

Enaminone substituted resorcin[4]arene – a scaffold with hydrogen-bond based motif for upper-rim sealing

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ELECTRONIC SUPPLEMENTARY INFORMATION

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Figure S1. Variable temperature ^1H NMR spectra of compound **4** (DMSO- d_6 , temperature range 303-343 K).

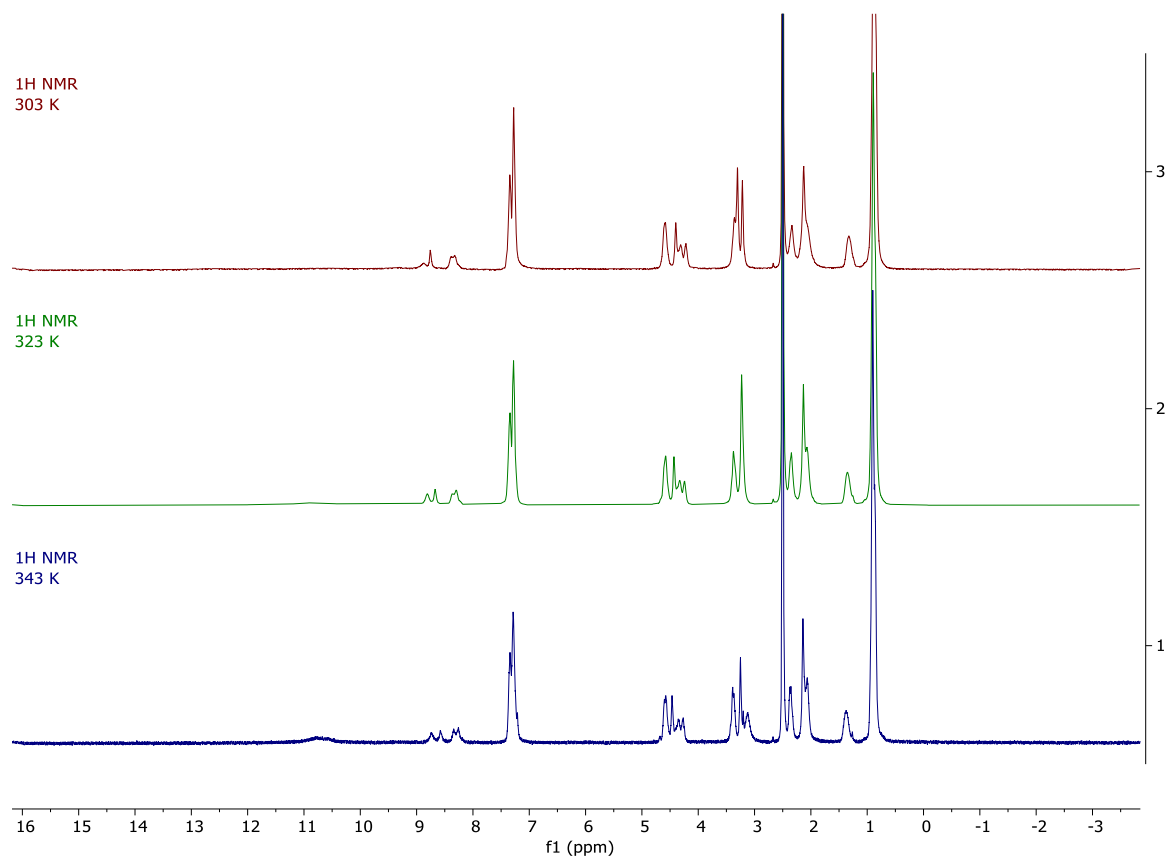


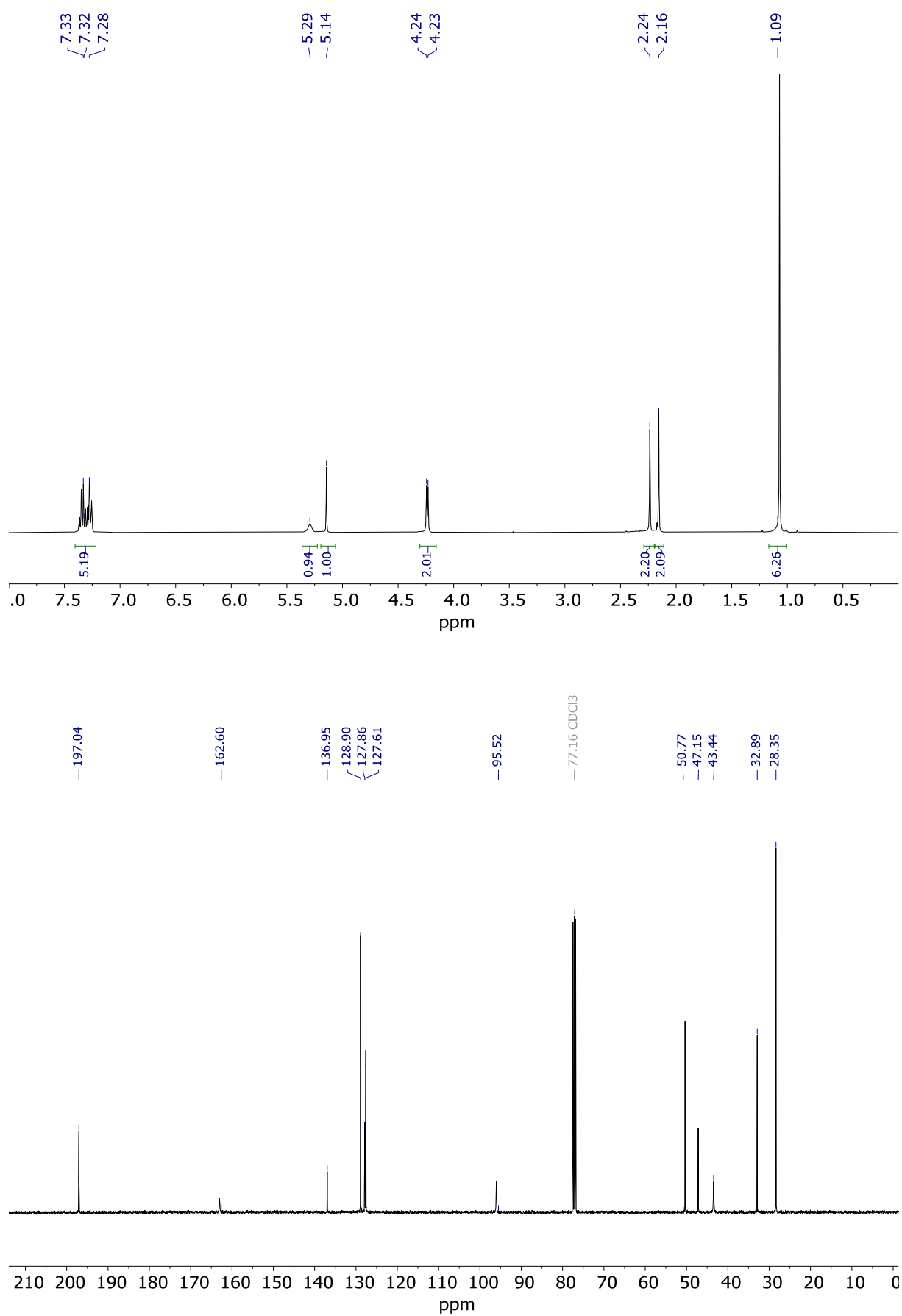
Figure 2. ^1H and ^{13}C NMR spectrum of compound **2** in CDCl_3 at 298 K

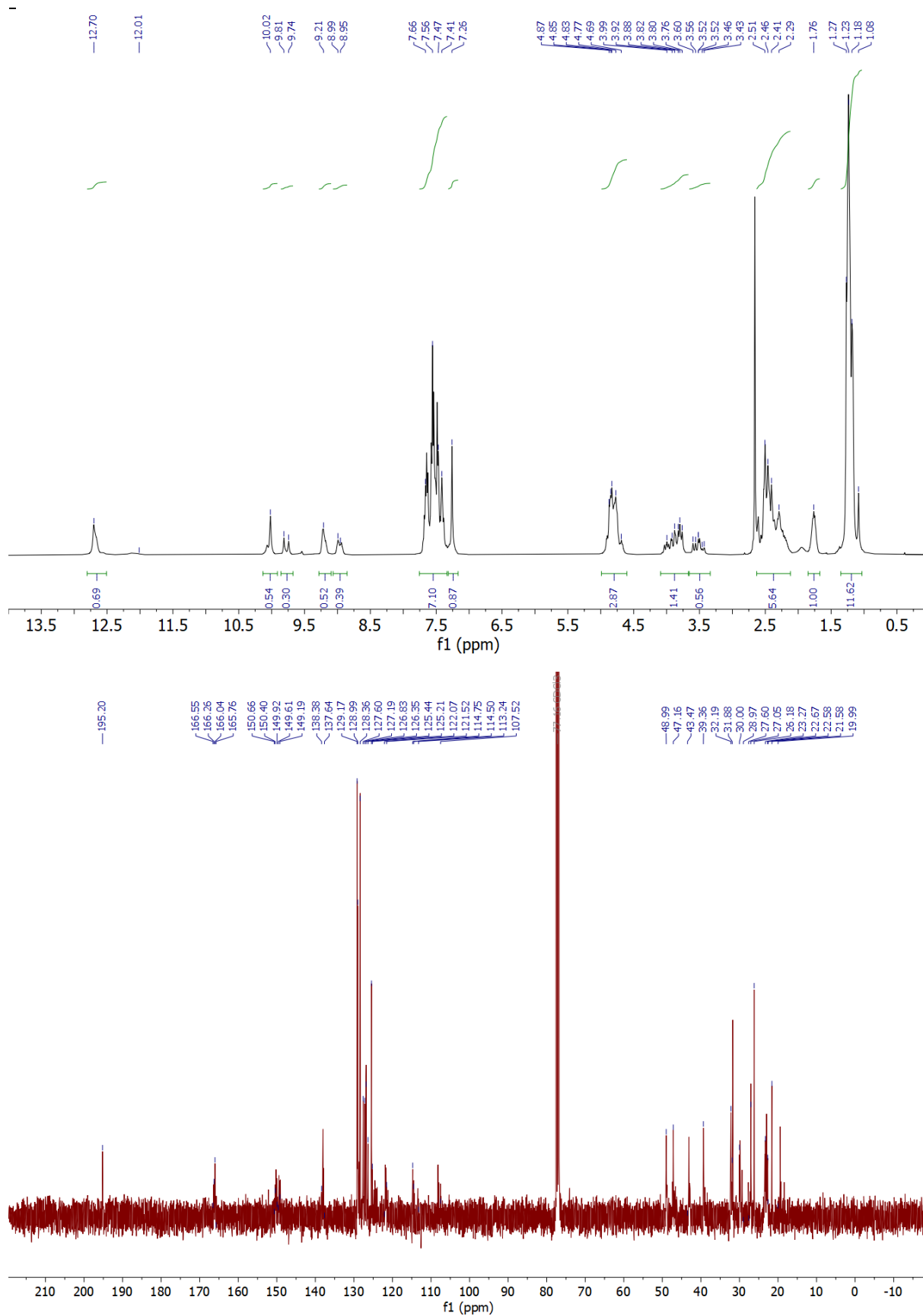
Figure 3. ^1H and ^{13}C NMR spectrum of compound **4** in CDCl_3 at 298 K

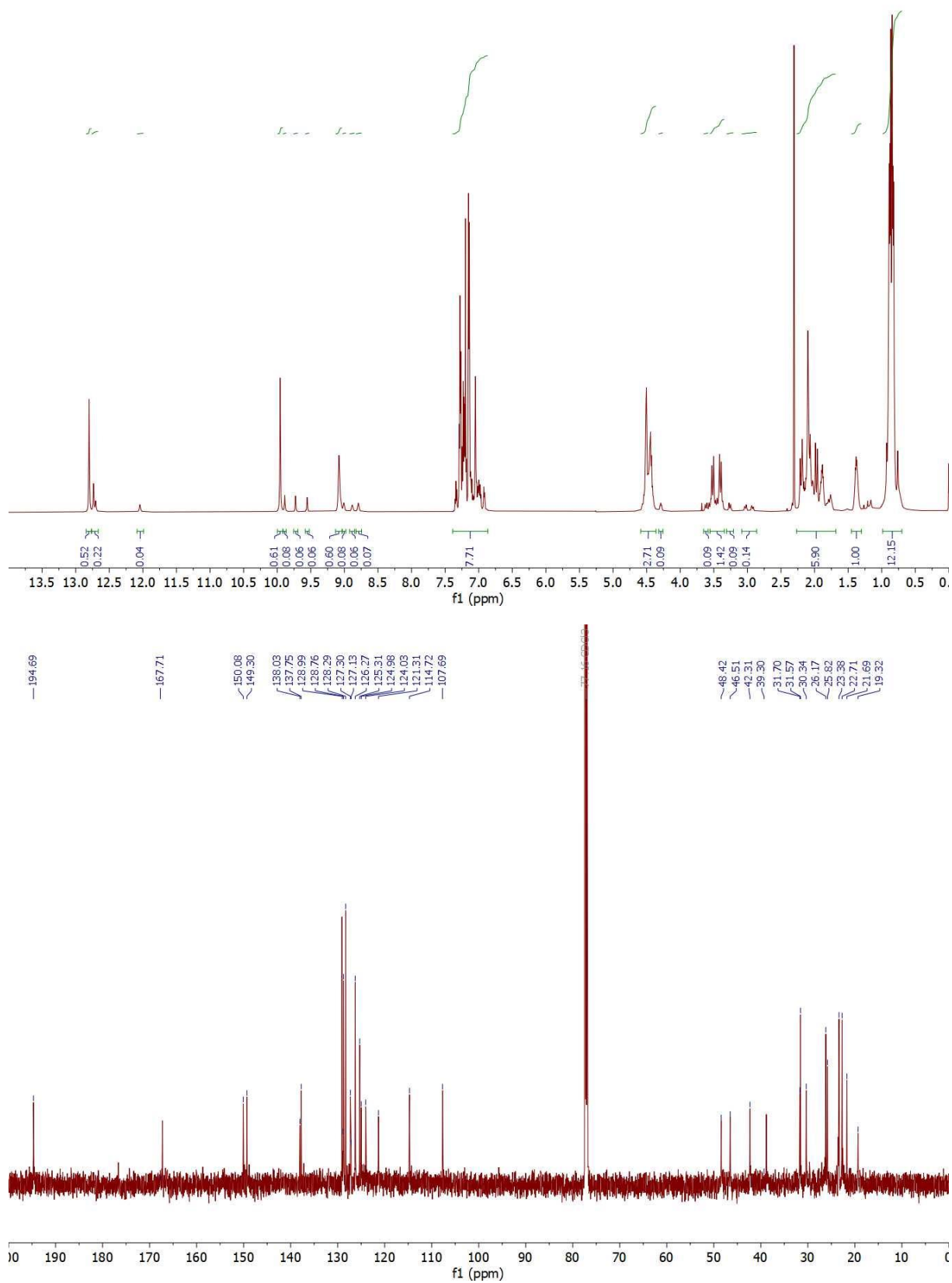
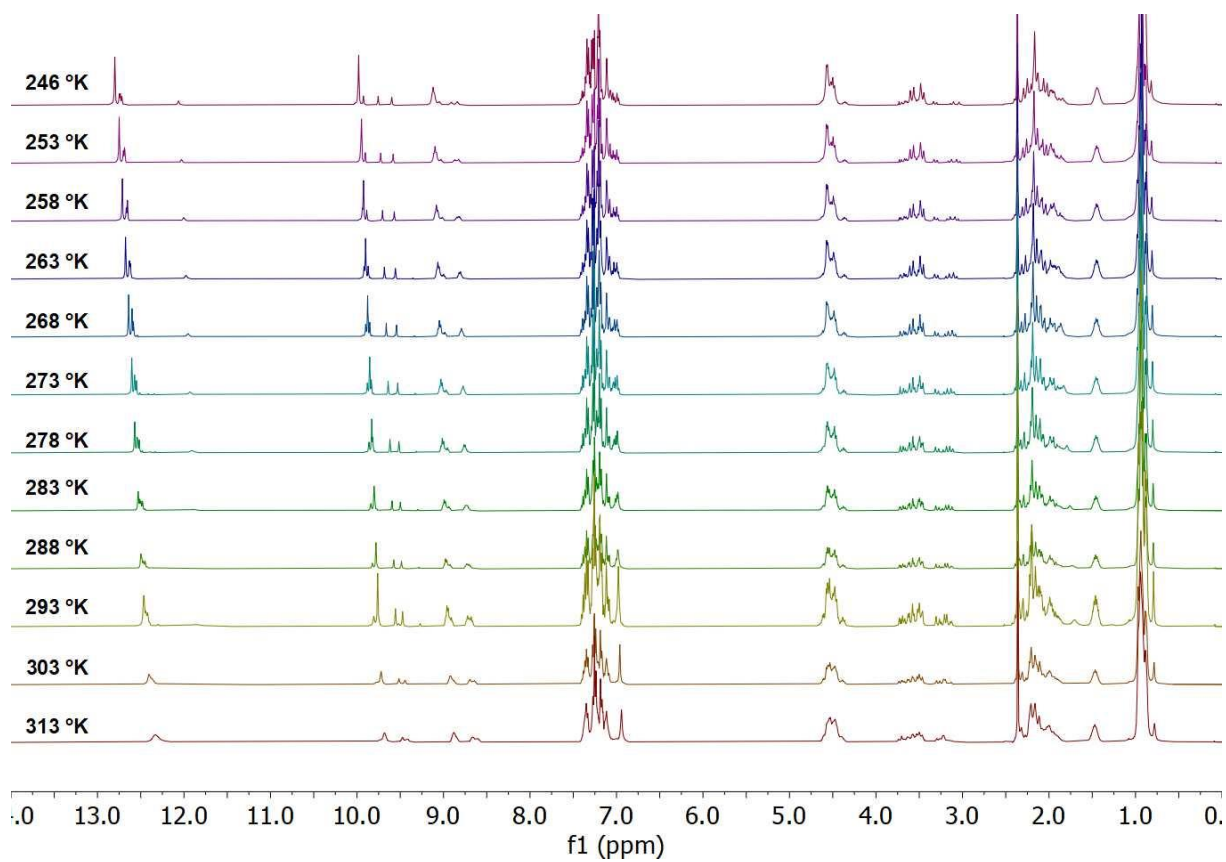
Figure 4. ^1H and ^{13}C NMR spectrum of compound **4** in CDCl_3 at 233 K

Figure 5. Variable temperature ^1H NMR spectra of compound **4** (in CDCl_3 , temperature range 246-313 K).



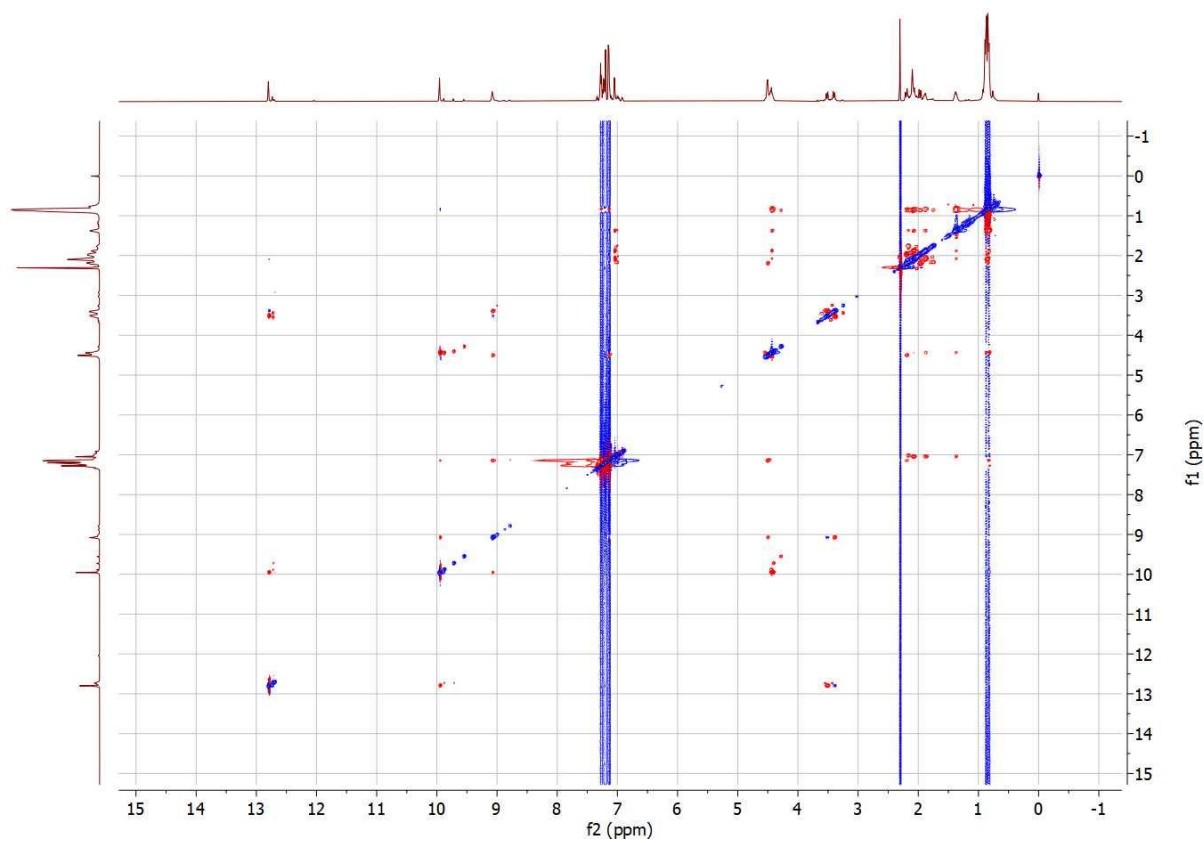
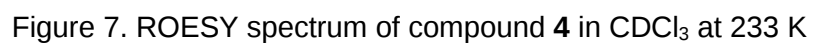


Figure 8. MS spectrum of compound **4**

Elements Used:

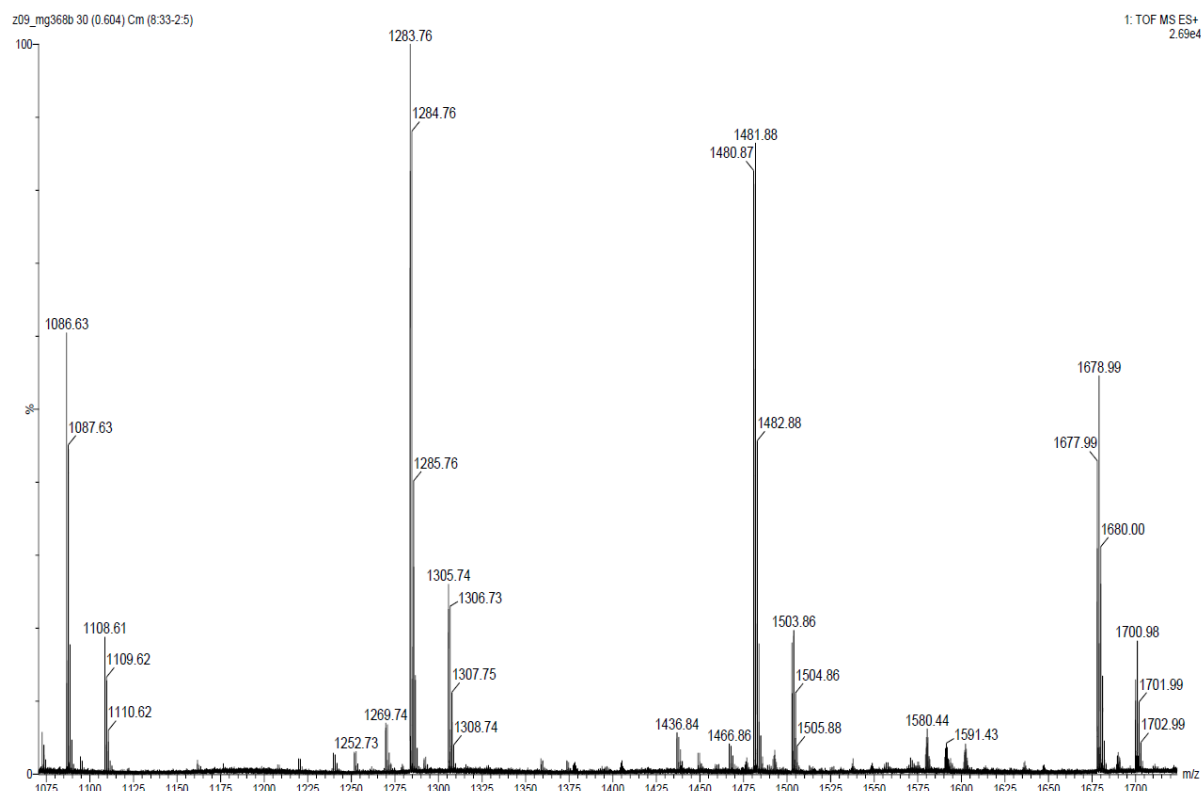
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8. DFT/B3LYP calculations

Atomic coordinates for all calculated geometries:

C₂ in chloroform

Energy total = -5317.11813806 a.u.

Symbol	X	Y	Z
C	-1.3491330	-2.9464780	2.1570030
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C	2.6046110	-0.0982320	2.6737750
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O	-2.2610350	4.1940890	0.4369670
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C₄ crown-*in* in chloroform

Energy total = -5317.12025046 a.u.

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C	1.1564500	3.9027730	1.4515960
C	2.4307770	3.6405550	0.9150080
C	3.1705140	2.5736440	1.4559150
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C	1.4442800	2.1533100	3.0617880
O	0.3713690	4.9042180	0.9274550
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C	-3.5509730	-0.7047140	3.1594640
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C	3.5427410	0.7569650	4.7121040
H	4.5864780	0.9097300	2.8735870
C	0.7569650	-3.5427410	4.7121040
H	0.9097300	-4.5864780	2.8735870
C	-3.5427410	-0.7569650	4.7121040
H	-4.5864780	-0.9097300	2.8735870
H	-1.8083380	3.4279210	5.0000740
H	-0.2374540	2.6689830	5.1250880
C	-0.2285540	4.8172850	5.4057050
H	3.4279210	1.8083380	5.0000740
H	2.6689830	0.2374540	5.1250880
C	4.8172850	0.2285540	5.4057050
H	1.8083380	-3.4279210	5.0000740
H	0.2374540	-2.6689830	5.1250880
C	0.2285540	-4.8172850	5.4057050
H	-3.4279210	-1.8083380	5.0000740
H	-2.6689830	-0.2374540	5.1250880
C	-4.8172850	-0.2285540	5.4057050
H	-0.9097300	4.5864780	2.8735870
C	-3.0460950	-4.5625830	-0.1339210
H	0.5830230	5.0480130	-0.0517280
H	5.0480130	-0.5830230	-0.0517280
H	1.3730540	-4.6326780	0.9730320
H	-0.5830230	-5.0480130	-0.0517280
H	-4.6326780	-1.3730540	0.9730320
H	-5.0480130	0.5830230	-0.0517280
O	4.4169470	2.3349290	0.9169050
C	-4.5625830	3.0460950	-0.1339210
H	-1.3730540	4.6326780	0.9730320
C	3.0460950	4.5625830	-0.1339210
H	4.6326780	1.3730540	0.9730320
C	-4.2363990	2.8717840	-1.6135060
C	-3.6238490	3.8773380	-2.3718280
C	-4.6590670	1.6705930	-2.2465820
O	-5.1903280	0.7155070	-1.6088910
C	2.8717840	4.2363990	-1.6135060
C	3.8773380	3.6238490	-2.3718280
C	1.6705930	4.6590670	-2.2465820
O	0.7155070	5.1903280	-1.6088910
C	4.5625830	-3.0460950	-0.1339210
C	4.2363990	-2.8717840	-1.6135060
C	4.6590670	-1.6705930	-2.2465820
O	5.1903280	-0.7155070	-1.6088910
C	3.6238490	-3.8773380	-2.3718280
C	-2.8717840	-4.2363990	-1.6135060
C	-1.6705930	-4.6590670	-2.2465820
O	-0.7155070	-5.1903280	-1.6088910
C	-3.8773380	-3.6238490	-2.3718280
H	-2.6217020	-5.5600500	0.0218880
H	-4.1130490	-4.6583730	0.0864900
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H	2.6217020	5.5600500	0.0218880
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H	5.5600500	-2.6217020	0.0218880
H	4.6583730	-4.1130490	0.0864900
C	1.2706670	5.0744470	5.1965020
C	-0.5559270	4.7664570	6.9066130
C	-4.7664570	-0.5559270	6.9066130
C	-5.0744470	1.2706670	5.1965020
C	0.5559270	-4.7664570	6.9066130
C	-1.2706670	-5.0744470	5.1965020
C	4.7664570	0.5559270	6.9066130
C	5.0744470	-1.2706670	5.1965020
H	-0.7769240	5.6691200	4.9754290

H	5.6691200	0.7769240	4.9754290
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H	-5.6691200	-0.7769240	4.9754290
H	1.5249530	5.1945230	4.1409210
H	1.8694970	4.2434120	5.5883760
H	1.5794160	5.9842970	5.7239360
H	-0.0382320	3.9299260	7.3924790
H	-1.6302090	4.6385440	7.0794780
H	-0.2409190	5.6866480	7.4106190
H	-3.9299260	-0.0382320	7.3924790
H	-4.6385440	-1.6302090	7.0794780
H	-5.6866480	-0.2409190	7.4106190
H	-5.1945230	1.5249530	4.1409210
H	-4.2434120	1.8694970	5.5883760
H	-5.9842970	1.5794160	5.7239360
H	0.0382320	-3.9299260	7.3924790
H	1.6302090	-4.6385440	7.0794780
H	0.2409190	-5.6866480	7.4106190
H	-1.5249530	-5.1945230	4.1409210
H	-1.8694970	-4.2434120	5.5883760
H	-1.5794160	-5.9842970	5.7239360
H	3.9299260	0.0382320	7.3924790
H	4.6385440	1.6302090	7.0794780
H	5.6866480	0.2409190	7.4106190
H	5.1945230	-1.5249530	4.1409210
H	4.2434120	-1.8694970	5.5883760
H	5.9842970	-1.5794160	5.7239360
C	4.4539920	-1.4727240	-3.7370080
H	5.2308580	-0.7878660	-4.0923870
H	3.4934930	-0.9527660	-3.8688850
C	1.4727240	4.4539920	-3.7370080
H	0.7878660	5.2308580	-4.0923870
H	0.9527660	3.4934930	-3.8688850
C	-4.4539920	1.4727240	-3.7370080
H	-5.2308580	0.7878660	-4.0923870
H	-3.4934930	0.9527660	-3.8688850
C	-1.4727240	-4.4539920	-3.7370080
H	-0.7878660	-5.2308580	-4.0923870
H	-0.9527660	-3.4934930	-3.8688850
C	-2.7789170	-4.4512080	-4.5472530
C	-3.7492150	-3.4628010	-3.8708800
H	-3.4189590	-2.4306860	-4.0611220
H	-4.7334320	-3.5509120	-4.3401860
C	-4.4512080	2.7789170	-4.5472530
C	-3.4628010	3.7492150	-3.8708800
H	-2.4306860	3.4189590	-4.0611220
H	-3.5509120	4.7334320	-4.3401860
C	2.7789170	4.4512080	-4.5472530
C	3.7492150	3.4628010	-3.8708800
H	3.4189590	2.4306860	-4.0611220
H	4.7334320	3.5509120	-4.3401860
C	4.4512080	-2.7789170	-4.5472530
C	3.4628010	-3.7492150	-3.8708800
H	2.4306860	-3.4189590	-4.0611220
H	3.5509120	-4.7334320	-4.3401860
C	5.8654600	-3.3928670	-4.5857980
H	5.8675850	-4.3229070	-5.1648550
H	6.5701320	-2.7020560	-5.0608260
H	6.2401860	-3.6186180	-3.5834440
C	3.9860310	-2.5038800	-5.9870180
H	2.9845830	-2.0597460	-6.0049780
H	4.6704900	-1.8122280	-6.4899020
H	3.9558170	-3.4283020	-6.5745390
C	-3.3928670	-5.8654600	-4.5857980
H	-4.3229070	-5.8675850	-5.1648550
H	-2.7020560	-6.5701320	-5.0608260
H	-3.6186180	-6.2401860	-3.5834440
C	-2.5038800	-3.9860310	-5.9870180
H	-2.0597460	-2.9845830	-6.0049780
H	-1.8122280	-4.6704900	-6.4899020
H	-3.4283020	-3.9558170	-6.5745390
C	-5.8654600	3.3928670	-4.5857980
H	-5.8675850	4.3229070	-5.1648550
H	-6.5701320	2.7020560	-5.0608260
H	-6.2401860	3.6186180	-3.5834440
C	-3.9860310	2.5038800	-5.9870180

H	-2.9845830	2.0597460	-6.0049780
H	-4.6704900	1.8122280	-6.4899020
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C	3.3928670	5.8654600	-4.5857980
H	4.3229070	5.8675850	-5.1648550
H	2.7020560	6.5701320	-5.0608260
H	3.6186180	6.2401860	-3.5834440
C	2.5038800	3.9860310	-5.9870180
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N	-3.1382420	4.9816550	-1.7789860
N	-4.9816550	-3.1382420	-1.7789860
N	3.1382420	-4.9816550	-1.7789860
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H	4.9221210	3.0045330	-0.7677160
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H	-4.9221210	-3.0045330	-0.7677160
H	3.0045330	-4.9221210	-0.7677160
C	2.4307770	-6.1047690	-2.4072250
H	1.3775310	-5.8424450	-2.5565330
H	2.8771080	-6.3105120	-3.3832150
C	6.1047690	2.4307770	-2.4072250
H	5.8424450	1.3775310	-2.5565330
H	6.3105120	2.8771080	-3.3832150
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H	-2.8771080	6.3105120	-3.3832150
C	-6.1047690	-2.4307770	-2.4072250
H	-5.8424450	-1.3775310	-2.5565330
H	-6.3105120	-2.8771080	-3.3832150
C	2.5290610	-7.3448770	-1.5399080
C	1.3889980	-7.8670580	-0.9187250
C	3.7620030	-7.9856330	-1.3515420
C	1.4785340	-9.0148220	-0.1262890
H	0.4343780	-7.3679400	-1.0571400
C	3.8526060	-9.1291140	-0.5594510
H	4.6530620	-7.5837380	-1.8272100
C	2.7085800	-9.6474830	0.0547800
H	0.5870190	-9.4103900	0.3516490
H	4.8129730	-9.6177780	-0.4225120
H	2.7785330	-10.5388020	0.6714740
C	7.3448770	2.5290610	-1.5399080
C	7.8670580	1.3889980	-0.9187250
C	7.9856330	3.7620030	-1.3515420
C	9.0148220	1.4785340	-0.1262890
H	7.3679400	0.4343780	-1.0571400
C	9.1291140	3.8526060	-0.5594510
H	7.5837380	4.6530620	-1.8272100
C	9.6474830	2.7085800	0.0547800
H	9.4103900	0.5870190	0.3516490
H	9.6177780	4.8129730	-0.4225120
H	10.5388020	2.7785330	0.6714740
C	-2.5290610	7.3448770	-1.5399080
C	-1.3889980	7.8670580	-0.9187250
C	-3.7620030	7.9856330	-1.3515420
C	-1.4785340	9.0148220	-0.1262890
H	-0.4343780	7.3679400	-1.0571400
C	-3.8526060	9.1291140	-0.5594510
H	-4.6530620	7.5837380	-1.8272100
C	-2.7085800	9.6474830	0.0547800
H	-0.5870190	9.4103900	0.3516490
H	-4.8129730	9.6177780	-0.4225120
H	-2.7785330	10.5388020	0.6714740
C	-7.3448770	-2.5290610	-1.5399080
C	-7.8670580	-1.3889980	-0.9187250
C	-7.9856330	-3.7620030	-1.3515420
C	-9.0148220	-1.4785340	-0.1262890
H	-7.3679400	-0.4343780	-1.0571400
C	-9.1291140	-3.8526060	-0.5594510
H	-7.5837380	-4.6530620	-1.8272100
C	-9.6474830	-2.7085800	0.0547800
H	-9.4103900	-0.5870190	0.3516490
H	-9.6177780	-4.8129730	-0.4225120
H	-10.5388020	-2.7785330	0.6714740

C₄ crown-out in chloroform

Energy total = -5317.11776943 a.u.

Symbol	X	Y	Z
C	2.9352710	-1.4179070	1.7840410
C	3.7806720	-1.4406180	0.6585130
C	4.3073730	-0.2637120	0.0972210
C	3.9461890	0.9666730	0.6733420
C	3.0864660	1.0368290	1.7840430
C	2.5944700	-0.1634840	2.2992010
O	4.1532500	-2.6261570	0.0637710
O	4.3826880	2.1495030	0.1351320
H	1.9310410	-0.1181490	3.1568270
C	2.7217020	2.3973210	2.3883550
C	1.4179070	2.9352710	1.7840410
C	1.4406180	3.7806720	0.6585130
C	0.2637120	4.3073730	0.0972210
C	-0.9666730	3.9461890	0.6733420
C	-1.0368290	3.0864660	1.7840430
C	0.1634840	2.5944700	2.2992010
O	2.6261570	4.1532500	0.0637710
H	0.1181490	1.9310410	3.1568270
C	-2.3973210	2.7217020	2.3883550
C	-2.9352710	1.4179070	1.7840410
C	-3.7806720	1.4406180	0.6585130
C	-4.3073730	0.2637120	0.0972210
C	-3.9461890	-0.9666730	0.6733420
C	-3.0864660	-1.0368290	1.7840430
C	-2.5944700	0.1634840	2.2992010
O	-4.1532500	2.6261570	0.0637710
O	-4.3826880	-2.1495030	0.1351320
H	-1.9310410	0.1181490	3.1568270
C	-2.7217020	-2.3973210	2.3883550
C	-1.4179070	-2.9352710	1.7840410
C	-1.4406180	-3.7806720	0.6585130
C	-0.2637120	-4.3073730	0.0972210
C	0.9666730	-3.9461890	0.6733420
C	1.0368290	-3.0864660	1.7840430
C	-0.1634840	-2.5944700	2.2992010
O	-2.6261570	-4.1532500	0.0637710
O	2.1495030	-4.3826880	0.1351320
H	-0.1181490	-1.9310410	3.1568270
C	2.3973210	-2.7217020	2.3883550
C	2.7616330	2.3785190	3.9405860
C	-2.3785190	2.7616330	3.9405860
H	-3.0836260	3.5169270	2.0824970
C	-2.7616330	-2.3785190	3.9405860
H	-3.5169270	-3.0836260	2.0824970
C	2.3785190	-2.7616330	3.9405860
H	3.0836260	-3.5169270	2.0824970
H	3.5169460	1.6416090	4.2373800
H	1.8141900	2.0190560	4.3610960
C	3.1359960	3.7156710	4.6155000
H	-1.6416090	3.5169460	4.2373800
H	-2.0190560	1.8141900	4.3610960
C	-3.7156710	3.1359960	4.6155000
H	-3.5169460	-1.6416090	4.2373800
H	-1.8141900	-2.0190560	4.3610960
C	-3.1359960	-3.7156710	4.6155000
H	1.6416090	-3.5169460	4.2373800
H	2.0190560	-1.8141900	4.3610960
C	3.7156710	-3.1359960	4.6155000
H	3.5169270	3.0836260	2.0824970
C	-0.3160020	-5.1834580	-1.1469810
H	3.2980180	3.4261310	0.0842600
H	-3.4261310	3.2980180	0.0842600
H	-5.2716140	-2.0761980	-0.3543160
H	-3.2980180	-3.4261310	0.0842600
H	2.0761980	-5.2716140	-0.3543160
H	3.4261310	-3.2980180	0.0842600
O	-2.1495030	4.3826880	0.1351320
C	5.1834580	-0.3160020	-1.1469810
H	5.2716140	2.0761980	-0.3543160
C	0.3160020	5.1834580	-1.1469810
H	-2.0761980	5.2716140	-0.3543160

C	6.6972570	-0.2816520	-0.9507770
C	7.4661790	-1.4386950	-0.8232880
C	7.3393350	0.9937920	-0.9229410
O	6.6972570	2.0794810	-0.9274220
C	0.2816520	6.6972570	-0.9507770
C	1.4386950	7.4661790	-0.8232880
C	-0.9937920	7.3393350	-0.9229410
O	-2.0794810	6.6972570	-0.9274220
C	-5.1834580	0.3160020	-1.1469810
C	-6.6972570	0.2816520	-0.9507770
C	-7.3393350	-0.9937920	-0.9229410
O	-6.6972570	-2.0794810	-0.9274220
C	-7.4661790	1.4386950	-0.8232880
C	-0.2816520	-6.6972570	-0.9507770
C	0.9937920	-7.3393350	-0.9229410
O	2.0794810	-6.6972570	-0.9274220
C	-1.4386950	-7.4661790	-0.8232880
H	0.5403930	-4.9261310	-1.7786720
H	-1.2103090	-4.9132520	-1.7150090
H	4.9261310	0.5403930	-1.7786720
H	4.9132520	-1.2103090	-1.7150090
H	-0.5403930	4.9261310	-1.7786720
H	1.2103090	4.9132520	-1.7150090
H	-4.9261310	-0.5403930	-1.7786720
H	-4.9132520	1.2103090	-1.7150090
C	2.1253990	4.8464680	4.3756020
C	3.3465750	3.4985740	6.1222010
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C	-2.1253990	-4.8464680	4.3756020
C	-3.4985740	3.3465750	6.1222010
C	-4.8464680	2.1253990	4.3756020
H	4.0995240	4.0333500	4.1882810
H	-4.0333500	4.0995240	4.1882810
H	-4.0995240	-4.0333500	4.1882810
H	4.0333500	-4.0995240	4.1882810
H	2.0096510	5.0757940	3.3135700
H	1.1357410	4.5777480	4.7645310
H	2.4462560	5.7614790	4.8867050
H	2.4156670	3.1758940	6.6049330
H	4.1046430	2.7316680	6.3157680
H	3.6701110	4.4226090	6.6137030
H	3.1758940	-2.4156670	6.6049330
H	2.7316680	-4.1046430	6.3157680
H	4.4226090	-3.6701110	6.6137030
H	5.0757940	-2.0096510	3.3135700
H	4.5777480	-1.1357410	4.7645310
H	5.7614790	-2.4462560	4.8867050
H	-2.4156670	-3.1758940	6.6049330
H	-4.1046430	-2.7316680	6.3157680
H	-3.6701110	-4.4226090	6.6137030
H	-2.0096510	-5.0757940	3.3135700
H	-1.1357410	-4.5777480	4.7645310
H	-2.4462560	-5.7614790	4.8867050
H	-3.1758940	2.4156670	6.6049330
H	-2.7316680	4.1046430	6.3157680
H	-4.4226090	3.6701110	6.6137030
H	-5.0757940	2.0096510	3.3135700
H	-4.5777480	1.1357410	4.7645310
H	-5.7614790	2.4462560	4.8867050
C	-8.8519720	-1.0910720	-0.8425030
H	-9.1077980	-1.2212600	0.2196420
H	-9.1515140	-2.0161120	-1.3462980
C	-9.5982490	0.1290960	-1.4051510
C	-8.9778320	1.3881340	-0.7663490
H	-9.3912660	2.2805990	-1.2453020
H	-9.2735660	1.4427530	0.2921830
C	0.1290960	9.5982490	-1.4051510
C	1.3881340	8.9778320	-0.7663490
H	2.2805990	9.3912660	-1.2453020
H	1.4427530	9.2735660	0.2921830
C	-1.0910720	8.8519720	-0.8425030
H	-1.2212600	9.1077980	0.2196420
H	-2.0161120	9.1515140	-1.3462980
C	-1.3881340	-8.9778320	-0.7663490

H	-2.2805990	-9.3912660	-1.2453020
H	-1.4427530	-9.2735660	0.2921830
C	-0.1290960	-9.5982490	-1.4051510
C	1.0910720	-8.8519720	-0.8425030
H	1.2212600	-9.1077980	0.2196420
H	2.0161120	-9.1515140	-1.3462980
C	8.8519720	1.0910720	-0.8425030
H	9.1077980	1.2212600	0.2196420
H	9.1515140	2.0161120	-1.3462980
C	9.5982490	-0.1290960	-1.4051510
C	8.9778320	-1.3881340	-0.7663490
H	9.3912660	-2.2805990	-1.2453020
H	9.2735660	-1.4427530	0.2921830
C	0.1831730	9.4713580	-2.9411390
H	-0.7128420	9.9107480	-3.3923740
H	1.0547710	9.9998170	-3.3421570
H	0.2441160	8.4282000	-3.2630920
C	0.0531140	11.0876610	-1.0296610
H	0.9262160	11.6328370	-1.4054290
H	-0.8405040	11.5504840	-1.4618990
H	0.0106380	11.2242250	0.0566350
C	9.4713580	-0.1831730	-2.9411390
H	9.9107480	0.7128420	-3.3923740
H	9.9998170	-1.0547710	-3.3421570
H	8.4282000	-0.2441160	-3.2630920
C	11.0876610	-0.0531140	-1.0296610
H	11.6328370	-0.9262160	-1.4054290
H	11.5504840	0.8405040	-1.4618990
H	11.2242250	-0.0106380	0.0566350
C	-9.4713580	0.1831730	-2.9411390
H	-9.9107480	-0.7128420	-3.3923740
H	-9.9998170	1.0547710	-3.3421570
H	-8.4282000	0.2441160	-3.2630920
C	-11.0876610	0.0531140	-1.0296610
H	-11.6328370	0.9262160	-1.4054290
H	-11.5504840	-0.8405040	-1.4618990
H	-11.2242250	0.0106380	0.0566350
C	-0.1831730	-9.4713580	-2.9411390
H	0.7128420	-9.9107480	-3.3923740
H	-1.0547710	-9.9998170	-3.3421570
H	-0.2441160	-8.4282000	-3.2630920
C	-0.0531140	-11.0876610	-1.0296610
H	-0.9262160	-11.6328370	-1.4054290
H	0.8405040	-11.5504840	-1.4618990
H	-0.0106380	-11.2242250	0.0566350
N	-6.8878370	2.6512760	-0.7100220
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N	-2.6512760	-6.8878370	-0.7100220
N	6.8878370	-2.6512760	-0.7100220
H	-5.8768870	2.6825700	-0.5717030
H	2.6825700	5.8768870	-0.5717030
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H	-2.6825700	-5.8768870	-0.5717030
C	-3.9288270	-7.5744230	-0.5470700
H	-3.8423770	-8.3820000	0.1874740
H	-4.6072210	-6.8358860	-0.1062080
C	-7.5744230	3.9288270	-0.5470700
H	-8.3820000	3.8423770	0.1874740
H	-6.8358860	4.6072210	-0.1062080
C	3.9288270	7.5744230	-0.5470700
H	3.8423770	8.3820000	0.1874740
H	4.6072210	6.8358860	-0.1062080
C	7.5744230	-3.9288270	-0.5470700
H	8.3820000	-3.8423770	0.1874740
H	6.8358860	-4.6072210	-0.1062080
C	-4.5464630	-8.1173620	-1.8300780
C	-5.3793330	-9.2420200	-1.7722560
C	-4.3427940	-7.4894400	-3.0643890
C	-6.0030380	-9.7266620	-2.9230870
H	-5.5410140	-9.7419150	-0.8200360
C	-4.9626150	-7.9749870	-4.2169660
H	-3.6930910	-6.6213600	-3.1220390
C	-5.7958150	-9.0937150	-4.1501990
H	-6.6438860	-10.6014840	-2.8615530
H	-4.7943230	-7.4778080	-5.1678940
H	-6.2764800	-9.4713190	-5.0478050

C	-8.1173620	4.5464630	-1.8300780
C	-9.2420200	5.3793330	-1.7722560
C	-7.4894400	4.3427940	-3.0643890
C	-9.7266620	6.0030380	-2.9230870
H	-9.7419150	5.5410140	-0.8200360
C	-7.9749870	4.9626150	-4.2169660
H	-6.6213600	3.6930910	-3.1220390
C	-9.0937150	5.7958150	-4.1501990
H	-10.6014840	6.6438860	-2.8615530
H	-7.4778080	4.7943230	-5.1678940
H	-9.4713190	6.2764800	-5.0478050
C	4.5464630	8.1173620	-1.8300780
C	5.3793330	9.2420200	-1.7722560
C	4.3427940	7.4894400	-3.0643890
C	6.0030380	9.7266620	-2.9230870
H	5.5410140	9.7419150	-0.8200360
C	4.9626150	7.9749870	-4.2169660
H	3.6930910	6.6213600	-3.1220390
C	5.7958150	9.0937150	-4.1501990
H	6.6438860	10.6014840	-2.8615530
H	4.7943230	7.4778080	-5.1678940
H	6.2764800	9.4713190	-5.0478050
C	8.1173620	-4.5464630	-1.8300780
C	9.2420200	-5.3793330	-1.7722560
C	7.4894400	-4.3427940	-3.0643890
C	9.7266620	-6.0030380	-2.9230870
H	9.7419150	-5.5410140	-0.8200360
C	7.9749870	-4.9626150	-4.2169660
H	6.6213600	-3.6930910	-3.1220390
C	9.0937150	-5.7958150	-4.1501990
H	10.6014840	-6.6438860	-2.8615530
H	7.4778080	-4.7943230	-5.1678940
H	9.4713190	-6.2764800	-5.0478050

C₂ in DMSO

Energy total = -5317.13125737 a.u.

Symbol	X	Y	Z
C	1.4239220	2.9068970	2.1341880
C	1.4362780	3.6866290	0.9623980
C	0.2542870	4.1602900	0.3654790
C	-0.9713690	3.8425870	0.9768720
C	-1.0317090	3.0589210	2.1449050
C	0.1732930	2.5968680	2.6782980
O	2.6121530	4.0422840	0.3456260
O	-2.1569170	4.2502830	0.4270500
H	0.1337230	1.9868180	3.5745310
C	-2.3884880	2.7214600	2.7759800
C	-2.9580980	1.4284580	2.1731210
C	-3.8501290	1.4673380	1.0842980
C	-4.3804090	0.2980980	0.5111740
C	-3.9868410	-0.9423550	1.0448650
C	-3.1091660	-1.0268660	2.1415040
C	-2.6027620	0.1664850	2.6599610
O	-4.2870300	2.6701850	0.5677300
H	-1.9132120	0.1084810	3.4961190
C	-2.7365070	-2.3913540	2.7376330
C	-1.4239220	-2.9068970	2.1341880
C	-1.4362780	-3.6866290	0.9623980
C	-0.2542870	-4.1602900	0.3654790
C	0.9713690	-3.8425870	0.9768720
C	1.0317090	-3.0589210	2.1449050
C	-0.1732930	-2.5968680	2.6782980
O	-2.6121530	-4.0422840	0.3456260
O	2.1569170	-4.2502830	0.4270500
H	-0.1337230	-1.9868180	3.5745310
C	2.3884880	-2.7214600	2.7759800
C	2.9580980	-1.4284580	2.1731210
C	3.8501290	-1.4673380	1.0842980
C	4.3804090	-0.2980980	0.5111740
C	3.9868410	0.9423550	1.0448650
C	3.1091660	1.0268660	2.1415040
C	2.6027620	-0.1664850	2.6599610
O	4.2870300	-2.6701850	0.5677300
O	4.4791330	2.1175920	0.5299250

H	1.9132120	-0.1084810	3.4961190
C	2.7365070	2.3913540	2.7376330
C	-2.3447310	2.7510870	4.3275560
C	-2.7915830	-2.3827300	4.2894540
H	-3.5222070	-3.0857430	2.4254360
C	2.3447310	-2.7510870	4.3275560
H	3.0655730	-3.5314150	2.4883450
C	2.7915830	2.3827300	4.2894540
H	3.5222070	3.0857430	2.4254360
H	-1.5893220	3.4898810	4.6192190
H	-1.9985280	1.7937220	4.7360950
C	-3.6638430	3.1478120	5.0249680
H	-3.5608180	-1.6589780	4.5825110
H	-1.8549910	-2.0096760	4.7216730
C	-3.1538380	-3.7292390	4.9524910
H	1.5893220	-3.4898810	4.6192190
H	1.9985280	-1.7937220	4.7360950
C	3.6638430	-3.1478120	5.0249680
H	3.5608180	1.6589780	4.5825110
H	1.8549910	2.0096760	4.7216730
C	3.1538380	3.7292390	4.9524910
H	-3.0655730	3.5314150	2.4883450
C	5.3994320	-0.3777920	-0.6196980
H	-3.5375980	3.3180110	0.5626090
H	-3.3202740	-3.3607520	0.4635900
H	2.0785030	-5.0476050	-0.2033990
H	3.5375980	-3.3180110	0.5626090
H	4.7741910	2.0270080	-0.4410310
H	3.3202740	3.3607520	0.4635900
O	-4.4791330	-2.1175920	0.5299250
C	0.3082970	4.8849350	-0.9736750
H	-2.0785030	5.0476050	-0.2033990
C	-5.3994320	0.3777920	-0.6196980
H	-4.7741910	-2.0270080	-0.4410310
C	0.2264430	6.4081840	-1.0010340
C	1.3624120	7.2275350	-0.9884870
C	-1.0608320	7.0028360	-1.1122570
O	-2.1279630	6.3220280	-1.0352720
C	-4.8866640	0.2758090	-2.0545960
C	-4.5971450	1.4051840	-2.8313760
C	-4.7993950	-1.0237280	-2.6309380
O	-5.0118440	-2.0769700	-1.9623820
C	-0.3082970	-4.8849350	-0.9736750
C	-0.2264430	-6.4081840	-1.0010340
C	1.0608320	-7.0028360	-1.1122570
O	2.1279630	-6.3220280	-1.0352720
C	-1.3624120	-7.2275350	-0.9884870
C	4.8866640	-0.2758090	-2.0545960
C	4.7993950	1.0237280	-2.6309380
O	5.0118440	2.0769700	-1.9623820
C	4.5971450	-1.4051840	-2.8313760
H	5.9702560	-1.3028620	-0.5044570
H	6.1198260	0.4351530	-0.4819450
H	-0.5241070	4.5173880	-1.5835130
H	1.2239610	4.5714200	-1.4815980
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H	-6.1198260	-0.4351530	-0.4819450
H	0.5241070	-4.5173880	-1.5835130
H	-1.2239610	-4.5714200	-1.4815980
C	-4.8196430	2.1640270	4.7926210
C	-3.4196450	3.3384680	6.5301570
C	3.3780920	3.5241020	6.4588890
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C	3.4196450	-3.3384680	6.5301570
C	4.8196430	-2.1640270	4.7926210
C	-3.3780920	-3.5241020	6.4588890
C	-2.1279630	-4.8464450	4.7136160
H	-3.9670710	4.1220330	4.6118290
H	-4.1099580	-4.0563960	4.5159960
H	3.9670710	-4.1220330	4.6118290
H	4.1099580	4.0563960	4.5159960
H	-5.0729020	2.0703550	3.7337250
H	-4.5638190	1.1637330	5.1626440
H	-5.7176890	2.4963440	5.3256230
H	-3.1120120	2.3955490	6.9990390
H	-2.6322510	4.0764380	6.7190060

H	-4.3287270	3.6790400	7.0375630
H	2.4545140	3.1939150	6.9503970
H	4.1464560	2.7672730	6.6513190
H	3.6947590	4.4552220	6.9412200
H	2.0036190	5.0700720	3.6511290
H	1.1444110	4.5680010	5.1111610
H	2.4418960	5.7675780	5.2176240
H	3.1120120	-2.3955490	6.9990390
H	2.6322510	-4.0764380	6.7190060
H	4.3287270	-3.6790400	7.0375630
H	5.0729020	-2.0703550	3.7337250
H	4.5638190	-1.1637330	5.1626440
H	5.7176890	-2.4963440	5.3256230
H	-2.4545140	-3.1939150	6.9503970
H	-4.1464560	-2.7672730	6.6513190
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H	-2.0036190	-5.0700720	3.6511290
H	-1.1444110	-4.5680010	5.1111610
H	-2.4418960	-5.7675780	5.2176240
C	1.2126410	-8.5000020	-1.2903890
H	1.3713470	-8.9311650	-0.2908170
H	2.1355140	-8.6775710	-1.8524350
C	0.0070140	-9.1778790	-1.9598830
C	-1.2605360	-8.7216750	-1.2102480
H	-2.1441880	-9.0739480	-1.7504600
H	-1.2982840	-9.2063500	-0.2232900
C	-3.6231120	-0.0729630	-4.6941320
C	-4.2535140	1.2805500	-4.3012490
H	-3.5724380	2.0833100	-4.5964680
H	-5.1785360	1.4292760	-4.8764400
C	-4.5020250	-1.1903220	-4.1083940
H	-5.4677510	-1.2102520	-4.6346790
H	-4.0451670	-2.1745200	-4.2533150
C	4.2535140	-1.2805500	-4.3012490
H	3.5724380	-2.0833100	-4.5964680
H	5.1785360	-1.4292760	-4.8764400
C	3.6231120	0.0729630	-4.6941320
C	4.5020250	1.1903220	-4.1083940
H	5.4677510	1.2102520	-4.6346790
H	4.0451670	2.1745200	-4.2533150
C	-1.2126410	8.5000020	-1.2903890
H	-1.3713470	8.9311650	-0.2908170
H	-2.1355140	8.6775710	-1.8524350
C	-0.0070140	9.1778790	-1.9598830
C	1.2605360	8.7216750	-1.2102480
H	2.1441880	9.0739480	-1.7504600
H	1.2982840	9.2063500	-0.2232900
C	-2.1848010	-0.1758100	-4.1478320
H	-1.7388910	-1.1361860	-4.4272490
H	-1.5563000	0.6195660	-4.5626320
H	-2.1544770	-0.0954810	-3.0574080
C	-3.5851110	-0.1837350	-6.2273430
H	-2.9796500	0.6186700	-6.6633070
H	-3.1450770	-1.1386890	-6.5338620
H	-4.5905970	-0.1213180	-6.6577000
C	0.0767830	8.7874890	-3.4496890
H	-0.8264430	9.1078220	-3.9797290
H	0.9351510	9.2721350	-3.9273570
H	0.1815150	7.7072710	-3.5846900
C	-0.1361540	10.7064680	-1.8509200
H	0.7268840	11.2063480	-2.3044880
H	-1.0354200	11.0556600	-2.3694750
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C	-0.0767830	-8.7874890	-3.4496890
H	0.8264430	-9.1078220	-3.9797290
H	-0.9351510	-9.2721350	-3.9273570
H	-0.1815150	-7.7072710	-3.5846900
C	0.1361540	-10.7064680	-1.8509200
H	-0.7268840	-11.2063480	-2.3044880
H	1.0354200	-11.0556600	-2.3694750
H	0.2024830	-11.0281770	-0.8058800
C	2.1848010	0.1758100	-4.1478320
H	1.7388910	1.1361860	-4.4272490
H	1.5563000	-0.6195660	-4.5626320
H	2.1544770	0.0954810	-3.0574080
C	3.5851110	0.1837350	-6.2273430

H	2.9796500	-0.6186700	-6.6633070
H	3.1450770	1.1386890	-6.5338620
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N	4.6511670	-2.6343690	-2.2918520
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H	-2.6670720	-5.7623710	-0.4335130
H	-4.7369440	2.6833310	-1.2753730
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C	4.5114830	-3.9381590	-2.9442060
H	3.5749130	-4.4069540	-2.6209060
H	4.4527170	-3.7969370	-4.0236890
C	-3.8327330	-7.5129890	-0.7417900
H	-4.0070440	-7.9214660	-1.7459040
H	-3.7386890	-8.3660260	-0.0617110
C	-4.5114830	3.9381590	-2.9442060
H	-3.5749130	4.4069540	-2.6209060
H	-4.4527170	3.7969370	-4.0236890
C	3.8327330	7.5129890	-0.7417900
H	4.0070440	7.9214660	-1.7459040
H	3.7386890	8.3660260	-0.0617110
C	5.6770870	-4.8552310	-2.6090130
C	5.4592970	-6.0593910	-1.9295840
C	6.9835230	-4.5085910	-2.9831510
C	6.5323360	-6.9061560	-1.6336800
H	4.4498730	-6.3334040	-1.6320970
C	8.0530520	-5.3520670	-2.6860780
H	7.1623280	-3.5733110	-3.5073330
C	7.8293300	-6.5555980	-2.0096430
H	6.3524250	-7.8382780	-1.1055470
H	9.0599780	-5.0734760	-2.9832500
H	8.6622370	-7.2130560	-1.7780810
C	-5.0246660	-6.6752610	-0.3288210
C	-5.3663510	-5.5069690	-1.0249000
C	-5.8315010	-7.0861340	0.7388610
C	-6.4880030	-4.7637960	-0.6562170
H	-4.7516530	-5.1643250	-1.8525510
C	-6.9627750	-6.3512020	1.1013460
H	-5.5748910	-7.9880880	1.2881400
C	-7.2925130	-5.1876640	0.4049170
H	-6.7190290	-3.8516830	-1.1962240
H	-7.5796130	-6.6854930	1.9303330
H	-8.1682670	-4.6116310	0.6891550
C	-5.6770870	4.8552310	-2.6090130
C	-5.4592970	6.0593910	-1.9295840
C	-6.9835230	4.5085910	-2.9831510
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H	-7.1623280	3.5733110	-3.5073330
C	-7.8293300	6.5555980	-2.0096430
H	-6.3524250	7.8382780	-1.1055470
H	-9.0599780	5.0734760	-2.9832500
H	-8.6622370	7.2130560	-1.7780810
C	5.0246660	6.6752610	-0.3288210
C	5.3663510	5.5069690	-1.0249000
C	5.8315010	7.0861340	0.7388610
C	6.4880030	4.7637960	-0.6562170
H	4.7516530	5.1643250	-1.8525510
C	6.9627750	6.3512020	1.1013460
H	5.5748910	7.9880880	1.2881400
C	7.2925130	5.1876640	0.4049170
H	6.7190290	3.8516830	-1.1962240
H	7.5796130	6.6854930	1.9303330
H	8.1682670	4.6116310	0.6891550

C₄ crown-*in* in DMSO

Energy total = -5317.13305223 a.u.

Symbol	X	Y	Z
C	-0.6603120	-3.1893160	2.5675030
C	-1.1554670	-3.8975210	1.4553820

C	-2.4285280	-3.6324330	0.9162370
C	-3.1700760	-2.5682520	1.4605400
C	-2.6999680	-1.8176190	2.5519110
C	-1.4463740	-2.1534260	3.0725260
O	-0.3713600	-4.8966900	0.9271150
O	-4.4158310	-2.3283650	0.9204340
H	-1.0788960	-1.5907430	3.9240610
C	-3.5523230	-0.7027470	3.1684330
C	-3.1893160	0.6603120	2.5675030
C	-3.8975210	1.1554670	1.4553820
C	-3.6324330	2.4285280	0.9162370
C	-2.5682520	3.1700760	1.4605400
C	-1.8176190	2.6999680	2.5519110
C	-2.1534260	1.4463740	3.0725260
O	-4.8966900	0.3713600	0.9271150
H	-1.5907430	1.0788960	3.9240610
C	-0.7027470	3.5523230	3.1684330
C	0.6603120	3.1893160	2.5675030
C	1.1554670	3.8975210	1.4553820
C	2.4285280	3.6324330	0.9162370
C	3.1700760	2.5682520	1.4605400
C	2.6999680	1.8176190	2.5519110
C	1.4463740	2.1534260	3.0725260
O	0.3713600	4.8966900	0.9271150
O	4.4158310	2.3283650	0.9204340
H	1.0788960	1.5907430	3.9240610
C	3.5523230	0.7027470	3.1684330
C	3.1893160	-0.6603120	2.5675030
C	3.8975210	-1.1554670	1.4553820
C	3.6324330	-2.4285280	0.9162370
C	2.5682520	-3.1700760	1.4605400
C	1.8176190	-2.6999680	2.5519110
C	2.1534260	-1.4463740	3.0725260
O	4.8966900	-0.3713600	0.9271150
O	2.3283650	-4.4158310	0.9204340
H	1.5907430	-1.0788960	3.9240610
C	0.7027470	-3.5523230	3.1684330
C	-3.5460420	-0.7548030	4.7211060
C	-0.7548030	3.5460420	4.7211060
H	-0.9068530	4.5873420	2.8799170
C	3.5460420	0.7548030	4.7211060
H	4.5873420	0.9068530	2.8799170
C	0.7548030	-3.5460420	4.7211060
H	0.9068530	-4.5873420	2.8799170
H	-3.4290100	-1.8056600	5.0099780
H	-2.6743810	-0.2334010	5.1355270
C	-4.8236450	-0.2300670	5.4119810
H	-1.8056600	3.4290100	5.0099780
H	-0.2334010	2.6743810	5.1355270
C	-0.2300670	4.8236450	5.4119810
H	3.4290100	1.8056600	5.0099780
H	2.6743810	0.2334010	5.1355270
C	4.8236450	0.2300670	5.4119810
H	1.8056600	-3.4290100	5.0099780
H	0.2334010	-2.6743810	5.1355270
C	0.2300670	-4.8236450	5.4119810
H	-4.5873420	-0.9068530	2.8799170
C	4.5460350	-3.0367690	-0.1439870
H	-5.0255960	0.5746830	-0.0613200
H	0.5746830	5.0255960	-0.0613200
H	4.6281150	1.3648580	0.9721160
H	5.0255960	-0.5746830	-0.0613200
H	1.3648580	-4.6281150	0.9721160
H	-0.5746830	-5.0255960	-0.0613200
O	-2.3283650	4.4158310	0.9204340
C	-3.0367690	-4.5460350	-0.1439870
H	-4.6281150	-1.3648580	0.9721160
C	-4.5460350	3.0367690	-0.1439870
H	-1.3648580	4.6281150	0.9721160
C	-2.8515780	-4.2055270	-1.6192130
C	-3.8584110	-3.6004530	-2.3836440
C	-1.6419260	-4.6113840	-2.2450240
O	-0.6863210	-5.1382190	-1.6004950
C	-4.2055270	2.8515780	-1.6192130
C	-3.6004530	3.8584110	-2.3836440
C	-4.6113840	1.6419260	-2.2450240

O	-5.1382190	0.6863210	-1.6004950
C	3.0367690	4.5460350	-0.1439870
C	2.8515780	4.2055270	-1.6192130
C	1.6419260	4.6113840	-2.2450240
O	0.6863210	5.1382190	-1.6004950
C	3.8584110	3.6004530	-2.3836440
C	4.2055270	-2.8515780	-1.6192130
C	4.6113840	-1.6419260	-2.2450240
O	5.1382190	-0.6863210	-1.6004950
C	3.6004530	-3.8584110	-2.3836440
H	5.5443400	-2.6122280	0.0063000
H	4.6455210	-4.1049330	0.0680860
H	-2.6122280	-5.5443400	0.0063000
H	-4.1049330	-4.6455210	0.0680860
H	-5.5443400	2.6122280	0.0063000
H	-4.6455210	4.1049330	0.0680860
H	2.6122280	5.5443400	0.0063000
H	4.1049330	4.6455210	0.0680860
C	-5.0854900	1.2681970	5.2010860
C	-4.7741520	-0.5554020	6.9133040
C	0.5554020	-4.7741520	6.9133040
C	-1.2681970	-5.0854900	5.2010860
C	4.7741520	0.5554020	6.9133040
C	5.0854900	-1.2681970	5.2010860
C	-0.5554020	4.7741520	6.9133040
C	1.2681970	5.0854900	5.2010860
H	-5.6731740	-0.7814880	4.9808870
H	-0.7814880	5.6731740	4.9808870
H	5.6731740	0.7814880	4.9808870
H	0.7814880	-5.6731740	4.9808870
H	-5.2054510	1.5209000	4.1448290
H	-4.2569720	1.8697650	5.5941720
H	-5.9971880	1.5742480	5.7266410
H	-3.9398570	-0.0345320	7.3993750
H	-4.6431860	-1.6290760	7.0873510
H	-5.6963320	-0.2427530	7.4150180
H	0.0345320	-3.9398570	7.3993750
H	1.6290760	-4.6431860	7.0873510
H	0.2427530	-5.6963320	7.4150180
H	-1.5209000	-5.2054510	4.1448290
H	-1.8697650	-4.2569720	5.5941720
H	-1.5742480	-5.9971880	5.7266410
H	3.9398570	0.0345320	7.3993750
H	4.6431860	1.6290760	7.0873510
H	5.6963320	0.2427530	7.4150180
H	5.2054510	-1.5209000	4.1448290
H	4.2569720	-1.8697650	5.5941720
H	5.9971880	-1.5742480	5.7266410
H	-0.0345320	3.9398570	7.3993750
H	-1.6290760	4.6431860	7.0873510
H	-0.2427530	5.6963320	7.4150180
H	1.5209000	5.2054510	4.1448290
H	1.8697650	4.2569720	5.5941720
H	1.5742480	5.9971880	5.7266410
C	1.4329940	4.3938270	-3.7310090
H	0.7334390	5.1571750	-4.0866830
H	0.9266280	3.4247930	-3.8522680
C	-4.3938270	1.4329940	-3.7310090
H	-5.1571750	0.7334390	-4.0866830
H	-3.4247930	0.9266280	-3.8522680
C	-1.4329940	-4.3938270	-3.7310090
H	-0.7334390	-5.1571750	-4.0866830
H	-0.9266280	-3.4247930	-3.8522680
C	4.3938270	-1.4329940	-3.7310090
H	5.1571750	-0.7334390	-4.0866830
H	3.4247930	-0.9266280	-3.8522680
C	4.4047540	-2.7324200	-4.5527890
C	3.4333920	-3.7227400	-3.8805390
H	2.3959210	-3.4065660	-4.0644560
H	3.5338180	-4.7026590	-4.3558850
C	-2.7324200	-4.4047540	-4.5527890
C	-3.7227400	-3.4333920	-3.8805390
H	-3.4065660	-2.3959210	-4.0644560
H	-4.7026590	-3.5338180	-4.3558850
C	-4.4047540	2.7324200	-4.5527890
C	-3.4333920	3.7227400	-3.8805390

H	-2.3959210	3.4065660	-4.0644560
H	-3.5338180	4.7026590	-4.3558850
C	2.7324200	4.4047540	-4.5527890
C	3.7227400	3.4333920	-3.8805390
H	3.4065660	2.3959210	-4.0644560
H	4.7026590	3.5338180	-4.3558850
C	3.3260830	5.8272620	-4.6053400
H	4.2503640	5.8379730	-5.1931510
H	2.6205570	6.5189000	-5.0779450
H	3.5571180	6.2114860	-3.6075780
C	2.4500240	3.9271510	-5.9869890
H	2.0192130	2.9199860	-5.9940030
H	1.7445810	4.5996840	-6.4866240
H	3.3699280	3.9056000	-6.5817200
C	5.8272620	-3.3260830	-4.6053400
H	5.8379730	-4.2503640	-5.1931510
H	6.5189000	-2.6205570	-5.0779450
H	6.2114860	-3.5571180	-3.6075780
C	3.9271510	-2.4500240	-5.9869890
H	2.9199860	-2.0192130	-5.9940030
H	4.5996840	-1.7445810	-6.4866240
H	3.9056000	-3.3699280	-6.5817200
C	-3.3260830	-5.8272620	-4.6053400
H	-4.2503640	-5.8379730	-5.1931510
H	-2.6205570	-6.5189000	-5.0779450
H	-3.5571180	-6.2114860	-3.6075780
C	-2.4500240	-3.9271510	-5.9869890
H	-2.0192130	-2.9199860	-5.9940030
H	-1.7445810	-4.5996840	-6.4866240
H	-3.3699280	-3.9056000	-6.5817200
C	-5.8272620	3.3260830	-4.6053400
H	-5.8379730	4.2503640	-5.1931510
H	-6.5189000	2.6205570	-5.0779450
H	-6.2114860	3.5571180	-3.6075780
C	-3.9271510	2.4500240	-5.9869890
H	-2.9199860	2.0192130	-5.9940030
H	-4.5996840	1.7445810	-6.4866240
H	-3.9056000	3.3699280	-6.5817200
N	-4.9699330	-3.1266950	-1.7960500
N	3.1266950	-4.9699330	-1.7960500
N	4.9699330	3.1266950	-1.7960500
N	-3.1266950	4.9699330	-1.7960500
H	-2.9984740	4.9204670	-0.7846820
H	-4.9204670	-2.9984740	-0.7846820
H	2.9984740	-4.9204670	-0.7846820
H	4.9204670	2.9984740	-0.7846820
C	6.1037370	2.4428260	-2.4323850
H	5.8510150	1.3914930	-2.6071030
H	6.3123510	2.9125650	-3.3963240
C	-2.4428260	6.1037370	-2.4323850
H	-1.3914930	5.8510150	-2.6071030
H	-2.9125650	6.3123510	-3.3963240
C	-6.1037370	-2.4428260	-2.4323850
H	-5.8510150	-1.3914930	-2.6071030
H	-6.3123510	-2.9125650	-3.3963240
C	2.4428260	-6.1037370	-2.4323850
H	1.3914930	-5.8510150	-2.6071030
H	2.9125650	-6.3123510	-3.3963240
C	7.3343880	2.5332950	-1.5512410
C	7.8463960	1.3891280	-0.9282800
C	7.9759580	3.7639470	-1.3493020
C	8.9846670	1.4718510	-0.1210070
H	7.3471880	0.4361910	-1.0779860
C	9.1097030	3.8481170	-0.5418980
H	7.5841950	4.6575760	-1.8283750
C	9.6179530	2.6999680	0.0737590
H	9.3737570	0.5769200	0.3559560
H	9.5996590	4.8063860	-0.3957310
H	10.5023380	2.7648030	0.7008150
C	-2.5332950	7.3343880	-1.5512410
C	-1.3891280	7.8463960	-0.9282800
C	-3.7639470	7.9759580	-1.3493020
C	-1.4718510	8.9846670	-0.1210070
H	-0.4361910	7.3471880	-1.0779860
C	-3.8481170	9.1097030	-0.5418980
H	-4.6575760	7.5841950	-1.8283750

C	-2.6999680	9.6179530	0.0737590
H	-0.5769200	9.3737570	0.3559560
H	-4.8063860	9.5996590	-0.3957310
H	-2.7648030	10.5023380	0.7008150
C	-7.3343880	-2.5332950	-1.5512410
C	-7.8463960	-1.3891280	-0.9282800
C	-7.9759580	-3.7639470	-1.3493020
C	-8.9846670	-1.4718510	-0.1210070
H	-7.3471880	-0.4361910	-1.0779860
C	-9.1097030	-3.8481170	-0.5418980
H	-7.5841950	-4.6575760	-1.8283750
C	-9.6179530	-2.6999680	0.0737590
H	-9.3737570	-0.5769200	0.3559560
H	-9.5996590	-4.8063860	-0.3957310
H	-10.5023380	-2.7648030	0.7008150
C	2.5332950	-7.3343880	-1.5512410
C	1.3891280	-7.8463960	-0.9282800
C	3.7639470	-7.9759580	-1.3493020
C	1.4718510	-8.9846670	-0.1210070
H	0.4361910	-7.3471880	-1.0779860
C	3.8481170	-9.1097030	-0.5418980
H	4.6575760	-7.5841950	-1.8283750
C	2.6999680	-9.6179530	0.0737590
H	0.5769200	-9.3737570	0.3559560
H	4.8063860	-9.5996590	-0.3957310
H	2.7648030	-10.5023380	0.7008150

C₄ crown-out in DMSO

Energy total = -5317.13032292 a.u.

Symbol	X	Y	Z
C	1.4287190	2.9294330	1.7741820
C	1.4545000	3.7753670	0.6484730
C	0.2792420	4.3081400	0.0884680
C	-0.9528750	3.9510760	0.6644860
C	-1.0261200	3.0906440	1.7750170
C	0.1728250	2.5935610	2.2901040
O	2.6396830	4.1437850	0.0521940
O	-2.1332880	4.3928190	0.1263610
H	0.1252070	1.9328410	3.1496980
C	-2.3877590	2.7305940	2.3800210
C	-2.9294330	1.4287190	1.7741820
C	-3.7753670	1.4545000	0.6484730
C	-4.3081400	0.2792420	0.0884680
C	-3.9510760	-0.9528750	0.6644860
C	-3.0906440	-1.0261200	1.7750170
C	-2.5935610	0.1728250	2.2901040
O	-4.1437850	2.6396830	0.0521940
H	-1.9328410	0.1252070	3.1496980
C	-2.7305940	-2.3877590	2.3800210
C	-1.4287190	-2.9294330	1.7741820
C	-1.4545000	-3.7753670	0.6484730
C	-0.2792420	-4.3081400	0.0884680
C	0.9528750	-3.9510760	0.6644860
C	1.0261200	-3.0906440	1.7750170
C	-0.1728250	-2.5935610	2.2901040
O	-2.6396830	-4.1437850	0.0521940
O	2.1332880	-4.3928190	0.1263610
H	-0.1252070	-1.9328410	3.1496980
C	2.3877590	-2.7305940	2.3800210
C	2.9294330	-1.4287190	1.7741820
C	3.7753670	-1.4545000	0.6484730
C	4.3081400	-0.2792420	0.0884680
C	3.9510760	0.9528750	0.6644860
C	3.0906440	1.0261200	1.7750170
C	2.5935610	-0.1728250	2.2901040
O	4.1437850	-2.6396830	0.0521940
O	4.3928190	2.1332880	0.1263610
H	1.9328410	-0.1252070	3.1496980
C	2.7305940	2.3877590	2.3800210
C	-2.3693870	2.7690670	3.9325280
C	-2.7690670	-2.3693870	3.9325280
H	-3.5280040	-3.0716020	2.0744960
C	2.3693870	-2.7690670	3.9325280

H	3.0716020	-3.5280040	2.0744960
C	2.7690670	2.3693870	3.9325280
H	3.5280040	3.0716020	2.0744960
H	-1.6261250	3.5172910	4.2312270
H	-2.0189500	1.8183150	4.3525430
C	-3.7038540	3.1562380	4.6056660
H	-3.5172910	-1.6261250	4.2312270
H	-1.8183150	-2.0189500	4.3525430
C	-3.1562380	-3.7038540	4.6056660
H	1.6261250	-3.5172910	4.2312270
H	2.0189500	-1.8183150	4.3525430
C	3.7038540	-3.1562380	4.6056660
H	3.5172910	1.6261250	4.2312270
H	1.8183150	2.0189500	4.3525430
C	3.1562380	3.7038540	4.6056660
H	-3.0716020	3.5280040	2.0744960
C	5.1900820	-0.3347170	-1.1516650
H	-3.4201230	3.3143110	0.0836880
H	-3.3143110	-3.4201230	0.0836880
H	2.0567290	-5.2838960	-0.3646920
H	3.4201230	-3.3143110	0.0836880
H	5.2838960	2.0567290	-0.3646920
H	3.3143110	3.4201230	0.0836880
O	-4.3928190	-2.1332880	0.1263610
C	0.3347170	5.1900820	-1.1516650
H	-2.0567290	5.2838960	-0.3646920
C	-5.1900820	0.3347170	-1.1516650
H	-5.2838960	-2.0567290	-0.3646920
C	0.2971710	6.7030190	-0.9480840
C	1.4545000	7.4740060	-0.8134830
C	-0.9767740	7.3433480	-0.9245140
O	-2.0638010	6.6981780	-0.9365210
C	-6.7030190	0.2971710	-0.9480840
C	-7.4740060	1.4545000	-0.8134830
C	-7.3433480	-0.9767740	-0.9245140
O	-6.6981780	-2.0638010	-0.9365210
C	-0.3347170	-5.1900820	-1.1516650
C	-0.2971710	-6.7030190	-0.9480840
C	0.9767740	-7.3433480	-0.9245140
O	2.0638010	-6.6981780	-0.9365210
C	-1.4545000	-7.4740060	-0.8134830
C	6.7030190	-0.2971710	-0.9480840
C	7.3433480	0.9767740	-0.9245140
O	6.6981780	2.0638010	-0.9365210
C	7.4740060	-1.4545000	-0.8134830
H	4.9347380	0.5195370	-1.7872180
H	4.9242200	-1.2308690	-1.7187350
H	-0.5195370	4.9347380	-1.7872180
H	1.2308690	4.9242200	-1.7187350
H	-4.9347380	-0.5195370	-1.7872180
H	-4.9242200	1.2308690	-1.7187350
H	0.5195370	-4.9347380	-1.7872180
H	-1.2308690	-4.9242200	-1.7187350
C	-4.8465520	2.1611970	4.3572230
C	-3.4878360	3.3555170	6.1140320
C	3.3555170	3.4878360	6.1140320
C	2.1611970	4.8465520	4.3572230
C	3.4878360	-3.3555170	6.1140320
C	4.8465520	-2.1611970	4.3572230
C	-3.3555170	-3.4878360	6.1140320
C	-2.1611970	-4.8465520	4.3572230
H	-4.0086690	4.1258440	4.1829530
H	-4.1258440	-4.0086690	4.1829530
H	4.0086690	-4.1258440	4.1829530
H	4.1258440	4.0086690	4.1829530
H	-5.0772530	2.0574630	3.2940060
H	-4.5903050	1.1657310	4.7396920
H	-5.7579860	2.4898780	4.8693570
H	-3.1778450	2.4179140	6.5919330
H	-2.7119990	4.1029000	6.3133140
H	-4.4091820	3.6879920	6.6044270
H	2.4179140	3.1778450	6.5919330
H	4.1029000	2.7119990	6.3133140
H	3.6879920	4.4091820	6.6044270
H	2.0574630	5.0772530	3.2940060
H	1.1657310	4.5903050	4.7396920

H	2.4898780	5.7579860	4.8693570
H	3.1778450	-2.4179140	6.5919330
H	2.7119990	-4.1029000	6.3133140
H	4.4091820	-3.6879920	6.6044270
H	5.0772530	-2.0574630	3.2940060
H	4.5903050	-1.1657310	4.7396920
H	5.7579860	-2.4898780	4.8693570
H	-2.4179140	-3.1778450	6.5919330
H	-4.1029000	-2.7119990	6.3133140
H	-3.6879920	-4.4091820	6.6044270
H	-2.0574630	-5.0772530	3.2940060
H	-1.1657310	-4.5903050	4.7396920
H	-2.4898780	-5.7579860	4.8693570
C	1.0777990	-8.8546120	-0.8410570
H	1.2136290	-9.1080960	0.2208780
H	2.0002300	-9.1546920	-1.3494890
C	-0.1437590	-9.6047340	-1.3958360
C	-1.4008420	-8.9849500	-0.7526970
H	-2.2947450	-9.4016290	-1.2256880
H	-1.4502470	-9.2767620	0.3068410
C	-9.6047340	0.1437590	-1.3958360
C	-8.9849500	1.4008420	-0.7526970
H	-9.4016290	2.2947450	-1.2256880
H	-9.2767620	1.4502470	0.3068410
C	-8.8546120	-1.0777990	-0.8410570
H	-9.1080960	-1.2136290	0.2208780
H	-9.1546920	-2.0002300	-1.3494890
C	8.9849500	-1.4008420	-0.7526970
H	9.4016290	-2.2947450	-1.2256880
H	9.2767620	-1.4502470	0.3068410
C	9.6047340	-0.1437590	-1.3958360
C	8.8546120	1.0777990	-0.8410570
H	9.1080960	1.2136290	0.2208780
H	9.1546920	2.0002300	-1.3494890
C	-1.0777990	8.8546120	-0.8410570
H	-1.2136290	9.1080960	0.2208780
H	-2.0002300	9.1546920	-1.3494890
C	0.1437590	9.6047340	-1.3958360
C	1.4008420	8.9849500	-0.7526970
H	2.2947450	9.4016290	-1.2256880
H	1.4502470	9.2767620	0.3068410
C	-9.4829000	0.2051540	-2.9319730
H	-9.9219550	-0.6897050	-3.3857440
H	-10.0154470	1.0772000	-3.3264420
H	-8.4409940	0.2706200	-3.2576850
C	-11.0927230	0.0628170	-1.0158450
H	-11.6401150	0.9368980	-1.3856830
H	-11.5545070	-0.8297330	-1.4513420
H	-11.2250690	0.0152210	0.0705790
C	0.2051540	9.4829000	-2.9319730
H	-0.6897050	9.9219550	-3.3857440
H	1.0772000	10.0154470	-3.3264420
H	0.2706200	8.4409940	-3.2576850
C	0.0628170	11.0927230	-1.0158450
H	0.9368980	11.6401150	-1.3856830
H	-0.8297330	11.5545070	-1.4513420
H	0.0152210	11.2250690	0.0705790
C	-0.2051540	-9.4829000	-2.9319730
H	0.6897050	-9.9219550	-3.3857440
H	-1.0772000	-10.0154470	-3.3264420
H	-0.2706200	-8.4409940	-3.2576850
C	-0.0628170	-11.0927230	-1.0158450
H	-0.9368980	-11.6401150	-1.3856830
H	0.8297330	-11.5545070	-1.4513420
H	-0.0152210	-11.2250690	0.0705790
C	9.4829000	-0.2051540	-2.9319730
H	9.9219550	0.6897050	-3.3857440
H	10.0154470	-1.0772000	-3.3264420
H	8.4409940	-0.2706200	-3.2576850
C	11.0927230	-0.0628170	-1.0158450
H	11.6401150	-0.9368980	-1.3856830
H	11.5545070	0.8297330	-1.4513420
H	11.2250690	-0.0152210	0.0705790
N	-2.6654290	-6.8972670	-0.6966110
N	-6.8972670	2.6654290	-0.6966110
N	6.8972670	-2.6654290	-0.6966110

N	2.6654290	6.8972670	-0.6966110
H	-2.6996620	-5.8851120	-0.5738610
H	-5.8851120	2.6996620	-0.5738610
H	2.6996620	5.8851120	-0.5738610
H	5.8851120	-2.6996620	-0.5738610
C	7.5844920	-3.9435900	-0.5327500
H	8.3977900	-3.8523260	0.1938260
H	6.8497890	-4.6189900	-0.0814310
C	-3.9435900	-7.5844920	-0.5327500
H	-3.8523260	-8.3977900	0.1938260
H	-4.6189900	-6.8497890	-0.0814310
C	-7.5844920	3.9435900	-0.5327500
H	-8.3977900	3.8523260	0.1938260
H	-6.8497890	4.6189900	-0.0814310
C	3.9435900	7.5844920	-0.5327500
H	3.8523260	8.3977900	0.1938260
H	4.6189900	6.8497890	-0.0814310
C	8.1144440	-4.5669400	-1.8184490
C	9.2293540	-5.4135290	-1.7640160
C	7.4851610	-4.3553050	-3.0509790
C	9.7028340	-6.0425330	-2.9168320
H	9.7305570	-5.5808420	-0.8137010
C	7.9599220	-4.9803810	-4.2056860
H	6.6249900	-3.6949420	-3.1066820
C	9.0687220	-5.8273560	-4.1424040
H	10.5702720	-6.6934950	-2.8581340
H	7.4624760	-4.8052290	-5.1552460
H	9.4381660	-6.3119310	-5.0412600
C	-4.5669400	-8.1144440	-1.8184490
C	-5.4135290	-9.2293540	-1.7640160
C	-4.3553050	-7.4851610	-3.0509790
C	-6.0425330	-9.7028340	-2.9168320
H	-5.5808420	-9.7305570	-0.8137010
C	-4.9803810	-7.9599220	-4.2056860
H	-3.6949420	-6.6249900	-3.1066820
C	-5.8273560	-9.0687220	-4.1424040
H	-6.6934950	-10.5702720	-2.8581340
H	-4.8052290	-7.4624760	-5.1552460
H	-6.3119310	-9.4381660	-5.0412600
C	-8.1144440	4.5669400	-1.8184490
C	-9.2293540	5.4135290	-1.7640160
C	-7.4851610	4.3553050	-3.0509790
C	-9.7028340	6.0425330	-2.9168320
H	-9.7305570	5.5808420	-0.8137010
C	-7.9599220	4.9803810	-4.2056860
H	-6.6249900	3.6949420	-3.1066820
C	-9.0687220	5.8273560	-4.1424040
H	-10.5702720	6.6934950	-2.8581340
H	-7.4624760	4.8052290	-5.1552460
H	-9.4381660	6.3119310	-5.0412600
C	4.5669400	8.1144440	-1.8184490
C	5.4135290	9.2293540	-1.7640160
C	4.3553050	7.4851610	-3.0509790
C	6.0425330	9.7028340	-2.9168320
H	5.5808420	9.7305570	-0.8137010
C	4.9803810	7.9599220	-4.2056860
H	3.6949420	6.6249900	-3.1066820
C	5.8273560	9.0687220	-4.1424040
H	6.6934950	10.5702720	-2.8581340
H	4.8052290	7.4624760	-5.1552460
H	6.3119310	9.4381660	-5.0412600

9. DFTB/GFN2-xTB calculations

Atomic coordinates for all calculated geometries:

C₂ in chloroform

Energy total = -359.525518333002 a.u.

Symbol	X	Y	Z
C	-1.39233440939539	-2.79621267988148	1.77205756126630
C	-1.40190189195070	-3.52889551534007	0.58368343005384
C	-0.21937296725526	-4.02270070520330	0.02338732597574
C	0.99253233702365	-3.74786181458977	0.65360461090755
C	1.03071321938180	-2.97206973876341	1.81743878952324
C	-0.16069290059559	-2.49958479042019	2.33564072207264
O	-2.56203105836668	-3.82488248436475	-0.08986763343585
O	2.18722096083988	-4.19890220573781	0.16356331882558
H	-0.12416798642093	-1.90087447998348	3.22786434666835
C	2.36790564628323	-2.69028918251522	2.47740101834871
C	2.95847231487840	-1.42391396336866	1.88486751921884
C	3.95870845969139	-1.47969028086596	0.91154639453439
C	4.54329937431824	-0.31948151523501	0.39619918089733
C	4.10742942530686	0.91764660478429	0.86926813485983
C	3.10234684135193	0.99704677609653	1.83881361430949
C	2.53096579253205	-0.17314838343817	2.30146321191118
O	4.43790822104035	-2.68213291050532	0.44173404728675
H	1.73729248133570	-0.10239127629611	3.02458637627207
C	2.70133338832501	2.35134813303880	2.39480107388988
C	1.39233427611225	2.79621264133396	1.77205757417079
C	1.40190168925219	3.52889560679196	0.58368354277525
C	0.21937267674166	4.02270092535784	0.02338768665334
C	-0.99253256661789	3.74786194949933	0.65360504049472
C	-1.03071340536906	2.97206972889442	1.81743910360685
C	0.16069281186938	2.49958476745346	2.33564088672304
O	2.56203073541237	3.82488249458854	-0.08986772907555
O	-2.18722127047680	4.19890251390836	0.16356386236737
H	0.12416793162961	1.90087418751633	3.22786433077673
C	-2.36790578121014	2.69028906775005	2.47740135945692
C	-2.95847226134812	1.42391378824536	1.88486781266582
C	-3.95870850737067	1.47969010613426	0.91154683051936
C	-4.54329936790956	0.31948136093621	0.39619950428079
C	-4.10742945627565	-0.91764677027824	0.86926847129545
C	-3.10234686803693	-0.99704696614642	1.83881394127558
C	-2.53096569990273	0.17314818459985	2.30146344206574
O	-4.43790852181031	2.68213280969804	0.44173485247692
O	-4.63568212934124	-2.09988745192320	0.42850225956685
H	-1.73729244497942	0.10239101693000	3.02458664378717
C	-2.70133339404904	-2.35134830312041	2.39480140188024
C	2.27017371003650	-2.67303042567003	4.01218239266834
C	2.73018352686613	2.34117861652455	3.93297194327296
H	3.48070136085489	3.06196988824904	2.09585690899360
C	-2.27017343173099	2.67303024725303	4.01218275274255
H	-3.02426833518725	3.53207438512860	2.23140945314609
C	-2.73018340348209	-2.34117866644768	3.93297228517364
H	-3.48070136790840	-3.06196998321160	2.09585708833282
H	1.53160672297305	-3.42577520576233	4.29717184293992
H	1.92406354290985	-1.70561937031887	4.37210609337446
C	3.58832795570937	-3.01193834205859	4.71954252446629
H	3.55855810120539	1.69236920932648	4.22798261415148
H	1.81775153328603	1.91731636149313	4.34782015557100
C	2.96726935334124	3.72453297913033	4.55052821212095
H	-1.53160645219971	3.42577505201783	4.29717222402730
H	-1.92406327757494	1.70561914427948	4.37210640554491
C	-3.58832768436343	3.01193818544145	4.71954287585243
H	-3.55855802713151	-1.69236927072550	4.22798298617216
H	-1.81775129366906	-1.91731643964742	4.34782040276518
C	-2.96726923647346	-3.72453323954466	4.55052815405165
H	3.02426818659731	-3.53207450024024	2.23140916738334
C	-5.67702836868773	0.42026698015024	-0.60195594639338
H	3.71677651816646	-3.34135307531433	0.47854386037162
H	3.30275721085819	3.25200732898925	0.19610443060520
H	-2.08071544048170	4.82001415423376	-0.60458890065190

H	-3.71677691903564	3.34135300009799	0.47854476807812
H	-5.20949083392764	-1.98965579261473	-0.37877441345153
H	-3.30275745407893	-3.25200721609152	0.19610454305633
O	4.63568217443433	2.09988730295773	0.42850198492041
C	-0.27458472097015	-4.80645936576091	-1.26969333402123
H	2.08071533089023	-4.82001392092087	-0.60458959728373
C	5.67702839483563	-0.42026697630775	-0.60195626760134
H	5.20949076785907	1.98965564123315	-0.37877480497769
C	-0.06565509163845	-6.30315520394108	-1.12029265731343
C	-1.07752024329908	-7.14960740937204	-0.69673547061553
C	1.21424444444705	-6.80709516467623	-1.44472404067519
O	2.17790942748484	-6.04496620374678	-1.71215064446643
C	5.28521392513466	-0.18978934550275	-2.05252916533415
C	4.82119961790336	-1.21412305466312	-2.86293056228056
C	5.50489738805968	1.11017861339365	-2.56988568442668
O	5.91529327860804	2.05585333635404	-1.85506082865953
C	0.27458436565872	4.80645970353414	-1.26969287933565
C	0.06565478000086	6.30315553478935	-1.12029233180280
C	-1.21424420562373	6.80709578015595	-1.44472490312075
O	2.17790976846254	6.04496691602630	-1.71215056437392
C	1.07752011575561	7.14960765384038	-0.69673500144155
C	-5.28521394623491	0.18978946834987	-2.05252898239217
C	-5.50489803653723	-1.11017872572962	-2.56988546015475
O	-5.91529329368431	-2.05585330990168	-1.85506088797002
C	-4.82119929482079	1.21412281160891	-2.86293022336659
H	-6.15008706773209	1.39774506464719	-0.49158367078538
H	-6.43270977731243	-0.33110397729507	-0.34907376494867
H	0.50406056207297	-4.43469374187605	-1.94409831771396
H	-1.23689504400652	-4.61240660672219	-1.74693287750697
H	6.15008711537841	-1.39774503928615	-0.49158388159269
H	6.43270977446909	0.33110400962609	-0.34907367847517
H	-0.50406088641497	4.43469408367459	-1.94409790657766
H	1.23689463310848	4.61240713385702	-1.74693250376392
C	4.63027591975153	-1.90789404203923	4.55793596586612
C	3.32179906008556	-3.26004869099519	6.20518119261464
C	-3.31815901426737	-3.57444540222325	6.03145272963834
C	-1.75850608315949	-4.64338008954200	4.39460988757769
C	-3.32179877721194	3.26004837988107	6.20518156874355
C	-4.63027577116597	1.90789396099395	4.55793650717399
C	3.31815935020902	3.57444526622292	6.03145273973609
C	1.75850631466330	4.64337992285382	4.39460976494073
H	3.99018835034795	-3.93474169411272	4.28407456806609
H	3.81964434424413	4.18434582432830	4.03755077547611
H	-3.99018813584706	3.93474155404824	4.28407498478017
H	-3.81964427473576	-4.18434612036066	4.03755076706192
H	4.89087753422326	-1.76370943190352	3.51321657609387
H	4.24654050068630	-0.96630373864255	4.94473251670083
H	5.53638283531621	-2.16130721319388	5.10479763817811
H	2.91523325311023	-2.36463582366480	6.67108344138553
H	2.61088277665315	-4.07257951358264	6.33974742479776
H	4.24360540835197	-3.52377187603561	6.71890846950380
H	-2.49908392901299	-3.10086332962205	6.56932062309191
H	-4.21004899897429	-2.96395488722487	6.15653002362975
H	-3.50387460617686	-4.54777204223515	6.48029665851157
H	-1.51828478499160	-4.79717784911904	3.34641220696112
H	-0.88898656136999	-4.20978129066630	4.88374207987977
H	-1.96014326810368	-5.61044230996149	4.85055645715598
H	-2.91523293419220	2.36463552449013	6.67108383506199
H	-2.61088250080105	4.07257920789105	6.33974773685006
H	-4.24360507930174	3.52377160189743	6.71890891220992
H	-4.89087744287229	1.76370936063445	3.51321715085795
H	-4.24654039458104	0.96630362240700	4.94473297043779
H	-5.53638267779556	2.16130707773197	5.10479821547303
H	2.49908423034814	3.10086318193786	6.56932053203883
H	4.21004927567199	2.96395465129918	6.15652999860513
H	3.50387495444897	4.54777189589851	6.48029673707046
H	1.51828496880904	4.79717776988098	3.34641209903545
H	0.88898682383479	4.20978113371491	4.88374196513544
H	1.96014353208186	5.61044207991233	4.85055642684553
C	-1.45552512508211	8.29607365770913	-1.42534538514051
H	-1.88392634426849	8.5334251307246	-0.44534984905699
H	-2.21793280714879	8.52733399052858	-2.17275152858492
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C	5.73237115179275	5.58999353619531	2.52204969585369
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C	6.38118504028498	4.75000039648968	1.63322098205901
H	6.55605174965753	4.13615955637591	-0.41353523044798
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C₄ crown-*in* in chloroform

Energy total = -359.518468104208 a.u.

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C	-1.81221054468751	2.65172291300436	2.43760962666376
C	-2.09778230308198	1.39205404107327	2.93822205633465
O	-4.86959314382787	0.31144307229268	0.85871252967214
O	-2.39043329538987	4.39379397353192	0.87015776586654
H	-1.49691508556819	1.01708101055255	3.74774217793408
C	-0.72252024553056	3.50701528703715	3.05930587700024
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C	1.10459921606415	3.87169998673706	1.36783071812481
C	2.37203882634278	3.62385381384917	0.83816380756597
C	3.13555250962454	2.58777619744748	1.38320475925422
C	2.65163411616666	1.81214516627064	2.43751280781505
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C	3.87180893869409	-1.10475280539994	1.36791624262743
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C	1.81221054489347	-2.65172291302683	2.43760962650533
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H	1.49691508559526	-1.01708101067140	3.74774217781270
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H	10.12877510834937	2.79786427149162	1.13867148027679
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C₄ crown-out in chloroform

Energy total = -359.525416637668 a.u.

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C	3.07120389292207	0.96150856334528	1.36742821064872
C	2.51229526179873	-0.20743006111476	1.84886593774108
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O	4.52589266519615	2.06082302628927	-0.12885835916556
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C	0.34652553759377	4.31851948420791	-0.25115867994427
C	-0.88291010236861	3.99425184208024	0.31907356894432
C	-0.96140196382020	3.07124382652021	1.36746218689076
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C₂ in DMSO

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C	1.04418919563475	-2.98669627269935	1.81915017922978
C	-0.15621723624293	-2.49509915346037	2.29679449667558
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H	-0.13404032716092	-1.85986720173421	3.16548902137768
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C	4.08205571078133	0.90261613465932	0.79125042523197
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C	5.80020053894745	5.59119064614835	2.54972168106422
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H	6.43466735228171	4.17370888674924	-0.44927277582847
H	6.11765533021456	5.55289539639894	3.58214366214632
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C₄ crown-*in* in DMSO

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C	-1.65153354106121	2.75307759079459	2.79717654373215
C	-2.00026267625565	1.50408301154189	3.28372664071138
O	-4.93279475428401	0.64361024588392	1.35172845264808
O	-2.13755436217638	4.53363864454613	1.24128915682896
H	-1.39973873368913	1.07752956834760	4.06858628395246
C	-0.51258903064294	3.53394703742590	3.42654091536656
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C	2.62015115005317	3.53720400204064	1.26123823192008
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C	1.50419214737392	2.00024945425351	3.28380841923185
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C	3.86015522739929	-1.36669517087186	1.78654218492521
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C₄ crown-out in DMSO

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C	2.51107981751967	-0.19769269035131	1.80383626786242
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