Supporting Information for "Improved electrostatic embedding for fragment-based chemical shift calculations in molecular crystals"

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This supporting info provides complete tables of the experimental and PBE0/SCRMP chemical shifts used for each test set. It also provides absolute shieldings and scaled ^{17}O isotropic chemical shifts for γ-glycine, along with the optimized GLYCIN34 crystal structure. Additional details regarding the composition of the ^{1}H, ^{13}C, ^{15}N and ^{17}O isotropic test sets have been provided previously.[1,2]

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1 Tabulated experimental and predicted chemical shifts

Table S1: Comparison of experimental, absolute and predicted isotropic ^{1}H chemical shifts for the 2-body fragment and combined cluster/2-body models with SCRMP charge embedding using the PBE0 density functional (in ppm). The predicted chemical shifts can be obtained from the absolute shieldings using the linear regression parameters reported in this work. All shifts are reported relative to TMS with adamantane at 1.87 ppm.

	Exp. Shifts	**2bd 6 Å Fragment**		**Cluster/Fragment**	
Crystal	Isotropic (ppm)	Absolute Shieldings	Predicted Shifts	Absolute Shieldings	Predicted Shifts
CIMETD	2.24	29.30	1.84	29.30	1.80
	2.24	29.16	1.97	29.14	1.95
	7.64	23.51	7.14	23.32	7.25
	8.44	22.17	8.36	22.12	8.34
	9.94	20.37	10.02	20.39	9.92
	11.84	18.74	11.51	18.63	11.53
INDMET	5.8	25.04	5.74	25.06	5.67
	6.1	24.64	6.11	24.62	6.07
	5.8	24.97	5.80	24.97	5.75
	1.7	29.43	1.72	29.41	1.70
	2.2	28.90	2.21	28.87	2.19
	1.8	29.24	1.89	29.28	1.82
	7.3	23.70	6.97	23.68	6.92
	5.7	25.03	5.75	24.98	5.74
	7.2	23.55	7.11	23.65	6.94
	7.3	23.16	7.46	23.24	7.32
URACIL	11.2	18.66	11.58	18.65	11.50
	10.8	19.34	10.96	19.18	11.02
	7.5	22.79	7.80	22.64	7.87
	6	24.33	6.39	24.15	6.50
4,5-Dimethylimidazole	4.8	26.37	4.52	26.27	4.56
Diazole	1.4	29.79	1.39	29.75	1.39
	0.7	29.68	1.49	29.62	1.51
	13	16.79	13.30	16.55	13.42
3,5-Dimethylpyrazole	5.2	25.23	5.57	25.20	5.53
Diazole	1.5	29.25	1.89	29.19	1.90
	1.4	28.95	2.16	28.91	2.16
	15	15.12	14.82	15.05	14.79
AMBACO05	5.8	24.90	5.87	24.83	5.87
	6.8	23.63	7.03	23.58	7.01
	5.4	25.03	5.74	24.92	5.79
PHBARB06	10.3	19.94	10.41	19.74	10.51
	8.1	22.49	8.07	22.45	8.05
	10.3	20.01	10.34	19.95	10.32

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Crystal	**Exp. Shifts** Isotropic (ppm)	**2bd 6 Å Fragment** Absolute Shieldings	Predicted Shifts	**Cluster/Fragment** Absolute Shieldings	Predicted Shifts
	6.9	23.73	6.94	23.63	6.97
	2.7	29.12	2.00	29.05	2.02
	1.7	29.42	1.73	29.41	1.70
	0.6	31.50	-0.17	31.43	-0.14
IPMEPL	5.4	25.78	5.06	25.62	5.16
	6.19	24.65	6.10	24.63	6.06
	7.08	23.72	6.95	23.73	6.88
	3.38	27.56	3.43	27.62	3.33
	1.05	30.11	1.09	30.05	1.11
	1.45	29.59	1.57	29.56	1.56
	0.42	30.70	0.56	30.66	0.56
	9.99	19.89	10.45	19.64	10.61
COYRUD11	7	23.09	7.52	23.05	7.50
	6.1	24.21	6.50	24.12	6.52
	3.8	27.23	3.74	27.24	3.68
	4.5	26.07	4.80	26.06	4.76
	4.1	26.47	4.43	26.40	4.44
	5.9	24.98	5.80	24.91	5.80
	3.2	27.11	3.84	27.02	3.87
	1.8	29.12	2.00	29.01	2.07
	2.3	28.87	2.23	28.76	2.29
FPAMCA11	8.3	22.45	8.11	22.41	8.08
	6	24.69	6.06	24.62	6.07
	5.4	25.50	5.32	25.37	5.38
	6.8	23.75	6.92	23.68	6.92
	9.6	20.86	9.57	20.83	9.52
	6.9	23.84	6.84	23.82	6.79
	6.2	24.30	6.42	24.27	6.38
	5.9	24.71	6.04	24.73	5.97
	7.3	23.33	7.30	23.25	7.31
BAPLOT01	14.6	15.37	14.59	15.28	14.58
	7.7	23.37	7.27	23.28	7.28
	3.4	27.68	3.33	27.59	3.36
WEZCOT	7.1	23.74	6.93	23.67	6.93
	9.9	20.88	9.55	20.84	9.51
	8	22.90	7.70	22.78	7.74
	8	22.34	8.21	22.29	8.19
	2	29.17	1.96	29.06	2.02
	1.2	30.12	1.09	29.97	1.19
FLUBIP	0.9	30.26	0.96	30.23	0.95
	2.9	28.38	2.68	28.34	2.68

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Table S1 – *Continued from previous page*

Crystal	**Exp. Shifts** Isotropic (ppm)	**2bd 6 Å Fragment** Absolute Shieldings	Predicted Shifts	**Cluster/Fragment** Absolute Shieldings	Predicted Shifts
	6.7	24.13	6.57	24.13	6.51
ZIVKAQ	1.33	30.19	1.03	30.02	1.14
	4.73	26.49	4.41	26.37	4.47
	6.83	24.10	6.60	24.02	6.62
	6.83	24.07	6.63	23.98	6.65
	6.83	23.98	6.71	23.98	6.65
	10.93	20.40	9.99	20.20	10.09

Table S2: Comparison of experimental, absolute and predicted isotropic ^{13}C chemical shifts for the 2-body fragment and combined cluster/2-body models with SCRMP charge embedding using the PBE0 density functional (in ppm). The predicted chemical shifts can be obtained from the absolute shieldings using the linear regression parameters reported in this work. All shifts are reported relative to TMS.

Crystal	**Exp. Shifts** Isotropic (ppm)	**2bd 6 Å Fragment** Absolute Shieldings	Predicted Shifts	**Cluster/Fragment** Absolute Shieldings	Predicted Shifts
GLYCIN03	176.2	0.5	179.1	0.6	178.8
	43.5	140.6	43.6	140.3	44.0
LALNIN12	176.8	-1.3	180.7	-1.0	180.4
	50.9	132.6	51.4	132.8	51.1
	19.8	164.2	20.8	164.4	20.6
LSERIN01	175.1	1.7	177.8	1.7	177.8
	55.6	128.3	55.5	128.2	55.7
	62.9	119.3	64.2	119.6	63.9
LTYROS11	176.0	0.7	178.9	1.0	178.4
	130.3	50.6	130.6	51.1	130.1
	117.2	64.8	116.8	65.4	116.3
	54.7	127.0	56.7	126.9	56.9
	131.0	50.4	130.8	50.1	131.1
	117.2	62.9	118.7	63.1	118.5
	155.7	25.0	155.4	24.6	155.7
	35.8	146.4	38.0	146.6	37.8
	123.0	59.5	122.0	59.7	121.8
LCYSTN21	35.4	152.3	32.3	152.7	32.0
	53.7	129.1	54.7	128.9	55.0
	175.1	4.4	175.3	4.3	175.3

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Table S2 – *Continued from previous page*

Crystal	**Exp. Shifts** Isotropic (ppm)	**2bd 6 Å Fragment** Absolute Shieldings	Predicted Shifts	**Cluster/Fragment** Absolute Shieldings	Predicted Shifts
MGLUCP11	101.0	82.0	100.3	81.9	100.4
	72.3	112.5	70.8	112.6	70.7
	74.6	109.4	73.8	109.3	73.9
	72.5	111.8	71.4	111.5	71.8
	75.3	109.6	73.6	109.6	73.6
	63.8	120.1	63.4	120.5	63.1
	56.5	126.4	57.3	126.7	57.0
MBDGAL02	105.7	77.1	105.0	77.2	104.8
	71.2	112.6	70.7	112.6	70.7
	72.1	111.1	72.2	110.9	72.3
	69.3	113.0	70.3	113.2	70.1
	75.6	108.7	74.4	108.6	74.5
	62.8	121.2	62.4	120.7	62.9
	57.6	124.7	59.0	124.5	59.2
MEMANP11	99.6	82.7	99.5	82.5	99.7
	71.3	112.2	71.0	112.4	70.9
	71.7	111.3	71.9	111.2	72.1
	64.8	119.0	64.5	118.8	64.8
	71.9	110.9	72.3	110.9	72.3
	58.9	125.2	58.5	125.2	58.5
	54.9	127.4	56.3	127.6	56.3
MGALPY01	100.4	82.2	100.1	82.1	100.2
	67.6	116.4	67.0	116.3	67.1
	72.6	110.4	72.8	109.9	73.3
	70.0	113.8	69.5	113.6	69.7
	72.9	110.8	72.5	110.7	72.6
	61.4	122.4	61.2	122.3	61.3
	55.2	127.7	56.0	128.0	55.9
XYLOBM01	104.2	78.8	103.3	78.8	103.3
	72.2	111.9	71.3	111.7	71.6
	78.2	105.9	77.1	106.0	77.1
	69.5	114.2	69.1	114.7	68.7
	66.9	116.7	66.7	117.0	66.5
	57.3	126.2	57.6	126.3	57.4
FRUCTO02	65.4	118.2	65.3	118.0	65.5
	99.7	80.8	101.4	80.7	101.5
	67.2	116.0	67.4	116.1	67.4
	69.0	115.7	67.7	115.8	67.6
	71.4	111.1	72.1	111.2	72.0
	64.9	117.8	65.7	117.9	65.6
RHAMAH12	94.5	88.0	94.5	87.8	94.7

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Table S2 – *Continued from previous page*

Crystal	**Exp. Shifts** Isotropic (ppm)	**2bd 6 Å Fragment** Absolute Shieldings	Predicted Shifts	**Cluster/Fragment** Absolute Shieldings	Predicted Shifts
	72.2	111.4	71.9	111.1	72.1
	71.0	113.6	69.7	113.3	70.0
	72.5	110.7	72.5	110.6	72.7
	69.8	112.9	70.4	112.8	70.5
	17.8	166.9	18.2	166.8	18.3
SUCROS04	93.3	89.8	92.7	89.6	92.9
	66.0	118.6	64.9	118.8	64.7
	73.7	110.1	73.1	110.0	73.2
	102.4	78.8	103.3	78.7	103.5
	72.8	111.2	72.0	111.1	72.1
	82.9	101.0	81.9	101.0	81.9
	67.9	116.0	67.4	115.8	67.6
	71.8	112.7	70.6	112.6	70.7
	73.6	109.8	73.4	109.6	73.6
	81.8	102.6	80.3	102.5	80.5
	60.0	124.8	58.9	124.7	59.0
	61.0	122.4	61.3	122.3	61.3
GLUTAM01	177.0	3.7	176.0	3.3	176.2
	54.0	129.6	54.2	129.5	54.3
	26.0	158.1	26.7	158.2	26.7
	29.0	154.0	30.6	154.4	30.3
	174.0	3.8	175.9	3.5	176.1
ASPARM03	176.4	1.5	178.1	0.9	178.6
	51.8	133.1	50.9	132.9	51.1
	36.1	148.5	35.9	149.1	35.5
	177.1	5.1	174.6	4.7	174.9
LSERMH10	175.6	1.5	178.1	0.9	178.5
	58.3	124.8	58.9	125.1	58.6
	61.8	122.2	61.4	122.1	61.5
LTHREO01	170.0	5.8	173.9	5.2	174.5
	60.2	123.7	59.9	123.1	60.5
	65.4	116.3	67.1	116.2	67.2
	18.9	163.4	21.6	163.8	21.3
NAPHTA36	126.0	55.4	125.9	55.5	125.8
	129.3	51.2	130.1	51.3	129.9
	134.9	47.8	133.3	47.8	133.3
	129.9	50.8	130.4	51.0	130.2
	125.4	56.2	125.2	56.3	125.1
ACENAP03	148.1	31.5	149.1	31.3	149.2
	120.3	61.4	120.1	61.7	119.9

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Table S2 – *Continued from previous page*

Crystal	**Exp. Shifts** Isotropic (ppm)	**2bd 6 Å Fragment** Absolute Shieldings	Predicted Shifts	**Cluster/Fragment** Absolute Shieldings	Predicted Shifts
	129.4	51.2	130.0	51.3	129.9
	122.3	59.3	122.2	59.1	122.3
	131.9	51.2	130.1	51.1	130.0
	139.9	43.0	137.9	43.1	137.8
	29.5	153.9	30.7	154.0	30.7
TRIPHE11	126.4	55.0	126.4	54.9	126.4
	129.5	52.6	128.6	52.7	128.6
	124.5	56.4	125.1	56.2	125.2
	125.9	55.8	125.5	55.7	125.7
	127.5	54.4	126.9	54.1	127.2
	122.3	59.4	122.2	59.3	122.2
	130.2	51.9	129.4	51.8	129.4
	129.5	53.1	128.2	53.1	128.1
	120.9	61.2	120.3	61.1	120.4
	125.9	55.6	125.8	55.7	125.6
	121.7	59.7	121.8	59.3	122.1
	129.5	52.6	128.7	52.8	128.4
	129.5	53.0	128.3	52.8	128.4
	122.3	58.7	122.7	58.8	122.6
	126.9	54.9	126.5	54.9	126.4
	126.9	53.0	128.3	53.1	128.2
	123.8	57.4	124.0	57.4	124.0
	129.8	52.1	129.1	52.1	129.2
HXACAN26[†]	152.3	28.4	152.1	28.2	152.2
	116.4	66.6	115.2	65.4	116.3
	120.6	61.1	120.4	60.9	120.6
	133.1	50.8	130.5	50.6	130.5
	123.4	58.3	123.2	58.6	122.8
	115.7	65.6	116.1	67.4	114.4
	169.8	10.6	169.2	10.2	169.5
	23.8	160.8	24.2	160.7	24.3
INDMET	167.7	10.1	169.8	10.5	169.3
	136.7	49.0	132.1	49.0	132.1
	134.4	48.3	132.8	48.2	132.9
	129.2	51.0	130.3	50.9	130.3
	140.3	36.8	144.0	36.6	144.1
	127.0	54.7	126.6	54.6	126.7
	132.0	48.3	132.9	48.5	132.6
	13.7	169.0	16.1	169.1	16.1
	28.2	154.3	30.3	154.6	30.1
	179.2	-4.7	184.0	-4.6	183.9
	138.0	43.3	137.7	42.6	138.3
	55.2	128.4	55.4	128.8	55.1
	112.6	68.7	113.1	68.9	112.9

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Table S2 – *Continued from previous page*

Crystal	**Exp. Shifts** Isotropic (ppm)	**2bd 6 Å Fragment** Absolute Shieldings	Predicted Shifts	**Cluster/Fragment** Absolute Shieldings	Predicted Shifts
	131.1	51.3	129.9	51.2	130.0
	97.9	84.8	97.5	85.2	97.2
	156.7	24.7	155.7	24.9	155.4
	112.6	70.2	111.7	70.8	111.0
	115.7	65.9	115.8	65.7	116.0
	131.1	52.1	129.2	52.4	128.9
SULAMD06	127.1	57.3	124.1	57.1	124.3
	129.5	51.2	130.0	51.4	129.8
	117.1	67.4	114.4	67.5	114.3
	153.4	29.8	150.7	30.0	150.5
	112.3	71.5	110.4	71.5	110.4
	129.5	49.4	131.8	49.8	131.3
ADENOS12	154.8	26.2	154.2	26.0	154.3
	148.5	34.6	146.1	34.4	146.3
	119.7	62.3	119.3	62.0	119.6
	155.2	28.4	152.1	28.3	152.1
	137.8	42.9	138.1	43.2	137.7
	92.3	90.3	92.2	90.1	92.4
	71.2	107.8	75.3	107.8	75.3
	75.0	111.8	71.5	111.6	71.6
	84.9	97.9	84.9	97.9	84.9
	62.7	121.0	62.6	121.0	62.6
PERYTO10	50.2	133.4	50.5	133.3	50.7
	58.4	125.4	58.3	125.2	58.5

[†]Previously the ^{13}C benchmark set used structures optimized from HXACAN09,[1] but HXACAN26 was used here instead. The former experimental structure was determined at 1 GPa of pressure while the latter was done at ambient pressure which is consistent with the NMR experiments.

Table S3: Comparison of experimental, absolute and predicted isotropic ^{15}N chemical shifts for the 2-body fragment and combined cluster/2-body models with SCRMP charge embedding using the PBE0 density functional (in ppm). The predicted chemical shifts can be obtained from the absolute shieldings using the linear regression parameters reported in this work. All shifts are reported relative to NH_4Cl with $NH_3(l)$ at 39.3 ppm.

Crystal	**Exp. Shifts** Isotropic (ppm)	**2bd 6 Å Fragment** Absolute Shieldings	Predicted Shifts	**Cluster/Fragment** Absolute Shieldings	Predicted Shifts
BITZAF	249.5	-46.8	244.8	-45.9	242.6
GEHHAD	261.8	-66.0	264.1	-65.9	262.6
	253.6	-50.6	248.6	-50.2	246.9
GEHHEH	187.4	19.4	177.9	18.4	178.3

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Table S3 – *Continued from previous page*

Crystal	**Exp. Shifts** Isotropic (ppm)	**2bd 6 Å Fragment** Absolute Shieldings	Predicted Shifts	**Cluster/Fragment** Absolute Shieldings	Predicted Shifts
	261.0	-55.5	253.5	-54.9	251.6
GEHHIL	268.5	-72.4	270.6	-71.6	268.3
	261.2	-61.2	259.3	-61.3	257.9
LHISTD02	210.8	-14.9	212.5	-13.8	210.5
	132.6	58.7	138.2	59.0	137.7
LHISTD13	210.6	-15.0	212.6	-14.2	210.9
	132.4	58.4	138.4	58.4	138.4
TEJWAG	143.9	50.7	146.2	50.9	145.9
GLYCIN03	-6.5	203.3	-8.0	207.0	-10.1
FUSVAQ01	183.2	16.3	181.0	16.3	180.4
	174.2	25.9	171.3	25.2	171.5
	192.2	5.4	192.0	7.4	189.3
	120.2	73.2	123.5	70.5	126.2
	50.2	148.2	47.7	146.4	50.5
CYTSIN	110.2	81.3	115.3	82.2	114.6
	165.2	34.3	162.8	35.6	161.1
	54.2	139.8	56.2	142.8	54.0
THYMIN01	90.2	101.7	94.6	102.1	94.7
	119.2	75.6	121.0	75.9	120.9
URACIL	96.2	91.3	105.2	91.5	105.3
	120.2	74.5	122.2	74.9	121.9
CIMETD	130.5	61.3	135.5	61.5	135.2
	213.1	-16.2	213.8	-15.9	212.6
	56.6	137.5	58.5	137.4	59.5
	43.5	151.2	44.6	151.7	45.1
	45.8	156.7	39.1	156.4	40.4
	149.9	49.5	147.5	49.1	147.6
BAPLOT01	114.7	74.7	122.0	74.5	122.3
	72.7	118.5	77.7	118.5	78.3
	122.7	71.0	125.7	70.6	126.2
	178.7	18.6	178.7	20.4	176.4
Structure 1	223.4	-22.1	219.8	-27.9	224.6
	202.5	-2.0	199.5	-9.6	206.3
	76.4	122.1	74.1	116.0	80.8
	285.1	-87.0	285.4	-93.8	290.4
	81.5	117.7	78.5	111.5	85.3
LTYRHC10	8.0	189.2	6.2	192.0	4.8
CYSCLM11	1.5	194.6	0.8	197.3	-0.4
LSERIN01	-4.1	201.5	-6.2	204.0	-7.1
GLUTAM01	-1.3	198.4	-3.1	200.7	-3.8
	72.1	119.6	76.6	122.5	74.4
ASPARM03	0.7	197.4	-2.0	199.8	-2.9
	74.9	117.8	78.4	121.0	75.8
LCYSTN21	-0.4	200.3	-5.0	201.7	-4.9
ALUCAL04	3.0	195.5	-0.1	197.0	-0.2
GLYHCL01	-1.7	199.3	-4.0	201.1	-4.2
LGLUAC11	-0.4	197.9	-2.6	200.1	-3.2

Table S4: Comparison of experimental, absolute and predicted isotropic ^{17}O chemical shifts for the 2-body fragment and combined cluster/2-body models with SCRMP charge embedding using the PBE0 density functional (in ppm). The predicted chemical shifts can be obtained from the absolute shieldings using the linear regression parameters reported in this work. All shifts are reported relative to liquid H_2O.

	Exp. Shifts	**2bd 6 Å Fragment**		**Cluster/Fragment**	
Crystal	Isotropic (ppm)	Absolute Shieldings	Predicted Shifts	Absolute Shieldings	Predicted Shifts
LALNIN12	285	-27.1	298.9	-23.8	296.6
	268	-3.1	273.6	-3.0	274.8
ALAHCL	327.8	-54.8	328.0	-54.1	328.3
	176.7	83.7	182.4	83.4	184.3
VALEHC11	351	-67.9	341.8	-68.8	343.7
	181	65.9	201.1	68.6	199.8
LTYRHC10	327	-57.8	331.1	-54.6	328.8
	183	83.4	182.7	84.7	183.0
	83	185.1	75.8	185.2	77.7
CYTSIN	230	55.9	211.6	50.4	218.9
ACANIL03	330	-49.7	322.6	-48.9	322.9
BZAMID07	300	-17.5	288.8	-18.8	291.4
GLYHCL01	336	-68.5	342.4	-66.1	340.9
	185	88.7	177.1	88.7	178.8
LGLUTA03	172.5	87.4	178.5	90.1	177.3
	322	-35.7	307.9	-35.3	308.7
	315	-28.5	300.3	-26.7	299.6
	187	77.3	189.1	79.5	188.4
MBNZAM10	287	-14.3	285.4	-13.2	285.5
FEQYUW	183.1	81.3	184.9	85.4	182.3
	342.7	-71.3	345.3	-70.1	345.0
LILEUC10	182.6	77.7	188.6	83.0	184.8
	347.1	-82.4	357.0	-82.2	357.8
PHALNC01	353.5	-75.9	350.2	-79.9	355.3
	178.8	79.5	186.8	83.1	184.7
CYSCLM11	174.9	78.4	188.0	84.4	183.3
	353.5	-78.0	352.4	-74.3	349.5
TPEPHO02	45	223.0	35.9	224.8	36.2

2 ^{17}O Isotropic shieldings for γ-Glycine

Table S5 provides the absolute shieldings along with the predicted ^{17}O isotropic chemical shifts for γ-glycine (in ppm) using each functional/model combination investigated in the paper.

Table S5: Absolute shieldings and predicted ^{17}O isotropic chemical shifts for γ-glycine (in ppm).

	Site O1		**Site O2**	
Functional/Method	Absolute Shielding	Chemical Shift	Absolute Shielding	Chemical Shift
PBE/GIPAW	-35.10	285.73	-28.12	278.29
PBE/Fragment	-21.66	285.16	-36.17	301.32
PBE/Cluster/Fragment	-20.65	286.78	-16.62	282.29
PBE0/Fragment	-13.15	282.06	-22.01	291.21
PBE0/Cluster/Fragment	-12.45	284.00	-5.18	276.48

3 Optimized γ-Glycine crystal structure

This section provides the fractional coordinates for the optimized GLYCIN34 crystal structure. The crystal structure was optimized with lattice parameters fixed at their experimental values.

```
O       1.006930389   0.550926531   1.005137642
O       0.981506158   0.219150722   0.987582393
C       1.001794262   0.392917313   0.890530341
H       1.205796308   0.532527784   0.574799610
H       0.934989498   0.486499507   0.536046429
C       1.031875042   0.418418242   0.614084264
N       0.968633132   0.207800372   0.492257551
H       0.979372964   0.224979626   0.299519575
H       1.068570215   0.145885686   0.548832143
H       0.804416521   0.096146049   0.538822871
```

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