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Supplementary Information

The equilibrium molecular structures of 2-deoxyribose and fructose by the semiexperimental mixed estimation method and coupled-cluster computations

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Table S1. Observed rotational transitions of fructose (ν_{obs}) and residuals ($\nu_{obs}-\nu_{calc}$) of the fit of Table S3 (^{18}O6 species), all values in MHz.

J′	*Ka′*	*Kc′*	*J″*	*Ka″*	*Kc″*	ν_{obs}	$\nu_{obs}-\nu_{calc}$
5	2	3	4	1	3	9097.689	0.001
4	4	0	3	3	0	10846.481	0.000
3	3	1	2	2	1	7957.144	-0.001
6	2	4	5	1	4	10656.749	0.000
4	2	3	3	1	3	8276.063	0.000
3	3	0	2	2	0	7933.932	0.002
3	2	1	2	1	1	6297.825	0.004
4	2	2	3	1	2	7653.897	0.000
4	3	2	3	2	2	9378.194	0.001
4	3	1	3	2	1	9271.084	0.000
5	3	2	4	2	2	10557.744	0.000
6	3	3	5	2	3	11811.065	0.001
5	4	1	4	3	1	12221.652	0.000
4	4	1	3	3	1	10848.864	0.001
6	4	2	5	3	2	13574.387	0.000
6	4	3	5	3	3	13634.508	-0.002
5	5	0	4	4	0	13749.327	0.000
5	5	1	4	4	1	13749.524	-0.002
6	1	6	5	1	5	7622.944	-0.001
6	0	6	5	0	5	7687.622	0.000

Table S2. Ground state rotational parameters of the isotopologues of deoxyribose (c-β-2-deoxy-D-ribopyranose, $^{1}C_{4}$-1 conformer) [a].

		Parent	^{13}C1	^{13}C2	^{13}C3	^{13}C4	^{13}C5	^{18}O6
A	MHz	2437.82519(13)	2432.6910(11)	2417.5851(11)	2428.91157(33)	2428.0033(29)	2410.4359(26)	2408.8515(21)
B	MHz	1510.728846(86)	1499.57261(13)	1508.36532(13)	1507.072715(39)	1505.32554(45)	1507.65494(30)	1495.28173(15)
C	MHz	1144.979958(82)	1139.153854(80)	1141.809999(90)	1141.768500(27)	1141.29514(20)	1139.73939(23)	1131.440878(75)
Δ_J	kHz	0.1067(10)	0.10540(19)	0.10606(95)	0.10654(27)	0.1064(11)	0.1048(20)	0.10224(12)
Δ_{JK}	kHz	-0.04349(42)	-0.043138(78)	-0.04221(38)	-0.04076(10)	0.3285(70)	0.3196(64)	0.30068(36)
Δ_K	kHz	0.3304(31)	0.33019(59)	0.3214(29)	0.32221(84)	-0.04547(48)	-0.04038(81)	-0.025270(30)
δ_J	kHz	0.01959(19)	0.019109(34)	0.01906(17)	0.019554(51)	0.01945(20)	0.01930(38)	0.018545(22)
δ_K	kHz	0.08343(81)	0.08220(14)	0.08150(74)	0.08469(22)	0.08159(86)	0.0823(16)	0.08621(10)

[a] This work, A-reduction, representation I^{r}.

Table S3. Ground state rotational parameters of the isotopologues of fructose (cc-β-D-fructopyranose, $^{2}C_{5}$ conformer)[a,b].

	A / MHz	B / MHz	C / MHz	Δ_J / kHz	Δ_{JK} / kHz	Δ_K / kHZ	δ_J / kHz	δ_K kHz
Parent	1 465.277876(82)	770.569989(50)	609.969040(48)	0.01858(16)	0.03115(28)	0.04752(43)	0.003177(28)	0.02417(22)
^{13}C1	1 461.73951(15)	764.21815(11)	606.47487(29)	0.01827(15)	0.02989(25)	0.04871(84)	0.003086(26)	0.02327(19)
^{13}C2	1 465.32193(13)	769.505785(98)	609.30340(25)	0.01855(26)	0.03086(44)	0.04808(69)	0.003172(45)	0.02399(34)
^{13}C3	1 461.35556(11)	770.379640(85)	609.36049(26)	0.01851(19)	0.03130(33)	0.04700(50)	0.003170(34)	0.02420(26)
^{13}C4	1 463.46908(13)	767.830223(93)	608.23584(16)	0.01832(31)	0.03196(54)	0.04610(78)	0.003127(53)	0.02431(41)
^{13}C5	1 460.57051(13)	767.00406(12)	607.07390(17)	0.01846(33)	0.02937(53)	0.04916(88)	0.003204(57)	0.02349(42)
^{13}C6	1 450.301268(80)	769.811572(69)	607.56700(10)	0.01847(19)	0.03018(31)	0.04582(47)	0.003193(33)	0.02404(25)
D_R-C2	1 450.487053(77)	762.129587(66)	607.20816(32)	0.01824(11)	0.02766(17)	0.04806(30)	0.002982(18)	0.02145(13)
D_S-C2	1 454.38676(21)	762.80239(18)	604.4125(10)	0.01796(31)	0.02729(47)	0.04931(85)	0.003065(53)	0.02191(38)
^{18}O6	1 450.793946(72)	769.50226(10)	606.801863(90)	0.01832(25)	0.03297(46)	0.04037(56)	0.003156(44)	0.02499(35)

[a] This work, A-reduction, representation I^{r}.

[b] For definition of labeling R and S for hydrogen atoms, see Fig. 1.

Table S4. DFT and *ab initio* structures of deoxyribose (in Å and degrees)

Method[a]	B3LYP	MP2	MP2	MP2	MP2_AE	MP2	CCSD	CCSD(T)
Basis set	6-311[b]	cc-pVTZ	6-311[b]	cc-pwCVTZ	cc-pwCVTZ	cc-pVQZ	cc-pVTZ	cc-pVTZ
C1C2	1.5255	1.5168	1.5177	1.5155	1.5123	1.5150	1.5205	1.5224
C1O6	1.4212	1.4207	1.4181	1.4194	1.4170	1.4177	1.4149	1.4224
C1O1	1.4106	1.4070	1.4054	1.4060	1.4036	1.4050	1.4043	1.4093
C1H1	1.0922	1.0905	1.0913	1.0903	1.0890	1.0897	1.0905	1.0925
C2C3	1.5340	1.5252	1.5252	1.5239	1.5207	1.5229	1.5285	1.5301
C2H2q	1.0886	1.0879	1.0884	1.0875	1.0861	1.0870	1.0883	1.0904
C2H2x	1.0917	1.0906	1.0910	1.0902	1.0888	1.0897	1.0916	1.0939
C3C4	1.5343	1.5238	1.5245	1.5224	1.5193	1.5219	1.5270	1.5290
C3O3	1.4167	1.4158	1.4137	1.4146	1.4122	1.4134	1.4122	1.4177
C3H3	1.0908	1.0897	1.0906	1.0895	1.0881	1.0891	1.0900	1.0924
C4C5	1.5204	1.5130	1.5141	1.5116	1.5084	1.5113	1.5167	1.5197
C4O4	1.4305	1.4281	1.4248	1.4270	1.4245	1.4250	1.4246	1.4305
C4H4	1.0910	1.0897	1.0906	1.0896	1.0882	1.0892	1.0898	1.0917
C5O6	1.4321	1.4310	1.4289	1.4299	1.4273	1.4283	1.4266	1.4339
C5H5q	1.0883	1.0872	1.0876	1.0869	1.0855	1.0863	1.0877	1.0896
C5H5x	1.0925	1.0909	1.0915	1.0905	1.0891	1.0902	1.0913	1.0935
O3H3	0.9651	0.9664	0.9650	0.9657	0.9649	0.9645	0.9620	0.9658
O4H4	0.9635	0.9655	0.9643	0.9648	0.9640	0.9636	0.9610	0.9649
O1H1	0.9625	0.9635	0.9623	0.9629	0.9620	0.9617	0.9596	0.9629
C2C1O6	111.78	111.64	111.58	111.67	111.66	111.63	111.70	111.59
C2C1O1	108.23	107.51	107.53	107.50	107.53	107.57	107.79	107.68
C2C1H1	111.01	111.39	111.47	111.39	111.35	111.43	111.03	111.25
O1C1O6	111.53	111.64	111.51	111.64	111.63	111.56	111.51	111.53
O1C1H1	103.84	103.76	103.91	103.76	103.79	103.81	104.09	103.93
H1C1O1	110.45	110.94	110.89	110.93	110.92	110.89	110.74	110.90
C1C2C3	112.34	111.66	111.50	111.67	111.68	111.73	111.72	112.12
C1C2H2q	109.78	109.84	109.89	109.81	109.82	109.84	109.78	109.84
C1C2H2x	108.13	108.41	108.40	108.42	108.44	108.37	108.35	108.18
C3C2H2q	110.10	110.25	110.22	110.24	110.23	110.19	110.26	109.84
C3C2H2x	109.00	108.76	108.89	108.79	108.79	108.81	108.87	110.20
H2qC2H2x	107.35	107.82	107.85	107.81	107.78	107.80	107.74	108.63
C2C3C4	110.29	109.52	109.51	109.55	109.55	109.61	109.69	110.03
O3C3C2	111.48	111.27	111.30	111.30	111.31	111.27	111.36	111.16
H3C3C2	109.45	109.77	109.83	109.75	109.73	109.79	109.56	109.62
C4C3O3	110.98	110.48	110.63	110.51	110.51	110.63	110.67	110.44
C4C3H3	108.31	108.97	108.86	108.93	108.90	108.82	108.74	108.74
O3C3H3	106.20	106.77	106.65	106.74	106.77	106.65	106.75	106.78
C3C4C5	109.97	109.95	109.76	109.94	109.94	109.81	109.89	109.85
O4C4C3	110.19	109.50	109.66	109.53	109.55	109.68	109.73	109.52
H4C4C3	109.27	109.51	109.49	109.50	109.46	109.48	109.46	109.60
C5C4O4	111.57	110.86	110.95	110.90	110.92	111.00	110.98	110.75
C5C4H4	109.96	110.56	110.55	110.53	110.50	110.44	110.31	110.60
O4C4H4	105.78	106.40	106.37	106.38	106.41	106.36	106.40	106.46
C4C5C6	110.60	109.82	109.77	109.84	109.86	109.92	110.07	109.88
C4C5H5q	110.79	110.72	110.78	110.74	110.73	110.77	110.60	110.69
C4C5H5x	110.16	110.44	110.34	110.42	110.41	110.30	110.30	110.41
O6C5H5q	105.83	105.75	105.79	105.75	105.80	105.77	105.96	105.79
O6C5H5x	110.45	110.60	110.56	110.59	110.60	110.56	110.61	110.52
H5C5H5x	108.92	109.43	109.51	109.41	109.36	109.44	109.22	109.45
C1O6C5	113.86	112.04	112.46	112.07	112.10	112.34	112.80	112.38

C3O3H3	106.94	104.80	105.71	104.87	104.96	105.45	105.66	104.98
C4O4H4	108.15	105.83	106.58	105.88	105.98	106.42	106.73	106.02
C1O1H1	108.56	107.18	107.78	107.21	107.31	107.57	107.58	107.21
C3C2C1O6	-50.33	-52.79	-52.76	-52.71	-52.70	-52.47	-52.15	-51.59
O6C1C2H2q	-173.19	-175.42	-175.27	-175.31	-175.30	-175.06	-174.79	-174.47
O6C1C2H2X	69.99	66.99	67.09	67.13	67.17	67.41	67.79	68.17
O1C1C2C3	72.87	69.98	69.82	70.06	70.08	70.23	70.69	71.11
O1C1C2H2q	-49.98	-52.65	-52.70	-52.54	-52.52	-52.36	-51.95	-51.77
O1C1C2H2x	-166.80	-170.23	-170.33	-170.09	-170.06	-169.89	-169.38	-169.12
H1C1C2C3	-165.77	-168.28	-168.45	-168.22	-168.21	-168.03	-167.85	-167.17
H1C1C2H2q	71.38	69.09	69.04	69.18	69.19	69.37	69.51	69.95
H1C1C2H2x	-45.44	-48.49	-48.60	-48.37	-48.35	-48.16	-47.92	-47.41
C2C1O6C5	56.83	59.23	59.00	59.14	59.08	58.79	58.65	58.94
O1C1O6C5	-64.49	-61.15	-61.27	-61.24	-61.33	-61.59	-62.04	-61.54
H1C1O6C5	176.57	179.31	179.23	179.23	179.14	178.94	178.53	178.92
C2C1O1H1	175.38	175.91	175.45	176.02	175.98	175.57	176.05	176.33
O6C1O1H1	-61.27	-61.32	-61.92	-61.19	-61.23	-61.69	-61.00	-60.93
H1C1O1H1	53.67	53.89	53.36	54.01	54.00	53.50	54.41	54.40
C1C2C3C4	48.83	50.20	50.65	50.16	50.21	50.26	49.87	48.95
O3C3C2C1	172.59	172.64	173.29	172.67	172.73	172.94	172.72	171.61
H3C3C2C1	-70.23	-69.39	-68.84	-69.39	-69.31	-69.22	-69.43	-70.58
H2qC2C3C4	171.51	172.60	172.98	172.52	172.57	172.66	172.24	171.62
H2qC2C3O3	-64.74	-64.96	-64.38	-64.98	-64.90	-64.66	-64.91	-65.72
H2qC2C3H3	52.44	53.00	53.48	52.96	53.06	53.18	52.95	52.09
Hx2C2C3C4	-70.99	-69.38	-68.91	-69.46	-69.45	-69.36	-69.76	-70.56
H2xC2C3O3	52.76	53.06	53.73	53.04	53.07	53.32	53.09	52.11
H2xC2C3H3	169.94	171.02	171.60	170.98	171.03	171.16	170.95	169.92
C2C3C4C5	-52.23	-53.71	-54.12	-53.70	-53.72	-53.77	-53.25	-52.69
O4C4C3C2	71.16	68.32	68.00	68.39	68.40	68.47	69.04	69.15
H4C4C3C2	-173.02	-175.37	-175.64	-175.31	-175.28	-175.18	-174.54	-174.40
O3C3C4C5	-176.28	-176.62	-177.16	-176.67	-176.72	-176.83	-176.51	-175.78
O3C3C4O4	-52.88	-54.59	-55.03	-54.58	-54.60	-54.59	-54.21	-53.93
O3C3C4H4	62.94	61.72	61.32	61.71	61.72	61.76	62.21	62.52
H3C3C4C5	67.52	66.38	65.97	66.36	66.30	66.31	66.55	67.37
H3C3C4O4	-169.08	-171.59	-171.91	-171.55	-171.57	-171.45	-171.16	-170.78
H3C3C4H4	-53.27	-55.28	-55.55	-55.25	-55.26	-55.10	-54.74	-54.34
C2C3O3H3	-80.63	-78.36	-77.74	-78.35	-78.40	-78.40	-78.67	-79.31
C4C3O3H3	42.73	43.52	44.26	43.61	43.57	43.70	43.62	43.11
H3C3O3H3	160.23	161.88	162.49	161.91	161.86	161.89	161.79	161.17
C3C4C5O6	57.84	59.88	59.77	59.85	59.82	59.73	59.13	59.54
C3C4C5H5q	174.87	176.28	176.23	176.28	176.31	176.25	175.88	176.03
C3C4C5H5x	-64.55	-62.35	-62.32	-62.37	-62.42	-62.43	-63.19	-62.62
O4C4C5O6	-64.74	-61.34	-61.58	-61.43	-61.49	-61.72	-62.42	-61.57
O4C4C5H5q	52.29	55.07	54.88	55.00	55.01	54.80	54.32	54.92
O4C4C5H5x	172.87	176.43	176.33	176.35	176.27	176.12	175.26	176.27
H4C4C5O6	178.21	-179.09	-179.35	-179.15	-179.24	-179.43	179.92	-179.35
H4C4C5H5q	-64.76	-62.68	-62.88	-62.72	-62.75	-62.91	-63.34	-62.86
H4C4C5H5x	55.82	58.68	58.56	58.62	58.51	58.40	57.59	58.49
H4O4C4C3	-86.07	-86.16	-86.09	-86.04	-86.14	-86.31	-86.15	-85.34
C5C4O4H4	36.39	35.32	35.32	35.48	35.39	35.21	35.50	35.96
H4C4O4H4	155.94	155.58	155.60	155.70	155.62	155.38	155.52	156.24
C4C5O6C1	-61.12	-62.90	-62.66	-62.84	-62.78	-62.66	-62.38	-63.26
C1O6C5H5q	178.83	177.61	177.78	177.63	177.66	177.72	178.01	177.22

C1O6C5H5x	61.10	59.24	59.30	59.28	59.34	59.35	59.76	58.83

[a] Frozen core, unless otherwise specified.
[b] 6-311+G(3df,2pd).

Table S5. DFT and *ab initio* structures of fructose (in Å and degrees)

Method	MP2[a]	MP2[a]	B3LYP	CCSD[a]
Basis set	cc-pVTZ	6-311[b]	6-311[b]	cc-pVTZ
O1H1'	0.9648	0.9633	0.9633	0.9607
C1O1	1.4221	1.4192	1.4223	1.4180
C2C1	1.5182	1.5198	1.5304	1.5213
$H1_SC1$	1.0858	1.0863	1.0870	1.0866
$H1_RC1$	1.0904	1.0908	1.0914	1.0911
O6C2	1.4122	1.4094	1.4137	1.4073
H2'O2	0.9698	0.9685	0.9676	0.9640
C3C2	1.5210	1.5238	1.5365	1.5251
O3C3	1.4216	1.4186	1.4220	1.4175
H3'O3	0.9670	0.9658	0.9655	0.9625
H3C3	1.0888	1.0899	1.0897	1.0888
C4C3	1.5183	1.5194	1.5297	1.5221
O4C4	1.4206	1.4180	1.4220	1.4166
H4'O4	0.9655	0.9643	0.9639	0.9609
H4C4	1.0950	1.0961	1.0959	1.0949
O2C2	1.4118	1.4093	1.4145	1.4084
C6O6	1.4267	1.4245	1.4277	1.4224
$H6_SC6$	1.0866	1.0871	1.0874	1.0869
$H6_RC6$	1.0921	1.0926	1.0930	1.0925
C5C6	1.5135	1.5140	1.5203	1.5170
O5C5	1.4152	1.4131	1.4175	1.4127
H5'O5	0.9660	0.9645	0.9643	0.9614
H5C5	1.0961	1.0969	1.0975	1.0958
C2C1O1H1'	-64.71	-65.83	-68.07	-65.36
$H1_SC1O1H1'$	176.56	175.41	172.93	175.71
$H1_RC1O1H1'$	56.33	55.10	53.51	55.80
O2C2C1O1	-52.00	-52.27	-50.91	-52.79
H2'O2C2C1	35.31	35.76	35.21	36.40
C3C2C1O1	-170.94	-171.17	-169.99	-171.78
O3C3C2C1	63.87	64.49	65.63	64.33
H3'O3C3C2	46.57	46.62	46.51	46.87
H3C3C2C1	-53.98	-53.29	-51.39	-53.37
C4C3C2C1	-173.18	-172.66	-170.60	-172.48
O4C4C3C2	173.99	173.85	173.19	173.72
H4'O4C4C3	43.29	44.42	44.43	43.89
H4C4C3C2	-64.39	-64.50	-65.88	-64.83
O6C2C1O1	68.43	68.30	69.52	67.63
C6O6C2C1	179.65	179.93	178.08	179.64
$H6_SC6O6C2$	-177.60	-177.86	-176.75	-177.46
$H6_RC6O6C2$	64.32	63.94	65.68	64.53
C5C6O6C2	-57.93	-58.17	-56.78	-57.72
O5C5C6O6	-66.40	-66.26	-69.27	-67.10
H5'O5C5C6	165.22	166.75	166.76	166.13
H5C5C6O6	172.98	173.27	170.92	172.51
C1O1H1'	105.70	106.50	107.72	106.37
C2C1O1	109.07	109.21	110.02	109.38
$H1_SC1O1$	107.12	107.06	106.81	107.21
$H1_RC1O1$	111.95	111.90	111.61	111.82
O2C2C1	109.60	109.94	109.76	109.75
H2'O2C2	104.81	105.60	106.72	105.79

C3C2C1	113.53	113.25	113.08	113.17
O3C3C2	111.81	111.76	112.04	111.82
H3'O3C3	105.08	105.84	107.06	105.93
H3C3C2	108.65	108.72	108.33	108.50
C4C3C2	110.11	109.99	110.79	110.34
O4C4C3	110.38	110.57	110.78	110.49
H4'O4C4	105.89	106.79	107.80	106.63
H4C4C3	108.73	108.70	108.61	108.71
O6C2C1	104.61	104.71	105.06	104.91
C6O6C2	113.93	114.31	115.93	114.69
$H6_SC6O6$	105.60	105.64	105.62	105.81
$H6_RC6O6$	110.16	110.14	110.06	110.15
C5C6O6	112.39	112.08	112.67	112.40
O5C5C6	108.98	108.78	109.23	108.95
H5'O5C5	105.24	106.12	107.09	106.00
H5C5C6	108.34	108.53	108.15	108.35

[a] Frozen core approximation.
[b] 6-311+G(3df,2pd).

Table S6. Cartesian coordinates in the principal axis system for deoxyribose (in Å).

atom	a_e^{SE}	b_e^{SE}	c_e^{SE}	r_e^{SE} [a]
O6 ring	-1.2422(10)	-1.0522(12)	-0.4195(19)	1.68110(70)
C1	-1.45958(89)	0.3398(13)	-0.58329(92)	1.60810(90)
O1	-2.1560(14)	0.8846(14)	0.5114(15)	2.3859(13)
H1′	-3.0083(22)	0.4446(35)	0.5610(40)	3.0923(23)
H1	-2.0481(46)	0.4107(39)	-1.4986(27)	2.5709(24)
C2	-0.1533(13)	1.1008(11)	-0.7225(12)	1.3256(10)
H2x	0.3080(38)	0.8208(42)	-1.6702(28)	1.8863(33)
H2q	-0.3515(38)	2.1700(13)	-0.7535(48)	2.3239(18)
C3	0.8155(11)	0.7727(13)	0.4097(13)	1.1958(11)
O3	2.0856(15)	1.3531(10)	0.1843(16)	2.4929(13)
H3′	2.5227(32)	0.7819(36)	-0.4565(35)	2.6802(31)
H3	0.4397(37)	1.1896(46)	1.3438(23)	1.8478(29)
C4	0.9289(11)	-0.7380(13)	0.5619(13)	1.3127(11)
O4	1.6090(24)	-1.2791(15)	-0.5690(16)	2.1328(20)
H4′	0.9425(46)	-1.4310(42)	-1.2464(30)	2.1189(40)
H4	1.5440(39)	-0.9701(38)	1.4309(29)	2.3179(17)
C5	-0.4465(17)	-1.3500(11)	0.7166(15)	1.5923(10)
H5q	-0.3808(42)	-2.4346(13)	0.7532(43)	2.5767(17)
H5x	-0.9215(41)	-0.9878(41)	1.6295(34)	2.1166(32)

[a] Distance from the center of mass.

Table S7. Cartesian coordinates in the principal axis system for fructose (in Å).

Atom	a_e^{SE}	b_e^{SE}	c_e^{SE}	r_e^{SE} [a]
H1'	-3.1014(35)	-1.3135(27)	-0.3608(46)	3.3874(32)
O1	-3.2958(16)	-0.3726(27)	-0.3188(26)	3.3321(16)
C1	-2.1681(13)	0.2937(26)	-0.8651(14)	2.3527(13)
C2	-0.9647(12)	0.0638(14)	0.0312(19)	0.9673(12)
$H1_S$	-2.4036(22)	1.3528(28)	-0.8940(38)	2.8994(18)
$H1_R$	-1.9384(23)	-0.0541(54)	-1.8741(14)	2.6968(19)
O2	-1.2842(32)	0.4178(45)	1.3599(20)	1.9165(26)
H2'	-2.2059(35)	0.1557(62)	1.4876(36)	2.6651(24)
C3	0.2483(14)	0.8935(19)	-0.3594(26)	0.9945(19)
O3	0.0062(32)	2.2834(19)	-0.2082(39)	2.2929(20)
H3'	-0.4009(54)	2.3882(43)	0.6592(49)	2.5098(35)
H3	0.4606(42)	0.7202(44)	-1.4131(31)	1.6516(30)
C4	1.4606(21)	0.4739(29)	0.4531(33)	1.6010(19)
O4	2.6236(21)	1.1421(31)	-0.0100(48)	2.8614(18)
H4'	2.3757(46)	2.0615(28)	-0.1493(69)	3.1490(31)
H4	1.2751(51)	0.7074(75)	1.5066(26)	2.0967(33)
O6	-0.6783(18)	-1.3109(12)	-0.0980(22)	1.4792(14)
C6	0.4324(16)	-1.7637(22)	0.6738(25)	1.9369(19)
$H6_S$	0.5505(40)	-2.8167(23)	0.4331(53)	2.9025(21)
$H6_R$	0.2177(49)	-1.6591(55)	1.7395(24)	2.4137(36)
C5	1.7037(16)	-1.0154(19)	0.3352(26)	2.0115(20)
O5	2.0900(29)	-1.3397(31)	-0.9864(28)	2.6714(25)
H5'	2.7559(42)	-0.6902(46)	-1.2353(51)	3.0980(36)
H5	2.4800(27)	-1.3132(53)	1.0494(43)	2.9960(27)

[a] Distance from the center of mass.

Table S8. Substitution coordinates of fructose compared to the equilibrium Cartesian coordinates (all values in Å).

	Substitution[a]			r_e^{SE}		
	$\|a\|$	$\|b\|$	$\|c\|$	a_e	b_e	c_e
C1	2.1672(7)	0.2822(53)	0.8750(17)	-2.1681	0.2937	-0.8651
C2	0.9557(16)	*i*[b]	*i*[b]	-0.9647	0.0638	0.0312
C3	0.1781(84)	0.8925(17)	0.3625(41)	0.2483	0.8935	-0.3594
C4	1.4627(10)	0.4744(32)	0.4525(33)	1.4606	0.4739	0.4531
C5	1.7149(9)	1.0090(15)	0.3259(46)	1.7037	-1.0154	0.3352
C6	0.4225(36)	1.7595(9)	0.6897(22)	0.4324	-1.7637	0.6738
O6 ring	0.6685(22)	1.3171(11)	0.0863(174)	-0.6783	-1.3109	-0.0980
$H1_R$	1.9305(17)	0.1016(315)	1.8793(17)	-1.9384	-0.0541	-1.8741
$H1_S$	2.4102(13)	1.3357(24)	0.9165(35)	-2.4036	1.3528	-0.8940

[a] The uncertainties are calculated using Costain's rule: $\delta z = C/|z|$ with $C = 0.0015$ Å^2 for heavy atoms and $C = 0.0032$ Å^2 for hydrogen atoms.[1]
[b] Imaginary value.

(1) Rudolph, H. D.; Demaison, J., In *Equilibrium Molecular Structures: From Spectroscopy to Quantum Chemistry*, Demaison, J.; Boggs, J. E.; Császár, A. G., Eds. CRS Press: Boca Raton, 2011; pp 125-158.

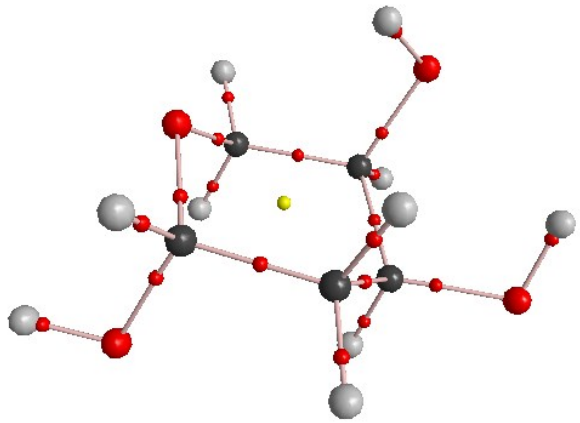

Fig. S1. Molecular graph for deoxyribose