   0.0216974868   -0.147766479    -1.6091077599
C  -0.5108552865    0.1095754303   -0.2021192265
O  -1.9334895405    0.0903886376   -0.1951007321
C  -0.0497090426   -0.9176479359    0.8117824716
H  -7.4610465258   -0.21659934      4.3078679229
H  -4.0568694719   -2.0709098833    2.4278511369
H  -8.6008667113    0.9818774124    1.203584973
H  -5.8339142811   -1.4236268634    5.3712480533
H  -5.127653405    -2.1962680065   -0.6118795394
H  -3.6164290483   -1.5031043447   -0.0006070384
H  -4.5203709738   -0.4862948675   -2.1498045671
H  -4.4317942006    1.9343208444   -1.3796643728
H  -4.1893218427    1.3545396314    0.2665453575
H  -2.1207584794    2.0626394821   -0.7315190792
H  -2.4906495907   -0.1145929201   -2.8384210875
H  -2.5381881447    1.6273624533   -3.1259805796
H  -0.2659406605    0.6043774967   -3.6256673052
H  -0.1947807229    1.8521075419   -2.3881929585
H  -0.245266612    -1.1726233414   -1.8978001599
H   1.1157691389   -0.0858503104   -1.6059324229
H  -0.1804651521    1.1131471298    0.1191493566
H  -0.3649547574   -1.9209056341    0.5092787344
H  -0.4786563626   -0.7037756904    1.7939230366
H   1.0404789487   -0.9104572325    0.8979190325
```

calc_**1c** conf_10

```
C  -7.8142626654   -0.1171483809    3.4386800573
C  -6.731993722    -0.6762385619    4.1067375596
C  -5.5151254059   -0.9170690674    3.4497523606
C  -5.4000527468   -0.6053421317    2.1107388742
C  -6.4883122388   -0.0575853259    1.4044364785
C  -7.6995455244    0.2113825957    2.0870204945
O  -8.7445374101    0.7710670823    1.4821588569
O  -6.7889928932   -1.0094520591    5.4144877322
C  -4.1217254732   -0.7912853818    1.3430891768
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S88

```
C   -4.4404392763   -1.126548554    -0.104499541
O   -5.2793794794   -0.1020776321   -0.6796096246
C   -6.3772458026    0.2830035016   -0.0091187135
O   -7.2315895161    0.9177856574   -0.6185326807
C   -3.2445698577   -1.3262504495   -1.0208871702
C   -2.1973144297   -0.2181132527   -1.097713709
C   -2.6483623944    1.0440759663   -1.8274073558
C   -1.4779790369    2.012666571    -1.9884923545
C   -0.2820399582    1.3025054209   -2.6180524729
C    0.0463241459    0.0279168334   -1.8464316446
O   -1.0946640433   -0.8141172994   -1.7657427923
C    1.1504356045   -0.7915101817   -2.4838168099
H   -8.7522058092    0.0879823435    3.945019922
H   -4.6897402406   -1.3419022623    4.0092416029
H   -8.4526543956    0.9856148439    0.5588190458
H   -7.6682386042   -0.8023198196    5.7577358661
H   -3.5125288721   -1.5877366678    1.7807187828
H   -3.5305137523    0.1315318357    1.3916737719
H   -5.027797957    -2.0540881334   -0.1186815891
H   -2.7275147869   -2.2332849566   -0.6881912608
H   -3.6154713218   -1.5311445826   -2.0306726762
H   -1.8712730217    0.0602177985   -0.079182751
H   -3.0315673744    0.7522032607   -2.8128581433
H   -3.4771656851    1.5151918994   -1.2925394618
H   -1.7775212933    2.8767943262   -2.5905703937
H   -1.1898542568    2.4037686951   -1.0027809578
H   -0.5138061403    1.0282708272   -3.6550640647
H    0.5961621589    1.9579795264   -2.6418030221
H    0.3456325173    0.3089354341   -0.8201622531
H    2.0766610047   -0.2124803747   -2.540228559
H    0.8641107432   -1.0888132268   -3.4969418432
H    1.339659211    -1.6973861174   -1.9023287373
```

calc_**1c** conf_11

```
C   -7.3872487536    0.6971484287    2.2474686633
C   -6.7090704648    0.486869927     3.4411119493
C   -5.568408246    -0.3288559026    3.4966846151
C   -5.1079415417   -0.921271148     2.3382459526
C   -5.7634176995   -0.7067051082    1.1115031644
C   -6.9295666799    0.0936298199    1.0742995191
O   -7.6142073876    0.2955122677   -0.0489962151
O   -7.1108565206    1.0462069742    4.6044516561
C   -3.9279206329   -1.8514033386    2.3191912328
C   -3.1907545166   -1.7423671212    0.9915213522
O   -4.1002896254   -1.9577573781   -0.1046875089
C   -5.2775282371   -1.318593504    -0.1214852795
O   -5.9159248761   -1.3087353142   -1.1691882826
C   -2.4223187097   -0.4289558411    0.8433102566
C   -1.9266493581   -0.141310583    -0.5689554581
C   -0.7083687372    0.7786797578    -0.6046286239
C   -0.3473036668    1.1154496266    -2.0512199687
C   -1.5736927815    1.6253030264    -2.8079791976
C   -2.7492369759    0.6658156855    -2.6401381117
O   -3.0078680709    0.4585268846    -1.2579041954
C   -4.0382175988    1.1676355286    -3.2574920396
H   -8.2792669553    1.3139385067    2.1998678441
H   -5.0750153622   -0.4801479475    4.4498544103
H   -7.1709064594   -0.2539912262   -0.7464911684
```

```
H  -7.8978649992   1.582810683    4.4423906829
H  -4.2765005184  -2.8834144345   2.4519725293
H  -3.2428021688  -1.6349171684   3.144348501
H  -2.4888092044  -2.5740704537   0.8887996628
H  -3.0410162974   0.4187551753   1.1561717818
H  -1.5711452428  -0.4780010733   1.533014667
H  -1.6646714413  -1.089948618   -1.0711326047
H  -0.9496361484   1.696279248   -0.0529973386
H   0.1372409281   0.3018007796  -0.0949175416
H   0.4627589518   1.8517968904  -2.0851836641
H   0.0313356634   0.2103049924  -2.5454647443
H  -1.8727802324   2.6065088313  -2.41785612
H  -1.3461473486   1.7533899629  -3.8724364276
H  -2.482907864   -0.3050254326  -3.0930666782
H  -3.9192733478   1.3091271017  -4.3356781876
H  -4.32520445     2.1247406021  -2.8113710536
H  -4.8405964223   0.4482408927  -3.0799380308

calc_1c conf_12

C  -7.7554800982  -1.076401486    3.1647219607
C  -6.992884387   -0.3442361131   4.0661564858
C  -5.9190777476   0.4497990563   3.6358204564
C  -5.6091291491   0.4905741566   2.2913531965
C  -6.3517341484  -0.2580975765   1.3599795257
C  -7.4528899573  -1.0294706247   1.8027294695
O  -8.2181543983  -1.7190950571   0.9599995766
O  -7.245996174   -0.3530580054   5.3939618873
C  -4.4987117409   1.3404922478   1.7430497111
C  -3.8945641329   0.6863000627   0.5112480907
O  -4.9247676238   0.4169281228  -0.4607402284
C  -6.0394299564  -0.2104642256  -0.0653881499
O  -6.7643005591  -0.7020957039  -0.924880518
C  -2.8429918382   1.5508817007  -0.1767673121
C  -1.7302467089   0.7658888841  -0.8562982359
C  -0.7129177944   1.6671243198  -1.552340015
C   0.3229697825   0.8222979125  -2.2923133483
C  -0.3729693061  -0.1941219617  -3.1958788064
C  -1.4073909804  -0.9947491491  -2.4091335278
O  -2.3313510687  -0.1209805709  -1.7752043455
C  -2.2204225349  -1.9377413861  -3.2724969514
H  -8.5980976549  -1.6790328488   3.4890878046
H  -5.3557515562   1.0160590259   4.3685672093
H  -7.8876846887  -1.5073893356   0.0478755531
H  -8.0016475537  -0.9293592091   5.5684700926
H  -3.7195646464   1.494027713    2.4958139564
H  -4.8844828302   2.3324226376   1.4703507895
H  -3.4608876599  -0.2810644272   0.7947156523
H  -3.3501888017   2.1852483388  -0.911085202
H  -2.3835126035   2.2150131382   0.5644925283
H  -1.1983086141   0.1729605143  -0.0869788021
H  -1.248590126    2.3074600693  -2.26443437
H  -0.2298811926   2.3237321562  -0.8192672594
H   0.9968231872   1.4607744428  -2.8732475921
H   0.9472105879   0.2913848542  -1.5606346516
H  -0.8892009494   0.3245474874  -4.0135721695
H   0.3558114797  -0.8752124811  -3.6497584055
H  -0.8810984604  -1.5728175375  -1.6278226659
H  -2.9632575371  -2.4630023774  -2.6675126166

S90
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H  -1.5723211731   -2.6756583151   -3.7540959483
H  -2.7499286848   -1.3778684491   -4.0485428248

calc_1c conf_13

C  -7.5876889952   -0.75212149     3.6003755176
C  -6.4039861811   -0.2923254145   4.1640807557
C  -5.3647603653    0.2124762422   3.3668373806
C  -5.5207523925    0.2385247063   1.9962927764
C  -6.7013056557   -0.2409229757   1.3982668758
C  -7.7547038856   -0.7175730894   2.2148569976
O  -8.9098697052   -1.1390445035   1.7058023341
O  -6.1930298854   -0.3006420637   5.4985429105
C  -4.4793377299    0.8003479163   1.0713453312
C  -4.500071867     0.0558394954  -0.2529277424
O  -5.8284318577    0.1172370981  -0.8196274457
C  -6.8780525724   -0.2079230119  -0.0491264975
O  -7.9459901992   -0.450320747   -0.6016506992
C  -3.5589573998    0.609337958   -1.3171803764
C  -2.2179067341   -0.1088318282  -1.4247805068
C  -1.3411221888   -0.0449418615  -0.1757097305
C   0.027524079    -0.6674851844  -0.4509651684
C   0.6481924817   -0.055294117   -1.7041825517
C  -0.3314246474   -0.125569162   -2.8716478805
O  -1.5608638933    0.495874167   -2.5236881686
C   0.1719781246    0.5696308034  -4.1203823341
H  -8.4019015928   -1.1277113103   4.2121577377
H  -4.4623725522    0.5752070431   3.8452910125
H  -8.8601120187   -0.9777850675   0.728149615
H  -6.9706364404   -0.6656978582   5.9410167731
H  -3.4846058041    0.7469258513   1.5208331594
H  -4.6868589375    1.8613502792   0.8775476941
H  -4.2850863798   -1.0068941358  -0.0735776749
H  -4.0563337132    0.5160638809  -2.2862560329
H  -3.3798662784    1.6781409262  -1.1545886417
H  -2.40529334     -1.1727179598  -1.6614078335
H  -1.2221304934    1.007200512    0.1141639831
H  -1.8286388605   -0.5655096148   0.6567744155
H   0.687756108    -0.5392888797   0.413132384
H  -0.0916106235   -1.7496781603  -0.5967017253
H   0.8959787855    0.9983924324   -1.5232101015
H   1.5792796101   -0.5691433027   -1.9686057836
H  -0.5291818774   -1.188331207    -3.0993345796
H   1.1017539361    0.1109582797   -4.4687752219
H   0.3612653452    1.6272921883   -3.9150173331
H  -0.5708434027    0.503953165    -4.9191236244

calc_1c conf_14

C  -7.5733800752   -0.7023863918   3.5974068427
C  -6.3252261167   -0.395695361    4.1248720588
C  -5.2674923663    0.0177608288   3.300350087
C  -5.471195805     0.1080926105   1.9385696797
C  -6.7197147351   -0.2167284369   1.3762415492
C  -7.7877114395   -0.6024370734   2.2217559714
O  -9.00107192     -0.8775805101   1.7494866918
O  -6.065666302    -0.4731802236   5.4485084998
C  -4.4025794642    0.5790539613   0.9930275878
C  -4.5655832768   -0.0945157505  -0.3580337456

S91
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```
O   -5.8997517934    0.121254373    -0.8637110639
C   -6.9476977915   -0.1167596389   -0.0607707991
O   -8.0559496641   -0.225230449    -0.5746636186
C   -3.6363587575    0.3955548945   -1.4562097063
C   -2.1552973725    0.0978554398   -1.2102983625
C   -1.365437261     1.2724555835   -0.6332301026
C    0.1148752444    0.917262145    -0.5180111701
C    0.6354984288    0.4033523203   -1.8579598968
C   -0.2575444349   -0.7154983384   -2.3861522215
O   -1.609921962    -0.2842418995   -2.4628422418
C    0.129816985    -1.1875091392   -3.7729949946
H   -8.4004955213   -1.0074719903    4.2307007129
H   -4.312204918     0.2600843675    3.7515215502
H   -8.9711514622   -0.6925739986    0.7752526955
H   -6.8609006243   -0.7680059998    5.9115858052
H   -3.4110520465    0.3614509599    1.3998986448
H   -4.4698541895    1.6676763156    0.8629069687
H   -4.4405776143   -1.178610703    -0.2316617599
H   -3.9237997697   -0.1118868741   -2.3809081786
H   -3.7982296571    1.4676580393   -1.615069502
H   -2.062286095    -0.7608320793   -0.5174839976
H   -1.491554523     2.1278244449   -1.3087299258
H   -1.7719055099    1.5680806673    0.3402012334
H    0.693895865     1.784317615    -0.1832273303
H    0.2448880605    0.1393790755    0.2468853728
H    0.6413626687    1.2180576383   -2.5931913444
H    1.6653783363    0.040749328    -1.764443093
H   -0.2037728949   -1.5657339057   -1.6821257951
H    0.0661311815   -0.3602808296   -4.4858858944
H   -0.5430733671   -1.9804818438   -4.1084663009
H    1.1535919605   -1.5722791717   -3.7771009062

calc_**1c** conf_15

C   -5.6452403417    0.0011588026    3.2361232899
C   -4.9803158058   -1.2133821803    3.1145861631
C   -4.8440134971   -1.8471819548    1.8719540301
C   -5.3689850325   -1.246760015     0.744456258
C   -6.0448120497   -0.0178704019    0.8394844386
C   -6.1940326004    0.6044191006    2.104218892
O   -6.8445417079    1.7560779775    2.2556854115
O   -4.4373926237   -1.8439245536    4.1803779778
C   -5.3256118477   -1.9174486302   -0.5976784524
C   -5.4227836725   -0.942643589    -1.7682994169
O   -6.4169373949    0.0817504405    -1.5454553435
C   -6.6234139222    0.618471764     -0.3373011381
O   -7.31627364      1.6308884633    -0.2774218802
C   -4.1267740158   -0.2907634005   -2.2490689689
C   -3.250126171     0.4265082167   -1.2320803626
C   -2.2707700558    1.3866585271   -1.9047318265
C   -1.3202205944    1.9867362934   -0.8721463654
C   -0.6702707667    0.8786248785   -0.0477406463
C   -1.7262876376   -0.0599440403    0.5301966342
O   -2.5521107183   -0.5758403429   -0.5086585917
C   -1.1227456397   -1.2499916936    1.2481929093
H   -5.7652946259    0.4926736927    4.196523834
H   -4.33135889     -2.8005279071    1.8193865411
H   -7.1983088113    1.9952639619    1.3590350368
H   -4.6018385092   -1.3202445583    4.9755507312
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S92

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H  -6.1706821107  -2.6153539598  -0.6552343371
H  -4.4106201698  -2.5052082119  -0.699138263
H  -5.8283326831  -1.4848024775  -2.6264014019
H  -3.5113970077  -1.0661409956  -2.7209983853
H  -4.4099500168   0.415255598   -3.0370939258
H  -3.872514488    1.0058082834  -0.5299534479
H  -1.7016912406   0.8323076989  -2.6625746346
H  -2.8282662102   2.1738738366  -2.4244944097
H  -0.5590524531   2.6042754111  -1.3605182109
H  -1.8847617946   2.6525600899  -0.2055919567
H   0.004654567    0.2889595117  -0.6814446276
H  -0.0681523362   1.2998250161   0.7653790677
H  -2.3630786759   0.5069394705   1.2306174083
H  -0.5243806471  -1.8467982667   0.5531955723
H  -1.906767138   -1.8845869024   1.6665307101
H  -0.4755470233  -0.9166229531   2.0645316871

calc_1c conf_16

C  -7.6970936644  -1.0327655031   3.4056697935
C  -7.2957565351   0.1459129588   4.0194291181
C  -6.3227341141   0.9754952298   3.4384973739
C  -5.745787238    0.6060001776   2.2379694291
C  -6.1217439544  -0.5908394128   1.6059647122
C  -7.1266656423  -1.4050417033   2.1896816188
O  -7.5479868748  -2.5259727063   1.6090986102
O  -7.8844207181   0.4600069282   5.1952453212
C  -4.7268673322   1.4566122056   1.534317051
C  -3.7674468303   0.5777788745   0.7482121154
O  -4.496860211   -0.2774632951  -0.1476525793
C  -5.5293171268  -0.985696464    0.3314822943
O  -5.9413753143  -1.9285604322  -0.33573616
C  -2.7629971579   1.3728195972  -0.0690974554
C  -1.7690767874   0.5394525523  -0.8737773464
C  -0.473524346    1.2928236955  -1.1762410748
C   0.4303286901   0.4511267895  -2.0773040566
C  -0.340389821   -0.0444104268  -3.3004597648
C  -1.6424335552  -0.7173525514  -2.8751113576
O  -2.409574865    0.1716124074  -2.0770873275
C  -2.5224601513  -1.1297619392  -4.0372352345
H  -8.4591568035  -1.6548229317   3.857578025
H  -6.0289654518   1.900469672    3.9285266161
H  -7.0785137574  -2.5851711559   0.7377723687
H  -7.5321029101   1.301851983    5.5113502679
H  -4.1679157455   2.0693349869   2.2483119707
H  -5.2291131249   2.1443557802   0.8407615467
H  -3.2292358446  -0.0760198131   1.4490841849
H  -3.2921545309   2.034080501   -0.7639084122
H  -2.2124125733   2.0092959106   0.633966911
H  -1.5143169241  -0.3747997498  -0.3061458251
H  -0.7305701611   2.2350587354  -1.6771818884
H   0.0402174503   1.547638504   -0.2415798099
H   1.313198182    1.0242883848  -2.3798578701
H   0.7985112297  -0.4135076911  -1.508222886
H  -0.587959686    0.8008997238  -3.9549953859
H   0.2688702965  -0.7427929422  -3.8855043046
H  -1.3975969153  -1.6083616805  -2.2699480842
H  -2.0081410489  -1.856083371   -4.6731954938
H  -2.7818831753  -0.2574558564  -4.6445001205
```

S93

```
H  -3.4475749564  -1.5770359723  -3.6661768909
```

calc_**1c** conf_17

```
C  -6.8324690593   0.3461196024   3.4544488479
C  -5.7402888705  -0.4567041367   3.7571197673
C  -5.0605901875  -1.169668687    2.7565514605
C  -5.4821835392  -1.0575541762   1.4473963146
C  -6.5727494383  -0.234279119    1.1107411415
C  -7.2677491785   0.4563381737   2.1320356094
O  -8.3298142699   1.2162381539   1.8777291939
O  -5.2810928226  -0.600056364    5.0196997922
C  -4.8565079863  -1.8287230862   0.3219664041
C  -4.9081877577  -1.0296772588  -0.9728549898
O  -6.2660496571  -0.627097022   -1.2522471201
C  -7.0131138112  -0.0942141041  -0.2739592458
O  -8.0484634397   0.4825280724  -0.5904940783
C  -4.0060542685   0.1996966511  -1.031750653
C  -2.5099508017  -0.1279563527  -0.9898898105
C  -1.8463813647   0.1855524098   0.349455598
C  -0.3456131482  -0.0862940938   0.2789388303
C   0.2619511994   0.6412261102  -0.9189697901
C  -0.516101759    0.3247490159  -2.1939154994
O  -1.89581923     0.6204284572  -2.0261434256
C  -0.0420113902   1.1163443127  -3.3960166643
H  -7.3724267928   0.8875158809   4.2249279272
H  -4.2251942463  -1.8016729543   3.0353098008
H  -8.5117339748   1.1257977765   0.9062217641
H  -5.8238526947  -0.0689581263   5.6172573458
H  -5.4095506391  -2.7654553043   0.1761715409
H  -3.8242372366  -2.1058838976   0.5532870344
H  -4.6610961228  -1.6853164475  -1.8118479233
H  -4.2066227386   0.7073024401  -1.9788817256
H  -4.2706113875   0.8952781889  -0.2280564827
H  -2.3597245461  -1.2031530944  -1.2100350126
H  -2.0235238028   1.2449779888   0.5729397784
H  -2.3159128449  -0.3919074287   1.1538925292
H   0.1464559349   0.2187738202   1.2083707774
H  -0.1754003082  -1.1667397111   0.173835415
H   0.2267425334   1.7254453535  -0.7530246765
H   1.314443483    0.3657647388  -1.0507622192
H  -0.4156000904  -0.755653728   -2.4046861512
H   1.010121608    0.9045714548  -3.6067488513
H  -0.1504192834   2.1887002991  -3.209216362
H  -0.6336160697   0.8616161922  -4.2787961913
```

calc_**1c** conf_18

```
C  -6.8886100406   0.1203256729   3.5431486779
C  -5.863528391   -0.7819705815   3.7966693068
C  -5.1861511564  -1.4285799533   2.7506346726
C  -5.5416493181  -1.1509167021   1.4466789915
C  -6.5616138738  -0.2247674914   1.1621798763
C  -7.2561643939   0.3996037621   2.2253395468
O  -8.2556178292   1.2525615125   2.0147909264
O  -5.4698868769  -1.088328272    5.0524311328
C  -4.9092795374  -1.8392143245   0.2707195749
C  -4.8559996777  -0.9049410321  -0.931580941
O  -6.1802989091  -0.397538463   -1.2136434328
```

```
C   -6.9316791848    0.0863360387   -0.2135434502
O   -7.9124792292    0.7622412911   -0.5072156863
C   -3.8736266878    0.2625949024   -0.7999774945
C   -2.498764146     0.0155523162   -1.4150432301
C   -1.6881811302   -1.1121258373   -0.7792858036
C   -0.2805595757   -1.1614923323   -1.3737582663
C    0.373570773     0.2162437803   -1.311393632
C   -0.543430421     1.2676597915   -1.9286734524
O   -1.8140079908    1.2490681274   -1.2931365226
C   -0.0101250542    2.6799006165   -1.7983419393
H   -7.4262302758    0.6126183196    4.347438975
H   -4.4013774553   -2.1368545815    2.9899572661
H   -8.3989720247    1.2779094191    1.0332615049
H   -6.0014474743   -0.5852392857    5.6833521011
H   -5.5038688962   -2.7231984248    0.0068057532
H   -3.9053631681   -2.19023005      0.5204540324
H   -4.6224972435   -1.4789065822   -1.8326244813
H   -4.3000364804    1.1245354791   -1.3207876473
H   -3.7481085408    0.5529857729    0.248853905
H   -2.6287757183   -0.2151135368   -2.4890667716
H   -1.6320447393   -0.9352035583    0.3026414039
H   -2.1924135743   -2.0735303535   -0.9320885185
H    0.3293836603   -1.9065214203   -0.8521892537
H   -0.3430032233   -1.4855277417   -2.4215077262
H    0.5649366211    0.4941717696   -0.2671695205
H    1.3385838889    0.2125868129   -1.8307034496
H   -0.683620743     1.02628219     -2.9976720242
H    0.9559028088    2.7753056981   -2.3022964189
H    0.1203198545    2.9389020864   -0.7436010599
H   -0.7082846255    3.393815165    -2.2420569248

calc_1c conf_19

C   -5.8220617114    0.4257152175    3.2700119386
C   -5.3669409366   -0.8822096315    3.3816304109
C   -5.2990986331   -1.7277279634    2.2636291317
C   -5.6830540902   -1.2424507378    1.0295729054
C   -6.1310747832    0.0821912773    0.8851860026
C   -6.2169063299    0.918866311     2.0249935204
O   -6.6576640019    2.1719522791    1.9534614796
O   -4.9746074424   -1.4079055289    4.5624378004
C   -5.7169400373   -2.1060117794   -0.1970776081
C   -5.4856545102   -1.3209159775   -1.4864543664
O   -6.2673615241   -0.1071500606   -1.5209106143
C   -6.4952357616    0.6182724568   -0.4204274528
O   -7.000131122     1.728639518    -0.5664479712
C   -4.0285479236   -1.063201722    -1.8656220836
C   -3.1104849428   -0.3080417256   -0.9036066227
C   -3.174519606     1.2123902346   -1.0324398744
C   -2.1209364887    1.8668347312   -0.1413068939
C   -0.7448794928    1.2680986366   -0.4217767142
C   -0.7987947023   -0.2551236125   -0.3479681887
O   -1.7994083496   -0.762943304    -1.2193263347
C    0.5043862402   -0.9203153639   -0.7436575709
H   -5.8889890906    1.0814663587    4.1324413969
H   -4.9529384837   -2.7465836881    2.3931976054
H   -6.9219121013    2.320854311     1.0077780939
H   -5.069585019    -0.7406353947    5.2548937519
H   -6.703933112    -2.5826215786   -0.2526056661
```

S95

```
H   -4.9820848158   -2.9133886712   -0.1293785311
H   -5.9098991254   -1.8998168655   -2.3107166667
H   -3.5745379888   -2.0493894342   -2.0174400671
H   -4.0160370756   -0.5644546317   -2.8410541772
H   -3.3323903835   -0.5924093831    0.1381005922
H   -2.9864430605    1.4688833388   -2.082776275
H   -4.1706742039    1.5895573629   -0.7868189723
H   -2.1103873136    2.9509631248   -0.294644619
H   -2.3852423776    1.7023187332    0.9121185611
H   -0.4120960296    1.5536172647   -1.4279497381
H   -0.0001200193    1.6466038719    0.2877939599
H   -1.0574674878   -0.5454952485    0.6864404525
H    1.316034863    -0.6021859484   -0.0830602498
H    0.7683561295   -0.6544327596   -1.7714919904
H    0.412262845    -2.0078140177   -0.684728355

calc_**1c** conf_20

C   -5.3228270666    0.1299785607    3.1837958212
C   -4.8788123361   -1.1853989271    3.2527719082
C   -4.8434312658   -1.9983539649    2.1118857781
C   -5.2521951506   -1.4766325296    0.8975547512
C   -5.7009346062   -0.151938334     0.8002173014
C   -5.7474353459    0.6540390351    1.9616352565
O   -6.1791847385    1.9148532518    1.9309764591
O   -4.4650927443   -1.7451301314    4.4124558595
C   -5.3002876191   -2.3162062232   -0.3458330895
C   -5.2210515262   -1.5088411873   -1.6417730749
O   -6.038037734    -0.325167386    -1.586901011
C   -6.1397421049    0.4086856377   -0.4745782182
O   -6.6549951493    1.5180035292   -0.5682855451
C   -3.8470487928   -1.1837714502   -2.2425616561
C   -2.7841250168   -0.3851772435   -1.4896831631
C   -2.0682836814   -1.1066131775   -0.3488248811
C   -1.033707589    -0.1731747657    0.2790382276
C   -1.688108781     1.1524915544    0.6640362304
C   -2.4253196751    1.7540128689   -0.5290367076
O   -3.3683795064    0.8247009461   -1.0507188596
C   -3.1871149177    3.0199963299   -0.1933194273
H   -5.3639644364    0.7648034998    4.0634334456
H   -4.4993332801   -3.0222576125    2.2047128349
H   -6.4832062745    2.0774146457    0.9975854015
H   -4.5419472577   -1.0946665648    5.122694489
H   -6.2527528889   -2.8615928698   -0.3458782885
H   -4.5115599048   -3.074485268    -0.3378056052
H   -5.7183292052   -2.1014445848   -2.4149796253
H   -3.3963748581   -2.1386273823   -2.5419803771
H   -4.0647556768   -0.6410862139   -3.1685885249
H   -2.0107643908   -0.1421339534   -2.2428528478
H   -2.7902699972   -1.4090868398    0.4148072219
H   -1.5877645919   -2.0141710012   -0.7339935046
H   -0.5702968744   -0.6449088873    1.1518564596
H   -0.2269218866    0.0156327922   -0.4427719587
H   -2.4124943744    0.9911479754    1.4719674735
H   -0.9400352192    1.8644967557    1.030903464
H   -1.6872853645    1.9708618765   -1.3223682758
H   -2.4988742266    3.800144242     0.1448652564
H   -3.916587253     2.8340486892    0.5994483356
H   -3.7253666914    3.3835543077   -1.0719073341
```

Table S32. Sampled and DFT geometry optimized conformers related to calc_**1d**, with energy values (Hartree) and related % contribution on the final Boltzmann distribution for the three employed functional/basis set combinations.

Conformer	MPW1PW91/6-31g(d,p)		MPW1PW91/6-311+g(d,p)		B97-2/cc-pVTZ	
	Energy (Hartree)	% contribution on the Boltzmann distribution	Energy (Hartree)	% contribution on the Boltzmann distribution	Energy (Hartree)	% contribution on the Boltzmann distribution
calc_**1d** conf_1	-997.7145519	69.45%	-997.9497948	79.39%	-997.9088768	81.25%
calc_**1d** conf_2	-997.7129280	12.44%	-997.9478343	9.95%	-997.9065739	7.09%
calc_**1d** conf_3	-997.7129263	12.41%	-997.9475148	7.10%	-997.9066714	7.86%
calc_**1d** conf_4	-997.7111995	1.99%	-997.9458455	1.21%	-997.9044298	0.73%
calc_**1d** conf_5	-997.7111538	1.90%	-997.9459094	1.30%	-997.9053266	1.89%
calc_**1d** conf_6	-997.7100113	0.57%	-997.9439393	0.16%	-997.9026267	0.11%
calc_**1d** conf_7	-997.7096731	0.40%	-997.9447707	0.39%	-997.9042392	0.60%
calc_**1d** conf_8	-997.7092679	0.26%	-997.9439922	0.17%	-997.9027621	0.13%
calc_**1d** conf_9	-997.7085747	0.12%	-997.9430913	0.07%	-997.9020797	0.06%
calc_**1d** conf_10	-997.7083106	0.09%	-997.9431711	0.07%	-997.9022704	0.07%
calc_**1d** conf_11	-997.7080874	0.07%	-997.9423688	0.03%	-997.9018509	0.05%
calc_**1d** conf_12	-997.7077698	0.05%	-997.9428325	0.05%	-997.9017539	0.04%
calc_**1d** conf_13	-997.7075785	0.04%	-997.9414658	0.01%	-997.8999649	0.01%
calc_**1d** conf_14	-997.7075210	0.04%	-997.9409407	0.01%	-997.8992183	0.00%
calc_**1d** conf_15	-997.7074126	0.04%	-997.9424322	0.03%	-997.9016501	0.04%
calc_**1d** conf_16	-997.7073787	0.03%	-997.9420120	0.02%	-997.9011330	0.02%
calc_**1d** conf_17	-997.7072016	0.03%	-997.9414065	0.01%	-997.8996308	0.00%
calc_**1d** conf_18	-997.7069172	0.02%	-997.9418101	0.02%	-997.9008934	0.02%
calc_**1d** conf_19	-997.7069151	0.02%	-997.9415833	0.01%	-997.9003288	0.01%
calc_**1d** conf_20	-997.7067265	0.02%	-997.9411055	0.01%	-997.9009285	0.02%
calc_**1d** conf_21	-997.7031610	0.00%	-997.9385785	0.00%	-997.8966992	0.00%

Table S33. Cartesian coordinates of the optimized geometries for the conformers related to calc_**1d**. The related energies and % contribution on the final Boltzmann distribution for the three employed functional/basis set combinations are reported in Table S32.

calc_**1d** conf_1

```
C  -7.7998868851  -0.9073248861   1.3262749071
C  -7.6726863531   0.4229759537   1.7061205275
C  -6.4127789054   1.0016176843   1.9229288898
C  -5.2794391032   0.2357601728   1.7407686565
C  -5.3794200913  -1.109171306    1.3362482676
C  -6.6573762969  -1.6898083263   1.1513081671
O  -6.812501915   -2.9677180606   0.8125022376
O  -8.7460771385   1.2227587777   1.8910335204
C  -3.8964532542   0.7688724944   1.9885468804
C  -2.9029960377   0.0924496384   1.061853545
O  -2.9865352586  -1.3433661457   1.2025930671
C  -4.1895045575  -1.9317680073   1.1487018077
O  -4.2321562616  -3.1438063333   0.9616009761
C  -1.4578954543   0.4638403555   1.3355628968
C  -0.4875610211  -0.092107393    0.3043259693
C   0.9707618847   0.2047617254   0.6402826841
C   1.8797738735  -0.273855046   -0.4909911646
C   1.3975330665   0.2805642207  -1.83073566
C  -0.0867103095  -0.0131008416  -2.0329784102
O  -0.8407363087   0.4936317909  -0.9394701404
C  -0.6553073549   0.6145267334  -3.2894761093
H  -8.7718071611  -1.3656808767   1.17277511
H  -6.3558173438   2.0395166625   2.2299419993
H  -5.9032778829  -3.3647752422   0.7967820183
H  -9.551243994    0.7199119795   1.7107973709
H  -3.8633466722   1.8514435715   1.8344918136
H  -3.6063862316   0.5809991902   3.0314088198
H  -3.1451255038   0.3306884454   0.0203860349
H  -1.3745371902   1.5567801801   1.3373868437
H  -1.1794104223   0.1063461797   2.3332359128
H  -0.6234160868  -1.1837731186   0.2369410764
H   1.0848762654   1.2876790254   0.7792671023
H   1.2403172282  -0.2780455409   1.5865415165
H   2.9180114344   0.0187114717  -0.3021591004
H   1.8638046485  -1.3713934409  -0.5260153792
H   1.5408209723   1.3684027553  -1.8587068601
H   1.9753578408  -0.1456169362  -2.658759963
H  -0.2259732037  -1.107453093   -2.0752275518
H  -0.5380030233   1.7018254761  -3.2571535587
H  -1.7202053823   0.3868290375  -3.3823709104
H  -0.1396846099   0.2358710722  -4.1765638105
```

calc_**1d** conf_2

```
C  -7.131285893   -0.5450466879   2.6435951439
C  -7.4836031782   0.3966120257   1.6851355258
C  -6.7468239365   0.5401749139   0.4989627546
C  -5.6462000732  -0.2648334117   0.2890131093
C  -5.2550518343  -1.2129931395   1.2534517715
C  -6.0214632982  -1.3659533846   2.4337450164
O  -5.720249746   -2.2706256121   3.3622291793
```
S98

```
O   -8.5487234677    1.2138599185    1.8384073247
C   -4.8398776382   -0.2242472125   -0.9768892822
C   -3.3809015077   -0.5574678912   -0.7031756257
O   -3.2765790191   -1.8135954551    0.0062825916
C   -4.0787921945   -2.0528574119    1.0527785851
O   -3.7882915464   -2.9846254849    1.7978323073
C   -2.6247310418    0.5282310196    0.0546567163
C   -1.1393046586    0.2309091158    0.190748399
C   -0.3961616123    1.2751509634    1.0184533703
C    1.103003748     0.9794528997    1.0157835642
C    1.6083546968    0.8109548284   -0.4161676765
C    0.7539549211   -0.2020432786   -1.1737213558
O   -0.6153614084    0.1779351361   -1.1277661654
C    1.1279174125   -0.3255106578   -2.6369395468
H   -7.7052721713   -0.6715710892    3.5561985229
H   -7.0621231338    1.2765258547   -0.2311997278
H   -4.943891353    -2.7807776647    3.0118673983
H   -8.9765388489    1.022464386     2.6834005787
H   -5.2443991611   -0.9610158359   -1.6827550894
H   -4.911923119     0.7536395425   -1.4615629003
H   -2.8564946523   -0.7505414736   -1.6396829169
H   -2.7390474429    1.4720234237   -0.4915303592
H   -3.0651514598    0.6718790003    1.0474669512
H   -1.0108896116   -0.7563768723    0.6644057314
H   -0.5829519514    2.2652305289    0.5829957502
H   -0.788489028     1.2872631966    2.0417085452
H    1.6542313756    1.7739381439    1.5297279872
H    1.2887374018    0.0541010873    1.5773876892
H    1.5570642489    1.7707176834   -0.9462295063
H    2.6562628497    0.4901104707   -0.4237693887
H    0.8589231197   -1.1861273602   -0.6846549476
H    2.1663116298   -0.6520082362   -2.7432420261
H    1.0138250788    0.6390800296   -3.1404899454
H    0.4819875042   -1.052036009    -3.1364580537

calc_**1d** conf_3

C   -7.7089809947   -0.5688712357    1.3053582625
C   -7.2318512235    0.6436330171    0.8226026828
C   -5.8558275598    0.9060908044    0.7421672526
C   -4.9602131496   -0.0662248913    1.1389332563
C   -5.4176715325   -1.3112897919    1.6115830098
C   -6.8084850436   -1.5520913569    1.7181444401
O   -7.2951129679   -2.6934506952    2.2012284337
O   -8.0617124631    1.6289977992    0.4132565825
C   -3.4742716932    0.1476879155    1.1234305621
C   -2.7645630537   -1.163357819     0.8435467285
O   -3.1719610956   -2.1639283933    1.8052778201
C   -4.4805297704   -2.3437709394    2.0387771774
O   -4.8270601331   -3.3709377197    2.614166636
C   -1.2457258799   -1.1135381809    0.9280543147
C   -0.5546265584   -0.5726589582   -0.3142475884
C    0.9650315135   -0.6910417621   -0.2240851549
C    1.624939111    -0.05543794     -1.4453480704
C    1.1024999345    1.3645642046    -1.6487148119
C   -0.4233203566    1.377700012     -1.6698467477
O   -0.9410590163    0.7827296035    -0.4847455053
C   -1.0075957812    2.7731036873    -1.7549004182
H   -8.7724090903   -0.7712313411    1.3860951054
```

```
H   -5.5230230704    1.8690699648    0.3726100803
H   -6.5124028726   -3.2279636938    2.4945659633
H   -8.9765587403    1.3351195373    0.5145667905
H   -3.1734322917    0.8839861899    0.3766582292
H   -3.1438344205    0.5263322722    2.1002544518
H   -3.0657481009   -1.5334070711   -0.1461393517
H   -0.9401993284   -0.5257707635    1.8010711066
H   -0.8958960913   -2.1382039331    1.0911604583
H   -0.8972540265   -1.1489166817   -1.1937060524
H    1.2992202513   -0.1821854191    0.688790498
H    1.2479127807   -1.7455987558   -0.1327017206
H    2.7145512125   -0.0555189235   -1.3377493123
H    1.397888411    -0.6575418895   -2.3355342571
H    1.4419012852    2.0098890464   -0.8285173048
H    1.4877155563    1.7923854052   -2.5811551786
H   -0.7666136778    0.7833554455   -2.5351590174
H   -2.0999253026    2.7341022586   -1.7727153504
H   -0.6651224625    3.2782836978   -2.6623588745
H   -0.6986723074    3.3669072942   -0.889675126

calc_**1d** conf_4

C   -6.9328357728    0.1651356259    2.1516654372
C   -6.6636609256    0.9060147722    1.0074830418
C   -5.6875976527    0.4966399173    0.0862309955
C   -4.9764758548   -0.6610530978    0.3284701125
C   -5.2150593986   -1.4182431776    1.4909499735
C   -6.2194953561   -1.0087505534    2.4001214765
O   -6.5117583432   -1.7066837817    3.4958077659
O   -7.3262878075    2.0490445413    0.7210742753
C   -3.9603308344   -1.2008862717   -0.6359079798
C   -2.8545587998   -1.9391111595    0.1021136741
O   -3.4135681262   -2.9419953796    0.9822477412
C   -4.4559135361   -2.6325339339    1.7666042591
O   -4.7300167682   -3.4007039488    2.6841907526
C   -1.9027102853   -1.050554336     0.9041319708
C   -0.7973795758   -0.3990835742    0.084948902
C    0.2100544589    0.3362788026    0.9659066599
C    1.2514939355    1.0501800579    0.1076892913
C    0.563218677     1.9193726324   -0.9424713683
C   -0.4592859739    1.1036166386   -1.7283624661
O   -1.3930438938    0.493370436    -0.8444544964
C   -1.2602084668    1.9356993066   -2.7094238392
H   -7.6964747155    0.4688883251    2.8609154735
H   -5.5122981992    1.0963681905   -0.7991762269
H   -5.9439519388   -2.520160947     3.4666240807
H   -7.9675282783    2.2269127637    1.4216312051
H   -4.4551259647   -1.8991864105   -1.3233864224
H   -3.5126291748   -0.4027863276   -1.2301531899
H   -2.2720231821   -2.531520141    -0.608453705
H   -2.4633882689   -0.2741538087    1.4364371343
H   -1.4263926605   -1.6845614102    1.6592823704
H   -0.2589072514   -1.1840207245   -0.4785101352
H   -0.3335807518    1.0660305391    1.5788772758
H    0.6887313949   -0.3733226432    1.6498595599
H    1.9183392481    1.6530273288    0.7327409359
H    1.8817599353    0.3036477154   -0.3944149988
H    0.0403604249    2.7520776337   -0.4551961266
H    1.2963973776    2.3531720892   -1.6318001514
```

S100

```
H   0.0746051696    0.3055713817   -2.2743481989
H  -1.8164651403    2.7143426362   -2.1793796205
H  -1.9749962521    1.3114316592   -3.2520960415
H  -0.599011472     2.4154886334   -3.4364693977
```

calc_**1d** conf_5

```
C  -7.8935127021   -1.4309898852    1.603007208
C  -8.0165800565   -0.0535878202    1.4687541501
C  -6.888056073     0.7687861597    1.3260324942
C  -5.6340857771    0.193899135     1.3067662078
C  -5.4825478488   -1.2015102048    1.4207823191
C  -6.62693863     -2.0171760074    1.5940990244
O  -6.5398925322   -3.3361359906    1.7493634611
O  -9.2177043861    0.5641202374    1.4733426089
C  -4.3755028438    1.0066147909    1.1954880526
C  -3.3032319851    0.215449977     0.465172534
O  -3.0978866304   -1.0554713265    1.1162746548
C  -4.163053762    -1.8196715998    1.4064139712
O  -3.9682885233   -3.0035822369    1.6611170006
C  -1.9672553604    0.9308230451    0.4100796456
C  -0.8965932452    0.2732412411   -0.4585754673
C  -0.1503399622   -0.8804691444    0.2062832056
C   0.9833094719   -1.3688345547   -0.6930395694
C   1.8674082068   -0.1984377131   -1.1159281017
C   1.0186715264    0.9211471924   -1.7103058194
O   0.0029518021    1.3184004917   -0.799732143
C   1.8162469838    2.1655224598   -2.0456322502
H  -8.7610520123   -2.0709571647    1.7295258106
H  -7.0256014645    1.8400683323    1.2356846494
H  -5.5725483043   -3.552877914     1.7750068045
H  -9.9151883454   -0.0967605975    1.5758932798
H  -4.5634702006    1.9457017792    0.6672647323
H  -4.0088103108    1.2664686432    2.1975733318
H  -3.6514503336   -0.0000896339   -0.5543556835
H  -2.146054665     1.9266838907   -0.0100582193
H  -1.5879346487    1.0751095589    1.4280674723
H  -1.3687391311   -0.0984726096   -1.3874866321
H   0.2606901435   -0.5162442968    1.1566763035
H  -0.8463890211   -1.688644153     0.4430464514
H   1.5731709572   -2.1364314747   -0.1813271684
H   0.5588929284   -1.8459012292   -1.5871614906
H   2.4038059099    0.1988706318   -0.2446971331
H   2.6206125319   -0.5175321812   -1.8455508333
H   0.5336770399    0.5399220124   -2.6273657974
H   2.2912657762    2.5643647667   -1.1444954393
H   1.1637611732    2.9387243953   -2.4591805719
H   2.5962443046    1.9378589976   -2.7778230534
```

calc_**1d** conf_6

```
C  -7.3935786474   -0.3422831099    1.979666225
C  -7.3291068686    0.4461239843    0.83721131
C  -6.1741489363    0.4839110282    0.0415487618
C  -5.0862437201   -0.2892030512    0.3936236134
C  -5.133904723    -1.113499875     1.5350476712
C  -6.2934086821   -1.117721236     2.3479478509
O  -6.3752904319   -1.8420836544    3.4621023045
O  -8.3652886836    1.2165884308    0.4382913859
```

S101

```
C    -3.7991851017    -0.2708508037    -0.3800134615
C    -3.1384577866    -1.6357016555    -0.298382001
O    -2.9518332025    -2.0278550469     1.0801201872
C    -3.9905482248    -1.9300688752     1.9241951406
O    -3.9207178464    -2.5275470897     2.9938895262
C    -1.796972666     -1.791475189     -1.001310729
C    -0.6637195456    -0.8141400758    -0.6980314902
C    -0.2355644745    -0.699262893      0.7624240946
C     0.912158901      0.3021977414     0.8823173068
C     0.5266986249     1.6269017311     0.2262074265
C     0.031498739      1.4000137517    -1.1997246346
O    -1.0324958329     0.456159582     -1.2178718736
C    -0.4843544447     2.6602795143    -1.8643282535
H    -8.2778772926    -0.3630136103     2.6088683812
H    -6.1584128189     1.1220299837    -0.8343934754
H    -5.4872095898    -2.2667702902     3.5849706375
H    -9.098704504      1.1067519495     1.0576832134
H    -3.97085376      -0.0116924637    -1.4282506672
H    -3.1211721765     0.4912505476     0.0165367928
H    -3.8230705511    -2.3747499195    -0.7366037091
H    -1.4389481795    -2.8056978897    -0.7932204312
H    -1.9895604423    -1.7383006704    -2.0787732366
H     0.2101386959    -1.1739235721    -1.2720565681
H    -1.0837613882    -0.3687118368     1.3691144184
H     0.0574755517    -1.6838655579     1.1414012541
H     1.1808935915     0.4558166579     1.9325098918
H     1.8045836569    -0.1031113281     0.3857045047
H    -0.2760815778     2.1073379289     0.8004796276
H     1.3759724284     2.3196772742     0.2141900489
H     0.8651232265     0.9878733638    -1.7962827952
H     0.3077239484     3.4114273742    -1.9314493194
H    -1.3135547522     3.0829459118    -1.2891684538
H    -0.8432405126     2.4412429386    -2.8731904759
```

calc_**1d** conf_7

```
C    -7.8797032857    -1.1376980819     1.2951402811
C    -7.6489825732    -0.0125146718     0.5136229965
C    -6.3548057767     0.5026932006     0.3422639827
C    -5.2919298512    -0.1303423889     0.9536565493
C    -5.4953980865    -1.2841653879     1.7334934794
C    -6.8093734428    -1.7762809567     1.9236549642
O    -7.0652755735    -2.8363900837     2.6861711377
O    -8.6496091494     0.6438962319    -0.1135198264
C    -3.882892134      0.3815681887     0.8532823268
C    -2.899057611     -0.7740461171     0.9163840691
O    -3.1306043279    -1.5648853787     2.1015056876
C    -4.3803880814    -1.957799285      2.3890103726
O    -4.5271851564    -2.8608104031     3.2060020828
C    -1.4381387958    -0.3655154577     0.9948840663
C    -0.9003311422     0.386945149     -0.2168821543
C    -0.9445267235    -0.4079969401    -1.520796511
C    -0.2393342159     0.3594968019    -2.638578238
C     1.1558464215     0.7889033015    -2.1907985973
C     1.0839876903     1.5254868849    -0.8564756777
O     0.4348504101     0.7211085952     0.1182845234
C     2.4448991749     1.8821607168    -0.2937173681
H    -8.8799882444    -1.5317823527     1.4450825828
H    -6.2176168688     1.3902928703    -0.2645323538
```

```
H   -6.1994553924   -3.1076150454    3.0879057844
H   -9.4875692332    0.2021415849    0.0771500347
H   -3.7437787066    0.9412764327   -0.0760625504
H   -3.6751823723    1.0737477167    1.6805176306
H   -3.0688517292   -1.4357673305    0.0576702807
H   -1.2919087814    0.2584675873    1.8828223076
H   -0.8345490688   -1.2673406849    1.1396440601
H   -1.4679220596    1.3244228678   -0.3606789195
H   -0.4473018277   -1.3722187592   -1.3553046693
H   -1.9818534894   -0.6205592599   -1.8045687242
H   -0.1862838894   -0.2491759117   -3.5471996779
H   -0.8285705094    1.2511872486   -2.8925837621
H    1.7967642383   -0.092785177    -2.0645629224
H    1.6266881099    1.4302388406   -2.944451378
H    0.4930285478    2.4485203584   -0.9976460826
H    3.0388529777    0.9770498713   -0.1368498507
H    2.3392907542    2.3923101741    0.6668902544
H    2.9861597748    2.5387750508   -0.9808301912

calc_1d conf_8

C   -6.9813488606   -0.1744873646    2.4480072324
C   -7.4584101115    0.1947107702    1.1967899422
C   -6.7865647034   -0.1769884144    0.0212591967
C   -5.6245070906   -0.9138120731    0.1155332321
C   -5.1088465035   -1.2850432223    1.3721438836
C   -5.8087741402   -0.9256280463    2.548848333
O   -5.3869308493   -1.2783946105    3.7606778694
O   -8.5874717094    0.9199619063    1.0433991318
C   -4.8749725004   -1.4044813786   -1.0896336519
C   -3.3793261138   -1.474039102    -0.807606156
O   -3.1364408114   -2.2605233404    0.3795782927
C   -3.8677337644   -2.0407400088    1.4833681084
O   -3.4525551193   -2.4997290512    2.5433704335
C   -2.7114900362   -0.1080672984   -0.7136994892
C   -1.1911376158   -0.131889036    -0.5656622275
C   -0.6879541644   -0.3626171472    0.8567374232
C    0.8323250258   -0.2248185675    0.91368975
C    1.2705009978    1.0974063425    0.2894596015
C    0.6647445299    1.255745402    -1.1019278036
O   -0.7491132738    1.1275830638   -1.0516264077
C    0.9585532111    2.601719953    -1.7336990187
H   -7.5033804089    0.0979248393    3.3598542062
H   -7.1973179157    0.1205492757   -0.9365534265
H   -4.5785741412   -1.8370219047    3.6243608492
H   -8.9583746379    1.1188764626    1.913245137
H   -5.2308448397   -2.4100255377   -1.347861357
H   -5.0604045469   -0.7661224683   -1.9579143148
H   -2.8896998751   -2.0554615582   -1.593473288
H   -2.9275863749    0.4237710571   -1.6470644627
H   -3.1576154761    0.4816179606    0.0947530174
H   -0.7787222767   -0.9236711695   -1.2193551803
H   -1.1518432871    0.3896888553    1.507983308
H   -1.0052033934   -1.3454587264    1.2144190266
H    1.1839116791   -0.3020295457    1.947782391
H    1.2933708284   -1.0571181211    0.3643271324
H    0.931519021     1.9354981653    0.9118831718
H    2.3630468138    1.1593582173    0.2257531072
H    1.0641272812    0.4536500208   -1.7490639667
```

S103

```
H   2.0369251934    2.7508670631   -1.8395949309
H   0.5555299221    3.4066662388   -1.1120926399
H   0.4975900381    2.6695720991   -2.7223954559
```

calc_**1d** conf_9

```
C  -7.5031310275   -0.2865922142    1.3610731373
C  -6.9015284313    0.9291606125    1.0600523491
C  -5.5055122021    1.0590913652    1.0129343019
C  -4.7167484419   -0.0469120168    1.2582419698
C  -5.301044539    -1.2942982874    1.5444355248
C  -6.7105741984   -1.405958079     1.619509792
O  -7.314521317    -2.5507986155    1.9303149698
O  -7.6232550119    2.0430674892     0.8038950087
C  -3.2153717054    0.0251517732     1.2656542654
C  -2.6243431683   -1.2989375952     0.8211438172
O  -3.1552834382   -2.3842917387     1.6180333202
C  -4.4775763945   -2.4675034574     1.8130638663
O  -4.934969803    -3.5285973368     2.2271417902
C  -1.1137870178   -1.4483604429     0.9499550156
C  -0.2734384724   -0.484204639      0.104751589
C   0.1059098591    0.8233147548     0.7999978304
C   0.894207977     1.7159764837    -0.1572477093
C   0.14109522      1.8779803407    -1.4763100076
C  -0.2369113231    0.5159988786    -2.0515448684
O  -0.9807083524   -0.2351584266    -1.0996671491
C  -1.0880651469    0.6060776062    -3.3016565388
H  -8.5823552669   -0.390454939      1.4149461126
H  -5.0738946736    2.0269236125     0.7854154108
H  -6.5920907105   -3.1998792186     2.1351628694
H  -8.5641164241    1.8305151975     0.8604887869
H  -2.8686013969    0.8086621043     0.5888097379
H  -2.8599634823    0.2710087367     2.2756025232
H  -2.916127628    -1.4840109019    -0.2171297531
H  -0.8333599759   -1.3488735605     2.0046151043
H  -0.8850620731   -2.4786744435     0.6620799531
H   0.670841418    -0.9975721276    -0.1479126104
H  -0.7969597737    1.3446532681     1.1359401789
H   0.6978941023    0.5971210204     1.6942719801
H   1.0920593635    2.6915375096     0.2988514612
H   1.8730891983    1.2579225945    -0.3540666144
H  -0.7798021896    2.4535164331    -1.3158689382
H   0.7458542235    2.4306958811    -2.2040654997
H   0.6910472714   -0.0381581467    -2.2778677653
H  -0.5523488697    1.1347331816    -4.0950549781
H  -2.0163740016    1.1452823569    -3.0909715452
H  -1.346172176    -0.393155013     -3.6610186889
```

calc_**1d** conf_10

```
C  -7.619897697    -0.5435134271    1.1217729405
C  -7.1991975618    0.7798600531     1.1656773096
C  -5.8522585834    1.1102146986     1.3810079039
C  -4.9281944046    0.0971116698     1.5370063455
C  -5.324676244    -1.2515057757     1.4748943417
C  -6.6907912575   -1.5716410085     1.2907467974
O  -7.1266630226   -2.8291357778     1.2721055432
O  -8.0583714491    1.8117070603     1.0105488905
C  -3.4739518498    0.3590020465     1.8100348369
```

```
C   -2.6224410062   -0.7301916792   1.1800757972
O   -3.0516582898   -2.0185878564   1.6831613858
C   -4.3549236262   -2.3276775431   1.6474497901
O   -4.6752163289   -3.5048917345   1.7790757483
C   -1.1292482542   -0.6510800186   1.4812669982
C   -0.2907980716    0.0904768852   0.4436364798
C   -0.5816804758    1.580146419    0.2738568701
C    0.3223154877    2.1619777703  -0.8122019101
C    0.1897363517    1.3433707415  -2.0950101119
C    0.4073492936   -0.1414725043  -1.8152021932
O   -0.4661019776   -0.5900105247  -0.7867099992
C    0.1539968696   -1.0224061208  -3.021441648
H   -8.6629847793   -0.8048169399   0.9731443437
H   -5.5663402606    2.1549326557   1.4220323984
H   -6.3393774616   -3.3997978685   1.4707732614
H   -8.948520633     1.4639112392   0.8680805995
H   -3.1793648406    1.3413605899   1.4338932719
H   -3.2945669457    0.3631496184   2.8940139074
H   -2.7716133051   -0.7455962452   0.0948640517
H   -0.9607009881   -0.2117054853   2.471300362
H   -0.7602514101   -1.6798306691   1.5170617343
H    0.7646794282   -0.0086503401   0.7545160603
H   -1.6284871171    1.713875019   -0.0241544413
H   -0.4390197057    2.101948775    1.2273347243
H    0.0781769744    3.2133134663  -0.9968238952
H    1.3650901314    2.1367989809  -0.4678267356
H   -0.8152986032    1.4727291001  -2.5167963335
H    0.9058228079    1.6843656825  -2.8511671357
H    1.4471748927   -0.2834958648  -1.4706259234
H    0.8321735414   -0.7613591967  -3.8388287023
H   -0.8752159392   -0.9003533501  -3.3714441051
H    0.3052963107   -2.0735325413  -2.764099559
```

calc_**1d** conf_11

```
C   -7.5241640742   -0.4241226331   1.836660622
C   -7.5563984077    0.0257246895   0.5226419574
C   -6.4088905167    0.0010886399  -0.2845281911
C   -5.2306340155   -0.4944232372   0.2362872699
C   -5.1757776224   -0.9764572695   1.5572892605
C   -6.3320340585   -0.9158037053   2.3716097728
O   -6.3251823937   -1.3153540419   3.6411568978
O   -8.6840868019    0.5127967267  -0.0419145576
C   -3.945368749    -0.5141726405  -0.5406044926
C   -3.1100378507   -1.7104395148  -0.1197991056
O   -2.8903627418   -1.6973321668   1.3050928564
C   -3.9349395456   -1.5037130092   2.1180163287
O   -3.8013301112   -1.775060831    3.3079135353
C   -1.7434207772   -1.829724036   -0.7866038664
C   -0.9647297983   -0.5396507035  -1.0111901007
C    0.4232593348   -0.8098446311  -1.5898966141
C    1.214166013     0.490997176   -1.711187942
C    1.1999699806    1.2401194856  -0.3803107233
C   -0.2295022651    1.4080487894   0.126216563
O   -0.874958991     0.1443538513   0.222746621
C   -0.3091720142    2.045046536    1.4986251717
H   -8.4041460851   -0.3920335652   2.4714845458
H   -6.4711449063    0.3741049433  -1.3003259405
H   -5.3871878692   -1.568755753    3.8470712771
```

S105

```
H   -9.4014528146    0.4791435942    0.6044804931
H   -4.1382080977   -0.5536487877   -1.6171721997
H   -3.3779966991    0.4007760661   -0.3352156271
H   -3.6764038955   -2.6266287472   -0.3342319108
H   -1.1445285046   -2.5154523934   -0.1781562162
H   -1.8825669485   -2.3079327648   -1.7631505162
H   -1.5153998678    0.0971358095   -1.7289215131
H    0.9474202065   -1.5023320741   -0.9193877044
H    0.3313162451   -1.3041314533   -2.5639807672
H    2.2413251601    0.2883670637   -2.0320790934
H    0.7613335064    1.1216957888   -2.4883762473
H    1.7681700192    0.6785508448    0.3718895465
H    1.6741354963    2.222971677    -0.4809898715
H   -0.7855179243    2.0285903772   -0.6002147647
H    0.2209266515    1.4303967064    2.2315149249
H   -1.3498181688    2.1339837134    1.8200168686
H    0.1403399026    3.0421214797    1.4875234532

calc_1d conf_12

C   -7.1946979261    0.0472167203    1.5974549378
C   -6.9963524361    0.2802058763    0.2426717328
C   -5.923471008    -0.3053323488   -0.4481107606
C   -5.0451599686   -1.1170410554    0.2391960617
C   -5.2101612508   -1.3517472732    1.6170852948
C   -6.3115901329   -0.7788036768    2.2961058855
O   -6.539423697    -0.997543306     3.5887386346
O   -7.8214679678    1.0698294512    -0.479395122
C   -3.9082013715   -1.8343487035   -0.42859218
C   -2.725447107    -1.9684838038    0.5213609202
O   -3.1473089839   -2.6010442234    1.7498557626
C   -4.2698320698   -2.1864663575    2.3574289624
O   -4.4598489289   -2.5424611899    3.5158285083
C   -2.0135493137   -0.6645490411    0.8678493888
C   -1.3133890047    0.0326367483   -0.293924537
C   -0.2109813192   -0.7941695025   -0.9533691468
C    0.5389900213    0.0430110349   -1.9887557767
C    1.0026477002    1.3606486576   -1.3726981234
C   -0.166199167     2.0744607218   -0.6997654821
O   -0.7798941503    1.223277961     0.2580353719
C    0.2433157841    3.3348706985    0.0349848707
H   -8.030526264     0.484682583     2.1344107266
H   -5.8118233666   -0.1119905758   -1.5087105405
H   -5.8441149192   -1.6379541867    3.8904312957
H   -8.5161755266    1.4143666678    0.0971199825
H   -4.2378362694   -2.8401494677   -0.7190569257
H   -3.6029240514   -1.3251054681   -1.3467976691
H   -2.0091620136   -2.6830202225    0.1104155524
H   -2.7265685437    0.0419736124    1.3047687337
H   -1.2670079401   -0.8822299552    1.6386098571
H   -2.054312574     0.3078551737   -1.0665930844
H    0.4816598126   -1.1331344244   -0.1723777788
H   -0.6329114206   -1.6887814112   -1.4262280984
H    1.3883676755   -0.5179853323   -2.3923206713
H   -0.1279439122    0.2538358766   -2.8359918788
H    1.7728484551    1.1693828069   -0.6147777763
H    1.4476048727    2.0117679959   -2.1336407931
H   -0.9137648215    2.3280331628   -1.4728652679
H   -0.6241926101    3.7967898146    0.5126508945
```

S106

```
H   0.6883235336    4.056734218    -0.6557579874
H   0.976482181     3.0987617441    0.8117262255
```

calc_**1d** conf_13

```
C   -6.7474625594   0.2386425027    1.9354200056
C   -7.343511065   -0.2086617281    0.7634025104
C   -6.6466223182  -1.0216501281   -0.1438443905
C   -5.3404200142  -1.3719980648    0.1320207675
C   -4.7062356773  -0.9146701217    1.3023160099
C   -5.4283866739  -0.1190237011    2.2223106464
O   -4.8918374931   0.3060067482    3.3638660538
O   -8.6173788679   0.1067435855    0.4385117744
C   -4.5412134818  -2.2810034831   -0.7592550667
C   -3.0646379266  -1.9106149968   -0.7038135044
O   -2.6082394177  -1.91036136      0.6628874285
C   -3.3223781218  -1.2716883903    1.5995816592
O   -2.7911490213  -1.0520691213    2.6828068331
C   -2.7709342418  -0.5895581911   -1.4179085058
C   -1.4056168015   0.0447653202   -1.1634324595
C   -0.220146769   -0.9165799899   -1.219770626
C   1.069157665    -0.1790097521   -0.8630487002
C   0.9000426434    0.5402409173    0.4733790441
C   -0.3356298431   1.4352245762    0.4468971836
O   -1.4909519085   0.6885647374    0.0939814585
C   -0.6345799821   2.0817991253    1.7844742087
H   -7.284989979    0.8553317975    2.6489193084
H   -7.1508997975  -1.3611565057   -1.0412446853
H   -3.9851267582  -0.0948534262    3.4104544575
H   -8.9917246829   0.6664981657    1.1314170751
H   -4.6620858598  -3.3184934727   -0.4227903113
H   -4.900000726   -2.234311149    -1.7918151091
H   -2.4698464626  -2.7063271201   -1.1579803351
H   -2.8796739962  -0.7833344689   -2.4919030279
H   -3.5257835291   0.1572347447   -1.1511846832
H   -1.2531961651   0.817757409    -1.9391934114
H   -0.3833712815  -1.7251430485   -0.4999542008
H   -0.1525197892  -1.3623496097   -2.2197993309
H   1.9126393968   -0.8763597685   -0.8251222053
H   1.3016188536    0.5551262267   -1.6469553736
H   0.7776609446   -0.193860404     1.27918884
H   1.7848492522    1.143260304     0.7072760648
H   -0.1814695898   2.2185555932   -0.3181087682
H   0.2121124669    2.688466199     2.1185346248
H   -0.8359275488   1.3101450405    2.5324933211
H   -1.5161328725   2.7237150086    1.70998542
```

calc_**1d** conf_14

```
C   -6.17695401     0.8831143423    0.9265396282
C   -6.4212820798   0.3134830065   -0.3173614868
C   -5.773691895   -0.8641825244   -0.7165433163
C   -4.8663114098  -1.4571935785    0.1411027723
C   -4.5838912249  -0.8900452939    1.3938938521
C   -5.2687232073   0.2799394088    1.7986170904
O   -5.0729471566   0.835758136     2.9936319402
O   -7.2941534741   0.8553424849   -1.1968789767
C   -4.1999813642  -2.7642492959   -0.1769579337
C   -2.8337776511  -2.905853387     0.4886978002
```

```
O   -2.8792582239   -2.5335194557    1.878739779
C   -3.6080950067   -1.4938422694    2.2969600611
O   -3.4489156335   -1.1112504726    3.4521979518
C   -1.6670219043   -2.2325491108   -0.2353800271
C   -1.7354112853   -0.7379182386   -0.5210039558
C   -0.6546584941   -0.3033012571   -1.5109853142
C   -0.6613740878    1.2152469417   -1.673221972
C   -0.5885515589    1.8907408189   -0.3064406428
C   -1.6689581425    1.3476456288    0.624351077
O   -1.5741289584   -0.070334683     0.7169361537
C   -1.5608375923    1.8886723507    2.0353438568
H   -6.6882054637    1.7842802138    1.2506360132
H   -6.00563083     -1.2913744588   -1.6854410756
H   -4.447803979     0.2315499925    3.4770026728
H   -7.6799798468    1.6518218954   -0.8093086358
H   -4.8467267322   -3.576149696     0.1793846641
H   -4.0950747677   -2.9007340757   -1.25770659
H   -2.5891667936   -3.9705696845    0.5341421993
H   -0.7575606158   -2.4218753426    0.345232848
H   -1.5508913353   -2.7610487152   -1.1900801937
H   -2.7197662159   -0.4760848929   -0.9457166936
H    0.3201503563   -0.6349017781   -1.1306403847
H   -0.8153104577   -0.7982874863   -2.4759739403
H    0.1678504499    1.538289659    -2.31158256
H   -1.5864716583    1.520353719    -2.1809169544
H    0.3900110829    1.7005338062    0.1526751096
H   -0.6975737413    2.977010412    -0.402121316
H   -2.6583773613    1.6023001403    0.2063578998
H   -1.644804564     2.9793356413    2.0334524081
H   -0.5962321586    1.6135176047    2.4715964873
H   -2.3515110073    1.4803294942    2.6667697043

calc_**1d** conf_15

C   -7.7370913546   -0.7446304562    2.0321583009
C   -7.8209819714    0.0492768964    0.8951641857
C   -6.6916160653    0.3106643998    0.1034515995
C   -5.4799881713   -0.2467104538    0.4562686333
C   -5.3718052815   -1.0733038537    1.5909211403
C   -6.5108985316   -1.3013586166    2.3999095561
O   -6.4567899303   -2.0354219889    3.5085487339
O   -8.9821738112    0.6132934322    0.4969486477
C   -4.2123578966    0.0147828591   -0.3070497792
C   -3.324094575    -1.2159682457   -0.25035471
O   -3.0596243566   -1.5666063672    1.125143642
C   -4.0944339293   -1.6648136395    1.9743154776
O   -3.9134220015   -2.2411842353    3.0415263213
C   -1.9737195209   -1.12650084     -0.9429749741
C   -1.0201092298   -0.0342206168   -0.4564594364
C   -1.1164242617    1.2835300271   -1.2253163356
C   -0.0423794274    2.2605004242   -0.7487911799
C    1.3327652212    1.59825116     -0.7971583448
C    1.3051607164    0.2577796839   -0.0682199209
O    0.2850050243   -0.5745063737   -0.6012027516
C    2.6042653386   -0.5141048289   -0.180860676
H   -8.6029362469   -0.9364210419    2.6581306607
H   -6.7950536048    0.9469040242   -0.767903001
H   -5.5049021135   -2.285747491     3.6323731851
H   -9.684114749     0.3642745779    1.1125645263
```

```
H   -4.4249942583    0.2745670157   -1.3482641527
H   -3.689985433     0.8680101245    0.1427281216
H   -3.8754349955   -2.0565881458   -0.6917501011
H   -1.4659500913   -2.0821376288   -0.783677231
H   -2.1439739721   -1.0318732291   -2.0219976371
H   -1.2036743313    0.1547329878    0.6150414313
H   -0.973058891     1.0651084989   -2.2914879412
H   -2.112154023     1.7265694759   -1.1180428966
H   -0.0559375636    3.1724854498   -1.355045306
H   -0.2628748903    2.5663095914    0.2829376041
H    1.6241690734    1.4189208668   -1.83989237
H    2.0949165135    2.2479773901   -0.3521078557
H    1.0819449054    0.443268208     0.997604426
H    3.4310782184    0.0558324403    0.2526786898
H    2.8350339022   -0.7175848298   -1.2307696297
H    2.5256165663   -1.4693566514    0.3439113472

calc_**1d** conf_16

C   -7.5042482974   -0.2791492712    1.366160629
C   -6.8996834687    0.9348030906    1.0693033896
C   -5.5021376311    1.0598589732    1.0202108312
C   -4.7119068927   -0.0489702035    1.2599131847
C   -5.3001857456   -1.2922854104    1.5422450981
C   -6.7133034191   -1.3983973815    1.6187305084
O   -7.3168881105   -2.5442480029    1.9264199061
O   -7.7146079498    1.988131319     0.8348275325
C   -3.2104905812    0.0220889328    1.2639109254
C   -2.62359767     -1.3022022153    0.8144027328
O   -3.1549879539   -2.3866645465    1.6100475505
C   -4.4780963137   -2.4679569815    1.8073967194
O   -4.9351543378   -3.5284954324    2.2208181007
C   -1.1130585387   -1.4554865465    0.939131527
C   -0.271431217    -0.4900671408    0.0968073481
C    0.1157625474    0.8118551514    0.7981574214
C    0.9067356708    1.7054831534   -0.1560320072
C    0.1527934661    1.8776558712   -1.473379065
C   -0.2344163843    0.5205382238   -2.0541379902
O   -0.9810506297   -0.2300565712   -1.1041171646
C   -1.0867973583    0.6210806245   -3.3025867961
H   -8.5828183851   -0.3577407035    1.4151439994
H   -5.0461519214    2.021130241     0.7966645995
H   -6.5977254533   -3.1955369267    2.1294543942
H   -7.1772215917    2.7689938023    0.6498800615
H   -2.8626708292    0.8061379146    0.5878454784
H   -2.8517170167    0.2644256501    2.2735549425
H   -2.9185153817   -1.4831284454   -0.2237806429
H   -0.8303611062   -1.3616481495    1.9936932623
H   -0.8878156292   -2.4851847897    0.6464713075
H    0.6697349453   -1.0059543003   -0.1619250825
H   -0.78417795     1.3355720441    1.138588625
H    0.7082571293    0.5783542948    1.6901661956
H    1.1104459949    2.6778153107    0.3044174959
H    1.8829679526    1.2435356734   -0.3565460273
H   -0.76459312      2.4579018388   -1.3091150779
H    0.7597172953    2.4301722285   -2.1994649288
H    0.6897593095   -0.0380781138   -2.2845268721
H   -0.5490379008    1.1495632857   -4.0946963392
H   -2.0115430141    1.1651467929   -3.0884843659
```

```
H  -1.351782512    -0.3749932843    -3.6655714071
```

calc_**1d** conf_17

```
C  -7.0042349774    0.0348018857     1.9373761032
C  -6.6490201414    0.8311172286     0.8560793439
C  -5.5551001835    0.5051236607     0.0390037366
C  -4.8135856256   -0.6230129737     0.3263458609
C  -5.1398680845   -1.4356276       1.4287017057
C  -6.2626955677   -1.1125615591    2.227209364
O  -6.6417697734   -1.8674194611    3.2556817619
O  -7.3358457556    1.9491418372     0.5312848617
C  -3.6654786707   -1.0846040999    -0.5217589812
C  -2.6075824325   -1.7717030745    0.3251876415
O  -3.2082521454   -2.8452030965    1.0885088049
C  -4.351858301    -2.6228083707    1.7500242557
O  -4.6955207423   -3.4409521381    2.598448173
C  -1.8202214965   -0.8959666163    1.3025541704
C  -0.9529221216    0.1966980546     0.6618494391
C  -1.6182765718    1.5695226062     0.575736037
C  -0.6951626097    2.5592719678    -0.1333068287
C  -0.219333697     1.9833057996    -1.4655460016
C   0.3799334518    0.5940113802    -1.2671599194
O  -0.5546697911   -0.2614654029    -0.6215067898
C   0.771914752    -0.0824941369    -2.5649491469
H  -7.8587548065    0.2723250517     2.5633341215
H  -5.3220259741    1.1404300959    -0.8077930549
H  -6.0337132302   -2.6524230218    3.2626228574
H  -8.0633266743    2.0665417903     1.1562872465
H  -4.0353359846   -1.8087392683    -1.2594370443
H  -3.2086296352   -0.2679366668    -1.082926918
H  -1.9002562799   -2.28017716      -0.3284406489
H  -2.504908139    -0.4333760022    2.0218749946
H  -1.1841505126   -1.5823082114    1.8693457279
H  -0.0467757611    0.3160513415     1.2811870059
H  -2.5703427966    1.4919834295     0.0390118825
H  -1.8544509203    1.9167278119     1.5880166783
H  -1.2003630175    3.5189820384    -0.2833712131
H   0.1767750098    2.7603931513     0.5040698234
H  -1.0639192897    1.8997669322    -2.1618772201
H   0.5219215534    2.641872868     -1.9322434773
H   1.2687959881    0.6852457142    -0.61813655
H   1.5280918273    0.5057169313    -3.0924509113
H  -0.1003645412   -0.1891502444    -3.2167076165
H   1.1782836691   -1.0781024721    -2.3701292756
```

calc_**1d** conf_18

```
C  -7.6470071758   -0.8324414368    2.2770009992
C  -7.8074566252    0.1778480827     1.336913968
C  -6.7528294742    0.5641752778     0.4955733897
C  -5.5380540115   -0.0825341029     0.5966454462
C  -5.3547211763   -1.124027        1.5268741947
C  -6.4178454224   -1.483315118     2.391305673
O  -6.2888200844   -2.4290159183    3.3188046403
O  -8.9747648619    0.8408065335     1.1869455235
C  -4.3505539574    0.302393752     -0.239819626
C  -3.4774632315   -0.9167014245    -0.4936275619
O  -3.115942336    -1.5582469041    0.7469299934
```

```
C   -4.0750938227   -1.8117298128    1.6514275407
O   -3.8196441365   -2.6034341655    2.5525794475
C   -2.1882967105   -0.6647863368   -1.27087124
C   -0.9541438436   -0.2316206751   -0.4801830247
C   -1.0668470565    1.0802274425    0.2910479027
C    0.2880300266    1.4604976278    0.8890473771
C    1.375182661     1.4375089001   -0.1814471674
C    1.3592476011    0.1039615027   -0.9236169015
O    0.0688135908   -0.1429064566   -1.4627043042
C    2.3359044683    0.049854978    -2.0809697979
H   -8.4533240859   -1.1256030436    2.9419431396
H   -6.9141644141    1.3651071656   -0.216651233
H   -5.3430964139   -2.7262164979    3.2873450211
H   -9.622277851     0.4904108812    1.81280318
H   -4.6725759833    0.714497825    -1.200969284
H   -3.7784277114    1.0870130458    0.2671006323
H   -4.0826478682   -1.6397921523   -1.0555185524
H   -1.9048743748   -1.5824638578   -1.7944832481
H   -2.389291645     0.083550758    -2.0461450938
H   -0.6976121456   -1.0300698766    0.233496388
H   -1.4101450003    1.8690249399   -0.3911867775
H   -1.8070674617    0.9782190475    1.0907209233
H    0.2325635049    2.4446056041    1.3662139092
H    0.5432960797    0.7425882686    1.6798836931
H    1.2033302311    2.2405050895   -0.9097236185
H    2.3630982593    1.6050777427    0.2626375652
H    1.5984364158   -0.6996168731   -0.2045492308
H    2.104147764     0.8328187743   -2.8090769471
H    2.2752042788   -0.916954912    -2.586898916
H    3.3607340001    0.1957833254   -1.7277980232

calc_**1d** conf_19

C   -7.436762891    -0.3116068365    1.9399609314
C   -7.3411115681    0.3738947727    0.7356305326
C   -6.2360490948    0.2051189528   -0.1134096175
C   -5.2222530919   -0.6519930375    0.2645013654
C   -5.2847403854   -1.3411569796    1.488985046
C   -6.4166452435   -1.1848524175    2.3233388708
O   -6.5457746539   -1.8436056537    3.47241366
O   -8.3005661115    1.2291200027    0.3172338622
C   -4.030165441    -0.933522492    -0.6049760819
C   -2.7953400152   -1.2017557673    0.245879971
O   -3.0785226627   -2.2665657844    1.1847825414
C   -4.2080491648   -2.2350518107    1.9028491521
O   -4.2929998122   -2.9750607379    2.8784745716
C   -2.2509304629    0.0126105604    1.0058297303
C   -1.145488906     0.7817579097    0.2864517929
C   -1.5248644203    1.4391593297   -1.0390899542
C   -0.3068192161    2.1463708187   -1.6320850832
C    0.8671455595    1.1732424919   -1.7255562904
C    1.1158570613    0.4949745299   -0.3808670407
O   -0.0721685512   -0.1244617565    0.0951774792
C    2.1797499515   -0.5821603016   -0.4397851969
H   -8.2956491589   -0.1973382577    2.5938991836
H   -6.2054483278    0.7463722373   -1.0520633886
H   -5.7582353341   -2.444639006     3.537553541
H   -9.0060917623    1.2615752891    0.9766634189
H   -4.2331919698   -1.8185650791   -1.2217900033
```

S111

```
H  -3.846302305    -0.102684564   -1.2895759658
H  -1.9929768149   -1.6184668148   -0.3642076441
H  -3.0609857196    0.7005721072    1.272412634
H  -1.817637       -0.3602169684    1.9383864094
H  -0.8130716003    1.5818829055    0.9716118366
H  -1.8650695916    0.6689033866   -1.7416669766
H  -2.353546237     2.140705151    -0.8880105521
H  -0.5427536732    2.564547166    -2.6162395579
H  -0.0303348778    2.9925287368   -0.98862043
H   0.6486797546    0.3968737479   -2.4701076139
H   1.7771001896    1.6894148916   -2.0518642364
H   1.4172601758    1.2676201467    0.3485533527
H   3.137040112    -0.1611081905   -0.7598791578
H   1.8895764328   -1.36370842     -1.1481431391
H   2.311136828    -1.0427242587    0.5423480474

calc_**1d** conf_20

C  -7.7172594296   -1.2931976791    1.2070203994
C  -7.8991523217    0.0784281939    1.3323290756
C  -6.8069465009    0.9592855887    1.3511358592
C  -5.5300142287    0.4501344411    1.2302781168
C  -5.3184166538   -0.9333986549    1.0821955598
C  -6.4270134258   -1.8140549625    1.0943426453
O  -6.2838690697   -3.1337872213    1.0005222887
O  -9.1263010346    0.6325698775    1.4466704238
C  -4.3056785629    1.3182169026    1.2805782136
C  -3.203293315     0.7190889723    0.4221282775
O  -2.9392879206   -0.6377668025    0.8227405104
C  -3.9717579013   -1.4823946766    0.9596397162
O  -3.7340719971   -2.6857490978    0.9892691166
C  -1.9065551906    1.5060490052    0.5115608294
C  -0.6991900299    0.978605119    -0.2658062126
C  -1.0083553485    0.4459247335   -1.6633562133
C   0.2706573972   -0.0762822228   -2.3158652319
C   0.9566519439   -1.0758144389   -1.3870947229
C   1.1552689732   -0.4710251788    0.0002755527
O  -0.0795498726   -0.0123686417    0.5293898425
C   1.7206816536   -1.4540452081    1.0053275459
H  -8.5565151866   -1.9817091935    1.2077159929
H  -6.9888715024    2.0219151264    1.4629056271
H  -5.3065773145   -3.3079222629    0.9906518775
H  -9.7933574296   -0.0660080852    1.4200124549
H  -4.5323577216    2.3323161287    0.9382121381
H  -3.9477792009    1.3982247753    2.3158189434
H  -3.5487484611    0.6846074844   -0.6193840672
H  -2.1322945723    2.5187964694    0.1566868862
H  -1.6064823605    1.5909428139    1.561436962
H   0.0062511709    1.8237018375   -0.3749990815
H  -1.729133956    -0.3745020919   -1.5769099079
H  -1.4661844173    1.2339885777   -2.2738069272
H   0.0481568236   -0.5359901342   -3.2845570689
H   0.9497655587    0.7642274011   -2.5146317993
H   0.3377699989   -1.975895872    -1.2856884561
H   1.9247696696   -1.3869225169   -1.7960381696
H   1.837735872     0.3942983309   -0.0926949593
H   2.6959046418   -1.8249616397    0.676835006
H   1.0425931168   -2.3042092844    1.1210050243
H   1.8388081062   -0.9763159137    1.9811479321
```

S112

calc_**1d** conf_21

```
C  -6.5533573767   0.5366852297   1.2263597118
C  -6.662736375    0.1861500608  -0.1135179534
C  -5.8572401112  -0.8183621478  -0.670586424
C  -4.9303786831  -1.4602705115   0.1280124265
C  -4.7916358627  -1.1168569242   1.4835557379
C  -5.6270948238  -0.1172126982   2.0405880283
O  -5.560315886    0.2280962721   3.3234122286
O  -7.5462722158   0.7833053146  -0.9428808207
C  -4.0899323059  -2.594896395   -0.3814980167
C  -2.7679268305  -2.7529059994   0.3662157014
O  -2.947668173   -2.6473098679   1.7949401116
C  -3.8137386389  -1.7837332069   2.3366030663
O  -3.753144198   -1.5999623361   3.5486988792
C  -1.5792762285  -1.8961640313  -0.0692696651
C  -1.6707227179  -0.3717840826  -0.005881669
C  -2.2512102856   0.283821317   -1.2571264991
C  -2.1634994181   1.805466919   -1.1518342153
C  -0.7362727495   2.2323406523  -0.8172699941
C  -0.2214836233   1.4677887642   0.3990903907
O  -0.333013028    0.0671350405   0.1893777086
C   1.2342534653   1.7492039845   0.7124388119
H  -7.1818220302   1.3035540642   1.6681599687
H  -5.9832462133  -1.0746735099  -1.7163361166
H  -4.8867261442  -0.3723976636   3.7387677132
H  -8.0447371153   1.4488005415  -0.4505737539
H  -4.6648772686  -3.5222659356  -0.2635084006
H  -3.8897044473  -2.4870829449  -1.4516833791
H  -2.4428260689  -3.7890258524   0.2419095921
H  -0.7440160515  -2.1810266653   0.5777977304
H  -1.3032322369  -2.2019444422  -1.0863979495
H  -2.2682023787  -0.0639235796   0.8682925701
H  -1.6694686832  -0.0624452637  -2.1214530136
H  -3.2892890207  -0.0263766932  -1.4078874065
H  -2.5003299017   2.273830282   -2.0827711402
H  -2.8441977264   2.1523542465  -0.3628338585
H  -0.0738498021   2.0178016467  -1.6657654665
H  -0.6844418739   3.3105014153  -0.6270482319
H  -0.84200984     1.7399560965   1.2715025066
H   1.5560507787   1.1699123197   1.5813717017
H   1.3842537892   2.811528673    0.9253212371
H   1.8653383011   1.4723879116  -0.1372918485
```

Table S34. Sampled and DFT geometry optimized conformers related to calc_**2a**, with energy values (Hartree) and related % contribution on the final Boltzmann distribution for the three employed functional/basis set combinations.

Conformer	MPW1PW91/6-31g(d,p)		MPW1PW91/6-311+g(d,p)		B97-2/cc-pVTZ	
	Energy (Hartree)	% contribution on the Boltzmann distribution	Energy (Hartree)	% contribution on the Boltzmann distribution	Energy (Hartree)	% contribution on the Boltzmann distribution
calc_**2a** conf_1	-916.6428199	47.75%	-916.8801926	15.17%	-916.8298210	48.81%
calc_**2a** conf_2	-916.6426963	41.89%	-916.8814972	60.41%	-916.8295482	36.56%
calc_**2a** conf_3	-916.6409860	6.85%	-916.8804583	20.10%	-916.8283295	10.06%
calc_**2a** conf_4	-916.6403030	3.32%	-916.8789241	3.96%	-916.8274255	3.86%
calc_**2a** conf_5	-916.6372323	0.13%	-916.8755818	0.11%	-916.8243186	0.14%
calc_**2a** conf_6	-916.6353451	0.02%	-916.8738058	0.02%	-916.8227599	0.03%
calc_**2a** conf_7	-916.6353118	0.02%	-916.8757050	0.13%	-916.8244998	0.17%
calc_**2a** conf_8	-916.6350563	0.01%	-916.8739557	0.02%	-916.8235548	0.06%
calc_**2a** conf_9	-916.6342671	0.01%	-916.8746861	0.04%	-916.8247115	0.22%
calc_**2a** conf_10	-916.6339973	0.00%	-916.8726469	0.01%	-916.8225701	0.02%
calc_**2a** conf_11	-916.6338765	0.00%	-916.8728533	0.01%	-916.8217229	0.01%
calc_**2a** conf_12	-916.6332930	0.00%	-916.8727808	0.01%	-916.8218994	0.01%
calc_**2a** conf_13	-916.6326067	0.00%	-916.8712038	0.00%	-916.8207010	0.00%
calc_**2a** conf_14	-916.6322320	0.00%	-916.8726368	0.01%	-916.8224439	0.02%
calc_**2a** conf_15	-916.6316901	0.00%	-916.8710877	0.00%	-916.8211578	0.01%
calc_**2a** conf_16	-916.6309166	0.00%	-916.8688316	0.00%	-916.8178010	0.00%
calc_**2a** conf_17	-916.6303572	0.00%	-916.8710994	0.00%	-916.8211567	0.01%

Table S35. Cartesian coordinates of the optimized geometries for the conformers related to calc_**2a**. The related energies and % contribution on the final Boltzmann distribution for the three employed functional/basis set combinations are reported in Table S34.

calc_**2a** conf_1

```
C  -9.0252381199   -1.7881653883   -0.8340015369
C  -8.9238618601   -0.291809802    -0.4272179486
C  -7.5642500875   -0.1647885362   0.2940965892
N  -6.9502011441   -1.5103604141   0.2626743554
C  -7.577111816    -2.2371786111   -0.8258827118
C  -5.5041333845   -1.6361879407   -0.0200156221
C  -5.3544704201   -1.7150888947   -1.5686017551
C  -6.7950979     -1.8294093483   -2.0807155869
O  -9.6564036524   -1.9205144199   -2.0943029598
O  -8.9593777057   0.5267787961    -1.5703677302
C  -4.5748083355   -0.6123064358   0.6263043268
C  -7.7016584877   0.2890026453    1.7497766721
O  -7.0579357614   -2.8039349737   -3.0875187481
O  -4.6298490006   0.6613932047    0.0360719763
N  -8.0795040973   1.6819110385    1.8762343934
O  -5.9544527089   2.4559794855    1.7372688796
C  -7.1620050594   2.6739830458    1.8232614211
C  -7.6955613695   4.0847687615    1.8903144489
H  -7.4670441167   -3.3218492086   -0.6930319835
H  -9.6025787066   -2.3401410309   -0.0849066504
H  -9.7532037384   -0.0212322161   0.2459875998
H  -6.9715623246   0.5770060492    -0.2506407566
H  -5.2138847062   -2.6078484041   0.4021486778
H  -4.7796482631   -2.5979653704   -1.8650389732
H  -4.8556840303   -0.8237148635   -1.9552472697
H  -7.1502971345   -0.848474263    -2.4180453022
H  -9.027190334    -2.3622921977   -2.691710041
H  -9.4623018481   0.0004101101    -2.2198532519
H  -3.5544457316   -1.001964572    0.5072334962
H  -4.7655185618   -0.5713852055   1.7064647669
H  -8.4422788662   -0.3278618861   2.2672290951
H  -6.7529038788   0.161087639     2.2717522379
H  -6.6548310904   -2.5043833515   -3.9122882833
H  -5.0533778978   1.2830478143    0.6574504372
H  -9.0558943554   1.9267095436    1.8425444651
H  -7.1360219625   4.6338656911    2.650022302
H  -7.5118561255   4.5751619188    0.9306786438
H  -8.7625554173   4.140751591     2.1178723266
```

calc_**2a** conf_2

```
C  -8.9091610546   -1.0652231709   -1.061132996
C  -8.606556514    0.2426218929    -0.3449356825
C  -7.0875593197   0.3437783976    -0.5200133663
N  -6.6903398594   -1.0021476989   -0.0808471435
C  -7.7016704791   -1.9324348669   -0.6731685038
C  -5.4047998589   -1.5653348708   -0.5325676356
C  -5.6466049015   -2.0034203345   -1.9729764484
C  -7.0039833171   -2.6938339507   -1.8435802948
O  -8.9408622414   -0.8374004415   -2.4556000059
O  -9.3297215892   1.300525271     -0.9035817301
C  -4.2412275081   -0.6658105846   -0.1808968141
C  -6.5051914474   1.5580495933    0.2026253616
```

S115

```
O   -6.7465779483    -4.0496815888    -1.5038245095
O   -4.3356495958    -0.3039837295     1.1901396226
N   -6.767226238      1.6425877156     1.6248781093
O   -8.7512091386     2.7246633783     1.418590544
C   -7.8449415457     2.2843512583     2.1274342671
C   -7.8844781582     2.449717176      3.6280488772
H   -7.9863046708    -2.6721621678     0.0833869799
H   -9.8564070571    -1.5120415445    -0.7307156184
H   -8.8234880193     0.1234901105     0.724351821
H   -6.8994240569     0.5152637496    -1.5928618671
H   -5.2751741309    -2.4857052116     0.0553044407
H   -4.8959246283    -2.6953061861    -2.3610295361
H   -5.7165614356    -1.1430527891    -2.6458348116
H   -7.5912152977    -2.628069462     -2.7627589943
H   -9.388145585      0.018013406     -2.5615080579
H   -9.2937276892     2.0173679495    -0.238806938
H   -3.2954224482    -1.1931345214    -0.3451779593
H   -4.2270592803     0.2324866079    -0.8143751343
H   -5.427842499      1.6339035794     0.0664133491
H   -6.9616104359     2.4345346431    -0.2679041964
H   -7.5950814127    -4.5078459486    -1.4628967692
H   -5.2200517833    -0.6081532401     1.4549316763
H   -6.0261431536     1.3591255085     2.2458858632
H   -7.0674829698     1.9433161497     4.1466829421
H   -7.8474989733     3.516516402      3.8633936603
H   -8.8376737582     2.0684295189     3.9999274985


calc_**2a** conf_3

C   -8.9959640431    -1.6193951558    -0.910622647
C   -8.8767397137    -0.359612495     -0.0104255835
C   -7.3902711901    -0.2768134808     0.408072903
N   -6.912388065     -1.6611619917     0.2694991253
C   -7.5727670741    -2.167445106     -0.9383703575
C   -5.4869948082    -1.8822798727    -0.0390224351
C   -5.3104077119    -1.6591159542    -1.5694088786
C   -6.7399978342    -1.6302489723    -2.1176550943
O   -9.4652392619    -1.3236883353    -2.2081892675
O   -9.3145800696     0.755890853     -0.7398660996
C   -4.4620510622    -1.1782694943     0.8387040236
C   -7.1947355465     0.2873196432     1.8270526077
O   -6.8771297719    -2.3948967428    -3.2895302073
O   -4.4258034658     0.2364160947     0.7354777686
N   -6.7704474649     1.6720836213     1.8444329296
O   -8.8053781805     2.5109493959     1.3090592666
C   -7.6072805441     2.6852402816     1.5493482419
C   -7.0093435216     4.0722083237     1.5529667215
H   -7.5308935717    -3.2633620153    -0.9658250549
H   -9.6782409135    -2.3402057777    -0.4473446575
H   -9.4963966004    -0.4937375254     0.8851686713
H   -6.8945338462     0.4120759943    -0.2926647307
H   -5.3229377965    -2.9513760639     0.1520705913
H   -4.7555656834    -2.481710325     -2.0282119887
H   -4.7734977245    -0.7352979121    -1.8134876011
H   -7.0413958026    -0.5933766058    -2.3162259114
H   -9.6905581552    -0.3762246019    -2.1878806348
H   -9.3183414356     1.5099782436    -0.1144809666
H   -3.4744282025    -1.6005847413     0.6047152598
H   -4.660570056     -1.3959699407     1.890661277
```

```
H   -8.1257169479    0.2136293231    2.3955262821
H   -6.4436464202   -0.2892171241    2.3640565478
H   -7.8057368603   -2.2801272109   -3.5439538643
H   -4.1835901792    0.4573128143   -0.1724836705
H   -5.7734977037    1.8272828364    1.8260415515
H   -5.9507107573    4.0931961961    1.8208990242
H   -7.1407529529    4.5183124416    0.5639951213
H   -7.567469061     4.6882213819    2.2619017369

calc_2a conf_4

C   -8.945953715    -1.6949082974   -0.6364476942
C   -8.7882312137   -0.3008487952    0.025238083
C   -7.2782987821   -0.1537527352    0.3508222841
N   -6.718733443    -1.5145109376    0.1755964308
C   -7.5098078545   -2.1112044561   -0.9057943905
C   -5.3510416566   -1.5969857054   -0.386165126
C   -5.464366166    -1.2595096947   -1.8881198992
C   -6.9409213054   -1.5308647848   -2.2204854829
O   -9.7249854459   -1.6636171732   -1.808956521
O   -9.2450699825    0.6674710364   -0.8873179786
C   -4.326177465    -0.8235071448    0.4122821063
C   -7.0012940003    0.4114478237    1.7575061507
O   -7.0772102749   -2.4170847745   -3.3073365463
O   -4.2733968114   -1.2707693638    1.75611044
N   -6.7597084739    1.8459109952    1.7832163643
O   -8.8224900463    2.4856555623    1.099169124
C   -7.6882594879    2.77621477      1.4802268114
C   -7.2681270978    4.218811477     1.6403597069
H   -7.3682813524   -3.1980268388   -0.9262206452
H   -9.4104271717   -2.385072168     0.0762903658
H   -9.3777350773   -0.2431869041    0.9465937952
H   -6.8667730157    0.5559969867   -0.3828775731
H   -5.077877686    -2.6576353223   -0.3010121242
H   -4.8189678113   -1.8984429775   -2.4954383342
H   -5.1909630893   -0.2199519379   -2.0955590298
H   -7.4512721371   -0.5859002364   -2.4464152429
H   -9.9374746486   -0.7226067928   -1.9445180712
H   -9.3011194059    1.495170134    -0.3721889562
H   -4.5515375336    0.2536296521    0.3794256299
H   -3.3355773952   -0.9577385032   -0.0360586616
H   -7.8373160947    0.1762199498    2.4251255445
H   -6.1076753586   -0.05282886      2.1732505366
H   -8.0329891451   -2.5093509179   -3.4357852133
H   -5.0561277076   -1.8263200272    1.8847027482
H   -5.8582478911    2.1600831519    2.1037883087
H   -7.9346595173    4.6972867497    2.3619141424
H   -6.2351459041    4.346666973     1.9716204723
H   -7.4027588352    4.732060087     0.6854584454

calc_2a conf_5

C   -8.9300797112   -1.5715042537   -0.4871691338
C   -8.6739907838   -0.1151911245   -0.0383440022
C   -7.1776485978   -0.0644980167    0.3513114492
N   -6.6569832509   -1.4439059621    0.1733445309
C   -7.5336003128   -2.0804222513   -0.8137673977
C   -5.3286321765   -1.5792842307   -0.4660159001
C   -5.5372943149   -1.2976675693   -1.9634408785
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S117

```
C   -7.0090982103   -1.6665578035   -2.2137666807
O   -9.8270696538   -1.6674319852   -1.5652810269
O   -8.9705275168    0.7143923444   -1.1379727939
C   -4.2472691016   -0.7961599908    0.2451300786
C   -6.9525520197    0.3614566303    1.803121061
O   -7.1134163965   -2.7165782947   -3.1532136033
O   -4.1366099569   -1.197215644     1.5988563179
N   -7.5267120999    1.6460234644    2.1993947702
O   -7.7436868079    2.7555429834    0.2107713495
C   -7.8148177356    2.7255416035    1.439536553
C   -8.2577297584    3.9551877432    2.2031530837
H   -7.4522666679   -3.1712863152   -0.7416536719
H   -9.3416383778   -2.143564581     0.3510169517
H   -9.3102484066    0.1540859489    0.816058339
H   -6.6881013138    0.6474718765   -0.3200851968
H   -5.0729403791   -2.641629279    -0.354388496
H   -4.8822275754   -1.903132037    -2.5940929245
H   -5.3503112139   -0.2453724327   -2.2013409283
H   -7.5580756195   -0.788377778    -2.5713816165
H   -9.8718258919   -0.7703389614   -1.9384214225
H   -8.6456870544    1.6042638175   -0.8973316514
H   -4.4469078419    0.2844641598    0.1779258982
H   -3.2834104238   -0.9747818236   -0.2429851298
H   -7.4085012654   -0.4038969429    2.4412783955
H   -5.8797480592    0.3639762802    2.023088746
H   -8.0615035683   -2.8766634515   -3.2615436131
H   -4.9737332393   -1.6345312965    1.8129158208
H   -7.5970900635    1.7799103942    3.1958055205
H   -8.3459217571    3.8093554381    3.2821396821
H   -7.539926758     4.7567274225    2.011637716
H   -9.2212161176    4.2825919182    1.8067098039

calc_2a conf_6

C   -9.0095328405   -1.4432301304   -0.7004649528
C   -8.673132616    -0.0483529952   -0.1157772281
C   -7.2261610508   -0.1572840526    0.420255519
N   -6.8521066941   -1.584231128     0.2816751552
C   -7.6449532926   -2.1008144748   -0.8312585337
C   -5.4786300756   -1.9135518734   -0.1372116177
C   -5.4175072944   -1.7015856517   -1.6730390926
C   -6.8864401528   -1.7134058547   -2.1187989785
O   -9.7010092557   -1.3734137988   -1.9262196172
O   -8.7852551303    0.881643606    -1.1698271377
C   -4.3445172812   -1.296390912     0.6668551061
C   -7.0811441672    0.2418466306    1.8884430988
O   -7.1059238005   -2.6204205754   -3.1755778293
O   -4.2080115311    0.1073005784    0.5695971524
N   -7.6493980533    1.5348489925    2.2687260534
O   -7.465515926     2.7380643273    0.3350346434
C   -7.7315456594    2.6655368441    1.5354851444
C   -8.1996202145    3.8949483634    2.2846639998
H   -7.693163416    -3.1962376548   -0.789046709
H   -9.6279802139   -2.000106141     0.0107274761
H   -9.3704687923    0.2164901862    0.6907159436
H   -6.5937788913    0.4963623295   -0.1861251518
H   -5.3881864625   -2.9940202323    0.0415183757
H   -4.8667755316   -2.5035926765   -2.1712659341
H   -4.9368641314   -0.7560275292   -1.9477401135
```

S118

```
H   -7.1892075425   -0.7030203334   -2.421862133
H   -9.615972422    -0.4452809387   -2.2079282387
H   -8.359643044     1.7047795109   -0.8556518354
H   -3.41104352     -1.7995366429    0.3736789647
H   -4.5018107115   -1.5054344595    1.728602995
H   -7.5865255105   -0.5185289126    2.4912681695
H   -6.0185850062    0.2315973138    2.1471565454
H   -8.057408089    -2.5708956953   -3.3515680953
H   -3.9956659066    0.3258219914   -0.3462041387
H   -7.8618762567    1.6294023411    3.2491489651
H   -7.4016193671    4.6411392138    2.2542370913
H   -9.0584938776    4.3180022044    1.7592537615
H   -8.4725262714    3.7115782297    3.3265231766
```

calc_**2a** conf_7

```
C   -9.0389938442   -1.6023677418   -0.8076975225
C   -8.8942408553   -0.2090541948   -0.1407805263
C   -7.4474239363   -0.1543536582    0.4160876571
N   -6.9541883753   -1.5411743247    0.3340042064
C   -7.6114109251   -2.1245969079   -0.8369306913
C   -5.5232204355   -1.7191408635    0.0130287319
C   -5.3751128977   -1.544623204    -1.5215845274
C   -6.8078132995   -1.6418048372   -2.0589735897
O   -9.6131403314   -1.5400039417   -2.0935568456
O   -9.136598499     0.7707022014   -1.1206905458
C   -4.5594158732   -0.8718796651    0.8309389781
C   -7.3616339902    0.3890520824    1.8561877173
O   -6.9063655556   -2.5179566976   -3.1575959642
O   -3.2188040065   -1.0917136522    0.4489361488
N   -6.9684763881    1.7863602403    1.9420921292
O   -8.7936434346    2.6092058969    0.8871762776
C   -7.7225386166    2.798347977     1.4629135405
C   -7.1869212311    4.1945548745    1.6768639783
H   -7.5511386934   -3.2192334952   -0.8017571209
H   -9.6644827991   -2.2432769844   -0.1771756353
H   -9.6166865006   -0.099172862     0.6758944969
H   -6.8867458003    0.5298374574   -0.2402007895
H   -5.3070862761   -2.7698418685    0.2578783463
H   -4.761775064    -2.3348856983   -1.9607234217
H   -4.901913594    -0.591781505    -1.7747740487
H   -7.1652510412   -0.6436326685   -2.3469097446
H   -9.7234933256   -0.5895886303   -2.2752591001
H   -9.1754991108    1.6159480587   -0.6346608919
H   -4.7015100083   -1.067659458     1.905251661
H   -4.7377023009    0.1940423147    0.6563013218
H   -8.3240661801    0.2583831423    2.3622659597
H   -6.6274288897   -0.1855834464    2.4201943523
H   -7.8459011741   -2.5062469442   -3.3956387727
H   -3.0275894166   -2.0298704948    0.5762754389
H   -6.1022404218    2.0111796559    2.403294825
H   -7.0742908063    4.6805170448    0.7049006124
H   -7.9253314551    4.7679582891    2.2421674516
H   -6.230924647     4.2273545085    2.2042559071
```

calc_**2a** conf_8

```
C   -8.9364183686   -1.26106666     -0.4254765719
C   -8.6525066805    0.1729288926   -0.9448394261
```

S119

```
C   -7.1530473372    0.422355723     -0.6577830258
N   -6.6578177862   -0.8171470137     0.0023263031
C   -7.5559030094   -1.8869243853    -0.4057809288
C   -5.3294695534   -1.3413646531    -0.385628424
C   -5.5362204186   -2.1052262047    -1.7188436474
C   -7.0579954844   -2.3338783732    -1.7920970608
O   -9.8538813631   -1.929264798     -1.2694009831
O   -8.8811410154    0.2409018826    -2.3334589614
C   -4.2227315708   -0.3044613204    -0.3917100308
C   -6.9026374054    1.6417847388     0.2285288693
O   -7.5056951623   -3.6691852604    -1.9867201761
O   -3.9432792971    0.2021219564     0.892390602
N   -7.3185278598    1.3550708403     1.5805426673
O   -7.8655545201    3.4896729061     2.1027007189
C   -7.7777268657    2.3167609915     2.427947558
C   -8.1697344279    1.8321154861     3.808526406
H   -7.4774944469   -2.7442725106     0.2745713773
H   -9.3484225465   -1.2125304758     0.5885072742
H   -9.2751332271    0.9114495297    -0.4228241247
H   -6.6779544735    0.5988668139    -1.6318435121
H   -5.0687140196   -2.0687145656     0.3925625597
H   -5.0008157635   -3.0587885334    -1.7149125748
H   -5.1806672436   -1.5245294507    -2.5765891966
H   -7.4943622415   -1.6825304467    -2.5570165629
H   -9.4287819098   -2.7440146793    -1.5839713153
H   -9.5931186638   -0.4052169131    -2.490986761
H   -4.4582452828    0.5007398451    -1.1054226399
H   -3.3004851018   -0.7772764717    -0.7412351677
H   -5.8445693652    1.934135941      0.1960764706
H   -7.4710774302    2.5017868793    -0.1341130173
H   -7.3232752571   -3.9226569043    -2.9005428009
H   -4.7831389988    0.4577698406     1.2960912926
H   -7.2500855029    0.3870192795     1.8629505229
H   -7.5198460153    2.3094569884     4.5463300068
H   -9.1909977887    2.1581583803     4.017298225
H   -8.1075265957    0.7479527046     3.9318460558
```

calc_**2a** conf_9

```
C   -8.8454894554   -1.0225025795    -0.6812051774
C   -8.1965345749    0.3667505145    -0.7140601033
C   -6.8847190564    0.1608237863     0.0476235806
N   -6.6357390955   -1.3060476932     0.0832401656
C   -7.6546792368   -1.9681762172    -0.7436646569
C   -5.366630498    -1.7842403623    -0.4987219472
C   -5.5882315165   -1.7153960831    -2.0094626736
C   -7.0224610659   -2.231060491     -2.1524061993
O   -9.7266724768   -1.2326836684    -1.7743378432
O   -7.9065233543    0.7181778029    -2.0531376653
C   -4.1575636208   -1.1071899055     0.1105712139
C   -6.9248275019    0.6939553038     1.4858987086
O   -6.9686201574   -3.6204360168    -2.4348523609
O   -4.1485642671   -1.2787771066     1.5154298082
N   -7.0890176199    2.1285070101     1.571610348
O   -9.3223232957    2.0798071948     1.9635498479
C   -8.2867851972    2.7183122075     1.8319002271
C   -8.2618344267    4.2273774816     1.948292518
H   -7.8983605629   -2.9487633129    -0.3190189053
H   -9.3692085845   -1.1626703071     0.2715651169
```

```
H  -8.8303093912    1.1260066715   -0.2420608348
H  -6.1045468404    0.6956374922   -0.5068459287
H  -5.3021550291   -2.846022103    -0.2225784719
H  -4.8961486      -2.3294247088   -2.5900270955
H  -5.5307014077   -0.6811651378   -2.3615491314
H  -7.5621272869   -1.7069366322   -2.944710004
H  -10.6009358269  -0.9139739719   -1.5173167744
H  -8.6420731299    0.3559786125   -2.5736693589
H  -4.1306846197   -0.0378490568   -0.1476801267
H  -3.2448211923   -1.5560823876   -0.2954072483
H  -7.7564924754    0.239506378     2.0287209806
H  -5.9950789069    0.4158868963    1.9894584212
H  -7.8771754777   -3.9204344172   -2.565305973
H  -5.0627054452   -1.4887911661    1.7584451155
H  -6.2755303388    2.7117756019    1.4620812649
H  -7.2729477585    4.6689374235    1.8025074546
H  -8.9502894109    4.6474948063    1.2114005334
H  -8.6334912979    4.5076881411    2.9367231747
```

calc_**2a** conf_10

```
C  -8.935405349    -1.8835560535   -0.5962126635
C  -8.9174379342   -0.4183917732   -0.0759531598
C  -7.4534308321   -0.1632771089    0.3538310248
N  -6.7428594136   -1.4546895612    0.1620895354
C  -7.473725145    -2.1457953559   -0.8896744947
C  -5.3750024034   -1.3960207215   -0.4008988715
C  -5.5360307902   -1.1051994119   -1.9117442048
C  -6.9921167712   -1.5125624163   -2.2115635328
O  -9.7777748287   -2.0028456593   -1.7279981575
O  -9.2968293118    0.4701879282   -1.0984778311
C  -4.4453890738   -0.4965817279    0.3864567078
C  -7.331546948     0.3246561327    1.7996506782
O  -7.2039590553   -2.4762479893   -3.2363796689
O  -4.2721702483   -0.9909751999    1.7025553417
N  -7.9142042663    1.6360654402    1.9848536369
O  -6.1401209888    2.7174836749    1.0847016148
C  -7.2685953908    2.7551384148    1.553288011
C  -8.0420072375    4.0489277504    1.68357371
H  -7.2192779637   -3.2126137318   -0.9104420637
H  -9.2948153927   -2.555659304     0.1895863638
H  -9.5992524181   -0.3085316748    0.7812668318
H  -7.0627955444    0.6286556172   -0.2977072109
H  -4.983211551    -2.4157224323   -0.2932275618
H  -4.8341949814   -1.6963685074   -2.5068135734
H  -5.3651959407   -0.0486139857   -2.1410378473
H  -7.5885257851   -0.6178259499   -2.422488127
H  -9.2393495453   -2.3399032359   -2.4630890924
H  -9.8632630059   -0.0676720274   -1.6823422651
H  -4.8146279517    0.5386315313    0.3980771169
H  -3.4585583273   -0.4899190079   -0.0871553875
H  -7.8287114115   -0.3800474333    2.4735386308
H  -6.2817184758    0.3841237025    2.0933288016
H  -7.0189446405   -2.059907024    -4.0879059445
H  -5.1082724443   -1.4139439343    1.9435495825
H  -8.8858888505    1.7057059949    2.2393512776
H  -8.8960318672    3.9812626423    2.3621633222
H  -7.3628173694    4.8273246166    2.0343567984
H  -8.4039405456    4.3457077813    0.6948926721
```

calc_**2a** conf_11

```
C  -8.9948258629  -1.4598172151  -0.6345882926
C  -8.6594651123  -0.0609527874  -0.0545972288
C  -7.1906437564  -0.1449517496   0.4218244718
N  -6.8151413159  -1.5738698287   0.3050392211
C  -7.6294910094  -2.1113219826  -0.782823291
C  -5.449457274   -1.9158845765  -0.1381890914
C  -5.4196307832  -1.7623222206  -1.680944202
C  -6.8979295764  -1.7408586213  -2.0888709941
O  -9.7014045193  -1.3936553951  -1.8525964454
O  -8.8351284245   0.8763300236  -1.0935209421
C  -4.3020386551  -1.2537522058   0.597203364
C  -6.9876928875   0.2921435296   1.8747449189
O  -7.1731132809  -2.6410760383  -3.1388414947
O  -4.2326510688   0.1250279447   0.2845873143
N  -7.6197319117   1.5488980512   2.2722402705
O  -7.4670048356   2.7648315383   0.3485405191
C  -7.7567082703   2.6762372309   1.5415865205
C  -8.3255237965   3.8689822861   2.2804135753
H  -7.6709356699  -3.2064914162  -0.722905233
H  -9.6041642463  -2.0183460185   0.0831536493
H  -9.3286724773   0.1820586124   0.7820745845
H  -6.5862192828   0.4949374035  -0.2265091655
H  -5.3480122497  -2.9845422776   0.0953153844
H  -4.9161298832  -2.6072682345  -2.1585719391
H  -4.9040857427  -0.8459925467  -1.9754734677
H  -7.1852050425  -0.7225434058  -2.3827663297
H  -9.6221185015  -0.4651140847  -2.1355218684
H  -8.376713764    1.6936806169  -0.8138962398
H  -3.3786628942  -1.7676533549   0.293694371
H  -4.4284283953  -1.4117112221   1.678966037
H  -7.4056510197  -0.4884988833   2.5164480848
H  -5.9124172897   0.3531650939   2.0688733864
H  -8.1294583962  -2.5695421017  -3.2785387666
H  -3.4063162999   0.4739558797   0.6384051072
H  -7.8707297424   1.6147894534   3.245586888
H  -8.5412361029   3.6850377799   3.3355431959
H  -7.614488889    4.6946745362   2.2015137895
H  -9.2437717701   4.1844161866   1.7794003382
```

calc_**2a** conf_12

```
C  -9.0203484916  -1.397402325   -0.6914499079
C  -8.7203904857   0.0257810319  -0.1583571334
C  -7.2930823426  -0.0460427783   0.4347909491
N  -6.8818155028  -1.4620047793   0.3388436602
C  -7.6433829246  -2.0397396336  -0.7659321428
C  -5.4866095196  -1.7589837937  -0.0352867532
C  -5.4057486735  -1.660418195   -1.5831247925
C  -6.8660189064  -1.6970527614  -2.0525993734
O  -9.6883042122  -1.3895210887  -1.9319100447
O  -8.8021013615   0.9100159025  -1.2530184604
C  -4.4193939672  -0.9563839267   0.6941484823
C  -7.2309374983   0.3746798029   1.9058854949
O  -7.0633941485  -2.6418560237  -3.0795284622
O  -3.1243478877  -1.4154787102   0.3703627356
N  -7.8264975247   1.6658732704   2.2410706079
```

```
O  -7.5736945389   2.8248020017   0.2908282602
C  -7.9047840868   2.7766452619   1.4757307187
C  -8.4517392746   4.007013128    2.166227601
H  -7.6773391575  -3.1324695658  -0.6751564372
H  -9.6461128139  -1.9332436266   0.0294056551
H  -9.4491261407   0.3160143152   0.6107127214
H  -6.6595508659   0.6178076179  -0.1633172189
H  -5.3222486616  -2.8063550212   0.2442575414
H  -4.8593214456  -2.5017331143  -2.0170902302
H  -4.9135413088  -0.7359885971  -1.9096582873
H  -7.1670481154  -0.6989970462  -2.3965700556
H  -9.6022430371  -0.4772519928  -2.2597219923
H  -8.4189245526   1.7568389665  -0.9509004167
H  -4.5198790662  -1.0919870486   1.774393432
H  -4.5211661062   0.1189939586   0.4776999192
H  -7.762912814   -0.3866495927   2.483787431
H  -6.1890334724   0.363350951    2.244408055
H  -8.012191966   -2.6070969912  -3.2725798532
H  -2.98872818    -1.2600744224  -0.5730028141
H  -8.1036815457   1.7689714048   3.2043956995
H  -9.3113198095   4.3718124307   1.5996406004
H  -8.7507122306   3.8458867472   3.2044778424
H  -7.6883273631   4.7882442431   2.1341369685
```

calc_**2a** conf_13

```
C  -8.9625560157  -1.4332445971  -0.5170484612
C  -8.6088695982   0.0209431887  -0.1826249012
C  -7.1757002644  -0.0337390022   0.3687392521
N  -6.6833355432  -1.4192899515   0.1452522751
C  -7.5983775412  -2.0694533255  -0.8102378416
C  -5.3730690807  -1.5160149385  -0.5302529044
C  -5.6638836579  -1.1619668193  -1.9891083702
C  -7.0107828288  -1.8687426552  -2.2424761868
O  -9.9193896317  -1.5450426523  -1.5279177056
O  -8.6721586191   0.7440880987  -1.3932644243
C  -4.2797709196  -0.7755231407   0.2101861108
C  -7.0788282599   0.2901260842   1.8586585435
O  -6.8804555722  -3.0896659419  -2.9431139087
O  -4.1595820188  -1.2645911123   1.5334505516
N  -7.586975831    1.6021652385   2.2532527849
O  -7.6938135527   2.7625973041   0.2794629276
C  -7.8012585162   2.7103218085   1.5022091192
C  -8.2213714383   3.9274824088   2.3046907443
H  -7.6303240888  -3.1493855105  -0.6187815334
H  -9.3714062779  -1.9132078136   0.3790997325
H  -9.3101079611   0.4451375313   0.5472828561
H  -6.5859863812   0.696260232   -0.1891514566
H  -5.1009139019  -2.5822583975  -0.482163043
H  -4.9023993763  -1.5046437462  -2.6942081624
H  -5.7713574155  -0.0784651623  -2.1071987512
H  -7.6691684995  -1.2630610891  -2.8638948027
H  -9.8214925954  -0.7428855661  -2.0658105508
H  -8.4181523906   1.6534452895  -1.1551125123
H  -4.4733639223   0.3074345617   0.2120713811
H  -3.3216198015  -0.9295163171  -0.296522703
H  -7.6498877165  -0.4657404318   2.4102613389
H  -6.0330725816   0.1996164575   2.1742681004
H  -6.3554195745  -3.6897578963  -2.3968879514
```

```
H  -5.0176524285  -1.6646383081   1.7402780982
H  -7.6855488724   1.7280819198   3.2492573023
H  -7.4734615812   4.1829444483   3.0615865437
H  -8.3393787393   4.7674501119   1.6221848558
H  -9.1721070044   3.7487396918   2.8165836529
```

calc_**2a** conf_14

```
C  -9.0500828562  -1.7721434218  -0.778782263
C  -8.9940485441  -0.2867717058  -0.3231123136
C  -7.615705539   -0.1289222415   0.3589372061
N  -6.9818237255  -1.4656901654   0.3169227663
C  -7.5879552344  -2.169278864   -0.800724759
C  -5.5405977111  -1.5375494566   0.0096202449
C  -5.4056985351  -1.4513529908  -1.5372143115
C  -6.836271186   -1.6768622524  -2.0486376874
O  -9.6903072019  -1.8853527134  -2.0367411478
O  -9.1010114142   0.5693093379  -1.4343895497
C  -4.674037877   -0.555264807    0.7740140657
C  -7.715752924    0.3611380212   1.8052646351
O  -7.0244965807  -2.6533301731  -3.0688199793
O  -3.3395639753  -0.8056950029   0.3712627302
N  -8.1804940861   1.7284738123   1.9001998153
O  -6.132742417    2.6211693916   1.5217546796
C  -7.3350458258   2.7739812124   1.6882796359
C  -7.9812681598   4.1420509256   1.6665135122
H  -7.4336692279  -3.2524507279  -0.7143312964
H  -9.5994481838  -2.3684516742  -0.0431540531
H  -9.8078288098  -0.0731825126   0.3873465119
H  -7.062958906    0.6237817725  -0.2189095562
H  -5.2199774168  -2.5400512251   0.3175024845
H  -4.730057167   -2.2224416078  -1.9155573301
H  -5.0082279909  -0.4819340021  -1.8508046067
H  -7.2697565264  -0.7235547618  -2.3735262065
H  -9.0568321379  -2.2922238827  -2.6529043174
H  -9.5934175089   0.0414227391  -2.0907125937
H  -4.7989537708  -0.7259981385   1.8536061368
H  -4.9668536328   0.4819116692   0.5661434798
H  -8.3910224477  -0.2871350223   2.3713829922
H  -6.7370433022   0.3146918339   2.2836649615
H  -6.6361359211  -2.3170185223  -3.8864914433
H  -2.7893067429  -0.1055485199   0.7410273771
H  -9.1723171623   1.9039483234   1.9035436596
H  -7.3220780211   4.8482758176   2.1730623341
H  -8.0837265154   4.4697093378   0.6276927143
H  -8.9674848152   4.1653401975   2.1370714714
```

calc_**2a** conf_15

```
C  -8.9439919306  -1.7557997992  -0.6930427533
C  -8.7617613403  -0.2347670347  -0.4357239497
C  -7.2828920487  -0.0643893324  -0.0092013905
N  -6.7375797543  -1.4381585112   0.1030873827
C  -7.5162657413  -2.2414139911  -0.8310269067
C  -5.3554317745  -1.6692159803  -0.3743842947
C  -5.4224173534  -1.7118514651  -1.9220919397
C  -6.9136416644  -1.9551322306  -2.219671275
O  -9.7390903682  -1.9713249086  -1.8440590364
O  -9.0103031564   0.5091060856  -1.606392951
```

S124

```
C   -4.3352799929   -0.7252894138    0.2266074237
C   -7.1566865725    0.7150667225    1.2931945186
O   -7.2415971551   -3.057923741    -3.0545648106
O   -4.2251724156   -0.891995437     1.6210290413
N   -7.6988863658    2.0441837509    1.1048762613
O   -7.2467796437    2.6844854318    3.2209664885
C   -7.7104519428    2.9459516789    2.1224046855
C   -8.328270925     4.2914454775    1.8032921869
H   -7.3967605087   -3.3110235605   -0.6205392219
H   -9.4278672607   -2.2226972997    0.1703229713
H   -9.4327098597    0.1012824097    0.3664281336
H   -6.7930441989    0.5095720312   -0.8115713584
H   -5.0969483213   -2.673135469    -0.0162278859
H   -4.8089637656   -2.5241312616   -2.3217572839
H   -5.073403271    -0.7759910474   -2.3710013562
H   -7.3651933069   -1.0422580376   -2.6258261246
H   -9.2257274858   -2.5173319922   -2.4627585167
H   -9.6229646482   -0.0482118441   -2.1214919854
H   -4.5772208603    0.3162330987   -0.0393747524
H   -3.3502097484   -0.9415870837   -0.1980477336
H   -7.7018393278    0.1911798011    2.0882695364
H   -6.1158683362    0.7937321419    1.6215000941
H   -6.9746440314   -2.8479114986   -3.9586761856
H   -5.1158973042   -1.0638905291    1.9565979261
H   -8.128372854     2.2717207757    0.220901075
H   -9.1534484252    4.472205462     2.4961883553
H   -7.5816823283    5.0697685396    1.9780147643
H   -8.6987340118    4.3784980618    0.7787508677

calc_**2a** conf_16

C   -8.9644114101   -0.8944784265   -0.5175079932
C   -8.4785861238    0.4518892069   -1.102766798
C   -6.989726908     0.5528160301   -0.6898763165
N   -6.6854364586   -0.6904253691    0.0591913402
C   -7.673170133    -1.6735502849   -0.3615609194
C   -5.4137563664   -1.3814662069   -0.2272969828
C   -5.605747431    -2.1136319363   -1.5715453366
C   -7.138726933    -2.2734369106   -1.6816517977
O   -9.8970692387   -1.5108873509   -1.3910464386
O   -8.5617788787    0.4279779631   -2.5155100257
C   -4.2253284259   -0.4587008373   -0.0665762011
C   -6.6128644956    1.8483564289    0.0692035321
O   -7.6378779081   -3.6019794994   -1.7664987465
O   -4.2486709653    0.1205124982    1.2234025921
N   -6.6774293066    1.8081059854    1.515777935
O   -8.9232069479    1.5657299588    1.6739891631
C   -7.8348549794    1.6943374649    2.215885684
C   -7.6941030325    1.7209102736    3.7232932878
H   -7.7436096984   -2.4885000802    0.3701034693
H   -9.4274548772   -0.7174652333    0.4562358619
H   -9.0566214244    1.2863379399   -0.6976938108
H   -6.4418435833    0.5977800724   -1.6426492982
H   -5.324258613    -2.1428680843    0.5594157856
H   -5.1071559106   -3.086982303    -1.5766842924
H   -5.211715778    -1.5289672109   -2.4094578738
H   -7.5092018862   -1.6828204968   -2.525576085
H   -9.5855771871   -2.4109655928   -1.5707122589
H   -9.3312048758   -0.1410095737   -2.6961069596
```

S125

```
H   -4.2327438346    0.317682585    -0.8477269849
H   -3.2919387159   -1.0202698418   -0.1783869058
H   -5.5825283775    2.1179952534   -0.1694179054
H   -7.2550907412    2.6522990146   -0.307495519
H   -7.4412001403   -3.9424191513   -2.6483542471
H   -5.1781030857    0.063381844     1.5033117404
H   -5.8226797862    1.9924524657    2.0157844022
H   -8.3749755708    2.4741129178    4.1252330505
H   -8.0091383762    0.7525637585    4.120374429
H   -6.680211595     1.9305827287    4.072897424

calc_2a conf_17

C   -8.9726266831   -1.8163430188   -0.9490636829
C   -8.9944051157   -0.6252996374    0.0434147369
C   -7.5166287435   -0.2231247779    0.2231923242
N   -6.8528837172   -1.5307890883    0.1228619407
C   -7.4943161891   -2.186007421    -1.0284252624
C   -5.4224647425   -1.591738583    -0.2552694576
C   -5.3543385557   -1.3115373594   -1.7671669057
C   -6.7522978701   -1.6667087678   -2.2918380411
O   -9.4481397595   -1.4279843007   -2.2337660605
O   -9.8548407853    0.4113355954   -0.3614313106
C   -4.5148546731   -0.752976027     0.6177653921
C   -7.3152904339    0.5132807782    1.5513646701
O   -6.6824208584   -2.6399477589   -3.3117066083
O   -4.6085050317   -1.1379820891    1.974677388
N   -7.9231650771    1.8238702343    1.5121466566
O   -5.9542243339    2.906273804     1.1631875426
C   -7.1726004501    2.9327273499    1.2471931451
C   -7.9530877849    4.2219342171    1.1007723236
H   -7.3251791997   -3.2675345188   -0.9840506097
H   -9.5754164529   -2.6499536922   -0.5747369806
H   -9.372306003    -0.9709918368    1.0104976137
H   -7.2304196379    0.4688353388   -0.5891138091
H   -5.1418253845   -2.639983683    -0.0878205511
H   -4.6019901718   -1.9288789079   -2.2634160427
H   -5.1103498688   -0.2639144264   -1.9687947788
H   -7.2475284272   -0.7697967444   -2.6776120013
H   -10.4132824626  -1.4409254993   -2.1956392339
H   -9.666486846     0.5528618541   -1.3021119558
H   -4.7326100182    0.3178610783    0.4897975354
H   -3.4773605773   -0.9089297598    0.3049214533
H   -7.7613023058   -0.0762628207    2.3617362634
H   -6.2644821105    0.6663865879    1.790618758
H   -7.5743166207   -2.712660734    -3.6768139071
H   -5.5071790088   -1.4730046349    2.1012685627
H   -8.9155624799    1.867052201     1.3328149343
H   -7.689737738     4.6879107798    0.1485564331
H   -9.0367206624    4.0912522644    1.1514937522
H   -7.6438532194    4.9076940044    1.8934957729
```

Table S36. Sampled and DFT geometry optimized conformers related to calc_**2b**, with energy values (Hartree) and related % contribution on the final Boltzmann distribution for the three employed functional/basis set combinations.

Conformer	MPW1PW91/6-31g(d,p)		MPW1PW91/6-311+g(d,p)		B97-2/cc-pVTZ	
	Energy (Hartree)	% contribution on the Boltzmann distribution	Energy (Hartree)	% contribution on the Boltzmann distribution	Energy (Hartree)	% contribution on the Boltzmann distribution
calc_**2b** conf_1	-916.6558506	66.58%	-916.8926282	19.95%	-916.8414899	26.77%
calc_**2b** conf_2	-916.6545098	16.09%	-916.8935168	51.14%	-916.8420943	50.77%
calc_**2b** conf_3	-916.6542962	12.83%	-916.8927758	23.33%	-916.8404895	9.28%
calc_**2b** conf_4	-916.6527150	2.40%	-916.8886848	0.31%	-916.8374863	0.39%
calc_**2b** conf_5	-916.6516843	0.81%	-916.8908171	2.93%	-916.8403837	8.29%
calc_**2b** conf_6	-916.6513944	0.59%	-916.8889588	0.41%	-916.8384095	1.02%
calc_**2b** conf_7	-916.6511811	0.47%	-916.8900930	1.36%	-916.8388397	1.62%
calc_**2b** conf_8	-916.6498398	0.11%	-916.8873110	0.07%	-916.8364653	0.13%
calc_**2b** conf_9	-916.6493910	0.07%	-916.8890092	0.43%	-916.8387838	1.52%
calc_**2b** conf_10	-916.6473366	0.01%	-916.8841813	0.00%	-916.8329573	0.00%
calc_**2b** conf_11	-916.6471566	0.01%	-916.8857487	0.01%	-916.8352583	0.04%
calc_**2b** conf_12	-916.6467867	0.00%	-916.8849720	0.01%	-916.8341934	0.01%
calc_**2b** conf_13	-916.6467284	0.00%	-916.8856732	0.01%	-916.8350680	0.03%
calc_**2b** conf_14	-916.6466014	0.00%	-916.8852076	0.01%	-916.8354701	0.05%
calc_**2b** conf_15	-916.6464851	0.00%	-916.8840561	0.00%	-916.8326546	0.00%
calc_**2b** conf_16	-916.6452414	0.00%	-916.8835624	0.00%	-916.8341376	0.01%
calc_**2b** conf_17	-916.6447394	0.00%	-916.8859038	0.02%	-916.8357834	0.06%
calc_**2b** conf_18	-916.6435924	0.00%	-916.8831703	0.00%	-916.8330099	0.00%
calc_**2b** conf_19	-916.6435609	0.00%	-916.8827571	0.00%	-916.8328211	0.00%
calc_**2b** conf_20	-916.6433206	0.00%	-916.8835240	0.00%	-916.8331326	0.00%
calc_**2b** conf_21	-916.6422478	0.00%	-916.8820942	0.00%	-916.8320366	0.00%
calc_**2b** conf_22	-916.6416031	0.00%	-916.8819705	0.00%	-916.8322649	0.00%
calc_**2b** conf_23	-916.6408353	0.00%	-916.8800713	0.00%	-916.8287722	0.00%
calc_**2b** conf_24	-916.6380444	0.00%	-916.8766959	0.00%	-916.8264854	0.00%

Table S37. Cartesian coordinates of the optimized geometries for the conformers related to calc_**2b**. The related energies and % contribution on the final Boltzmann distribution for the three employed functional/basis set combinations are reported in Table S36.

calc_**2b** conf_1

```
C  -6.8075237742   -1.5203746315   -1.692037999
C  -7.6191987634   -0.8858882976   -0.56727615
C  -6.581974372     0.041774871     0.0961781365
N  -5.3349084474   -0.7256721602    0.0236376069
C  -5.4807780387   -1.8000679438   -1.0030273798
C  -4.1092991292    0.0494561195   -0.2594844501
C  -3.7151822452   -0.3329055522   -1.6930986438
C  -4.2079038224   -1.7710618226   -1.8714369634
O  -6.6384471252   -0.5796564967   -2.7320250464
O  -8.7316069063   -0.2367976838   -1.1147382967
C  -3.0651863108   -0.2913727507    0.8141387799
C  -6.8821010552    0.4415244932    1.5489181032
O  -3.2676912123   -2.7451004369   -1.4868629739
O  -3.0785261749   -1.6763639748    1.1070625828
N  -7.7383715298    1.605977508     1.7052144703
O  -9.696073753     0.5434742718    1.3106124739
C  -9.0837396968    1.5696303716    1.6087683202
C  -9.8140736157    2.8602565732    1.8939882499
H  -5.5414059147   -2.7827504959   -0.5198032007
H  -7.2767530975   -2.4381996317   -2.071556434
H  -7.9215550748   -1.6638677909    0.1493488504
H  -6.5249195476    0.954958447    -0.5159432868
H  -4.327664788     1.1224634593   -0.1914404961
H  -4.2561900489    0.3104940419   -2.3912121449
H  -2.6433047942   -0.2491173684   -1.8925677217
H  -4.4499726636   -1.979608061    -2.9151001208
H  -7.5005878126   -0.1424016302   -2.8202077091
H  -9.2985768899    0.0248475707   -0.3628970019
H  -3.274406827     0.2814682738    1.7299809383
H  -2.0543407358   -0.0384884667    0.4846666517
H  -5.9396704443    0.6765371772    2.0496886994
H  -7.3346944788   -0.3994907       2.083247507
H  -3.0017516268   -2.5403559504   -0.5697015708
H  -4.0265381042   -1.8551232846    1.2551706674
H  -7.3011476228    2.4869259121    1.9212562788
H  -10.386136178    3.144511506     1.00753463
H  -10.5313277039   2.6811209106    2.698280526
H  -9.1604696743    3.6882436239    2.1777241174
```

calc_**2b** conf_2

```
C  -6.9389606379   -1.839455981    -1.2721040309
C  -7.6643916      -0.7270460284   -0.5172259632
C  -6.683556628     0.4379975352   -0.6773121372
N  -5.425638052    -0.2159527286   -0.3500246069
C  -5.4970903486   -1.6320150334   -0.797669786
C  -4.1692956724    0.3933204573   -0.8067922099
C  -3.3197217889   -0.8123920443   -1.2113322464
C  -4.3437483078   -1.7784758096   -1.7952163786
O  -7.0424630926   -1.6312697578   -2.6653900863
O  -8.9397584633   -0.4896157829   -1.0357888864
C  -3.5864128341    1.2555389255    0.3404498571
C  -7.0072273806    1.6668622773    0.1631086458
```

S128

```
O   -3.8145843815   -3.0806406646   -1.8830376119
O   -4.0001352933    0.7460678757    1.5869940198
N   -7.1409369391    1.4160551705    1.5807626077
O   -9.3396936944    0.8868101273    1.4423064299
C   -8.3263605318    1.0563129132    2.122472709
C   -8.3516877528    0.8870070285    3.6224976283
H   -5.2922865702   -2.3034225192    0.0462794793
H   -7.3188255583   -2.8343150537   -1.004133733
H   -7.7074021724   -1.0063365411    0.5438478937
H   -6.7102826136    0.7544656105   -1.7335573394
H   -4.3445046021    1.0305279116   -1.6866554493
H   -2.5243146642   -0.5528428712   -1.9136536928
H   -2.8610511811   -1.2715736863   -0.3276041451
H   -4.6754310276   -1.4197033271   -2.7774743209
H   -7.9634430919   -1.3697015885   -2.8216995201
H   -9.3984947843    0.0356801209   -0.3525887745
H   -3.9142596707    2.2994224861    0.2267608238
H   -2.491045148     1.256701104     0.2901123808
H   -7.9556482368    2.0785195256   -0.1923283337
H   -6.2438235161    2.4367969317    0.0229072592
H   -4.4157950009   -3.6003035764   -2.4308024794
H   -4.7144767021    0.1200714281    1.3231505469
H   -6.3059019756    1.4636850552    2.1469886859
H   -8.7217239227   -0.1127852516    3.8603437418
H   -7.3782788871    1.0335442573    4.0954372286
H   -9.0623472755    1.6034615044    4.0419717942

calc_2b conf_3

C   -6.8665426371   -1.9521762691   -1.1442396092
C   -7.5843345575   -0.8237112527   -0.3971881649
C   -6.618325309     0.3449010962   -0.589820495
N   -5.3561149999   -0.3030517478   -0.2375425611
C   -5.3805222042   -1.6281353845   -0.9007687544
C   -4.1078998756    0.3910155101   -0.6200883662
C   -3.3841108758   -0.5513863185   -1.5960449074
C   -4.4970401078   -1.4389446947   -2.1406044317
O   -7.1685717011   -1.8907644382   -2.523153709
O   -8.8671774741   -0.6233873339   -0.9141112405
C   -3.3233369926    0.7095637308    0.669840099
C   -6.9538142489    1.6112603009    0.1868363287
O   -3.9849173428   -2.6343129206   -2.6769891636
O   -4.2221643818    0.9874732152    1.7209595982
N   -7.1666286883    1.4435551192    1.6089596454
O   -9.3510317921    0.8715669626    1.4101073345
C   -8.3779811606    1.1310933113    2.1197715583
C   -8.4870582043    1.1254451948    3.6257482244
H   -4.9113225322   -2.3838270301   -0.2601088141
H   -7.1375858821   -2.9386835919   -0.7472719004
H   -7.6131738573   -1.0745301634    0.6710890874
H   -6.6460189652    0.6258806152   -1.6576241265
H   -4.367118168     1.3331155197   -1.1198444117
H   -2.8442296139   -0.0200361359   -2.3830757029
H   -2.663175592    -1.185173249    -1.0661854339
H   -5.0705087612   -0.8920282475   -2.8981418641
H   -8.105588133    -1.6405996418   -2.5704559856
H   -9.3262091991   -0.0656315584   -0.2553808501
H   -2.673830589     1.5785909819    0.5347350524
H   -2.6842129826   -0.1479967134    0.9314002437
```

```
H  -7.868824643     2.028217815    -0.2438434113
H  -6.1587735641    2.3499567723    0.0588628761
H  -4.715549544    -3.0569181322   -3.1475095872
H  -4.8981510221    0.2925112091    1.5712355586
H  -6.3948180946    1.6639006006    2.2204803741
H  -9.194560119     1.9017643639    3.9282735993
H  -8.9014568555    0.16709694      3.9456617991
H  -7.5353193285    1.294385565     4.1340321117
```

calc_**2b** conf_4

```
C  -6.9454285826   -1.5962470955   -1.4525350484
C  -7.7020871632   -0.7980389477   -0.3813418488
C  -6.6200641575    0.1400963137    0.2041748072
N  -5.3285716924   -0.4882687582   -0.0925036855
C  -5.5741254736   -1.7608995152   -0.8102763205
C  -4.3189477212    0.3088636215   -0.8236196746
C  -3.9600950849   -0.520477894    -2.068498622
C  -4.3616118715   -1.9579662519   -1.730666486
O  -6.8685017511   -0.8190246037   -2.6223579318
O  -8.7786229448   -0.1225465562   -0.9885652265
C  -3.1389401219    0.5508274477    0.1259111798
C  -6.7303546616    0.3496501435    1.7221799525
O  -3.3335194263   -2.689982267    -1.1042733151
O  -2.8038154556   -0.6480171188    0.8007433753
N  -8.0598691316    0.6259489266    2.2533227565
O  -8.7644152419    2.0898632108    0.6726429279
C  -8.9426847702    1.5123714368    1.7465231395
C  -10.195918577    1.7450635385    2.557373268
H  -5.6179029209   -2.5994193733   -0.1038471903
H  -7.4218017453   -2.5659161001   -1.6567875684
H  -8.0718881422   -1.4811345835    0.3984968245
H  -6.6949944711    1.1077337733   -0.2996749859
H  -4.7395258355    1.2789020027   -1.1158503774
H  -4.5566594827   -0.174218228    -2.9131480525
H  -2.9006363568   -0.4624981981   -2.3336860576
H  -4.6409370437   -2.5211674987   -2.6238710466
H  -7.7038282833   -0.3170492435   -2.626432313
H  -8.8558495824    0.7592643796   -0.5743168842
H  -3.3993767072    1.33170601      0.8562444564
H  -2.2508961099    0.8823534895   -0.4178246302
H  -6.0390789954    1.1481360338    2.0190286754
H  -6.3894815494   -0.5697455202    2.2051580208
H  -2.9124504666   -2.0943423959   -0.4553897956
H  -3.6759629191   -0.9542226171    1.1183332084
H  -8.2778452185    0.2181638785    3.1483564247
H  -10.2745831546   2.8129496534    2.7738710408
H  -11.0613091086   1.4731604315    1.9483296784
H  -10.2314180779   1.1871284751    3.4957773246
```

calc_**2b** conf_5

```
C  -6.7825739263   -1.7426225167   -1.5318658426
C  -7.5158053712   -1.191293345    -0.3110484506
C  -6.5906368096   -0.0443975341    0.1520302395
N  -5.2475636134   -0.5418203151   -0.1492806356
C  -5.3276688178   -1.6943381984   -1.0801430769
C  -4.27921142      0.4319192744   -0.6744512773
C  -3.3257839517   -0.4431580865   -1.4795789466
```

S130

```
C    -4.2532106109    -1.4447053792    -2.1531571207
O    -6.9872649152    -0.8669691933    -2.6188018638
O    -8.7988095648    -0.7958968096    -0.6996052958
C    -3.6234129514     1.1778275681     0.4910803878
C    -6.7426129805     0.3361550779     1.642174229
O    -3.5364128721    -2.6025833964    -2.5261551058
O    -3.2967994206     0.2845613804     1.5257439645
N    -7.5414987659     1.5226563676     1.8898064285
O    -9.5477579447     0.5320982123     1.5550079474
C    -8.8896040392     1.5288430501     1.8567625093
C    -9.5682476657     2.8257394199     2.2262186318
H    -5.0761334377    -2.6233734555    -0.5521434546
H    -7.1123810615    -2.7611968487    -1.7816061264
H    -7.5503210091    -1.9640152578     0.4736548489
H    -6.8231148521     0.8404254188    -0.4608168284
H    -4.7737119172     1.1597635656    -1.3392444396
H    -2.7259133284     0.128157053     -2.1918391917
H    -2.6476428247    -0.9776911884    -0.8054790271
H    -4.7259588442    -0.9794634746    -3.0255862063
H    -7.9055619009    -0.5632067874    -2.5187949978
H    -9.2186768437    -0.3631794905     0.0738853534
H    -4.3065412206     1.9654978226     0.8528131629
H    -2.7096352009     1.679164622      0.1541090988
H    -5.7548978502     0.5206979778     2.0674903729
H    -7.1859234297    -0.4957917541     2.1988714925
H    -4.0829468116    -3.1005319826    -3.1458196174
H    -3.9166336559    -0.4585027595     1.3839256382
H    -7.0623065327     2.3751942123     2.1297075326
H    -8.8755963834     3.6323587464     2.476616264
H    -10.2004797485    3.141895855      1.3933448879
H    -10.2247475061    2.6427821491     3.0801745152
```

calc_**2b** conf_6

```
C    -6.5767415182    -1.9398427352    -1.5604375083
C    -7.4736655297    -1.3879157914    -0.4534155569
C    -6.6976758772    -0.1418093715     0.0046955261
N    -5.2992481762    -0.5638022284    -0.0605105899
C    -5.1841656164    -1.7442166485    -0.9615285098
C    -4.3332706093     0.4680875957    -0.4834114389
C    -3.9241130538     0.0670346832    -1.9079995737
C    -4.0147185945    -1.4614409573    -1.9297891709
O    -6.843091169     -1.1148054346    -2.6905152969
O    -8.792784055     -1.1313965855    -0.8641490497
C    -3.1878283287     0.5129107974     0.5347656522
C    -7.0946855214     0.345788497      1.3914580923
O    -2.8292005456    -2.1076328581    -1.5480944255
O    -2.7888366103    -0.7957347211     0.9096676997
N    -8.4765834347     0.7660536843     1.4047166989
O    -8.1301749414     2.5564017466     2.7534644928
C    -8.8879197128     1.8692862227     2.0848185115
C    -10.364101368     2.1884712131     1.9684292742
H    -4.9317185768    -2.6447633112    -0.3874034075
H    -6.7909654626    -2.9889172567    -1.7935756768
H    -7.526293069     -2.1122824889     0.3667445998
H    -6.9081693652     0.6610331051    -0.7212390974
H    -4.8216877247     1.4493432674    -0.4820703516
H    -4.6546714648     0.4793026798    -2.610224331
H    -2.9282569325     0.4115030043    -2.1989370462
```

```
H   -4.2357466686   -1.8313361447   -2.9360917645
H   -6.5095059056   -1.5531851678   -3.4817697437
H   -8.709754399    -0.7715690718   -1.7625737494
H   -3.5094532532    1.0689545063    1.4252697286
H   -2.3065762261    1.0109865596    0.1233542189
H   -6.4932394414    1.2047868174    1.7002184484
H   -6.9096496785   -0.4579448076    2.1182628632
H   -2.5826710767   -1.7510165674   -0.6705958045
H   -3.6195012854   -1.2046611606    1.2109382858
H   -9.1229079276    0.2535115683    0.8206694377
H   -10.8208623736   2.101620098     2.957672875
H   -10.4739722599   3.2277015792    1.6509554747
H   -10.9035922464   1.5404956833    1.2732302132
```

calc_**2b** conf_7

```
C   -6.68367873     -2.0734876136   -1.1824130631
C   -7.3750501844   -1.2714673245   -0.0614807053
C   -6.4668177379   -0.0483406862    0.1470105273
N   -5.135642442    -0.647328554     0.0011858894
C   -5.2279385466   -1.5894504296   -1.1318823041
C   -4.0215706956    0.2842947058   -0.3060003243
C   -3.5954506036    0.0042159177   -1.7614661851
C   -4.7753156372   -0.7610906122   -2.3406029447
O   -7.2564432595   -1.7879805556   -2.4409616886
O   -8.6874064943   -1.0001839245   -0.4564537296
C   -2.8997901437    0.0614070178    0.7067904331
C   -6.6106005332    0.6445106796    1.5107019136
O   -4.4199276916   -1.524860907    -3.4633798466
O   -3.3965309511    0.0877597301    2.0241915342
N   -7.5637455553    1.7395458626    1.5403271881
O   -9.4207109738    0.4566923128    1.7069150576
C   -8.8949103654    1.5706549299    1.675463921
C   -9.7245106872    2.8258391931    1.7996494167
H   -4.5215926268   -2.4174409114   -1.000327317
H   -6.7581237475   -3.1500875988   -0.9861710049
H   -7.349862218    -1.8678641642    0.8619942006
H   -6.6884847366    0.6880226586   -0.6451708958
H   -4.3833315315    1.3137726302   -0.1941539332
H   -3.3614941425    0.9136788433   -2.3193798611
H   -2.7100064045   -0.6424134212   -1.7917723599
H   -5.5774364908   -0.0577863651   -2.5969951457
H   -8.1722212283   -1.5208074422   -2.2506902278
H   -9.1348197166   -0.5643464942    0.2988046787
H   -2.1439790723    0.848014737     0.6256443266
H   -2.4053261667   -0.8990154549    0.491822852
H   -5.6423772956    1.0512391368    1.8124111094
H   -6.905261146    -0.0890860976    2.2683998659
H   -5.2535500301   -1.8807392842   -3.8031518282
H   -4.1128469055   -0.5689766204    2.0054765282
H   -7.2024127898    2.6790404376    1.5122429221
H   -10.4593281525   2.8429357974    0.991369694
H   -10.2786310036   2.783351148     2.7402669367
H   -9.1408733628    3.7487787231    1.7717843696
```

calc_**2b** conf_8

```
C   -6.8140483469   -1.8719041619   -2.0699457526
C   -7.9100716628   -0.8359618986   -1.8090415256
```

S132

```
C   -7.2052863147    0.2248985022   -0.9170043031
N   -6.0723885629   -0.4558073618   -0.310476889
C   -6.054464409    -1.8598509655   -0.7441081235
C   -4.7292551007    0.1262043057   -0.3862348935
C   -3.8592306253   -0.9591600352   -1.0445182002
C   -4.5755193572   -2.2760393636   -0.7326660147
O   -6.0703654552   -1.3505638038   -3.1684942797
O   -8.4912536095   -0.3186694263   -2.9729339626
C   -4.2469031852    0.5255874546    1.0162900559
C   -8.2010270651    0.7619449047    0.114585197
O   -4.1929092519   -2.8348998254    0.4953385675
O   -4.5013659371   -0.4765583482    1.9766760608
N   -7.7039473765    1.8325219591    0.953676968
O   -7.0981281501    0.5103161105    2.6970873652
C   -7.2300951928    1.6282382256    2.2074724286
C   -6.8882018917    2.8746358774    2.9944944493
H   -6.5963110203   -2.5016308517   -0.0356654757
H   -7.2255469427   -2.856815234    -2.3211496642
H   -8.713873944    -1.313685213    -1.2362900262
H   -6.8683798449    1.0494670132   -1.5625752253
H   -4.7412641891    1.0326508973   -1.0083132739
H   -3.8394604889   -0.7931367615   -2.1241901838
H   -2.8302582167   -0.9791146784   -0.6755756772
H   -4.3705221167   -3.0432811168   -1.4877812394
H   -5.5146897478   -2.0529284075   -3.5255050985
H   -7.7655394015   -0.2827019376   -3.6170781872
H   -4.7297163812    1.4648640939    1.3155947947
H   -3.1664208544    0.7026071353    1.0089685743
H   -8.4850709307   -0.0544808274    0.7831778232
H   -9.0989518541    1.1166021031   -0.4040557674
H   -4.2585412518   -2.1200761102    1.1641353564
H   -5.458915462    -0.4249134673    2.1662771209
H   -7.7931540715    2.7800557988    0.6242373149
H   -6.9570224252    3.7992732822    2.4159914381
H   -7.5665019493    2.94191558      3.8491670669
H   -5.8763974124    2.7733965522    3.3924331819

calc_2b conf_9

C   -6.8419608461   -1.7519588169   -1.7003288569
C   -7.6095191294   -1.3222091149   -0.4520827964
C   -6.6316442673   -0.3368318234    0.2197166153
N   -5.3056112009   -0.8546366028   -0.1065303266
C   -5.4289572112   -1.8995874968   -1.1454040614
C   -4.304209041     0.1152422968   -0.5405780482
C   -3.330630328    -0.7402914704   -1.3424060195
C   -4.2584818371   -1.6799067895   -2.1200706403
O   -6.885255592    -0.6986287687   -2.6371271063
O   -8.8296478343   -0.7459604196   -0.826732576
C   -3.649863154     0.8693617895    0.6069396111
C   -6.8655397304   -0.1721942315    1.7377107555
O   -3.6540923545   -2.8619687295   -2.5882045722
O   -4.5157155474    1.8103952136    1.231230852
N   -7.2969903757    1.1520901669    2.1280561492
O   -9.4046531663    0.8791606794    1.3504125619
C   -8.5447307781    1.5914598052    1.8748360647
C   -8.8599893054    3.0071316133    2.2954387775
H   -5.3358707667   -2.8981999758   -0.6901813378
H   -7.2256535971   -2.6850630604   -2.1347484117
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S133

```
H  -7.7616059048  -2.1958666001   0.2032647865
H  -6.7848923629   0.6434813179  -0.2573650617
H  -4.7575423397   0.8638166253  -1.222459716
H  -2.6726696059  -0.1571336895  -1.9910680507
H  -2.7026286471  -1.3274423589  -0.6578932142
H  -4.6305721176  -1.1726815993  -3.0122293622
H  -7.7750919487  -0.3197012655  -2.5286972851
H  -9.1528832125  -0.208171062   -0.0719070609
H  -2.7423975458   1.3745827535   0.245109863
H  -3.3578162969   0.1623316686   1.3869096884
H  -5.9340922327  -0.3834294786   2.2618209759
H  -7.6183547408  -0.8842430775   2.0893422847
H  -3.3186339771  -3.3419334191  -1.8191263365
H  -4.7625040039   2.4531905236   0.553396579
H  -6.5693900479   1.8036635034   2.3803854133
H  -8.0114678991   3.5290654409   2.743583857
H  -9.2124679606   3.5667148645   1.4257875301
H  -9.6799730928   2.9813515882   3.0171984754

calc_2b conf_10

C  -7.0754529885  -1.2147352621  -1.0376276931
C  -7.2430362325   0.3173168345  -0.9212526647
C  -6.253868544    0.68976625     0.1825084699
N  -5.1160207824  -0.2144672175   0.0026704978
C  -5.6595487891  -1.5112611741  -0.4675628199
C  -4.0415562319   0.2324965837  -0.9204567615
C  -4.0068352049  -0.8136261507  -2.044081202
C  -4.6061260824  -2.0811438697  -1.4330394941
O  -7.2046681717  -1.6241359295  -2.3964799566
O  -6.8323119124   0.9353324891  -2.1215214442
C  -2.748743967    0.329834308   -0.0969916079
C  -6.815391256    0.5037110195   1.5994705288
O  -3.6604230499  -2.8859932026  -0.7723658687
O  -2.6425145749  -0.7722038377   0.7850333367
N  -7.9602337561   1.333294016    1.9011582758
O  -9.4979444132  -0.2671562575   1.4442370645
C  -9.2361178046   0.8674415027   1.8202628833
C  -10.3187635682  1.8444519134   2.2235806288
H  -5.7558421244  -2.2069365673   0.3718234746
H  -7.8327711053  -1.7125720022  -0.4263100615
H  -8.276598067    0.5908272127  -0.6805312728
H  -5.9296865289   1.727723328    0.0573603354
H  -4.2791357779   1.2183791253  -1.3293652504
H  -4.6412008114  -0.4713035906  -2.8652754339
H  -3.0040037704  -0.9987759841  -2.4381290701
H  -5.0783976506  -2.714385569   -2.1847331809
H  -8.107583473   -1.9347538577  -2.5317801689
H  -6.9943583836   0.2661958184  -2.8096021792
H  -2.7451119681   1.2679541035   0.4775128864
H  -1.8649113396   0.3262858258  -0.7398571102
H  -6.0173408056   0.7156124252   2.3168549292
H  -7.1286264329  -0.5318918012   1.7504096676
H  -3.1159998636  -2.2982062199  -0.2123535049
H  -3.5360033095  -0.7945512562   1.1845543188
H  -7.8053882888   2.2836281812   2.1955521644
H  -10.902961988   1.4028182192   3.034247352
H  -9.9412856699   2.817582808    2.5470750461
H  -10.9952353116  1.9894477853   1.3780048855
```

S134

calc_**2b** conf_11

```
C   -6.9327349157    -1.6318355617    -1.5156860139
C   -7.663895802     -0.8719537647    -0.4015862099
C   -6.5667123964     0.0474383173     0.1866153342
N   -5.2849011443    -0.5785470525    -0.1557008287
C   -5.5377598835    -1.8128365345    -0.9276086424
C   -4.3204804134     0.2471375229    -0.8987059991
C   -3.426365592     -0.8088648559    -1.5388380831
C   -4.3879587336    -1.9352645782    -1.9352978575
O   -6.8722344317    -0.8026571103    -2.6519541191
O   -8.7568053168    -0.1837030829    -0.9619480138
C   -3.5966208968     1.1672144873     0.0830315712
C   -6.6311891365     0.2025859572     1.7121996323
O   -3.8349240597    -3.2352789067    -1.8354673163
O   -3.1361238331     0.4400708908     1.1954465117
N   -7.9272566271     0.5407553638     2.290454103
O   -8.6872501278     1.9915439192     0.7168764062
C   -8.8087094179     1.4455732229     1.8151626385
C   -9.994978296      1.7471408251     2.7016631451
H   -5.5254000657    -2.6899693563    -0.2688664526
H   -7.4156609875    -2.5907614265    -1.7509480152
H   -8.0114129884    -1.5795078123     0.3669461691
H   -6.6457125849     1.0306907839    -0.2867667237
H   -4.8211877021     0.8484003367    -1.6729708333
H   -2.8525649778    -0.4119574385    -2.3813557881
H   -2.7284402697    -1.1933059646    -0.78804921
H   -4.7784510989    -1.7600558359    -2.9439643156
H   -7.7049043215    -0.2968426545    -2.6165763089
H   -8.8276404265     0.6840857032    -0.5159287182
H   -4.2787564391     1.9765212276     0.3930336823
H   -2.7366658831     1.6401375696    -0.4026833893
H   -5.8804940636     0.938314777      2.0250255557
H   -6.3398403923    -0.7571043625     2.1485375537
H   -3.1988480284    -3.3365278962    -2.5539139274
H   -3.7882660365    -0.2807084036     1.278002373
H   -8.1036891679     0.1754604407     3.2127880976
H   -10.0014150808    1.1955436231     3.6444587873
H   -10.0016610158    2.8184874683     2.9162026506
H   -10.910087445     1.5215801618     2.1493725546
```

calc_**2b** conf_12

```
C   -6.2288353468    -2.6407197421    -0.9094431273
C   -7.4923459948    -1.8561088308    -0.4740284837
C   -6.9766550827    -0.5289738008     0.1181374122
N   -5.5009457887    -0.5735803124     0.0191758276
C   -5.1416074405    -1.5765965195    -0.9831690269
C   -4.8510108532     0.6902059586    -0.409202261
C   -4.3855458016     0.4856961429    -1.86945276
C   -5.0667967956    -0.8092553397    -2.3066987513
O   -6.3987907168    -3.3280989243    -2.1274860754
O   -8.2691479958    -1.6588978173    -1.6479392507
C   -3.7063560855     0.993130783      0.562765182
C   -7.4411184768    -0.2865638874     1.5539667471
O   -4.3371662538    -1.4782299461    -3.3023481084
O   -4.1236801571     0.786137128      1.8979397988
N   -7.0895492806     1.0219071996     2.0487992853
```

S135

```
O  -9.1869272014   1.8612989029   1.8113017928
C  -8.0120869837   2.0212233462   2.1125402723
C  -7.4868884297   3.352234719    2.6063130946
H  -4.1476250683  -1.9958214365  -0.7822380426
H  -5.9815992453  -3.3726848778  -0.1332406475
H  -8.0749625104  -2.4276811862   0.2586070961
H  -7.3853523718   0.2799530848  -0.5037266142
H  -5.5879808738   1.4957614081  -0.3318063643
H  -4.6282167092   1.3331860176  -2.5138740947
H  -3.3012912909   0.3303147497  -1.9175886154
H  -6.0893812896  -0.5906914635  -2.6517532454
H  -7.2319795837  -2.9885499263  -2.4988932283
H  -9.1654645152  -1.4066025059  -1.3959339919
H  -3.3814289036   2.0329300111   0.4741463386
H  -2.842527984    0.3517991193   0.3318606975
H  -7.0144517574  -1.0572798761   2.2078913661
H  -8.531227573   -0.3503625876   1.6075017687
H  -4.7887836324  -2.3292183799  -3.4131203095
H  -4.5046547739  -0.1114167428   1.8564659857
H  -6.1072605384   1.2236340761   2.2063960915
H  -7.7450554799   4.1247551458   1.8783246792
H  -7.9963080703   3.6047701398   3.5397896491
H  -6.407993144    3.3623961707   2.7780199136

calc_**2b** conf_13

C  -6.4317990895  -2.4728624896  -1.3430893019
C  -7.2681817166  -2.0852505268  -0.1040193035
C  -6.7688634939  -0.6952245648   0.2701901471
N  -5.3319947314  -0.7710034167   0.0033809379
C  -5.1630741509  -1.6132185022  -1.2059201508
C  -4.6444506205   0.5214507947  -0.254844523
C  -4.0388545013   0.4146632313  -1.6628326227
C  -4.9275848386  -0.6118537155  -2.3422523993
O  -7.1311565383  -2.1485729052  -2.5220471016
O  -8.6515699609  -2.1312097354  -0.3976875469
C  -3.6016828217   0.7865482783   0.8266725333
C  -7.1450917273  -0.3397457828   1.7073252415
O  -4.3245200845  -1.1645456362  -3.4837925682
O  -4.1483001649   0.6314222567   2.1227692239
N  -7.0769635203   1.0694598695   2.0050865882
O  -9.0888853047   1.4358836579   1.0419120651
C  -8.0871187306   1.8792802176   1.5946794863
C  -7.9106112481   3.3541987283   1.8731724611
H  -4.2663190344  -2.2364439677  -1.1095060372
H  -6.19176016    -3.5434450929  -1.3387640436
H  -7.0551274482  -2.7852589888   0.7138429878
H  -7.2678348381   0.03299804    -0.3943794986
H  -5.3896252737   1.3266812709  -0.2225003531
H  -4.013329401    1.3727580459  -2.1868297235
H  -3.0141847672   0.0249439946  -1.6228070395
H  -5.8882341086  -0.1493360662  -2.5992178747
H  -8.07142765    -2.2156519325  -2.2765368224
H  -9.0371968368  -1.2628985968  -0.2097140902
H  -3.2245573661   1.8105813339   0.7579073473
H  -2.7500143114   0.1046782588   0.689679643
H  -6.5082383102  -0.8908900027   2.4054490406
H  -8.1765499996  -0.6566334119   1.8857751497
H  -5.0123798151  -1.6844867095  -3.9216282574
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S136

```
H   -4.4655586445   -0.286043688    2.1232191987
H   -6.1767258224    1.4369191708    2.286936274
H   -7.9300194178    3.8998731023    0.9264303034
H   -8.7608124729    3.7023024674    2.4643159182
H   -6.986401078     3.5899330133    2.4056247112
```

calc_**2b** conf_14

```
C   -6.5354555209   -2.201367372    -1.8058537946
C   -7.653096493    -1.6705506776   -0.9046169271
C   -7.049179126    -0.4080581765   -0.2633299399
N   -5.5925724952   -0.6269720388   -0.2829308644
C   -5.2993759796   -1.9090434758   -0.9634931476
C   -4.765181638     0.4187163769   -0.9045093468
C   -3.4892872128   -0.3437116607   -1.2478411731
C   -3.9871422347   -1.7094206067   -1.7302743434
O   -6.5109719077   -1.4350994747   -2.9882873194
O   -8.8126476136   -1.3143844096   -1.6363259861
C   -4.5579447937    1.5558102771    0.0976390545
C   -7.6299844065   -0.1941175065    1.135193886
O   -3.1218129163   -2.7886734061   -1.4340638459
O   -4.3207483609    1.0257444878    1.3890109935
N   -7.2452342727    1.0441207846    1.7633333507
O   -9.3652723077    1.8454249232    1.9586713837
C   -8.1639906147    1.9766311675    2.1402530006
C   -7.5876822514    3.2045498921    2.8143174376
H   -5.1585262875   -2.7112001884   -0.2287680077
H   -6.6404235945   -3.2726040934   -2.032646164
H   -7.893745529    -2.406750877    -0.1252825988
H   -7.3124024958    0.4522401524   -0.8923373861
H   -5.2325105395    0.8132233244   -1.8194075919
H   -2.8779440286    0.1825180161   -1.9865601795
H   -2.8913044172   -0.4901088062   -0.3416318906
H   -4.2027198727   -1.6710255145   -2.8042163709
H   -7.4357892319   -1.1771385079   -3.1436016806
H   -9.379226348    -2.0920764249   -1.7151111554
H   -5.4473259932    2.2006558504    0.1130118753
H   -3.7033822868    2.1742998682   -0.1967531998
H   -7.33811939     -1.0438678722    1.7678974792
H   -8.7210968433   -0.1754306218    1.0678761239
H   -2.3569648494   -2.7203903063   -2.0183630018
H   -4.6162759445    0.0942926426    1.3020872059
H   -6.2615948467    1.1965353731    1.9620169209
H   -7.9330419482    4.0921808047    2.2792611576
H   -7.9841404632    3.2655749516    3.831107274
H   -6.4958849447    3.2114731254    2.857528772
```

calc_**2b** conf_15

```
C   -6.6562235621   -2.1598478158   -0.8617009442
C   -7.5046303845   -1.0018979589   -0.2770771102
C   -6.4874692415    0.0073042853    0.2978490161
N   -5.146376412    -0.5757396353    0.0867094263
C   -5.2569310051   -1.5683412673   -0.9825635252
C   -4.1027272345    0.3866112942    -0.3492596803
C   -3.8654201622    0.1404918869    -1.8572999085
C   -5.0029816103   -0.7870692232   -2.2756642599
O   -7.1522843264   -2.6255498416   -2.0971332729
O   -8.2485320153   -0.4585651359   -1.3410866205
```

```
C   -2.8569165216    0.1698128505    0.5079341216
C   -6.6333454182    0.2827657825    1.7922399411
O   -4.6501672854   -1.6038222445   -3.3624322014
O   -3.1913839551    0.1630711251    1.8747166881
N   -7.8846242848    0.8867762211    2.2421653496
O   -8.8848203882    1.6064164268    0.3099545434
C   -8.8519398902    1.5140469909    1.5364079944
C   -9.9550442048    2.1336444008    2.3679668708
H   -4.4762790822   -2.33385867     -0.8905919357
H   -6.6507881779   -2.9997574384   -0.1593453325
H   -8.1812724016   -1.3696665195    0.5068766926
H   -6.6020715664    0.943679068    -0.2578146451
H   -4.4701343524    1.400658308    -0.1566785354
H   -3.8342939861    1.0653564492   -2.437252603
H   -2.9185038127   -0.3874149317   -2.0223378655
H   -5.8993587873   -0.1924218734   -2.5093414151
H   -7.7970182557   -1.9513390676   -2.3782163352
H   -8.6649384672    0.3511795577   -0.9851460148
H   -2.1344141639    0.9751854478    0.34682491
H   -2.3721616664   -0.774960919     0.2129473543
H   -5.7962530126    0.9194407145    2.1041406543
H   -6.520253849    -0.6722518779    2.3195347302
H   -5.3957254062   -2.2171625577   -3.459143956
H   -3.9221339042   -0.4769925479    1.914055702
H   -7.9872224066    0.9200633318    3.2443164628
H   -9.9563161415    3.2118391988    2.1897997783
H   -10.9139898403   1.7465893405    2.016939634
H   -9.8680528174    1.9527268452    3.4417062918

calc_2b conf_16

C   -6.6697376016   -2.0736884741   -1.9458820629
C   -7.8009213761   -1.4103194651   -1.16207246
C   -7.0894279222   -0.2630190416   -0.405114541
N   -5.7175359884   -0.7596426616   -0.18382695
C   -5.5158419862   -2.0156658      -0.9455546505
C   -4.6000090755    0.1500848395   -0.4890385092
C   -3.4449538667   -0.8161576281   -0.7294260123
C   -4.0912686541   -1.9480901413   -1.5233673886
O   -6.4581675686   -1.2380035511   -3.0789140917
O   -8.8783508622   -1.006883446    -1.9509142021
C   -4.3717170855    1.1012499992    0.688986464
C   -7.8643871041    0.067323378     0.8710724843
O   -3.401255145    -3.1742248284   -1.5268795296
O   -4.543477751     0.4066356953    1.9093305331
N   -7.3754522639    1.1940078506    1.6256353724
O   -9.1442236488    2.5472113775    1.1661771947
C   -8.0711059014    2.3617280347    1.7189603672
C   -7.4173183805    3.4300928386    2.57162414
H   -5.5942695317   -2.8836676627   -0.2748405296
H   -6.9159527515   -3.0945592682   -2.2554445692
H   -8.1942229164   -2.1278198953   -0.4318571502
H   -7.0704251112    0.625247504    -1.052267703
H   -4.7961152998    0.7381447139   -1.3993374181
H   -2.6025842217   -0.3551442334   -1.2499906766
H   -3.0836352242   -1.1939548539    0.2364968889
H   -4.1488484207   -1.6522474419   -2.5741080828
H   -6.0913560639   -1.7701212489   -3.7939236853
H   -8.4794162453   -0.6195201096   -2.7459763901
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S138

```
H   -5.0751761417    1.9417514305    0.6272351553
H   -3.357193646     1.5122330331    0.6527887037
H   -7.8756052366   -0.824279189     1.511952069
H   -8.8950786302    0.3017292084    0.5917917239
H   -3.2371650478   -3.4227039461   -0.607266655
H   -5.0339729456   -0.3979245465    1.6337312849
H   -6.4863186224    1.0962321942    2.1024102175
H   -7.2944274023    4.33327246      1.9691094249
H   -8.0904330125    3.680853305     3.3952377336
H   -6.4476513468    3.1368395702    2.9814635004

calc_2b conf_17

C   -6.8973764431   -1.8138260195   -1.4150402913
C   -7.5575143158   -1.1394876066   -0.2083102055
C   -6.5651891263   -0.0172253797    0.1383803186
N   -5.2921746534   -0.7143697121    0.0043168385
C   -5.3997110454   -1.6577980766   -1.1284900132
C   -4.0775117463    0.100845579    -0.1691754151
C   -3.397305375    -0.4430296347   -1.4375120445
C   -4.5485099494   -1.0297517167   -2.237328164
O   -7.2528217396   -1.1272093695   -2.5974827265
O   -8.8460356872   -0.7369294857   -0.573416447
C   -3.1671793241    0.0130476992    1.0547097801
C   -6.7208187304    0.5773716635    1.5441361657
O   -4.088187993    -1.9382681912   -3.2094098124
O   -1.9992253316    0.7945110557    0.9149762484
N   -7.6881697871    1.6572241228    1.6481924453
O   -9.5293851777    0.3522555169    1.8195146814
C   -9.0130056137    1.471000764     1.8175759018
C   -9.8452977832    2.7153238167    2.0166943142
H   -4.9520393416   -2.6244331772   -0.86381733
H   -7.1913834564   -2.8686561467   -1.4934807069
H   -7.5781644488   -1.8466826868    0.6332799477
H   -6.6877460916    0.7945566772   -0.602034278
H   -4.345893606     1.1572463048   -0.3233983077
H   -2.8430343802    0.3212254278   -1.987294483
H   -2.7030634506   -1.2581949805   -1.1901587351
H   -5.1252704035   -0.222086644    -2.7024577046
H   -8.1760641606   -0.8562752072   -2.4610881879
H   -9.2937194524   -0.4341718394    0.2425715794
H   -2.9367462305   -1.0458119095    1.2469093448
H   -3.6768987619    0.3947653956    1.9433895505
H   -5.7635342831    0.9906386763    1.868451366
H   -6.9954012492   -0.208254067     2.2539431357
H   -4.8431632785   -2.1365716966   -3.7785583788
H   -1.4634530706    0.3944545745    0.218640044
H   -7.3410509583    2.6021967324    1.6222337388
H   -9.2646910072    3.6405284508    2.028153953
H   -10.5916958963   2.7715755537    1.2207616405
H   -10.3855666501   2.6222655362    2.9616222371

calc_2b conf_18

C   -6.5193844578   -2.2452481528   -1.4121000295
C   -7.3246183735   -1.6167199099   -0.2613871435
C   -6.5830381004   -0.3017443675    0.0271216544
N   -5.1894119617   -0.73795884     -0.0659525733
C   -5.1203183037   -1.6306653193   -1.2350467282
```

```
C    -4.1586648796     0.3111922895    -0.254127092
C    -3.6034360889     0.1311953597    -1.6848604803
C    -4.6728587557    -0.7122896603    -2.369543952
O    -7.1580658465    -1.8488063804    -2.6137770908
O    -8.6927277162    -1.4784766662    -0.5438618801
C    -3.0888159445     0.1531581824     0.823886134
C    -6.9410408259     0.3014459611     1.3793077037
O    -4.2748391659    -1.504183636     -3.4733589404
O    -3.6607124866     0.1298643426     2.1042286536
N    -8.319059446      0.7307514374     1.3870874675
O    -7.8946656941     2.821004362      2.1702795
C    -8.6866927402     1.9875622633     1.7581292112
C   -10.1678888164     2.2845600868     1.6412436143
H    -4.3529978891    -2.4014140367    -1.0952324383
H    -6.5000096774    -3.3386835337    -1.348490331
H    -7.2380113755    -2.2550525302     0.6245240128
H    -6.8507500755     0.4308137261    -0.7557881683
H    -4.6289827049     1.2929625874    -0.1302613222
H    -3.4170470029     1.0861213419    -2.1840756746
H    -2.6627052849    -0.4328372348    -1.6681956233
H    -5.515877777     -0.0694616386    -2.6552368457
H    -6.5468434567    -2.0293762424    -3.3437136188
H    -8.7468867583    -1.3075938291    -1.4982560661
H    -2.3882624152     0.9930943107     0.7934114531
H    -2.5144985621    -0.7670331064     0.6234622277
H    -6.3289954614     1.1753736223     1.6138275371
H    -6.7601178281    -0.4470598487     2.1643529884
H    -3.9893913322    -0.9150763743    -4.1833009915
H    -4.3435203652    -0.557280372      2.0471905789
H    -8.9937281007     0.1120090069     0.9588254651
H   -10.7491597651     1.4723372485     1.197807057
H   -10.5619934251     2.4966492601     2.6383536224
H   -10.297981139      3.1888662905     1.0425281086
```

calc_**2b** conf_19

```
C    -6.5376228404    -2.3211741446    -1.1438365085
C    -7.2694671874    -1.6569042886     0.0341846995
C    -6.5813133782    -0.2885605117     0.1591708615
N    -5.1778032953    -0.6622890648    -0.0208163011
C    -5.1531710417    -1.6492876833    -1.1128575473
C    -4.2245021638     0.418608267     -0.3760928268
C    -3.7552238443     0.1396570168    -1.8190586082
C    -4.8111330626    -0.8207991484    -2.355729405
O    -7.2917347873    -2.0084068957    -2.3016440822
O    -8.6629934223    -1.6112506865    -0.1254150958
C    -3.0785433337     0.4193738212     0.6334879937
C    -6.8602040692     0.4011146427     1.4887171516
O    -4.4860541083    -1.5899165759    -3.4936761819
O    -3.5590292937     0.4734947384     1.9494520598
N    -8.253907278      0.7631856983     1.5833231145
O    -7.8793427664     2.9236449188     2.1782450979
C    -8.6569734744     2.0252649416     1.8959354847
C   -10.1564518594     2.2419550899     1.8857645611
H    -4.3557950103    -2.3879758561    -0.9440737476
H    -6.4734443324    -3.4088593618    -1.0267072392
H    -7.0645895384    -2.2241350785     0.9485493825
H    -6.9515993499     0.3654419186    -0.6507223171
H    -4.7437759206     1.381096572     -0.3092511346
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S140

```
H   -3.6596429248    1.0455592711   -2.4210835501
H   -2.7746814538   -0.3576446274   -1.8113590642
H   -5.697442076    -0.2544794509   -2.6509599932
H   -6.7597479315   -2.2313278577   -3.0796437442
H   -8.8136951432   -1.4983924166   -1.0781203783
H   -2.4373330134    1.2929528875    0.4824937124
H   -2.4594191738   -0.4794216978    0.4695141717
H   -6.2793423645    1.3190308197    1.6044255582
H   -6.5750594428   -0.2740883994    2.3087650729
H   -3.6845042236   -2.0933569827   -3.2946942457
H   -4.201809444    -0.2518382703    1.9987339971
H   -8.927313096     0.0802421432    1.264828284
H   -10.72829391     1.3684705144    1.5629184884
H   -10.4765210311   2.5209479494    2.8927923133
H   -10.3845194134   3.0840677878    1.2284399662
```

calc_**2b** conf_20

```
C   -6.3794813935   -2.6002444532   -0.8847284408
C   -7.6003725815   -1.6779146461   -0.6965787158
C   -7.0509610335   -0.4304220964    0.0189739061
N   -5.5799448365   -0.5087785866   -0.0670944005
C   -5.2007675101   -1.6328828967   -0.9169304073
C   -4.8357453524    0.6678956483   -0.5502851016
C   -4.1876700278    0.2618280276   -1.8990533083
C   -4.902720711    -1.0233615309   -2.2909371357
O   -6.4676595955   -3.4009226116   -2.0419108641
O   -8.0870448375   -1.3982623173   -2.0055771783
C   -3.7518078179    1.1017542243    0.4249346208
C   -7.5234006635   -0.3497052436    1.4723685877
O   -4.1028376877   -1.8424653417   -3.1068871344
O   -4.335602489     1.6555412921    1.5951955491
N   -7.0903252461    0.8660182328    2.1092431712
O   -9.1806296387    1.7514554067    2.2717248065
C   -7.9691899991    1.8605606238    2.4088263153
C   -7.3364387525    3.1141002032    2.9781299101
H   -4.2788352342   -2.1135995906   -0.5615453369
H   -6.2975600231   -3.2638412618   -0.0178088596
H   -8.3880247909   -2.1687260567   -0.1122966248
H   -7.426230373     0.4607561472   -0.5040014159
H   -5.5295180928    1.5075702885   -0.6782371302
H   -4.2622665752    1.0476604373   -2.6538322264
H   -3.1238311484    0.0274589958   -1.767777415
H   -5.8522187314   -0.7786040622   -2.7883540953
H   -7.146803885    -2.9719710592   -2.590998037
H   -8.9738736613   -1.0256729653   -1.9339347564
H   -3.1088936377    1.8477380675   -0.0643913076
H   -3.1347040205    0.2276603563    0.6725995502
H   -7.1441413039   -1.2200065667    2.0227629754
H   -8.6155347942   -0.3543384596    1.520842375
H   -4.5940113503   -2.6750049876   -3.1813291518
H   -3.6459955488    1.7543117874    2.2620621893
H   -6.0935227992    1.063718807     2.1036894342
H   -7.3959795881    3.0831806866    4.0705664745
H   -6.2893983978    3.2276510293    2.6873932983
H   -7.9090558706    3.9788644722    2.6401758803
```

calc_**2b** conf_21

S141

```
C    -6.8706444466    -1.7248768251    -0.912581398
C    -7.4262068504    -0.2911688396    -0.814738339
C    -6.34231908      0.4639527449     -0.0356811506
N    -5.1224715855    -0.369880122     -0.0849940288
C    -5.3611248419    -1.5403942838    -0.9261981074
C    -3.8691574193    0.2640230836     -0.5488353984
C    -3.4806594784    -0.4363243751    -1.8676987246
C    -4.7322549568    -1.1996537071    -2.2876667423
O    -7.2932174505    -2.3797185678    -2.1060849646
O    -7.552289813     0.2701753662     -2.1060235496
C    -2.7995286173    0.117398459      0.5354037977
C    -6.7104249603    0.7357890822     1.4283807106
O    -4.4067481983    -2.3312021848    -3.0589861322
O    -3.2902322626    0.5081947542     1.794244286
N    -7.8682472177    1.584726563      1.5994114682
O    -9.3261847218    -0.1088730976    1.9830512484
C    -9.1011118425    1.090616046      1.8947619344
C    -10.186061469    2.1226504414     2.1143519931
H    -4.8449732146    -2.4279335242    -0.5371482486
H    -7.1746638272    -2.2998179976    -0.0313286827
H    -8.3897946251    -0.2715058208    -0.2932018971
H    -6.1822014467    1.4235653708     -0.544388025
H    -4.0579218615    1.3330696431     -0.7005440607
H    -3.1383658986    0.2633828507     -2.6329779363
H    -2.6785220586    -1.1653761272    -1.7009575632
H    -5.4058043996    -0.5281527348    -2.8338375474
H    -8.1038601451    -2.868087256     -1.9176292767
H    -7.7648983955    -0.4769617934    -2.6891710608
H    -1.9357565319    0.7494416135     0.3087537806
H    -2.4494360133    -0.9273397443    0.5571578566
H    -5.8509778466    1.2027710543     1.9189118664
H    -6.9247099344    -0.2072244599    1.9368132912
H    -5.2486026777    -2.7666429181    -3.2522281555
H    -4.0933183405    -0.0275785633    1.8974641352
H    -7.7491946582    2.5819200755     1.5264607781
H    -9.858347648     3.153536683      1.9592698709
H    -11.0166419829   1.9076804309     1.4384631917
H    -10.5631232821   2.0208186798     3.1350007805
```

calc_**2b** conf_22

```
C    -6.5032116316    -2.2800054016    -1.3684617081
C    -7.3503508264    -1.5923495516    -0.2722166264
C    -6.5894387489    -0.2959449513    0.0320191442
N    -5.2014731115    -0.7446006439    -0.0509705228
C    -5.1225352319    -1.6345630377    -1.2229468285
C    -4.1734096545    0.3091559054     -0.242980208
C    -3.6450182422    0.1552741651     -1.6834385473
C    -4.6863838117    -0.7133807731    -2.3739678753
O    -7.0349312952    -1.9959045234    -2.66269525
O    -8.6973452509    -1.4176448643    -0.6443561515
C    -3.0905736323    0.1348181037     0.8189738727
C    -6.9488511985    0.3080536055     1.3844777547
O    -4.1546491673    -1.3924365086    -3.4827238604
O    -3.6487874712    0.0857670232     2.1060683457
N    -8.3210483932    0.7557716199     1.3937765448
O    -7.8662125665    2.8544231442     2.1361416823
C    -8.6720226888    2.0232928203     1.7493075529
C    -10.1515613091   2.3333158264     1.6468725064
```

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H   -4.3374808706   -2.386941056    -1.084630703
H   -6.4649863824   -3.3641475057   -1.2242846513
H   -7.3571618902   -2.2162139905    0.6266827474
H   -6.8387726754    0.4483414306   -0.7481867167
H   -4.6444797711    1.2866343949   -0.0918766366
H   -3.4940768747    1.1131743046   -2.1853313442
H   -2.6881162354   -0.3807761071   -1.6936172603
H   -5.53811424     -0.0910213445   -2.6783857793
H   -7.73516152     -2.6399281517   -2.8295721546
H   -8.6687191945   -0.992796808    -1.5157243833
H   -2.3934768912    0.9775914518    0.7952811168
H   -2.514807927    -0.7790816856    0.5960258394
H   -6.3266169833    1.1738474311    1.6211868796
H   -6.7771912456   -0.4440550623    2.1675760434
H   -4.9064677946   -1.8277960641   -3.9071874798
H   -4.3350316731   -0.5970147041    2.0373125808
H   -9.0133786009    0.1360676714    0.9985782918
H  -10.5302312179    2.5654733114    2.6454422453
H  -10.2803728667    3.2291943256    1.0354356544
H  -10.7475509143    1.5204062002    1.2243958846

calc_2b conf_23

C   -7.110479108    -1.6175104069   -0.6852964058
C   -7.6806549415   -0.2923643254   -1.2283825977
C   -6.6760279708    0.7754059218   -0.7595747616
N   -5.5031085986    0.0492539702   -0.2447633925
C   -5.6153864679   -1.366532706    -0.5794804163
C   -4.1710312822    0.5057906493   -0.6944728682
C   -3.6046032974   -0.6122811679   -1.5956937732
C   -4.7923080351   -1.535289694    -1.8660100482
O   -7.3581876171   -2.7072888862   -1.5733173893
O   -7.6834885151   -0.3144143729   -2.6441164481
C   -3.3233775988    0.7922658318    0.554018119
C   -7.2007505581    1.8355908909    0.2331283091
O   -4.3674832754   -2.8564932821   -2.1007737886
O   -4.1067358481    1.4559042167    1.5158025504
N   -7.1825519443    1.4917141709    1.6413543782
O   -8.8254690331   -0.0647026992    1.5660368509
C   -8.0219269047    0.594688306     2.214090979
C   -7.9093547494    0.4565402428    3.7174959303
H   -5.1550758455   -1.9962500719    0.1934268079
H   -7.537559593    -1.8151108822    0.3006359247
H   -8.6867622372   -0.1014118297   -0.8428418419
H   -6.4190939282    1.3385470238   -1.6676637822
H   -4.2986798386    1.4440497366   -1.2460058414
H   -3.1543102705   -0.2293785883   -2.5139069605
H   -2.8387811179   -1.1922412176   -1.0670944533
H   -5.3749665607   -1.1510283324   -2.7132626487
H   -8.1670464809   -3.1509380685   -1.2909052917
H   -7.7988989921   -1.2495227159   -2.8817572758
H   -2.4658632179    1.4262012743    0.3098837466
H   -2.9314599131   -0.1573357204    0.9541727286
H   -8.2165522764    2.1185683191   -0.0649709696
H   -6.5716001227    2.7238312173    0.1421080731
H   -5.1768325918   -3.372916961    -2.2201951872
H   -4.9326855274    0.9323314928    1.4834353282
H   -6.5758884559    2.0317196823    2.2377757141
H   -7.0987693051    1.0416058622    4.1581335226
```

S143

```
H   -8.8557554209    0.7642654697    4.1695381973
H   -7.7604925585   -0.5972623498    3.9624489819


calc_2b conf_24

C   -6.6444574678   -2.184341141    -1.5439792899
C   -7.7928595229   -1.1185926758   -1.4549436698
C   -7.3553356382   -0.1617549613   -0.3157641831
N   -5.9426902933   -0.4177609088   -0.0656946333
C   -5.7566591962   -1.8507396361   -0.33097286
C   -5.0211422642    0.287580397    -0.9839211187
C   -3.7975846082   -0.6373112487   -1.0594031117
C   -4.2428899206   -1.9986582863   -0.4864316395
O   -5.9317006264   -2.0470110343   -2.7470612587
O   -7.9711114456   -0.4793417766   -2.7120528839
C   -4.7097950079    1.7055582195   -0.5238291728
C   -8.2094961868   -0.4101778553    0.9423620856
O   -3.635236822    -2.2804181905    0.7633866897
O   -5.7865411953    2.5958040036   -0.703537772
N   -7.6466964902    0.1091651217    2.1708914593
O   -7.5528050665    2.2580502278    1.4806799047
C   -7.3141297762    1.4064011284    2.3357093169
C   -6.6406337932    1.7639015378    3.6403802555
H   -6.0913547113   -2.4444337333    0.5290134776
H   -7.0516408249   -3.2025030179   -1.4681548209
H   -8.7477565978   -1.6044467593   -1.227923814
H   -7.4886439553    0.8811861311   -0.6059830586
H   -5.4572319267    0.3700045766   -1.9904684662
H   -3.4491321485   -0.7294912364   -2.0891319789
H   -2.961877657    -0.2628374861   -0.457386619
H   -3.9771819182   -2.8304550254   -1.1388352875
H   -6.5287609583   -1.5477445166   -3.3345378499
H   -7.5811836235    0.4030331147   -2.6631745497
H   -3.877710357     2.0879738174   -1.126618764
H   -4.3710758003    1.6737124163    0.5228812824
H   -8.3571844808   -1.4823201379    1.0997726838
H   -9.1986939395    0.029945397     0.7780981128
H   -3.8839912593   -1.5521111049    1.3495889664
H   -6.3551753718    2.5694336504    0.0867969677
H   -7.3118668615   -0.5539209268    2.8499126183
H   -5.6168630144    2.0866238198    3.4328119476
H   -7.1658617496    2.6135602514    4.0810030993
H   -6.6140475228    0.9454378489    4.3635179347
```

Table S38. Sampled and DFT geometry optimized conformers related to calc_**2c**, with energy values (Hartree) and related % contribution on the final Boltzmann distribution for the three employed functional/basis set combinations.

Conformer	MPW1PW91/6-31g(d,p)		MPW1PW91/6-311+g(d,p)		B97-2/cc-pVTZ	
	Energy (Hartree)	% contribution on the Boltzmann distribution	Energy (Hartree)	% contribution on the Boltzmann distribution	Energy (Hartree)	% contribution on the Boltzmann distribution
calc_**2c** conf_1	-916.6593144	93.88%	-916.8940084	88.54%	-916.8411975	73.40%
calc_**2c** conf_2	-916.6561823	3.40%	-916.8918926	9.42%	-916.8399559	19.71%
calc_**2c** conf_3	-916.6553274	1.38%	-916.8898102	1.04%	-916.8382855	3.36%
calc_**2c** conf_4	-916.6552247	1.23%	-916.8894586	0.71%	-916.8381521	2.92%
calc_**2c** conf_5	-916.6523443	0.06%	-916.8866502	0.04%	-916.8339035	0.03%
calc_**2c** conf_6	-916.6511297	0.02%	-916.8883109	0.21%	-916.8362275	0.38%
calc_**2c** conf_7	-916.6510022	0.01%	-916.8856609	0.01%	-916.8346381	0.07%
calc_**2c** conf_8	-916.6507502	0.01%	-916.8850608	0.01%	-916.8344792	0.06%
calc_**2c** conf_9	-916.6496278	0.00%	-916.8839994	0.00%	-916.8329005	0.01%
calc_**2c** conf_10	-916.6487700	0.00%	-916.8857021	0.01%	-916.8337733	0.03%
calc_**2c** conf_11	-916.6487010	0.00%	-916.8832926	0.00%	-916.8332605	0.02%
calc_**2c** conf_12	-916.6468637	0.00%	-916.8815696	0.00%	-916.8310224	0.00%
calc_**2c** conf_13	-916.6457891	0.00%	-916.8846577	0.00%	-916.8328106	0.01%
calc_**2c** conf_14	-916.6445246	0.00%	-916.8827466	0.00%	-916.8317578	0.00%
calc_**2c** conf_15	-916.6441171	0.00%	-916.8810170	0.00%	-916.8291855	0.00%
calc_**2c** conf_16	-916.6436037	0.00%	-916.8797328	0.00%	-916.8289386	0.00%
calc_**2c** conf_17	-916.6434575	0.00%	-916.8820410	0.00%	-916.8310253	0.00%
calc_**2c** conf_18	-916.6429565	0.00%	-916.8777842	0.00%	-916.8273620	0.00%
calc_**2c** conf_19	-916.6428849	0.00%	-916.8786364	0.00%	-916.8278920	0.00%
calc_**2c** conf_20	-916.6425687	0.00%	-916.8787206	0.00%	-916.8274909	0.00%
calc_**2c** conf_21	-916.6424392	0.00%	-916.8778239	0.00%	-916.8258961	0.00%
calc_**2c** conf_22	-916.6423425	0.00%	-916.8785005	0.00%	-916.8281990	0.00%
calc_**2c** conf_23	-916.6422630	0.00%	-916.8760118	0.00%	-916.8255323	0.00%
calc_**2c** conf_24	-916.6422249	0.00%	-916.8773204	0.00%	-916.8270534	0.00%
calc_**2c** conf_25	-916.6421984	0.00%	-916.8772600	0.00%	-916.8268987	0.00%
calc_**2c** conf_26	-916.6421715	0.00%	-916.8781638	0.00%	-916.8280307	0.00%
calc_**2c** conf_27	-916.6420646	0.00%	-916.8772723	0.00%	-916.8268253	0.00%
calc_**2c** conf_28	-916.6419182	0.00%	-916.8790238	0.00%	-916.8283886	0.00%

calc_**2c** conf_29	-916.6414649	0.00%	-916.8763347	0.00%	-916.8263286	0.00%
calc_**2c** conf_30	-916.6413011	0.00%	-916.8762497	0.00%	-916.8250859	0.00%
calc_**2c** conf_31	-916.6409741	0.00%	-916.8755981	0.00%	-916.8241265	0.00%
calc_**2c** conf_32	-916.6408285	0.00%	-916.8778290	0.00%	-916.8273658	0.00%
calc_**2c** conf_33	-916.6407598	0.00%	-916.8769028	0.00%	-916.8266625	0.00%
calc_**2c** conf_34	-916.6401777	0.00%	-916.8778566	0.00%	-916.8273923	0.00%
calc_**2c** conf_35	-916.6401356	0.00%	-916.8744093	0.00%	-916.8230158	0.00%
calc_**2c** conf_36	-916.6398480	0.00%	-916.8748831	0.00%	-916.8243886	0.00%
calc_**2c** conf_37	-916.6397383	0.00%	-916.8757712	0.00%	-916.8254365	0.00%
calc_**2c** conf_38	-916.6396444	0.00%	-916.8767428	0.00%	-916.8261981	0.00%
calc_**2c** conf_39	-916.6392437	0.00%	-916.8793164	0.00%	-916.8282140	0.00%
calc_**2c** conf_40	-916.6392215	0.00%	-916.8762287	0.00%	-916.8262948	0.00%
calc_**2c** conf_41	-916.6387064	0.00%	-916.8780046	0.00%	-916.8274347	0.00%
calc_**2c** conf_42	-916.6386646	0.00%	-916.8756762	0.00%	-916.8253078	0.00%
calc_**2c** conf_43	-916.6382805	0.00%	-916.8747320	0.00%	-916.8248691	0.00%
calc_**2c** conf_44	-916.6374710	0.00%	-916.8750000	0.00%	-916.8236343	0.00%
calc_**2c** conf_45	-916.6373683	0.00%	-916.8729987	0.00%	-916.8230565	0.00%
calc_**2c** conf_46	-916.6368994	0.00%	-916.8726268	0.00%	-916.8215026	0.00%
calc_**2c** conf_47	-916.6364445	0.00%	-916.8725305	0.00%	-916.8229899	0.00%
calc_**2c** conf_48	-916.6363982	0.00%	-916.8750007	0.00%	-916.8236258	0.00%
calc_**2c** conf_49	-916.6348422	0.00%	-916.8716995	0.00%	-916.8210615	0.00%
calc_**2c** conf_50	-916.6347653	0.00%	-916.8732921	0.00%	-916.8227527	0.00%
calc_**2c** conf_51	-916.6329818	0.00%	-916.8725001	0.00%	-916.8220643	0.00%
calc_**2c** conf_52	-916.6306019	0.00%	-916.8703707	0.00%	-916.8204293	0.00%

Table S39. Cartesian coordinates of the optimized geometries for the conformers related to calc_**2c**. The related energies and % contribution on the final Boltzmann distribution for the three employed functional/basis set combinations are reported in Table S38.

```
calc_2c conf_1

C   -6.8736049234   -2.3148339446   -4.1837253314
C   -8.0757480558   -1.9796885431   -3.2814986425
C   -8.190143612    -3.2301994749   -2.3993650546
N   -8.0247543195   -4.2884271867   -3.3833464889
C   -6.9897673352   -3.8416360554   -4.3431241493
C   -7.7611583704   -5.6992180736   -3.0309292397
C   -6.455190287    -6.0594485708   -3.7924294181
C   -5.770681964    -4.7193089385   -4.0199086973
O   -5.6998886066   -1.8453259514   -3.5510546216
O   -7.8915021957   -0.7857121277   -2.5736938295
C   -7.6657274605   -6.0556036914   -1.5468125968
C   -9.503476252    -3.25968671     -1.6178102405
O   -5.077914424    -4.2903146342   -2.8543984408
O   -6.6206345504   -5.3765095523   -0.8716686891
N   -9.4298184646   -2.3751636908   -0.4695926922
O   -8.2779043008   -3.8756751952    0.7843221316
C   -8.7411927982   -2.741802114     0.6338883656
C   -8.5916844641   -1.694506271     1.7096425452
H   -7.30850659     -4.0806830652   -5.3675563628
H   -6.9394893521   -1.8030930557   -5.148106047
H   -8.9885357742   -1.8903336579   -3.8826456665
H   -7.3724835236   -3.1877027572   -1.6639354509
H   -8.5799048134   -6.3209946135   -3.4210584089
H   -6.6915622235   -6.5205945177   -4.7560172733
H   -5.8153456349   -6.7508310333   -3.2372583721
H   -5.0399144243   -4.7401375829   -4.8323353752
H   -5.2859795765   -2.6151897148   -3.0994390807
H   -6.9191197143   -0.7165804525   -2.5050440189
H   -7.4769089273   -7.135360732    -1.4908795786
H   -8.6106513084   -5.8753183863   -1.029428366
H   -10.336216103   -2.9425174877   -2.2518454058
H   -9.7385151673   -4.2562731906   -1.246240565
H   -5.5496234312   -4.6419091476   -2.0620111652
H   -7.0492278493   -4.7928709975   -0.2124764999
H   -9.5254658639   -1.3869793366   -0.6533718704
H   -9.1092737222   -0.7598832099    1.4845825177
H   -8.9779995757   -2.1011884061    2.6469243632
H   -7.5284840407   -1.4894979295    1.8586477163

calc_2c conf_2

C   -6.6615626247   -2.4177208805   -3.8469617348
C   -7.7869842054   -2.1179710375   -2.8491860751
C   -8.0074381884   -3.4643641146   -2.1334346733
N   -7.8660398941   -4.4012607085   -3.2354556211
C   -6.946328571    -3.8691123963   -4.25126095
C   -7.6243864916   -5.833053238    -3.0236081316
C   -6.5827508483   -6.1887182062   -4.1138315938
C   -5.8080013813   -4.8977559239   -4.3499462165
O   -5.4131241098   -2.2551023349   -3.1898771438
O   -7.3682233932   -1.0595921069   -2.0368620115
C   -7.2070935217   -6.2534341728   -1.6072569973
C   -9.389985811    -3.5873189563   -1.4583106875
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S147

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O   -4.8297510425   -4.7865984028   -3.3302963895
O   -6.0796282003   -5.6187499325   -1.0775978645
N   -9.3754177649   -3.3780793508   -0.0220789377
O   -9.2785639815   -1.1193327946   -0.1177791882
C   -9.3134818938   -2.157817928     0.5464368395
C   -9.3084715099   -2.1160060869    2.0549739907
H   -7.442808665    -3.857314269    -5.2342567872
H   -6.6916188295   -1.7435547814   -4.7103167895
H   -8.700677055    -1.8640981769   -3.4073059702
H   -7.2327803519   -3.5939934244   -1.3623961145
H   -8.5454972225   -6.4016448496   -3.2261231843
H   -7.0914296315   -6.4871236786   -5.0359413787
H   -5.917028568    -7.0040615052   -3.8179867959
H   -5.322933716    -4.8722575888   -5.3338001085
H   -5.5997054502   -1.6448622095   -2.4505986811
H   -8.0388911339   -0.9413149697   -1.3282733647
H   -7.0857255709   -7.3508704333   -1.6318942172
H   -8.0383976207   -6.0612724759   -0.9154469179
H   -10.0973158739  -2.8773116061   -1.8970996967
H   -9.7902841087   -4.5879145692   -1.6317851489
H   -4.7265516445   -3.8281073963   -3.1495295389
H   -5.4740091105   -5.4149873476   -1.8227566018
H   -9.2940619176   -4.1866077821    0.5733816936
H   -8.3754652822   -1.6572614286    2.3914850759
H   -10.1255243044  -1.4716812266    2.3869615877
H   -9.4130605098   -3.096771709     2.5240163248

calc_2c conf_3

C   -6.4171740365   -2.5713102188   -3.8546736011
C   -7.3414695056   -1.9677100613   -2.7971445632
C   -7.8724773911   -3.2143941952   -2.0563197843
N   -7.9794591984   -4.199324267    -3.1148684624
C   -7.2444422302   -3.7696978872   -4.3158569461
C   -7.8304982262   -5.6314769017   -2.8742965
C   -7.4047617742   -6.1469680963   -4.2619624979
C   -6.5517837223   -5.0306052315   -4.8778894398
O   -5.2314704002   -2.9344040315   -3.1601259803
O   -6.7203150225   -1.0227228231   -1.9633344374
C   -6.8633713729   -6.0013254896   -1.744910966
C   -9.1895672477   -2.9640946864   -1.3272079231
O   -5.1705676468   -5.1568909246   -4.5651638915
O   -5.5330650574   -5.5480155265   -1.9456042685
N   -9.0036622484   -2.0035906325   -0.2640172949
O   -10.1841578334  -3.1727125029    1.2827113614
C   -9.4983898726   -2.2053688559    0.9874143921
C   -9.1490207227   -1.1353117166    2.0009637516
H   -7.9520082131   -3.4075015795   -5.0789659192
H   -6.1839060666   -1.8705219622   -4.6649921198
H   -8.1740758551   -1.4544719709   -3.2907907067
H   -7.124479443    -3.4768761505   -1.2868999652
H   -8.7976747085   -6.0741542524   -2.5951783522
H   -8.2986717538   -6.2932927533   -4.8756182223
H   -6.8637593916   -7.0968175256   -4.2286089379
H   -6.6024070395   -5.0366478459   -5.9688614462
H   -4.7774234529   -3.5682702631   -3.7547726985
H   -5.835688226    -1.3763671382   -1.7791276505
H   -6.8069732938   -7.0903223685   -1.6658119686
H   -7.2460193334   -5.6306483114   -0.7853513076
```

```
H   -9.9421489928    -2.6241904457    -2.0514286698
H   -9.5716790181    -3.8781247405    -0.8659384647
H   -5.122478791     -5.5665205783    -3.6721152326
H   -5.5362808814    -4.5726952781    -1.9718661142
H   -8.3703122835    -1.2358129512    -0.4388120126
H   -10.0743121811   -0.6822830508     2.3653006175
H   -8.6615401525    -1.6083772656     2.856592208
H   -8.500507413     -0.3481795197     1.6085340148
```

calc_**2c** conf_4

```
C   -6.727583951     -2.4814269701    -3.9696822434
C   -7.8267375142    -1.9397592954    -3.0531785659
C   -8.1711603647    -3.1685744001    -2.1875653217
N   -8.0378437597    -4.2715700928    -3.1182549064
C   -7.2855291847    -3.8615109558    -4.3160482416
C   -7.659398608     -5.6127429175    -2.6774352421
C   -7.0274891003    -6.2034759196    -3.9519222941
C   -6.3340484302    -5.0303464966    -4.6562699263
O   -5.5554203207    -2.5283563148    -3.1682011646
O   -7.4574989378    -0.7998889843    -2.3240412841
C   -6.750568236     -5.6584507914    -1.4448263127
C   -9.549041133     -3.1025004804    -1.5273332808
O   -4.9852284111    -4.8599081587    -4.2398420132
O   -5.4992403403    -5.0059981602    -1.6253608684
N   -9.5773950642    -2.1589162234    -0.4317346773
O   -9.1123720865    -3.7437874779     1.1283228835
C   -9.2685526501    -2.5669618432     0.8328107557
C   -9.159601544     -1.4654229908     1.8646922106
H   -7.9754025622    -3.7345120077    -5.1658849659
H   -6.5607540931    -1.8511391374    -4.8515875392
H   -8.6985298519    -1.6618042088    -3.6565142035
H   -7.4380036266    -3.2026667994    -1.3633115649
H   -8.5551599987    -6.1903191524    -2.4067100039
H   -7.8221310338    -6.5886803237    -4.5980581611
H   -6.3313140471    -7.0233758779    -3.7540736672
H   -6.2859803333    -5.1777018734    -5.7375359577
H   -4.9564147461    -3.1470140666    -3.6373799492
H   -6.5406328535    -0.9539868027    -2.0471407587
H   -6.5178742146    -6.7016277089    -1.2143289303
H   -7.2720695004    -5.2432846266    -0.5735892357
H   -10.312244986    -2.8386092587    -2.2670495892
H   -9.8065360064    -4.0763335602    -1.1074241191
H   -4.9477148891    -5.140477452     -3.2967211464
H   -5.6624888044    -4.0542794372    -1.7583447168
H   -9.441438475     -1.1852180896    -0.6598585053
H   -9.3881933072    -0.4712986424     1.4735533421
H   -9.8425220484    -1.690057113      2.6870110904
H   -8.1468849855    -1.4640153884     2.2758190747
```

calc_**2c** conf_5

```
C   -7.2014432377    -2.3144769854    -4.3652207606
C   -7.4757635893    -1.9542237828    -2.8875337085
C   -8.0850199733    -3.2357690556    -2.2790763789
N   -8.0479861437    -4.262892433     -3.3355896027
C   -7.0783658451    -3.8365828716    -4.3456989877
C   -7.7063338365    -5.6662701518    -3.0037095268
C   -6.3094531717    -5.9233142949    -3.6513585756
```

S149

```
C   -5.7711775291   -4.5210835566   -3.9157551686
O   -6.1002683798   -1.6291648557   -4.8871965076
O   -6.2766122128   -1.5492446564   -2.2618367545
C   -7.7298968413   -6.0520956591   -1.5292524786
C   -9.507849986    -3.0628479267   -1.7428920204
O   -5.2195575532   -3.9815303963   -2.7137518143
O   -6.6651518125   -5.466949656    -0.7878576682
N   -9.5276452754   -2.3158154602   -0.4961404674
O   -8.5139110617   -3.9360863252    0.7225487162
C   -8.9980858763   -2.8055966327    0.646046492
C   -9.0347501884   -1.8912553013    1.8472145488
H   -7.3444649052   -4.2518550825   -5.328300087
H   -8.0847346457   -2.0662568368   -4.9663731555
H   -8.1510936298   -1.097433236    -2.8039686463
H   -7.4623335785   -3.4936205621   -1.423909764
H   -8.4472590364   -6.316509555    -3.4880161741
H   -6.4185194787   -6.4667952001   -4.5941365262
H   -5.6395989257   -6.502780611    -3.0094310407
H   -4.9937611105   -4.478313657    -4.681695193
H   -5.6445581137   -1.2740622389   -4.1021075052
H   -5.7015398399   -2.3495493777   -2.2765758821
H   -7.6302296408   -7.1432845077   -1.4772864226
H   -8.6852232758   -5.7899286835   -1.0669694032
H   -10.1410770269  -2.5422325252   -2.4662646563
H   -9.9563179436   -4.0441601285   -1.5690591012
H   -5.5718571227   -4.5057927065   -1.9618449685
H   -7.0864888815   -4.9290692347   -0.09162718
H   -9.8470897287   -1.36125629     -0.5048515372
H   -9.5960561072   -0.9688588425    1.6823902729
H   -9.4746364227   -2.4343836627    2.6860621335
H   -8.008888072    -1.6356570603    2.1250255
```

calc_**2c** conf_6

```
C   -6.7767353238   -2.3396637531   -3.9914167253
C   -7.9638045582   -2.0062621222   -3.0937844449
C   -8.1095145358   -3.2830266789   -2.2569143141
N   -7.8201457853   -4.3586634489   -3.2028261332
C   -7.038079973    -3.8044416274   -4.3358752037
C   -7.1099626071   -5.561686799    -2.7248062181
C   -5.6465705221   -5.3484281546   -3.1124565167
C   -5.7672472926   -4.6849827758   -4.4871164178
O   -5.5973984383   -2.1983746997   -3.2149565419
O   -7.6720197846   -0.8660581169   -2.3299479179
C   -7.2799013947   -5.9213616322   -1.25901736
C   -9.4977949914   -3.3994066749   -1.5917708365
O   -4.6309585242   -4.0096680316   -4.948697762
O   -8.6143372063   -6.2033781635   -0.8640786819
N   -9.443249675    -3.5310107659   -0.1531736686
O   -8.8561389405   -1.3674804656    0.1484336295
C   -9.0859468062   -2.4859675356    0.617761554
C   -9.0026618436   -2.7365945845    2.1037468513
H   -7.633018685    -3.8372564407   -5.2575107943
H   -6.7192669144   -1.7062686167   -4.8847703526
H   -8.8649788304   -1.8582238751   -3.7088104512
H   -7.352771309    -3.2061548493   -1.4612018806
H   -7.4944601517   -6.4169059335   -3.3086910317
H   -5.0586087938   -6.2700058767   -3.1403695334
H   -5.1721013691   -4.646457343    -2.4171374494
```

S150

```
H   -5.9659699941    -5.4614367768    -5.2341069954
H   -5.7922704151    -1.4492109057    -2.6203816899
H   -8.1318846965    -0.9446311677    -1.4647125906
H   -6.9492102769    -5.1044889172    -0.6135742172
H   -6.6283598458    -6.780880172     -1.047508782
H   -10.1002148055   -2.5145936381    -1.8199859515
H   -10.0113474192   -4.2718164874    -1.9920449107
H   -4.4948541013    -3.2656560769    -4.3382228222
H   -8.9645894977    -6.8779443869    -1.4598026793
H   -9.4454293914    -4.472037975      0.2145877336
H   -9.2181850473    -3.7701881437     2.3830760681
H   -8.0034576103    -2.4676933428     2.4542723443
H   -9.7115526429    -2.0766930443     2.6097926936

calc_2c conf_7

C   -6.5099237508    -2.5215859594    -4.1339453034
C   -6.8936606868    -1.5646215217    -3.0036938247
C   -7.3981490681    -2.5240346956    -1.8999149688
N   -7.9931977978    -3.6095990138    -2.6506825665
C   -7.653507676     -3.5289520035    -4.075643792
C   -8.079557692     -4.9846528566    -2.1807299773
C   -8.2479739762    -5.7621857558    -3.5001612266
C   -7.446160496     -4.9837264375    -4.5505443006
O   -5.2574455824    -3.0768008419    -3.7509636706
O   -5.8547628831    -0.7220319021    -2.5930547417
C   -6.8865763873    -5.4399961433    -1.3353897641
C   -8.3517945822    -1.8188235147    -0.9321789052
O   -6.0897742085    -5.4084917951    -4.6340213839
O   -5.6336211924    -5.342617371     -1.9971848522
N   -8.5455771331    -2.5098665304     0.3269015061
O   -10.5506276177   -3.4432866045    -0.1910897465
C   -9.6577159425    -3.2418293851     0.6166947476
C   -9.7177562985    -3.7983110317     2.0254518222
H   -8.4971247129    -3.1069008661    -4.647155703
H   -6.4209395337    -2.0178766142    -5.1037188231
H   -7.7177521969    -0.9218195445    -3.333764185
H   -6.5110314944    -2.8348767569    -1.3179475105
H   -8.9729619108    -5.1145906964    -1.5555053363
H   -9.30540617      -5.7547946397    -3.7804810005
H   -7.9261648503    -6.8057921056    -3.4381265753
H   -7.8527029243    -5.1185957881    -5.5552849316
H   -5.1624557661    -3.8786304992    -4.308041526
H   -5.0514328484    -1.2643612889    -2.6323778527
H   -7.0114079363    -6.4931606087    -1.068627945
H   -6.8594699156    -4.8705131173    -0.397127579
H   -7.9527071108    -0.8211766429    -0.7171765197
H   -9.3320263736    -1.7192262554    -1.4032608551
H   -5.8320087742    -5.7013213715    -3.7312028762
H   -5.4860230665    -4.4099802885    -2.2472761262
H   -7.8696924915    -2.3567937043     1.0576923059
H   -10.5836465201   -3.3674472025     2.5344580505
H   -9.8795606461    -4.8770458486     1.9699033968
H   -8.8237017861    -3.6026827969     2.6231725403

calc_2c conf_8

C   -7.1587817012    -2.3314264424    -4.3489187981
C   -7.2527184753    -2.0171172751    -2.8352914139

S151
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C  -7.8807907449  -3.2603092074  -2.2000926619
N  -7.992726737   -4.2667918068  -3.2759782639
C  -7.1415036279  -3.8639521412  -4.3928111626
C  -7.5621088882  -5.6404512304  -2.9700391119
C  -6.0336646389  -5.6219150866  -3.117742827
C  -5.7547042719  -4.5709761734  -4.2023064687
O  -6.0732363256  -1.6821887523  -4.963114182
O  -5.9516911787  -1.8076906936  -2.3036690019
C  -8.0550726673  -6.2488803949  -1.6585317736
C  -9.2813212557  -3.0014794348  -1.6319099701
O  -4.6804539281  -3.6950847218  -3.87381861
O  -7.4053372429  -5.7462396904  -0.5179468698
N  -9.2804750958  -2.2319944328  -0.404994782
O  -9.0677561     -4.0382136727   0.9465641458
C  -9.1575356194  -2.8197993831   0.8073386761
C  -9.1512555243  -1.8977071538   2.002685639
H  -7.5790828548  -4.2279490758  -5.3301010743
H  -8.0693649579  -1.9753227069  -4.8401126921
H  -7.8534008798  -1.1135575306  -2.6583922922
H  -7.2320514017  -3.5958869103  -1.3838268101
H  -7.9890947529  -6.2651700797  -3.7689055977
H  -5.6149745733  -6.6029020282  -3.3567754717
H  -5.5884080236  -5.2981803574  -2.1709153559
H  -5.4463274547  -5.0320831201  -5.1431681295
H  -5.3061216286  -2.2772983697  -4.8277785834
H  -5.5382228112  -1.1868054876  -2.9296389786
H  -7.8564330214  -7.3274377079  -1.7193551226
H  -9.1449558405  -6.1354920568  -1.5923720753
H  -9.8979363054  -2.486550298   -2.3748001588
H  -9.7648267517  -3.9550877515  -1.4178193931
H  -4.9184490781  -3.2521870375  -3.0346947757
H  -8.0327796199  -5.2088083615   0.0008511698
H  -9.2891803206  -1.2264251834  -0.4554140339
H  -9.3399620718  -0.8509379318   1.7535483324
H  -9.9088174695  -2.2401985137   2.7106006478
H  -8.1814761594  -1.9755017981   2.5006478316

calc_**2c** conf_9

C  -6.716259386   -2.3627110181  -3.6896297955
C  -7.7037752979  -2.1181408066  -2.5228160772
C  -8.0094333475  -3.5158864072  -1.9573730598
N  -7.8772689398  -4.3867639581  -3.114364075
C  -7.0877738138  -3.7665496544  -4.1822398887
C  -7.5839695737  -5.8159731985  -2.9937138231
C  -6.7330016284  -6.0988301455  -4.253360769
C  -5.996083608   -4.7937829866  -4.5355403271
O  -5.3952046318  -2.2669516864  -3.1942799866
O  -7.0924533139  -1.2442002364  -1.6036738416
C  -6.9344065753  -6.260179429   -1.674398872
C  -9.4377357906  -3.6573620662  -1.4059332582
O  -4.8465526661  -4.7514358391  -3.7088566487
O  -5.7747532248  -5.5742553582  -1.3035622024
N  -9.9231541972  -2.6223552186  -0.4970513091
O  -8.0471959231  -2.257525636    0.7282669339
C  -9.2516618775  -2.0789118166   0.5397773278
C  -10.056402701  -1.1968990762   1.4662813093
H  -7.7071992413  -3.6499797216  -5.0866716004
H  -6.84500349    -1.618599715   -4.484516442
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S152

```
H   -8.6246805745    -1.6662435981    -2.9174536876
H   -7.2769793065    -3.754274024     -1.1772548595
H   -8.5143036812    -6.4012906947    -3.0649288717
H   -7.3865271932    -6.341950927     -5.0973437934
H   -6.0329457465    -6.9277126908    -4.1189868903
H   -5.694226053     -4.7046460102    -5.5868039182
H   -5.4945068641    -1.7735785172    -2.3525250603
H   -7.2567784352    -1.5885024276    -0.6991943988
H   -6.7644323688    -7.3482826486    -1.759267333
H   -7.6536459793    -6.1289783711    -0.8561649329
H   -10.1105362333   -3.6555461171    -2.2674632916
H   -9.532106173     -4.6364139578    -0.9197161938
H   -4.7169325237    -3.8107131041    -3.4617018056
H   -5.2655572369    -5.3901152747    -2.1211080339
H   -10.9114676174   -2.4320823325    -0.5452522401
H   -9.5990728718    -0.2051854518     1.4896400566
H   -11.1089405884   -1.0991448251     1.1906691142
H   -9.9900713253    -1.6080450535     2.4765125452

calc_2c conf_10

C   -6.622332946     -2.4156912325    -3.8349604814
C   -7.766437461     -2.0461008462    -2.8983075912
C   -8.0552100857    -3.3942671617    -2.2243647534
N   -8.0033249417    -4.3298371681    -3.3504767749
C   -7.0593970072    -3.7814247352    -4.3632400809
C   -7.5604643454    -5.711523423     -3.0979259272
C   -6.0408174147    -5.678451177     -3.2701183668
C   -5.9187095823    -4.830395043     -4.5419501619
O   -5.4442119796    -2.5200050321    -3.0452252139
O   -7.329462409     -1.0336087303    -2.035541484
C   -8.0956429072    -6.4141540633    -1.8582871781
C   -9.3949364196    -3.4357368119    -1.4646322337
O   -4.6563621877    -4.3083191321    -4.837586059
O   -7.7014639042    -5.8770367694    -0.6063078974
N   -9.2405924365    -3.404982813     -0.025389024
O   -9.0543057258    -1.1494342718     0.0956956368
C   -9.0418952913    -2.2539622163     0.6469407668
C   -8.8331247245    -2.3745323377     2.1371147757
H   -7.5818787236    -3.6325139446    -5.315694724
H   -6.4704879912    -1.6864550344    -4.639089068
H   -8.6443024023    -1.7346937973    -3.48464603
H   -7.2518887641    -3.5633765857    -1.4930335169
H   -7.9605232205    -6.3164311327    -3.9284056673
H   -5.5833310908    -6.6662340481    -3.3784344409
H   -5.5553923729    -5.1486182963    -2.4408505486
H   -6.1719286087    -5.469939612     -5.395199145
H   -5.5409898602    -1.8217165725    -2.3718401229
H   -7.9705570994    -0.9535623801    -1.2942027687
H   -7.7971583756    -7.4699471025    -1.9286564396
H   -9.1880120287    -6.3928275242    -1.8578365815
H   -10.0278514476   -2.590046953     -1.7464845495
H   -9.9395786722    -4.3433346186    -1.725149655
H   -4.4685934321    -3.643556087     -4.1535231985
H   -6.736031331     -5.8688123746    -0.5804392885
H   -8.9781618531    -4.2804862966     0.4056160512
H   -9.6091382465    -1.7959575041     2.6439755654
H   -8.8633860808    -3.4038949622     2.5007042958
H   -7.8721166291    -1.9251322089     2.398751881
```

S153

calc_**2c** conf_11

```
C  -7.3462853727   -2.4343435998   -4.3594814932
C  -7.4024804158   -2.0180040318   -2.8709722304
C  -7.8955112802   -3.2593372861   -2.1281071238
N  -7.7958501732   -4.3708376324   -3.0790242792
C  -7.1164071221   -3.9535084303   -4.2967309089
C  -7.16508744     -5.6339500917   -2.6765003891
C  -5.6787840176   -5.4852466203   -3.0582209189
C  -5.6392613035   -4.4584248435   -4.2045310132
O  -6.3989669168   -1.6931090399   -5.0874281341
O  -6.0991307932   -1.6682348099   -2.4196977994
C  -7.3470237157   -6.0556718685   -1.2233376311
C  -9.3569138617   -3.1484806144   -1.6619743273
O  -4.6750972153   -3.4321402037   -3.98942322
O  -8.6925352504   -6.2302490854   -0.8613728251
N  -9.521743852    -2.3711926784   -0.4499666362
O  -9.0137864792   -4.087257822     0.9434890001
C  -9.3128017975   -2.9065153635    0.7743611117
C  -9.4767577953   -1.9739433521    1.951213155
H  -7.5794051846   -4.444533433    -5.1622046447
H  -8.3236904087   -2.2454142607   -4.8144225213
H  -8.067441041    -1.1564835616   -2.7207949975
H  -7.266626013    -3.3915362275   -1.2394662782
H  -7.6219346379   -6.4158897798   -3.298277999
H  -5.2109251572   -6.4359474566   -3.3261317863
H  -5.1103417443   -5.0753919233   -2.2134589234
H  -5.3412122357   -4.9159391118   -5.1501070019
H  -5.5511613778   -2.1709865425   -4.9762427842
H  -5.7861489218   -1.023033536    -3.077608809
H  -6.8475808401   -5.3382643582   -0.5583849456
H  -6.8097952989   -7.0076962045   -1.1043177589
H  -9.9750998056   -2.7061084141   -2.4486327058
H  -9.7256750712   -4.158367171    -1.4861983509
H  -4.9358510695   -2.9706110276   -3.166830942
H  -8.8918492436   -5.5714124822   -0.1712664765
H  -9.7100338046   -1.384524074    -0.5179820097
H  -10.2432202625  -2.3810080377    2.6146819885
H  -8.5403206536   -1.9490723081    2.5132882117
H  -9.7522624263   -0.9543327162    1.6720643978
```

calc_**2c** conf_12

```
C  -7.0776509013   -1.9221148945   -3.370140069
C  -6.2310269962   -2.1564019854   -2.0942504782
C  -6.7339404998   -3.4993269876   -1.5234130004
N  -7.7613128389   -3.9807151192   -2.4581892494
C  -7.5592814185   -3.3229858896   -3.7491976643
C  -7.7456196853   -5.4142524475   -2.7953926049
C  -6.616860367    -5.5638564282   -3.8332515121
C  -6.584524278    -4.2219095167   -4.5716142823
O  -6.3334154325   -1.2613439946   -4.3771802876
O  -4.8532743698   -2.1440222118   -2.3976491365
C  -7.6464085416   -6.3692563573   -1.6158219831
C  -7.2910299031   -3.3799987139   -0.0990553143
O  -5.2435184181   -3.7348692668   -4.6037140008
O  -8.796543042    -6.4407646936   -0.8261131672
N  -8.4075680638   -2.4678209705    0.007955745
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S154

```
O   -10.0451851437   -4.0429688413   -0.0866616873
C   -9.7032336564    -2.8693014313   -0.0141189194
C   -10.7325166624   -1.7648182637    0.0652159916
H   -8.516228231     -3.2850168449   -4.2831339015
H   -7.9550855706    -1.3159385421   -3.1161835392
H   -6.3646547586    -1.3345435159   -1.384694816
H   -5.857543347     -4.1641196928   -1.4677496261
H   -8.707543958     -5.6194900372   -3.2832573543
H   -6.7709224256    -6.4152787439   -4.5002543978
H   -5.6484715014    -5.7062013318   -3.3393392723
H   -6.9425147629    -4.3178354597   -5.6033933272
H   -5.5010056732    -1.010259691    -3.9348545783
H   -4.7118997012    -2.883774444    -3.0278723328
H   -6.7460199694    -6.1273659033   -1.0226696195
H   -7.4776133894    -7.3746917301   -2.01759703
H   -7.6340403449    -4.3533592524    0.2554725018
H   -6.4941943005    -3.0450685154    0.57384948
H   -5.3213258803    -2.8558235451   -5.0157810852
H   -9.1479702194    -5.5461316443   -0.6480605512
H   -8.2181653171    -1.4828686013    0.0939180741
H   -11.2497009709   -1.6996656736   -0.8958215528
H   -11.4756859412   -2.0332282328    0.8180314388
H   -10.313503519    -0.7846105847    0.3059831095
```

calc_**2c** conf_13

```
C   -6.8213471006    -2.3001204701   -3.5216872072
C   -7.3355465181    -2.1050751042   -2.0985022439
C   -7.2618389432    -3.5228050779   -1.519024773
N   -7.801583547     -4.3088480959   -2.6138351508
C   -7.4566008561    -3.6455248664   -3.8935308264
C   -7.5602405943    -5.7571971853   -2.7221119904
C   -7.4061922074    -5.9621261487   -4.2407482619
C   -6.6978058915    -4.6977330558   -4.7174530153
O   -5.4026889824    -2.3402755633   -3.5066374526
O   -6.5592615264    -1.1571886267   -1.4229988899
C   -6.3552283083    -6.2806073531   -1.9234935642
C   -8.0038961781    -3.6782230635   -0.1908889436
O   -5.3287538384    -4.8315413096   -4.4092685101
O   -6.2203630491    -7.6822676483   -2.063912302
N   -9.3366289685    -3.1130214279   -0.156457561
O   -8.6370403201    -1.0514916693    0.4719144332
C   -9.5544179341    -1.8265417993    0.1980623839
C   -10.9962646348   -1.3832627337    0.2655562162
H   -8.3822537524    -3.4252934543   -4.4471972421
H   -7.1488763443    -1.4978458319   -4.1936672891
H   -8.3886081525    -1.8009965834   -2.1551197283
H   -6.1993704834    -3.7332718612   -1.3116079828
H   -8.4360366278    -6.3151150438   -2.3637857932
H   -8.3919323277    -6.0417419579   -4.7112327932
H   -6.8453927565    -6.8633562197   -4.4989007144
H   -6.8366237174    -4.5228057875   -5.7944759067
H   -5.126587696     -1.758799255    -2.7785414877
H   -7.0563598104    -0.9361979583   -0.6108665331
H   -6.5097155939    -6.1049905066   -0.8540348179
H   -5.4450038478    -5.7581347249   -2.2297108859
H   -8.0777503735    -4.7345419353    0.081047344
H   -7.4253618599    -3.1768221075    0.5891482568
H   -4.998238425     -3.9473245449   -4.172469401
```

```
H   -5.7297736411    -7.8398444503    -2.8790089625
H  -10.1078468849    -3.6749946444    -0.4769374158
H  -11.708675652     -2.1541293106    -0.0367945238
H  -11.2180199979    -1.0799261187     1.291770186
H  -11.1268726575    -0.5030165047    -0.3675966504
```

calc_**2c** conf_14

```
C   -6.6714499758    -2.3052590389    -3.8683590479
C   -7.7402512583    -1.9973557647    -2.8128647986
C   -7.9338568264    -3.3475805702    -2.0961143133
N   -7.8901885198    -4.2707297504    -3.2139413166
C   -6.9909220715    -3.7518336139    -4.2627027269
C   -7.660616241     -5.7105025551    -3.0321886503
C   -6.6943618474    -6.0772054767    -4.176713244
C   -5.8788979474    -4.8050564168    -4.3869082956
O   -5.3874691548    -2.1548122731    -3.2835639125
O   -7.2758358805    -0.9453931037    -2.0180881872
C   -7.0976123213    -6.1355735248    -1.6696313567
C   -9.266523792     -3.4680785883    -1.3293733603
O   -4.9168752096    -4.7441381217    -3.3610634861
O   -7.0066440023    -7.5422748928    -1.5747309128
N   -9.1776912806    -3.1921512671     0.0934691472
O   -9.1853151921    -0.9370392089    -0.092607704
C   -9.1596891987    -1.947600729      0.6122378164
C   -9.1224833159    -1.8454333381     2.1177846154
H   -7.5252865068    -3.7334840648    -5.2245200315
H   -6.7467559634    -1.6286611353    -4.7276752465
H   -8.6806246465    -1.73825543      -3.3213346076
H   -7.1027669814    -3.4700931432    -1.3801329006
H   -8.6134106361    -6.2525197929    -3.1639323419
H   -7.2491992081    -6.3234874698    -5.0879533617
H   -6.0637564515    -6.928664274     -3.9132074312
H   -5.4059883124    -4.7707387459    -5.3797562863
H   -5.5138046058    -1.5064590615    -2.5666719923
H   -7.9439052863    -0.782503809     -1.3178790205
H   -7.7157610911    -5.7339729659    -0.8499028253
H   -6.0838295772    -5.7528236571    -1.5538989668
H  -10.0142427152    -2.7979816296    -1.7635468838
H   -9.6496014553    -4.4853673294    -1.4317943667
H   -4.7351198625    -3.7985658861    -3.2107162759
H   -7.8869798545    -7.9036374289    -1.7423803412
H   -9.1019104924    -3.9734675675     0.7245307175
H   -9.9789318212    -1.2523024449     2.4464391119
H   -9.1406935906    -2.8110570543     2.6280044547
H   -8.2207469061    -1.3029388757     2.4116883295
```

calc_**2c** conf_15

```
C   -6.2417042566    -2.6029405763    -3.717873018
C   -7.2770248313    -1.966808115     -2.7851662108
C   -7.8770602612    -3.1865108831    -2.0498287823
N   -7.8768629825    -4.225479672     -3.0663339565
C   -7.0142638679    -3.8289496121    -4.2020239523
C   -7.6330973657    -5.6270388403    -2.7313486038
C   -7.231495717     -6.1824964643    -4.1050263196
C   -6.2873611571    -5.1103776382    -4.6478104734
O   -5.1259896598    -2.8940648838    -2.9017063864
O   -6.732815243     -0.9985833139    -1.9230535502
```

S156

```
C   -6.5380324601   -5.8372489317   -1.654069407
C   -9.2626120726   -2.9165753087   -1.4724004626
O   -4.9723406768   -5.2415610001   -4.1045459647
O   -5.7006660585   -6.9352708842   -2.0308644528
N   -9.1844866447   -1.89080851    -0.4561436429
O   -10.6451993801  -2.8865157796   0.9670688593
C   -9.8734877644   -1.9732242202   0.7119885951
C   -9.626915942    -0.8413933618   1.6890731011
H   -7.6466589375   -3.5024161552   -5.0423267192
H   -5.9552074178   -1.937037679    -4.5427201491
H   -8.056104831    -1.4685502539   -3.3732067764
H   -7.2033292573   -3.4117917054   -1.2082473488
H   -8.5603974327   -6.0982338702   -2.3894259496
H   -8.125576992    -6.229400353    -4.7333274922
H   -6.7808485318   -7.1751461202   -4.0694132643
H   -6.1880969935   -5.1462228883   -5.7365581879
H   -4.7240409094   -3.7048919763   -3.2768476019
H   -5.8755359458   -1.3652177658   -1.6493688356
H   -6.9957020834   -6.0367062758   -0.6784275599
H   -5.9308060154   -4.9289149509   -1.5721758438
H   -9.9438530894   -2.6277990567   -2.2842133195
H   -9.6823935399   -3.8083367092   -1.0002024863
H   -4.9880314997   -5.9738665674   -3.4554180854
H   -5.0946610871   -7.1117145264   -1.2994447643
H   -8.5018194198   -1.1576716071   -0.5932208196
H   -10.5718573949  -0.3236653257   1.8716217245
H   -9.3007960933   -1.2648832106   2.6419514121
H   -8.8858661869   -0.1146850075   1.3470366948

calc_**2c** conf_16

C   -7.4816816338   -2.1858258081   -3.4047906644
C   -6.7415461771   -2.3642794306   -2.0598187458
C   -7.1368905405   -3.7529164013   -1.5491830537
N   -7.9725481097   -4.363339653    -2.6198116772
C   -7.7360152321   -3.626262893    -3.8632296721
C   -7.6902059976   -5.7562541921   -2.9932822498
C   -6.4356266366   -5.6927408625   -3.8770019285
C   -6.5677385827   -4.3511843298   -4.6202362508
O   -6.7909501226   -1.36644266     -4.3130859283
O   -5.3308486772   -2.3400585027   -2.2720150956
C   -7.657284322    -6.7704261931   -1.86561311
C   -7.9297073762   -3.702901232    -0.2449593766
O   -5.3523811917   -3.6200651402   -4.686000782
O   -6.4941688791   -6.6089261418   -1.0786949886
N   -9.2040836759   -3.0527856507   -0.4308398097
O   -8.8622135222   -1.3846578133   1.0731727138
C   -9.5647157566   -1.917798766    0.2271151841
C   -10.9188708265  -1.3534325818   -0.1522498831
H   -8.6326080594   -3.6826175834   -4.4919878469
H   -8.4452258818   -1.7070652512   -3.2055785605
H   -7.0050507332   -1.5765039205   -1.3454717594
H   -6.2209374058   -4.3235394462   -1.3657410588
H   -8.5391606836   -6.0640232837   -3.6218910168
H   -6.3458900949   -6.5470828894   -4.553130068
H   -5.538273253    -5.6758870186   -3.2507698212
H   -6.8506010554   -4.5025807097   -5.6644341161
H   -6.1489140056   -1.9539084819   -4.7601941503
H   -5.1666793225   -1.5038185771   -2.7392843609
```

```
H   -7.6827752218   -7.7715172036   -2.3204789942
H   -8.569914184    -6.6562771381   -1.2627663938
H   -8.0742406264   -4.7224089051    0.1288224481
H   -7.3882196104   -3.1401638479    0.5181468204
H   -5.0880525226   -3.4080881983   -3.7651152543
H   -6.4951258866   -7.2897464313   -0.3955411793
H   -9.7663166291   -3.4022653908   -1.1921673415
H  -11.5511288919   -1.3334301473    0.7387302584
H  -10.7895414577   -0.3192613621   -0.4799369035
H  -11.4308672143   -1.9165159617   -0.9366853831
```

calc_**2c** conf_17

```
C   -6.6750942072   -2.3507917887   -3.8877847348
C   -7.7453035248   -1.9215536686   -2.8917137134
C   -8.0478919826   -3.2385504137   -2.1561917208
N   -8.0100242703   -4.2352567417   -3.2270042521
C   -7.1850724061   -3.7136974024   -4.3447360165
C   -7.5150602423   -5.5924368108   -2.9224151729
C   -6.040585224    -5.577537671    -3.3258239436
C   -6.0829381869   -4.7734803501   -4.6304491746
O   -5.451750899    -2.4746011502   -3.1765433466
O   -7.2243037358   -0.9038698236   -2.0838527953
C   -7.7852378912   -6.0843997116   -1.5052042708
C   -9.4057343386   -3.2279455076   -1.4139587298
O   -4.8645639178   -4.2561870778   -5.0846942011
O   -7.3869124049   -7.4274984032   -1.3380966462
N   -9.3064964415   -3.2441085403    0.0331496798
O   -8.6998109478   -1.0727696524    0.2149677389
C   -8.9699713701   -2.1499738331    0.7473186293
C   -8.9533403431   -2.3004836009    2.2489018826
H   -7.8076854543   -3.5676599519   -5.2361740177
H   -6.5582463149   -1.6467372961   -4.7201661665
H   -8.6451495194   -1.591407684    -3.433802802
H   -7.2467043322   -3.3706853195   -1.4122447409
H   -8.0424208085   -6.2911041656   -3.5878604659
H   -5.6081995248   -6.571497168    -3.4747883883
H   -5.4437769489   -5.0308007981   -2.5854309113
H   -6.4342177332   -5.4327892734   -5.4314350643
H   -5.4792217697   -1.7542409949   -2.5201114842
H   -7.7641164174   -0.850277924    -1.2653292279
H   -8.8603824551   -6.0739140009   -1.3013942631
H   -7.2952733012   -5.4334329256   -0.7659849933
H   -9.9837633682   -2.3428555361   -1.6987188245
H   -9.9847244553   -4.1000302434   -1.7197046202
H   -4.585615635    -3.6025366301   -4.4216851312
H   -6.430895739    -7.4639016887   -1.4678338124
H   -9.4836596418   -4.1067061897    0.5214516352
H   -7.9527509439   -2.0610368441    2.6163900772
H   -9.6403726843   -1.5683271079    2.6794037333
H   -9.232730619    -3.29791611      2.5955502564
```

calc_**2c** conf_18

```
C   -7.2459899791   -2.4653046733   -4.5053771967
C   -7.0338454379   -1.8665982356   -3.0973965848
C   -7.5270658067   -2.9608957192   -2.1249149478
N   -7.7871904212   -4.1659951757   -2.9550107395
C   -7.1668636251   -3.9744664815   -4.2735478612
```

```
C   -7.2417156673   -5.4610212373   -2.5299326272
C   -5.756882357    -5.4346471022   -2.9243397953
C   -5.7418167222   -4.6208769374   -4.2194262475
O   -6.303142231    -1.9648443089   -5.4371107054
O   -5.6922317845   -1.4703972195   -2.9208880588
C   -7.4950820235   -5.898114065    -1.0998541386
C   -8.7890444917   -2.4748014687   -1.4056236683
O   -4.6707448931   -3.6880971818   -4.1642665154
O   -8.864442149    -6.1350424857   -0.8128530636
N   -9.2580324976   -3.35001236     -0.3654721496
O   -9.1847077056   -1.7732407104    1.2740301202
C   -9.4145720434   -2.9198663875    0.9174458396
C   -9.9211468716   -3.9708433009    1.8839837174
H   -7.7521478796   -4.5196105606   -5.0239897354
H   -8.2563170034   -2.2240311111   -4.8553017645
H   -7.6136707657   -0.9481573728   -2.9747374885
H   -6.7398582076   -3.1267036233   -1.3766203368
H   -7.7346597221   -6.2081455562   -3.1758805568
H   -5.3221711636   -6.4310402389   -3.0355342247
H   -5.1674355618   -4.896263262    -2.1730907199
H   -5.5999248357   -5.2666000861   -5.094851228
H   -5.8305274349   -1.2661618867   -4.9471921691
H   -5.1382830548   -2.2667471776   -3.0674273332
H   -7.1702737542   -5.1380748458   -0.3857922967
H   -6.9035602987   -6.8039208755   -0.9076516706
H   -8.5862237183   -1.516112796    -0.9212283345
H   -9.5725753758   -2.3198453264   -2.1602074006
H   -4.8008711458   -3.1202858775   -4.9460498153
H   -9.2208878766   -6.7175358244   -1.4960225694
H   -9.4444785848   -4.3209626379   -0.593386582
H   -9.3317548939   -3.9131657485    2.8011667732
H   -10.9566711545  -3.7377173832    2.1485586567
H   -9.8771908607   -4.9858527589    1.4827934189
```

calc_**2c** conf_19

```
C   -7.4768563454   -2.2378111632   -3.702420941
C   -6.758046429    -2.1371007271   -2.3318543598
C   -6.9302804079   -3.5257290136   -1.6789707413
N   -7.7277974125   -4.3288212534   -2.6374637383
C   -7.5485806948   -3.7408225541   -3.9717780532
C   -7.3212994553   -5.7328717716   -2.8397426614
C   -6.076405498    -5.669207652    -3.7392414759
C   -6.2880556549   -4.4146646713   -4.596445939
O   -6.8005937357   -1.5030934345   -4.7055452632
O   -5.410574159    -1.7562950696   -2.5002380597
C   -7.1687811784   -6.5358007271   -1.5620202419
C   -7.6280525463   -3.4516925831   -0.3213165924
O   -5.1172740729   -3.6064895506   -4.5361396901
O   -8.3865302306   -6.6928975426   -0.8712362574
N   -9.0049365666   -3.0581574211   -0.5003504487
O   -9.1422137514   -1.840430324     1.4057384163
C   -9.6690700412   -2.2734483284    0.3940428499
C   -11.1138201025  -1.9782988849    0.0489003861
H   -8.4148575548   -3.9999212985   -4.5914515614
H   -8.4990299894   -1.8537538116   -3.6030984978
H   -7.2059576094   -1.3546428884   -1.7157513067
H   -5.9235928324   -3.9379154776   -1.5212217565
H   -8.1402304247   -6.1976458699   -3.4048385632
```

```
H   -5.9454519744   -6.5758412388   -4.3342865565
H   -5.1644125495   -5.5299064697   -3.1483642112
H   -6.4834568542   -4.6702469412   -5.6444902413
H   -6.1424490516   -0.9759155905   -4.2145145071
H   -4.9925983827   -2.4773992983   -3.015483036
H   -6.3919085515   -6.090286311    -0.9209068206
H   -6.8273380924   -7.5430248081   -1.8169595671
H   -7.5599435608   -4.4135119318    0.203280104
H   -7.1439483501   -2.710705759     0.3194033738
H   -5.3589688804   -2.804428197    -5.0344004754
H   -8.8094510838   -5.8251579207   -0.8318031362
H   -9.459435003    -3.4056493026   -1.3329924373
H   -11.4192572769  -2.3476083175   -0.9333746339
H   -11.755792446   -2.429341469     0.8100257749
H   -11.2707512494  -0.8984644268    0.0913108667

calc_2c conf_20

C   -7.1685462742   -2.4095061601   -4.1921687604
C   -7.8955671769   -2.2084557727   -2.8383358362
C   -7.8163167015   -3.5682450473   -2.1111406772
N   -7.8440868985   -4.5016607324   -3.2570164414
C   -6.9124088501   -3.9192107155   -4.2444831957
C   -7.3050858068   -5.8673317779   -3.1109477016
C   -5.7705146834   -5.7596529875   -3.1542074982
C   -5.489479193    -4.4165222926   -3.8460861038
O   -5.9860262034   -1.6317017502   -4.2711410045
O   -7.2990540637   -1.132043362    -2.1721355185
C   -7.8725846656   -6.6504211599   -1.9498617367
C   -8.9934433927   -3.7633989266   -1.1340329239
O   -4.8350024072   -3.5914301493   -2.9102890547
O   -9.2788487339   -6.7875361509   -2.0417189589
N   -8.6999763007   -3.3498082063    0.2277628962
O   -9.0221182782   -1.1308590843   -0.0924003304
C   -8.7593919396   -2.0738476835    0.6574056802
C   -8.4940820182   -1.847122573     2.1265306926
H   -7.1464130441   -4.3367216108   -5.2315715734
H   -7.8286913637   -2.1140181169   -5.0151137861
H   -8.9538957868   -1.9958579084   -3.0389474265
H   -6.8677142082   -3.603511226    -1.5574693223
H   -7.6307706127   -6.3900053157   -4.0226566506
H   -5.3276250421   -6.6113529462   -3.6765527985
H   -5.3318779992   -5.7143818712   -2.1529660332
H   -4.8733164326   -4.5386877035   -4.748713188
H   -6.1269886422   -0.9195131281   -3.6175970818
H   -7.8939366416   -0.8928257743   -1.4308859397
H   -7.5923757086   -6.1712727881   -0.9989370127
H   -7.4331961616   -7.6537076208   -1.9422856718
H   -9.858681963    -3.1884781987   -1.478378057
H   -9.3026103696   -4.8073137132   -1.0869469695
H   -4.8882979917   -2.695137487    -3.2916431218
H   -9.5756055129   -6.1292643351   -2.6865245044
H   -8.4547549383   -4.0644868244    0.8936180711
H   -9.3416636282   -1.3058922148    2.5527823653
H   -8.3344165979   -2.7660607022    2.6950955459
H   -7.6146337674   -1.2067559827    2.2299596278

calc_2c conf_21
```

```
C   -7.4359554683   -2.3492301146   -3.9937547643
C   -7.5283450146   -2.2213448754   -2.4589429596
C   -7.9740357897   -3.6207221156   -1.9902448623
N   -7.8990689278   -4.5221371866   -3.1716713622
C   -7.1099216272   -3.8297385158   -4.2028383132
C   -7.1438561983   -5.7758244428   -2.9678631738
C   -5.6742108077   -5.3584304213   -2.9347127566
C   -5.6054199229   -4.2429059326   -3.9990672525
O   -6.6041234125   -1.4445252797   -4.6473927341
O   -6.2644142589   -1.8863045957   -1.913164436
C   -7.6958920882   -6.604288299    -1.8264398035
C   -9.3944688835   -3.6597621438   -1.4267847523
O   -4.7241737785   -3.1894576871   -3.6648453838
O   -9.0620200719   -6.9000897621   -2.0489075987
N   -9.6529806448   -2.7520632924   -0.3111946644
O   -7.5558201903   -2.3352083989    0.5087526785
C   -8.7789655276   -2.2145471914    0.5707188375
C   -9.4048303629   -1.4076637918    1.6883625158
H   -7.4370429411   -4.1622500436   -5.1932934911
H   -8.4472846582   -2.1791376943   -4.3799431368
H   -8.252136397    -1.4466247426   -2.1809886208
H   -7.2832486863   -3.9361714239   -1.2055117582
H   -7.3113129312   -6.3637705117   -3.8823047475
H   -4.984255861    -6.1812841696   -3.1371674969
H   -5.4085861601   -4.9402909946   -1.9565900345
H   -5.2189085912   -4.6398806492   -4.9409202776
H   -5.6936729678   -1.7294338054   -4.447098983
H   -6.3969324045   -1.9280177646   -0.9465014176
H   -7.5623793533   -6.0843863533   -0.8661497064
H   -7.1497039752   -7.5506639208   -1.7579481058
H   -10.0889693027  -3.3941956933   -2.2315959561
H   -9.6289941615   -4.6860421003   -1.1213113159
H   -5.0458956128   -2.791745415    -2.8262829022
H   -9.3786499972   -6.2171991666   -2.6594578604
H   -10.6288217671  -2.597586848    -0.1128105642
H   -8.9756929663   -0.4033543041    1.6737806378
H   -10.493271991   -1.331187548     1.6358771975
H   -9.1267362986   -1.8645328041    2.6412093255


calc_2c conf_22

C   -7.5713198783   -2.2681069679   -3.4441407678
C   -6.8176896331   -2.271478091    -2.0895335447
C   -6.9648715512   -3.7097163833   -1.549899528
N   -7.7403022802   -4.4480215468   -2.5665908206
C   -7.6250438998   -3.7437116741   -3.8443428367
C   -7.3206627286   -5.8154437236   -2.8905437303
C   -6.1267410455   -5.6619447725   -3.8542615331
C   -6.3858279968   -4.335911614    -4.5805890446
O   -6.9330884004   -1.4347120746   -4.3963139984
O   -5.4745240598   -1.868987316    -2.269377268
C   -7.0393168443   -6.7201576754   -1.7110106326
C   -7.6800530568   -3.7622855862   -0.1970828573
O   -5.2224596238   -3.5204369311   -4.4887363836
O   -8.2343048915   -6.9020212706   -0.9790067869
N   -9.0582354179   -3.3571307688   -0.3188149551
O   -8.8670632786   -1.4274573351    0.8642755814
C   -9.5492867373   -2.2080020582    0.2148780714
C   -11.0233675712  -1.9590804365   -0.0319274697
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S161

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H   -8.5120908403    -3.9613787858    -4.452237071
H   -8.5963989187    -1.914967998     -3.2854195899
H   -7.2449466685    -1.5445222242    -1.3958947863
H   -5.9470868199    -4.1085073437    -1.4164300699
H   -8.1589379634    -6.2681445754    -3.4371478807
H   -6.0253332302    -6.5097837981    -4.5360740643
H   -5.1838866834    -5.5671259342    -3.3039422719
H   -6.6189318932    -4.4950155091    -5.6403754599
H   -6.2655174198    -0.9488770174    -3.8757249669
H   -5.0679209781    -2.5398094434    -2.8555477505
H   -6.2415427033    -6.2935495577    -1.0847172795
H   -6.663663928     -7.6759466548    -2.1054058339
H   -7.6455694409    -4.7793053046     0.2031343914
H   -7.2014339756    -3.0853373791     0.5133649423
H   -5.5027271469    -2.6721154204    -4.8801423452
H   -8.0524135677    -7.516462946     -0.2575716859
H   -9.6265282145    -3.9214334596    -0.9312662528
H  -11.1458806933    -0.958414246     -0.452014508
H  -11.4906088163    -2.6896634969    -0.6969016952
H  -11.5454212031    -1.9730326799     0.9283326829

calc_2c conf_23

C   -7.36793157      -2.6465208664    -4.6215955006
C   -7.4414976165    -1.949584423     -3.2415598021
C   -7.7125917851    -3.0805837295    -2.2192132579
N   -7.7672490138    -4.3387826773    -3.0195209596
C   -7.0414388203    -4.0956326137    -4.2784597895
C   -7.0531600878    -5.5215014709    -2.5006958334
C   -5.5625574924    -5.2370138455    -2.7032878334
C   -5.5374778351    -4.4407873263    -4.0144429386
O   -6.4245153687    -2.0242090959    -5.4746263165
O   -6.2710362762    -1.2066583031    -2.988193705
C   -7.5189265115    -5.9505693827    -1.1303607737
C   -9.0072661049    -2.7688256991    -1.4527972404
O   -4.6993063722    -3.3048627371    -3.8513833678
O   -8.9231693113    -6.1846202725    -1.1472208582
N   -9.2279285101    -3.5057411042    -0.234967535
O   -9.1661820373    -1.6742960197     1.1155539616
C   -9.3083612402    -2.8791518015     0.9733748743
C   -9.596917368     -3.7925358899     2.14664322
H   -7.4194939815    -4.7858349283    -5.0412197811
H   -8.3555409852    -2.6176873014    -5.0962812025
H   -8.2480170386    -1.2124189301    -3.2303524218
H   -6.8827021215    -3.0828988071    -1.4989518194
H   -7.33002171      -6.3370373838    -3.1864240439
H   -4.9581614647    -6.1460995707    -2.7417247854
H   -5.16168564      -4.6042722146    -1.9044540902
H   -5.1505618586    -5.0476925681    -4.8420529083
H   -6.1867509474    -1.2004537002    -5.0083563435
H   -5.5369285105    -1.8548170364    -2.961945917
H   -7.2788618944    -5.187159835     -0.3793293467
H   -7.0189101942    -6.8793339697    -0.8383888805
H   -8.9779427938    -1.7197145909    -1.1468818954
H   -9.8527966915    -2.9018721387    -2.1415339637
H   -4.813905368     -2.8035246385    -4.6795650057
H   -9.2438050999    -5.8002144002    -1.979154025
H   -9.3899529867    -4.5056476061    -0.2943536376
H   -8.838405841     -3.6261646383     2.9147799445
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H   -10.5615197324   -3.5143175258    2.5791713282
H    -9.6185218185   -4.8529609576    1.8837724508
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calc_**2c** conf_24

```
C    -7.3845072046   -2.1450618701   -3.3301354947
C    -6.703964265    -2.4141708172   -1.9641964348
C    -7.1417849601   -3.8368028023   -1.5644736693
N    -7.9971360224   -4.3284915881   -2.6742409447
C    -7.6925809627   -3.5420585051   -3.8730121881
C    -7.8160386685   -5.7127879048   -3.124306792
C    -6.5615584265   -5.6925873154   -4.0182091418
C    -6.5488126156   -4.2866640846   -4.6292854861
O    -6.5628033711   -1.36277744     -4.1790710518
O    -5.3030441633   -2.2599068887   -2.0729675259
C    -7.8473332017   -6.7925576956   -2.0489671046
C    -7.9214110063   -3.8588609119   -0.2503157479
O    -5.2625319776   -3.7096109671   -4.4368181836
O    -6.7433427472   -6.8106604445   -1.1684544615
N    -9.1825529456   -3.1703042866   -0.3853063791
O    -8.7907011398   -1.594463339     1.2043834443
C    -9.5136436033   -2.0682314964    0.3406440075
C   -10.8650324555   -1.4638562481    0.0158001752
H    -8.5742170912   -3.5322050901   -4.5259793128
H    -8.3326977053   -1.6210917107   -3.1643339225
H    -7.0150742261   -1.6795772645   -1.2184607793
H    -6.2431492665   -4.4493357034   -1.4295223883
H    -8.682701259    -5.9265518726   -3.7679613538
H    -6.5616556199   -6.4873779384   -4.7686326075
H    -5.6501267646   -5.7971425077   -3.419248917
H    -6.7658697015   -4.3116262263   -5.7040613264
H    -5.8363588244   -1.0691301047   -3.5964348201
H    -5.0045542836   -2.9466961803   -2.7035024438
H    -7.9645031213   -7.7652022882   -2.548242386
H    -8.7304307972   -6.6458089206   -1.4218040676
H    -8.0827923983   -4.8936266664    0.0686385995
H    -7.3587945062   -3.3522977379    0.536539324
H    -5.3702128826   -2.7910014363   -4.7470893713
H    -5.978125947    -7.1463354089   -1.650657303
H    -9.7584533291   -3.4586953549   -1.1616058822
H   -11.3827450427   -1.953437217    -0.8130315889
H   -11.495599016    -1.5193147485    0.9066822558
H   -10.7301584809   -0.405691017    -0.21935873
```

calc_**2c** conf_25

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C    -7.3054715723   -2.3213517297   -3.8385549614
C    -7.2120284058   -2.311596067    -2.2916792505
C    -7.5980931681   -3.7447594907   -1.8661960092
N    -7.8517738753   -4.5007443376   -3.1148193376
C    -7.1689429144   -3.7980786375   -4.2103757603
C    -7.2860597146   -5.8591842811   -3.202021231
C    -5.7853481413   -5.6645150605   -3.4486415671
C    -5.7199526885   -4.3841096038   -4.2914864026
O    -6.3258065296   -1.4830320501   -4.427598712
O    -5.9225604454   -1.9153403313   -1.8719403004
C    -7.6992358197   -6.7529877919   -2.0521456053
C    -8.8446772289   -3.7728139697   -0.9723712688
O    -4.7171009804   -3.5277256178   -3.758534355
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O   -9.1013906268   -6.9169093831   -2.0145256302
N   -8.6568161027   -3.0919066507    0.2880620756
O   -9.7347702193   -1.1890853672   -0.3160014357
C   -9.1328696572   -1.8381077594    0.5272147738
C   -8.8557212551   -1.2891443629    1.9097535114
H   -7.6824504756   -4.0250487567   -5.1515048894
H   -8.300402865    -1.9787355722   -4.1435019203
H   -7.8969356181   -1.5764142146   -1.8665684211
H   -6.7473703092   -4.15060901     -1.2974540926
H   -7.7267428134   -6.3004168483   -4.1075511614
H   -5.3227748882   -6.524138768    -3.9391118219
H   -5.2451649566   -5.4888378678   -2.5116917434
H   -5.4717782086   -4.6065584056   -5.3364273341
H   -5.9539181767   -0.9860448355   -3.6749002805
H   -5.3005238988   -2.5751618932   -2.2439441103
H   -7.3220260231   -6.3500264194   -1.0991044112
H   -7.2529038191   -7.7444046694   -2.1783240341
H   -9.6660766851   -3.2711606779   -1.4888464479
H   -9.1472992707   -4.805684705    -0.7771306139
H   -4.8250625418   -2.6967494829   -4.2584654786
H   -9.4774423094   -6.1179863896   -2.4120175133
H   -8.148540319    -3.5630913776    1.0185449862
H   -8.1535139348   -0.4559024972    1.8220127
H   -9.7860359448   -0.8907877047    2.3191023011
H   -8.4434175969   -2.0248474122    2.6047457529

calc_2c conf_26

C   -7.201144057    -2.2422100028   -3.8116053501
C   -7.180345366    -2.3536517594   -2.2697143977
C   -7.7993626364   -3.7188743396   -1.9578992803
N   -7.9989668885   -4.3970428481   -3.2609090101
C   -7.2053028513   -3.7041048556   -4.2737260947
C   -7.5697212723   -5.7937127687   -3.3718299132
C   -6.0455434201   -5.7324517267   -3.5608390941
C   -5.8166035785   -4.4331899396   -4.3572175086
O   -6.1651421012   -1.4401882205   -4.321442973
O   -5.8283603237   -2.3361206221   -1.8008329353
C   -8.0803024855   -6.7515165053   -2.3017580127
C   -9.1414479529   -3.6183747308   -1.227257761
O   -4.7105577237   -3.679364039    -3.8869744631
O   -7.5612415601   -6.559628682    -0.9987394222
N   -9.0024259008   -3.1836867269    0.1439328852
O   -9.5814711949   -1.0196986301   -0.2215769542
C   -9.2316608458   -1.9050217477    0.5464254226
C   -9.026183122    -1.640844262     2.0234083227
H   -7.6970682596   -3.8010971501   -5.2488351087
H   -8.1454768224   -1.7792731623   -4.1122009529
H   -7.7308799031   -1.5361351337   -1.7950392868
H   -7.1047436952   -4.265850753    -1.310628947
H   -8.0093645199   -6.1643008694   -4.3104393313
H   -5.631980115    -6.615044655    -4.0566450514
H   -5.5380090583   -5.6303373796   -2.593646978
H   -5.5790672716   -4.649631309    -5.4012864645
H   -5.3898701734   -2.0298928304   -4.4009915414
H   -5.4603959177   -1.5092991115   -2.1551302273
H   -7.8894688279   -7.7781902868   -2.6458272152
H   -9.1635822602   -6.6392201434   -2.2119989231
H   -9.7970045373   -2.9072057507   -1.7337004903
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H  -9.6311081604   -4.5952189117   -1.2398275996
H  -4.9218678523   -3.4046172581   -2.9675979725
H  -6.6312832584   -6.8174843829   -1.0096937485
H  -8.6626889604   -3.8546846294    0.8141800902
H  -9.9369783246   -1.1933795024    2.4273173765
H  -8.7790336245   -2.5328005884    2.6045840454
H  -8.2243451771   -0.9076537854    2.1409648665

calc_2c conf_27

C  -7.2008588926   -2.5030069594   -4.4603115548
C  -7.4070558746   -2.073860517    -2.9831367209
C  -7.827476514    -3.3621275892   -2.2474933869
N  -7.8889448576   -4.423055788    -3.2791413662
C  -7.0008813847   -4.01437498     -4.37468155
C  -7.336334076    -5.7368350046   -2.8937220572
C  -5.8122023073   -5.555854574    -2.8989040475
C  -5.5694477278   -4.524778127    -4.009282437
O  -6.128576156    -1.8018776043   -5.0629542399
O  -6.240422206    -1.4670677588   -2.4707102551
C  -7.9764604719   -6.3079320999   -1.6452472421
C  -9.1747668386   -3.2212670472   -1.5298283472
O  -4.7020492773   -3.5056088844   -3.521666832
O  -9.3588334791   -6.5341400658   -1.8578895288
N  -9.1280915978   -2.2640916326   -0.4458417354
O  -8.0225703457   -3.6648264599    0.9443399981
C  -8.5106192404   -2.5646844045    0.7297058796
C  -8.4547471327   -1.4470257521    1.7476666356
H  -7.3187419787   -4.5156709809   -5.2959263857
H  -8.1185190855   -2.3095430624   -5.0277732033
H  -8.1781480166   -1.3011068627   -2.9130411482
H  -7.0719743353   -3.5686084192   -1.4781228482
H  -7.6043004582   -6.4148763666   -3.7164643877
H  -5.2797947389   -6.4949223996   -3.0657784211
H  -5.4550189104   -5.1387706786   -1.9515690279
H  -5.105308885    -4.9849327017   -4.8899238202
H  -5.8979967928   -1.1136144656   -4.4102904501
H  -5.55370224     -2.1668154467   -2.4779374158
H  -7.8118412015   -5.6499166884   -0.7804239667
H  -7.5223688228   -7.2763072579   -1.4131122099
H  -9.9409552803   -2.9050659824   -2.244371423
H  -9.4815398236   -4.1847969984   -1.1170723057
H  -4.6689427722   -2.8565901565   -4.2474168286
H  -9.6488603293   -5.850478103    -2.4784195245
H  -9.4331899852   -1.3190915143   -0.6096094302
H  -8.6599150955   -1.8646545113    2.7344259233
H  -7.4416914647   -1.0348704488    1.7669885713
H  -9.1578514035   -0.6349517064    1.5459370901

calc_2c conf_28

C  -7.5915148903   -2.2067132225   -3.4149825542
C  -6.7852825103   -2.2475199764   -2.0971949388
C  -7.0690902395   -3.6235063734   -1.484979288
N  -7.8839386933   -4.3622661961   -2.4820828106
C  -7.7537357013   -3.6876604332   -3.7780962561
C  -7.4903990143   -5.7474099342   -2.7750917167
C  -6.2825418422   -5.6371966859   -3.7145512422
C  -6.5669597823   -4.371611561    -4.5434629629
```

S165

```
O  -7.0018215686   -1.3937673194   -4.396320034
O  -5.3899321209   -2.1478484691   -2.3745416534
C  -7.291147552    -6.6290957842   -1.5574023984
C  -7.8279658786   -3.5314473222   -0.1602068858
O  -5.4221262862   -3.5506548006   -4.7276190434
O  -7.0441105689   -7.9321373297   -2.0434541025
N  -9.1403704687   -2.966502192    -0.3498708623
O  -8.8101498635   -1.1386724034    0.9568695652
C  -9.5289244959   -1.7887677087    0.212806846
C  -10.9328890943  -1.3390821405   -0.1337574007
H  -8.6697227618   -3.8486201131   -4.3579141411
H  -8.5796936441   -1.7892930812   -3.1993760611
H  -7.0710963004   -1.4352962251   -1.4199843907
H  -6.0972744219   -4.1015002266   -1.2979343221
H  -8.3245745658   -6.1901330281   -3.3361275715
H  -6.1352529812   -6.5310987447   -4.3221140794
H  -5.3622572138   -5.4842488675   -3.1371636736
H  -6.8863390916   -4.6244498989   -5.556764329
H  -6.3449477955   -1.9613607093   -4.8477979411
H  -5.3024551538   -1.333520497    -2.8980952422
H  -8.1961135126   -6.5953630345   -0.9325520419
H  -6.4476020291   -6.2675674736   -0.9502872485
H  -7.9148278704   -4.5274894675    0.2896530833
H  -7.2991569045   -2.8882308928    0.546334432
H  -5.1226107344   -3.2701210097   -3.837379719
H  -6.876728137    -8.507433224    -1.2879023579
H  -9.7207278607   -3.4209879055   -1.0383033048
H  -11.4389767307  -1.9829895694   -0.8573509359
H  -11.5255482403  -1.3064300292    0.7839322588
H  -10.8891934793  -0.3210061497   -0.5269346758

calc_2c conf_29

C  -7.1711550698   -2.3362184186   -4.3944905008
C  -6.8006562419   -1.8612083848   -2.9727408664
C  -7.3905680147   -2.9398968667   -2.040532805
N  -7.8044471361   -4.0659415269   -2.9116105386
C  -7.2559015735   -3.85856094     -4.2577108433
C  -7.3787331804   -5.4346979675   -2.5886591178
C  -5.9322452417   -5.5427336419   -3.0935436337
C  -5.9172128182   -4.6665120222   -4.3462448217
O  -6.237820566    -1.8828545157   -5.3601837931
O  -5.4093249799   -1.6631705218   -2.8602563276
C  -7.5644544171   -5.9096353724   -1.1642524298
C  -8.5864892032   -2.3587653649   -1.2825672868
O  -4.7403250918   -3.8678996548   -4.3332246212
O  -8.9490495416   -6.1321384996   -0.9308467215
N  -9.199778925    -3.2832874406   -0.3656614581
O  -9.1672033874   -1.8621335813    1.4116656297
C  -9.4502918357   -2.94848445      0.9279090426
C  -10.1126426384  -4.0305853554    1.7584811387
H  -7.9493875327   -4.2806872608   -4.9946768873
H  -8.16622081     -1.95928739     -4.6571289925
H  -7.2401143817   -0.8827763302   -2.7606783043
H  -6.6149550426   -3.2261932584   -1.317539646
H  -8.006929001    -6.0939786427   -3.2037238795
H  -5.620917828    -6.5726832152   -3.2850523984
H  -5.2328869085   -5.1131301716   -2.3663172149
H  -5.9173396104   -5.2747403963   -5.2589719214
```

```
H  -5.6496284274   -1.2849565212   -4.8628322637
H  -4.97591898     -2.5061993475   -3.1159723802
H  -7.1537295578   -5.186706674    -0.4470693904
H  -7.0055975389   -6.8480265465   -1.0505869231
H  -8.272094354    -1.4977003926   -0.687435318
H  -9.322785239    -2.0120389547   -2.0212848088
H  -4.8626847447   -3.2394094689   -5.0684537899
H  -9.0388314178   -6.5582745456   -0.0692765104
H  -9.4471265941   -4.207072393    -0.704694716
H  -9.4470752746   -4.3012943745    2.5825348419
H  -11.0230807852  -3.6213070019    2.2017979669
H  -10.3693961093  -4.926812589     1.1888324902
```

calc_**2c** conf_30

```
C   -7.3809918266   -2.0626296438   -3.4377893032
C   -6.5628873709   -2.1131313231   -2.1220634429
C   -6.8187727086   -3.520841033    -1.5362567103
N   -7.7709106746   -4.1673339757   -2.4551011196
C   -7.6476077319   -3.5310099205   -3.7672587235
C   -7.5687775561   -5.5851321373   -2.7482730618
C   -6.4247239581   -5.6370471639   -3.7842668602
C   -6.5381890807   -4.305691528    -4.5408587856
O   -6.684625261    -1.367357056    -4.4611167639
O   -5.1932918234   -1.8603082803   -2.3734616026
C   -7.3657704583   -6.4833135776   -1.5418758206
C   -7.322304903    -3.5171533419   -0.0695568137
O   -5.2741356265   -3.6516736043   -4.525272813
O   -8.4634163387   -6.4830943647   -0.6427332384
N   -8.7538161112   -3.5710927063    0.0834154073
O   -9.0906564943   -1.3892890084   -0.4464357626
C   -9.5390037381   -2.5053543014   -0.2110039051
C   -11.0289465545  -2.7764442775   -0.2106050544
H   -8.5914809601   -3.6579215936   -4.3126921315
H   -8.3347585006   -1.5640676802   -3.2412073629
H   -6.8938136298   -1.3335573092   -1.4375352597
H   -5.8366563809   -4.0214615216   -1.5317890937
H   -8.4896077581   -5.9237980443   -3.251591374
H   -6.4887173958   -6.5091271885   -4.4397468727
H   -5.4461359534   -5.6660628335   -3.2927551071
H   -6.841841131    -4.4597114749   -5.583763247
H   -5.95316832     -0.9256668888   -3.9897822927
H   -4.8871893717   -2.5965276179   -2.9399810473
H   -6.5000277489   -6.1626160019   -0.9574835641
H   -7.1525301058   -7.5025110818   -1.8937329357
H   -6.9202128924   -4.3793336657    0.4676617492
H   -6.9477105058   -2.6206060086    0.4306968622
H   -5.4661537645   -2.779223621    -4.9199516583
H   -9.2261037365   -6.8386168389   -1.1171659434
H   -9.1417015954   -4.5006776291   -0.0043476393
H   -11.5314052988  -1.9728025198    0.3305062703
H   -11.3928750177  -2.7550496637   -1.2419649218
H   -11.2960817162  -3.7357635731    0.2391399437
```

calc_**2c** conf_31

```
C   -7.4623705903   -2.0697959916   -3.3816244403
C   -6.617381178    -2.1942521192   -2.095276824
C   -6.8833055286   -3.6083230216   -1.5573032226
```

```
N   -7.8061685918    -4.2477798705    -2.5243310932
C   -7.6890918995    -3.5261719117    -3.7961776782
C   -7.5015095532    -5.6374202822    -2.9094767818
C   -6.2962511106    -5.5467685347    -3.8472530722
C   -6.5389473571    -4.2247812706    -4.6105799138
O   -6.8686819311    -1.242165661     -4.3521577918
O   -5.2256165451    -2.0939941635    -2.4122111543
C   -7.443256594     -6.5458754203    -1.6992617119
C   -7.3768492621    -3.6618907292    -0.0902730426
O   -5.3626631542    -3.4510659664    -4.7768580825
O   -8.6356125171    -6.3953261805    -0.9512367369
N   -8.8050405843    -3.5975541545     0.1273549031
O   -9.0549191796    -1.4325277698    -0.4805006075
C   -9.5409671959    -2.4734493983    -0.0594218779
C   -11.0114076884   -2.5853343681     0.2811772495
H   -8.6235245776    -3.6379162384    -4.3570014706
H   -8.4213622419    -1.6235378545    -3.1109513168
H   -6.8832190639    -1.4233014537    -1.3704675226
H   -5.8999221654    -4.1024585773    -1.5454815786
H   -8.3684768694    -5.9671798655    -3.5007054561
H   -6.2031805082    -6.4087505809    -4.5122565513
H   -5.3583287618    -5.4672021259    -3.2855268932
H   -6.8838330405    -4.4212972817    -5.6283020835
H   -6.2397590625    -1.8103111042    -4.8383246988
H   -5.1530707073    -1.2630718451    -2.9120851204
H   -6.5609655918    -6.3158013185    -1.0822848906
H   -7.3547505667    -7.591432234     -2.0117883855
H   -7.0513228634    -4.5997913119     0.3621416805
H   -6.8859704748    -2.8484149805     0.4550963862
H   -5.0568637077    -3.1807025321    -3.8835962159
H   -8.9952221064    -5.5386757464    -1.2396654376
H   -9.2439334364    -4.4127377932     0.5239430905
H   -11.5956052171   -2.3962813378    -0.6227313122
H   -11.3006003429   -3.555606958      0.6920710826
H   -11.2640482334   -1.8030520468     1.0003285728
```

calc_**2c** conf_32

```
C   -7.1541395484    -2.1317418374    -4.0763696303
C   -6.3604573686    -1.7811091159    -2.7733991931
C   -6.909816687     -2.7358227152    -1.7033645708
N   -7.1338897709    -3.9085193476    -2.5179300753
C   -7.6972048592    -3.5526248217    -3.8023245325
C   -7.5307168073    -5.2627113356    -2.207324096
C   -7.4938488846    -5.9131582312    -3.6262467498
C   -7.1853602651    -4.7552804612    -4.5981834772
O   -6.3337175672    -2.0028799143    -5.2178579909
O   -4.9984431894    -2.0747489339    -2.9805741545
C   -6.6085153611    -5.9550349914    -1.2244176892
C   -8.1403240766    -2.1588218122    -0.9973887453
O   -5.7821579679    -4.6108210463    -4.8040437276
O   -6.7990532604    -5.3869819323     0.0653268115
N   -8.6854881142    -3.113928993     -0.0616822483
O   -10.768759137    -2.2236970786    -0.0858226743
C   -9.9897816201    -3.0779077717     0.3124913069
C   -10.4143338374   -4.1714102591     1.2726496389
H   -8.802527378     -3.5483922025    -3.8080158804
H   -7.9844306913    -1.4336215085    -4.206705072
H   -6.4900163312    -0.7273331941    -2.4904128663
```

```
H   -6.1299374672    -2.9405847456    -0.9635842952
H   -8.5556495089    -5.3188041554    -1.8042891699
H   -8.4523585813    -6.3836758991    -3.8606071974
H   -6.7154321191    -6.6765562409    -3.7180736167
H   -7.6340403415    -4.8882931799    -5.58323868
H   -5.9523584804    -2.8896475321    -5.3822176849
H   -4.8329128519    -1.7816589626    -3.8944935298
H   -5.5696374292    -5.8318899938    -1.5597081232
H   -6.8437516172    -7.0284074515    -1.2069845202
H   -7.8559553759    -1.2275457496    -0.4872883164
H   -8.9310272423    -1.8940396783    -1.7075772898
H   -5.44618075     -4.3117109508    -3.9343676281
H   -6.1398085247    -5.7527683173     0.6668249835
H   -8.0829081806    -3.8634142766     0.2559483978
H   -9.6643427572    -4.9567817117     1.3959456949
H  -10.6245239641    -3.7262615363     2.2491282563
H  -11.3451920859    -4.6124121147     0.9101783358

calc_2c conf_33

C   -7.4618764893    -2.1573976316    -3.3468940611
C   -6.7068490579    -2.3092936793    -2.002853161
C   -7.0630026165    -3.724757727     -1.5021624839
N   -7.9203602384    -4.3299133482    -2.5470054856
C   -7.7065601589    -3.5985358308    -3.8004974616
C   -7.6572621947    -5.7263750109    -2.9156702235
C   -6.4376077381    -5.6778404867    -3.8559639214
C   -6.5489895635    -4.319438178     -4.5588436606
O   -6.7306367661    -1.3754666009    -4.2747041453
O   -5.3225864989    -2.0996046404    -2.1843589198
C   -7.5321147493    -6.7008195259    -1.7520227477
C   -7.8053334087    -3.6962656302    -0.1644380845
O   -5.2965438543    -3.6489377073    -4.4712820854
O   -7.4141899849    -8.0308822197    -2.2109572018
N   -9.0923224787    -3.0623654045    -0.3032856155
O   -8.6948019171    -1.3715301719     1.1599653294
C   -9.437616329     -1.9272871708     0.3651605047
C  -10.8276355621    -1.4025908667     0.0705993069
H   -8.6112163564    -3.6769142661    -4.4152014958
H   -8.4327745169    -1.6832010514    -3.1633295911
H   -7.0207711626    -1.5480396005    -1.2855141818
H   -6.1168289046    -4.2679400696    -1.3632965597
H   -8.5249161347    -6.0603187121    -3.5000509075
H   -6.4091656279    -6.515286777     -4.5569706198
H   -5.5000070432    -5.6841259857    -3.2861787023
H   -6.8118791914    -4.4331665385    -5.6172651662
H   -6.0007308498    -1.0001674656    -3.7471919296
H   -5.0229926303    -2.7880981278    -2.814243398
H   -8.4402957915    -6.669704534     -1.144653478
H   -6.68712389      -6.4313572321    -1.1013824925
H   -7.9311130701    -4.7144618236     0.2218590696
H   -7.2419386333    -3.1245014862     0.576159377
H   -5.4774332178    -2.7633840141    -4.8377484612
H   -6.537830697     -8.1316789214    -2.602327389
H   -9.6923526833    -3.4336745257    -1.0238731712
H  -10.757146648     -0.3429931888    -0.1837348348
H  -11.3407251484    -1.9341748173    -0.734803491
H  -11.4294681967    -1.4785090318     0.9799615407
```

calc_**2c** conf_34

```
C   -6.9800979585    -2.0270218101    -3.944401896
C   -6.2396115153    -1.7884313567    -2.5900160104
C   -6.9188754728    -2.7495068724    -1.599476938
N   -7.0145458077    -3.8905828596    -2.4916618782
C   -7.5683131966    -3.4452039842    -3.7576343269
C   -7.5015708954    -5.234414937     -2.2717689099
C   -7.4142461904    -5.8241959819    -3.70798076
C   -7.2031811268    -4.6264746998    -4.6609285118
O   -6.079429313     -1.8837456473    -5.0269819159
O   -4.8852154066    -2.1694705708    -2.7677737951
C   -6.6889208679    -6.0158271669    -1.263070739
C   -8.2229260338    -2.2075459862    -1.0141617298
O   -5.846301993     -4.5980072145    -5.0436615443
O   -6.9296252882    -5.4759918404     0.0319893724
N   -8.7915461927    -3.1642690745    -0.0929175203
O   -10.7823784544   -2.0979624967     0.0236602807
C   -10.0638112421   -3.0287105033     0.358802966
C   -10.5295284025   -4.1074777651     1.3157844031
H   -8.6723487794    -3.3752010245    -3.7178208726
H   -7.7867083472    -1.3021670893    -4.0857688757
H   -6.2344695385    -0.7435871905    -2.2749434405
H   -6.2260128105    -2.9691960209    -0.7812113724
H   -8.5531936108    -5.2392065989    -1.9378787629
H   -8.318744188     -6.3860334993    -3.9516584654
H   -6.558574669     -6.4963872164    -3.8197370195
H   -7.8565037836    -4.6881139288    -5.5411805297
H   -5.2052425966    -1.8112626499    -4.5939842456
H   -4.9322497754    -3.1396814802    -2.881256031
H   -5.6259989946    -5.9441792525    -1.5295217525
H   -6.9875908573    -7.072659298     -1.2991068223
H   -8.0205723525    -1.2554445383    -0.5042125783
H   -8.9614890307    -1.9871720753    -1.7924480413
H   -5.7266858784    -3.7219979764    -5.4524470349
H   -6.3599369877    -5.9245850951     0.6678735295
H   -8.2221990775    -3.9527286756     0.1910939401
H   -10.6737892361   -3.6663030619     2.3058265998
H   -11.5009256187   -4.4770405144     0.9807177772
H   -9.8326385099    -4.9452120463     1.3988634517
```

calc_**2c** conf_35

```
C   -7.3759240601    -2.0810828614    -3.4076500372
C   -6.5893505623    -2.1851707302    -2.0788653248
C   -6.8630108014    -3.6175928102    -1.5624825904
N   -7.7790486672    -4.2388599023    -2.5413913356
C   -7.6042579231    -3.5345489384    -3.8184454502
C   -7.5123654399    -5.6383875575    -2.9143628624
C   -6.2869914938    -5.5974708443    -3.8353936388
C   -6.4395103611    -4.2568640349    -4.5724404865
O   -6.6730842985    -1.318314842     -4.3771295605
O   -5.2144900407    -1.9227975057    -2.2809989783
C   -7.496274876     -6.5483498043    -1.7046483459
C   -7.363593603     -3.679138442     -0.0984280595
O   -5.2036331616    -3.5552164519    -4.5254282523
O   -8.6981415251    -6.3767764198    -0.9772083692
N   -8.7933564096    -3.6077658565     0.1141651024
O   -9.0492027633    -1.4398412136    -0.4898949867
```

```
C   -9.5295327444    -2.4827829337   -0.0677635117
C   -10.9977891803   -2.5953545736    0.2834811101
H   -8.5185428031    -3.6493986102   -4.412134999
H   -8.3448667352    -1.6143508514   -3.2071414777
H   -6.9396373759    -1.4370746557   -1.3701949905
H   -5.8811501695    -4.1158518935   -1.5483187444
H   -8.3797476056    -5.943628789    -3.5179613929
H   -6.2388059699    -6.4538912956   -4.5118602963
H   -5.3526955977    -5.5736452699   -3.2646874419
H   -6.7179059599    -4.4088653345   -5.622613526
H   -5.9618572191    -0.8859636969   -3.8688705826
H   -4.8951491785    -2.613343118    -2.8973596438
H   -6.619983808     -6.3378467633   -1.0724129276
H   -7.4238571802    -7.594951343    -2.0180610788
H   -7.0457242192    -4.6202084599    0.3531500351
H   -6.869146689     -2.8712496567    0.4524270604
H   -5.4219954222    -2.6773957539   -4.8936419444
H   -9.0328527558    -5.5089014506   -1.2610212141
H   -9.2331216269    -4.4203171561    0.5152560843
H   -11.5888876961   -2.3759055977   -0.6088257156
H   -11.2903771694   -3.5746454519    0.6698636482
H   -11.2381369076   -1.83224913      1.0272947254

calc_2c conf_36

C   -7.2108539764    -2.31735667     -4.3714986137
C   -6.719121814     -1.8840660861   -2.9715899347
C   -7.2685248328    -2.9563582546   -2.0054586046
N   -7.8943099172    -3.9960886462   -2.8554923028
C   -7.4209932338    -3.824221727    -4.2331736691
C   -7.6181405587    -5.4129819806   -2.5990123425
C   -6.2256988638    -5.6756811516   -3.2000087799
C   -6.1690482668    -4.7446079037   -4.4140439515
O   -6.2925667825    -1.9470788267   -5.3867635416
O   -5.314001351     -1.7477559057   -2.9565640671
C   -7.8509788646    -5.9401068229   -1.1936600362
C   -8.2585638769    -2.310276213    -1.0331696447
O   -4.9265697816    -4.0507929278   -4.4093576408
O   -6.9595936921    -5.4649032911   -0.1965125568
N   -8.690388908     -3.19210413      0.0214410084
O   -10.7671449995   -2.2935592273    0.2009898596
C   -9.92686524      -3.0962429241    0.5784496405
C   -10.1975974147   -4.0650146517    1.712853202
H   -8.1971108105    -4.180281382    -4.921614731
H   -8.1802510499    -1.8505222784   -4.5779206854
H   -7.0988399145    -0.891044498    -2.7180332818
H   -6.420022012     -3.3488231361   -1.4297394046
H   -8.3477819744    -5.9610357696   -3.2148175746
H   -6.0563376871    -6.7256363597   -3.4532279384
H   -5.4326980937    -5.3645239246   -2.5094495926
H   -6.2534418689    -5.3047495143   -5.3532181507
H   -5.6475719353    -1.3760382924   -4.9296345689
H   -4.9497658093    -2.6241195825   -3.2046172363
H   -7.8252794131    -7.037783246    -1.2314666504
H   -8.8468369045    -5.6392446457   -0.8663935755
H   -7.7787257969    -1.4177612944   -0.6053463492
H   -9.1516131118    -1.9782234154   -1.5684871216
H   -5.0178668793    -3.3966070191   -5.1271271862
H   -6.0791172847    -5.8186873865   -0.3717634559
```

```
H   -8.0094279551   -3.8367464132    0.3998771212
H  -11.1291330539   -4.596022755     1.5044608094
H   -9.3959548013   -4.7906273657    1.8729445786
H  -10.3492612694   -3.4963243813    2.6341469693
```

calc_**2c** conf_37

```
C   -7.2611510423   -2.4007147704   -4.256152297
C   -7.2781414032   -2.1372810516   -2.7276263942
C   -7.586022363    -3.5071014047   -2.0829893357
N   -7.8360563515   -4.4346717795   -3.2040631002
C   -7.0943489522   -3.9132146201   -4.3618246421
C   -7.2799577245   -5.7954519722   -3.0652668001
C   -5.7652493112   -5.646727364    -3.2809579678
C   -5.639962414    -4.4663251797   -4.2525707235
O   -6.2444018934   -1.6627292984   -4.9110267949
O   -6.0622599087   -1.5730203982   -2.28092456
C   -7.7221298923   -6.5078114528   -1.804018404
C   -8.7698305778   -3.4196928763   -1.1268059857
O   -4.7097459141   -3.522584272    -3.7257191301
O   -9.1177621299   -6.6981790972   -1.7775645105
N   -8.4467737092   -2.5029586781   -0.0536642003
O  -10.4498702057   -2.7541666634    0.9536968581
C   -9.3476715141   -2.2308146456    0.9287022025
C   -8.8926583798   -1.2466281344    1.9857874205
H   -7.5462826367   -4.3094663525   -5.2779156023
H   -8.2340844854   -2.1270660366   -4.679322161
H   -8.044215677    -1.4005134052   -2.4740535996
H   -6.695138248    -3.7962525255   -1.5013439237
H   -7.6970021342   -6.3651552354   -3.9066026164
H   -5.3074279851   -6.5626933039   -3.6610621205
H   -5.2499816295   -5.3843786213   -2.3505918158
H   -5.2872383093   -4.7899011225   -5.2387473496
H   -5.9672279003   -0.9912942551   -4.2620123076
H   -5.3815349581   -2.2561200873   -2.4575758179
H   -7.3713144973   -5.9607465481   -0.914373739
H   -7.262499079    -7.5001190597   -1.7680450568
H   -9.6541844511   -3.0678745051   -1.6724957194
H   -9.026564362    -4.3970512523   -0.7071729253
H   -4.7420319237   -2.7855525055   -4.3630372399
H   -9.5145709518   -5.9116767785   -2.17776821
H   -7.5565032427   -2.0291794015   -0.0717363717
H   -8.9192634718   -1.7414013013    2.9596674974
H   -7.8891551748   -0.8472680263    1.8185692181
H   -9.603785195    -0.4182160177    2.023608226
```

calc_**2c** conf_38

```
C   -7.2258213663   -2.3167433429   -4.3449165361
C   -7.4405085771   -1.9375880939   -2.8558954756
C   -7.9877650848   -3.2182464903   -2.1954582757
N   -8.0515404087   -4.2366585298   -3.2602985626
C   -7.1187755354   -3.8416364438   -4.3197316378
C   -7.598439464    -5.5884097782   -2.9032190109
C   -6.0615287267   -5.5190350397   -2.9035407971
C   -5.7312618808   -4.4607067057   -3.9610537919
O   -6.1014366004   -1.6540181168   -4.8934326343
O   -6.240627555    -1.4581024809   -2.2872563773
C   -8.2146701414   -6.158422364    -1.6398521507
```

```
C   -9.3757621471   -3.0242745429   -1.5754859129
O   -4.8097221243   -3.5196423096   -3.4109041199
O   -7.6829332168   -7.4622700145   -1.4883397063
N   -9.3604374629   -2.159654707    -0.4150964013
O   -8.6657774234   -3.7919605945    0.9916725321
C   -8.957182576    -2.6192628906    0.8003554859
C   -8.8909160241   -1.5877422503    1.9050904587
H   -7.4523751781   -4.2810448758   -5.2673402346
H   -8.1167428953   -2.0442454317   -4.9225208766
H   -8.1447495005   -1.1045683126   -2.7686209891
H   -7.2985030992   -3.4904031131   -1.3838087046
H   -7.9124165943   -6.2421897886   -3.728239654
H   -5.6016107291   -6.48846517     -3.0978024941
H   -5.6874353887   -5.1690429334   -1.9352669893
H   -5.2786122843   -4.9052223229   -4.8553421137
H   -5.8301658371   -1.02990395     -4.1936932871
H   -5.6083571811   -2.2078833754   -2.3318094509
H   -9.3089845343   -6.1885112094   -1.7536290058
H   -7.9869442593   -5.5302369059   -0.7691750238
H   -10.0587674484  -2.608574779    -2.3219769966
H   -9.7772742844   -3.9899341278   -1.2651365453
H   -4.7137598881   -2.8475147181   -4.1089635365
H   -7.9341624313   -7.7785635918   -0.6129116504
H   -9.4928549596   -1.1695094474   -0.5397634566
H   -9.3605847852   -0.6352197993    1.6475005883
H   -9.3733921826   -1.9971107298    2.7944356151
H   -7.842200224    -1.4054807231    2.1554277192

calc_2c conf_39

C   -6.5273232674   -2.382541197    -3.9497267023
C   -7.5761404072   -1.902439148    -2.9532343645
C   -7.8981900546   -3.1888726589   -2.1735782395
N   -7.9393241204   -4.2028635096   -3.2276192539
C   -7.0979960064   -3.7446845481   -4.3625767013
C   -7.5151851222   -5.5788080855   -2.9185506667
C   -6.034030086    -5.6292233053   -3.2974398796
C   -6.0554776041   -4.8608245318   -4.6126757917
O   -5.3280782715   -2.4539527304   -3.201459741
O   -7.1356185209   -0.8330588007   -2.1527850744
C   -7.8295178802   -6.067834899    -1.5168513428
C   -9.2131280932   -3.0769261386   -1.4052315357
O   -4.8158925386   -4.2910968216   -5.0280988401
O   -7.3539715802   -7.3986099169   -1.4467393527
N   -9.1170922139   -2.0646136373   -0.3777021918
O   -9.9504263502   -3.3709461145    1.2842635222
C   -9.4644634184   -2.3115752641    0.9126213798
C   -9.2270708917   -1.1658159271    1.8751124125
H   -7.7154824432   -3.6046478264   -5.2585390638
H   -6.4087277181   -1.7093852383   -4.8077524305
H   -8.4723991399   -1.5623204862   -3.4832281168
H   -7.0772481782   -3.3420737842   -1.4541715954
H   -8.0596647874   -6.249446276    -3.599593393
H   -5.649079345    -6.6480509542   -3.3833420319
H   -5.4380111431   -5.0787429523   -2.5606087383
H   -6.4222734512   -5.5191558181   -5.4115127705
H   -4.7014432243   -2.954860694    -3.7530799191
H   -6.2020992084   -1.0291563475   -1.9678482749
H   -8.9132782854   -6.0255548491   -1.3464091553
```

```
H   -7.3426989676    -5.4336184477    -0.7630508753
H  -10.0186223743    -2.8496592539    -2.1162936669
H   -9.4794601514    -4.0048583162    -0.8979231697
H   -4.1830085464    -5.0109363469    -5.1437818024
H   -7.5801291147    -7.7439832624    -0.5751355218
H   -8.6123953324    -1.2205681534    -0.6130018939
H   -8.726239764     -0.3058499075     1.4237282846
H  -10.1899573687    -0.8414126658     2.2780115435
H   -8.6308550293    -1.5300311859     2.7148049549
```

calc_**2c** conf_40

```
C   -7.349733894     -2.2651927463    -3.9184157945
C   -7.1616530817    -2.2221266465    -2.38540561
C   -7.7108963462    -3.5592188792    -1.8783430779
N   -8.0045112209    -4.3748685853    -3.0769021314
C   -7.3501037744    -3.7653938873    -4.2352207281
C   -7.5334092363    -5.7634488105    -3.0923202298
C   -6.04153011      -5.6742936778    -3.4519422121
C   -5.9553265133    -4.4653627834    -4.4035639354
O   -6.4026363815    -1.4888452232    -4.6080947237
O   -5.7710635305    -2.1355116523    -2.0669326608
C   -7.8550370269    -6.5763173434    -1.8456459187
C   -8.9963700942    -3.3974308404    -1.0574516773
O   -4.8304508832    -3.6381341509    -4.149115957
O   -7.4794264063    -7.9285856531    -1.9975509547
N   -8.7932251833    -2.7301184878     0.2086039977
O   -9.5626708037    -0.7054517434    -0.4681015374
C   -9.1093755458    -1.4206437427     0.4130733496
C   -8.8634161073    -0.901439954      1.813566354
H   -7.9438555503    -3.9725191179    -5.132813357
H   -8.3366639385    -1.8580362956    -4.1565145124
H   -7.6840074538    -1.3705520609    -1.9401293565
H   -6.9338344647    -4.0060227996    -1.2400895677
H   -8.0568391643    -6.2593458513    -3.9208564394
H   -5.6431943515    -6.5884610964    -3.8998925319
H   -5.4434069347    -5.4543791536    -2.5571852116
H   -5.8314569881    -4.7876554508    -5.4396761101
H   -5.6221516637    -2.0650970537    -4.7273740651
H   -5.4642689834    -1.3454159316    -2.5429316123
H   -8.935286975     -6.5811385759    -1.6795849839
H   -7.3814549816    -6.1351342745    -0.9552720967
H   -9.7182939604    -2.8064440438    -1.6241816716
H   -9.4415378403    -4.3809222817    -0.8798604354
H   -4.9348948331    -3.291563618     -3.2371794112
H   -6.5155205174    -7.9634897529    -2.0319330512
H   -8.396049321     -3.2545271423     0.9710439263
H   -9.8032434517    -0.5104733858     2.2101657331
H   -8.4706392477    -1.6515006701     2.5044968828
H   -8.1615632393    -0.0659366362     1.7595313193
```

calc_**2c** conf_41

```
C   -6.4019146377    -2.4279168373    -3.9246330969
C   -7.3707830018    -1.9169050618    -2.8652997495
C   -7.7887232369    -3.2118545855    -2.1445293394
N   -7.9292561399    -4.1673891197    -3.244970153
C   -7.1047203391    -3.7076676673    -4.3904361466
C   -7.5967372671    -5.5838582296    -3.0192538223
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S174

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C   -6.1494641137    -5.7297930047    -3.492426236
C   -6.1723188641    -4.8852105182    -4.7592154767
O   -5.1907653503    -2.6506489284    -3.2273897778
O   -6.80834341      -0.9415228786    -2.0222268515
C   -7.8533554733    -6.126826541     -1.6179062628
C   -9.0809088297    -3.0289607947    -1.3526048661
O   -4.9114595165    -4.3898948621    -5.2032438631
O   -7.4844176522    -7.4897457175    -1.5366999248
N   -8.8933507661    -2.051337277     -0.3044737327
O   -10.145960889    -3.1570190027     1.2308925972
C   -9.4340044356    -2.2089140173     0.9314595435
C   -9.0964341989    -1.1198700297     1.9294327586
H   -7.7468681634    -3.4586769376    -5.2447214153
H   -6.2508493636    -1.7182111749    -4.7472562222
H   -8.2470377399    -1.4651664716    -3.3426924619
H   -6.9739698066    -3.4689061169    -1.4486932563
H   -8.2342109597    -6.1734338445    -3.7008236145
H   -5.8514102764    -6.7687188331    -3.653289895
H   -5.472863322     -5.2723211837    -2.7618861793
H   -6.6295053313    -5.4615289901    -5.5749378586
H   -4.6238869094    -3.1541368257    -3.8375880585
H   -5.8909561246    -1.2302176263    -1.8836254005
H   -8.9042107417    -5.983393384     -1.3374989624
H   -7.2386146981    -5.6086560596    -0.8782802765
H   -9.8776060158    -2.7289445387    -2.0473542778
H   -9.4086815393    -3.950135844     -0.8681844981
H   -4.3456862109    -5.1481192981    -5.3958605814
H   -8.1405360744    -7.9997856181    -2.0278578906
H   -8.2655001999    -1.2823143002    -0.4974060465
H   -10.0262556787   -0.6684099511     2.2837347535
H   -8.6078669867    -1.5755481942     2.7941389019
H   -8.4515657357    -0.3350397342     1.5266076397

calc_2c conf_42

C   -6.7431511087    -2.2700889027    -3.7552381991
C   -7.7155552337    -2.0052957416    -2.5810010318
C   -7.9674865523    -3.3918187916    -1.9699500791
N   -7.9162103803    -4.2747839699    -3.1223243525
C   -7.0947155601    -3.6950610579    -4.1983048678
C   -7.6508554361    -5.7143230621    -3.0022552688
C   -6.7802645073    -6.0230753348    -4.2357301275
C   -5.9926077929    -4.7358901413    -4.4611021582
O   -5.4164562237    -2.1351109155    -3.2861112249
O   -7.1218123182    -1.0776168936    -1.7025071575
C   -6.9683904191    -6.1689410093    -1.7050966335
C   -9.3453022351    -3.5387160398    -1.3039600827
O   -4.9426937812    -4.7105206721    -3.5253598838
O   -6.84048413      -7.5770386845    -1.6722361124
N   -9.7831959068    -2.4780936623    -0.4021826998
O   -7.8443836495    -2.1270672188     0.7174987965
C   -9.0530109868    -1.9218514708     0.5859056417
C   -9.7885821045    -0.9902820469     1.5200725997
H   -7.6949765518    -3.626893467     -5.1187926765
H   -6.9015144668    -1.553933753     -4.5707537994
H   -8.6579131482    -1.5986978794    -2.9725454009
H   -7.1768513285    -3.5889040137    -1.2336977615
H   -8.6020087116    -6.2695253073    -3.0716433699
H   -7.4073596305    -6.2378843023    -5.1074364467
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S175

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H  -6.1241440264   -6.8777597844   -4.0600348689
H  -5.6109856089   -4.6545804597   -5.4900410377
H  -5.504444627    -1.5548170548   -2.5024974875
H  -7.1926078042   -1.4268621672   -0.7895896455
H  -7.5228265217   -5.8120044227   -0.8234200162
H  -5.9561922687   -5.767516531    -1.6621110324
H  -10.0770586039  -3.5831934381   -2.1140673778
H  -9.3842465638   -4.4991282207   -0.7748533884
H  -4.7583801458   -3.7704593293   -3.3448034462
H  -7.7301844592   -7.951766971    -1.7060624621
H  -10.7675835152  -2.2643571107   -0.4203300967
H  -9.6375205328   -1.3392782114    2.5441365836
H  -9.3406928468    0.0036585188    1.4468862438
H  -10.8603503118  -0.9135204795    1.3235403283

calc_2c conf_43

C  -7.2202292355   -2.2259283371   -3.7564117622
C  -7.1241717724   -2.2907843261   -2.2116257614
C  -7.7234569472   -3.6644254383   -1.8422717694
N  -8.024357911    -4.3479025894   -3.1156167363
C  -7.268919727    -3.6929990511   -4.1881393013
C  -7.6433848472   -5.758102241    -3.2404766526
C  -6.1363628772   -5.7547123129   -3.5461371778
C  -5.9122903797   -4.4541594544   -4.3248533255
O  -6.1448564947   -1.4910218044   -4.31611144
O  -5.7874335374   -2.1126493135   -1.7901615231
C  -8.060602245    -6.653884458    -2.0828976358
C  -9.0094899875   -3.5396003848   -1.0163638738
O  -4.8019452259   -3.762043974    -3.7620524115
O  -7.670479328    -7.9938449303   -2.2984294848
N  -8.8002006738   -2.9440706271    0.2835485317
O  -9.6106525305   -0.8980678383   -0.2708323742
C  -9.1205970233   -1.6487282571    0.5599889927
C  -8.8230228281   -1.1910756147    1.9714997419
H  -7.818273961    -3.8116562121   -5.1300110107
H  -8.1650139649   -1.7498773741   -4.0410040953
H  -7.6872084298   -1.4765615094   -1.7523888116
H  -6.9651325532   -4.1936515106   -1.2439943747
H  -8.1723813321   -6.1287638578   -4.1337069704
H  -5.8086006555   -6.6465755374   -4.0823708346
H  -5.5564358261   -5.7037895991   -2.6176477788
H  -5.7014994457   -4.6473018958   -5.3837779442
H  -5.7005794632   -1.0940688626   -3.5438116466
H  -5.2687350322   -2.8316519373   -2.2102605112
H  -9.1449008343   -6.5711780087   -1.9194212788
H  -7.5597513493   -6.3524039624   -1.1586342302
H  -9.7202371162   -2.9054266647   -1.5494212855
H  -9.4716930924   -4.5238947383   -0.8930604236
H  -4.7986740976   -2.9037168349   -4.2249323947
H  -8.1671335402   -8.3250745174   -3.0573878506
H  -8.3539261578   -3.4934938568    0.999983865
H  -8.0501946944   -0.4190759939    1.9339940185
H  -9.7228474488   -0.7317105813    2.3856836831
H  -8.490327434    -1.9911255928    2.6375138381

calc_2c conf_44

C  -7.4105200644   -2.272158779    -4.2110713398

S176
```

```
C   -7.5969405271   -2.0264583443   -2.695966258
C   -8.0907706636   -3.3827112286   -2.1362154037
N   -8.0671470348   -4.3356180886   -3.2681934239
C   -7.1819574344   -3.7815253161   -4.297686964
C   -7.4644019342   -5.6446586406   -2.9761997879
C   -5.9472964955   -5.4015843126   -2.9541325901
C   -5.728895226    -4.2851553465   -3.9974408394
O   -6.4645376632   -1.4790375848   -4.8555795252
O   -6.364379664    -1.6581564095   -2.1066797396
C   -8.033966393    -6.3544080319   -1.7560527729
C   -9.4865514948   -3.3355815204   -1.490677766
O   -4.8137990479   -3.2877008435   -3.5812341153
O   -7.4185367001   -7.6062793214   -1.5388686826
N   -9.4584705175   -3.2636680087   -0.0357874051
O   -7.9888975202   -1.5431680376    0.1588233616
C   -8.7429941492   -2.3640325511    0.6766551365
C   -8.9158835697   -2.418935568     2.1777536957
H   -7.4879796506   -4.166207115    -5.2770613398
H   -8.3734750676   -2.0568468553   -4.6856959357
H   -8.3231941901   -1.2286107865   -2.5152497076
H   -7.3759747306   -3.6739515216   -1.3550959775
H   -7.6973611428   -6.275914308    -3.8491698632
H   -5.3667768836   -6.3037801981   -3.1555842808
H   -5.6308012385   -5.0365891881   -1.9697475877
H   -5.2920216522   -4.6887098505   -4.9139071787
H   -5.5982085476   -1.7867295623   -4.5327087395
H   -6.5906902375   -1.4841581473   -1.1747987338
H   -9.1248991613   -6.4573223161   -1.8659543322
H   -7.846051415    -5.7769716668   -0.8462246551
H   -10.0625151968  -2.4941683764   -1.8955977616
H   -10.0261027184  -4.246568391    -1.7528628353
H   -5.1853381953   -2.8287106287   -2.798214592
H   -7.6050198181   -8.161470015    -2.3067245718
H   -10.0797873253  -3.8732468579    0.4702516991
H   -7.934246757    -2.5499125338    2.6384342645
H   -9.3076621494   -1.4573231684    2.5181661195
H   -9.5799478229   -3.2149705801    2.5223004289
```

calc_**2c** conf_45

```
C   -7.1931761584   -2.2269001034   -3.7556701947
C   -7.1679707944   -2.3582491583   -2.2111812899
C   -7.7306803164   -3.7673233643   -1.9288030746
N   -7.9952667976   -4.3856124918   -3.2428884876
C   -7.2054041369   -3.6724720865   -4.2505222303
C   -7.6059194046   -5.7868862944   -3.4476198788
C   -6.0867614973   -5.7592896782   -3.6849481797
C   -5.8322369558   -4.4079341964   -4.3590426016
O   -6.0989610767   -1.46053802     -4.2309914694
O   -5.861950482    -2.1540915079   -1.7129635441
C   -8.0823731789   -6.8065979602   -2.4220672038
C   -9.0305839435   -3.711110212    -1.1169342448
O   -4.7685677245   -3.7396622297   -3.6866245086
O   -7.4226581314   -6.7619741093   -1.1698986785
N   -8.8611178253   -3.1304918733    0.1955020366
O   -9.8772099656   -1.1637372866   -0.3085370093
C   -9.2798905953   -1.8652369731    0.4929272216
C   -8.9391412849   -1.3809425682    1.885260701
H   -7.7108705962   -3.7580443449   -5.2201893116
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S177

```
H  -8.1279195023   -1.7452554459   -4.0626932035
H  -7.7811449338   -1.5834476837   -1.7480850929
H  -6.9663152774   -4.3127708485   -1.3562380466
H  -8.0962731693   -6.0847564479   -4.3869004408
H  -5.7373479287   -6.6075447094   -4.2789715427
H  -5.5561565493   -5.7830289352   -2.7284333844
H  -5.5569500733   -4.5259564179   -5.4140931579
H  -5.7039385063   -1.0824493656   -3.4232088071
H  -5.3061873056   -2.8544285838   -2.1168206907
H  -7.8785014001   -7.8007115194   -2.8317567515
H  -9.1707752154   -6.7239158126   -2.304861898
H  -9.7589991179   -3.092703461    -1.644217429
H  -9.4731045806   -4.7116253685   -1.0262527569
H  -4.7444842081   -2.8599228423   -4.1065842612
H  -7.9030694828   -6.1502695842   -0.602295916
H  -8.2872071438   -3.6106245973    0.8704861491
H  -9.8132011712   -0.8788983554    2.3030240855
H  -8.6216004323   -2.1768021414    2.5636684052
H  -8.1370831362   -0.6407934215    1.8144266875

calc_**2c** conf_46

C  -7.3818274985   -2.3993469581   -4.1475722005
C  -8.008644803    -2.2392941148   -2.7282103
C  -7.8901860901   -3.6190477458   -2.058401928
N  -7.8688735329   -4.5412094248   -3.2153101175
C  -7.0138625527   -3.8845707232   -4.2236810626
C  -7.2109738062   -5.8570693293   -3.0747955384
C  -5.6942384059   -5.6134285696   -3.1461890147
C  -5.5458226836   -4.2696834433   -3.8750551106
O  -6.2888824416   -1.5190779208   -4.3223037712
O  -7.3656513079   -1.1886664125   -2.043732473
C  -7.6874866931   -6.6718520648   -1.8940659724
C  -9.0917113979   -3.8969292233   -1.1457163627
O  -4.9235878419   -3.3693192532   -2.9863046403
O  -9.0815062204   -6.9028187211   -1.947189691
N  -9.4391306303   -2.811520206    -0.2339143789
O  -7.3569262727   -2.2744526516    0.4914486597
C  -8.5791418331   -2.1484787228    0.5700193306
C  -9.2008860107   -1.1916992793    1.5610383562
H  -7.2508413632   -4.3109542938   -5.2061745218
H  -8.1347757047   -2.1697605993   -4.9092710214
H  -9.0692761577   -1.978734371    -2.8318682704
H  -6.9590761039   -3.6514957976   -1.4821589646
H  -7.5111767626   -6.409524808    -3.9768873567
H  -5.1811883152   -6.4340583382   -3.6535864722
H  -5.2499466726   -5.5034905404   -2.1523360921
H  -4.9565619721   -4.3653985565   -4.7982261509
H  -6.3594078378   -0.9179564954   -3.5503288245
H  -7.0241980501   -1.5329413757   -1.1947126511
H  -7.4058125393   -6.1743309142   -0.9532806583
H  -7.1836473826   -7.6443132128   -1.9020935008
H  -9.962451129    -4.0432565333   -1.7918889784
H  -8.9507499753   -4.8183550252   -0.5750822155
H  -5.0107150636   -2.503291322    -3.4235545198
H  -9.4442613105   -6.2174580695   -2.5253618883
H  -10.4226658465  -2.6710338655   -0.0684632649
H  -8.8045910788   -1.4167333392    2.5534301705
H  -8.8870868809   -0.175966589     1.307477344
```

S178

```
H  -10.2922298312  -1.227481189    1.5943040525
```

calc_**2c** conf_47

```
C  -7.3778266214  -2.315082544   -4.3241512547
C  -6.8526490612  -1.8033148251  -2.967686116
C  -7.4747382781  -2.7780064849  -1.9529317081
N  -7.9037822746  -3.9736671457  -2.7150229008
C  -7.4935680933  -3.8328011537  -4.1192709486
C  -7.4263887382  -5.3073651758  -2.3238918251
C  -6.0642009797  -5.4734705966  -3.0108670671
C  -6.1990865417  -4.6919862724  -4.3175455922
O  -6.5411136377  -1.9230702925  -5.399474154
O  -5.4462729121  -1.7259424971  -2.9733691375
C  -7.4084417461  -5.6188515942  -0.8313866033
C  -8.6874717662  -2.108088749   -1.2895942336
O  -5.0105773613  -3.9377373982  -4.5181691894
O  -7.0798020751  -6.9752013293  -0.6092065962
N  -9.5096801193  -3.0205002778  -0.5417539021
O  -9.2249175097  -2.0095329152   1.4713174333
C  -9.7218351363  -2.8992212863   0.7995748159
C  -10.6153894036 -3.9582083675   1.4106532573
H  -8.2724421865  -4.2516382786  -4.7674073705
H  -8.3840295996  -1.916954372   -4.4993152116
H  -7.1890737327  -0.7801847896  -2.7742720161
H  -6.7304386564  -3.0164826246  -1.1862867615
H  -8.1230949038  -6.0291895406  -2.7727869233
H  -5.7834003474  -6.5174425051  -3.1692825848
H  -5.2756853668  -4.9956018306  -2.4146931837
H  -6.3377221497  -5.3631264488  -5.1736868019
H  -5.8720395063  -1.3453339907  -4.9900304046
H  -5.0959207418  -2.587006028   -3.2906768525
H  -8.400530861   -5.4722966208  -0.4017556471
H  -6.7196647859  -4.9527467856  -0.2938237774
H  -8.3605222758  -1.3333784911  -0.5925241781
H  -9.2961755156  -1.6299953394  -2.0693595587
H  -5.2197099099  -3.3339059467  -5.2544573771
H  -6.1367698973  -7.0834118111  -0.7819882874
H  -9.9377999812  -3.7726589981  -1.0575580568
H  -10.0255137789 -4.5563233818   2.110227491
H  -11.3989345441 -3.4628171593   1.9877173786
H  -11.0777890037 -4.625456152    0.6787358457
```

calc_**2c** conf_48

```
C  -7.3863935362  -2.1642257645  -3.870037857
C  -6.7210684161  -2.0132187761  -2.4748371724
C  -6.8792720566  -3.3968078563  -1.7922026812
N  -7.7335021338  -4.1762060717  -2.7178172224
C  -7.4527901584  -3.6799500044  -4.0656915878
C  -7.5176027897  -5.6260823492  -2.8380281043
C  -6.3200780194  -5.7962303862  -3.8065244055
C  -6.2090577574  -4.4514082037  -4.5579675276
O  -6.7364294323  -1.4438156269  -4.8714741302
O  -5.3764556866  -1.6071324911  -2.5952116369
C  -7.3823027928  -6.374334919   -1.5228847338
C  -7.4903602382  -3.3099727648  -0.3904003271
O  -5.0127683055  -3.7544713782  -4.1992875062
O  -8.5579601415  -6.3658043181  -0.7527823231
```

```
N   -8.9218763945    -3.1372104189    -0.4957255081
O   -9.1537215686    -2.1676663312     1.5359080087
C   -9.6518305247    -2.5277351439     0.4826212226
C  -11.1243072286    -2.3479691798     0.1792652549
H   -8.2784733918    -3.9638753931    -4.7293621894
H   -8.422869749     -1.811272003     -3.8027136451
H   -7.2108833691    -1.2273951264    -1.895965734
H   -5.8714589348    -3.8241242113    -1.6921180116
H   -8.4183368524    -6.0172651664    -3.3277468565
H   -6.4719864048    -6.6442218601    -4.47968731
H   -5.3893306129    -5.9767245277    -3.2563590754
H   -6.2320366448    -4.5683052776    -5.6461824517
H   -5.8920399625    -1.1691222518    -4.4730913693
H   -4.9177025708    -2.3523786549    -3.027754341
H   -6.5149873566    -5.9940633725    -0.9592017112
H   -7.1741753852    -7.4251896268    -1.7453787764
H   -7.2534602777    -4.2024872335     0.2015649213
H   -7.062081335     -2.463601763      0.1543861545
H   -4.2583171304    -4.2703255111    -4.5091784808
H   -8.8125503785    -5.4456755839    -0.5901267223
H   -9.3159416969    -3.3441036105    -1.4054163302
H  -11.7055944875    -2.9252786099     0.9026861679
H  -11.3849998646    -1.2965633791     0.31898105
H  -11.4089964136    -2.6577848536    -0.8292570516
```

calc_**2c** conf_49

```
C   -7.3673156967    -2.6343971485    -4.6602840259
C   -7.4616292636    -1.9287336433    -3.2857366002
C   -7.6978520316    -3.0657257954    -2.2522778574
N   -7.7884382189    -4.3127620054    -3.0691177145
C   -7.00409359      -4.07091609      -4.2882280195
C   -7.1775293886    -5.557141235     -2.5753571226
C   -5.6592691804    -5.400251924     -2.7580142666
C   -5.5293709644    -4.4315238365    -3.9547291204
O   -6.5174285436    -1.9894742573    -5.5574649061
O   -6.3170297006    -1.1507457561    -3.0265120104
C   -7.6718078504    -5.9877203969    -1.2160953009
C   -8.9568237108    -2.7382077505    -1.4359442343
O   -4.7755030083    -3.2704292179    -3.6034716558
O   -9.0880050122    -6.1239306753    -1.2317473418
N   -9.1595031666    -3.4745067377    -0.2134873228
O   -8.8416432937    -1.6851228782     1.1571969646
C   -9.1055209359    -2.868085948      1.0059961305
C   -9.4081422834    -3.7739773635     2.1821936543
H   -7.328693903     -4.7757497008    -5.0625872377
H   -8.3699369686    -2.6737472353    -5.1019510946
H   -8.2918156761    -1.2185548766    -3.2805001641
H   -6.8389434295    -3.0801251609    -1.5657033013
H   -7.5132837062    -6.3300464343    -3.282995234
H   -5.1636909717    -6.3608364344    -2.922759813
H   -5.2053054653    -4.9350822887    -1.875912592
H   -5.0549383107    -4.9013008808    -4.8226402562
H   -5.9774902664    -1.3961455716    -5.0073348764
H   -5.5749691128    -1.7807985152    -2.9567159744
H   -7.3753490851    -5.2609513382    -0.4488669455
H   -7.2379927447    -6.9567947932    -0.9493505927
H   -8.8882608768    -1.6910354033    -1.1299685111
H   -9.8295265233    -2.8469188984    -2.0936883725
```

```
H   -3.8786120782    -3.5492117869    -3.3807193079
H   -9.38713802      -5.6866744186    -2.0450970033
H   -9.4154740577    -4.4537694831    -0.2773287232
H   -8.6013071943    -3.681847204      2.9125543311
H  -10.3241347899    -3.4257431498     2.6668076113
H   -9.5302309803    -4.8250137664     1.9088388073
```

calc_**2c** conf_50

```
C   -7.1716362517    -2.4555349858    -4.4168736742
C   -8.1137412384    -2.1566649323    -3.2144089853
C   -7.9842425955    -3.3736560458    -2.2800327166
N   -7.8273955505    -4.4550830553    -3.269985115
C   -6.8366336804    -3.9486955369    -4.2311142467
C   -7.2594091892    -5.7547956228    -2.8781116404
C   -5.73442808      -5.5539797695    -2.7744949034
C   -5.4400140886    -4.3315496369    -3.6600067778
O   -6.0843815052    -1.5583941437    -4.4610242443
O   -7.8242413138    -0.9281608052    -2.6089868148
C   -7.9050056863    -6.3973844935    -1.6677430368
C   -9.2149447586    -3.4823232431    -1.3757646242
O   -4.9091652339    -3.2514304286    -2.8807930751
O   -9.2719818708    -6.6697426131    -1.8911678481
N   -9.2099449016    -2.4241561153    -0.3895652542
O   -8.2877625796    -3.7426333809     1.2176336851
C   -8.6423134715    -2.6374202194     0.8334994148
C   -8.4896259664    -1.4036167272     1.6968569675
H   -6.9422629773    -4.5019169837    -5.1716851617
H   -7.7091828428    -2.3080543764    -5.3554760636
H   -9.1487800535    -2.136818741     -3.5830634568
H   -7.0976131765    -3.2409958839    -1.6422867113
H   -7.4587244382    -6.4197053561    -3.7300215948
H   -5.1870504876    -6.4476413576    -3.085587917
H   -5.4419673154    -5.3216287719    -1.7447824029
H   -4.7434765529    -4.5565911247    -4.4758894291
H   -5.4035510552    -1.9150380662    -3.8572254514
H   -7.0326179541    -0.6045398339    -3.0801818445
H   -7.7534967882    -5.7753357821    -0.7734235449
H   -7.4191488113    -7.3595269932    -1.4767797012
H  -10.1243944214    -3.4090022909    -1.9844538258
H   -9.2553797841    -4.4169354      -0.819130664
H   -4.0283597353    -3.5001050303    -2.5729011855
H   -9.6200904884    -5.9348420382    -2.4140624373
H   -9.2165125737    -1.4762089353    -0.7399987303
H   -9.0739208526    -0.5511278627     1.3429121359
H   -8.7905360483    -1.6510906194     2.7161436272
H   -7.434065681     -1.117672797      1.7249772484
```

calc_**2c** conf_51

```
C   -7.2593902024    -2.3107148429    -4.3637692889
C   -7.5595736886    -1.920136164     -2.8922302695
C   -8.0163446495    -3.2367495931    -2.221470911
N   -8.0269875913    -4.2489582045    -3.2959075938
C   -7.0372828103    -3.8251399341    -4.285368844
C   -7.6083650773    -5.6120038274    -2.9568598496
C   -6.0611940472    -5.5820535876    -2.9268026897
C   -5.6686337972    -4.3858416717    -3.819298838
O   -6.2399385395    -1.5524673306    -4.9388690847
```

S181

```
O   -6.4364795537    -1.3258441841    -2.2794463967
C   -8.252865175     -6.2217166344    -1.7181964555
C   -9.396345192     -3.1192039818    -1.5701070708
O   -4.9345381622    -3.4016543154    -3.0820822685
O   -7.8098737518    -7.5558938871    -1.5383540586
N   -9.3897556215    -2.2341713338    -0.4235642164
O   -8.4130382462    -3.7556359664     0.9396801414
C   -8.8312743579    -2.620204031      0.7552006554
C   -8.748119444     -1.5493308711     1.8208224995
H   -7.2616543496    -4.3072522448    -5.2443640089
H   -8.1686259578    -2.1639579665    -4.9576123862
H   -8.3398438683    -1.1545299195    -2.8530773911
H   -7.2958585145    -3.4728585149    -1.4250023175
H   -7.9097172088    -6.2418228138    -3.8039427108
H   -5.6290040147    -6.5278659549    -3.2625047676
H   -5.6976829657    -5.3893790863    -1.9090790847
H   -5.0657351423    -4.6841269495    -4.6834775966
H   -5.7505163654    -1.1800138436    -4.1859204124
H   -5.7574518334    -2.0272826988    -2.2443401936
H   -9.3355572161    -6.2760920204    -1.8626347842
H   -8.0672320556    -5.6140570789    -0.8229598325
H   -10.1207020091   -2.7483297414    -2.3005913071
H   -9.7412226465    -4.0978707094    -1.2336206563
H   -4.1312320741    -3.8190386954    -2.7471297019
H   -6.9693832392    -7.522491558     -1.0673872657
H   -9.5949418348    -1.2579808933    -0.5623640267
H   -9.4690987176    -0.7403023552     1.6783659451
H   -8.9100909713    -2.0118833512     2.7950004038
H   -7.7414491073    -1.1201432432     1.8172666342
```

calc_**2c** conf_52

```
C   -7.3218466809    -2.2075823081    -4.027475607
C   -6.9735601141    -1.9018473738    -2.5352375939
C   -6.9741003014    -3.2591042029    -1.8116866082
N   -7.8266696508    -4.1035528994    -2.6768233147
C   -7.5305297217    -3.7301145285    -4.0597906665
C   -7.660101483     -5.5602329688    -2.670457942
C   -6.4717974115    -5.8650591761    -3.6187825219
C   -6.3430037401    -4.6180188421    -4.5116137705
O   -6.3603387851    -1.6992566325    -4.9207323801
O   -5.7303171233    -1.2684286672    -2.4089057132
C   -7.5455054892    -6.2251081319    -1.3055521707
C   -7.5188285554    -3.1437597146    -0.3877104129
O   -5.1147407233    -3.9267523356    -4.2672094026
O   -7.5954033571    -7.632118163     -1.4300978528
N   -8.9451139437    -2.9334825592    -0.4208659209
O   -9.0636298166    -1.9649517318     1.6211571003
C   -9.6198399522    -2.3563218904     0.6065023512
C   -11.1165075565   -2.2215509195     0.4088327932
H   -8.3825072172    -4.0070196583    -4.6928037991
H   -8.2587269657    -1.7121986398    -4.2899453161
H   -7.7638359064    -1.2703882819    -2.1052279091
H   -5.9305211248    -3.6010116795    -1.7705656582
H   -8.567116907     -5.9735272516    -3.1306962059
H   -6.6356270712    -6.7806478943    -4.1930123647
H   -5.5388018527    -5.98113041      -3.0537401254
H   -6.4198171481    -4.8530924801    -5.5794327294
H   -5.6031109671    -2.3132894745    -4.864747976
```

```
H  -5.5652063342   -0.8671359216   -3.2794160098
H  -8.3951582072   -5.943962675    -0.6788623531
H  -6.62785059     -5.905828204    -0.7917182951
H  -7.2698501557   -4.0262328399   0.2130942679
H  -7.0471531485   -2.2908070528   0.10835275
H  -4.3863362045   -4.470449761    -4.5932645486
H  -6.7486998612   -7.9287310302   -1.7848712743
H  -9.4224683131   -3.2931149365   -1.235319571
H  -11.4746638326  -2.6142190663   -0.5462473897
H  -11.6272550484  -2.7429217679   1.2219154514
H  -11.3854587388  -1.1650479296   0.4819586898
```

Table S40. Sampled and DFT geometry optimized conformers related to calc_**2d**, with energy values (Hartree) and related % contribution on the final Boltzmann distribution for the three employed functional/basis set combinations.

Conformer	MPW1PW91/6-31g(d,p)		MPW1PW91/6-311+g(d,p)		B97-2/cc-pVTZ	
	Energy (Hartree)	% contribution on the Boltzmann distribution	Energy (Hartree)	% contribution on the Boltzmann distribution	Energy (Hartree)	% contribution on the Boltzmann distribution
calc_**2d** conf_1	-916.6602254	86.03%	-916.8959853	48.60%	-916.8428697	23.79%
calc_**2d** conf_2	-916.6579264	7.54%	-916.8953805	25.61%	-916.8432410	35.25%
calc_**2d** conf_3	-916.6567706	2.22%	-916.8949115	15.58%	-916.8424834	15.80%
calc_**2d** conf_4	-916.6567506	2.17%	-916.8935842	3.82%	-916.8421527	11.13%
calc_**2d** conf_5	-916.6563070	1.36%	-916.8938544	5.09%	-916.8420066	9.54%
calc_**2d** conf_6	-916.6551986	0.42%	-916.8892291	0.04%	-916.8386682	0.28%
calc_**2d** conf_7	-916.6539039	0.11%	-916.8919865	0.70%	-916.8405758	2.10%
calc_**2d** conf_8	-916.6529672	0.04%	-916.8897929	0.07%	-916.8385423	0.24%
calc_**2d** conf_9	-916.6528236	0.03%	-916.8896250	0.06%	-916.8385582	0.25%
calc_**2d** conf_10	-916.6522584	0.02%	-916.8861748	0.00%	-916.8354509	0.01%
calc_**2d** conf_11	-916.6522133	0.02%	-916.8876632	0.01%	-916.8369902	0.05%
calc_**2d** conf_12	-916.6521418	0.02%	-916.8896318	0.06%	-916.8385297	0.24%
calc_**2d** conf_13	-916.6520655	0.02%	-916.8860581	0.00%	-916.8354306	0.01%
calc_**2d** conf_14	-916.6514534	0.01%	-916.8909015	0.22%	-916.8396257	0.77%
calc_**2d** conf_15	-916.6510172	0.01%	-916.8873766	0.01%	-916.8361109	0.02%
calc_**2d** conf_16	-916.6509492	0.00%	-916.8897769	0.07%	-916.8384907	0.23%
calc_**2d** conf_17	-916.6505226	0.00%	-916.8869896	0.00%	-916.8357173	0.01%
calc_**2d** conf_18	-916.6504742	0.00%	-916.8892337	0.04%	-916.8381284	0.16%
calc_**2d** conf_19	-916.6494853	0.00%	-916.8866687	0.00%	-916.8355612	0.01%
calc_**2d** conf_20	-916.6492676	0.00%	-916.8875793	0.01%	-916.8364101	0.03%
calc_**2d** conf_21	-916.6491423	0.00%	-916.8830372	0.00%	-916.8330498	0.00%
calc_**2d** conf_22	-916.6488090	0.00%	-916.8882200	0.01%	-916.8370444	0.05%
calc_**2d** conf_23	-916.6486700	0.00%	-916.8842583	0.00%	-916.8340766	0.00%
calc_**2d** conf_24	-916.6482572	0.00%	-916.8852167	0.00%	-916.8344317	0.00%
calc_**2d** conf_25	-916.6480039	0.00%	-916.8832578	0.00%	-916.8323040	0.00%
calc_**2d** conf_26	-916.6474383	0.00%	-916.8837327	0.00%	-916.8334163	0.00%
calc_**2d** conf_27	-916.6473577	0.00%	-916.8855042	0.00%	-916.8348847	0.01%
calc_**2d** conf_28	-916.6468530	0.00%	-916.8860622	0.00%	-916.8350201	0.01%

calc_**2d** conf_29	-916.6468474	0.00%	-916.8846051	0.00%	-916.8337990	0.00%
calc_**2d** conf_30	-916.6465621	0.00%	-916.8853328	0.00%	-916.8343019	0.00%
calc_**2d** conf_31	-916.6464920	0.00%	-916.8859177	0.00%	-916.8352544	0.01%
calc_**2d** conf_32	-916.6461138	0.00%	-916.8845756	0.00%	-916.8332151	0.00%
calc_**2d** conf_33	-916.6458219	0.00%	-916.8842265	0.00%	-916.8334170	0.00%
calc_**2d** conf_34	-916.6457829	0.00%	-916.8852733	0.00%	-916.8346174	0.00%
calc_**2d** conf_35	-916.6454169	0.00%	-916.8854930	0.00%	-916.8350438	0.01%
calc_**2d** conf_36	-916.6444355	0.00%	-916.8845010	0.00%	-916.8338331	0.00%
calc_**2d** conf_37	-916.6438194	0.00%	-916.8820646	0.00%	-916.8314767	0.00%
calc_**2d** conf_38	-916.6437971	0.00%	-916.8827304	0.00%	-916.8319925	0.00%
calc_**2d** conf_39	-916.6435138	0.00%	-916.8823569	0.00%	-916.8321443	0.00%
calc_**2d** conf_40	-916.6433259	0.00%	-916.8847580	0.00%	-916.8338578	0.00%
calc_**2d** conf_41	-916.6428984	0.00%	-916.8838123	0.00%	-916.8334919	0.00%
calc_**2d** conf_42	-916.6426125	0.00%	-916.8795741	0.00%	-916.8299328	0.00%
calc_**2d** conf_43	-916.6425132	0.00%	-916.8798507	0.00%	-916.8302082	0.00%
calc_**2d** conf_44	-916.6420538	0.00%	-916.8792092	0.00%	-916.8282448	0.00%
calc_**2d** conf_45	-916.6412700	0.00%	-916.8800598	0.00%	-916.8291861	0.00%
calc_**2d** conf_46	-916.6390525	0.00%	-916.8774673	0.00%	-916.8267158	0.00%
calc_**2d** conf_47	-916.6385838	0.00%	-916.8775320	0.00%	-916.8267990	0.00%

Table S41. Cartesian coordinates of the optimized geometries for the conformers related to calc_**2d**. The related energies and % contribution on the final Boltzmann distribution for the three employed functional/basis set combinations are reported in Table S40.

calc_**2d** conf_1

```
C  -5.6312983065  -2.1941409735   0.1640601368
C  -6.7619517758  -1.2695529933   0.6331875336
C  -6.7760044328  -0.195787355   -0.4528002485
N  -5.3454024628   0.0985583804  -0.5334142966
C  -4.6629229912  -1.2199128964  -0.5403515664
C  -4.8799650274   0.8759594357  -1.6965388589
C  -3.8728947539  -0.0350052024  -2.4237719253
C  -4.29013101    -1.4449412867  -2.0188500836
O  -6.1547831214  -3.1819336565  -0.7134138549
O  -7.9519729961  -1.9895392527   0.773415285
C  -4.2832407027   2.2045869871  -1.1831078884
C  -7.6861661745   0.9942648803  -0.1805694176
O  -5.3908448933  -1.7912071424  -2.8245735802
O  -4.955161443    2.619032791   -0.0131301111
N  -7.5240966963   1.6370901066   1.1068271191
O  -8.8939029621   0.2069680879   2.2102375532
C  -8.190740216    1.2195294111   2.2044293299
C  -8.0411809477   2.0704028772   3.4426239248
H  -3.7308048229  -1.1500002323   0.0337275355
H  -5.1442002775  -2.7014070907   1.0044304951
H  -6.4600154738  -0.8019827845   1.5789977793
H  -7.1357574753  -0.6535185021  -1.3883333994
H  -5.7343477445   1.0860363779  -2.3498098631
H  -3.90018945     0.079618323   -3.5092325117
H  -2.851788203    0.1707380345  -2.0821326103
H  -3.4700128008  -2.1712206985  -2.1223507035
H  -7.0678032213  -3.3315604375  -0.4107199283
H  -8.5525746299  -1.4003633952   1.2735938175
H  -4.3778623279   2.9961644534  -1.9313344017
H  -3.2098579581   2.0707084934  -0.9751481673
H  -8.7191061251   0.6414126229  -0.2521689271
H  -7.5421945437   1.7564544287  -0.9498918133
H  -5.8349448756  -2.5226322154  -2.356734282
H  -5.0584939806   1.760983276    0.4512766685
H  -6.9611983864   2.4743013929   1.1357126453
H  -7.3397512842   2.8987089185   3.3219108945
H  -9.0218978503   2.4710481318   3.7114877364
H  -7.7125376555   1.4371387047   4.2694599846
```

calc_**2d** conf_2

```
C  -5.7843527184  -2.2654769481   0.1057620243
C  -6.8974402203  -1.3155122821   0.5507346533
C  -6.8085482602  -0.2092039355  -0.5003130981
N  -5.3771281828   0.0426019629  -0.466902641
C  -4.7218972104  -1.2865695214  -0.4339991491
C  -4.775160546    0.8385726483  -1.5380753308
C  -3.6560802139  -0.0482615362  -2.1230930751
C  -4.1503564509  -1.4643104319  -1.8519057904
O  -6.2814971643  -3.1499059043  -0.8915462784
O  -8.1269078608  -1.9793223476   0.6184226862
C  -4.2353921749   2.1578765027  -0.9980342411
```

S186

```
C   -7.6880259844    0.996552408    -0.2132776722
O   -5.1361646242   -1.7400608249   -2.8177196944
O   -5.2391103902    3.015385925    -0.4682941058
N   -7.4663139038    1.6092890787    1.0741031554
O   -8.9431056952    0.2679178303    2.1525398795
C   -8.1169351973    1.1848000744    2.1762999499
C   -7.802180021     1.9140597959    3.4609143552
H   -3.8741030412   -1.2621972337    0.2644145734
H   -5.394215529    -2.8641790791    0.9366245624
H   -6.6160323466   -0.8883418874    1.5205387305
H   -7.1365031107   -0.6217510989   -1.47086748
H   -5.5209981118    1.0430499527   -2.3210482385
H   -3.4969569872    0.117933681    -3.1904939918
H   -2.7082504815    0.1302894685   -1.6002819986
H   -3.3382571352   -2.2064256131   -1.8770761793
H   -7.220965098    -3.2782747859   -0.6752028609
H   -8.7101627532   -1.3838487526    1.1296560554
H   -3.6581774219    2.6797008029   -1.7753131901
H   -3.5608784198    1.9454707202   -0.1646252726
H   -8.7328239923    0.6791643446   -0.2611362364
H   -7.5392381666    1.7598665902   -0.9808440032
H   -5.6892238796   -2.445835825    -2.4349550446
H   -5.7135224167    3.4056893864   -1.2127283929
H   -6.6877080106    2.2515588518    1.1317746189
H   -8.7191544491    2.3788281434    3.8318518925
H   -7.0343186084    2.682415792     3.3484856642
H   -7.4809132218    1.1884540481    4.2116111642
```

calc_**2d** conf_3

```
C   -5.8290489521   -2.0252499695   -0.0559874865
C   -6.93862182     -1.1686749759    0.539005382
C   -6.9391633649    0.0264634469   -0.4174228463
N   -5.5117545463    0.2946415651   -0.6051303451
C   -4.7661083903   -0.9710309728   -0.3638199159
C   -5.1458189459    0.8152224415   -1.9390926397
C   -4.5686425412   -0.3728050442   -2.7033706703
C   -3.8874619673   -1.2188210159   -1.617459235
O   -6.3026382609   -2.6297686009   -1.2522665948
O   -8.1465923119   -1.8718940577    0.5821712422
C   -4.1734050289    1.9851207661   -1.736789128
C   -7.7508409789    1.2360725822    0.0380530135
O   -3.6861831058   -2.5683801248   -1.9354972334
O   -4.6432176733    2.8043760478   -0.693436262
N   -7.5360626045    1.6515851273    1.4106060652
O   -9.0273322436    0.1826278367    2.27585804
C   -8.2458737536    1.1208267364    2.4327049379
C   -8.0435094323    1.7512900494    3.7896492166
H   -4.1340620733   -0.8671537312    0.5255439975
H   -5.465950695    -2.7932822936    0.6367552854
H   -6.6250735415   -0.8389992219    1.5387216954
H   -7.4003294287   -0.3211263927   -1.3558883747
H   -6.049494003     1.2123628047   -2.4143552297
H   -5.3755412374   -0.9620530434   -3.1502304703
H   -3.8765275811   -0.0833556417   -3.4998412244
H   -2.8871281863   -0.8195203842   -1.4241991901
H   -7.2019948101   -2.9386474278   -1.0564972491
H   -8.7428428253   -1.3261075832    1.1310939806
H   -4.1058575281    2.5912461503   -2.6448000459
```

S187

```
H   -3.1617557295    1.6046104152   -1.5180393463
H   -8.8132329297    0.9992351401   -0.0703550344
H   -7.5269918119    2.0894526454   -0.6077363475
H   -4.5706359147   -2.9606689528   -2.0244701209
H   -4.9277641909    2.1334221764   -0.0411580798
H   -6.9256876116    2.43205762      1.5900133682
H   -7.2564951119    2.5084607105    3.8097390428
H   -8.9841331571    2.2102318955    4.1050984617
H   -7.8072257115    0.9672332766    4.511829341
```

calc_**2d** conf_4

```
C   -5.7682599365   -2.1544457518   -0.282312966
C   -6.4344751139   -1.3426213985    0.8247892922
C   -6.4173892825    0.0768554711    0.2284464386
N   -5.1120891606    0.1445337797   -0.4387815684
C   -4.6420756341   -1.2317749734   -0.733119338
C   -5.0862506444    0.935834635    -1.6862516822
C   -5.0777852105   -0.0855197957   -2.8208550319
C   -4.2898402654   -1.2708342032   -2.2435479799
O   -6.7154659654   -2.3400622227   -1.3249539957
O   -7.7042009883   -1.8786464324    1.0612819683
C   -3.8585397338    1.8521149889   -1.6586674687
C   -6.5627603555    1.2401754323    1.2233556789
O   -4.5104106536   -2.5066885939   -2.8653688181
O   -3.7666766312    2.5002863035   -0.4133389106
N   -7.9241346004    1.6942797281    1.4500318033
O   -8.5345897841    0.0039340232    2.8232432697
C   -8.79894792      1.0693358161    2.2631146785
C  -10.1310041383    1.7489944716    2.4707679316
H   -3.7555518274   -1.4623222099   -0.1307783582
H   -5.3991781843   -3.1247317733    0.0703799384
H   -5.8074302116   -1.3671757479    1.7288020711
H   -7.2423994802    0.134007586    -0.499093349
H   -5.976366489     1.5745353332   -1.709912082
H   -6.0973715724   -0.4182168761   -3.0368842067
H   -4.6370292657    0.2957370764   -3.7469702757
H   -3.2176836686   -1.0827288444   -2.3562595064
H   -7.5620110118   -2.4994563537   -0.8729773521
H   -8.1142814961   -1.3408038806    1.7709436898
H   -3.9410957494    2.6224427586   -2.4309199296
H   -2.9464083732    1.2707236917   -1.8707034541
H   -6.0073405628    2.0951053084    0.8306037912
H   -6.1166990983    0.9700956923    2.1862519927
H   -5.441942072    -2.7290885309   -2.7000723242
H   -3.9048417402    1.7692880294    0.2164837675
H   -8.2078495021    2.5585115898    1.0178779558
H  -10.2480210788    2.6776354025    1.9076206559
H  -10.9272371861    1.0563445121    2.1889018646
H  -10.2493654116    1.9623459588    3.5358718097
```

calc_**2d** conf_5

```
C   -5.577889399    -2.2199369409   -0.107679016
C   -6.2537967973   -1.2839267045    0.9052247635
C   -6.3776544508    0.0385203183    0.131999337
N   -5.0673746771    0.1084753613   -0.5106180255
C   -4.7257996643   -1.2674809646   -0.9603567721
C   -4.9221348771    1.0230347913   -1.6656433523
```

```
C   -4.3545611823    0.1441640758   -2.7918686409
C   -4.920876169    -1.232050305    -2.4856193411
O   -6.5704566654   -2.8972624193   -0.8649670024
O   -7.449398305    -1.8782959529    1.3186458037
C   -3.9801868405    2.1702750568   -1.287598067
C   -6.6441351191    1.2738086445    1.0021858652
O   -6.2768257481   -1.2087755839   -2.8665724379
O   -2.8436497523    1.6699724129   -0.6311580245
N   -8.050209188     1.5577707044    1.2330696017
O   -8.3325409232    0.0984030721    2.9388707309
C   -8.7864577651    0.9754144531    2.2009962469
C   -10.2081574249   1.4601585998    2.3495052502
H   -3.6620450265   -1.4530472905   -0.7667783985
H   -4.9562349568   -2.9688765058    0.3960711622
H   -5.5712006014   -1.120251976     1.7515724522
H   -7.1877590317   -0.0595190131   -0.6095579751
H   -5.9035863592    1.4166141331   -1.9612643363
H   -4.6564633662    0.4907932185   -3.7825813649
H   -3.2612974429    0.1348047401   -2.7339761746
H   -4.3716431553   -2.0441305587   -2.9843411734
H   -7.3375210041   -2.9587069168   -0.266808124
H   -7.8305825847   -1.3151051577    2.0251183785
H   -4.5074478678    2.9080040557   -0.6593327198
H   -3.6417504875    2.6965030432   -2.1859317316
H   -6.2246955954    2.1571246524    0.5162576021
H   -6.1488175411    1.1683809452    1.9718359807
H   -6.6927031488   -1.9422583838   -2.3768031604
H   -3.2193516067    1.0283039322   -0.0014321517
H   -8.4982376012    2.2321100681    0.6340510936
H   -10.4805843452   2.2571992439    1.6540275791
H   -10.8849587301   0.614374945     2.2069505087
H   -10.3470145985   1.8174142056    3.3725056339
```

calc_**2d** conf_6

```
C   -5.9770038731   -2.5419160341   -0.2758372687
C   -7.305603866    -1.7923890231   -0.5061141412
C   -7.024202007    -0.3637777711   -0.0577246032
N   -5.5881808041   -0.1506694469   -0.3113670478
C   -4.8962826892   -1.4486368194   -0.4748494044
C   -5.2251781385    0.7619297016   -1.4107431194
C   -3.9532863126    0.1321437876   -1.9795400911
C   -4.2147750462   -1.3666110688   -1.8529428168
O   -5.8448136676   -3.6789761399   -1.0912853738
O   -7.6035839766   -1.7746058088   -1.8993796246
C   -5.0472497835    2.1683938463   -0.8267987821
C   -7.3713468233   -0.1148601158    1.4111327822
O   -5.0316191765   -1.8553945358   -2.9102647974
O   -4.3428129635    2.0949569033    0.3949795105
N   -7.1177513122    1.2527634277    1.7903039615
O   -9.2474539618    1.6804103264    2.4581676019
C   -8.1022945782    2.0629835403    2.2750959071
C   -7.6671636653    3.4784461382    2.589415632
H   -4.1138402856   -1.5595603069    0.2849483504
H   -5.9484913029   -2.894449476     0.7599532746
H   -8.138019261    -2.2519822135    0.0394732639
H   -7.6105335981    0.3326620504   -0.6662328167
H   -6.0083158699    0.7924255302   -2.1828822145
H   -3.7583348499    0.4229034913   -3.0137947678
```

```
H   -3.0923631661    0.4202927334    -1.3658763943
H   -3.2996829452   -1.9608239756    -1.8921892904
H   -5.4830900115   -3.3608770832    -1.9421415985
H   -7.636758234    -2.7098342045    -2.1597479701
H   -6.0356416761    2.6258659531    -0.6732764545
H   -4.4895008514    2.8075672221    -1.5188792288
H   -6.8017206136   -0.8010719704     2.0526073392
H   -8.434686101    -0.2897206707     1.5916221661
H   -5.9392443531   -1.51275175      -2.7763055283
H   -4.4953600563    1.1681796506     0.673066004
H   -6.2002335478    1.6420438511     1.6204585702
H   -7.7496749162    3.6397958272     3.6675244509
H   -6.6457715415    3.7054403045     2.2744079485
H   -8.3581341734    4.1717041291     2.1050165714
```

calc_**2d** conf_7

```
C   -5.9184358948   -2.516593991     -0.259362422
C   -6.5093533434   -1.70602221       0.9019404998
C   -6.2814635091   -0.2501921616     0.4776319795
N   -4.9828100933   -0.2844274928    -0.1673603963
C   -4.7205003474   -1.6529397755    -0.6789305964
C   -4.6962891764    0.6796263511    -1.2288987595
C   -3.7071066138   -0.0842437109    -2.1124019189
C   -4.3505567209   -1.4687851397    -2.1628273857
O   -6.9099167284   -2.6376479976    -1.2624353766
O   -7.8612278838   -2.0418004801     1.0647355587
C   -4.1785206577    2.0231580428    -0.7359458979
C   -6.3591313105    0.7217035209     1.6756309873
O   -5.4452853267   -1.3685409363    -3.0397285445
O   -5.2093950009    2.8817075856    -0.2505847803
N   -7.3487500331    1.7626557267     1.521725749
O   -9.0852663737    0.3409131385     1.7950212405
C   -8.6634915193    1.4786884923     1.5673050762
C   -9.6158109552    2.6280605675     1.3453421587
H   -3.832756306    -2.0593351058    -0.1725942537
H   -5.5991287972   -3.5183934102     0.0526471425
H   -5.9340517055   -1.9109120392     1.8177651784
H   -7.0779287709    0.0187646245    -0.2392882259
H   -5.6010830527    0.8692525536    -1.8366454168
H   -3.6105593164    0.3464597188    -3.1114864875
H   -2.7173631874   -0.1241783715    -1.6416952781
H   -3.6513764141   -2.2500814542    -2.4946876992
H   -7.7537962218   -2.5388496909    -0.7778175763
H   -8.3412168143   -1.2466225728     1.3897303736
H   -3.6314238407    2.5265163235    -1.5458468538
H   -3.4877632352    1.8726038411     0.0965791715
H   -5.390579538     1.2000054292     1.8126118496
H   -6.5946577849    0.1727920564     2.5931906503
H   -6.171504637    -1.8968219681    -2.6620600367
H   -5.7644840955    3.0943965112    -1.0121475672
H   -7.0180357368    2.6509176482     1.1767744968
H   -9.1138949148    3.5863762329     1.1944657448
H   -10.2432132206   2.4079696451     0.4781097747
H   -10.2768709219   2.7058204988     2.2115378414
```

calc_**2d** conf_8

```
C   -6.2945318769   -2.4218033696    -1.0605008557
```

```
C   -6.9074687226   -1.9226700604    0.2638478562
C   -6.380447981    -0.5018731704    0.3888591587
N   -5.0044710193   -0.5975239854   -0.0742145291
C   -4.9923846654   -1.5988883229   -1.1781995657
C   -4.4096016683    0.6545456055   -0.5812678236
C   -3.7769884728    0.2698282019   -1.9265758726
C   -4.7429141036   -0.7779038137   -2.4570483553
O   -7.2173667026   -2.1853876372   -2.1098302484
O   -8.3147005386   -1.9769457858    0.2114588441
C   -3.3921747718    1.2799205742    0.3584355702
C   -6.5666072614    0.0325668053    1.8156441515
O   -5.8789406944   -0.0781723674   -2.9018789066
O   -3.9496832773    1.7485031629    1.5821148922
N   -7.0667513209    1.3864510536    1.8522090293
O   -9.0991800623    0.6734758125    1.172456509
C   -8.3413234521    1.6043047869    1.4570505403
C   -8.799128372     3.0393858188    1.392719789
H   -4.1341666255   -2.2697171259   -1.0412717153
H   -6.0746460436   -3.4949483906   -1.0298893099
H   -6.5328753706   -2.5356393533    1.095243859
H   -6.9779280533    0.1255905946   -0.2943850612
H   -5.2050667724    1.3910222369   -0.763525382
H   -3.6931328944    1.1180045641   -2.6093002345
H   -2.7792643738   -0.1620306267   -1.7793541836
H   -4.3068251147   -1.396914771    -3.2553143767
H   -8.0772088933   -2.1087613401   -1.6461582538
H   -8.6701693495   -1.1249603948    0.5435101566
H   -2.9517171057    2.1541413855   -0.1327897232
H   -2.583049597     0.5649455556    0.5546079758
H   -5.6250891961   -0.019194361     2.3595500134
H   -7.2887562986   -0.5907316833    2.3510864842
H   -6.6042618266   -0.731299996    -2.8947536894
H   -3.8722557451    1.0285558004    2.2176199526
H   -6.390585761     2.1366844163    1.8738308664
H   -9.0314099226    3.2915737377    0.3546992529
H   -9.7230100263    3.1388643716    1.9663276418
H   -8.0599160667    3.7460020713    1.7759855434
```

calc_**2d** conf_9

```
C   -6.2712963749   -2.3002254859   -1.090847792
C   -7.1496761756   -1.9365934586    0.1091257919
C   -6.6978008432   -0.5132287744    0.4331526607
N   -5.2750723995   -0.462663225     0.0914978998
C   -4.9378057899   -1.6590405373   -0.7100214582
C   -4.8328010131    0.7573166581   -0.6188078767
C   -4.4532400674    0.3159054571   -2.0306276561
C   -4.0681325241   -1.1650816161   -1.8895939913
O   -6.8081412075   -1.6785293838   -2.2443930827
O   -8.5160337996   -2.0012491715   -0.2485178363
C   -3.6930699641    1.3961527453    0.1781071066
C   -7.0063445699   -0.0942684685    1.8716650999
O   -4.196548031    -1.9275054604   -3.0589272139
O   -4.0342650567    1.4415127038    1.5487840273
N   -7.1509747146    1.3365597093    2.0138753326
O   -9.2352064519    1.234287887     1.1437200305
C   -8.2963552214    1.9094412168    1.558039405
C   -8.3583019074    3.4172476428    1.6153492006
H   -4.3810227188   -2.3803826605   -0.0992122969
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S191

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H   -6.1826598918   -3.3824585916   -1.2451034007
H   -6.9431402181   -2.619052822     0.946026584
H   -7.2696744129    0.1478134915   -0.2338147017
H   -5.6650363359    1.4699394836   -0.6305989644
H   -5.3232499044    0.3832559304   -2.688886068
H   -3.6467671069    0.9123640676   -2.4680819608
H   -3.0141693527   -1.2462484531   -1.6065351514
H   -7.7739746825   -1.7335861977   -2.1322560032
H   -8.9695805875   -1.2319296432    0.1306186164
H   -3.5153546007    2.42285291     -0.1528894917
H   -2.7597224868    0.8306849993    0.0297399796
H   -6.2186369672   -0.4481408329    2.5422464789
H   -7.948536303    -0.5447595394    2.1961590325
H   -5.1373119361   -1.8945650397   -3.2987768593
H   -4.3051711656    0.5206460328    1.7196008552
H   -6.3045134069    1.8835293461    2.1083868231
H   -9.2018736755    3.7086582937    2.2457431246
H   -7.4476556537    3.8753374572    2.007568256
H   -8.554882481     3.8040033287    0.6124855003

calc_2d conf_10

C   -6.0318715848   -2.5578783302   -0.2608322411
C   -7.3589589265   -1.817863771    -0.5340352615
C   -7.1205032273   -0.4272230275    0.0579031048
N   -5.6867917292   -0.1651762392   -0.1055892084
C   -4.9583119155   -1.4403923966   -0.3122295381
C   -5.3004095886    0.8061954218   -1.1488355456
C   -3.9752362027    0.2503063998   -1.6652478451
C   -4.1856179344   -1.2528905841   -1.6285639935
O   -5.8303991338   -3.613414479    -1.1881642488
O   -7.6277068212   -1.828353798    -1.9210379298
C   -5.194100448     2.1963312317   -0.519482282
C   -7.5540037325   -0.3654073774    1.5324739465
O   -4.9625816696   -1.6102716383   -2.7665013942
O   -4.4558346522    2.1237204819    0.6789510301
N   -7.1925050461    0.8672782029    2.1898589491
O   -8.7821681179    2.0901341718    1.1467817205
C   -7.8228179557    2.0439478961    1.9016561691
C   -7.2301887245    3.2595738106    2.5793190753
H   -4.2286027917   -1.5910667994    0.4931494242
H   -6.0470955762   -2.990947569     0.7457773775
H   -8.2100760762   -2.3245582105   -0.0695965236
H   -7.7030239466    0.3219190714   -0.4847091086
H   -6.0389064057    0.8364498376   -1.9629271329
H   -3.7292698085    0.5987100603   -2.6704692726
H   -3.1692090417    0.5368138936   -0.9820648203
H   -3.2464278521   -1.8176897271   -1.6322771578
H   -6.6382414387   -3.6095253589   -1.7340320986
H   -6.8408761661   -1.4585411509   -2.37367048
H   -6.2041495303    2.5945006974   -0.3416010985
H   -4.680986636     2.8856737795   -1.1972142895
H   -7.1076033166   -1.1873537795    2.1014144649
H   -8.6411479655   -0.4772036083    1.5805581097
H   -5.0882237562   -2.5704969821   -2.6679338478
H   -4.7362641904    1.2573867995    1.0335190317
H   -6.3400172586    0.8982990681    2.7242410495
H   -7.199315195     3.133198364     3.6659683513
H   -6.2054414748    3.4162191251    2.2258974088
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```
H   -7.8381141627   4.1295965141    2.3355461053
```

calc_**2d** conf_11

```
C   -5.7683826807   -1.657155312     0.5094066485
C   -7.1060694313   -0.9870048314    0.1410577704
C   -6.7013337097    0.4558461776    -0.1751138848
N   -5.349087722     0.3769300729    -0.7358370836
C   -4.7170644233   -0.9074792356    -0.3481158778
C   -5.1986967603    0.5972911926    -2.1857171723
C   -4.0597106008   -0.3470220802    -2.5659455547
C   -4.2864752159   -1.5555097809    -1.6750457594
O   -5.8046276156   -3.060384036     0.2756648956
O   -7.7026946196   -1.6573547461    -0.9517397714
C   -4.8871770792    2.0739940843    -2.4324601407
C   -6.6847950371    1.3732730182     1.0576716599
O   -5.3253690328   -2.336959051     -2.255562904
O   -3.8400102678    2.5010251103    -1.6005780356
N   -7.9766418951    1.5647671079     1.6763761744
O   -7.6653709388   -0.0049439955     3.2794844407
C   -8.3627877714    0.86663332       2.7802828844
C   -9.7127058131    1.2380012364     3.3537042874
H   -3.8172893573   -0.7160065781     0.2487961339
H   -5.5631036313   -1.490663329      1.571565409
H   -7.8208402373   -1.0512166779     0.9621894739
H   -7.3930698975    0.8691476939    -0.9183833722
H   -6.1143137084    0.3237698775    -2.7310904118
H   -4.0666480066   -0.6188552543    -3.6235627846
H   -3.1032129706    0.1274432159    -2.3257128939
H   -3.3878792782   -2.1708976411    -1.552553266
H   -6.7334233238   -3.2501760134     0.0566155423
H   -7.0262011569   -1.7239959666    -1.6580479236
H   -5.7999717925    2.6708100534    -2.2660725624
H   -4.580852824     2.2320500263    -3.4712742254
H   -6.2807045988    2.3450881262     0.7577738779
H   -6.0233219831    0.9602717171     1.822748691
H   -5.4572350289   -3.0538414801    -1.6078347122
H   -4.0376324425    2.0628411938    -0.7525248635
H   -8.5960254757    2.2633105811     1.299241285
H   -9.5721873426    1.5857622509     4.3800194535
H  -10.2392405263    2.0098841232     2.7870438196
H  -10.3348458036    0.3413258297     3.3975307526
```

calc_**2d** conf_12

```
C   -5.7990352927   -2.0470213663    -0.2931833045
C   -6.51906256     -1.2639294865     0.7981493045
C   -6.51169215      0.1683547679     0.2265407871
N   -5.2112042537    0.2696494813    -0.4402405976
C   -4.6785464938   -1.09396489      -0.6822686215
C   -5.1890153305    1.0346632414    -1.707077602
C   -5.0176511464   -0.0116663286    -2.8117620138
C   -4.2176993932   -1.1440372523    -2.1589595064
O   -6.6953340101   -2.2372690729    -1.378773373
O   -7.7873260761   -1.8232610211     0.9900990728
C   -4.0668136982    2.0755581361    -1.6271264172
C   -6.6740692228    1.2982979375     1.2562790255
O   -4.35346826     -2.4036496905    -2.7619862691
O   -2.8783103227    1.5182677314    -1.1199741131
```

```
N    -8.0471091328    1.676034083     1.5498273522
O    -8.504530907    -0.0598169173    2.9258682472
C    -8.8527124947    0.9926299843    2.3881429545
C    -10.2153864357   1.5883915593    2.6493260725
H    -3.8298314064   -1.2920307788   -0.0152302387
H    -5.4227700075   -3.0136835194    0.0624925599
H    -5.9228506731   -1.2919305426    1.722098877
H    -7.3393621621    0.2338790216   -0.4972183158
H    -6.1402004278    1.5696773707   -1.8250507951
H    -5.9982384501   -0.4042625189   -3.0984578653
H    -4.5289743666    0.3819557967   -3.7069055347
H    -3.1534709366   -0.9042398349   -2.2026018044
H    -7.5510726892   -2.4516294458   -0.971234473
H    -8.1816255159   -1.3642202199    1.7590696296
H    -4.4024161122    2.9164489106   -0.9969238729
H    -3.8382713131    2.4781323338   -2.6182932016
H    -6.1789393231    2.1923168018    0.870569004
H    -6.1761154546    1.0284704386    2.1927728408
H    -5.290014789    -2.6454713705   -2.672947914
H    -3.1580428188    1.0952852162   -0.2917403339
H    -8.4061821245    2.5148242241    1.1238569787
H    -10.3976500646   2.529227811     2.1250884687
H    -10.9785864753   0.8630662836    2.3576573482
H    -10.3204177093   1.7539531252    3.7241176444
```

calc_**2d** conf_13

```
C    -5.6439979524   -2.5800717405   -0.5602794989
C    -7.0476137636   -2.0315615209   -0.1714249164
C    -6.8367820144   -0.5414372622    0.1461219586
N    -5.4038968851   -0.2707490757   -0.0859348504
C    -4.8211601579   -1.3361781826   -0.9099360584
C    -5.0963045309    1.0041788213   -0.7512550404
C    -4.8123149571    0.6833533945   -2.2370765942
C    -4.8848649859   -0.8413876374   -2.3680651199
O    -5.7335058789   -3.5125225369   -1.62057079
O    -7.9754650402   -2.2588823974   -1.2111655729
C    -3.9032516593    1.6425960368   -0.0317365133
C    -7.2510722598   -0.1776521268    1.5714123935
O    -6.1073303331   -1.1952460479   -3.0109568648
O    -4.0853881757    1.5807624919    1.3668252138
N    -7.0681040396    1.2204969561    1.8751239301
O    -9.2677218966    1.6358468555    2.2764213333
C    -8.1117939784    2.0264656737    2.2205748511
C    -7.7349208328    3.4582276623    2.5396749287
H    -3.7656312498   -1.4724077073   -0.6431742687
H    -5.1929557826   -3.0689388005    0.3111785322
H    -7.4461875715   -2.5749522791    0.689215577
H    -7.4620264696    0.0428290336   -0.5438656317
H    -5.9568472703    1.668766556    -0.6346884812
H    -5.5458969087    1.1318023986   -2.9103391373
H    -3.8259947353    1.0528618108   -2.5360736967
H    -4.0504508644   -1.2403864608   -2.9558638211
H    -6.6903400598   -3.6890452135   -1.70191236
H    -7.6945407764   -1.6760245882   -1.9432718073
H    -3.8008839578    2.6953440349   -0.3075379214
H    -2.971011263     1.1312662461   -0.3206684629
H    -6.6774159799   -0.7960417787    2.2757144297
H    -8.3136847937   -0.3878450412    1.7163016347
```

S194

```
H   -6.0473515848   -2.1642493093   -3.0817664738
H   -4.3083138953    0.6413077929    1.508094567
H   -6.1277339302    1.5990547399    1.8580767881
H   -8.0022190707    3.6669873134    3.5787027923
H   -6.6743275358    3.6777496431    2.3953017674
H   -8.3306969588    4.1256822455    1.9128231841
```

calc_**2d** conf_14

```
C   -6.2417416242   -2.4163489056   -0.5422873218
C   -7.5760802063   -1.734839331    -0.2368565563
C   -7.295111789    -0.2671922677   -0.6364739634
N   -5.8784809381   -0.0588782656   -0.3549313914
C   -5.2683163089   -1.3597281295   -0.0099137577
C   -5.0698159833    0.5630351949   -1.4038446808
C   -3.6632638059    0.1303365064   -1.0067348407
C   -3.8228822304   -1.3155596714   -0.5432374427
O   -6.2414158896   -2.5604786045   -1.9470292258
O   -8.6684057251   -2.3013194067   -0.9035379768
C   -5.2249089965    2.0828357311   -1.4632261006
C   -8.2227688197    0.7295625933    0.0626045463
O   -3.6726573516   -2.2583150742   -1.6099646175
O   -4.7962489917    2.7366723249   -0.3060805961
N   -8.1142342703    0.7237450825    1.5059434119
O   -6.7726001256    2.5502015517    1.6752146768
C   -7.3966823821    1.6354665495    2.2028061635
C   -7.4221299437    1.4831368851    3.7074419971
H   -5.2376894379   -1.4723779932    1.0833032945
H   -6.1311494589   -3.3872906595   -0.0402677916
H   -7.7834262598   -1.8051817851    0.8373509879
H   -7.4915512715   -0.1886704401   -1.7177406784
H   -5.3284099041    0.1514354127   -2.3981975806
H   -2.9334687368    0.2321761264   -1.8173274327
H   -3.3402757607    0.7649491589   -0.1763698433
H   -3.1076945419   -1.5793221703    0.2445058154
H   -5.3086169062   -2.6407269921   -2.2126700551
H   -8.3284801776   -2.5238357886   -1.7857181502
H   -6.2680540802    2.3318011765   -1.7158113767
H   -4.6105583629    2.4533945081   -2.2927671472
H   -9.2559050893    0.4920873112   -0.2126649982
H   -8.0099570467    1.7479969939   -0.2662173861
H   -2.8324650239   -2.0816367484   -2.0505958764
H   -5.4653921363    2.5864895085    0.3885504969
H   -8.629797894     0.0298471249    2.0216490247
H   -8.0478808759    0.6602837245    4.0617690943
H   -6.3993363242    1.3286436022    4.0594802967
H   -7.7781453294    2.4176051658    4.146846982
```

calc_**2d** conf_15

```
C   -5.5292574003   -2.1852861326    0.0560162221
C   -6.3275581143   -1.224666259     0.9783098443
C   -6.388631898     0.0858236889    0.188821423
N   -5.0841415139    0.1353033471   -0.4701400812
C   -4.6809600614   -1.2501753525   -0.8183748892
C   -4.980320502     0.9754453993   -1.6851932645
C   -4.3062388623    0.0661362764   -2.7219413172
C   -4.8129443022   -1.3176781771   -2.3493516338
O   -6.4356126961   -2.974918433    -0.6898489515
```

S195

```
O    -7.5783876783    -1.8032936057     1.2686093432
C    -4.1625859119     2.2290913081    -1.3659318765
C    -6.5633196817     1.3523184606     1.0374047894
O    -6.1506349731    -1.3901957188    -2.7807333582
O    -2.9986303431     1.8859182715    -0.655696192
N    -7.5586809796     1.3188417463     2.1027383984
O    -9.2494279838     0.3312703137     0.9660498567
C    -8.8382382766     0.912353305      1.9727052171
C    -9.7479627027     1.1719757649     3.1495576013
H    -3.6198061348    -1.3835997376    -0.572080976
H    -4.8912670404    -2.853157301      0.6467010826
H    -5.7707587672    -1.0677914615     1.9115069847
H    -7.2025595835     0.0133440859    -0.5462395284
H    -5.9825003804     1.2547633383    -2.0359745273
H    -4.5790817855     0.3311636812    -3.745656879
H    -3.2181623849     0.1258135489    -2.6142250757
H    -4.2023258795    -2.1289288673    -2.772451349
H    -7.2469557639    -2.9656753255    -0.1402956084
H    -8.2804664834    -1.1643503913     1.0238212446
H    -4.7773954737     2.945868925     -0.7967575149
H    -3.8558315982     2.729044791     -2.290131563
H    -6.7756372694     2.1967332565     0.3703601229
H    -5.6018831501     1.5486841377     1.5183920286
H    -6.5434160479    -2.1228960758    -2.2712632125
H    -3.3189373721     1.2191466272    -0.0215598224
H    -7.3133503484     1.8049024175     2.9503808977
H    -9.2741450385     1.7177673628     3.9685286392
H    -10.6143467884    1.7368483493     2.7979084258
H    -10.1156388287    0.2140544353     3.5250354993

calc_2d conf_16

C    -5.822369136     -2.4696726217    -0.5847750635
C    -6.4488669734    -1.7106828566     0.6056345102
C    -6.3989528487    -0.2466773739     0.1495435967
N    -5.0588953882    -0.1742164344    -0.42111217
C    -4.8061768443    -1.4482722258    -1.1377597359
C    -4.7557660106     0.953603991     -1.3220944166
C    -4.1316633966     0.2943555452    -2.563148469
C    -4.8068526185    -1.0675694631    -2.6201651459
O    -6.8568562523    -2.8772131762    -1.4592749329
O    -7.729511688     -2.1897564381     0.9149229438
C    -3.7911917099     1.9159273263    -0.6266022778
C    -6.6278627345     0.7485515223     1.2777811557
O    -6.1631983887    -0.9214052844    -3.0558392365
O    -2.7038803041     1.2053598855    -0.0870467505
N    -7.959141643      0.589939261      1.8142968012
O    -8.3563271376     2.8133209425     2.0318318267
C    -8.7384360083     1.6563714128     2.1331835058
C    -10.1244455148    1.3145770058     2.6400612466
H    -3.7903310924    -1.7950747943    -0.9118525747
H    -5.3233591189    -3.3844664448    -0.2550117703
H    -5.8187623647    -1.8204399303     1.4959817968
H    -7.179335294     -0.0923409717    -0.6172204104
H    -5.6812051634     1.4784926092    -1.5957385498
H    -4.2830256422     0.8813134122    -3.4743235576
H    -3.0544542733     0.174372111     -2.4065637214
H    -4.2838090942    -1.8034547725    -3.2421433257
H    -6.9157161459    -2.2224099094    -2.1803275188
```

S196

```
H   -8.0581257563   -2.5409125727    0.0652181551
H   -4.325470574     2.4807962546    0.1513769344
H   -3.3882810787    2.6397338338   -1.3418527718
H   -6.5451325881    1.7834286247    0.9351854424
H   -5.8611370164    0.5965186716    2.0510158919
H   -6.1659279407   -0.6847771137   -3.9917201757
H   -3.1299716617    0.4880427418    0.4128869383
H   -8.3315397634   -0.3498741673    1.8480091297
H  -10.8599415959    1.8587733378    2.0433933724
H  -10.3549123262    0.2468831805    2.6097565416
H  -10.2181669121    1.6668548812    3.6704927852


calc_2d conf_17

C   -6.0924638137   -2.154971053    -0.2477241113
C   -6.9269471053   -1.2566389283    0.6732732929
C   -6.4827886149    0.1741011958    0.2746216687
N   -5.1826467546    0.03340915     -0.3948430934
C   -4.7801080668   -1.3834457328   -0.3350062018
C   -5.1205129384    0.4716051039   -1.8011159162
C   -3.9083191988   -0.2912871296   -2.3269950813
C   -3.88590536     -1.6406325259   -1.5774899933
O   -6.7354126917   -2.1846000519   -1.5082352494
O   -8.2903079551   -1.522030552     0.442826279
C   -4.9625262224    1.9912736375   -1.829552436
C   -6.3085638884    1.1349215292    1.4571233754
O   -4.2740449164   -2.7525258873   -2.3438114862
O   -3.9375412875    2.399750133    -0.9560550328
N   -7.4024079655    1.2040923958    2.4198957099
O   -9.1756836014    1.0097496959    1.0124401677
C   -8.7227554494    1.2220236878    2.1389304388
C   -9.6459180568    1.5002349915    3.302460067
H   -4.2235242595   -1.5719854037    0.5930679611
H   -5.9662994939   -3.1702163427    0.1485073492
H   -6.6686127481   -1.4555265506    1.7244087457
H   -7.2184874525    0.5842782293   -0.4221445085
H   -6.0283209663    0.1817807939   -2.349879137
H   -3.943472693    -0.4548414238   -3.4061926678
H   -3.0058661406    0.2837736612   -2.0962574348
H   -2.866220362    -1.8690350215   -1.2582170472
H   -7.6866406795   -2.1203993986   -1.2975762025
H   -8.7782257869   -0.6789588663    0.5413852915
H   -5.9220292383    2.465088393    -1.5618309503
H   -4.7092998267    2.3267908554   -2.8405029605
H   -6.0924986955    2.1355018515    1.0633494021
H   -5.4247550978    0.813217339     2.015762203
H   -5.2329135994   -2.6872070171   -2.485800733
H   -3.9651489729    1.7284291273   -0.2493491502
H   -7.1377003417    1.4244227445    3.3669151614
H   -9.1345148248    1.6354401641    4.258067379
H  -10.2221678793    2.4010955564    3.0773811404
H  -10.3564470542    0.6753216493    3.3901637611


calc_2d conf_18

C   -5.8083007856   -2.3600850022   -0.2509769972
C   -6.4452268333   -1.4665821354    0.8246668733
C   -6.3423803066   -0.0583361286    0.2184453318
N   -4.9900377057   -0.0931745462   -0.3260080259
```

S197

```
C   -4.7915092912    -1.4290003987    -0.9315026545
C   -4.6364377735     0.9287487294    -1.3239001344
C   -4.152149915      0.1404004445    -2.5584095247
C   -4.8907226139    -1.1855657393    -2.4485814786
O   -6.8144814206    -2.82392146      -1.1410971631
O   -7.7345454219    -1.9444766026     1.0799457325
C   -3.5651292684     1.8767168694    -0.7894651686
C   -6.5054404893     1.0897913001     1.2230250468
O   -6.206834349     -0.9513756465    -2.8876400014
O   -3.2239847278     2.8852487715    -1.7177168451
N   -7.8733625766     1.542536249      1.412588227
O   -8.483589123     -0.0694985398     2.8790415234
C   -8.7532665839     0.9541468502     2.2468244636
C   -10.1007239246    1.6210399612     2.383671032
H   -3.7732794017    -1.7793473524    -0.7161145844
H   -5.3159329254    -3.2312644111     0.1957550023
H   -5.8195258343    -1.4941927995     1.7278846458
H   -7.1064457429     0.0470312514    -0.5709719141
H   -5.5224126709     1.5171692253    -1.5983330176
H   -4.3840290545     0.6399668357    -3.5014882664
H   -3.0682365744    -0.030405175     -2.5067991653
H   -4.4072224742    -1.9896157624    -3.0236372389
H   -7.6270864947    -2.8424624593    -0.6024486773
H   -8.1011689742    -1.4177039626     1.8214455482
H   -2.688596362      1.2855921454    -0.4811003778
H   -3.9222773602     2.401121074      0.1009745027
H   -5.9407518526     1.9564811621     0.8736407981
H   -6.0954114737     0.8033469763     2.19581766
H   -6.7332281565    -1.6805829833    -2.5094086944
H   -2.8205670103     2.453915183     -2.4813583172
H   -8.1773855977     2.3486489726     0.8910221779
H   -10.8762512852    0.9143940296     2.0786862193
H   -10.2677605348    1.8498353552     3.4387457599
H   -10.2033071099    2.5384597191     1.7997777023
```

calc_**2d** conf_19

```
C   -6.1688490112    -2.5258952433    -0.9973415445
C   -7.2379841881    -2.0304222508    -0.0241756826
C   -6.9220877869    -0.5171182075     0.1003324569
N   -5.4699345061    -0.4009885561    -0.1619033292
C   -4.9494547711    -1.7452836458    -0.5013522242
C   -5.0554353749     0.521227296     -1.2272199764
C   -3.6602784595     0.0015481131    -1.5681407294
C   -3.7682210215    -1.5231591124    -1.4673392775
O   -6.6306216469    -2.1152815266    -2.2676585166
O   -8.5428325884    -2.3078223729    -0.4357569254
C   -5.0518362039     1.947073743     -0.6744698725
C   -7.3536839592     0.0115981339     1.4660563751
O   -4.0539139863    -2.1510140813    -2.7170514998
O   -4.4839891732     1.9530489429     0.622163509
N   -7.2408666527     1.4411757458     1.6256890438
O   -9.4592563355     1.8005420353     1.9819872807
C   -8.3207591049     2.2311609208     1.8828120254
C   -8.0081215729     3.7049509894     2.0466574382
H   -4.592458421     -2.2391288496     0.4116459638
H   -6.0218221439    -3.6127553833    -0.9546644234
H   -7.1042113988    -2.5141397561     0.9508751292
H   -7.4819675921     0.0136592487    -0.6797744136
```

```
H   -5.7181601305   0.45865167     -2.1029075051
H   -3.3142406024   0.3286990066   -2.553343346
H   -2.9501093448   0.3734043921   -0.8220761118
H   -2.8504301813  -1.9651620747   -1.0632016721
H   -5.877508905   -2.2120356223   -2.8737518313
H   -8.5493669538  -2.141083635    -1.3917342955
H   -6.0799622841   2.3317557397   -0.6429221106
H   -4.4664816778   2.6097636182   -1.3206286087
H   -6.7692503994  -0.4994825336    2.2435956441
H   -8.4081868064  -0.2333887898    1.6182626377
H   -3.3151809342  -1.9858785362   -3.3155672332
H   -4.5539147212   1.0120098992    0.8926351424
H   -6.3203786666   1.861462813     1.5682916964
H   -8.2827182802   4.010845607     3.0594733178
H   -6.9589191045   3.9558545338    1.8720730118
H   -8.6346051089   4.2746077287    1.3564304571
```

calc_**2d** conf_20

```
C   -5.9762194467  -2.2194552154   -0.7668002244
C   -6.6819883319  -1.6276166645    0.4512249744
C   -6.5117986478  -0.1161879859    0.2249364738
N   -5.1584219397   0.0021390286   -0.3190590926
C   -4.7498386797  -1.3094806043   -0.8793131956
C   -4.9648458005   1.0511684106   -1.3378679581
C   -4.8769379736   0.298829312    -2.6716352432
C   -4.2309665478  -1.034687818    -2.3023578258
O   -6.898340861   -2.0778590487   -1.8305945824
O   -8.020132063   -2.0412721257    0.5789327019
C   -3.7165650493   1.8613882687   -0.9826850955
C   -6.7069943294   0.7143274519    1.4859554284
O   -4.5830798318  -2.1260414702   -3.1516476564
O   -2.6300071698   1.0207427465   -0.6601721887
N   -8.0596162466   0.5702787555    1.9736474462
O   -8.2803236008   2.7341700836    2.6175474692
C   -8.756939272    1.6157699826    2.4901929828
C   -10.1784670389  1.3006006051    2.9095222717
H   -3.9490514381  -1.7495529495   -0.2713852188
H   -5.6977325825  -3.2715919737   -0.6309316052
H   -6.1627590491  -1.9276156292    1.368203193
H   -7.2691834717   0.1883629831   -0.5156714636
H   -5.8262966695   1.7290834425   -1.3318876945
H   -5.8864111965   0.0985911146   -3.0443733591
H   -4.3233626058   0.8480573794   -3.4394934441
H   -3.1426332224  -0.9282858318   -2.2748206808
H   -6.4028590788  -2.2965938763   -2.6389713645
H   -8.3584287703  -2.0803191048   -0.3311070873
H   -3.9535496759   2.5310072902   -0.1429214449
H   -3.4009311687   2.4825347647   -1.8261640822
H   -6.5408809394   1.7780222037    1.2958380102
H   -5.9701444626   0.4012321684    2.2389945998
H   -4.1879472448  -1.9712606116   -4.0184185195
H   -2.953763858    0.4965542826    0.0889822201
H   -8.507203656   -0.3254843703    1.8331414773
H   -10.2760869678  1.4809102969    3.9830004205
H   -10.8550622774  1.9921183966    2.4021433305
H   -10.4862288344  0.2744163121    2.6940160275
```

calc_**2d** conf_21

S199

```
C   -5.9101259237   -2.4665492471   -0.2756871712
C   -7.3324875582   -1.9380036472   -0.5833534188
C   -7.2392114508   -0.4163720686   -0.357677574
N   -5.8176584155   -0.1106913777   -0.1253403631
C   -4.9981853174   -1.2606121675   -0.5243692607
C   -5.2682035764    1.0428032699   -0.8433843626
C   -4.7480724588    0.5014304373   -2.1923445378
C   -4.5291994048   -1.001961218    -1.9838932897
O   -5.5982213429   -3.6053607362   -1.0590726491
O   -7.7362528307   -2.3118189241   -1.8824798409
C   -4.1526494678    1.6829264657   -0.0184051462
C   -8.1133627085    0.0082003253    0.8270870786
O   -5.2886576991   -1.7118363975   -2.9611206457
O   -4.5964113604    2.1582827845    1.2208466698
N   -8.0998157881    1.4244762004    1.1021206123
O   -6.8089706946    1.2621022398    2.957398907
C   -7.4407822847    1.9544771541    2.1696760582
C   -7.4979007913    3.4576451436    2.2936771277
H   -4.1080256353   -1.314062004     0.1120367666
H   -5.8448715306   -2.7341617594    0.7849900062
H   -8.0681804243   -2.3964318056    0.0836116576
H   -7.6132917924    0.0785461228   -1.2675322812
H   -6.0567003796    1.7906785851   -0.9690551714
H   -5.4920816959    0.6241882779   -2.9845123149
H   -3.8387885914    1.0130640355   -2.5211613674
H   -3.475526164    -1.2818498843   -2.096665417
H   -6.4375537405   -3.8308915786   -1.5013241259
H   -7.0769205214   -1.9202426573   -2.4955178034
H   -3.7528301114    2.5436416012   -0.5648448303
H   -3.3223554291    0.9650415717    0.0962221092
H   -7.7520432631   -0.4803746912    1.7350356375
H   -9.1453470101   -0.3149085742    0.6430984315
H   -5.1593960962   -2.647984142    -2.722751473
H   -5.0651751604    1.4345209703    1.670185301
H   -8.6087738084    2.0431488919    0.4914595379
H   -6.5341843769    3.8473960411    1.9543488779
H   -8.2983336054    3.919065083     1.709107973
H   -7.61745159      3.7204776793    3.3455902923
```

calc_**2d** conf_22

```
C   -6.2090323806   -2.3729013744   -0.7122601086
C   -6.9617465513   -1.6340572537    0.395344118
C   -6.526249093    -0.1689883179    0.1715590406
N   -5.1260418209   -0.279605731    -0.239047723
C   -4.8419538268   -1.6858730312   -0.616879644
C   -4.6518448697    0.6052679014   -1.3073297598
C   -3.4534877292   -0.1698183227   -1.8499557315
C   -3.9046819972   -1.6276033546   -1.8371373966
O   -6.9541364851   -2.0925954654   -1.8771377826
O   -8.3527307269   -1.8261941942    0.3477701821
C   -4.2660219953    1.9668668852   -0.7293268379
C   -6.729711859     0.6912796458    1.4157762026
O   -4.6214422541   -1.9793705235   -3.0206610586
O   -3.4116157123    1.80768905      0.3745528214
N   -8.1355533145    0.7696271712    1.7405431214
O   -8.0984460349    2.9711382065    2.290095621
C   -8.7216772788    1.9317726636    2.1338197055
```

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C   -10.2149230276    1.851755803     2.3774295015
H   -4.2993774943    -2.1765666618    0.2027917554
H   -6.1401818545    -3.4547007249   -0.5360319423
H   -6.6262602046    -1.9757570981    1.3810206152
H   -7.1412059894     0.2389259493   -0.6457996157
H   -5.4156257171     0.7355422833   -2.0925190178
H   -3.1404725031     0.1638048725   -2.8446204827
H   -2.6119726209    -0.0288934393   -1.1643210753
H   -3.0666304996    -2.3242038995   -1.7180917476
H   -6.3423589165    -2.1438997527   -2.6307711188
H   -8.5738249982    -1.796721983    -0.5982917587
H   -5.174159394      2.527100548    -0.4607518272
H   -3.7333594626     2.5568114693   -1.4820730815
H   -6.3761013336     1.7147653464    1.2740505719
H   -6.1523687236     0.2611698592    2.2472615041
H   -4.0551908522    -1.8150574185   -3.7843835455
H   -3.7871469408     1.0489591518    0.8549366091
H   -8.6988274472    -0.0494922542    1.5556312994
H   -10.7101407129    2.612586429     1.7697283528
H   -10.6485064228    0.8741907439    2.1525438663
H   -10.4129909548    2.0940468212    3.4245363673

calc_**2d** conf_23

C   -5.5629187627    -2.0753975513    0.0414990775
C   -6.8704985612    -1.2828870057    0.3223956183
C   -6.5388658965     0.1742307053   -0.0456719756
N   -5.1786300018     0.1710739246   -0.6045331558
C   -4.7713784193    -1.1976500146   -0.9362728146
C   -4.9624415658     0.9939353544   -1.801192542
C   -4.9735092143     0.0345256018   -3.0139422077
C   -5.0544634994    -1.3848420625   -2.442104673
O   -5.8441702982    -3.3688525169   -0.4646408039
O   -7.945825551     -1.8195539761   -0.4231591367
C   -3.6389504643     1.7428607912   -1.6455847302
C   -6.5913010052     1.1416467503    1.1415234278
O   -6.354552645     -1.9134079626   -2.6968132745
O   -3.6013195113     2.4328284837   -0.4243472569
N   -7.9147002813     1.3120145376    1.6950289334
O   -7.6174316468    -0.1277355234    3.4223717212
C   -8.331913209      0.6553906659    2.8134185712
C   -9.7500849399     0.9488813627    3.2517513478
H   -3.6914349724    -1.3085290871   -0.7784634084
H   -4.9924792341    -2.1706319972    0.9721496825
H   -7.1628261242    -1.3757137857    1.369302398
H   -7.2780594066     0.5008130562   -0.7939177292
H   -5.760681123      1.7413657741   -1.8571688522
H   -5.8321332441     0.1977828801   -3.6690421596
H   -4.0718507695     0.162403253    -3.6217034033
H   -4.3124500739    -2.0508164471   -2.897157148
H   -6.8045773918    -3.4740332095   -0.3285054261
H   -7.7169494032    -1.6686437111   -1.3622833728
H   -3.5223135612     2.4789068942   -2.4468368281
H   -2.802244426      1.0283255355   -1.7315857092
H   -6.1982000657     2.1145950655    0.8272291493
H   -5.9527697199     0.7647304633    1.9439570607
H   -6.3119342007    -2.802143967    -2.2988479425
H   -3.8784725202     1.7635053218    0.2241384485
H   -8.5632749942     1.917310258     1.2186285446
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S201

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H   -9.7446459828    1.1736386619    4.3199887262
H  -10.2192147425    1.7760877233    2.7132309847
H  -10.3545325709    0.0489857535    3.1101608585

calc_2d conf_24

C   -5.9161705488   -2.6309320839   -1.0348949114
C   -6.8598739484   -2.1869187109    0.1096384641
C   -6.6906515814   -0.6620525708    0.160069946
N   -5.2343457932   -0.5369586957   -0.0257992292
C   -4.8498659528   -1.5148865492   -1.067593382
C   -4.6952880798    0.7779475333   -0.4221324964
C   -4.0249474578    0.577197197    -1.7979123273
C   -4.6802777831   -0.6831620377   -2.3459050827
O   -6.6501626012   -2.8206726807   -2.2276912769
O   -8.1657580226   -2.6326190431   -0.0805711147
C   -3.6999614074    1.2594148243    0.6363110449
C   -7.2326961504   -0.0970551059    1.4673010036
O   -5.9745281032   -0.3713236344   -2.8696186317
O   -4.2284462186    1.1211511863    1.9374851576
N   -7.1129093736    1.3334313524    1.6254955159
O   -9.2911887144    1.796112203     1.1698990877
C   -8.1726418572    2.174163886     1.4831610052
C   -7.8712408254    3.6362912827    1.7475850936
H   -3.8610492543   -1.9298771779   -0.8361525439
H   -5.4643587336   -3.6004952101   -0.8144045572
H   -6.4885149977   -2.5958505891    1.0586966586
H   -7.2450334677   -0.2041332476   -0.6736443702
H   -5.5215651456    1.492529347    -0.4934284793
H   -4.1553444325    1.4348448568   -2.4644718409
H   -2.9468211807    0.4125639088   -1.6828932421
H   -4.0780883097   -1.2002123956   -3.1024189284
H   -6.7061393532   -1.9557903035   -2.6758485634
H   -8.2271509066   -2.8013647244   -1.0384310867
H   -3.4556952269    2.3160075647    0.4943621131
H   -2.7648523929    0.6850379623    0.5459495501
H   -6.7343289602   -0.5940179097    2.3103603454
H   -8.2969137183   -0.3412417355    1.5120200447
H   -5.8662578759    0.1442403819   -3.6787851377
H   -4.5127618686    0.1899559743    1.9628211796
H   -6.2032482527    1.6876169751    1.8958088976
H   -6.8208618718    3.838034347     1.9722490921
H   -8.1716902249    4.2213311398    0.8751809933
H   -8.4833694067    3.9726924829    2.5882020091

calc_2d conf_25

C   -5.5780346943   -1.8133931026    0.4026930847
C   -7.0759386899   -1.4806999631    0.1328518883
C   -7.069056912    -0.1219523968   -0.5933815804
N   -5.6742702187    0.3323646102   -0.5748807082
C   -4.7940806619   -0.8354901699   -0.4773658015
C   -5.2458074432    1.0774711593   -1.762379434
C   -4.6342300895    0.0386024429   -2.7321644018
C   -4.4986622459   -1.2652859459   -1.9291293268
O   -5.2887747729   -3.1708273585    0.1199023283
O   -7.6784747201   -2.4999378415   -0.6425443502
C   -4.2559651208    2.1546120244   -1.2950785901
C   -8.028880309     0.9386178252   -0.034363244
```

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O   -5.4456400136   -2.2153455156   -2.4121887459
O   -4.7400696649    2.7666375941   -0.1246809243
N   -7.5908989829    1.5948971689    1.1753235228
O   -8.5610518228    0.1311487258    2.6084999162
C   -7.9189714327    1.1548527201    2.4191159004
C   -7.4507623777    2.027473923     3.5638140112
H   -3.8486598673   -0.5414691879   -0.005476221
H   -5.3473408105   -1.6069026993    1.453784964
H   -7.6446821855   -1.4371301674    1.0622107812
H   -7.4074302114   -0.3197499684   -1.6240245849
H   -6.1179798716    1.5817598563   -2.190018261
H   -5.2748424201   -0.1511879473   -3.5963511062
H   -3.6649039416    0.3753746763   -3.1129732847
H   -3.4930359695   -1.693241114    -2.0156103447
H   -6.1665354376   -3.5938779682    0.0623416619
H   -7.2642700429   -2.4332683862   -1.5234564542
H   -4.1314204839    2.9244196203   -2.0620375264
H   -3.2658701887    1.6995504618   -1.1228862241
H   -8.9974708046    0.4698173841    0.1592780604
H   -8.1821790432    1.7163615809   -0.7890826205
H   -5.2904348625   -2.9874078853   -1.8373237267
H   -5.0776251547    1.9956820208    0.3740764872
H   -7.0440873138    2.4351014957    1.0738415038
H   -6.8036589693    2.852518513     3.2565467508
H   -8.3275054989    2.4369666973    4.0723039418
H   -6.9194967499    1.4039371174    4.2858126588

calc_**2d** conf_26

C   -5.4670990404   -2.3552447145   -0.3476703062
C   -6.6541608154   -1.6909972695    0.407888456
C   -6.3289311642   -0.1880031402    0.4211473206
N   -5.0404719028   -0.0372227007   -0.2757449615
C   -4.8248009096   -1.2070316963   -1.1326923203
C   -4.9664145476    1.1396811659   -1.154367374
C   -5.4565829211    0.6741710081   -2.5422671295
C   -5.430978266    -0.8610362417   -2.5145705697
O   -5.9067029232   -3.4320449117   -1.1529498876
O   -7.8785776012   -2.0040443165   -0.2229651183
C   -3.5230050715    1.6438418512   -1.156868998
C   -6.2269701177    0.4361968275    1.8146538267
O   -6.76364718     -1.3469370148   -2.6771674648
O   -3.0616529005    1.8123433771    0.1568422303
N   -7.5068419041    0.5702382974    2.4720827319
O   -8.0722864516    2.4081848239    1.2833010816
C   -8.3676597573    1.5653121275    2.1173213106
C   -9.7073586999    1.5605115189    2.8200668343
H   -3.749211783    -1.3727461096   -1.2626832568
H   -4.7369185372   -2.7280810719    0.3801539145
H   -6.7435935385   -2.1005785381    1.4181871623
H   -7.1360256121    0.3361668576   -0.1090424453
H   -5.59928096      1.9254179685   -0.7309431901
H   -6.4831965182    0.9935909134   -2.7374235128
H   -4.8334276776    1.0772626697   -3.3464035111
H   -4.8119772014   -1.2744709368   -3.3189628058
H   -6.8412359952   -3.5524040637   -0.8968122718
H   -7.837275873    -1.5660055604   -1.0980240542
H   -3.4652676722    2.6126808438   -1.662123815
H   -2.8846852832    0.9425436874   -1.7232715804

S203
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H   -5.7884046268    1.4328668953    1.71851444
H   -5.5618347471   -0.1604300129    2.4465163213
H   -6.6609112647   -2.3143557691   -2.6394000442
H   -3.3960661317    1.0221566215    0.6161361304
H   -7.823829996    -0.1571112893    3.0912720904
H   -9.8998366208    2.5620671573    3.2095496591
H  -10.4891442086    1.3386446201    2.0888023185
H   -9.7747335787    0.8388661257    3.6379187885
```

calc_**2d** conf_27

```
C   -5.946048462    -2.4270695024   -0.7774102027
C   -6.4896020628   -1.7497059987    0.5026016114
C   -6.3456816641   -0.2506971487    0.2096475535
N   -5.0177111382   -0.2240740314   -0.4077111776
C   -4.952992104    -1.3780895826   -1.3276847797
C   -4.6312810713    0.9835766316   -1.1603468315
C   -4.4237847907    0.5310649903   -2.6220811666
C   -5.1868147257   -0.7831527885   -2.7237099984
O   -7.0208267445   -2.7780621041   -1.6269150958
O   -7.7896947104   -2.1753115744    0.8079994336
C   -3.3592487061    1.5791923681   -0.5599470606
C   -6.4635620145    0.6106922692    1.4600755473
O   -6.585895677    -0.5268215338   -2.8880738913
O   -3.4909895618    1.8065748407    0.817014022
N   -7.8043121137    0.52018972      1.9881739727
O   -8.0638378527    2.7527575683    2.3181313734
C   -8.5171013421    1.6187964259    2.3544972443
C   -9.9275278685    1.3392026868    2.8332579921
H   -3.9361377575   -1.7894145045   -1.3337294785
H   -5.4393178883   -3.3651491899   -0.5407359194
H   -5.8393390302   -1.9934027524    1.3514597224
H   -7.1362248738    0.0537529252   -0.496549826
H   -5.4364786047    1.7232790985   -1.0880785902
H   -4.773405586     1.2688461574   -3.3502562391
H   -3.3595985385    0.3549604653   -2.8208657491
H   -4.8269396491   -1.4418768736   -3.5230305435
H   -7.1956717322   -2.0127656064   -2.2076900639
H   -8.1393491545   -2.5002522052   -0.0436948712
H   -3.1322055483    2.5426334618   -1.0268730641
H   -2.5160999737    0.8999318932   -0.7734653976
H   -6.2617525057    1.665745377     1.2610278041
H   -5.7272801787    0.2703308089    2.2038105511
H   -6.730361389    -0.1489038801   -3.7648222174
H   -3.7724142313    0.9524278164    1.1796579341
H   -8.2492843325   -0.3871639837    1.9541603815
H  -10.0088639025    1.6433031925    3.8799579352
H  -10.6211426649    1.9592868676    2.2609630131
H  -10.2252198485    0.2913676956    2.7462360727
```

calc_**2d** conf_28

```
C   -5.8290899899   -2.4473049411   -0.5654778865
C   -6.449089333    -1.6916801757    0.6232998443
C   -6.417606393    -0.2291248607    0.1599292783
N   -5.0875052059   -0.154878729    -0.4305522837
C   -4.8473106599   -1.4234795848   -1.1601909889
C   -4.8105760657    0.9726771055   -1.3479771349
C   -4.240430644     0.3103102609   -2.6119596301
```

S204

```
C    -4.9352145681   -1.0407971079   -2.6480280439
O    -6.9103741143   -2.8111298627   -1.4426150581
O    -7.7064359607   -2.1887796973    0.9987244477
C    -3.8212067552    1.9303544298   -0.6824996757
C    -6.6194883067    0.7647567138    1.2956367604
O    -6.2536976457   -0.8046239919   -3.087935375
O    -2.7292175645    1.2154885159   -0.1554708737
N    -7.9345792336    0.6173822202    1.8732309782
O    -8.3254683755    2.8442340188    2.0678068743
C    -8.7018364303    1.6900252576    2.2049784886
C   -10.0677632213    1.3571836359    2.7693443588
H    -3.8198448621   -1.7611027414   -0.9707238852
H    -5.3228898041   -3.3610703969   -0.2450003846
H    -5.7887406899   -1.7903411353    1.4914880648
H    -7.2096459564   -0.0746817089   -0.5940751666
H    -5.7435030908    1.4978131656   -1.5889256624
H    -4.446983423     0.8876537652   -3.5154985918
H    -3.1579764925    0.1866261946   -2.5049729188
H    -4.4194689132   -1.7724322876   -3.288801558
H    -6.8009287583   -3.7328389772   -1.700767764
H    -8.1466031862   -2.4187422365    0.1639835584
H    -4.3308380605    2.511652812     0.100813415
H    -3.4266616963    2.640836673    -1.4153285058
H    -6.5423050717    1.79707593      0.9456638292
H    -5.8303440168    0.613166764     2.0461642732
H    -6.7776641373   -1.5723309754   -2.8112113985
H    -3.1547993187    0.4976680779    0.3440442631
H    -8.2976679141   -0.3210489519    1.9643187114
H   -10.2898484665    0.2873288962    2.7894540692
H   -10.1325589216    1.7509884696    3.7867238696
H   -10.8268367526    1.8701654558    2.1744077018
```

calc_**2d** conf_29

```
C    -5.7092967461   -2.364273284     0.0974676663
C    -6.9974271933   -1.5874053243    0.4601523402
C    -6.9591771908   -0.3967064428   -0.505940788
N    -5.5501817011   -0.0144382337   -0.4582319425
C    -4.7284093534   -1.234995659    -0.2691715585
C    -4.9906501182    0.8036318265   -1.5399222551
C    -3.6018207263    0.1898519669   -1.7672944089
C    -3.8427175296   -1.2953740059   -1.5159401737
O    -6.0246294703   -3.2888568537   -0.9257691095
O    -8.1364029181   -2.3806379288    0.3442671344
C    -4.9503586139    2.2703341698   -1.0801191307
C    -7.9288051495    0.7329585369   -0.1654704849
O    -4.5960587352   -1.847434057    -2.5989937106
O    -4.5917764165    2.3262121769    0.2833367049
N    -7.5778327632    1.4653842526    1.0272199755
O    -9.5794902581    1.1723684152    2.0687193867
C    -8.463975876     1.6647699565    2.0466466055
C    -7.9544645868    2.5424834056    3.1721066022
H    -4.0485059592   -1.0860235421    0.5800253065
H    -5.3398220146   -2.9451637544    0.9476039218
H    -6.941228036    -1.2114096353    1.487503999
H    -7.2329939878   -0.7711769581   -1.5089156582
H    -5.5921855369    0.7101973078   -2.454513199
H    -3.2096514887    0.3935767349   -2.7680395956
H    -2.8917396023    0.5890891315   -1.0342563823
```

```
H  -2.9284626486  -1.876459856   -1.3495793961
H  -5.6587527392  -2.9545543533  -1.7636700931
H  -7.9183855628  -3.0061046619  -0.3698439703
H  -5.9315164388   2.7393041552  -1.2436870796
H  -4.2166637924   2.8389080338  -1.6616674466
H  -8.9177517356   0.300415783    0.0058433367
H  -8.0131580159   1.419946041   -1.0182490652
H  -4.0119210792  -1.9666645233  -3.3578786225
H  -4.8591587982   1.4367723268   0.6041218523
H  -6.7183175424   1.9961439154   1.0230109473
H  -6.9343261664   2.9055925394   3.0247015896
H  -8.6255251067   3.3980184988   3.2803554283
H  -8.0004584022   1.9757198989   4.1050712737

calc_2d conf_30

C  -6.0653929182  -1.989323005   -0.0264388785
C  -6.9726287785  -0.9710961214   0.6687852872
C  -6.6579697913   0.3419950455  -0.0966832186
N  -5.291573431    0.1889092553  -0.6155303732
C  -4.8010318258  -1.1550235505  -0.2462355377
C  -5.0981743305   0.3680471757  -2.0576031939
C  -3.7720538542  -0.3522292793  -2.2865329511
C  -3.8164084361  -1.570668788   -1.3585994478
O  -6.7513462959  -2.3084924624  -1.222071305
O  -8.327186271   -1.3348672132   0.6314285752
C  -5.0443814379   1.8618195468  -2.372355913
C  -6.7792413922   1.5851737898   0.7885714375
O  -4.298935407   -2.7515217197  -2.003008561
O  -4.1349693444   2.5148470333  -1.5239230233
N  -8.0624841744   1.6771024981   1.4470353989
O  -7.2897716971   1.0217374049   3.4828552556
C  -8.2282991899   1.2793020973   2.7446857014
C  -9.6690068409   1.1646869591   3.1899057803
H  -4.272594265   -1.1007753099   0.7143375629
H  -5.8831031683  -2.8851027491   0.5809784874
H  -6.6956820856  -0.8627579967   1.7217491348
H  -7.368709043    0.4113562263  -0.9331921242
H  -5.9040808089  -0.109171252   -2.638069577
H  -3.6145931941  -0.6350643815  -3.3320247705
H  -2.958383937    0.3160350132  -1.9883536869
H  -2.8293106744  -1.7919446536  -0.9372871933
H  -6.106444014   -2.7587683925  -1.793371722
H  -8.4423307886  -1.7709856127  -0.2289518655
H  -6.0570037841   2.2875814147  -2.2787060193
H  -4.7211748138   2.0233757365  -3.4057814385
H  -6.5933767738   2.491850314    0.20130516
H  -6.0297535172   1.5411540375   1.5816202779
H  -3.6923789878  -2.9732755352  -2.7200167429
H  -4.2436914249   2.0560742559  -0.6707454099
H  -8.8855214469   1.6908780057   0.8641296099
H  -9.7128738568   1.2514717802   4.2751469688
H  -10.3118438482  1.9231159449   2.7343716069
H  -10.0452941511  0.177554488    2.9025767083

calc_2d conf_31

C  -6.6496554516  -2.0651289004  -1.1387503033
C  -7.4045908078  -1.4484756313   0.0344853538
```

S206

```
C    -6.5290939206    -0.2197915711     0.3852711161
N    -5.1646859251    -0.6203762902     0.0349970174
C    -5.2069117581    -1.9220916808    -0.6677677651
C    -4.4119225881     0.3211096624    -0.794926763
C    -3.3460311234    -0.5733378348    -1.4177114577
C    -4.073599488     -1.8968855616    -1.7277611331
O    -6.8971230505    -1.248075193     -2.2718592023
O    -8.7035475222    -1.1372938534    -0.3835733643
C    -3.8458370317     1.4669071958     0.0348441378
C    -6.6482433012     0.2425131935     1.8562908858
O    -4.4970040811    -2.0104303141    -3.0614500808
O    -3.1238416235     2.3989567559    -0.7395736733
N    -7.3997111569     1.4704779538     2.0460715019
O    -9.4235117629     0.5481407919     1.6377299627
C    -8.742544923      1.5302029383     1.936263709
C    -9.3853278432     2.8669647993     2.2159559061
H    -5.0222181371    -2.7301436576     0.0535086878
H    -6.939759007     -3.1041625436    -1.3376673946
H    -7.4124661054    -2.1534060884     0.8808654277
H    -6.8576350868     0.6091479609    -0.2596727077
H    -5.0448740737     0.7509144814    -1.5909384014
H    -2.9028483834    -0.1661272063    -2.3293119587
H    -2.5490847549    -0.7526504131    -0.6838078142
H    -3.3955143888    -2.7401534961    -1.5709379424
H    -7.8193236995    -0.9505061785    -2.1734669776
H    -9.1055469096    -0.5707668938     0.3090296332
H    -3.2378107737     1.0439525528     0.8507132961
H    -4.6585823752     2.040351837      0.4933866908
H    -5.6442574452     0.4098417838     2.2480346488
H    -7.1124099381    -0.5385741298     2.4677367992
H    -5.3416926445    -1.5391667008    -3.1516780303
H    -2.366416398      1.9354025462    -1.1183352855
H    -6.8955452293     2.3136299587     2.2669201887
H    -8.6730285202     3.6554025351     2.469090807
H    -9.9598239986     3.1720178523     1.3383491145
H    -10.091978772     2.7476093397     3.0406453709
```

calc_**2d** conf_32

```
C    -5.9930970126    -2.3858075241    -0.4821548234
C    -6.7149433199    -1.7055423443     0.6775784644
C    -6.3274588926    -0.2210942723     0.4966745102
N    -5.0310326472    -0.2230510195    -0.1822211477
C    -4.6685099202    -1.6260024036    -0.4791761666
C    -4.9337077945     0.5378041604    -1.4366712599
C    -3.7144381142    -0.0981554509    -2.0927689082
C    -3.832181599     -1.6027694715    -1.7850325355
O    -6.732437513     -2.1113678676    -1.658903729
O    -8.0975520079    -1.9340276071     0.5788947554
C    -4.7798645138     2.0373696545    -1.2221342789
C    -6.3231371025     0.5483739545     1.8381599181
O    -4.3667771904    -2.3631683022    -2.8393074767
O    -5.980243588      2.7094056944    -0.8971398889
N    -7.1620460828     1.7394559595     1.8112054225
O    -9.0584111643     0.5238005023     1.6006829529
C    -8.5169641718     1.6143329131     1.7563521034
C    -9.3190622936     2.8870170817     1.8544071466
H    -4.0679738451    -2.0306968162     0.347559487
H    -5.8700111788    -3.4667569799    -0.3409332732
```

```
H   -6.3191410644   -2.087696799    1.6319188479
H   -7.0862117055    0.2281692545   -0.1578659456
H   -5.8256788545    0.378477809    -2.0658222421
H   -3.6641878341    0.0720703303   -3.1702663364
H   -2.8041824464    0.3079935026   -1.6345373847
H   -2.8422597272   -2.0298002425   -1.6051229534
H   -7.66424508     -2.1023873242   -1.3728698923
H   -8.5529034294   -1.1649684535    0.9750776001
H   -4.4376627077    2.4951064855   -2.1550624483
H   -3.998800943     2.2033784856   -0.4631093334
H   -5.3013536833    0.8619256357    2.0558338688
H   -6.6636309932   -0.099713551     2.6541856388
H   -5.3290360834   -2.23208181     -2.8452425519
H   -6.3391232294    2.3290783573   -0.0834055048
H   -6.7795320926    2.6102183044    2.1474325933
H   -8.7224929367    3.7623590422    2.1199375303
H   -9.7983633804    3.0717473281    0.8894346526
H   -10.1113438566   2.7480037838    2.5924125884

calc_2d conf_33

C   -6.1419698968   -2.4843683935   -0.8050300283
C   -7.5610627393   -2.0075434327   -0.4752176282
C   -7.4277872035   -0.4600611009   -0.3527622728
N   -6.0063226519   -0.1770653516   -0.2182986302
C   -5.2752536335   -1.4368713901   -0.1037933321
C   -5.345363169     0.7445466807   -1.1476094752
C   -4.1564738909   -0.0383140533   -1.7257860533
C   -3.9048109849   -1.1750901096   -0.7340187706
O   -6.031892793    -2.4335303258   -2.2164229396
O   -8.5170982958   -2.4335434497   -1.4067079913
C   -4.9160419847    2.0130068236   -0.405157509
C   -8.2339700343    0.0279504711    0.8561266354
O   -3.440756347    -2.3824857636   -1.3372708365
O   -4.1932804312    1.7206262293    0.761432806
N   -8.1852509785    1.4552955415    1.0851012259
O   -6.5127285612    1.3758179513    2.6174969975
C   -7.3306132821    2.0239453219    1.9737672572
C   -7.4509487013    3.5229288476    2.1412515525
H   -5.1646123396   -1.7303738455    0.9495450845
H   -5.9494565141   -3.5007621537   -0.4413830294
H   -7.85850031     -2.4205556668    0.4963676602
H   -7.8258891134   -0.0017201826   -1.2680787282
H   -6.0357046302    1.0330214026   -1.9537798175
H   -4.4345887835   -0.475023625    -2.6880844522
H   -3.2731476778    0.5904983856   -1.8707217327
H   -3.2034331802   -0.8497095138    0.0410826988
H   -5.1105951311   -2.6764997462   -2.4075585965
H   -8.0401989999   -2.4773825035   -2.2516727635
H   -5.8097270343    2.6171557378   -0.1853850836
H   -4.2669647787    2.6201490556   -1.0465360434
H   -7.835186367    -0.4430111395    1.7581251746
H   -9.2804958965   -0.2768425983    0.7419994154
H   -2.5448540429   -2.2268797109   -1.6606452832
H   -4.8317575818    1.3145488566    1.3750607781
H   -8.8266419956    2.0481476313    0.5839472854
H   -8.1700074105    3.992390451     1.4649751375
H   -7.7430390166    3.7364369561    3.1725947255
H   -6.4655736174    3.9671677128    1.984046563
```

calc_**2d** conf_34

```
C   -6.0426694448   -2.308324148    -0.413987464
C   -6.7525319323   -1.599886451    0.7353940151
C   -6.3780440999   -0.1161160794   0.4949865744
N   -5.0592195483   -0.1586637394   -0.1395739029
C   -4.7117317126   -1.5661016645   -0.440070402
C   -4.904146007    0.6142984565    -1.3714453074
C   -3.7028572888   -0.0492811699   -2.0303903975
C   -3.888232374    -1.5532081234   -1.7560271835
O   -6.7924531908   -2.0477679104   -1.5905768711
O   -8.1234871089   -1.8721150548   0.6528863808
C   -4.7177563731   2.0987149644    -1.0899597749
C   -6.3891552028   0.7526721346    1.7748055278
O   -4.4633376906   -2.2620949925   -2.8251227738
O   -4.4853318093   2.8496266973    -2.2616189971
N   -7.4879309666   1.6986546983    1.8551825434
O   -9.0812283584   0.1398247184    2.2363970521
C   -8.7591597484   1.3207147407    2.1006225221
C   -9.7823716311   2.4242236915    2.2195075818
H   -4.1010370341   -1.9710818033   0.3785557097
H   -5.9342819565   -3.3879113567   -0.2529366662
H   -6.3325650876   -1.9398442873   1.6952271367
H   -7.121383639    0.2971018144    -0.2035212462
H   -5.7941833763   0.4920896785    -2.0214817067
H   -3.6242408871   0.1472954408    -3.100300801
H   -2.7875412293   0.3118672618    -1.5471380992
H   -2.9161944545   -2.0263428765   -1.5930114327
H   -7.7223972045   -2.047327898    -1.3003318555
H   -8.5834310314   -1.2397132705   1.2448447369
H   -3.837857221    2.2347857224    -0.4545929949
H   -5.5893258581   2.4910130843    -0.5377339897
H   -5.461726038    1.3252516857    1.8087349217
H   -6.4175558951   0.119796189     2.6683622686
H   -5.4255610817   -2.1381305317   -2.786732137
H   -5.2290407068   2.6961959366    -2.8584840575
H   -7.2886989455   2.6785603235    1.7378998157
H   -9.3715605596   3.4255610472    2.0720016236
H   -10.5748182203  2.2506601762    1.4879763193
H   -10.2389550855  2.3700028949    3.2106533307
```

calc_**2d** conf_35

```
C   -6.0490635234   -2.5035971429   -0.8684991064
C   -6.5454842935   -1.8802201993   0.4547269652
C   -6.3629038728   -0.376065721    0.2192786056
N   -5.0498919995   -0.3476142272   -0.4082739138
C   -4.9648094192   -1.5040854164   -1.326025574
C   -4.6659566686   0.8683024298    -1.1334893273
C   -4.1989126252   0.377614649     -2.5163580885
C   -5.0128416897   -0.8915038217   -2.729267961
O   -7.1547807896   -2.6831417992   -1.7333662999
O   -7.8553700778   -2.2764122111   0.7615828745
C   -3.5778435079   1.6420536116    -0.3942754891
C   -6.4373558471   0.449317999     1.495702524
O   -6.3700243027   -0.5506556932   -3.0344569653
O   -3.1256082694   2.7609289241    -1.1307493541
N   -7.7615214295   0.3643798629    2.0668603667
```

S209

```
O   -7.966031239    2.5931656711    2.4493732241
C   -8.4445309918   1.467677445     2.4696239001
C   -9.8531103062   1.2103737627    2.9642338197
H   -3.978916471   -1.9772402118   -1.2302170644
H   -5.627447327   -3.4986446655   -0.705510125
H   -5.8930501616  -2.1851373436    1.2811049844
H   -7.1600220081  -0.0276016874   -0.4641554329
H   -5.5467646771   1.5181882472   -1.2591496086
H   -4.3489059223   1.1202666718   -3.3040397235
H   -3.1295868214   0.13873893     -2.4950060427
H   -4.6062464702  -1.5611211854   -3.4964262036
H   -7.1943895763  -1.9125165689   -2.3307129431
H   -8.2493430517  -2.4698309099   -0.1104799523
H   -2.7105753949   0.9897870866   -0.2567907228
H   -3.9296554558   1.9293541437    0.6058060334
H   -6.245364841    1.5089446606    1.3076235417
H   -5.6720731825   0.0930689792    2.19885016
H   -6.4007664261  -0.1606629915   -3.9169569234
H   -3.8176784961   3.433082101    -1.0972288988
H   -8.2284375808  -0.5306858631    2.0039698662
H   -10.1609507214  0.1640887607    2.8970724507
H   -9.9237535267   1.5341677264    4.0055705334
H   -10.5460310352  1.8262359969    2.3860558709


calc_2d conf_36

C   -6.0873007394  -2.2393437744   -0.4301355422
C   -6.8031149682  -1.4909392464    0.6879494615
C   -6.3842449203  -0.0216068199    0.4251245755
N   -5.0493263578  -0.1125726972   -0.1718280527
C   -4.7360753743  -1.5353504823   -0.4360907567
C   -4.8488262928   0.6300220483   -1.4187014662
C   -3.6661221911  -0.0886637084   -2.054870286
C   -3.8830811415  -1.578581561    -1.7320341267
O   -6.7968442354  -1.9817460655   -1.6324543377
O   -8.1771210779  -1.7380960257    0.5847432587
C   -4.5925942526   2.1023275788   -1.1514257379
C   -6.3947922247   0.8752441544    1.6827964424
O   -4.4413690546  -2.3237268373   -2.7849327684
O   -4.3952372218   2.7396630963   -2.3955629828
N   -7.574534253    1.7118210637    1.8258526726
O   -8.9653574903   0.0526414351    2.4807450561
C   -8.7723459144   1.2433269268    2.2307694847
C   -9.8789253952   2.2596655897    2.3809970409
H   -4.1585734138  -1.942018205     0.4055095692
H   -6.0138996772  -3.3180412303   -0.2451510337
H   -6.4101084304  -1.8190465879    1.6626408504
H   -7.0980431364   0.3980402291   -0.2999227559
H   -5.7315375472   0.5490025613   -2.0763100983
H   -3.5891320931   0.0752922584   -3.1300540437
H   -2.7389542931   0.2627422803   -1.5862583782
H   -2.9224411812  -2.0592380414   -1.5285503955
H   -7.7359685235  -1.9674670368   -1.3790661319
H   -8.6162403041  -1.1990809781    1.2750322253
H   -3.7124195506   2.1882696092   -0.4957384838
H   -5.4514217151   2.5428833612   -0.6165502972
H   -5.5307559299   1.5398098517    1.642301678
H   -6.2956802519   0.2674690853    2.5879427262
H   -5.3975121952  -2.1553758617   -2.7971560928
```

S210

```
H   -4.148027069    3.6562888268   -2.2284009091
H   -7.4944932442   2.6901260808    1.6015565198
H   -9.5740685724   3.2838665264    2.1543790497
H   -10.7062200879  1.9794327961    1.724680428
H   -10.2512896786  2.2179597995    3.4071736382
```

calc_**2d** conf_37

```
C   -6.2606958986   -2.1180172632   -0.347343491
C   -7.067594402    -1.2308180028    0.6063024784
C   -6.4415380678    0.1735502605    0.4033857353
N   -5.1164299513   -0.0392222048   -0.1850750419
C   -4.8730223921   -1.491030328    -0.2530814057
C   -4.8877799137    0.5191689578   -1.5212813873
C   -3.7184086559   -0.3115939824   -2.0388538994
C   -3.9100507569   -1.7244533703   -1.4472490105
O   -6.7986101278   -1.9444994585   -1.6458818582
O   -8.4296964014   -1.3116239735    0.2538257096
C   -4.5922795153    2.0111760003   -1.4502587622
C   -6.2705813943    0.9722682556    1.7031813297
O   -4.3512725837   -2.6960728815   -2.3624008816
O   -4.2914277339    2.563662458    -2.7142685925
N   -7.4119572503    1.002149814     2.6122574116
O   -9.0833820245    1.2268304331    1.0930174006
C   -8.700757195    1.1998210035    2.2646837638
C   -9.6808187224   1.3656185722    3.4029548522
H   -4.4195102965   -1.8363511734    0.6866842376
H   -6.2744957534   -3.1768455351   -0.0598994486
H   -6.919578151    -1.5667497587    1.6437080122
H   -7.0768492434    0.7373431165   -0.2864873261
H   -5.7694869109    0.3609915407   -2.168972254
H   -3.6644283347   -0.3504798086   -3.1277349466
H   -2.7808828999    0.1225994392   -1.6741400477
H   -2.9524200861   -2.1042757136   -1.0831358048
H   -7.751240046    -1.7931059268   -1.4957057862
H   -8.8302214381   -0.4339049777    0.4164180484
H   -3.7089858389    2.1686866029   -0.824821203
H   -5.4322930703    2.5440291281   -0.9749177125
H   -5.972797716    1.996143022     1.4480480681
H   -5.4404185947    0.5269561349    2.2573243559
H   -5.2834914337   -2.5067266675   -2.5591553614
H   -5.0662407628    2.4403469919   -3.2772920247
H   -7.1950801066    1.0258934782    3.5959073872
H   -10.4429627498  0.5868147249    3.3248298084
H   -9.2263020695   1.3220228383    4.395269666
H   -10.1870115108  2.3266982536    3.2851579808
```

calc_**2d** conf_38

```
C   -6.1321059088   -2.5583991595   -1.0243446451
C   -7.3522645926   -2.0785397613   -0.2330274138
C   -7.0694836792   -0.5647090439   -0.0209337768
N   -5.6152569417   -0.3946957532   -0.1623945333
C   -5.0196712378   -1.7253839891   -0.3795896047
C   -5.1342539001    0.4724960669   -1.23624833
C   -3.6767042829    0.0358806751   -1.353784672
C   -3.7210103046   -1.4857792457   -1.1761908196
O   -6.4099282237   -2.1945666889   -2.3628133869
O   -8.5663130549   -2.3573564897   -0.8688452135
```

S211

```
C   -5.3116341873    1.9525792251   -0.947639901
C   -7.5510731578   -0.0897229404    1.3472526885
O   -3.7882713945   -2.1971458805   -2.4142058889
O   -4.646423762     2.2933977192    0.2605254312
N   -7.1730593185    1.2769371776    1.6056031852
O   -9.2227525842    1.9684282746    2.3118453904
C   -8.0456593914    2.2027359504    2.0801901948
C   -7.4537490345    3.5799739002    2.3138862466
H   -4.783229209    -2.1867155142    0.5890075384
H   -5.9643067761   -3.6395075595   -0.9330684236
H   -7.3816495134   -2.5840773025    0.7393890019
H   -7.5931573135   -0.0024537004   -0.8046708349
H   -5.662006114     0.2710861319   -2.1848927241
H   -3.2149896706    0.3283654022   -2.3025728499
H   -3.1095165152    0.4908930138   -0.5373911908
H   -2.8505679768   -1.8503265425   -0.6193528661
H   -5.5705857568   -2.2875460818   -2.8439789273
H   -8.3911748133   -2.2214260571   -1.8138858555
H   -6.3821841114    2.187972105    -0.8767777554
H   -4.8992022079    2.51801539     -1.7949897116
H   -7.1269512761   -0.7475949575    2.1191866603
H   -8.6393705813   -0.1514214006    1.4170702889
H   -2.9830504382   -2.0110251447   -2.9123927228
H   -4.597481045     3.2556109401    0.3088272069
H   -6.2016575009    1.5238478576    1.4467061244
H   -6.4144713756    3.6674175548    1.988141775
H   -8.0638614091    4.3185675402    1.7888795138
H   -7.5099714391    3.8121882883    3.3804808015

calc_**2d** conf_39

C   -6.1715936243   -2.4790635999   -1.0653475296
C   -7.4265365183   -1.9164285263   -0.3983594332
C   -7.0613850794   -0.4237629769   -0.157070357
N   -5.5918928968   -0.3516081109   -0.1562042502
C   -5.0773136378   -1.7243905956   -0.3075018472
C   -4.942201478     0.4772872748   -1.1679040801
C   -3.5243656338   -0.0941035817   -1.1971783019
C   -3.6945075785   -1.5972894354   -0.9863405399
O   -6.2749407064   -2.0967421723   -2.4238700092
O   -8.5894875454   -2.1102499692   -1.1517098274
C   -4.929073953     1.9617665659   -0.8356238229
C   -7.6945743345    0.0654338086    1.139583642
O   -3.6134863919   -2.2530991175   -2.2595213761
O   -6.1909908278    2.6009850147   -0.9714566409
N   -7.4975183225    1.4783185126    1.3507543857
O   -7.8040835521    1.3685582876    3.5939350984
C   -7.5515412515    2.0221618491    2.5906107189
C   -7.2844424493    3.5140175608    2.6519749545
H   -4.9749018165   -2.1899414544    0.6830288382
H   -6.0961185779   -3.5716453487   -0.9630429443
H   -7.5878825053   -2.4149242638    0.5644607831
H   -7.4598835905    0.1548604681   -1.0006633994
H   -5.412978464     0.3453640816   -2.1610522428
H   -2.9883407632    0.1123558079   -2.126012226
H   -2.9482258646    0.3257887928   -0.3658805204
H   -2.9019940955   -1.9979898602   -0.3469385234
H   -5.3765398235   -2.1725824872   -2.7927618525
H   -8.3187585929   -1.9729433123   -2.0734537052
```

```
H   -4.1846373964    2.4697933718   -1.4653499875
H   -4.6417967727    2.0898138337    0.2104384523
H   -7.2675147341   -0.472080051    1.9923668562
H   -8.7656531041   -0.1798059141   1.1109887304
H   -3.4652038276   -3.1941726293   -2.0998506579
H   -6.4842501473    2.500299073    -1.8863501517
H   -7.2338197321    2.0453820498    0.5530103464
H   -6.9853254257    3.9448967959    1.6932083602
H   -8.187760024     4.0205721381    3.0022264706
H   -6.5024789609    3.7001681201    3.3918565898

calc_2d conf_40

C   -6.2305595872   -2.3930119586   -0.7951928462
C   -6.9784188983   -1.6964611378    0.3427911625
C   -6.514845576    -0.2288830483    0.1970558521
N   -5.1230976604   -0.3369663688   -0.2290365892
C   -4.855601012    -1.7290557444   -0.6610617901
C   -4.6516720516    0.5674682908   -1.2708882147
C   -3.4382257301   -0.1805887518   -1.8153555391
C   -3.9075298096   -1.6325803906   -1.8706030523
O   -6.9630257927   -2.047043667    -1.9507749347
O   -8.3734587454   -1.8582211897    0.2729361164
C   -4.3061164273    1.9452507747   -0.7349472747
C   -6.6872266952    0.5598419386    1.4913723948
O   -4.6156828888   -1.9220390422   -3.0773326556
O   -3.7407587985    2.6790765799   -1.8040923827
N   -8.0866905782    0.6285540578    1.8489861843
O   -7.9755843351    2.7320099684    2.6898165441
C   -8.631302991     1.7377959117    2.411445097
C   -10.1207057339   1.6640540464    2.6802095318
H   -4.3260768508   -2.2614182199    0.1420004344
H   -6.1792977954   -3.4830921833   -0.6702901326
H   -6.6598029998   -2.0946501782    1.3127468357
H   -7.1324644434    0.2367070032   -0.5883162219
H   -5.3995519328    0.6873960783   -2.0749364352
H   -3.0938542022    0.2010551938   -2.7803162115
H   -2.6083533722   -0.0906246483   -1.105594425
H   -3.0787595978   -2.3441112125   -1.7779049199
H   -6.336604684    -2.0437769949   -2.6951246607
H   -8.5814726944   -1.7776457557   -0.6733473136
H   -3.6044910918    1.8289409669    0.1047090312
H   -5.2101057196    2.438470384    -0.3518221596
H   -6.3264854635    1.5861895165    1.3977683208
H   -6.0934765081    0.0827818906    2.2835675733
H   -4.1056964009   -1.5804236051   -3.8219554587
H   -3.5886147849    3.5807485507   -1.4983842109
H   -8.6709508239   -0.152816938    1.5824963575
H   -10.5839813166   0.7304856315    2.3516119391
H   -10.290021589    1.7849270971    3.7530610387
H   -10.6094344175   2.5026571541    2.1787030152

calc_2d conf_41

C   -6.3659501088   -2.3802829183   -0.8753400789
C   -7.1058044039   -1.8137675258    0.3392509818
C   -6.5392564379   -0.3812791714    0.4304703248
N   -5.143328687    -0.5211133601    0.0310479972
C   -4.9537537019   -1.8471456494   -0.6024941612
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S213

```
C   -4.5991918277    0.4957633734   -0.8629538417
C   -3.4132373749   -0.2331464024   -1.485261158
C   -3.9556697192   -1.6357320177   -1.7569774769
O   -7.0281095226   -1.8051334942   -1.9815351739
O   -8.5038164636   -1.8684998641    0.2250630968
C   -4.2068108544    1.7787837629   -0.1392033036
C   -6.7202964983    0.2352203349    1.8181880316
O   -4.6330440961   -1.7172119731   -3.0123588151
O   -3.5603207242    2.686842644    -1.0128969179
N   -8.1013596328    0.5911768852    2.0603021813
O   -7.7617420734    2.8092168177    1.6882848573
C   -8.5259137056    1.8753330219    1.8892695025
C  -10.0216559385    2.0832981667    1.9986306251
H   -4.4929504098   -2.5324093916    0.123160833
H   -6.3950551993   -3.4774566271   -0.9220136027
H   -6.8386247368   -2.3778576645    1.24064767
H   -7.0888057715    0.2421205396   -0.2931791287
H   -5.3254348015    0.7501917185   -1.6597964348
H   -3.022920885     0.2600160618   -2.3795780535
H   -2.598695922    -0.2892757782   -0.7543670319
H   -3.168631172    -2.3987233556   -1.7389699927
H   -6.3827376041   -1.7606949894   -2.7074458263
H   -8.6837722919   -1.6262029247   -0.6984490575
H   -3.4909326417    1.5340736271    0.6513153428
H   -5.0824065693    2.2424307325    0.3332725307
H   -6.1423919218    1.1536324662    1.9163502639
H   -6.3722280708   -0.4630078484    2.5881035938
H   -4.0445746367   -1.380961333    -3.6992416753
H   -4.2446215495    3.1315075827   -1.5273667835
H   -8.782229262    -0.1502948456    1.9778916801
H  -10.3846262353    2.5329337381    1.071155395
H  -10.5812365508    1.1657726078    2.1953914478
H  -10.2168619975    2.7968830539    2.8026321585
```

calc_**2d** conf_42

```
C   -5.7661892523   -2.4928316375   -0.5006309051
C   -6.9484409956   -1.7615954592    0.1956337856
C   -6.4248822054   -0.3438777335    0.4812927101
N   -5.0519846397   -0.2961853168   -0.0411083842
C   -4.8801121914   -1.3604763599   -1.0311666777
C   -4.7151062057    0.9575476219   -0.7187774659
C   -5.0755258829    0.7586992101   -2.2097216773
C   -5.2407732458   -0.7530975858   -2.4102534608
O   -6.2264503471   -3.3872049889   -1.4961366192
O   -8.0990154       -1.7901906829   -0.6229612066
C   -3.2334448645    1.2792502867   -0.5145331618
C   -6.4129987964    0.0494884599    1.9609029828
O   -6.5881749424   -1.0242399837   -2.8035347709
O   -2.8293067607    2.4401479415   -1.2091812408
N   -7.7269671771    0.3453623113    2.4854164457
O   -7.7187944508    2.4541921789    1.6659175168
C   -8.3072831231    1.5552010995    2.2495773567
C   -9.7236019409    1.7162154114    2.7566296306
H   -3.8284284012   -1.6694762761   -1.0587608733
H   -5.1960939444   -3.0549103507    0.2482199104
H   -7.2387211972   -2.284930127     1.1115283411
H   -7.0853536329    0.3659764898   -0.0382584788
H   -5.3027659088    1.7677229761   -0.2693955146
```

```
H   -6.0236171021    1.2387106749   -2.4663439268
H   -4.306700536     1.1914098544   -2.8538281555
H   -4.5723606029   -1.1399974641   -3.1877799127
H   -7.1954300145   -3.3946823609   -1.3785958981
H   -7.8630396046   -1.2653947904   -1.417034599
H   -2.6123610688    0.4688604676   -0.908569276
H   -3.0289276547    1.3516886939    0.562743593
H   -5.8043897625    0.9486709285    2.0761908607
H   -5.952649737    -0.7419294225    2.55984309
H   -6.6100484415   -1.9931805729   -2.8939826219
H   -3.308041435     3.1888118829   -0.8308168415
H   -8.2855523912   -0.3987850202    2.8698932405
H  -10.4024246215    1.7682892284    1.9009757431
H  -10.0498137923    0.9073365775    3.4150901406
H   -9.7972277294    2.665403838     3.2905163209
```

calc_**2d** conf_43

```
C   -6.2612228921   -2.4872152827   -0.9576251495
C   -7.6191601618   -1.9235863284   -0.521663556
C   -7.339070302    -0.4119886439   -0.2862231215
N   -5.8848590321   -0.2658422977   -0.1790919237
C   -5.2957735296   -1.6123616714   -0.1651112307
C   -5.2170259692    0.5162660925   -1.2322191291
C   -3.7850330186   -0.0192368446   -1.2185148761
C   -3.8515500064   -1.4748779863   -0.7081241608
O   -6.1097629239   -2.2584059239   -2.3665603929
O   -8.6596711754   -2.1821133807   -1.4327534298
C   -5.3021615816    2.0004012567   -0.8894216089
C   -8.096257706     0.0733189532    0.9529017161
O   -3.5077411193   -2.4584890648   -1.6541389404
O   -4.7766255194    2.2679900906    0.384882306
N   -8.0307885625    1.4959317899    1.1825419774
O   -6.565188272     1.361362788     2.9063397877
C   -7.2581354683    2.0434452673    2.1655040002
C   -7.2779194304    3.5518075732    2.2436579391
H   -5.2924592223   -2.0010667327    0.8616607813
H   -6.1435958877   -3.5527257577   -0.737318914
H   -7.9248182693   -2.3974279061    0.4173088384
H   -7.6990356489    0.1476862317   -1.1624611913
H   -5.6848143752    0.3476374573   -2.2165864897
H   -3.316265837     0.0146098579   -2.204697818
H   -3.1876850208    0.5919616451   -0.5366231726
H   -3.1390743654   -1.6143548313    0.107362188
H   -6.5825511766   -2.970499293    -2.8176543671
H   -8.4051436171   -1.7374181847   -2.2538181198
H   -6.3513701532    2.3316413116   -0.9645883826
H   -4.7249676677    2.5839763546   -1.61400793
H   -7.6713665287   -0.3983990653    1.8422026905
H   -9.1453544277   -0.2346263621    0.8645174785
H   -4.2111077782   -2.441877027    -2.3231642555
H   -5.1050267036    1.5542574385    0.9608860898
H   -8.5863210477    2.1073132839    0.6063902109
H   -7.2355302497    3.8509075736    3.2915685013
H   -6.374546682     3.9170515914    1.7467173145
H   -8.1530186705    4.0049460271    1.7699263404
```

calc_**2d** conf_44

```
C   -6.30723933     -2.3558560508    -0.8909111236
C   -7.6360985904   -1.5228979765    -0.8383191228
C   -7.2819377599   -0.2714890761    -0.0010299378
N   -5.8299390047   -0.1935521339     0.0588487908
C   -5.358571211    -1.5789708745     0.0528930973
C   -5.1895845551    0.4583232154     -1.1021033458
C   -3.772754468    -0.1163365903     -1.0747161689
C   -3.8730450656   -1.4922212816     -0.3650372567
O   -5.8243521011   -2.3966340667     -2.2169283492
O   -8.0676100625   -1.2151618455     -2.16008108
C   -5.2481227893    1.9778022442     -1.0343168548
C   -7.9051771586   -0.3655664779      1.4033275239
O   -3.4075941756   -2.591356985      -1.0995142987
O   -6.5373147534    2.496959681      -1.2831417461
N   -7.3523317675    0.5634346458      2.3666414851
O   -7.8933463616    2.4255953408      1.2045954848
C   -7.3367390836    1.8987433892      2.1673755543
C   -6.6084069359    2.7200224178      3.2056569241
H   -5.4590198154   -2.0121098781      1.0569375511
H   -6.4684377672   -3.3812773052     -0.5370238326
H   -8.4407233239   -2.108532295      -0.3817632223
H   -7.6722473481    0.6320280003     -0.4695954429
H   -5.6763126692    0.1599859612     -2.0446244376
H   -3.3583419102   -0.2373614454     -2.0779306559
H   -3.1026696845    0.5494807753     -0.5193706053
H   -3.2574703196   -1.4762446211      0.5378013186
H   -6.5638041458   -2.0709016392     -2.7672617964
H   -7.9131614973   -0.2740691127     -2.3181410943
H   -4.5842595393    2.3812196611     -1.8081857489
H   -4.8564214884    2.3048463063     -0.0603673593
H   -7.7687172563   -1.3668164744      1.8217938485
H   -8.9834143071   -0.1973322707      1.3140691674
H   -4.0073008787   -2.6811396537     -1.8587090168
H   -6.9982890909    2.6089692218     -0.4324946058
H   -6.7440081665    0.1904549764      3.0766361922
H   -6.3028484412    2.1481950403      4.0848029543
H   -5.7209036816    3.1645906296      2.7472670195
H   -7.258483495     3.5391765478      3.5189201904

calc_2d conf_45

C   -6.1122945284   -2.3623711316    -0.4481618525
C   -7.4594993204   -1.6423387851    -0.7279505487
C   -7.2776750161   -0.2691404437    -0.0784196306
N   -5.8594615041    0.0622028818    -0.2567155818
C   -5.119917153    -1.1999220964    -0.1050959344
C   -5.4827346387    0.699193547     -1.539971592
C   -4.4686781913   -0.2426832195    -2.197173639
C   -3.9008948647   -1.0138472627    -1.0108358514
O   -5.801454786    -3.1482870109    -1.5795092147
O   -7.6271830441   -1.4634704269    -2.1129462195
C   -4.9027622377    2.085930237     -1.2574816089
C   -7.6409293233   -0.2725746024     1.407295839
O   -3.3113192637   -2.2744256072    -1.3114858675
O   -4.4791917755    2.7551163996    -2.4259868919
N   -7.2107752682    0.9557778113     2.0212413885
O   -8.9963435744    1.1694711652     3.4013188363
C   -7.9317890703    1.5948816884     2.9786751099
C   -7.3243027738    2.8839560324     3.4938469723
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H   -4.798754889    -1.3245128065    0.9343958141
H   -6.2104197789   -3.014315128     0.4287365584
H   -8.3074766571   -2.1991675223   -0.3035270291
H   -7.8909722547    0.4794250908   -0.5873695916
H   -6.36488183      0.8040961135   -2.1806066269
H   -4.9821606931   -0.945253766    -2.8589284766
H   -3.7173474649    0.3064466888   -2.7716193554
H   -3.1648321401   -0.3980313798   -0.4776372439
H   -4.8299062355   -3.1550338288   -1.6669750516
H   -7.1311724876   -2.2006735609   -2.5136217751
H   -4.0156901653    1.9933124144   -0.6233495704
H   -5.6425756111    2.6747054967   -0.6941256039
H   -7.1903349462   -1.1385423007    1.9150932293
H   -8.7216790141   -0.3558617788    1.5411484297
H   -2.6097102724   -2.1330570891   -1.9596296979
H   -5.2615031265    2.932025063    -2.9638130858
H   -6.3322759287    1.3237248069    1.6858201822
H   -7.1406797236    2.7820167953    4.5662800195
H   -6.3904934323    3.1627878562    2.9990433407
H   -8.0509270151    3.6894396589    3.3650418213

calc_**2d** conf_46

C   -6.3115887871   -2.2585162277   -0.3125425798
C   -7.5914965994   -1.6370961682   -0.9388834552
C   -7.6133869123   -0.2154617683   -0.3636833091
N   -6.2163719327    0.1782867088   -0.2482312564
C   -5.4841471122   -1.0212290977    0.1753036804
C   -5.5782100876    0.7560430573   -1.4480713823
C   -4.3847015905   -0.152080269    -1.765683711
C   -4.0920267634   -0.8186749773   -0.4248438762
O   -5.7102179959   -3.0783067041   -1.295492135
O   -7.4536064385   -1.5577843103   -2.3364429244
C   -5.1596709025    2.195561874    -1.1460789044
C   -8.3206009806   -0.1767000481    1.0007640015
O   -3.3966354458   -2.0607376118   -0.4944403058
O   -4.5072095534    2.8228103735   -2.231111158
N   -8.1809818885    1.0839100189    1.6848902475
O   -6.548489599     0.3588875092    3.0916711075
C   -7.2068535144    1.2741524524    2.6219928404
C   -7.006605301     2.7104063029    3.0563661372
H   -5.4331646761   -1.0473214013    1.2673950943
H   -6.5780387303   -2.8740523149    0.5553788058
H   -8.4890924804   -2.2159624734   -0.674015049
H   -8.1291330143    0.4592893042   -1.0553828952
H   -6.2794245597    0.7569112424   -2.291221798
H   -4.6810409357   -0.92433264     -2.4809725974
H   -3.5416351635    0.4103503125   -2.1773689862
H   -3.5321970939   -0.1354833651    0.2264038286
H   -4.7457749343   -3.0287462119   -1.1544847156
H   -6.8202671854   -2.2670413407   -2.5540785806
H   -4.4479770252    2.2060122088   -0.3154212018
H   -6.0442583836    2.7628059217   -0.8181838674
H   -7.9051318181   -0.929213374     1.6751208634
H   -9.3825518572   -0.4069192317    0.8617410557
H   -2.5569082811   -1.9114094375   -0.9467060852
H   -5.1345697385    2.8655572066   -2.9640626144
H   -8.5788882679    1.9017202583    1.2499787511
H   -7.8794953831    3.3434574686    2.8754575583
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H   -6.7622322534    2.7253971294    4.118946608
H   -6.1554168133    3.1295096237    2.510992809
```

calc_**2d** conf_47

```
C   -6.1101356391   -1.6428247685    0.2096249742
C   -7.3173104531   -0.7051504784   -0.0476903158
C   -6.7062139613    0.6975767841    0.0102605229
N   -5.3581091023    0.5608750205   -0.5379545662
C   -4.8599922742   -0.7452956394   -0.083322348
C   -5.2148014791    0.6581832386   -2.0063177808
C   -4.6219398562   -0.6795084813   -2.4613606542
C   -3.9155029297   -1.1792194189   -1.2064827406
O   -6.2706601147   -2.7845085081   -0.6108207618
O   -7.8161827763   -0.9092813895   -1.3513118837
C   -4.3132941489    1.8475834126   -2.3413280691
C   -6.6104385178    1.2797440023    1.4273867704
O   -3.6766240185   -2.5819187       -1.1427469357
O   -4.0884727172    1.9965043625   -3.728887692
N   -7.8900564608    1.4811720401    2.0675493111
O   -7.7679345208   -0.3762629076    3.3620787565
C   -8.3762277199    0.6222814776    3.0061820659
C   -9.7304620958    0.9791256196    3.5806954288
H   -4.2989273599   -0.6307554881    0.8504030641
H   -6.0983829338   -1.946323859     1.2622807765
H   -8.1053840686   -0.8626645439    0.6974406114
H   -7.2933580486    1.378897612    -0.6144179444
H   -6.1943462426    0.8108116532   -2.473886573
H   -5.4241100164   -1.3785318656   -2.7127331488
H   -3.9629410516   -0.5608408      -3.3262393255
H   -2.9604551463   -0.6532984268   -1.0772289229
H   -5.3772472028   -3.0822830329   -0.8629154589
H   -7.5818750627   -1.8338787627   -1.5526564158
H   -3.3278103578    1.7062979127   -1.8881477702
H   -4.7418897251    2.7577348174   -1.8960558859
H   -6.0705289143    2.2297236009    1.3726287576
H   -6.0432638879    0.613267287     2.080770269
H   -3.1674569134   -2.8353572462   -1.9228717811
H   -4.9390544396    2.1891193298   -4.1435630308
H   -8.4522846431    2.2690954137    1.7900649054
H   -10.1168846831   1.9438636722    3.2423520737
H   -10.4446727415   0.1976098687    3.3091019574
H   -9.6557677752    0.9864371912    4.6701197599
```