Electronic Supplementary Material (ESI) for RSC Advances

Supplementary information

A rule to distinguish diastereomeric bianthrones by ^{1}H NMR

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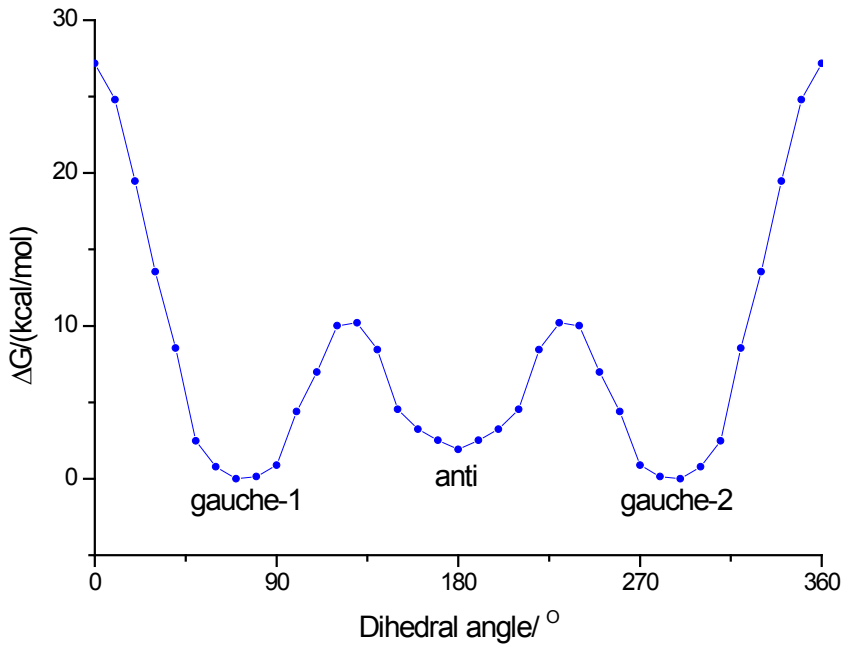


Figure S1. Relationship between relative free energy (ΔG) and dihedral angle (∠H-10–C-10–C-10'–H-10', 0–360°) of 1,1',8,8'-tetrahydroxybianthrone with conformers being produced by rotating the vicinal lowest-energy gauche or anti form.

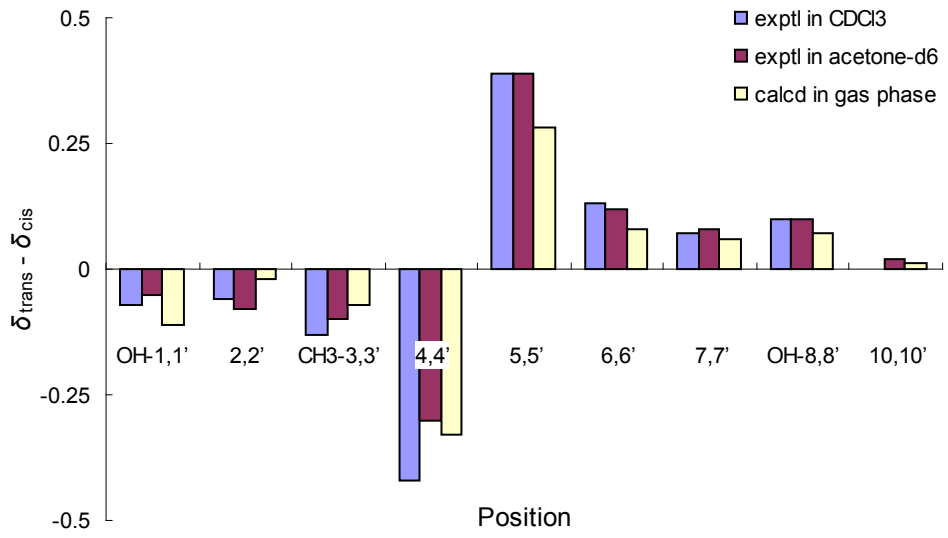


Figure S2. Experimental and calculated differences of ^{1}H NMR shifts for chrysophanol bianthrone (**1**).

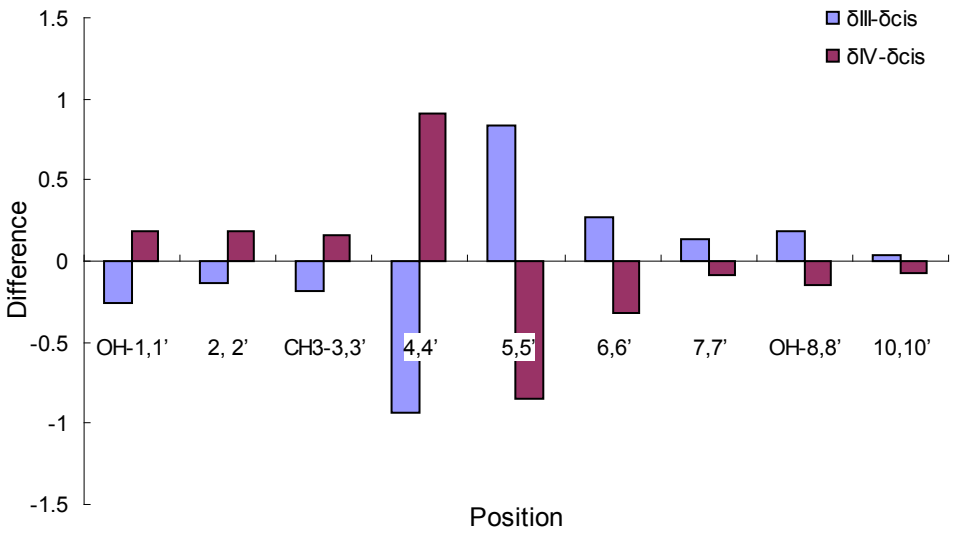


Figure S3. Differences of the calculated ^{1}H NMR data for *cis* (*meso*) and *trans* chrysophanol bianthrone (**1**).

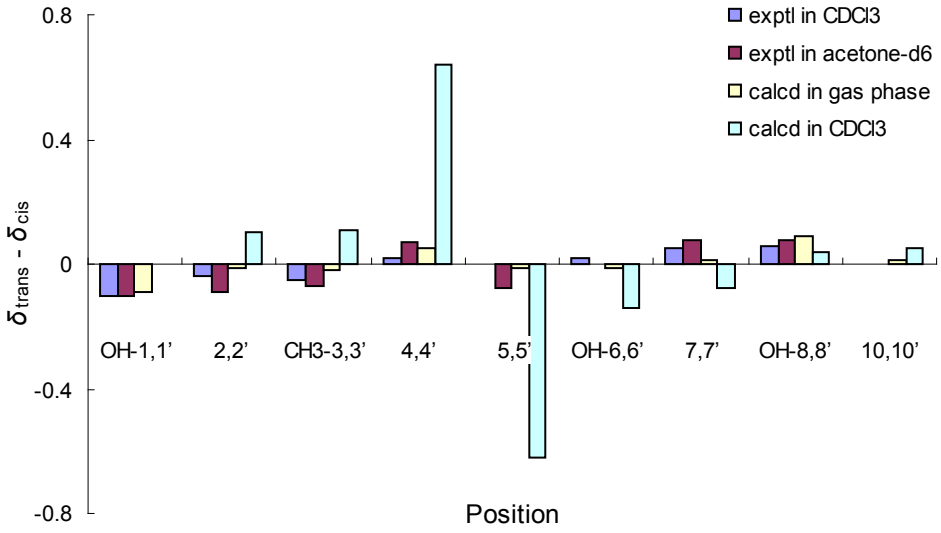


Figure S4. Experimental and calculated differences of ^{1}H NMR shifts for emodin bianthrone (**2**).

Table S1. Calculated degrees for the dihedral angles ∠H-10–C-10–C-10'–H-10' at the gas-phase B3LYP/6-31G(d) level[a]

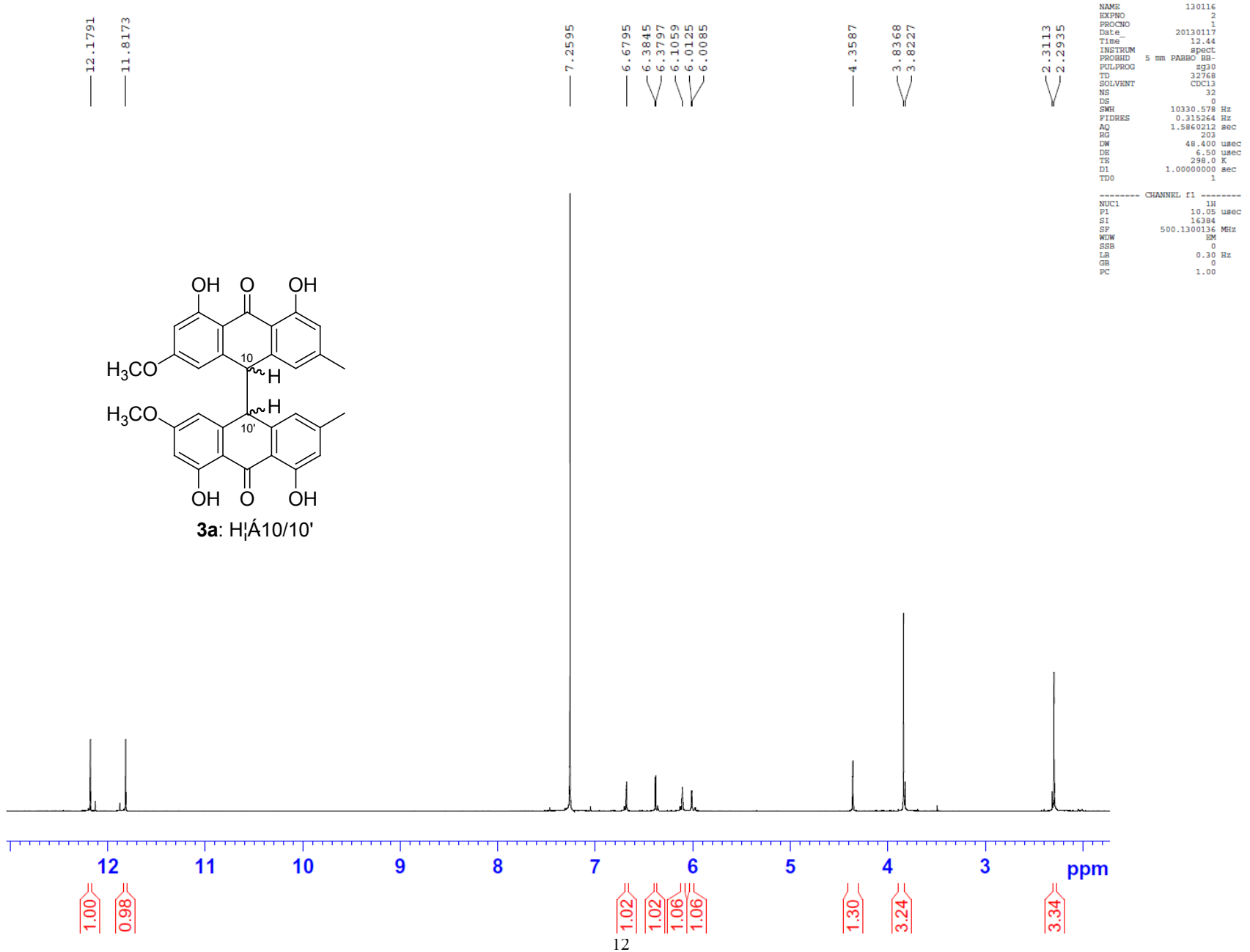
1,1'	2,2'	3,3'	5,5'	6,6'	7,7'	8,8'	I/°	II/°	III/°	IV/°
OH	H	H	H	H	H	OH		71.9		
OCH_3	H	CH_3	H	OH	H	OH	76.5	76.5	70.8	69.3
OCH_3	H	CH_3	Cl	OH	H	OH	73.0	73.0	55.3	69.3
OAc	H	CH_3	H	OCH_3	H	OCH_3	72.5	72.5	79.0	68.3
OH	COOH	CH_3	H	OH	H	OH	71.7	71.7	71.2	70.1
OH	H	CH_3	H	H	H	OH	71.6	71.6	70.8	72.0
OH	H	CH_3	Cl	H	H	OH	71.5	71.5	54.6	72.6
OH	H	CH_3	H	OH	H	OH	71.2	71.2	71.0	71.6
OH	H	CH_3	H	OH	CH_3	OH	71.3	71.3	70.9	71.3
OH	H	CH_3	H	OCH_3	H	OH	71.4	71.4	70.7	72.1
OH	H	CH_3	H	OCH_3	H	OCH_3	73.6	73.6	78.1	71.6
OH	H	CH_3	H	H	CH_3	OH	71.7	71.7	71.1	71.3
OH	H	CH_3	H	H	OCH_3	OH	71.1	71.1	70.7	70.4
OH	H	COOH	H	H	H	OH	71.7	71.7	70.4	69.7
OH	H	CH_3	Cl,H	H	H	OH	69.6	74.8	70.0	74.5
OH	H	CH_3	H	H,OH	H	OH	71.8	71.5	72.0	71.9
OH	H	CH_3	H	H,OCH_3	H	OH	72.0	72.2	72.1	71.8
OH	H	CH_3	H	OH,OCH_3	H	OH	72.3	71.9	71.9	72.6
OH	H	CH_3	H	H	H,OCH_3	OH	70.7	72.0	71.5	71.8

[a]Without groups at 4/4' and 10/10' positions.

Table S2. Calculated ^{1}H NMR data for the conformers of *cis* (*meso*) and *trans* chrysophanol bianthrone (**1**)

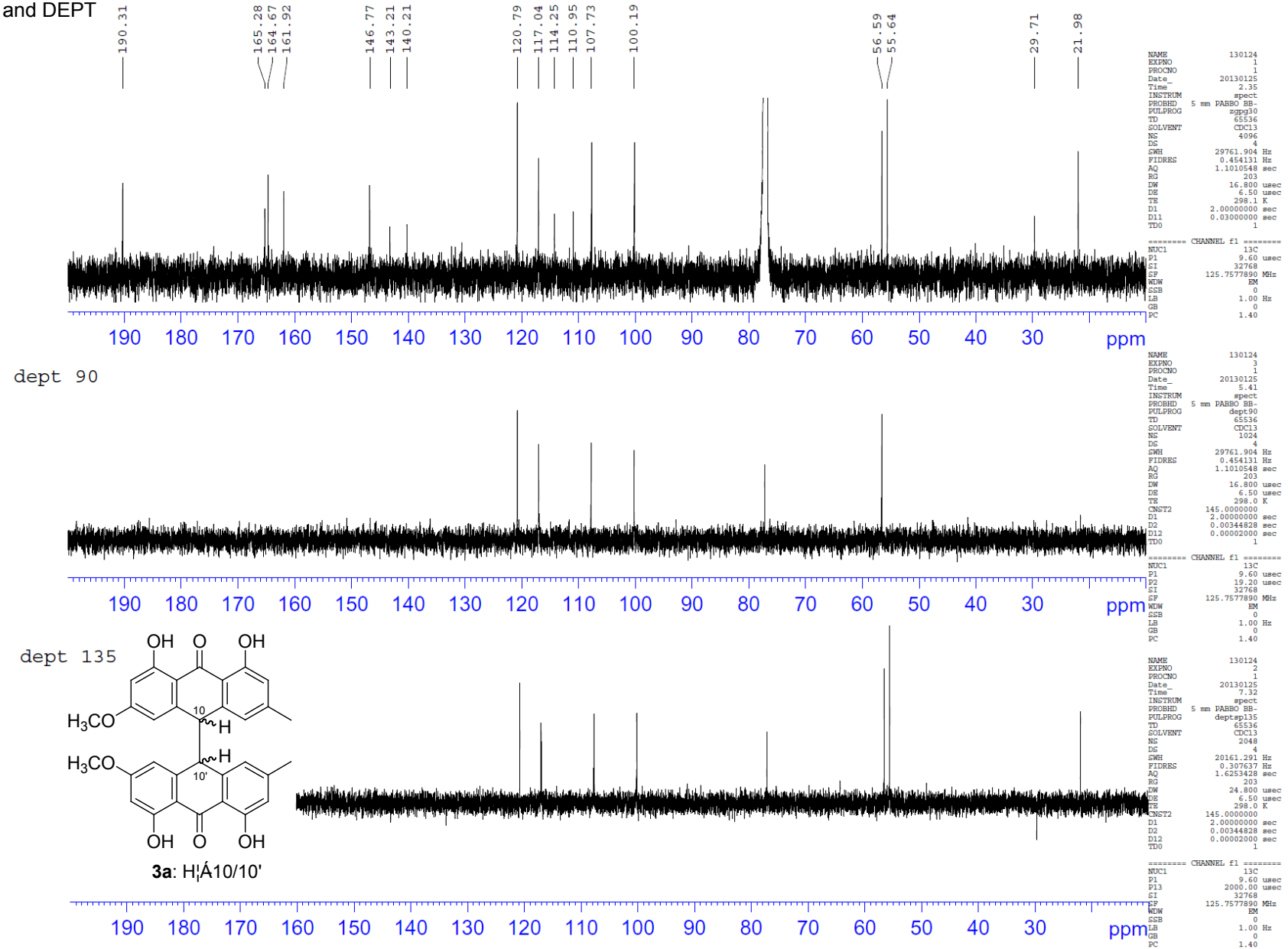
pos.	δ_{I}	δ_{II}	δ_{III}	δ_{IV}
OH-1	12.21	12.34	12.02	12.47
2	6.83	7.19	6.88	7.20
CH_3-3	2.16	2.48	2.13	2.48
4	5.38	7.28	5.39	7.25
5	7.38	5.68	7.37	5.67
6	7.80	7.25	7.79	7.21
7	7.18	6.92	7.19	6.97
OH-8	12.49	12.08	12.46	12.13
10	4.53	4.62	4.62	4.51
OH-1’	12.34	12.21	12.02	12.47
2’	7.20	6.83	6.88	7.20
CH_3-3’	2.48	2.16	2.13	2.48
4’	7.28	5.38	5.39	7.25
5’	5.68	7.38	7.37	5.67
6’	7.25	7.80	7.79	7.21
7’	6.92	7.18	7.19	6.97
OH-8’	12.08	12.49	12.47	12.13
10’	4.62	4.53	4.62	4.50

^{1}H NMR



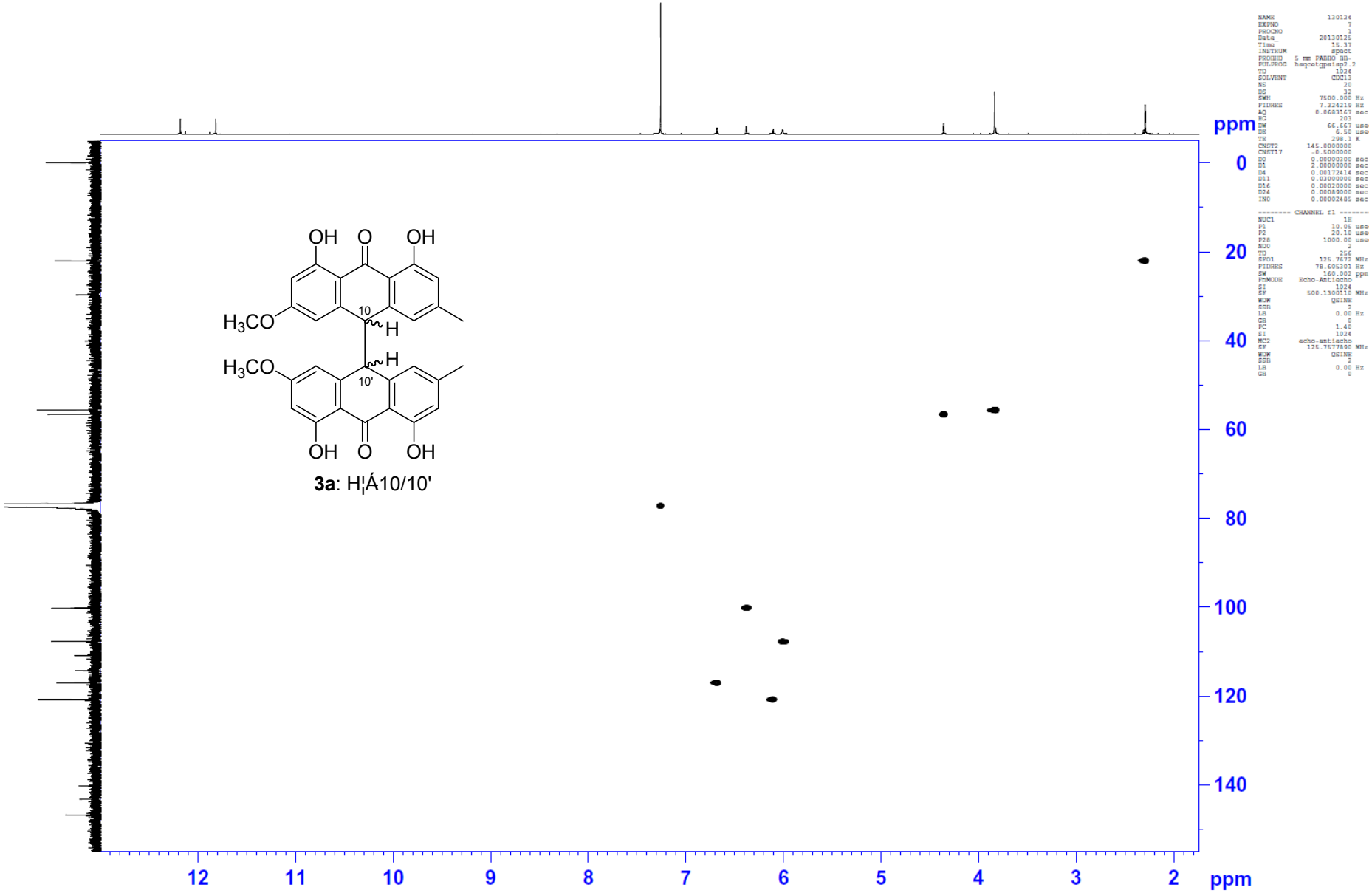
3a: H¦Á10/10'

^{13}C NMR and DEPT

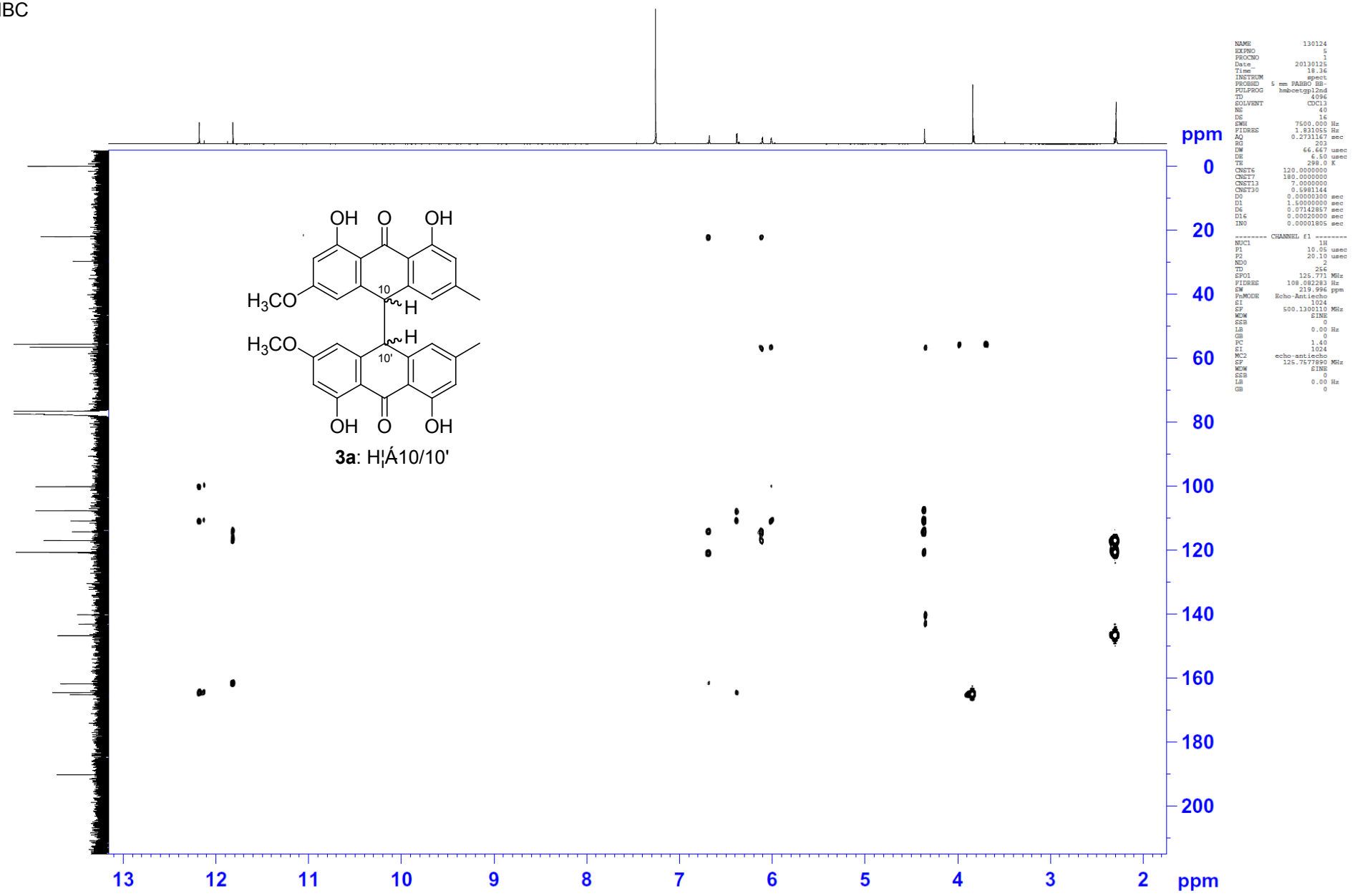


3a: H¦Á10/10'

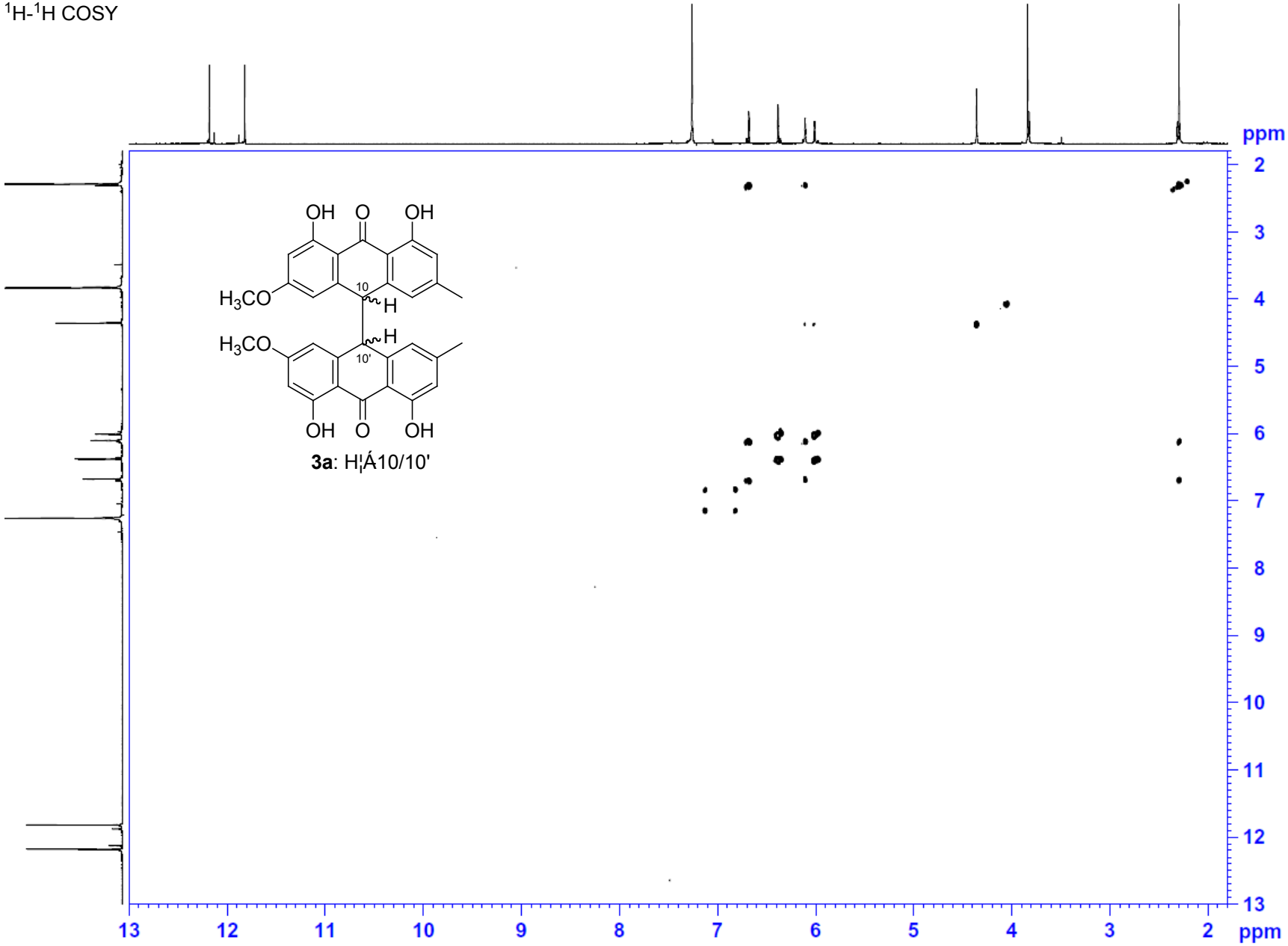
HSQC



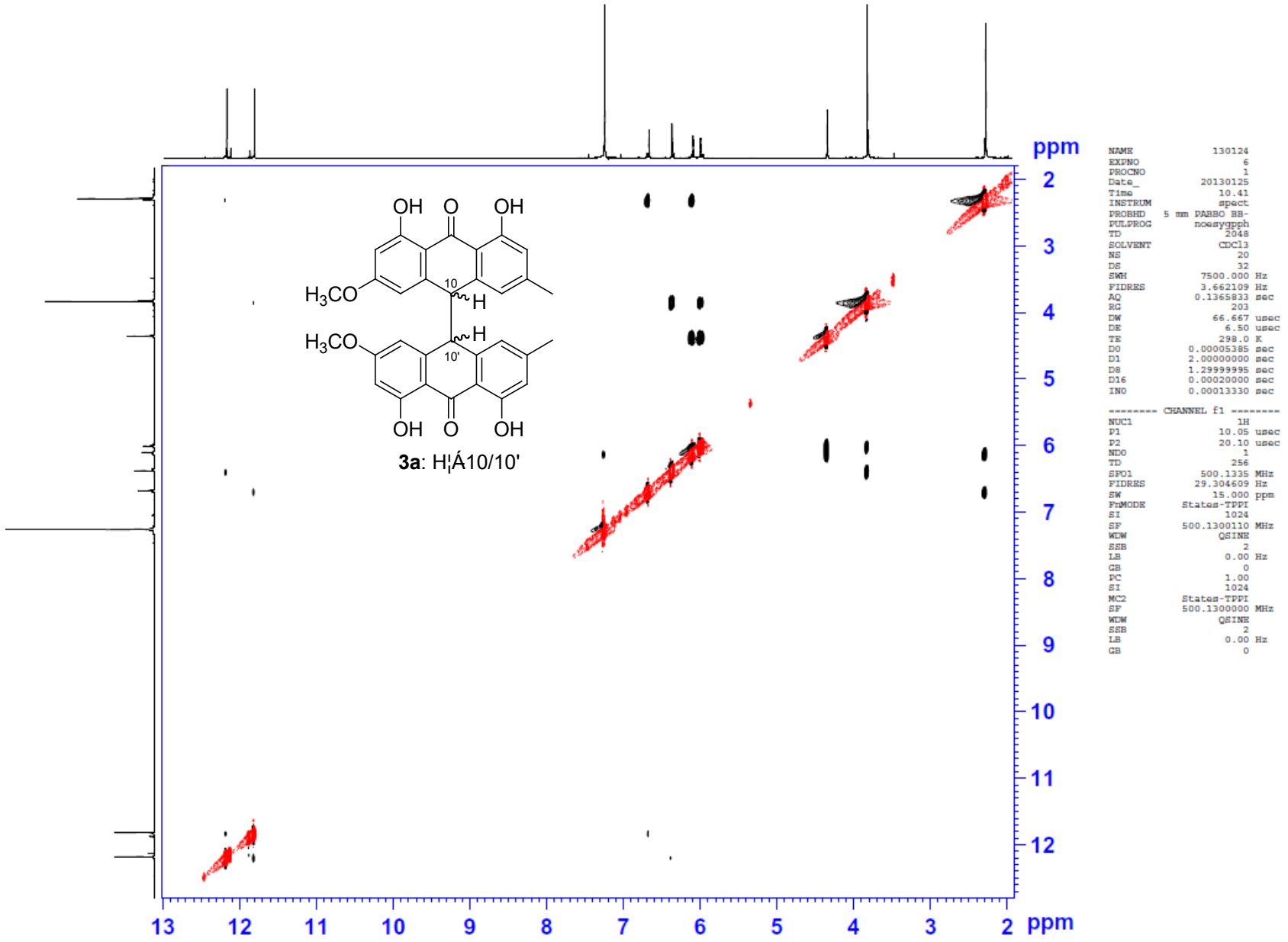
HMBC



^{1}H-^{1}H COSY



NOESY

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SSB                      2
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GB                       0
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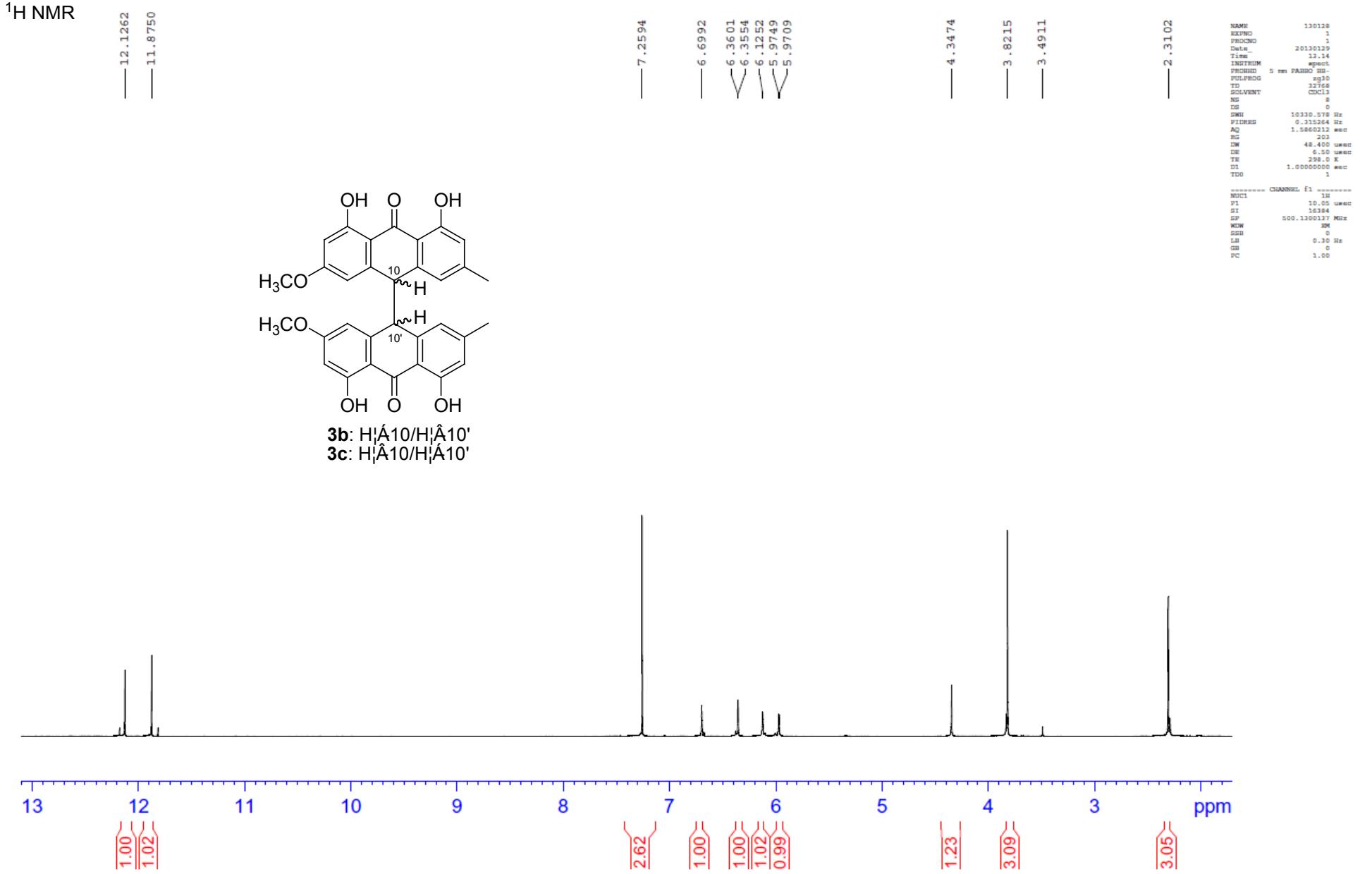
^{1}H NMR



3b: H¦Á10/H¦Â10'
3c: H¦Â10/H¦Á10'

Cartesian coordinates of gauche-1 form of 1,1',8,8'-tetrahydroxybianthrone optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	2.8502	0.6031	0.2596
C	1.9048	1.6533	0.2902
C	2.2872	2.9366	-0.0903
C	3.5989	3.1857	-0.5141
C	4.5361	2.1650	-0.5740
C	4.1756	0.8639	-0.1932
C	2.4888	-0.7306	0.7430
C	1.2196	-0.9159	1.4409
C	0.2750	0.1398	1.5095
C	0.4646	1.3805	0.6661
C	0.9773	-2.1223	2.1592
C	-0.1725	-2.2386	2.9552
C	-1.0594	-1.1783	3.0415
C	-0.8445	0.0079	2.3239
C	-1.9049	1.6532	-0.2901
C	-2.8502	0.6030	-0.2597
C	-4.1757	0.8638	0.1930
C	-4.5363	2.1648	0.5738
C	-3.5991	3.1856	0.5141
C	-2.2874	2.9365	0.0904
C	-0.4646	1.3805	-0.6659
C	-0.2750	0.1398	-1.5093
C	-1.2196	-0.9160	-1.4409
C	-2.4889	-0.7307	-0.7431
C	0.8447	0.0079	-2.3237
C	1.0597	-1.1782	-3.0412
C	0.1727	-2.2386	-2.9551
C	-0.9772	-2.1223	-2.1592
O	3.3082	-1.6881	0.6337
O	-3.3082	-1.6882	-0.6339
H	-0.0989	2.2420	-1.2341
H	0.0988	2.2420	1.2343
O	1.8175	-3.1660	2.1267
O	5.1132	-0.0912	-0.2703
O	-1.8173	-3.1660	-2.1267
O	-5.1133	-0.0914	0.2700
H	2.5705	-2.9136	1.5338
H	4.6857	-0.9374	0.0225
H	-2.5705	-2.9137	-1.5340
H	-4.6857	-0.9375	-0.0228
H	1.5663	3.7494	-0.0557
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H	-5.5542	2.3398	0.9060
H	-3.8879	4.1936	0.8002
H	-1.5665	3.7493	0.0558
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H	0.3301	-3.1646	-3.4980

Cartesian coordinates of gauche-2 form of 1,1',8,8'-tetrahydroxybianthrone optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	-1.2199	-0.9160	1.4406
C	-0.2751	0.1395	1.5092
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C	1.0592	-1.1790	3.0409
C	0.1721	-2.2392	2.9546
C	-0.9778	-2.1226	2.1587
C	-2.4892	-0.7306	0.7428
C	-2.8504	0.6032	0.2595
C	-1.9048	1.6533	0.2900
C	-0.4647	1.3803	0.6660
C	-4.1758	0.8643	-0.1933
C	-4.5361	2.1655	-0.5739
C	-3.5987	3.1861	-0.5140
C	-2.2871	2.9366	-0.0903
C	0.2751	0.1395	-1.5092
C	1.2199	-0.9161	-1.4406
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C	2.2871	2.9366	0.0903
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O	3.3085	-1.6881	-0.6335
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H	-0.0989	2.2418	1.2343
O	-5.1138	-0.0905	-0.2706
O	-1.8183	-3.1659	2.1260
O	5.1138	-0.0905	0.2706
O	1.8183	-3.1659	-2.1260
H	-4.6866	-0.9370	0.0216
H	-2.5713	-2.9128	1.5332
H	4.6867	-0.9370	-0.0216
H	2.5713	-2.9128	-1.5333
H	1.5553	0.8224	2.4042
H	1.9385	-1.2679	3.6732
H	0.3293	-3.1653	3.4973
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H	-3.8873	4.1941	-0.8001
H	-1.5661	3.7493	-0.0556
H	-0.3293	-3.1654	-3.4972
H	-1.9386	-1.2680	-3.6732
H	-1.5553	0.8224	-2.4042
H	1.5661	3.7493	0.0556
H	3.8873	4.1941	0.8001
H	5.5540	2.3406	0.9062

Cartesian coordinates of anti form of 1,1',8,8'-tetrahydroxybianthrone optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	-2.5640	1.2555	-0.1157
C	-1.2967	1.2509	-0.7528
C	-0.8305	2.4064	-1.3639
C	-1.6002	3.5798	-1.3301
C	-2.8196	3.6199	-0.6734
C	-3.3160	2.4614	-0.0539
C	-3.1632	0.0001	0.3353
C	-2.5641	-1.2554	-0.1157
C	-1.2968	-1.2510	-0.7527
C	-0.4494	-0.0001	-0.6811
C	-3.3162	-2.4613	-0.0538
C	-2.8198	-3.6199	-0.6732
C	-1.6004	-3.5799	-1.3300
C	-0.8307	-2.4065	-1.3639
C	1.2967	1.2509	0.7528
C	2.5640	1.2555	0.1157
C	3.3161	2.4614	0.0539
C	2.8196	3.6199	0.6734
C	1.6002	3.5797	1.3302
C	0.8305	2.4064	1.3640
C	0.4494	-0.0001	0.6811
C	1.2968	-1.2510	0.7527
C	2.5641	-1.2555	0.1157
C	3.1632	0.0000	-0.3353
C	0.8307	-2.4065	1.3639
C	1.6004	-3.5799	1.3300
C	2.8198	-3.6199	0.6732
C	3.3162	-2.4613	0.0538
O	-4.2430	0.0001	0.9943
O	4.2430	0.0001	-0.9944
H	-0.2696	-0.0001	1.5064
H	0.2696	-0.0001	-1.5064
O	-4.5069	-2.5392	0.5584
O	-4.5067	2.5393	0.5583
O	4.5069	-2.5393	-0.5584
O	4.5067	2.5394	-0.5583
H	-4.7067	-1.6377	0.9187
H	-4.7064	1.6377	0.9186
H	4.7066	-1.6377	-0.9187
H	4.7065	1.6378	-0.9186
H	0.1382	2.4078	-1.8537
H	-1.2277	4.4756	-1.8197
H	-3.4186	4.5235	-0.6296
H	-3.4189	-4.5234	-0.6294
H	-1.2280	-4.4757	-1.8196
H	0.1380	-2.4080	-1.8536
H	3.4186	4.5235	0.6296
H	1.2277	4.4756	1.8198
H	-0.1382	2.4078	1.8538
H	-0.1380	-2.4080	1.8537
H	1.2280	-4.4757	1.8196
H	3.4188	-4.5235	0.6294

Cartesian coordinates of **1**-I optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	-1.4192	-0.9390	1.3367
C	-0.3468	-0.0108	1.3793
C	0.8222	-0.3427	2.0481
C	0.9915	-1.6097	2.6447
C	-0.0408	-2.5360	2.5745
C	-1.2485	-2.2190	1.9352
C	-2.7159	-0.5537	0.7971
C	-2.9518	0.8462	0.4350
C	-1.8850	1.7734	0.4354
C	-0.4605	1.3080	0.6486
C	-4.2705	1.2930	0.1338
C	-4.5007	2.6514	-0.1302
C	-3.4431	3.5485	-0.1014
C	-2.1393	3.1170	0.1741
C	1.8289	1.3632	-0.5163
C	2.6148	0.1931	-0.6225
C	3.9878	0.2473	-0.2540
C	4.5495	1.4607	0.1657
C	3.7798	2.6180	0.2346
C	2.4138	2.5526	-0.0998
C	0.3381	1.3040	-0.7678
C	-0.0861	0.1652	-1.6671
C	0.7071	-1.0079	-1.7457
C	2.0379	-1.0432	-1.1446
C	-1.2736	0.2406	-2.3868
C	-1.7021	-0.8510	-3.1567
C	-0.9636	-2.0216	-3.2146
C	0.2483	-2.1162	-2.5135
O	-3.6573	-1.3965	0.7180
O	2.7209	-2.1093	-1.1542
H	0.0364	2.2462	-1.2365
H	0.0585	2.0744	1.2336
C	2.2955	-1.9461	3.3249
C	4.3989	3.9324	0.6440
O	-5.3223	0.4625	0.0938
O	-2.2102	-3.1526	1.9286
O	0.9388	-3.2608	-2.6161
O	4.7852	-0.8319	-0.2868
H	-4.9767	-0.4463	0.2941
H	-2.9851	-2.7639	1.4473
H	1.7589	-3.1530	-2.0697
H	4.2279	-1.5884	-0.6065
H	1.6315	0.3785	2.1049
H	0.0555	-3.5225	3.0174
H	-5.5152	2.9679	-0.3485
H	-3.6300	4.6015	-0.2956
H	-1.3233	3.8350	0.1864
H	5.6024	1.4687	0.4310
H	1.8071	3.4531	-0.0289
H	-1.8724	1.1443	-2.3512
H	-2.6318	-0.7776	-3.7146
H	-1.2873	-2.8764	-3.7990
H	2.2608	-2.9305	3.8001
H	3.1206	-1.9470	2.6013
H	2.5437	-1.2036	4.0929
H	5.3621	3.7853	1.1414
H	3.7430	4.4888	1.3229
H	4.5721	4.5707	-0.2323

Cartesian coordinates of **1**-II optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	-2.6149	0.1931	-0.6224
C	-1.8290	1.3631	-0.5162
C	-2.4138	2.5526	-0.0997
C	-3.7798	2.6180	0.2347
C	-4.5496	1.4608	0.1658
C	-3.9879	0.2473	-0.2539
C	-2.0381	-1.0432	-1.1446
C	-0.7073	-1.0080	-1.7457
C	0.0860	0.1651	-1.6671
C	-0.3382	1.3039	-0.7678
C	-0.2485	-2.1163	-2.5136
C	0.9634	-2.0217	-3.2146
C	1.7020	-0.8511	-3.1568
C	1.2735	0.2405	-2.3868
C	0.3469	-0.0109	1.3793
C	1.4194	-0.9390	1.3367
C	1.2487	-2.2190	1.9352
C	0.0411	-2.5361	2.5746
C	-0.9912	-1.6097	2.6448
C	-0.8221	-0.3428	2.0482
C	0.4605	1.3079	0.6486
C	1.8850	1.7734	0.4353
C	2.9518	0.8462	0.4349
C	2.7159	-0.5537	0.7971
C	2.1393	3.1171	0.1741
C	3.4430	3.5486	-0.1015
C	4.5006	2.6515	-0.1304
C	4.2705	1.2931	0.1336
O	-2.7211	-2.1092	-1.1543
O	3.6575	-1.3964	0.7179
H	-0.0585	2.0743	1.2336
H	-0.0365	2.2461	-1.2365
C	-4.3989	3.9324	0.6442
C	-2.2952	-1.9463	3.3251
O	-0.9390	-3.2608	-2.6161
O	-4.7853	-0.8318	-0.2867
O	5.3223	0.4626	0.0935
O	2.2105	-3.1526	1.9286
H	-1.7591	-3.1530	-2.0698
H	-4.2281	-1.5884	-0.6065
H	4.9767	-0.4462	0.2939
H	2.9853	-2.7638	1.4473
H	-1.8070	3.4531	-0.0288
H	-5.6024	1.4688	0.4311
H	1.2871	-2.8765	-3.7991
H	2.6317	-0.7777	-3.7146
H	1.8723	1.1442	-2.3512
H	-0.0551	-3.5226	3.0175
H	-1.6314	0.3783	2.1050
H	1.3232	3.8350	0.1864
H	3.6298	4.6015	-0.2957
H	5.5151	2.9680	-0.3488
H	-4.5721	4.5708	-0.2321
H	-5.3620	3.7854	1.1416
H	-3.7429	4.4888	1.3231
H	-3.1204	-1.9470	2.6016
H	-2.2605	-2.9307	3.8002
H	-2.5433	-1.2039	4.0933

Cartesian coordinates of **1**-III optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	0.8968	-0.8205	-1.6019
C	-0.0258	0.2553	-1.5282
C	-1.2713	0.1345	-2.1260
C	-1.6639	-1.0602	-2.7657
C	-0.7791	-2.1298	-2.8086
C	0.4994	-2.0284	-2.2402
C	2.2663	-0.6581	-1.1350
C	2.7333	0.6744	-0.7433
C	1.8195	1.7473	-0.6378
C	0.3314	1.4965	-0.7437
C	4.1190	0.9071	-0.5132
C	4.5672	2.2047	-0.2253
C	3.6568	3.2494	-0.1563
C	2.2880	3.0271	-0.3534
C	0.0258	0.2555	1.5281
C	-0.8968	-0.8203	1.6020
C	-0.4994	-2.0282	2.2404
C	0.7791	-2.1295	2.8088
C	1.6639	-1.0598	2.7658
C	1.2713	0.1348	2.1259
C	-0.3314	1.4966	0.7435
C	-1.8195	1.7474	0.6376
C	-2.7334	0.6745	0.7432
C	-2.2663	-0.6580	1.1350
C	-2.2880	3.0271	0.3531
C	-3.6569	3.2495	0.1559
C	-4.5673	2.2048	0.2251
C	-4.1190	0.9072	0.5131
O	3.0723	-1.6347	-1.1461
O	-3.0723	-1.6346	1.1463
H	0.1261	2.3636	1.2308
H	-0.1261	2.3635	-1.2311
C	-3.0436	-1.1666	-3.3666
C	3.0436	-1.1662	3.3668
O	5.0323	-0.0753	-0.5572
O	1.3085	-3.0925	-2.3387
O	-5.0323	-0.0752	0.5573
O	-1.3085	-3.0922	2.3391
H	4.5419	-0.9107	-0.7754
H	2.1592	-2.8498	-1.8913
H	-4.5419	-0.9106	0.7755
H	-2.1592	-2.8495	1.8917
H	-1.9665	0.9678	-2.0926
H	-1.0492	-3.0661	-3.2870
H	5.6292	2.3586	-0.0650
H	4.0120	4.2544	0.0563
H	1.5888	3.8565	-0.2837
H	1.0492	-3.0657	3.2874
H	1.9665	0.9681	2.0924
H	-1.5888	3.8565	0.2832
H	-4.0120	4.2544	-0.0568
H	-5.6293	2.3586	0.0648
H	-3.8115	-1.1112	-2.5844
H	-3.1778	-2.1087	-3.9057
H	-3.2362	-0.3423	-4.0638
H	3.2360	-0.3420	4.0641
H	3.8115	-1.1104	2.5846
H	3.1779	-2.1084	3.9056

Cartesian coordinates of **1**-IV optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	2.8371	0.2915	0.3809
C	1.8922	1.3428	0.3683
C	2.2878	2.6225	-0.0008
C	3.6163	2.898	-0.3765
C	4.5437	1.8612	-0.3924
C	4.1755	0.5605	-0.0212
C	2.4619	-1.0389	0.8529
C	1.1632	-1.2257	1.4959
C	0.2138	-0.1725	1.5192
C	0.4371	1.0689	0.684
C	0.893	-2.4305	2.2061
C	-0.2913	-2.5492	2.9493
C	-1.1849	-1.4917	2.9923
C	-0.9412	-0.3066	2.2826
C	-1.8922	1.3428	-0.3682
C	-2.8371	0.2915	-0.3808
C	-4.1755	0.5605	0.0212
C	-4.5438	1.8611	0.3924
C	-3.6164	2.8979	0.3766
C	-2.2878	2.6225	0.0008
C	-0.4371	1.069	-0.6839
C	-0.2137	-0.1724	-1.5191
C	-1.1632	-1.2256	-1.4959
C	-2.4618	-1.0389	-0.8529
C	0.9412	-0.3065	-2.2826
C	1.1849	-1.4915	-2.9924
C	0.2914	-2.549	-2.9495
C	-0.893	-2.4304	-2.2062
O	3.2889	-1.9945	0.784
O	-3.2888	-1.9946	-0.784
H	-0.0478	1.9298	-1.2371
H	0.0478	1.9298	1.2372
C	4.026	4.3054	-0.7371
C	-4.0261	4.3053	0.7371
O	1.7383	-3.471	2.2142
O	5.1208	-0.3897	-0.0599
O	-1.7382	-3.4709	-2.2143
O	-5.1208	-0.3898	0.0599
H	2.5156	-3.2159	1.654
H	4.6859	-1.2365	0.2206
H	-2.5155	-3.2158	-1.6541
H	-4.6859	-1.2366	-0.2206
H	1.5595	3.431	0.0015
H	5.5746	2.0327	-0.6868
H	-0.4701	-3.4745	3.4867
H	-2.0922	-1.582	3.5837
H	-1.6582	0.506	2.3278
H	-5.5746	2.0326	0.6868
H	-1.5595	3.4311	-0.0014
H	1.6582	0.5061	-2.3278
H	2.0922	-1.5818	-3.5838
H	0.4701	-3.4743	-3.4869
H	3.2912	4.778	-1.3987
H	4.999	4.3253	-1.2364
H	4.1006	4.9321	0.1612
H	-4.1002	4.9322	-0.1611
H	-4.9994	4.3253	1.236
H	-3.2915	4.7777	1.3993

Cartesian coordinates of anti form of **1a** optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	2.8533	-0.1155	0.0526
C	1.7276	-0.6818	-0.6001
C	1.7922	-1.9768	-1.0845
C	2.9536	-2.7614	-0.9177
C	4.043	-2.2287	-0.2398
C	4.0114	-0.9143	0.2523
C	2.8819	1.3074	0.3712
C	1.8529	2.1697	-0.2127
C	0.7274	1.5971	-0.858
C	0.4488	0.1221	-0.6712
C	2.0545	3.5766	-0.2659
C	1.1658	4.3766	-1.0024
C	0.0989	3.7894	-1.6647
C	-0.1327	2.4074	-1.5871
C	-1.7279	0.682	0.5997
C	-2.8536	0.1153	-0.0526
C	-4.0119	0.9138	-0.2521
C	-4.0438	2.2283	0.2395
C	-2.9543	2.7614	0.9171
C	-1.7927	1.9771	1.0839
C	-0.4489	-0.1216	0.6708
C	-0.7271	-1.5967	0.8578
C	-1.8525	-2.1696	0.2129
C	-2.882	-1.3077	-0.3708
C	0.1335	-2.4066	1.5868
C	-0.0977	-3.7887	1.6646
C	-1.1647	-4.3762	1.0027
C	-2.0537	-3.5766	0.2663
O	3.8397	1.8035	1.0342
O	-3.8399	-1.8042	-1.0335
H	0.1634	0.2403	1.5027
H	-0.1636	-0.2396	-1.5032
C	2.988	-4.169	-1.4592
C	-2.989	4.1691	1.4584
O	3.0834	4.1823	0.3457
O	5.103	-0.4544	0.8811
O	-3.0827	-4.1826	-0.3449
O	-5.1036	0.4535	-0.8806
H	3.611	3.4724	0.7938
H	4.9121	0.4842	1.1386
H	-3.6106	-3.4728	-0.7929
H	-4.9126	-0.4851	-1.138
H	0.9274	-2.4086	-1.581
H	4.9479	-2.8082	-0.0842
H	1.3506	5.4449	-1.0458
H	-0.575	4.4112	-2.2482
H	-0.9947	1.9736	-2.0842
H	-4.9488	2.8076	0.084
H	-0.9278	2.4092	1.58
H	0.9956	-1.9726	2.0835
H	0.5765	-4.4102	2.2479
H	-1.3492	-5.4446	1.0463
H	2.8467	-4.1751	-2.5471
H	3.938	-4.6639	-1.2385
H	2.179	-4.7717	-1.0284
H	-2.8502	4.1751	2.5467
H	-3.9381	4.6646	1.2355
H	-2.1786	4.7712	1.0295

Cartesian coordinates of anti form of **1b** optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	2.5349	0.9411	0.0924
C	1.2812	0.8977	0.7544
C	0.7976	2.029	1.3891
C	1.5179	3.2423	1.3668
C	2.7234	3.3052	0.6778
C	3.2452	2.1705	0.0367
C	3.1581	-0.2883	-0.3857
C	2.5937	-1.5663	0.0507
C	1.3366	-1.6029	0.7068
C	0.4604	-0.3699	0.6737
C	3.3716	-2.753	-0.046
C	2.9107	-3.9346	0.5571
C	1.701	-3.9354	1.2331
C	0.9059	-2.7807	1.302
C	-1.2812	0.8977	-0.7544
C	-2.5349	0.9411	-0.0924
C	-3.2452	2.1705	-0.0367
C	-2.7234	3.3052	-0.6778
C	-1.5179	3.2423	-1.3668
C	-0.7976	2.0289	-1.3891
C	-0.4603	-0.3699	-0.6737
C	-1.3366	-1.6029	-0.7068
C	-2.5937	-1.5663	-0.0507
C	-3.1581	-0.2883	0.3858
C	-0.9059	-2.7807	-1.302
C	-1.701	-3.9354	-1.2331
C	-2.9107	-3.9346	-0.5571
C	-3.3716	-2.753	0.046
O	4.2302	-0.2512	-1.0582
O	-4.2302	-0.2512	1.0582
H	0.2444	-0.4004	-1.5106
H	-0.2444	-0.4004	1.5106
C	0.9658	4.4522	2.0797
C	-0.9658	4.4522	-2.0797
O	4.5546	-2.7905	-0.6769
O	4.423	2.2932	-0.5933
O	-4.5546	-2.7905	0.6769
O	-4.423	2.2932	0.5933
H	4.7269	-1.8764	-1.0203
H	4.6442	1.4012	-0.9655
H	-4.7269	-1.8764	1.0203
H	-4.6442	1.4012	0.9656
H	-0.1645	1.9919	1.893
H	3.2984	4.225	0.6313
H	3.529	-4.8234	0.4863
H	1.3566	-4.8491	1.7102
H	-0.054	-2.8129	1.8076
H	-3.2984	4.225	-0.6313
H	0.1645	1.9918	-1.893
H	0.054	-2.8129	-1.8076
H	-1.3566	-4.8491	-1.7102
H	-3.529	-4.8234	-0.4863
H	0.911	4.2774	3.1616
H	1.5856	5.3377	1.9128
H	-0.0528	4.6758	1.7404
H	0.0528	4.6757	-1.7405
H	-1.5856	5.3377	-1.9128
H	-0.911	4.2774	-3.1616

Cartesian coordinates of **2**-I optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	-0.9462	-1.1108	1.6021
C	-0.0097	-0.049	1.5137
C	1.2384	-0.1825	2.1044
C	1.6222	-1.3798	2.7434
C	0.7232	-2.4369	2.7993
C	-0.5604	-2.3189	2.2457
C	-2.3218	-0.9282	1.1537
C	-2.7652	0.3979	0.7449
C	-1.8395	1.4595	0.6097
C	-0.3526	1.1962	0.7267
C	-4.1509	0.6574	0.5298
C	-4.582	1.9501	0.2156
C	-3.6515	2.9802	0.1113
C	-2.2805	2.7382	0.3019
C	1.8164	1.4566	-0.6226
C	2.7294	0.3826	-0.7167
C	4.1066	0.6224	-0.4576
C	4.5435	1.9198	-0.1568
C	3.6452	2.9814	-0.1009
C	2.278	2.7333	-0.3259
C	0.329	1.2044	-0.7483
C	-0.0128	-0.0334	-1.5475
C	0.9142	-1.1074	-1.6096
C	2.272	-0.947	-1.1197
C	-1.2444	-0.139	-2.1718
C	-1.5926	-1.3289	-2.8385
C	-0.7216	-2.4125	-2.8788
C	0.5337	-2.3122	-2.2708
O	-3.1457	-1.8921	1.1965
O	3.0819	-1.9237	-1.1212
H	-0.123	2.0716	-1.2398
H	0.1029	2.0587	1.2239
C	3.0076	-1.5026	3.3284
C	4.1266	4.3848	0.1776
O	-5.0808	-0.3016	0.6233
O	-1.3858	-3.3697	2.3621
O	1.3488	-3.3713	-2.3535
O	5.0246	-0.3573	-0.4835
H	-4.5972	-1.1439	0.8382
H	-2.2408	-3.1102	1.931
H	2.1879	-3.1226	-1.8827
H	4.5405	-1.1923	-0.7182
O	-4.0113	4.2586	-0.1796
H	-5.6442	2.121	0.0632
O	-2.8153	-1.3563	-3.4288
H	-0.9826	-3.339	-3.3827
H	-4.9754	4.3039	-0.2819
H	-2.9528	-2.2238	-3.8417
H	1.9433	0.6421	2.0637
H	0.9849	-3.3748	3.2793
H	-1.5884	3.5691	0.2053
H	5.6032	2.0697	0.0266
H	1.5716	3.5587	-0.2643
H	-1.9604	0.6744	-2.1561
H	3.2172	-0.6825	4.0257
H	3.7669	-1.4531	2.5375
H	3.1377	-2.4475	3.8636
H	4.1746	4.9715	-0.7492
H	5.1268	4.3859	0.6209
H	3.4488	4.9127	0.8577

Cartesian coordinates of **2**-II optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	-2.7295	0.3825	-0.7168
C	-1.8164	1.4565	-0.6226
C	-2.2781	2.7332	-0.326
C	-3.6453	2.9813	-0.1011
C	-4.5436	1.9197	-0.1569
C	-4.1066	0.6223	-0.4577
C	-2.2719	-0.9471	-1.1197
C	-0.9141	-1.1074	-1.6096
C	0.0128	-0.0333	-1.5475
C	-0.329	1.2044	-0.7484
C	-0.5334	-2.3121	-2.2707
C	0.7219	-2.4124	-2.8788
C	1.5928	-1.3286	-2.8385
C	1.2445	-0.1388	-2.1719
C	0.0096	-0.0491	1.5137
C	0.946	-1.1108	1.602
C	0.5604	-2.319	2.2456
C	-0.7231	-2.4369	2.7994
C	-1.6222	-1.3798	2.7435
C	-1.2385	-0.1826	2.1045
C	0.3525	1.1962	0.7267
C	1.8394	1.4595	0.6098
C	2.7651	0.398	0.745
C	2.3217	-0.9283	1.1535
C	2.2804	2.7383	0.3022
C	3.6514	2.9804	0.1116
C	4.5819	1.9502	0.2158
C	4.1508	0.6574	0.5299
O	-3.0818	-1.9238	-1.1215
O	3.1455	-1.8922	1.1961
H	-0.1031	2.0586	1.2239
H	0.1229	2.0717	-1.2398
C	-4.1268	4.3847	0.1772
C	-3.0075	-1.5027	3.3288
O	-1.3484	-3.3714	-2.3535
O	-5.0247	-0.3574	-0.4835
O	5.0806	-0.3015	0.6232
O	1.3859	-3.3696	2.362
H	-2.1874	-3.1228	-1.8825
H	-4.5407	-1.1925	-0.7175
H	4.597	-1.1439	0.838
H	2.2408	-3.1099	1.9308
O	2.8155	-1.356	-3.4288
H	0.983	-3.3388	-3.3827
O	4.0112	4.2588	-0.1792
H	5.6441	2.1211	0.0634
H	2.953	-2.2236	-3.8416
H	4.9753	4.3039	-0.2815
H	-1.5717	3.5586	-0.2644
H	-5.6033	2.0695	0.0264
H	1.9603	0.6747	-2.1562
H	-0.9847	-3.3749	3.2795
H	-1.9434	0.6421	2.0638
H	1.5883	3.5692	0.2057
H	-4.1758	4.971	-0.7498
H	-5.1266	4.3857	0.6214
H	-3.4485	4.913	0.8566
H	-3.7669	-1.4538	2.5379
H	-3.1372	-2.4474	3.8645
H	-3.2172	-0.6822	4.0256

Cartesian coordinates of **2**-III optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	0.8985	-1.0967	-1.614
C	-0.0279	-0.026	-1.5287
C	-1.2775	-0.1495	-2.118
C	-1.6694	-1.3427	-2.7597
C	-0.7796	-2.4077	-2.8144
C	0.5029	-2.3025	-2.2556
C	2.2727	-0.928	-1.1576
C	2.7303	0.3973	-0.7601
C	1.8171	1.4714	-0.6428
C	0.328	1.2168	-0.7439
C	4.1161	0.6401	-0.531
C	4.5624	1.9318	-0.2348
C	3.6449	2.9768	-0.1582
C	2.272	2.7493	-0.3523
C	0.0277	-0.0253	1.5288
C	-0.8985	-1.0962	1.6143
C	-0.5025	-2.3017	2.2564
C	0.78	-2.4062	2.8154
C	1.6695	-1.341	2.7605
C	1.2773	-0.1482	2.1183
C	-0.3283	1.2171	0.7435
C	-1.8173	1.4715	0.6423
C	-2.7305	0.3974	0.7598
C	-2.2727	-0.9278	1.1575
C	-2.2722	2.7494	0.3515
C	-3.6451	2.9768	0.1574
C	-4.5626	1.9318	0.2341
C	-4.1163	0.6402	0.5306
O	3.0852	-1.902	-1.185
O	-3.0851	-1.9019	1.1848
H	0.1311	2.083	1.2307
H	-0.1314	2.0825	-1.2315
C	-3.0534	-1.4536	-3.3506
C	3.0534	-1.4513	3.3517
O	5.0311	-0.3379	-0.5857
O	1.3176	-3.3618	-2.3665
O	-5.0315	-0.3376	0.5853
O	-1.3165	-3.3616	2.3678
H	4.5379	-1.1723	-0.8126
H	2.1712	-3.1139	-1.9265
H	-4.5386	-1.1722	0.8121
H	-2.1701	-3.1151	1.9277
O	4.0203	4.2549	0.112
H	5.6254	2.091	-0.075
O	-4.0206	4.2549	-0.1131
H	-5.6255	2.0909	0.0742
H	4.9849	4.2907	0.2131
H	-4.9852	4.2906	-0.2142
H	-1.9756	0.6811	-2.0762
H	-1.0486	-3.343	-3.2955
H	1.5894	3.5894	-0.2701
H	1.0492	-3.3413	3.2968
H	1.9752	0.6826	2.0762
H	-1.5896	3.5895	0.2691
H	-3.2567	-0.6262	-4.0411
H	-3.1859	-2.393	-3.8949
H	-3.8156	-1.4086	-2.5621
H	3.1863	-2.3907	3.8958
H	3.8158	-1.4057	2.5634
H	3.256	-0.6239	4.0424

Cartesian coordinates of **2**-IV optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	-2.77	0.3839	-0.6942
C	-1.8406	1.4425	-0.5822
C	-2.2837	2.7213	-0.2673
C	-3.648	2.9882	-0.0449
C	-4.5635	1.9443	-0.1291
C	-4.1466	0.6445	-0.4494
C	-2.3319	-0.9474	-1.1111
C	-0.974	-1.1245	-1.5967
C	-0.0334	-0.0625	-1.5322
C	-0.3564	1.1782	-0.7291
C	-0.6101	-2.3306	-2.2653
C	0.6428	-2.4447	-2.8757
C	1.5266	-1.3714	-2.8346
C	1.1942	-0.18	-2.1629
C	1.8406	1.4426	0.5823
C	2.77	0.384	0.6942
C	4.1466	0.6446	0.4494
C	4.5635	1.9444	0.1292
C	3.648	2.9882	0.045
C	2.2837	2.7213	0.2674
C	0.3564	1.1782	0.7292
C	0.0334	-0.0626	1.5323
C	0.974	-1.1246	1.5967
C	2.3319	-0.9474	1.1109
C	-1.1942	-0.1801	2.163
C	-1.5266	-1.3715	2.8346
C	-0.6427	-2.4448	2.8757
C	0.6102	-2.3306	2.2654
O	-3.1564	-1.9115	-1.1279
O	3.1564	-1.9115	1.1275
H	-0.0906	2.041	1.233
H	0.0906	2.041	-1.2329
C	-4.1067	4.394	0.2589
C	4.1066	4.3941	-0.2589
O	-1.4396	-3.3783	-2.3529
O	-5.0841	-0.3121	-0.5169
O	1.4397	-3.3784	2.3529
O	5.084	-0.3121	0.5169
H	-2.2779	-3.1163	-1.8871
H	-4.6122	-1.1573	-0.7364
H	2.2781	-3.1163	1.8873
H	4.612	-1.1572	0.7367
O	2.7465	-1.4105	-3.4297
H	0.8906	-3.3718	-3.385
O	-2.7465	-1.4106	3.4297
H	-0.8905	-3.372	3.385
H	2.8732	-2.2783	-3.8455
H	-2.8733	-2.2785	3.8454
H	-1.5652	3.5351	-0.192
H	-5.6222	2.1089	0.0467
H	1.9194	0.6249	-2.1481
H	5.6222	2.109	-0.0466
H	1.5651	3.5352	0.1922
H	-1.9194	0.6248	2.1482
H	-4.1152	5.0074	-0.6517
H	-5.1186	4.4051	0.6744
H	-3.4374	4.8871	0.9729
H	3.4386	4.8863	-0.9748
H	5.1193	4.4053	-0.6724
H	4.1128	5.0082	0.6512

Cartesian coordinates of **3**-I optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	−2.8781	0.5382	−0.8890
C	−1.8507	1.5082	−0.8818
C	−2.1748	2.8587	−0.8288
C	−3.5142	3.2866	−0.7674
C	−4.5280	2.3337	−0.7379
C	−4.2310	0.9650	−0.7945
C	−2.5586	−0.8817	−1.0411
C	−1.2003	−1.2661	−1.3773
C	−0.1556	−0.3025	−1.4019
C	−0.3989	1.0804	−0.8381
C	−0.9185	−2.5955	−1.8017
C	0.3567	−2.9386	−2.2698
C	1.3491	−1.9639	−2.3238
C	1.0922	−0.6459	−1.8869
C	−0.3606	0.1884	1.6121
C	0.4373	−0.9351	1.9483
C	−0.1300	−1.9719	2.7395
C	−1.4536	−1.8621	3.1910
C	−2.2174	−0.7418	2.8902
C	−1.6536	0.2855	2.1059
C	0.1777	1.2436	0.6709
C	1.6898	1.3267	0.6420
C	2.4739	0.2104	1.0232
C	1.8522	−0.9750	1.5962
C	2.2998	2.4800	0.1791
C	3.7036	2.5505	0.0721
C	4.4970	1.4589	0.4185
C	3.8893	0.2882	0.8910
O	−3.4799	−1.7514	−0.9637
O	2.5526	−1.9996	1.8617
H	−0.2056	2.2190	0.9878
H	0.1851	1.8011	−1.4192
C	−3.8403	4.7606	−0.7532
C	−3.6456	−0.6223	3.3625
O	−1.8473	−3.5609	−1.7912
O	−5.2568	0.0993	−0.7514
O	4.6936	−0.7339	1.2133
O	0.5580	−3.0680	3.0926
H	−2.6826	−3.1487	−1.4448
H	−4.8609	−0.8101	−0.8093
H	4.1015	−1.4739	1.5156
H	1.4646	−2.9735	2.7004
O	2.6064	−2.1797	−2.7786
H	0.5194	−3.9605	−2.5873
O	4.1880	3.7321	−0.3843
H	5.5768	1.4715	0.3436
C	2.9587	−3.4877	−3.2152
C	5.5968	3.8853	−0.5152
H	2.3418	−3.8039	−4.0654
H	6.0120	3.1637	−1.2294
H	−1.3798	3.6018	−0.8335
H	−5.5722	2.6250	−0.6754
H	1.9004	0.0746	−1.9332
H	−1.8553	−2.6746	3.7886
H	−2.2534	1.1598	1.8729
H	1.7197	3.3516	−0.1086
H	−3.7386	5.1921	−1.7577
H	−4.8659	4.9421	−0.4183
H	−3.1610	5.3140	−0.0951
H	−4.3372	−0.6431	2.5106
H	−3.9171	−1.4385	4.0381
H	−3.8115	0.3263	3.8871
H	4.0026	−3.4245	−3.5257
H	2.8620	−4.2178	−2.4026
H	5.7508	4.8983	−0.8901
H	6.1020	3.7722	0.4519

Cartesian coordinates of **3**-II optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	-0.4372	-0.9355	1.9481
C	0.3607	0.1881	1.6122
C	1.6537	0.2850	2.1060
C	2.2175	-0.7426	2.8899
C	1.4536	-1.8630	3.1904
C	0.1300	-1.9725	2.7390
C	-1.8522	-0.9751	1.5961
C	-2.4738	0.2104	1.0234
C	-1.6896	1.3267	0.6423
C	-0.1775	1.2436	0.6713
C	-3.8892	0.2881	0.8912
C	-4.4969	1.4588	0.4188
C	-3.7035	2.5505	0.0726
C	-2.2997	2.4800	0.1795
C	1.8509	1.5083	-0.8815
C	2.8782	0.5383	-0.8889
C	4.2311	0.9649	-0.7945
C	4.5282	2.3336	-0.7378
C	3.5145	3.2867	-0.7670
C	2.1750	2.8588	-0.8283
C	0.3990	1.0806	-0.8378
C	0.1556	-0.3021	-1.4019
C	1.2002	-1.2658	-1.3775
C	2.5585	-0.8816	-1.0411
C	-1.0923	-0.6453	-1.8869
C	-1.3494	-1.9631	-2.3241
C	-0.3571	-2.9380	-2.2703
C	0.9181	-2.5951	-1.8021
O	-2.5526	-1.9997	1.8615
O	3.4796	-1.7515	-0.9637
H	-0.1849	1.8015	-1.4187
H	0.2058	2.2189	0.9883
C	3.6458	-0.6235	3.3620
C	3.8406	4.7606	-0.7522
O	-4.6933	-0.7341	1.2135
O	-0.5581	-3.0687	3.0918
O	1.8468	-3.5607	-1.7919
O	5.2569	0.0993	-0.7518
H	-4.1008	-1.4739	1.5160
H	-1.4648	-2.9738	2.6998
H	2.6821	-3.1490	-1.4455
H	4.8612	-0.8101	-0.8099
O	-4.1879	3.7322	-0.3837
H	-5.5767	1.4715	0.3440
O	-2.6068	-2.1786	-2.7789
H	-0.5199	-3.9598	-2.5880
C	-5.5967	3.8853	-0.5149
C	-2.9593	-3.4866	-3.2153
H	-6.0116	3.1639	-1.2294
H	-2.3428	-3.8030	-4.0657
H	2.2536	1.1593	1.8734
H	1.8553	-2.6757	3.7878
H	-1.7196	3.3517	-0.1080
H	5.5724	2.6249	-0.6754
H	1.3801	3.6020	-0.8329
H	-1.9004	0.0754	-1.9330
H	3.8129	0.3264	3.8839
H	4.3373	-0.6475	2.5100
H	3.9164	-1.4382	4.0398
H	3.7339	5.1936	-1.7555
H	4.8677	4.9417	-0.4218
H	3.1644	5.3129	-0.0900
H	-6.1021	3.7720	0.4519
H	-5.7506	4.8983	-0.8897
H	-2.8624	-4.2167	-2.4027
H	-4.0034	-3.4233	-3.5253

Cartesian coordinates of **3**-III optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	−0.8660	−1.3582	1.6359
C	0.0567	−0.2862	1.5296
C	1.3177	−0.4060	2.0954
C	1.7238	−1.5963	2.7332
C	0.8368	−2.6624	2.8088
C	−0.4561	−2.5611	2.2739
C	−2.2491	−1.1942	1.2038
C	−2.7161	0.1281	0.8103
C	−1.8070	1.2054	0.6737
C	−0.3155	0.9545	0.7482
C	−4.1033	0.3699	0.6044
C	−4.5654	1.6597	0.3114
C	−3.6527	2.7085	0.2153
C	−2.2729	2.4774	0.3883
C	−0.0566	−0.2869	−1.5298
C	0.8662	−1.3589	−1.6358
C	0.4561	−2.5622	−2.2731
C	−0.8370	−2.6639	−2.8074
C	−1.7240	−1.5977	−2.7322
C	−1.3177	−0.4070	−2.0952
C	0.3156	0.9542	−0.7491
C	1.8071	1.2051	−0.6745
C	2.7162	0.1278	−0.8108
C	2.2494	−1.1945	−1.2042
C	2.2729	2.4772	−0.3893
C	3.6526	2.7084	−0.2160
C	4.5654	1.6595	−0.3117
C	4.1034	0.3697	−0.6045
O	−3.0585	−2.1705	1.2491
O	3.0591	−2.1706	−1.2499
H	−0.1509	1.8212	−1.2276
H	0.1510	1.8218	1.2264
C	3.1195	−1.7034	3.2969
C	−3.1198	−1.7052	−3.2956
O	−5.0169	−0.6091	0.6776
O	−1.2669	−3.6217	2.4036
O	5.0169	−0.6095	−0.6772
O	1.2667	−3.6229	−2.4023
H	−4.5192	−1.4425	0.8979
H	−2.1287	−3.3762	1.9782
H	4.5191	−1.4427	−0.8976
H	2.1288	−3.3772	−1.9777
O	−3.9928	3.9941	−0.0501
H	−5.6304	1.7955	0.1739
O	3.9927	3.9939	0.0492
H	5.6304	1.7953	−0.1739
C	−5.3682	4.3119	−0.2310
C	5.3681	4.3117	0.2306
H	−5.7927	3.7750	−1.0882
H	5.7922	3.7749	1.0881
H	2.0139	0.4251	2.0360
H	1.1165	−3.5958	3.2876
H	−1.5956	3.3203	0.2895
H	−1.1168	−3.5975	−3.2855
H	−2.0140	0.4240	−2.0362
H	1.5956	3.3201	−0.2908
H	3.3355	−0.8733	3.9802
H	3.2637	−2.6407	3.8419
H	3.8658	−1.6605	2.4934
H	−3.2645	−2.6432	−3.8392
H	−3.8660	−1.6608	−2.4920
H	−3.3356	−0.8760	−3.9801
H	−5.9525	4.0816	0.6682
H	−5.4012	5.3856	−0.4219
H	5.9527	4.0812	−0.6683
H	5.4010	5.3854	0.4212

Cartesian coordinates of **3**-IV optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	-2.6206	0.5425	-1.1401
C	-1.7183	1.5982	-0.8781
C	-2.2027	2.8794	-0.6436
C	-3.5838	3.1517	-0.6507
C	-4.4768	2.1108	-0.8829
C	-4.0175	0.8087	-1.1264
C	-2.1253	-0.7922	-1.4764
C	-0.7078	-0.9749	-1.7314
C	0.2144	0.0849	-1.5153
C	-0.2309	1.3290	-0.7779
C	-0.2396	-2.1821	-2.3241
C	1.0983	-2.3102	-2.7192
C	1.9691	-1.2395	-2.5368
C	1.5258	-0.0423	-1.9335
C	1.7184	1.5984	0.8777
C	2.6207	0.5427	1.1400
C	4.0175	0.8090	1.1266
C	4.4768	2.1111	0.8828
C	3.5839	3.1519	0.6502
C	2.2028	2.8795	0.6431
C	0.2309	1.3292	0.7776
C	-0.2143	0.0852	1.5152
C	0.7079	-0.9746	1.7314
C	2.1254	-0.7919	1.4765
C	-1.5257	-0.0418	1.9335
C	-1.9690	-1.2389	2.5372
C	-1.0982	-2.3095	2.7198
C	0.2397	-2.1816	2.3244
O	-2.9407	-1.7534	-1.6263
O	2.9407	-1.7531	1.6265
H	-0.2958	2.1896	1.2024
H	0.2959	2.1894	-1.2029
C	-4.0806	4.5597	-0.4271
C	4.0806	4.5598	0.4258
O	-1.0465	-3.2290	-2.5441
O	-4.9345	-0.1458	-1.3450
O	1.0465	-3.2285	2.5447
O	4.9345	-0.1454	1.3456
H	-1.9493	-2.9631	-2.2242
H	-4.4341	-0.9924	-1.4824
H	1.9492	-2.9628	2.2243
H	4.4343	-0.9920	1.4833
O	3.2730	-1.2460	-2.9022
H	1.4044	-3.2455	-3.1699
O	-3.2729	-1.2451	2.9025
H	-1.4042	-3.2447	3.1708
C	3.8094	-2.4243	-3.4934
C	-3.8101	-2.4231	3.4937
H	3.2997	-2.6657	-4.4343
H	-3.3030	-2.6630	4.4363
H	-1.5032	3.6907	-0.4519
H	-5.5493	2.2796	-0.8853
H	2.2439	0.7581	-1.7996
H	5.5494	2.2800	0.8855
H	1.5033	3.6908	0.4511
H	-2.2437	0.7586	1.7995
H	-5.1557	4.5789	-0.2262
H	-3.8960	5.1845	-1.3108
H	-3.5662	5.0352	0.4159
H	5.1571	4.5797	0.2329
H	3.5721	5.0317	-0.4229
H	3.8882	5.1874	1.3057
H	4.8589	-2.2033	-3.6931
H	3.7387	-3.2793	-2.8104
H	-4.8603	-2.2025	3.6902
H	-3.7370	-3.2789	2.8118

Cartesian coordinates of **4**-I optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	1.3647	-1.1751	-1.2286
C	0.3299	-0.2260	-1.3944
C	-0.8734	-0.5881	-1.9984
C	-1.1240	-1.9087	-2.3804
C	-0.1218	-2.8618	-2.1976
C	1.1180	-2.5156	-1.6441
C	2.6862	-0.7393	-0.7170
C	2.9357	0.7051	-0.5937
C	1.8988	1.6499	-0.7283
C	0.4693	1.1805	-0.8568
C	4.2639	1.1724	-0.3644
C	4.5266	2.5463	-0.3192
C	3.4847	3.4549	-0.4830
C	2.1680	3.0124	-0.6797
C	-1.7968	1.5410	0.3195
C	-2.6910	0.4712	0.5112
C	-4.0710	0.6849	0.2216
C	-4.5037	1.9313	-0.2413
C	-3.6053	2.9891	-0.4255
C	-2.2569	2.7774	-0.1444
C	-0.3096	1.3764	0.5558
C	0.0204	0.2940	1.5535
C	-0.8566	-0.8089	1.6786
C	-2.1771	-0.8188	1.0437
C	1.2013	0.3442	2.2782
C	1.5450	-0.7284	3.1202
C	0.7276	-1.8497	3.2247
C	-0.4681	-1.9057	2.5003
O	3.5989	-1.5507	-0.4643
O	-2.8645	-1.8602	1.0197
H	0.0711	2.3307	0.9330
H	-0.0491	1.8627	-1.5387
C	-2.4769	-2.3022	-2.9188
C	-4.1046	4.3334	-0.8983
O	5.2916	0.3332	-0.1920
O	2.1138	-3.4168	-1.4903
O	-1.2264	-3.0036	2.6237
O	-4.9215	-0.3490	0.4234
H	4.8951	-0.5861	-0.2223
H	-2.0069	-2.8628	2.0163
H	-1.6432	0.1628	-2.1454
H	-0.3157	-3.8856	-2.4939
H	5.5494	2.8737	-0.1520
H	1.3801	3.7506	-0.7937
H	-5.5530	2.0949	-0.4581
H	-1.5487	3.5921	-0.2788
H	1.8797	1.1858	2.2008
H	0.9931	-2.6930	3.8566
H	-2.4440	-3.2635	-3.4412
H	-3.1934	-2.3917	-2.0915
H	-2.8678	-1.5478	-3.6106
H	-4.7385	4.2336	-1.7873
H	-3.2761	5.0035	-1.1464
H	-4.7097	4.8240	-0.1251
C	-6.3105	-0.1549	0.2067
H	-6.7793	-1.1077	0.4579
H	-6.7156	0.6331	0.8547
H	-6.5268	0.0909	-0.8413
C	1.9058	-4.7596	-1.9006
H	1.6944	-4.8276	-2.9757
H	2.8415	-5.2766	-1.6822
H	1.0898	-5.2320	-1.3388
O	3.6841	4.8027	-0.4557
H	4.6286	4.9784	-0.3190
O	2.7106	-0.6116	3.8110
H	2.8597	-1.4230	4.3218

Cartesian coordinates of **4**-II optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	2.6910	0.4711	0.5112
C	1.7969	1.5409	0.3194
C	2.2570	2.7774	-0.1445
C	3.6054	2.9890	-0.4256
C	4.5038	1.9312	-0.2415
C	4.0710	0.6847	0.2214
C	2.1771	-0.8188	1.0438
C	0.8566	-0.8089	1.6787
C	-0.0203	0.2941	1.5535
C	0.3097	1.3764	0.5557
C	0.4681	-1.9056	2.5005
C	-0.7275	-1.8496	3.2249
C	-1.5449	-0.7282	3.1202
C	-1.2012	0.3443	2.2783
C	-0.3299	-0.2261	-1.3943
C	-1.3648	-1.1751	-1.2285
C	-1.1182	-2.5156	-1.6441
C	0.1216	-2.8619	-2.1976
C	1.1238	-1.9089	-2.3803
C	0.8734	-0.5883	-1.9983
C	-0.4692	1.1804	-0.8568
C	-1.8988	1.6499	-0.7284
C	-2.9356	0.7051	-0.5937
C	-2.6862	-0.7393	-0.7168
C	-2.1679	3.0124	-0.6798
C	-3.4846	3.4549	-0.4831
C	-4.5265	2.5464	-0.3192
C	-4.2638	1.1725	-0.3644
O	2.8645	-1.8602	1.0199
O	-3.5989	-1.5507	-0.4638
H	0.0492	1.8626	-1.5388
H	-0.0710	2.3307	0.9329
C	4.1047	4.3334	-0.8984
C	2.4768	-2.3025	-2.9186
O	1.2265	-3.0035	2.6239
O	4.9214	-0.3492	0.4230
O	-5.2916	0.3333	-0.1919
O	-2.1142	-3.4167	-1.4904
H	2.0070	-2.8626	2.0166
H	-4.8951	-0.5859	-0.2221
H	1.5489	3.5921	-0.2788
H	5.5531	2.0946	-0.4585
H	-0.9930	-2.6928	3.8569
H	-1.8797	1.1859	2.2008
H	0.3154	-3.8858	-2.4939
H	1.6432	0.1626	-2.1454
H	-1.3800	3.7506	-0.7939
H	-5.5493	2.8738	-0.1521
H	4.7102	4.8238	-0.1254
H	4.7382	4.2336	-1.7877
H	3.2762	5.0036	-1.1461
H	3.1932	-2.3919	-2.0913
H	2.8678	-1.5481	-3.6105
H	2.4438	-3.2639	-3.4409
C	-1.9063	-4.7594	-1.9009
H	-2.8422	-5.2763	-1.6827
H	-1.6948	-4.8273	-2.9760
H	-1.0906	-5.2321	-1.3392
C	6.3105	-0.1550	0.2066
H	6.7154	0.6330	0.8547
H	6.7793	-1.1077	0.4579
H	6.5271	0.0907	-0.8413
O	-2.7105	-0.6114	3.8111
H	-2.8597	-1.4229	4.3218
O	-3.6840	4.8027	-0.4559
H	-4.6285	4.9785	-0.3194

Cartesian coordinates of **4**-III optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	-4.5574	2.1466	0.2017
C	-3.6613	3.2126	0.1712
C	-2.2883	3.0062	0.3762
C	-1.8176	1.7263	0.6416
C	-2.7051	0.6342	0.7224
C	-4.0891	0.8540	0.4629
C	-0.3312	1.4814	0.7420
C	0.0275	0.2462	1.5374
C	-0.8655	-0.8474	1.6220
C	-2.2381	-0.7140	1.0801
C	1.2792	0.1865	2.1472
C	1.7095	-0.9679	2.8076
C	0.8456	-2.0609	2.8817
C	-0.4331	-2.0166	2.3104
C	0.3313	1.4814	-0.7420
C	1.8176	1.7263	-0.6417
C	2.7052	0.6341	-0.7225
C	2.2381	-0.7140	-1.0801
C	0.8655	-0.8475	-1.6220
C	-0.0275	0.2462	-1.5374
C	0.4330	-2.0166	-2.3103
C	-0.8457	-2.0610	-2.8815
C	-1.7096	-0.9680	-2.8075
C	-1.2792	0.1865	-2.1472
C	2.2884	3.0062	-0.3763
C	3.6614	3.2125	-0.1712
C	4.5575	2.1465	-0.2018
C	4.0891	0.8539	-0.4630
O	-3.0160	-1.6855	0.9909
O	3.0160	-1.6856	-0.9909
C	3.0992	-1.0361	3.3920
C	-3.0993	-1.0361	-3.3918
O	-4.9765	-0.1502	0.4535
O	-1.2986	-3.0526	2.3978
O	4.9765	-0.1503	-0.4537
O	1.2985	-3.0527	-2.3977
H	-4.4438	-0.9782	0.6409
C	-0.9156	-4.2181	3.1115
H	4.4439	-0.9783	-0.6412
C	0.9155	-4.2182	-3.1115
H	0.1273	2.3489	1.2275
H	-0.1273	2.3489	-1.2276
H	1.1794	-2.9555	3.3935
H	-1.1795	-2.9556	-3.3933
H	0.0460	-4.7063	-2.6528
H	-0.0461	-4.7062	2.6529
H	-5.6200	2.2885	0.0227
H	-1.6170	3.8577	0.3209
H	1.9402	1.0459	2.0915
H	-1.9402	1.0459	-2.0914
H	1.6171	3.8577	-0.3209
H	5.6201	2.2883	-0.0228
H	3.3262	-0.1426	3.9849
H	3.8483	-1.0909	2.5915
H	3.2277	-1.9137	4.0329
H	-3.8484	-1.0909	-2.5913
H	-3.2279	-1.9137	-4.0327
H	-3.3263	-0.1426	-3.9848
H	-0.6939	-3.9954	4.1634
H	-1.7761	-4.8869	3.0565
H	0.6937	-3.9954	-4.1633
H	1.7759	-4.8870	-3.0565
O	-4.0626	4.4919	-0.0687
H	-5.0263	4.5053	-0.1812
O	4.0627	4.4918	0.0688
H	5.0264	4.5051	0.1812

Cartesian coordinates of **4**-IV optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	0.6278	-2.4250	-2.8979
C	1.4896	-1.3335	-2.9033
C	1.1619	-0.1479	-2.2234
C	-0.0443	-0.0574	-1.5438
C	-0.9638	-1.1311	-1.5628
C	-0.5976	-2.3374	-2.2274
C	-0.3658	1.1667	-0.7232
C	-1.8511	1.4123	-0.5557
C	-2.7824	0.3607	-0.6399
C	-2.3125	-1.0035	-1.0010
C	-2.2716	2.7129	-0.2603
C	-3.6152	3.0066	-0.0364
C	-4.5502	1.9681	-0.1117
C	-4.1588	0.6597	-0.4136
C	0.3658	1.1667	0.7232
C	0.0443	-0.0574	1.5438
C	0.9638	-1.1311	1.5628
C	2.3125	-1.0035	1.0009
C	2.7824	0.3607	0.6399
C	1.8511	1.4123	0.5558
C	4.1588	0.6597	0.4137
C	4.5502	1.9681	0.1118
C	3.6152	3.0066	0.0364
C	2.2716	2.7129	0.2603
C	-1.1619	-0.1479	2.2234
C	-1.4895	-1.3335	2.9033
C	-0.6278	-2.4251	2.8979
C	0.5976	-2.3375	2.2274
O	-3.0559	-1.9998	-0.9085
O	3.0559	-1.9999	0.9085
C	-4.0701	4.4158	0.2597
C	4.0701	4.4158	-0.2597
O	-1.4021	-3.4072	-2.2530
O	-5.0460	-0.3554	-0.5171
O	1.4021	-3.4072	2.2530
O	5.0460	-0.3554	0.5171
H	-2.2038	-3.1559	-1.7110
C	-6.4260	-0.0933	-0.3176
H	2.2038	-3.1559	1.7110
C	6.4260	-0.0933	0.3176
H	0.0578	2.0425	-1.2261
H	-0.0578	2.0425	1.2261
H	-5.5959	2.1944	0.0616
H	5.5959	2.1944	-0.0615
H	6.6252	0.2739	-0.6975
H	-6.6252	0.2739	0.6975
H	0.8767	-3.3530	-3.4057
H	1.8716	0.6711	-2.2330
H	-1.5349	3.5119	-0.2097
H	1.5349	3.5119	0.2097
H	-1.8716	0.6711	2.2330
H	-0.8767	-3.3531	3.4056
H	-3.2214	5.0769	0.4594
H	-4.7353	4.4452	1.1307
H	-4.6285	4.8372	-0.5861
H	4.7348	4.4452	-1.1310
H	4.6290	4.8370	0.5859
H	3.2214	5.0771	-0.4588
H	-6.8119	0.6300	-1.0479
H	-6.9264	-1.0525	-0.4591
H	6.8119	0.6300	1.0480
H	6.9264	-1.0525	0.4591
O	2.6848	-1.3540	-3.5547
H	2.8134	-2.2315	-3.9485
O	-2.6848	-1.3541	3.5547
H	-2.8134	-2.2316	3.9485

Cartesian coordinates of **5**-I optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	-4.4719	1.4634	0.1043
C	-3.6870	2.5489	-0.2962
C	-2.3007	2.5140	-0.1244
C	-1.6904	1.4014	0.4453
C	-2.4533	0.2875	0.8627
C	-3.8649	0.3399	0.6822
C	-0.1789	1.4076	0.5572
C	0.3539	0.4778	1.6188
C	-0.3943	-0.6674	1.9738
C	-1.7770	-0.8613	1.5101
C	1.6006	0.6997	2.1891
C	2.1691	-0.2316	3.0799
C	1.4563	-1.3794	3.4046
C	0.1834	-1.6143	2.8635
C	0.4950	1.1486	-0.8964
C	1.8996	1.7026	-0.9214
C	2.9923	0.8339	-0.7388
C	2.8119	-0.6310	-0.6884
C	1.5082	-1.1761	-1.1188
C	0.4114	-0.3009	-1.3203
C	1.3289	-2.5526	-1.4350
C	0.1128	-3.0146	-1.9575
C	-0.9337	-2.1168	-2.1789
C	-0.7814	-0.7623	-1.8608
C	2.1057	3.0740	-1.0363
C	3.3984	3.6221	-0.9630
C	4.4798	2.7730	-0.7441
C	4.2963	1.3885	-0.6191
O	-2.3682	-1.9379	1.7262
O	3.7714	-1.3606	-0.3690
C	3.5561	0.0056	3.6252
O	-4.5906	-0.7208	1.1013
O	-0.4531	-2.7404	3.2209
O	5.3765	0.6275	-0.3829
O	2.3742	-3.3833	-1.2311
C	-6.0032	-0.6936	0.9802
H	0.1267	2.4303	0.8012
H	-0.1182	1.7426	-1.5818
H	5.4909	3.1607	-0.6604
H	-6.3187	-0.6206	-0.0690
H	-5.5439	1.4909	-0.0228
H	-1.7182	3.3749	-0.4378
H	2.1605	1.5919	1.9259
H	1.8672	-2.1252	4.0786
H	-0.0079	-4.0609	-2.1953
H	-1.6157	-0.0927	-2.0343
H	1.2538	3.7350	-1.1852
H	3.6529	1.0141	4.0447
H	4.3011	-0.0834	2.8240
H	3.8124	-0.7168	4.4057
H	-6.3480	-1.6422	1.3946
H	-6.4440	0.1340	1.5515
O	-4.1852	3.6831	-0.8565
C	-5.5884	3.7944	-1.0475
H	-5.9652	3.0172	-1.7248
H	-6.1294	3.7401	-0.0941
H	-5.7499	4.7748	-1.4986
C	3.6076	5.1076	-1.1366
H	2.8215	5.6839	-0.6356
H	4.5742	5.4263	-0.7346
H	3.5842	5.3854	-2.1987
C	2.2452	-4.7615	-1.5420
H	3.2094	-5.2061	-1.2912
H	1.4591	-5.2385	-0.9427
H	2.0386	-4.9194	-2.6089
C	-2.3866	-3.8328	-2.9952
H	-3.4087	-3.8734	-3.3754
H	-1.6997	-4.2120	-3.7630
H	-2.3087	-4.4550	-2.0949
O	-2.1374	-2.4652	-2.7024
H	-1.3152	-2.7337	2.7185
H	5.0338	-0.3081	-0.3041

Cartesian coordinates of **5**-II optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	-1.9239	-2.2860	1.9536
C	-2.5432	-1.5225	0.9595
C	-1.9673	-0.3221	0.5355
C	-0.7753	0.1232	1.0973
C	-0.1232	-0.6226	2.1051
C	-0.7243	-1.8427	2.5271
C	-0.1789	1.4076	0.5572
C	0.7601	2.0913	1.5196
C	1.4536	1.3168	2.4770
C	1.1197	-0.0958	2.7166
C	1.0012	3.4554	1.4202
C	1.9754	4.0821	2.2215
C	2.6892	3.3204	3.1388
C	2.4459	1.9457	3.2781
C	0.4950	1.1486	-0.8964
C	1.5263	0.0497	-0.8000
C	1.1891	-1.2566	-1.2023
C	-0.0942	-1.5494	-1.8720
C	-0.8861	-0.4046	-2.3663
C	-0.5373	0.9130	-1.9764
C	-1.9433	-0.5633	-3.3065
C	-2.5935	0.5544	-3.8481
C	-2.1976	1.8390	-3.4697
C	-1.1700	2.0150	-2.5358
C	2.7712	0.3101	-0.2353
C	3.7109	-0.7182	-0.0448
C	3.3698	-2.0191	-0.4049
C	2.1192	-2.3070	-0.9700
O	1.8307	-0.7918	3.4686
O	-0.4300	-2.7335	-2.0722
C	2.2626	5.5521	2.0372
O	-0.1055	-2.5413	3.5050
O	3.1672	1.2688	4.1850
O	1.8419	-3.5853	-1.2710
O	-2.2779	-1.8215	-3.6661
C	-0.6909	-3.7401	3.9859
H	-1.0094	2.0859	0.3359
H	1.0153	2.0862	-1.1175
H	4.0605	-2.8436	-0.2537
H	-0.7662	-4.4994	3.1963
H	-2.3704	-3.2113	2.2863
H	-2.4753	0.2531	-0.2325
H	0.4500	4.0468	0.6955
H	3.4558	3.7665	3.7653
H	-3.3918	0.4188	-4.5623
H	-0.8931	3.0244	-2.2547
H	3.0236	1.3256	0.0646
H	1.3401	6.1446	2.0583
H	2.7372	5.7287	1.0634
H	2.9330	5.9332	2.8131
H	-0.0182	-4.0982	4.7667
H	-1.6852	-3.5623	4.4163
O	-3.7104	-1.8656	0.3523
C	-4.3602	-3.0663	0.7443
H	-3.7320	-3.9454	0.5511
H	-4.6393	-3.0443	1.8056
H	-5.2634	-3.1278	0.1350
C	5.0743	-0.4089	0.5263
H	5.0120	0.3292	1.3340
H	5.5573	-1.3080	0.9211
H	5.7359	0.0102	-0.2434
C	-3.3182	-2.0279	-4.6083
H	-3.3921	-3.1101	-4.7252
H	-4.2765	-1.6363	-4.2436
H	-3.0826	-1.5727	-5.5795
C	-3.8384	2.8804	-4.8644
H	-4.1275	3.9071	-5.0950
H	-3.5446	2.3706	-5.7912
H	-4.6895	2.3560	-4.4122
O	-2.7502	2.9800	-3.9567
H	2.8676	0.3197	4.1136
H	0.9102	-3.5799	-1.6329

Cartesian coordinates of **5**-III optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	4.5040	1.9338	-0.1368
C	3.4930	2.8996	-0.1300
C	2.1631	2.5255	-0.3400
C	1.8343	1.1919	-0.5595
C	2.8309	0.1906	-0.5776
C	4.1807	0.5883	-0.3601
C	0.3689	0.8428	-0.7241
C	0.1345	-0.4389	-1.4831
C	1.1178	-1.4524	-1.4439
C	2.4511	-1.2122	-0.8697
C	-1.0702	-0.6600	-2.1380
C	-1.3593	-1.9075	-2.7243
C	-0.4100	-2.9205	-2.6630
C	0.8240	-2.7151	-2.0275
C	-0.3689	0.8428	0.7241
C	-1.8343	1.1919	0.5595
C	-2.8309	0.1906	0.5776
C	-2.4511	-1.2121	0.8696
C	-1.1178	-1.4523	1.4439
C	-0.1345	-0.4389	1.4831
C	-0.8240	-2.7151	2.0275
C	0.4099	-2.9205	2.6630
C	1.3592	-1.9075	2.7244
C	1.0702	-0.6600	2.1381
C	-2.1631	2.5255	0.3400
C	-3.4929	2.8996	0.1300
C	-4.5040	1.9338	0.1368
C	-4.1807	0.5883	0.3600
O	3.2475	-2.1578	-0.7074
O	-3.2475	-2.1578	0.7073
C	-2.7104	-2.1464	-3.3522
C	2.7103	-2.1464	3.3523
O	5.1302	-0.3740	-0.3910
O	1.6949	-3.7345	-2.0036
O	-5.1302	-0.3740	0.3910
O	-1.6949	-3.7345	2.0036
C	6.4942	-0.0174	-0.2348
C	-6.4942	-0.0173	0.2348
H	-0.1056	1.6670	-1.2660
H	0.1056	1.6670	1.2660
H	-6.6865	0.4301	-0.7493
H	-5.5327	2.2215	-0.0223
H	6.6865	0.4301	0.7493
H	5.5327	2.2214	0.0223
H	1.4011	3.2988	-0.3353
H	-1.8143	0.1303	-2.1765
H	-0.6021	-3.8985	-3.0939
H	0.6021	-3.8985	3.0940
H	1.8142	0.1303	2.1766
H	-1.4011	3.2988	0.3353
H	-3.0147	-1.3017	-3.9814
H	-3.4725	-2.2634	-2.5705
H	-2.7166	-3.0522	-3.9661
H	3.4724	-2.2634	2.5706
H	2.7165	-3.0522	3.9662
H	3.0146	-1.3017	3.9815
H	7.0496	-0.9526	-0.3192
H	6.8253	0.6746	-1.0204
H	-7.0496	-0.9526	0.3191
H	-6.8253	0.6746	1.0203
O	-3.7094	4.2272	-0.0687
O	3.7094	4.2272	0.0687
C	5.0392	4.6823	0.2740
H	5.4823	4.2385	1.1749
H	5.6776	4.4630	-0.5915
H	4.9664	5.7633	0.4037
C	-5.0392	4.6823	-0.2740
H	-5.4822	4.2386	-1.1749
H	-5.6775	4.4630	0.5915
H	-4.9663	5.7634	-0.4037
H	-2.4761	-3.4128	1.4741
H	2.4761	-3.4128	-1.4742

Cartesian coordinates of **5**-IV optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	1.2609	-1.9870	-2.7422
C	2.0890	-0.8804	-2.5402
C	1.5868	0.2759	-1.9319
C	0.2628	0.3303	-1.5178
C	-0.6157	-0.7608	-1.7390
C	-0.0831	-1.9317	-2.3494
C	-0.2101	1.5658	-0.7832
C	-1.6914	1.8218	-0.9300
C	-2.5645	0.7440	-1.1719
C	-2.0550	-0.6154	-1.4404
C	-2.1962	3.1060	-0.7488
C	-3.5791	3.3553	-0.7956
C	-4.4504	2.2894	-1.0017
C	-3.9664	0.9857	-1.1807
C	0.2098	1.5657	0.7834
C	-0.2629	0.3301	1.5179
C	0.6158	-0.7610	1.7388
C	2.0550	-0.6154	1.4401
C	2.5644	0.7441	1.1718
C	1.6912	1.8219	0.9301
C	3.9662	0.9859	1.1805
C	4.4501	2.2897	1.0017
C	3.5788	3.3556	0.7958
C	2.1958	3.1061	0.7491
C	-1.5868	0.2756	1.9322
C	-2.0888	-0.8809	2.5405
C	-1.2606	-1.9874	2.7422
C	0.0833	-1.9319	2.3492
O	-2.8494	-1.5757	-1.4885
O	2.8496	-1.5756	1.4879
C	-4.1060	4.7628	-0.6458
C	4.1055	4.7631	0.6462
O	-0.9233	-2.9722	-2.5494
O	-4.8594	0.0011	-1.3598
O	0.9236	-2.9724	2.5490
O	4.8593	0.0013	1.3595
C	-0.4486	-4.1389	-3.2016
C	0.4491	-4.1392	3.2011
H	0.3266	2.4293	-1.1892
H	-0.3269	2.4292	1.1895
H	-0.3523	-4.6255	2.6297
H	-1.6507	-2.8816	3.2051
H	0.3528	-4.6252	-2.6301
H	1.6512	-2.8811	-3.2052
H	2.2583	1.1126	-1.7798
H	-1.5109	3.9322	-0.5689
H	-5.5258	2.4392	-1.0252
H	5.5255	2.4395	1.0252
H	1.5105	3.9323	0.5693
H	-2.2584	1.1123	1.7803
H	-4.0355	5.3106	-1.5950
H	-3.5319	5.3288	0.0963
H	-5.1572	4.7672	-0.3415
H	3.5314	5.3291	-0.0959
H	5.1567	4.7676	0.3418
H	4.0350	5.3107	1.5955
H	-1.3081	-4.8087	-3.2587
H	-0.0909	-3.9201	-4.2164
H	1.3086	-4.8090	3.2580
H	0.0915	-3.9205	4.2159
O	-3.3955	-0.8320	2.9023
O	3.3958	-0.8314	-2.9018
C	3.9964	-1.9876	-3.4684
H	3.9512	-2.8400	-2.7791
H	3.5235	-2.2611	-4.4206
H	5.0395	-1.7221	-3.6467
C	-3.9960	-1.9883	3.4688
H	-3.9508	-2.8405	2.7794
H	-3.5229	-2.2619	4.4209
H	-5.0391	-1.7229	3.6474
H	4.3229	-0.8390	1.4220
H	-4.3230	-0.8392	-1.4222

Cartesian coordinates of 1,1'-acetylated **5**-I optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	4.5841	2.0550	0.2043
C	3.7157	3.1456	0.0893
C	2.3766	2.9452	-0.2550
C	1.8991	1.6581	-0.4844
C	2.7444	0.5368	-0.3678
C	4.1052	0.7571	-0.0212
C	0.4315	1.4859	-0.8148
C	0.1434	0.2359	-1.6114
C	0.9769	-0.8929	-1.4779
C	2.2077	-0.8281	-0.6261
C	-0.9864	0.1865	-2.4301
C	-1.3600	-0.9863	-3.0930
C	-0.5369	-2.1067	-2.9612
C	0.6097	-2.0581	-2.1780
C	-0.4718	1.6053	0.5214
C	-1.8946	1.9788	0.1694
C	-2.8934	0.9929	0.1153
C	-2.5587	-0.4350	0.4425
C	-1.3666	-0.6329	1.3044
C	-0.3878	0.3825	1.4063
C	-1.1990	-1.8041	2.0912
C	-0.1037	-1.9323	2.9562
C	0.8333	-0.9001	3.0484
C	0.6884	0.2574	2.2757
C	-2.1901	3.3070	-0.1580
C	-3.4728	3.6985	-0.5429
C	-4.4695	2.7162	-0.6006
C	-4.1862	1.3958	-0.2812
O	2.7494	-1.8425	-0.1997
O	-3.2630	-1.3568	0.0415
C	-2.6464	-1.0480	-3.8773
O	4.9114	-0.3261	0.0562
O	1.3260	-3.2433	-2.0724
O	-5.2259	0.4916	-0.4473
O	-2.1475	-2.7629	1.9909
C	6.2943	-0.1477	0.3115
H	0.1273	2.3516	-1.4133
H	-0.0302	2.4491	1.0618
H	-5.4849	2.9679	-0.8928
H	6.4702	0.3000	1.2988
H	5.6217	2.2107	0.4603
H	1.7289	3.8117	-0.3478
H	-1.6067	1.0723	-2.5321
H	-0.7771	-3.0382	-3.4648
H	0.0102	-2.8252	3.5526
H	1.4371	1.0364	2.3612
H	-1.3998	4.0535	-0.1056
H	-2.8187	-0.1245	-4.4411
H	-3.4931	-1.1763	-3.1902
H	-2.6530	-1.8868	-4.5804
H	6.7260	-1.1496	0.2900
H	6.7731	0.4706	-0.4593
C	2.5990	-3.3002	-2.5841
C	3.2770	-4.5605	-2.1181
H	3.5509	-4.4198	-1.0670
H	2.6012	-5.4180	-2.1802
H	4.1751	-4.7359	-2.7119
O	3.0726	-2.4514	-3.2962
O	4.0883	4.4396	0.2874
C	5.4376	4.7184	0.6308
H	5.7187	4.2420	1.5790
H	6.1293	4.3944	-0.1576
H	5.4986	5.8025	0.7403
C	-3.7942	5.1379	-0.8659
H	-2.8866	5.7460	-0.9303
H	-4.3284	5.2233	-1.8194
H	-4.4381	5.5814	-0.0958
C	-2.0512	-3.9244	2.7982
H	-2.9270	-4.5255	2.5485
H	-1.1426	-4.4984	2.5736
H	-2.0725	-3.6788	3.8683
C	2.1732	-2.1015	4.6235
H	3.0973	-1.9069	5.1706
H	1.3662	-2.3057	5.3395
H	2.3130	-2.9729	3.9717
O	1.9166	-0.9270	3.8680
C	-5.7134	-0.1698	0.6571
O	-5.4450	0.1409	1.7893
C	-6.6044	-1.3004	0.2209
H	-7.1910	-1.6543	1.0697
H	-7.2600	-0.9934	-0.5987
H	-5.9592	-2.1070	-0.1435

Cartesian coordinates of 1,1'-acetylated **5**-II optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	0.1037	-1.9323	2.9561
C	-0.8334	-0.9001	3.0483
C	-0.6884	0.2574	2.2757
C	0.3877	0.3825	1.4063
C	1.3665	-0.6329	1.3044
C	1.1990	-1.8040	2.0912
C	0.4718	1.6053	0.5215
C	1.8946	1.9788	0.1695
C	2.8934	0.9929	0.1154
C	2.5587	-0.4350	0.4425
C	2.1901	3.3070	-0.1579
C	3.4729	3.6985	-0.5429
C	4.4695	2.7162	-0.6005
C	4.1862	1.3958	-0.2811
C	-0.4314	1.4861	-0.8148
C	-0.1434	0.2360	-1.6114
C	-0.9768	-0.8927	-1.4779
C	-2.2075	-0.8281	-0.6261
C	-2.7443	0.5367	-0.3677
C	-1.8991	1.6582	-0.4844
C	-4.1051	0.7569	-0.0211
C	-4.5841	2.0548	0.2043
C	-3.7158	3.1455	0.0893
C	-2.3767	2.9452	-0.2550
C	0.9863	0.1868	-2.4302
C	1.3600	-0.9859	-3.0933
C	0.5369	-2.1064	-2.9615
C	-0.6096	-2.0579	-2.1782
O	3.2628	-1.3568	0.0414
O	-2.7492	-1.8425	-0.1998
C	3.7943	5.1379	-0.8657
O	2.1475	-2.7628	1.9909
O	5.2259	0.4916	-0.4471
O	-1.3257	-3.2431	-2.0725
O	-4.9113	-0.3263	0.0565
C	2.0513	-3.9244	2.7982
H	0.0302	2.4491	1.0619
H	-0.1273	2.3518	-1.4132
H	0.7771	-3.0378	-3.4652
H	1.1428	-4.4984	2.5737
H	-0.0103	-2.8252	3.5526
H	-1.4371	1.0364	2.3611
H	1.3998	4.0535	-0.1055
H	5.4850	2.9678	-0.8928
H	-5.6218	2.2104	0.4604
H	-1.7290	3.8118	-0.3479
H	1.6067	1.0726	-2.5322
H	2.8868	5.7459	-0.9306
H	4.3291	5.2234	-1.8189
H	4.4378	5.5814	-0.0952
H	2.9271	-4.5254	2.5486
H	2.0726	-3.6787	3.8683
C	5.7132	-0.1701	0.6573
C	6.6041	-1.3007	0.2211
H	5.9588	-2.1072	-0.1436
H	7.2599	-0.9937	-0.5984
H	7.1904	-1.6549	1.0699
O	5.4447	0.1406	1.7894
O	-1.9167	-0.9270	3.8680
C	-2.1734	-2.1016	4.6232
H	-2.3131	-2.9730	3.9713
H	-1.3666	-2.3060	5.3393
H	-3.0976	-1.9071	5.1701
C	2.6463	-1.0475	-3.8776
H	2.8186	-0.1239	-4.4413
H	3.4931	-1.1759	-3.1906
H	2.6529	-1.8862	-4.5808
C	-6.2943	-0.1480	0.3107
H	-6.7260	-1.1498	0.2888
H	-6.4710	0.2996	1.2980
H	-6.7725	0.4705	-0.4603
C	-5.4377	4.7181	0.6315
H	-5.4986	5.8022	0.7414
H	-6.1298	4.3943	-0.1566
H	-5.7182	4.2414	1.5797
O	-4.0885	4.4395	0.2873
C	-2.5988	-3.3002	-2.5841
O	-3.0726	-2.4513	-3.2960
C	-3.2767	-4.5605	-2.1181
H	-4.1745	-4.7363	-2.7123
H	-2.6006	-5.4178	-2.1795
H	-3.5512	-4.4195	-1.0671

Cartesian coordinates of 1,1'-acetylated **5**-III optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	-4.4877	2.4165	-0.5475
C	-3.4943	3.3882	-0.3847
C	-2.2064	3.0185	0.0112
C	-1.9049	1.6804	0.2481
C	-2.8796	0.6758	0.0838
C	-4.1857	1.0673	-0.3181
C	-0.4875	1.3233	0.6458
C	-0.4010	0.0447	1.4461
C	-1.3652	-0.9685	1.2647
C	-2.5305	-0.7465	0.3510
C	0.6772	-0.1533	2.3096
C	0.8685	-1.3677	2.9760
C	-0.0855	-2.3722	2.7995
C	-1.1812	-2.1743	1.9679
C	0.4875	1.3234	-0.6459
C	1.9049	1.6804	-0.2481
C	2.8795	0.6758	-0.0838
C	2.5304	-0.7464	-0.3511
C	1.3652	-0.9685	-1.2648
C	0.4010	0.0447	-1.4462
C	1.1812	-2.1743	-1.9680
C	0.0856	-2.3721	-2.7996
C	-0.8685	-1.3676	-2.9761
C	-0.6771	-0.1532	-2.3097
C	2.2063	3.0185	-0.0111
C	3.4943	3.3882	0.3848
C	4.4877	2.4165	0.5476
C	4.1856	1.0673	0.3181
O	-3.1681	-1.6819	-0.1233
O	3.1680	-1.6819	0.1233
C	2.1029	-1.5972	3.8107
C	-2.1029	-1.5971	-3.8109
O	-5.1169	0.0939	-0.4442
O	-2.0357	-3.2581	1.8193
O	5.1168	0.0939	0.4442
O	2.0357	-3.2580	-1.8194
C	-6.4600	0.4484	-0.7291
C	6.4600	0.4484	0.7292
H	-0.1087	2.1429	1.2654
H	0.1087	2.1429	-1.2654
H	6.5539	0.9266	1.7134
H	5.4863	2.7029	0.8432
H	-6.5539	0.9266	-1.7134
H	-5.4863	2.7029	-0.8431
H	-1.4598	3.7960	0.1413
H	1.4022	0.6444	2.4437
H	0.0114	-3.3290	3.3035
H	-0.0114	-3.3289	-3.3037
H	-1.4021	0.6445	-2.4438
H	1.4598	3.7960	-0.1413
H	2.3459	-0.7189	4.4195
H	2.9610	-1.7905	3.1536
H	1.9872	-2.4567	4.4783
H	-2.9610	-1.7903	-3.1538
H	-1.9871	-2.4566	-4.4785
H	-2.3458	-0.7188	-4.4197
H	-7.0145	-0.4913	-0.7327
H	-6.8755	1.1131	0.0396
H	7.0145	-0.4913	0.7328
H	6.8754	1.1131	-0.0395
C	3.3330	-3.1520	-2.2579
C	-3.3330	-3.1521	2.2579
C	4.1364	-4.3191	-1.7509
H	4.3316	-4.1495	-0.6865
H	3.5774	-5.2541	-1.8469
H	5.0809	-4.3786	-2.2933
C	-4.1363	-4.3194	1.7512
H	-4.3324	-4.1494	0.6869
H	-3.5770	-5.2542	1.8463
H	-5.0804	-4.3793	2.2942
O	3.7353	-2.2464	-2.9435
O	-3.7353	-2.2465	2.9435
O	3.6931	4.7196	0.5826
O	-3.6931	4.7196	-0.5825
C	-4.9851	5.1705	-0.9620
H	-5.2921	4.7478	-1.9274
H	-5.7371	4.9239	-0.2015
H	-4.9064	6.2552	-1.0529
C	4.9850	5.1705	0.9622
H	5.2921	4.7477	1.9276
H	5.7370	4.9239	0.2017
H	4.9064	6.2552	1.0531

Cartesian coordinates of 1,1'-acetylated **5**-IV optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	-0.4364	-1.7789	3.0632
C	-1.2576	-0.6505	3.1265
C	-0.9524	0.4885	2.3737
C	0.1668	0.4991	1.5507
C	1.0307	-0.6175	1.4789
C	0.7023	-1.7671	2.2462
C	0.4250	1.7120	0.6864
C	1.8947	1.9314	0.4066
C	2.7822	0.8433	0.3895
C	2.2778	-0.5430	0.6769
C	2.3490	3.2227	0.1163
C	3.6857	3.4765	-0.1936
C	4.5727	2.3930	-0.2088
C	4.1313	1.1083	0.0747
C	-0.4250	1.7120	-0.6866
C	-0.1668	0.4990	-1.5507
C	-1.0308	-0.6175	-1.4789
C	-2.2778	-0.5430	-0.6769
C	-2.7822	0.8433	-0.3895
C	-1.8947	1.9315	-0.4067
C	-4.1313	1.1083	-0.0747
C	-4.5726	2.3930	0.2088
C	-3.6856	3.4766	0.1935
C	-2.3489	3.2228	-0.1165
C	0.9524	0.4884	-2.3738
C	1.2576	-0.6506	-3.1266
C	0.4363	-1.7791	-3.0632
C	-0.7023	-1.7672	-2.2461
O	2.8961	-1.5330	0.2994
O	-2.8961	-1.5330	-0.2993
C	4.1769	4.8749	-0.4806
C	-4.1768	4.8750	0.4804
O	1.5427	-2.8253	2.1766
O	5.0778	0.0997	-0.0367
O	-1.5428	-2.8254	-2.1765
O	-5.0777	0.0998	0.0369
C	1.2987	-3.9608	2.9895
C	-1.2988	-3.9609	-2.9893
H	0.0528	2.5932	1.2204
H	-0.0527	2.5931	-1.2206
H	-0.3457	-4.4435	-2.7355
H	0.6743	-2.6578	-3.6440
H	0.3457	-4.4434	2.7357
H	-0.6744	-2.6577	3.6441
H	-1.6139	1.3448	2.4382
H	1.6422	4.0503	0.1393
H	5.6246	2.5358	-0.4388
H	-5.6246	2.5359	0.4388
H	-1.6421	4.0503	-0.1396
H	1.6139	1.3447	-2.4384
H	3.3461	5.5833	-0.5554
H	4.7412	4.9145	-1.4198
H	4.8473	5.2296	0.3125
H	-4.7408	4.9147	1.4198
H	-4.8475	5.2296	-0.3125
H	-3.3460	5.5834	0.5548
H	2.1178	-4.6506	2.7794
H	1.3047	-3.7049	4.0572
H	-2.1179	-4.6507	-2.7792
H	-1.3047	-3.7051	-4.0571
C	-5.4212	-0.6163	-1.0857
C	5.4212	-0.6163	1.0859
C	-6.2169	-1.8302	-0.6900
H	-5.5169	-2.5602	-0.2692
H	-6.9545	-1.5850	0.0792
H	-6.7048	-2.2528	-1.5693
C	6.2171	-1.8301	0.6902
H	5.5177	-2.5592	0.2671
H	6.9564	-1.5842	-0.0772
H	6.7031	-2.2539	1.5700
O	-5.1142	-0.2902	-2.2039
O	5.1142	-0.2901	2.2041
O	2.3724	-0.5636	-3.8982
O	-2.3725	-0.5634	3.8981
C	-2.7879	-1.7066	4.6305
H	-2.9869	-2.5564	3.9656
H	-2.0421	-1.9971	5.3822
H	-3.7117	-1.4170	5.1341
C	2.7878	-1.7068	-4.6305
H	2.9869	-2.5566	-3.9656
H	2.0420	-1.9974	-5.3822
H	3.7116	-1.4173	-5.1342

Cartesian coordinates of 3,3'-dicarboxyl-1,1',8,8'-tetrahydroxybianthrone-I optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	-0.3147	-0.6705	2.2275
C	0.4865	-0.0042	1.2716
C	1.6211	-0.6269	0.7701
C	1.9690	-1.9188	1.1981
C	1.1821	-2.5997	2.1204
C	0.0320	-1.9878	2.6405
C	-1.4616	0.0127	2.8344
C	-1.6373	1.4436	2.6068
C	-0.8161	2.1313	1.6760
C	0.0809	1.3535	0.7405
C	-2.5557	2.1786	3.4111
C	-2.6100	3.5769	3.3029
C	-1.7687	4.2309	2.4183
C	-0.8755	3.5185	1.6033
C	-1.7436	0.2683	-0.7084
C	-1.6295	-1.0662	-1.1643
C	-2.7350	-1.9544	-1.0225
C	-3.9328	-1.4874	-0.4615
C	-4.0299	-0.1689	-0.0424
C	-2.9430	0.7082	-0.1574
C	-0.5513	1.1982	-0.7485
C	0.4873	0.8178	-1.7782
C	0.6078	-0.5302	-2.1996
C	-0.4079	-1.5179	-1.8264
C	1.3556	1.7750	-2.2846
C	2.3763	1.4055	-3.1779
C	2.5399	0.0817	-3.5671
C	1.6581	-0.8982	-3.0868
O	-2.2313	-0.6160	3.6152
O	-0.2679	-2.7303	-2.1539
H	-0.9165	2.2037	-0.9802
H	0.9938	1.9338	0.5737
O	-3.3731	1.5923	4.2958
O	-0.6909	-2.6832	3.5275
O	1.8446	-2.1553	-3.5105
O	-2.6861	-3.2366	-1.4102
H	-3.1995	0.6177	4.2517
H	-1.4682	-2.1193	3.7727
H	1.1394	-2.7107	-3.0904
H	-1.7757	-3.3972	-1.7674
H	2.2600	-0.1336	0.0447
H	1.4334	-3.5998	2.4509
H	-3.3110	4.1141	3.9328
H	-1.8021	5.3149	2.3514
H	-0.2307	4.0535	0.9145
H	-4.7634	-2.1797	-0.3727
H	-3.0387	1.7361	0.1823
H	1.2656	2.8184	-2.0072
H	3.3278	-0.2165	-4.2478
C	3.2059	-2.5225	0.6214
O	3.9227	-1.9754	-0.1923
O	3.4632	-3.7634	1.0975
H	4.2805	-4.0566	0.6535
C	3.2712	2.4894	-3.6800
O	4.2312	2.0380	-4.5218
H	4.7522	2.8216	-4.7779
O	3.1678	3.6606	-3.3775
H	-4.9641	0.1893	0.3818

Cartesian coordinates of 3,3'-dicarboxyl-1,1',8,8'-tetrahydroxybianthrone-II optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	2.1231	-0.1090	1.1339
C	1.5748	1.1175	0.6925
C	2.4067	2.0890	0.1533
C	3.7864	1.8544	0.0329
C	4.3417	0.6464	0.4403
C	3.5188	-0.3482	0.9891
C	1.2704	-1.1047	1.7910
C	-0.0875	-0.7333	2.1758
C	-0.6371	0.5102	1.7691
C	0.0809	1.3535	0.7405
C	-0.8223	-1.5690	3.0660
C	-2.0620	-1.1362	3.5618
C	-2.5592	0.1002	3.1848
C	-1.8577	0.9238	2.2909
C	-1.8760	1.9243	-0.8249
C	-3.0933	1.2047	-0.7796
C	-4.3288	1.9146	-0.7493
C	-4.3249	3.3165	-0.7961
C	-3.1204	4.0008	-0.8634
C	-1.8986	3.3146	-0.8727
C	-0.5513	1.1982	-0.7485
C	-0.6162	-0.2428	-1.1990
C	-1.8377	-0.9573	-1.1167
C	-3.0891	-0.2558	-0.8196
C	0.5258	-0.8868	-1.6547
C	0.4841	-2.2506	-1.9932
C	-0.6927	-2.9800	-1.8753
C	-1.8647	-2.3430	-1.4404
O	1.7414	-2.2368	2.0975
O	-4.1665	-0.9030	-0.6892
H	0.1608	1.7292	-1.3881
H	-0.0836	2.4084	0.9816
O	-0.3722	-2.7623	3.4759
O	4.1012	-1.4926	1.3687
O	-2.9775	-3.0851	-1.3661
O	-5.5160	1.2961	-0.6814
H	0.5085	-2.9054	3.0448
H	3.3825	-2.0838	1.7095
H	-3.7049	-2.4871	-1.0569
H	-5.3343	0.3225	-0.6444
H	2.0139	3.0435	-0.1822
H	5.4020	0.4488	0.3436
H	-2.5974	-1.7866	4.2453
H	-3.5109	0.4382	3.5856
H	-2.2708	1.8856	2.0068
H	-5.2782	3.8342	-0.7814
H	-0.9659	3.8705	-0.9204
H	1.4651	-0.3575	-1.7606
H	-0.7351	-4.0331	-2.1247
C	4.6197	2.9468	-0.5493
O	4.1845	4.0156	-0.9283
O	5.9346	2.6325	-0.6189
H	6.3749	3.4077	-1.0142
C	1.7514	-2.8747	-2.4752
O	1.6189	-4.1914	-2.7629
H	2.4989	-4.4903	-3.0586
O	2.8034	-2.2823	-2.6029
H	-3.1248	5.0865	-0.9099

Cartesian coordinates of 3,3'-dicarboxyl-1,1',8,8'-tetrahydroxybianthrone-III optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	0.3511	1.8389	-0.6971
C	-0.4938	1.4577	0.3753
C	-1.8643	1.6541	0.2718
C	-2.4175	2.1894	-0.9043
C	-1.6102	2.5263	-1.9843
C	-0.2204	2.3587	-1.8923
C	1.8082	1.8192	-0.5373
C	2.3747	1.5737	0.7858
C	1.5429	1.1614	1.8543
C	0.0931	0.8067	1.6064
C	3.7614	1.8044	1.0227
C	4.2793	1.6505	2.3174
C	3.4419	1.2672	3.3531
C	2.0805	1.0183	3.1285
C	0.4938	-1.4577	0.3751
C	-0.3511	-1.8388	-0.6973
C	0.2204	-2.3585	-1.8925
C	1.6102	-2.5260	-1.9845
C	2.4175	-2.1892	-0.9045
C	1.8643	-1.6540	0.2717
C	-0.0932	-0.8069	1.6063
C	-1.5430	-1.1616	1.8542
C	-2.3747	-1.5739	0.7856
C	-1.8082	-1.8192	-0.5375
C	-2.0806	-1.0187	3.1284
C	-3.4420	-1.2676	3.3530
C	-4.2793	-1.6508	2.3172
C	-3.7614	-1.8047	1.0225
O	2.5587	2.0996	-1.5147
O	-2.5587	-2.0996	-1.5149
H	0.4868	-1.1314	2.4762
H	-0.4869	1.1312	2.4763
O	4.6066	2.1804	0.0545
O	0.5151	2.7215	-2.9518
O	-4.6066	-2.1806	0.0542
O	-0.5150	-2.7213	-2.9521
H	4.0852	2.2235	-0.7867
H	1.4634	2.5523	-2.7177
H	-4.0852	-2.2236	-0.7869
H	-1.4633	-2.5521	-2.7180
H	-2.5306	1.4036	1.0884
H	-2.0256	2.9321	-2.8985
H	5.3364	1.8365	2.4734
H	3.8478	1.1568	4.3551
H	1.4434	0.7131	3.9546
H	2.0256	-2.9318	-2.8987
H	2.5306	-1.4036	1.0883
H	-1.4435	-0.7134	3.9545
H	-3.8479	-1.1573	4.3549
H	-5.3365	-1.8369	2.4731
C	-3.8975	2.3771	-0.9417
C	3.8976	-2.3768	-0.9419
O	-4.6466	2.1218	-0.0210
O	4.6466	-2.1215	-0.0212
O	-4.3402	2.8701	-2.1230
H	-5.3084	2.9464	-2.0343
O	4.3403	-2.8697	-2.1233
H	5.3084	-2.9460	-2.0345

Cartesian coordinates of 3,3'-dicarboxyl-1,1',8,8'-tetrahydroxybianthrone-IV optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	-2.7887	-0.2082	-0.5690
C	-1.8649	0.8594	-0.4973
C	-2.3075	2.1328	-0.1635
C	-3.6653	2.3609	0.1129
C	-4.5863	1.3189	0.0693
C	-4.1594	0.0261	-0.2660
C	-2.3501	-1.5375	-1.0098
C	-1.0139	-1.6928	-1.5728
C	-0.0885	-0.6171	-1.5401
C	-0.3879	0.6128	-0.7141
C	-0.6769	-2.8898	-2.2694
C	0.5480	-2.9774	-2.9486
C	1.4164	-1.8986	-2.9406
C	1.1080	-0.7222	-2.2400
C	1.8649	0.8594	0.4974
C	2.7887	-0.2082	0.5690
C	4.1594	0.0261	0.2660
C	4.5863	1.3190	-0.0693
C	3.6652	2.3610	-0.1129
C	2.3075	2.1328	0.1635
C	0.3879	0.6127	0.7141
C	0.0885	-0.6172	1.5401
C	1.0139	-1.6928	1.5728
C	2.3501	-1.5375	1.0098
C	-1.1080	-0.7223	2.2400
C	-1.4163	-1.8986	2.9406
C	-0.5480	-2.9774	2.9486
C	0.6769	-2.8898	2.2694
O	-3.1576	-2.5092	-0.9823
O	3.1576	-2.5092	0.9823
H	-0.0240	1.4858	1.2303
H	0.0240	1.4858	-1.2303
O	-1.4944	-3.9494	-2.3250
O	-5.0835	-0.9443	-0.2889
O	1.4944	-3.9495	2.3249
O	5.0835	-0.9443	0.2889
H	-2.3076	-3.7181	-1.8087
H	-4.6139	-1.7841	-0.5290
H	2.3077	-3.7181	1.8086
H	4.6139	-1.7841	0.5290
H	-1.6212	2.9721	-0.1131
H	-5.6349	1.4810	0.2868
H	0.7772	-3.8956	-3.4789
H	2.3550	-1.9641	-3.4842
H	1.8070	0.1072	-2.2465
H	5.6348	1.4810	-0.2868
H	1.6211	2.9722	0.1131
H	-1.8070	0.1071	2.2466
H	-2.3550	-1.9641	3.4842
H	-0.7772	-3.8956	3.4788
C	-4.0729	3.7551	0.4559
C	4.0728	3.7552	-0.4558
O	-3.3110	4.6982	0.5193
O	3.3110	4.6982	-0.5194
O	-5.4003	3.8755	0.6975
H	-5.5495	4.8160	0.9079
O	5.4002	3.8755	-0.6975
H	5.5494	4.8161	-0.9080

Cartesian coordinates of **9**-I optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	0.5984	0.3656	1.9726
C	-0.2619	-0.6633	1.5081
C	-1.5202	-0.8131	2.0722
C	-1.9884	0.0707	3.0667
C	-1.1655	1.1027	3.4988
C	0.1244	1.2624	2.9713
C	1.9818	0.4417	1.5229
C	2.5292	-0.6492	0.7112
C	1.6715	-1.6631	0.2144
C	0.1712	-1.5440	0.3585
C	3.9247	-0.7141	0.4777
C	4.4641	-1.8180	-0.2338
C	3.6105	-2.8142	-0.6919
C	2.2259	-2.7317	-0.4723
C	-1.9571	-1.4411	-1.0762
C	-2.9369	-0.4510	-0.8347
C	-4.3003	-0.8418	-0.7202
C	-4.6570	-2.1860	-0.8921
C	-3.6929	-3.1512	-1.1678
C	-2.3415	-2.7659	-1.2458
C	-0.4886	-1.0788	-1.0547
C	-0.2170	0.3715	-1.3758
C	-1.2064	1.3589	-1.1119
C	-2.5642	0.9596	-0.7483
C	1.0090	0.7736	-1.8787
C	1.2939	2.1334	-2.0945
C	0.3570	3.1153	-1.8040
C	-0.9179	2.7321	-1.3083
O	2.7287	1.3934	1.8973
O	-3.4346	1.8282	-0.4456
H	0.0252	-1.7030	-1.7930
H	-0.2364	-2.5481	0.5166
C	-3.3800	-0.1016	3.6240
C	-4.0880	-4.5895	-1.4002
O	4.7857	0.2198	0.9014
O	0.8704	2.2668	3.4530
O	-1.7978	3.7114	-1.0689
O	-5.2801	0.0339	-0.4460
H	4.2401	0.9084	1.3644
H	1.7398	2.2319	2.9774
H	-2.6217	3.2716	-0.7355
H	-4.8498	0.9250	-0.3644
H	-2.1675	-1.6159	1.7328
H	-1.4941	1.8065	4.2573
H	4.0095	-3.6699	-1.2250
H	1.5858	-3.5245	-0.8516
H	-5.7074	-2.4478	-0.8079
H	-1.5843	-3.5227	-1.4405
H	1.7714	0.0360	-2.1060
H	2.2657	2.4087	-2.4885
H	-3.5854	0.6141	4.4251
H	-4.1325	0.0422	2.8384
H	-3.5231	-1.1130	4.0236
H	-5.0812	-4.8038	-0.9947
H	-3.3724	-5.2804	-0.9408
H	-4.1131	-4.8175	-2.4740
O	0.5353	4.4533	-1.9624
C	1.7953	4.9022	-2.4338
H	2.0096	4.5192	-3.4408
H	1.7288	5.9908	-2.4685
H	2.6072	4.6079	-1.7554
O	5.8141	-1.7934	-0.4001
C	6.4161	-2.8716	-1.0961
H	7.4854	-2.6544	-1.1136
H	6.2483	-3.8282	-0.5830
H	6.0436	-2.9458	-2.1270

Cartesian coordinates of **9**-II optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	2.9369	-0.4510	-0.8346
C	1.9571	-1.4411	-1.0762
C	2.3415	-2.7659	-1.2458
C	3.6929	-3.1512	-1.1677
C	4.6570	-2.1860	-0.8921
C	4.3003	-0.8419	-0.7202
C	2.5642	0.9596	-0.7483
C	1.2064	1.3589	-1.1119
C	0.2170	0.3715	-1.3758
C	0.4886	-1.0789	-1.0546
C	0.9180	2.7321	-1.3084
C	-0.3570	3.1153	-1.8040
C	-1.2939	2.1334	-2.0945
C	-1.0089	0.7736	-1.8786
C	0.2619	-0.6633	1.5081
C	-0.5984	0.3656	1.9726
C	-0.1244	1.2624	2.9713
C	1.1655	1.1027	3.4988
C	1.9884	0.0708	3.0667
C	1.5202	-0.8130	2.0722
C	-0.1712	-1.5440	0.3586
C	-1.6715	-1.6631	0.2144
C	-2.5292	-0.6492	0.7112
C	-1.9818	0.4417	1.5229
C	-2.2259	-2.7317	-0.4723
C	-3.6105	-2.8141	-0.6920
C	-4.4641	-1.8180	-0.2338
C	-3.9247	-0.7141	0.4777
O	3.4346	1.8281	-0.4457
O	-2.7288	1.3935	1.8973
H	0.2364	-2.5480	0.5166
H	-0.0252	-1.7030	-1.7930
C	4.0879	-4.5895	-1.4002
C	3.3799	-0.1016	3.6240
O	1.7978	3.7114	-1.0689
O	5.2801	0.0339	-0.4460
O	-4.7857	0.2199	0.9014
O	-0.8704	2.2668	3.4530
H	2.6218	3.2716	-0.7355
H	4.8498	0.9249	-0.3644
H	-4.2401	0.9084	1.3644
H	-1.7398	2.2320	2.9774
H	1.5843	-3.5227	-1.4404
H	5.7074	-2.4479	-0.8079
H	-2.2656	2.4087	-2.4885
H	-1.7714	0.0360	-2.1060
H	1.4941	1.8065	4.2573
H	2.1675	-1.6158	1.7328
H	-1.5858	-3.5244	-0.8516
H	-4.0095	-3.6699	-1.2250
H	4.1131	-4.8175	-2.4740
H	5.0812	-4.8039	-0.9946
H	3.3723	-5.2804	-0.9408
H	4.1325	0.0423	2.8384
H	3.5854	0.6141	4.4251
H	3.5231	-1.1129	4.0236
O	-5.8141	-1.7934	-0.4002
C	-6.4161	-2.8715	-1.0961
H	-6.2483	-3.8282	-0.5830
H	-7.4854	-2.6544	-1.1136
H	-6.0436	-2.9458	-2.1270
O	-0.5352	4.4533	-1.9624
C	-1.7953	4.9022	-2.4338
H	-1.7288	5.9908	-2.4685
H	-2.0096	4.5192	-3.4408
H	-2.6072	4.6080	-1.7554

Cartesian coordinates of **9**-III optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	−0.8693	−1.1602	1.6165
C	0.0479	−0.0804	1.5282
C	1.3034	−0.1970	2.1061
C	1.7114	−1.3897	2.7391
C	0.8313	−2.4626	2.7970
C	−0.4561	−2.3666	2.2486
C	−2.2462	−1.0078	1.1666
C	−2.7269	0.3218	0.7790
C	−1.8140	1.4009	0.6665
C	−0.3244	1.1583	0.7470
C	−4.1115	0.5309	0.5692
C	−4.5861	1.8385	0.2854
C	−3.6796	2.8892	0.2100
C	−2.3048	2.6675	0.3924
C	−0.0480	−0.0804	−1.5282
C	0.8693	−1.1602	−1.6165
C	0.4561	−2.3666	−2.2486
C	−0.8313	−2.4626	−2.7971
C	−1.7114	−1.3897	−2.7391
C	−1.3034	−0.1970	−2.1061
C	0.3243	1.1583	−0.7470
C	1.8140	1.4009	−0.6665
C	2.7269	0.3218	−0.7789
C	2.2462	−1.0078	−1.1665
C	2.3048	2.6676	−0.3924
C	3.6796	2.8892	−0.2100
C	4.5861	1.8385	−0.2854
C	4.1115	0.5309	−0.5692
O	−3.0435	−1.9916	1.1884
O	3.0436	−1.9916	−1.1885
H	−0.1395	2.0266	−1.2265
H	0.1395	2.0266	1.2265
C	3.1024	−1.4918	3.3146
C	−3.1023	−1.4918	−3.3146
O	−5.0202	−0.4522	0.6243
O	−1.2582	−3.4351	2.3597
O	5.0202	−0.4522	−0.6242
O	1.2582	−3.4351	−2.3597
H	−4.5164	−1.2818	0.8360
H	−2.1158	−3.1971	1.9228
H	4.5164	−1.2818	−0.8359
H	2.1158	−3.1971	−1.9227
H	1.9952	0.6384	2.0586
H	1.1129	−3.3981	3.2705
H	−4.0290	3.8952	0.0069
H	−1.6212	3.5090	0.3118
H	−1.1128	−3.3981	−3.2706
H	−1.9952	0.6385	−2.0587
H	1.6211	3.5090	−0.3119
H	4.0290	3.8952	−0.0069
H	3.3064	−0.6653	4.0059
H	3.8554	−1.4368	2.5180
H	3.2484	−2.4322	3.8535
H	−3.3063	−0.6652	−4.0059
H	−3.8554	−1.4369	−2.5181
H	−3.2484	−2.4321	−3.8536
O	5.9314	1.9388	−0.1107
O	−5.9315	1.9388	0.1107
C	6.4710	3.2202	0.1656
H	6.0714	3.6342	1.1016
H	7.5477	3.0742	0.2665
H	6.2753	3.9263	−0.6528
C	−6.4710	3.2202	−0.1656
H	−6.0715	3.6342	−1.1016
H	−7.5477	3.0741	−0.2664
H	−6.2753	3.9263	0.6528

Cartesian coordinates of **9**-IV optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	2.6974	0.7156	0.8770
C	1.7891	1.7869	0.7160
C	2.2676	3.0627	0.4430
C	3.6461	3.3151	0.3120
C	4.5424	2.2586	0.4408
C	4.0904	0.9614	0.7191
C	2.2221	-0.6136	1.2552
C	0.8299	-0.7789	1.6679
C	-0.0872	0.3005	1.5380
C	0.2976	1.5343	0.7566
C	0.4371	-1.9795	2.3094
C	-0.8700	-2.0861	2.8553
C	-1.7358	-1.0060	2.7550
C	-1.3472	0.1752	2.0992
C	-1.7892	1.7869	-0.7159
C	-2.6975	0.7156	-0.8770
C	-4.0905	0.9613	-0.7191
C	-4.5426	2.2584	-0.4407
C	-3.6463	3.3149	-0.3116
C	-2.2678	3.0627	-0.4427
C	-0.2978	1.5345	-0.7565
C	0.0872	0.3008	-1.5380
C	-0.8299	-0.7788	-1.6678
C	-2.2221	-0.6136	-1.2552
C	1.3471	0.1756	-2.0993
C	1.7358	-1.0056	-2.7552
C	0.8702	-2.0857	-2.8554
C	-0.4369	-1.9794	-2.3094
O	3.0322	-1.5853	1.3092
O	-3.0321	-1.5852	-1.3094
H	0.1783	2.4042	-1.2214
H	-0.1785	2.4039	1.2217
C	4.1402	4.7185	0.0566
C	-4.1406	4.7182	-0.0561
O	1.2457	-3.0356	2.4553
O	5.0107	-0.0087	0.8287
O	-1.2454	-3.0356	-2.4552
O	-5.0106	-0.0089	-0.8289
H	2.1070	-2.7888	2.0297
H	4.5165	-0.8490	1.0154
H	-2.1067	-2.7887	-2.0298
H	-4.5164	-0.8492	-1.0156
H	1.5646	3.8853	0.3287
H	5.6121	2.4119	0.3349
H	-2.7309	-1.0652	3.1811
H	-2.0557	0.9942	2.0325
H	-5.6123	2.4116	-0.3346
H	-1.5648	3.8854	-0.3284
H	2.0555	0.9947	-2.0327
H	2.7310	-1.0647	-3.1812
H	4.1142	5.3144	0.9784
H	3.5133	5.2354	-0.6786
H	5.1712	4.7212	-0.3094
H	-4.1147	5.3143	-0.9779
H	-5.1715	4.7209	0.3100
H	-3.5137	5.2352	0.6791
O	1.1490	-3.2728	-3.4556
O	-1.1487	-3.2732	3.4556
C	2.4433	-3.4481	-4.0080
H	2.6395	-2.7277	-4.8137
H	3.2245	-3.3545	-3.2418
H	2.4569	-4.4596	-4.4172
C	-2.4431	-3.4488	4.0074
H	-2.6398	-2.7286	4.8133
H	-3.2241	-3.3550	3.2410
H	-2.4570	-4.4604	4.4162

Cartesian coordinates of 7,7'-methylated **1**-I optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	−1.0283	−0.6305	1.7145
C	−0.0580	0.3749	1.4680
C	1.1605	0.3308	2.1295
C	1.4820	−0.7275	3.0048
C	0.5515	−1.7360	3.2197
C	−0.7033	−1.7014	2.5938
C	−2.3766	−0.5132	1.1751
C	−2.7713	0.7265	0.5022
C	−1.8046	1.7172	0.2137
C	−0.3332	1.4521	0.4435
C	−4.1379	0.9638	0.1890
C	−4.5463	2.1882	−0.3815
C	−3.5688	3.1457	−0.6311
C	−2.2159	2.9213	−0.3459
C	1.8918	1.4129	−0.8395
C	2.7856	0.3282	−0.6889
C	4.1579	0.5959	−0.4265
C	4.6107	1.9208	−0.3653
C	3.7332	2.9847	−0.5516
C	2.3699	2.7160	−0.7774
C	0.4065	1.1598	−0.9750
C	0.0703	−0.2042	−1.5315
C	0.9708	−1.2862	−1.3559
C	2.3176	−1.0475	−0.8442
C	−1.1401	−0.4316	−2.1725
C	−1.4810	−1.7217	−2.6052
C	−0.6456	−2.8150	−2.4137
C	0.5969	−2.5901	−1.7822
O	−3.2252	−1.4354	1.3594
O	3.1047	−2.0145	−0.6201
H	−0.0084	1.9209	−1.6437
H	0.1274	2.3842	0.7869
C	2.8355	−0.7608	3.6706
C	4.2331	4.4089	−0.5302
O	−5.0961	0.0512	0.4220
O	−1.5609	−2.6945	2.8695
O	1.4001	−3.6550	−1.6252
O	5.0567	−0.3811	−0.2266
H	−4.6443	−0.7432	0.8114
H	−2.3888	−2.5090	2.3559
H	2.2232	−3.3309	−1.1759
H	4.5659	−1.2400	−0.3097
H	1.8905	1.1166	1.9618
H	0.7654	−2.5691	3.8820
H	−3.8694	4.0987	−1.0608
H	−1.4854	3.6968	−0.5627
H	5.6659	2.0889	−0.1726
H	1.6792	3.5472	−0.9040
H	−1.8307	0.3891	−2.3352
H	−2.4349	−1.8755	−3.1045
H	2.9192	−1.5942	4.3738
H	3.6323	−0.8656	2.9232
H	3.0298	0.1696	4.2177
H	5.2230	4.4804	−0.0703
H	3.5498	5.0641	0.0216
H	4.3111	4.8096	−1.5495
C	−6.0034	2.4127	−0.6898
H	−6.6179	2.3246	0.2139
H	−6.1632	3.4049	−1.1224
H	−6.3805	1.6619	−1.3941
C	−1.0094	−4.2068	−2.8593
H	−1.9928	−4.2186	−3.3388
H	−0.2721	−4.6030	−3.5673
H	−1.0292	−4.9009	−2.0109

Cartesian coordinates of 7,7'-methylated **1**-II optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	-2.7856	0.3282	-0.6889
C	-1.8918	1.4129	-0.8396
C	-2.3699	2.7160	-0.7774
C	-3.7332	2.9847	-0.5516
C	-4.6107	1.9207	-0.3654
C	-4.1579	0.5958	-0.4265
C	-2.3176	-1.0476	-0.8442
C	-0.9708	-1.2862	-1.3559
C	-0.0703	-0.2042	-1.5315
C	-0.4065	1.1598	-0.9750
C	-0.5969	-2.5901	-1.7822
C	0.6457	-2.8150	-2.4137
C	1.4810	-1.7217	-2.6052
C	1.1401	-0.4316	-2.1725
C	0.0580	0.3749	1.4680
C	1.0283	-0.6305	1.7145
C	0.7033	-1.7013	2.5938
C	-0.5516	-1.7359	3.2197
C	-1.4820	-0.7274	3.0048
C	-1.1605	0.3308	2.1295
C	0.3332	1.4521	0.4434
C	1.8046	1.7172	0.2137
C	2.7713	0.7266	0.5022
C	2.3766	-0.5132	1.1751
C	2.2159	2.9213	-0.3459
C	3.5688	3.1457	-0.6311
C	4.5463	2.1882	-0.3815
C	4.1379	0.9638	0.1890
O	-3.1046	-2.0146	-0.6200
O	3.2252	-1.4354	1.3594
H	-0.1275	2.3843	0.7869
H	0.0084	1.9209	-1.6437
C	-4.2331	4.4089	-0.5303
C	-2.8355	-0.7608	3.6706
O	-1.4001	-3.6550	-1.6252
O	-5.0567	-0.3811	-0.2267
O	5.0961	0.0512	0.4220
O	1.5609	-2.6944	2.8695
H	-2.2232	-3.3309	-1.1759
H	-4.5659	-1.2400	-0.3097
H	4.6443	-0.7432	0.8114
H	2.3887	-2.5090	2.3560
H	-1.6792	3.5472	-0.9041
H	-5.6659	2.0888	-0.1726
H	2.4350	-1.8754	-3.1045
H	1.8307	0.3891	-2.3352
H	-0.7655	-2.5691	3.8820
H	-1.8905	1.1167	1.9618
H	1.4854	3.6968	-0.5628
H	3.8694	4.0987	-1.0608
H	-4.3111	4.8096	-1.5495
H	-5.2231	4.4804	-0.0704
H	-3.5498	5.0641	0.0216
H	-3.6323	-0.8653	2.9232
H	-2.9193	-1.5943	4.3737
H	-3.0297	0.1696	4.2178
C	1.0095	-4.2068	-2.8592
H	0.2721	-4.6030	-3.5672
H	1.9928	-4.2186	-3.3388
H	1.0293	-4.9009	-2.0108
C	6.0034	2.4127	-0.6898
H	6.1632	3.4049	-1.1225
H	6.6179	2.3247	0.2139
H	6.3805	1.6618	-1.3941

Cartesian coordinates of 7,7'-methylated **1**-III optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	0.9063	-0.9659	-1.6023
C	-0.0201	0.1067	-1.5263
C	-1.2667	-0.0185	-2.1212
C	-1.6569	-1.2144	-2.7596
C	-0.7683	-2.2808	-2.8053
C	0.5112	-2.1750	-2.2401
C	2.2765	-0.8002	-1.1367
C	2.7403	0.5321	-0.7422
C	1.8210	1.6009	-0.6357
C	0.3339	1.3490	-0.7423
C	4.1232	0.7672	-0.5116
C	4.5960	2.0636	-0.2169
C	3.6641	3.0944	-0.1500
C	2.2948	2.8754	-0.3477
C	0.0201	0.1065	1.5264
C	-0.9063	-0.9661	1.6021
C	-0.5112	-2.1754	2.2398
C	0.7682	-2.2813	2.8050
C	1.6568	-1.2148	2.7596
C	1.2666	-0.0189	2.1214
C	-0.3339	1.3489	0.7426
C	-1.8209	1.6008	0.6360
C	-2.7403	0.5320	0.7422
C	-2.2765	-0.8004	1.1366
C	-2.2947	2.8754	0.3482
C	-3.6640	3.0944	0.1504
C	-4.5959	2.0636	0.2171
C	-4.1231	0.7672	0.5116
O	3.0839	-1.7765	-1.1512
O	-3.0839	-1.7767	1.1510
H	0.1246	2.2146	1.2315
H	-0.1246	2.2148	-1.2311
C	-3.0384	-1.3264	-3.3556
C	3.0383	-1.3269	3.3556
O	5.0359	-0.2189	-0.5610
O	1.3234	-3.2367	-2.3413
O	-5.0359	-0.2189	0.5607
O	-1.3235	-3.2371	2.3408
H	4.5419	-1.0526	-0.7811
H	2.1741	-2.9911	-1.8953
H	-4.5419	-1.0527	0.7808
H	-2.1741	-2.9914	1.8948
C	6.0691	2.2827	0.0085
C	-6.0690	2.2827	-0.0084
H	-1.9644	0.8125	-2.0854
H	-1.0363	-3.2182	-3.2830
H	4.0146	4.1013	0.0657
H	1.6005	3.7088	-0.2736
H	1.0362	-3.2187	3.2826
H	1.9644	0.8122	2.0857
H	-1.6005	3.7088	0.2743
H	-4.0145	4.1013	-0.0652
H	-3.2385	-0.5007	-4.0490
H	-3.8033	-1.2783	-2.5699
H	-3.1696	-2.2673	-3.8975
H	3.2384	-0.5013	4.0491
H	3.8032	-1.2789	2.5699
H	3.1694	-2.2679	3.8974
H	6.6543	1.9759	-0.8663
H	6.2805	3.3362	0.2149
H	6.4355	1.6839	0.8508
H	-6.6542	1.9758	0.8663
H	-6.2804	3.3363	-0.2146
H	-6.4353	1.6842	-0.8508

Cartesian coordinates of 7,7'-methylated **1**-IV optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	-2.8160	0.5287	-0.4764
C	-1.8792	1.5864	-0.4321
C	-2.2952	2.8632	-0.0750
C	-3.6369	3.1295	0.2577
C	-4.5572	2.0863	0.2429
C	-4.1684	0.7886	-0.1171
C	-2.4171	-0.7991	-0.9378
C	-1.0979	-0.9769	-1.5395
C	-0.1568	0.0844	-1.5289
C	-0.4130	1.3218	-0.6992
C	-0.7984	-2.1768	-2.2418
C	0.4098	-2.3123	-2.9591
C	1.2858	-1.2342	-2.9593
C	1.0179	-0.0500	-2.2573
C	1.8792	1.5864	0.4321
C	2.8160	0.5287	0.4764
C	4.1684	0.7886	0.1171
C	4.5572	2.0863	-0.2429
C	3.6369	3.1295	-0.2577
C	2.2952	2.8632	0.0750
C	0.4130	1.3217	0.6992
C	0.1568	0.0844	1.5289
C	1.0979	-0.9769	1.5395
C	2.4171	-0.7991	0.9378
C	-1.0179	-0.0500	2.2573
C	-1.2858	-1.2342	2.9593
C	-0.4098	-2.3123	2.9591
C	0.7984	-2.1768	2.2418
O	-3.2416	-1.7595	-0.8948
O	3.2416	-1.7595	0.8948
H	0.0094	2.1866	1.2360
H	-0.0094	2.1866	-1.2360
C	-4.0680	4.5338	0.6053
C	4.0680	4.5338	-0.6053
O	-1.6431	-3.2207	-2.2741
O	-5.1086	-0.1679	-0.1097
O	1.6431	-3.2207	2.2741
O	5.1086	-0.1679	0.1097
H	-2.4382	-2.9638	-1.7386
H	-4.6586	-1.0114	-0.3760
H	2.4382	-2.9638	1.7386
H	4.6586	-1.0114	0.3760
C	0.6938	-3.5935	-3.6979
C	-0.6938	-3.5935	3.6979
H	-1.5723	3.6763	-0.0529
H	-5.5981	2.2505	0.5041
H	2.2133	-1.3152	-3.5217
H	1.7373	0.7616	-2.2826
H	5.5982	2.2505	-0.5041
H	1.5723	3.6763	0.0529
H	-1.7373	0.7616	2.2826
H	-2.2132	-1.3152	3.5217
H	-4.1276	5.1580	-0.2959
H	-3.3535	5.0147	1.2829
H	-5.0528	4.5455	1.0814
H	4.1271	5.1581	0.2959
H	5.0530	4.5456	-1.0810
H	3.3537	5.0146	-1.2833
H	-0.0861	-3.8059	-4.4386
H	1.6576	-3.5415	-4.2130
H	0.7124	-4.4494	-3.0130
H	-1.6576	-3.5415	4.2130
H	0.0861	-3.8059	4.4386
H	-0.7124	-4.4494	3.0130

Cartesian coordinates of 7,7'-methylated **2**-I optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	-0.6492	-0.7018	1.9273
C	0.2176	0.3654	1.5787
C	1.4795	0.4420	2.1500
C	1.9459	-0.5544	3.0319
C	1.1159	-1.6224	3.3475
C	-0.1789	-1.7089	2.8149
C	-2.0384	-0.7096	1.4815
C	-2.5734	0.4602	0.7979
C	-1.7169	1.5163	0.4103
C	-0.2154	1.3814	0.5459
C	-3.9756	0.5776	0.5603
C	-4.5175	1.7331	-0.0285
C	-3.6332	2.7634	-0.3706
C	-2.2493	2.6599	-0.1629
C	1.9171	1.4803	-0.8841
C	2.9034	0.4738	-0.7817
C	4.2647	0.8554	-0.6284
C	4.6118	2.2134	-0.6248
C	3.6401	3.2001	-0.7613
C	2.2904	2.8189	-0.8794
C	0.4501	1.1085	-0.9103
C	0.1881	-0.2941	-1.4101
C	1.1846	-1.2947	-1.2725
C	2.5359	-0.9397	-0.8763
C	-1.0425	-0.6221	-1.9505
C	-1.3154	-1.9499	-2.3221
C	-0.3820	-2.9796	-2.1612
C	0.8768	-2.6397	-1.6367
O	-2.7933	-1.6920	1.7595
O	3.4183	-1.8345	-0.6945
H	-0.0666	1.8143	-1.5685
H	0.1851	2.3596	0.8314
C	3.3421	-0.4591	3.5962
C	4.0229	4.6598	-0.8022
O	-4.8261	-0.4059	0.8951
O	-0.9334	-2.7543	3.1862
O	1.7807	-3.6241	-1.5072
O	5.2522	-0.0424	-0.4797
H	-4.2735	-1.1401	1.2793
H	-1.8080	-2.6503	2.7295
H	2.6045	-3.2086	-1.1345
H	4.8256	-0.9388	-0.5093
H	2.1303	1.2757	1.9054
H	1.4419	-2.4102	4.0196
H	-1.6194	3.4931	-0.4596
H	5.6615	2.4691	-0.5158
H	1.5269	3.5892	-0.9683
H	-1.8191	0.1211	-2.0881
H	3.5418	-1.2573	4.3168
H	4.0891	-0.5299	2.7954
H	3.5011	0.5028	4.0986
H	5.0360	4.8206	-0.4218
H	3.3326	5.2708	-0.2098
H	3.9905	5.0426	-1.8308
C	-6.0008	1.8616	-0.2772
H	-6.4458	2.6856	0.2995
H	-6.2244	2.0361	-1.3396
H	-6.5136	0.9453	0.0172
C	-0.7097	-4.4006	-2.5505
H	-0.9215	-4.4950	-3.6255
H	0.1314	-5.0575	-2.3261
H	-1.5810	-4.7847	-2.0008
O	-2.5485	-2.1812	-2.8453
H	-2.6386	-3.1245	-3.0535
O	-4.0723	3.9234	-0.9303
H	-5.0380	3.8925	-1.0178

Cartesian coordinates of 7,7'-methylated **2**-II optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	-2.9032	0.4743	-0.7814
C	-1.9168	1.4808	-0.8838
C	-2.2901	2.8194	-0.8791
C	-3.6397	3.2007	-0.7609
C	-4.6115	2.2141	-0.6243
C	-4.2644	0.8560	-0.6278
C	-2.5359	-0.9392	-0.8762
C	-1.1846	-1.2943	-1.2726
C	-0.1880	-0.2938	-1.4100
C	-0.4500	1.1088	-0.9101
C	-0.8770	-2.6392	-1.6371
C	0.3818	-2.9791	-2.1615
C	1.3153	-1.9495	-2.3222
C	1.0426	-0.6218	-1.9505
C	-0.2176	0.3650	1.5787
C	0.6491	-0.7023	1.9271
C	0.1785	-1.7098	2.8140
C	-1.1165	-1.6237	3.3461
C	-1.9464	-0.5556	3.0307
C	-1.4797	0.4414	2.1497
C	0.2156	1.3814	0.5463
C	1.7171	1.5162	0.4108
C	2.5735	0.4601	0.7983
C	2.0385	-0.7099	1.4818
C	2.2495	2.6599	-0.1622
C	3.6334	2.7633	-0.3700
C	4.5177	1.7329	-0.0280
C	3.9757	0.5774	0.5607
O	-3.4183	-1.8340	-0.6946
O	2.7932	-1.6924	1.7592
H	-0.1849	2.3595	0.8320
H	0.0669	1.8147	-1.5680
C	-4.0222	4.6605	-0.8012
C	-3.3430	-0.4607	3.5942
O	-1.7809	-3.6235	-1.5077
O	-5.2520	-0.0417	-0.4789
O	4.8262	-0.4061	0.8953
O	0.9330	-2.7553	3.1853
H	-2.6047	-3.2080	-1.1351
H	-4.8255	-0.9381	-0.5089
H	4.2737	-1.1403	1.2797
H	1.8078	-2.6508	2.7293
H	-1.5265	3.5896	-0.9681
H	-5.6611	2.4698	-0.5152
H	1.8192	0.1214	-2.0880
H	-1.4427	-2.4119	4.0177
H	-2.1303	1.2753	1.9053
H	1.6196	3.4931	-0.4588
H	-5.0389	4.8202	-0.4299
H	-3.3376	5.2696	-0.2001
H	-3.9797	5.0465	-1.8281
H	-3.5423	-1.2582	4.3158
H	-4.0895	-0.5334	2.7931
H	-3.5033	0.5017	4.0951
C	0.7093	-4.4001	-2.5511
H	0.9223	-4.4940	-3.6259
H	1.5799	-4.7849	-2.0006
H	-0.1323	-5.0567	-2.3279
C	6.0010	1.8614	-0.2766
H	6.4456	2.6862	0.2991
H	6.5139	0.9456	0.0190
H	6.2248	2.0345	-1.3392
O	4.0726	3.9232	-0.9296
H	5.0382	3.8922	-1.0175
O	2.5484	-2.1809	-2.8454
H	2.6384	-3.1242	-3.0536

Cartesian coordinates of 7,7'-methylated **2**-III optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	0.8978	-1.2186	-1.6162
C	-0.0300	-0.1495	-1.5282
C	-1.2816	-0.2742	-2.1131
C	-1.6746	-1.4677	-2.7529
C	-0.7833	-2.5313	-2.8111
C	0.5009	-2.4248	-2.2567
C	2.2731	-1.0496	-1.1610
C	2.7329	0.2749	-0.7632
C	1.8164	1.3449	-0.6463
C	0.3277	1.0927	-0.7444
C	4.1195	0.5171	-0.5331
C	4.5910	1.8069	-0.2344
C	3.6496	2.8419	-0.1628
C	2.2776	2.6187	-0.3553
C	0.0300	-0.1492	1.5279
C	-0.8978	-1.2184	1.6162
C	-0.5007	-2.4245	2.2569
C	0.7837	-2.5309	2.8109
C	1.6749	-1.4673	2.7525
C	1.2817	-0.2739	2.1126
C	-0.3278	1.0928	0.7440
C	-1.8164	1.3449	0.6459
C	-2.7329	0.2750	0.7634
C	-2.2732	-1.0495	1.1613
C	-2.2778	2.6187	0.3545
C	-3.6499	2.8417	0.1623
C	-4.5912	1.8066	0.2343
C	-4.1196	0.5171	0.5336
O	3.0822	-2.0276	-1.1901
O	-3.0826	-2.0271	1.1908
H	0.1324	1.9592	1.2299
H	-0.1325	1.9590	-1.2304
C	-3.0614	-1.5813	-3.3368
C	3.0618	-1.5807	3.3361
O	5.0214	-0.4776	-0.5911
O	1.3154	-3.4844	-2.3709
O	-5.0213	-0.4778	0.5927
O	-1.3150	-3.4842	2.3713
H	4.5145	-1.3053	-0.8182
H	2.1695	-3.2369	-1.9319
H	-4.5141	-1.3054	0.8196
H	-2.1692	-3.2368	1.9324
C	6.0600	2.0684	-0.0054
C	-6.0603	2.0680	0.0056
H	-1.9804	0.5556	-2.0677
H	-1.0528	-3.4672	-3.2908
H	1.6003	3.4629	-0.2702
H	1.0533	-3.4668	3.2907
H	1.9804	0.5560	2.0670
H	-1.6005	3.4629	0.2690
H	-3.2714	-0.7521	-4.0232
H	-3.8192	-1.5419	-2.5438
H	-3.1937	-2.5192	-3.8837
H	3.2719	-0.7516	4.0225
H	3.8194	-1.5412	2.5429
H	3.1944	-2.5186	3.8829
H	6.4715	2.7756	-0.7403
H	6.2543	2.4762	0.9971
H	6.6270	1.1412	-0.0960
H	-6.4734	2.7695	0.7450
H	-6.2539	2.4827	-0.9942
H	-6.6262	1.1395	0.0888
O	-4.0192	4.1229	-0.1078
H	-4.9831	4.1659	-0.2083
O	4.0187	4.1231	0.1075
H	4.9827	4.1662	0.2083

Cartesian coordinates of 7,7'-methylated **2**-IV optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	2.7148	0.6005	0.8585
C	1.8011	1.6659	0.6944
C	2.2700	2.9430	0.4119
C	3.6468	3.2023	0.2748
C	4.5488	2.1522	0.4105
C	4.1053	0.8537	0.6986
C	2.2441	-0.7300	1.2430
C	0.8601	-0.9009	1.6511
C	-0.0638	0.1695	1.5325
C	0.3102	1.4080	0.7500
C	0.4504	-2.1069	2.2946
C	-0.8367	-2.2360	2.8438
C	-1.6961	-1.1366	2.7430
C	-1.3232	0.0528	2.0935
C	-1.8010	1.6659	-0.6944
C	-2.7148	0.6006	-0.8585
C	-4.1053	0.8537	-0.6985
C	-4.5487	2.1523	-0.4105
C	-3.6467	3.2024	-0.2748
C	-2.2699	2.9430	-0.4119
C	-0.3101	1.4080	-0.7501
C	0.0638	0.1695	-1.5326
C	-0.8601	-0.9009	-1.6511
C	-2.2441	-0.7299	-1.2429
C	1.3232	0.0528	-2.0935
C	1.6961	-1.1366	-2.7431
C	0.8367	-2.2360	-2.8438
C	-0.4505	-2.1069	-2.2946
O	3.0634	-1.6983	1.2998
O	-3.0634	-1.6983	-1.2997
H	0.1647	2.2730	-1.2242
H	-0.1647	2.2730	1.2241
C	4.1315	4.6064	0.0050
C	-4.1314	4.6064	-0.0051
O	1.2836	-3.1532	2.4143
O	5.0324	-0.1085	0.8182
O	-1.2836	-3.1532	-2.4143
O	-5.0323	-0.1084	-0.8181
H	2.1441	-2.8810	1.9941
H	4.5429	-0.9519	1.0028
H	-2.1441	-2.8810	-1.9941
H	-4.5429	-0.9519	-1.0027
C	-1.2683	-3.5065	3.5350
C	1.2682	-3.5066	-3.5350
H	1.5618	3.7611	0.2958
H	5.6173	2.3106	0.3005
H	-2.0466	0.8580	2.0409
H	-5.6172	2.3107	-0.3005
H	-1.5617	3.7611	-0.2958
H	2.0466	0.8580	-2.0410
H	4.0775	5.2196	0.9141
H	3.5165	5.1022	-0.7545
H	5.1703	4.6136	-0.3379
H	-4.0772	5.2197	-0.9141
H	-5.1703	4.6137	0.3377
H	-3.5165	5.1022	0.7546
H	-1.5088	-3.3369	4.5946
H	-2.1519	-3.9538	3.0573
H	-0.4687	-4.2471	3.4980
H	2.1521	-3.9536	-3.0576
H	1.5083	-3.3371	-4.5946
H	0.4688	-4.2474	-3.4975
O	2.9489	-1.1608	-3.2691
H	3.1111	-2.0259	-3.6772
O	-2.9490	-1.1608	3.2690
H	-3.1112	-2.0259	3.6771

Cartesian coordinates of **12**-I optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	−1.6609	1.1745	−0.9352
C	−0.5521	0.3481	−1.2057
C	0.6349	0.9322	−1.6261
C	0.7974	2.3228	−1.7447
C	−0.2854	3.1788	−1.4244
C	−1.5092	2.5839	−1.0338
C	−2.9789	0.5885	−0.6883
C	−3.1656	−0.8390	−0.8701
C	−2.0558	−1.6889	−1.1028
C	−0.6453	−1.1464	−1.0052
C	−4.4783	−1.4010	−0.8724
C	−4.6568	−2.7638	−1.1277
C	−3.5493	−3.5700	−1.3756
C	−2.2473	−3.0366	−1.3574
C	1.5466	−1.5630	0.2633
C	2.2756	−0.5294	0.8739
C	3.6771	−0.4505	0.6514
C	4.3622	−1.3995	−0.1463
C	3.6062	−2.4520	−0.7250
C	2.2210	−2.5000	−0.5090
C	0.0406	−1.6295	0.3841
C	−0.5068	−0.8999	1.5906
C	0.2342	0.1692	2.1648
C	1.6055	0.4180	1.7700
C	−1.7447	−1.2440	2.1036
C	−2.2918	−0.5072	3.1728
C	−1.6103	0.5717	3.7251
C	−0.3467	0.9156	3.2346
O	−3.9679	1.3336	−0.4024
O	2.2523	1.3974	2.2560
H	−0.2429	−2.6842	0.4576
H	−0.0428	−1.6359	−1.7768
C	2.1442	2.8145	−2.2148
C	4.2029	−3.5469	−1.5756
O	−5.5738	−0.6679	−0.6433
O	−2.5641	3.3803	−0.7558
O	0.2792	1.9431	3.8181
O	4.3741	0.5578	1.2174
H	−5.2713	0.2606	−0.4710
H	−3.3435	2.7845	−0.5343
H	1.1588	2.0432	3.3717
H	3.7230	1.1277	1.7323
H	1.4766	0.2957	−1.8774
H	−5.6671	−3.1629	−1.1302
H	−1.4123	−3.7028	−1.5505
H	1.6590	−3.3115	−0.9646
H	−2.3161	−2.0721	1.7015
H	−2.0234	1.1523	4.5451
H	2.7742	1.9643	−2.4929
H	2.0528	3.4908	−3.0683
H	2.6473	3.3935	−1.4356
H	3.4211	−4.2524	−1.8737
H	4.9896	−4.0863	−1.0421
H	4.6828	−3.1422	−2.4703
C	−0.1060	4.6805	−1.5126
C	5.8552	−1.3249	−0.3948
O	0.9806	5.1919	−1.6857
O	6.4303	−2.1167	−1.1128
O	−1.1948	5.4622	−1.4092
H	−1.9890	4.9243	−1.2131
O	6.5573	−0.3492	0.2046
H	5.9703	0.2260	0.7374
O	−3.6576	−4.8952	−1.6409
H	−4.5938	−5.1519	−1.6370
O	−3.5076	−0.9073	3.6189
H	−3.7903	−0.3343	4.3499

Cartesian coordinates of **12**-II optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	0.6340	0.6530	-2.2495
C	0.3746	-0.7149	-2.0329
C	1.0943	-1.6580	-2.7536
C	2.1125	-1.3093	-3.6569
C	2.4312	0.0577	-3.8509
C	1.6717	1.0230	-3.1470
C	-0.2364	1.6738	-1.6649
C	-1.4513	1.2649	-0.9848
C	-1.7073	-0.1042	-0.7238
C	-0.6453	-1.1464	-1.0052
C	-2.4342	2.2336	-0.6177
C	-3.6375	1.8249	-0.0353
C	-3.8709	0.4709	0.1883
C	-2.9050	-0.4953	-0.1490
C	0.6429	-0.4411	1.0996
C	0.0112	0.1246	2.2192
C	0.5602	1.3003	2.7990
C	1.7400	1.9013	2.2961
C	2.3758	1.2906	1.1839
C	1.8064	0.1421	0.6144
C	0.0406	-1.6295	0.3841
C	-0.8960	-2.4482	1.2444
C	-1.5531	-1.8396	2.3487
C	-1.1641	-0.5228	2.8102
C	-1.1452	-3.7719	0.9286
C	-2.0834	-4.5087	1.6785
C	-2.7746	-3.9270	2.7356
C	-2.5148	-2.5977	3.0833
O	0.0245	2.9071	-1.8263
O	-1.7787	0.0345	3.7722
H	0.8623	-2.2734	0.0548
H	-1.1471	-2.0464	-1.3743
C	2.8085	-2.4419	-4.3706
C	3.6501	1.8032	0.5577
O	-2.2587	3.5452	-0.8150
O	1.9369	2.3330	-3.3421
O	-3.1851	-2.0936	4.1247
O	-0.0612	1.8589	3.8595
H	-1.3607	3.6606	-1.2194
H	1.2812	2.8602	-2.7912
H	-2.8754	-1.1600	4.2495
H	-0.8757	1.3032	4.0637
H	0.8663	-2.7103	-2.6214
H	-4.3701	2.5828	0.2274
H	-3.1266	-1.5395	0.0481
H	2.3061	-0.3082	-0.2397
H	-0.6366	-4.2661	0.1094
H	-3.5052	-4.4815	3.3177
H	2.3186	-3.3901	-4.1299
H	2.8070	-2.2993	-5.4540
H	3.8623	-2.5004	-4.0850
H	3.9530	1.1423	-0.2604
H	4.4602	1.8650	1.2887
H	3.5268	2.8188	0.1732
C	3.5536	0.4398	-4.7939
C	2.3338	3.1569	2.9022
O	4.3079	-0.3843	-5.2674
O	3.3215	3.6911	2.4415
O	3.7006	1.7352	-5.1221
H	3.0670	2.2917	-4.6247
O	1.7428	3.6877	3.9853
H	0.9509	3.1703	4.2393
O	-5.0215	0.0110	0.7385
H	-5.6149	0.7571	0.9219
O	-2.2703	-5.7988	1.3071
H	-2.9341	-6.2102	1.8840

Cartesian coordinates of **12**-III optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	0.5340	-0.5160	-1.8173
C	-0.3430	0.5386	-1.4955
C	-1.6901	0.4105	-1.8045
C	-2.2300	-0.7497	-2.3839
C	-1.3786	-1.8458	-2.6688
C	0.0021	-1.7044	-2.3871
C	1.9817	-0.3412	-1.6908
C	2.5118	0.9713	-1.3695
C	1.6455	2.0336	-1.0106
C	0.1691	1.7751	-0.7935
C	3.9135	1.2265	-1.4679
C	4.4095	2.5133	-1.2373
C	3.5312	3.5431	-0.9117
C	2.1497	3.3049	-0.7917
C	0.3428	0.5390	1.4953
C	-0.5340	-0.5157	1.8175
C	-0.0017	-1.7038	2.3876
C	1.3790	-1.8449	2.6690
C	2.2303	-0.7487	2.3836
C	1.6900	0.4112	1.8040
C	-0.1696	1.7752	0.7930
C	-1.6461	2.0335	1.0102
C	-2.5121	0.9711	1.3695
C	-1.9817	-0.3412	1.6911
C	-2.1505	3.3046	0.7910
C	-3.5321	3.5425	0.9111
C	-4.4101	2.5126	1.2371
C	-3.9138	1.2260	1.4679
O	2.7679	-1.3064	-1.9420
O	-2.7677	-1.3064	1.9426
H	0.3825	2.6402	1.1739
H	-0.3832	2.6399	-1.1746
C	-3.7125	-0.7424	-2.6668
C	3.7128	-0.7411	2.6662
O	4.7974	0.2732	-1.7824
O	0.8361	-2.7257	-2.6777
O	-4.7974	0.2725	1.7828
O	-0.8355	-2.7252	2.6786
H	4.2882	-0.5694	-1.9023
H	1.7691	-2.4356	-2.4400
H	-4.2880	-0.5699	1.9029
H	-1.7686	-2.4352	2.4412
O	3.9486	4.8140	-0.6903
H	5.4793	2.6798	-1.3258
O	-3.9499	4.8133	0.6894
H	-5.4800	2.6789	1.3257
H	4.9108	4.8654	-0.8097
H	-4.9120	4.8645	0.8089
H	-2.3603	1.2370	-1.5940
H	1.5022	4.1360	-0.5301
H	2.3600	1.2378	1.5932
H	-1.5032	4.1357	0.5291
H	-4.1292	0.2426	-2.4351
H	-3.9262	-0.9891	-3.7097
H	-4.2328	-1.4997	-2.0744
H	3.9268	-0.9878	3.7090
H	4.2331	-1.4984	2.0737
H	4.1292	0.2440	2.4345
C	1.9608	-3.1105	3.2650
C	-1.9599	-3.1117	-3.2647
O	-3.1561	-3.2792	-3.3823
O	3.1571	-3.2780	3.3819
O	1.1166	-4.0666	3.6876
H	0.1892	-3.8236	3.4880
O	-1.1154	-4.0679	-3.6862
H	-0.1882	-3.8247	-3.4864

Cartesian coordinates of **12**-IV optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	2.7385	0.0698	0.7566
C	1.8228	1.1269	0.6258
C	2.2962	2.3970	0.3228
C	3.6571	2.6728	0.1222
C	4.6002	1.6166	0.2183
C	4.1194	0.3236	0.5380
C	2.2781	-1.2602	1.1660
C	0.9134	-1.4265	1.6203
C	-0.0169	-0.3543	1.5375
C	0.3353	0.8811	0.7399
C	0.5229	-2.6298	2.2828
C	-0.7426	-2.7299	2.8686
C	-1.6139	-1.6475	2.8111
C	-1.2556	-0.4588	2.1439
C	-1.8228	1.1269	-0.6258
C	-2.7386	0.0698	-0.7566
C	-4.1194	0.3237	-0.5380
C	-4.6002	1.6166	-0.2183
C	-3.6571	2.6728	-0.1221
C	-2.2961	2.3970	-0.3228
C	-0.3353	0.8811	-0.7399
C	0.0169	-0.3543	-1.5375
C	-0.9134	-1.4265	-1.6204
C	-2.2782	-1.2602	-1.1661
C	1.2556	-0.4588	-2.1439
C	1.6139	-1.6475	-2.8111
C	0.7426	-2.7299	-2.8686
C	-0.5229	-2.6298	-2.2828
O	3.0961	-2.2328	1.1998
O	-3.0961	-2.2328	-1.1997
H	0.1137	1.7517	-1.2284
H	-0.1137	1.7516	1.2284
C	4.0270	4.1029	-0.1871
C	-4.0270	4.1030	0.1872
O	1.3349	-3.6878	2.3883
O	4.9967	-0.6978	0.6393
O	-1.3349	-3.6878	-2.3884
O	-4.9968	-0.6977	-0.6394
H	2.1879	-3.4462	1.9445
H	4.4714	-1.5282	0.8586
H	-2.1879	-3.4461	-1.9446
H	-4.4716	-1.5281	-0.8588
O	-2.8439	-1.6697	3.3783
H	-1.0091	-3.6542	3.3733
O	2.8439	-1.6696	-3.3783
H	1.0091	-3.6542	-3.3732
H	-2.9887	-2.5264	3.8116
H	2.9888	-2.5264	-3.8115
H	1.5887	3.2183	0.2401
H	-1.9706	0.3552	2.1215
H	-1.5886	3.2183	-0.2400
H	1.9706	0.3552	-2.1214
H	3.1318	4.7320	-0.1602
H	4.7607	4.4912	0.5238
H	4.4986	4.1897	-1.1693
H	-4.7606	4.4913	-0.5237
H	-4.4986	4.1897	1.1694
H	-3.1317	4.7320	0.1604
C	-6.0691	1.8988	0.0236
C	6.0691	1.8988	-0.0236
O	6.4687	2.9905	-0.3724
O	-6.4689	2.9905	0.3722
O	-6.9520	0.9033	-0.1632
H	-6.4934	0.0743	-0.4113
O	6.9521	0.9034	0.1633
H	6.4937	0.0744	0.4115

Cartesian coordinates of **13**-I optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	0.7053	-1.6325	-1.3372
C	-0.0721	-0.4622	-1.4807
C	-1.3295	-0.5177	-2.0788
C	-1.8840	-1.7354	-2.4848
C	-1.1336	-2.9012	-2.3305
C	0.1538	-2.8685	-1.7774
C	2.0890	-1.5213	-0.8254
C	2.6974	-0.1800	-0.7879
C	1.9162	0.9872	-0.9376
C	0.4118	0.8600	-0.9311
C	4.1100	-0.0669	-0.6635
C	4.7177	1.1880	-0.7642
C	3.9486	2.3290	-0.9591
C	2.5445	2.2264	-1.0348
C	-1.6470	1.5894	0.4219
C	-2.6738	0.6390	0.5787
C	-4.0199	1.0566	0.3739
C	-4.2932	2.3864	0.0368
C	-3.2644	3.3240	-0.1084
C	-1.9449	2.9097	0.0782
C	-0.1918	1.1879	0.5510
C	0.0062	0.0631	1.5389
C	-0.9948	-0.9379	1.6076
C	-2.3175	-0.7395	0.9933
C	1.1411	-0.0499	2.3384
C	1.3365	-1.1954	3.1448
C	0.3987	-2.2201	3.1430
C	-0.7706	-2.1056	2.3855
O	2.7682	-2.5210	-0.5201
O	-3.1282	-1.6840	0.9220
H	0.3702	2.0630	0.8814
H	-0.0023	1.6586	-1.5505
C	-3.2932	-1.7889	-3.0193
C	-3.5880	4.7631	-0.4307
O	4.8993	-1.1289	-0.4700
O	0.9157	-3.9777	-1.6520
O	-1.6539	-3.1098	2.4423
O	-4.9943	0.1283	0.5261
H	4.2821	-1.9133	-0.3950
H	-2.4048	-2.8450	1.8380
H	-1.9013	0.3962	-2.2059
H	-1.5633	-3.8439	-2.6473
H	5.7997	1.2495	-0.6829
H	-5.3174	2.7079	-0.1133
H	-1.1338	3.6228	-0.0399
H	0.5473	-3.1165	3.7388
H	-3.4821	-2.7093	-3.5807
H	-4.0062	-1.7505	-2.1850
H	-3.5064	-0.9363	-3.6735
H	-4.4157	4.8383	-1.1447
H	-2.7228	5.2822	-0.8538
H	-3.8893	5.3086	0.4733
C	-6.3521	0.5253	0.4067
H	-6.9362	-0.3752	0.6032
H	-6.6143	1.2978	1.1411
H	-6.5800	0.8924	-0.6025
C	0.4067	-5.2246	-2.1015
H	0.1837	-5.2080	-3.1762
H	1.2003	-5.9478	-1.9071
H	-0.4942	-5.5160	-1.5469
O	4.5012	3.5624	-1.0726
H	5.4652	3.4788	-0.9988
O	2.4606	-1.2481	3.8985
H	2.4748	-2.0908	4.3795
Cl	1.6321	3.7172	-1.2450
Cl	2.3456	1.2216	2.4438

Cartesian coordinates of **13**-II optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	2.6738	0.6389	0.5787
C	1.6469	1.5893	0.4222
C	1.9449	2.9097	0.0788
C	3.2643	3.3240	-0.1080
C	4.2931	2.3864	0.0368
C	4.0198	1.0565	0.3736
C	2.3176	-0.7396	0.9935
C	0.9949	-0.9381	1.6078
C	-0.0062	0.0629	1.5390
C	0.1918	1.1877	0.5513
C	0.7708	-2.1058	2.3857
C	-0.3985	-2.2204	3.1432
C	-1.3365	-1.1958	3.1449
C	-1.1412	-0.0503	2.3384
C	0.0721	-0.4621	-1.4806
C	-0.7055	-1.6325	-1.3374
C	-0.1540	-2.8684	-1.7775
C	1.1335	-2.9012	-2.3306
C	1.8840	-1.7355	-2.4848
C	1.3296	-0.5177	-2.0787
C	-0.4117	0.8600	-0.9310
C	-1.9161	0.9874	-0.9376
C	-2.6975	-0.1797	-0.7880
C	-2.0892	-1.5211	-0.8258
C	-2.5443	2.2266	-1.0346
C	-3.9484	2.3294	-0.9590
C	-4.7176	1.1885	-0.7642
C	-4.1101	-0.0666	-0.6636
O	3.1284	-1.6840	0.9225
O	-2.7686	-2.5208	-0.5208
H	0.0025	1.6587	-1.5501
H	-0.3703	2.0628	0.8817
C	3.5881	4.7629	-0.4309
C	3.2932	-1.7889	-3.0192
O	1.6542	-3.1099	2.4426
O	4.9944	0.1281	0.5251
O	-4.8994	-1.1284	-0.4701
O	-0.9158	-3.9776	-1.6522
H	2.4051	-2.8449	1.8382
H	-4.2823	-1.9128	-0.3950
H	1.1337	3.6229	-0.0388
H	5.3173	2.7079	-0.1134
H	-0.5471	-3.1168	3.7390
H	1.5632	-3.8440	-2.6473
H	1.9015	0.3961	-2.2057
H	-5.7995	1.2501	-0.6829
H	3.9057	5.3046	0.4699
H	4.4049	4.8372	-1.1575
H	2.7184	5.2864	-0.8392
H	3.4823	-2.7097	-3.5799
H	4.0061	-1.7498	-2.1849
H	3.5061	-0.9367	-3.6740
C	-0.4071	-5.2244	-2.1025
H	-1.2008	-5.9475	-1.9086
H	-0.1840	-5.2070	-3.1772
H	0.4938	-5.5163	-1.5480
C	6.3521	0.5257	0.4066
H	6.6136	1.2980	1.1413
H	6.9363	-0.3747	0.6031
H	6.5804	0.8931	-0.6024
O	-2.4606	-1.2486	3.8985
H	-2.4748	-2.0914	4.3794
O	-4.5009	3.5629	-1.0724
H	-5.4648	3.4793	-0.9988
Cl	-2.3459	1.2210	2.4438
Cl	-1.6318	3.7175	-1.2447

Cartesian coordinates of **13**-III optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	-4.5622	1.1514	0.8246
C	-3.8845	2.3625	0.7553
C	-2.4726	2.3849	0.7628
C	-1.7444	1.2019	0.8786
C	-2.4335	-0.0261	1.0094
C	-3.8529	-0.0481	0.9367
C	-0.2346	1.1695	0.7825
C	0.3719	0.0350	1.5784
C	-0.3111	-1.1916	1.7225
C	-1.7145	-1.2882	1.2678
C	1.6416	0.2046	2.1287
C	2.2866	-0.8408	2.7941
C	1.6307	-2.0675	2.9195
C	0.3458	-2.2595	2.3979
C	0.2345	1.1694	-0.7827
C	1.7442	1.2020	-0.8787
C	2.4334	-0.0260	-1.0094
C	1.7146	-1.2882	-1.2676
C	0.3112	-1.1918	-1.7224
C	-0.3719	0.0348	-1.5784
C	-0.3456	-2.2598	-2.3977
C	-1.6305	-2.0679	-2.9194
C	-2.2866	-0.8412	-2.7941
C	-1.6417	0.2043	-2.1288
C	2.4724	2.3849	-0.7630
C	3.8843	2.3626	-0.7554
C	4.5621	1.1515	-0.8247
C	3.8528	-0.0480	-0.9367
O	-2.3202	-2.3751	1.1948
O	2.3205	-2.3750	-1.1945
C	3.6880	-0.6639	3.3259
C	-3.6879	-0.6645	-3.3260
O	-4.5558	-1.1870	0.9751
O	-0.3236	-3.4265	2.5264
O	4.5556	-1.1870	-0.9752
O	0.3239	-3.4267	-2.5261
H	-3.8749	-1.9200	1.0311
C	0.3001	-4.5130	3.1945
H	3.8746	-1.9199	-1.0314
C	-0.2998	-4.5133	-3.1942
H	0.1647	2.1110	1.1666
H	-0.1649	2.1109	-1.1668
H	2.1334	-2.8775	3.4343
H	-2.1332	-2.8780	-3.4341
H	-1.2211	-4.8228	-2.6850
H	1.2215	-4.8225	2.6853
H	-5.6479	1.1133	0.7936
H	2.1462	1.1605	2.0206
H	-2.1463	1.1601	-2.0208
H	5.6478	1.1134	-0.7936
H	3.8565	0.3601	3.6752
H	4.4247	-0.8653	2.5368
H	3.8965	-1.3486	4.1543
H	-4.4246	-0.8655	-2.5368
H	-3.8965	-1.3495	-4.1541
H	-3.8564	0.3594	-3.6757
H	0.5253	-4.2707	4.2413
H	-0.4242	-5.3282	3.1600
H	-0.5249	-4.2711	-4.2410
H	0.4246	-5.3285	-3.1595
O	-4.5340	3.5493	0.6633
H	-5.4900	3.3844	0.6894
O	4.5339	3.5494	-0.6635
H	5.4898	3.3845	-0.6895
Cl	-1.6903	3.9506	0.6363
Cl	1.6901	3.9506	-0.6365

Cartesian coordinates of **13**-IV optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	-0.9004	-2.5770	2.7504
C	-1.7060	-1.4534	2.8808
C	-1.3237	-0.2309	2.2815
C	-0.1379	-0.1434	1.5553
C	0.7286	-1.2619	1.5028
C	0.3197	-2.4974	2.0709
C	0.2619	1.0847	0.7724
C	1.7564	1.3196	0.8145
C	2.6492	0.2328	0.8457
C	2.1033	-1.1382	0.9851
C	2.2295	2.6314	0.7754
C	3.5979	2.9014	0.7536
C	4.4964	1.8293	0.7715
C	4.0462	0.5052	0.8143
C	-0.2619	1.0848	-0.7723
C	0.1379	-0.1433	-1.5553
C	-0.7286	-1.2618	-1.5029
C	-2.1033	-1.1382	-0.9853
C	-2.6493	0.2328	-0.8457
C	-1.7564	1.3196	-0.8144
C	-4.0462	0.5052	-0.8143
C	-4.4964	1.8294	-0.7714
C	-3.5980	2.9015	-0.7534
C	-2.2295	2.6315	-0.7751
C	1.3237	-0.2306	-2.2816
C	1.7060	-1.4530	-2.8810
C	0.9005	-2.5768	-2.7506
C	-0.3196	-2.4972	-2.0711
O	2.7927	-2.1564	0.7862
O	-2.7927	-2.1563	-0.7864
C	4.1110	4.3201	0.6932
C	-4.1111	4.3202	-0.6928
O	1.0712	-3.6020	2.0013
O	4.8895	-0.5509	0.8563
O	-1.0709	-3.6019	-2.0015
O	-4.8895	-0.5508	-0.8564
H	1.8803	-3.3472	1.4723
C	6.2897	-0.3192	0.8464
H	-1.8799	-3.3474	-1.4722
C	-6.2897	-0.3191	-0.8465
H	-0.2299	1.9590	1.2045
H	0.2298	1.9591	-1.2043
H	5.5595	2.0392	0.7585
H	-5.5596	2.0392	-0.7584
H	-6.6068	0.1934	0.0707
H	6.6067	0.1935	-0.0707
H	-1.1926	-3.5292	3.1849
H	1.5191	3.4549	0.7619
H	-1.5192	3.4549	-0.7616
H	1.1928	-3.5288	-3.1851
H	3.3325	5.0389	0.9665
H	4.4519	4.5709	-0.3199
H	4.9629	4.4681	1.3665
H	-4.4517	4.5709	0.3204
H	-4.9631	4.4682	-1.3658
H	-3.3326	5.0390	-0.9662
H	6.6105	0.2644	1.7193
H	6.7479	-1.3086	0.8844
H	-6.6105	0.2645	-1.7193
H	-6.7479	-1.3086	-0.8846
O	-2.8725	-1.4782	3.5701
H	-3.0193	-2.3794	3.8989
O	2.8725	-1.4778	-3.5703
H	3.0193	-2.3789	-3.8992
Cl	-2.3672	1.1556	2.5502
Cl	2.3671	1.1559	-2.5501

Cartesian coordinates of **14**-I optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	-1.2350	-0.7417	1.6085
C	-0.1464	0.1614	1.4977
C	1.0598	-0.1373	2.1138
C	1.2493	-1.3536	2.8025
C	0.1998	-2.2599	2.8805
C	-1.0441	-1.9703	2.3007
C	-2.5599	-0.3721	1.1297
C	-2.7959	0.9975	0.6671
C	-1.7136	1.8925	0.5060
C	-0.2866	1.4106	0.6574
C	-4.1248	1.4525	0.4302
C	-4.3472	2.7894	0.0675
C	-3.2726	3.6561	-0.0648
C	-1.9601	3.2147	0.1471
C	1.9131	1.2966	-0.6638
C	2.6645	0.1008	-0.7016
C	4.0601	0.1540	-0.4348
C	4.6746	1.3875	-0.1791
C	3.9361	2.5670	-0.1774
C	2.5494	2.5060	-0.4112
C	0.4065	1.2543	-0.8041
C	-0.1018	0.0439	-1.5553
C	0.6632	-1.1526	-1.5597
C	2.0262	-1.1661	-1.0585
C	-1.3319	0.0873	-2.1900
C	-1.8426	-1.0696	-2.8089
C	-1.1350	-2.2670	-2.7907
C	0.1183	-2.3192	-2.1726
O	-3.5192	-1.1968	1.1887
O	2.6889	-2.2469	-1.0094
H	0.0896	2.1545	-1.3401
H	0.2903	2.2130	1.1288
C	2.5928	-1.6617	3.4160
C	4.6101	3.8982	0.0518
O	-5.1933	0.6513	0.5461
O	-2.0203	-2.8788	2.4400
O	0.7742	-3.4862	-2.1996
O	4.8306	-0.9455	-0.4113
H	-4.8513	-0.2478	0.7898
H	-2.8212	-2.5113	1.9850
H	1.6380	-3.3390	-1.7309
H	4.2357	-1.7132	-0.6188
H	-5.3691	3.1132	-0.0999
O	-3.0526	-0.9485	-3.4125
H	-1.5225	-3.1686	-3.2571
H	-3.3109	-1.8048	-3.7896
H	1.8830	0.5677	2.0532
H	0.3104	-3.2075	3.3985
H	-1.1311	3.9087	0.0341
H	5.7434	1.3928	0.0121
H	1.9672	3.4252	-0.3920
H	-1.9244	0.9942	-2.2186
H	2.9150	-0.8565	4.0872
H	3.3603	-1.7563	2.6372
H	2.5724	-2.5946	3.9863
H	4.7514	4.4319	-0.8973
H	5.5954	3.7758	0.5112
H	4.0076	4.5457	0.6986
H	-3.4524	4.6929	-0.3366

Cartesian coordinates of **14**-II optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	2.6743	0.4941	0.6179
C	1.7149	1.5241	0.4886
C	2.1075	2.7837	0.0536
C	3.4482	3.0569	-0.2785
C	4.3894	2.0358	-0.1888
C	4.0231	0.7564	0.2507
C	2.2966	-0.8066	1.1656
C	0.9751	-0.9669	1.7672
C	0.0068	0.0637	1.6587
C	0.2502	1.2327	0.7311
C	0.6934	-2.1150	2.5611
C	-0.5211	-2.1962	3.2592
C	-1.4356	-1.1592	3.1709
C	-1.1816	-0.0330	2.3741
C	-0.1850	-0.2338	-1.3829
C	-1.0919	-1.3225	-1.3221
C	-0.7072	-2.5725	-1.8812
C	0.5456	-2.7064	-2.4983
C	1.4142	-1.6265	-2.5874
C	1.0313	-0.3878	-2.0324
C	-0.5196	1.0692	-0.6912
C	-2.0039	1.3017	-0.5018
C	-2.9020	0.2086	-0.4855
C	-2.4434	-1.1367	-0.8075
C	-2.4660	2.5910	-0.2798
C	-3.8297	2.8132	-0.0255
C	-4.7316	1.7535	0.0214
C	-4.2795	0.4497	-0.2058
O	3.1384	-1.7517	1.1978
O	-3.2393	-2.1204	-0.7189
H	-0.1249	1.8941	-1.2931
H	-0.2045	2.1259	1.1714
C	3.8551	4.4452	-0.7090
C	2.7669	-1.7658	-3.2412
O	1.5555	-3.1336	2.6912
O	4.9791	-0.1846	0.3029
O	-5.1815	-0.5387	-0.1533
O	-1.5053	-3.6497	-1.8575
H	2.3494	-2.9116	2.1408
H	4.5453	-1.0126	0.6371
H	-4.6859	-1.3830	-0.3316
H	-2.3413	-3.3766	-1.3987
H	-0.7083	-3.0770	3.8643
O	-4.2120	4.1027	0.1732
H	-5.7877	1.9094	0.2242
H	-5.1702	4.1325	0.3246
H	1.3669	3.5760	-0.0343
H	5.4292	2.2047	-0.4518
H	-1.9167	0.7626	2.3139
H	0.8075	-3.6761	-2.9103
H	1.7113	0.4552	-2.1058
H	-1.7958	3.4448	-0.3010
H	3.8985	5.1232	0.1534
H	4.8419	4.4468	-1.1811
H	3.1350	4.8712	-1.4168
H	3.5686	-1.6298	-2.5041
H	2.8939	-2.7500	-3.7009
H	2.9122	-1.0042	-4.0169
H	-2.3683	-1.2207	3.7253

Cartesian coordinates of **14**-III optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	0.6697	-1.1326	-1.5689
C	-0.1065	0.0542	-1.5312
C	-1.3581	0.0770	-2.1291
C	-1.9023	-1.0760	-2.7327
C	-1.1625	-2.2513	-2.7390
C	0.1198	-2.2975	-2.1715
C	2.0506	-1.1331	-1.1020
C	2.6772	0.1315	-0.7383
C	1.9143	1.3206	-0.6658
C	0.4061	1.2666	-0.7863
C	4.0815	0.1960	-0.5015
C	4.6933	1.4255	-0.2378
C	3.9223	2.5847	-0.2029
C	2.5331	2.5351	-0.4073
C	-0.1186	0.1636	1.5162
C	-1.2007	-0.7486	1.6168
C	-1.0034	-1.9803	2.3015
C	0.2392	-2.2618	2.8881
C	1.2825	-1.3478	2.8184
C	1.0886	-0.1308	2.1319
C	-0.2678	1.4178	0.6854
C	-1.6972	1.8942	0.5463
C	-2.7710	0.9855	0.6828
C	-2.5244	-0.3881	1.1293
C	-1.9541	3.2197	0.2071
C	-3.2689	3.6493	-0.0135
C	-4.3348	2.7668	0.0864
C	-4.1009	1.4270	0.4294
O	2.7266	-2.2067	-1.0892
O	-3.4759	-1.2230	1.1676
H	0.3114	2.2192	1.1554
H	0.0781	2.1667	-1.3160
C	-3.2833	-1.0216	-3.3381
C	2.6233	-1.6479	3.4418
O	4.8597	-0.8950	-0.5188
O	0.7859	-3.4594	-2.2371
O	-5.1597	0.6057	0.5035
O	-1.9719	-2.8985	2.4289
H	4.2628	-1.6641	-0.7259
H	1.6633	-3.3123	-1.7990
H	-4.8102	-0.2879	0.7584
H	-2.7715	-2.5398	1.9655
O	4.4615	3.8097	0.0340
H	5.7667	1.4470	-0.0708
H	-5.3579	3.0813	-0.0911
H	-1.9393	0.9939	-2.1238
H	-1.5510	-3.1597	-3.1891
H	1.9678	3.4607	-0.3595
H	0.3542	-3.2105	3.4032
H	1.9073	0.5801	2.0759
H	-1.1314	3.9238	0.1132
H	-3.3573	-0.2197	-4.0826
H	-3.5478	-1.9645	-3.8248
H	-4.0367	-0.8141	-2.5676
H	2.6042	-2.5815	4.0112
H	3.3979	-1.7375	2.6695
H	2.9348	-0.8414	4.1165
H	5.4216	3.7211	0.1453
H	-3.4579	4.6888	-0.2688

Cartesian coordinates of **14**-IV optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	-2.8998	0.1932	-0.4394
C	-2.0011	1.2827	-0.4807
C	-2.4668	2.5722	-0.2534
C	-3.8229	2.8205	0.0305
C	-4.7064	1.7480	0.0993
C	-4.2667	0.4367	-0.1305
C	-2.4448	-1.1580	-0.7661
C	-1.1124	-1.3416	-1.3149
C	-0.2038	-0.2539	-1.3998
C	-0.5208	1.0479	-0.6971
C	-0.7480	-2.5933	-1.8938
C	0.4735	-2.7297	-2.5609
C	1.3251	-1.6350	-2.6647
C	0.9919	-0.3966	-2.0847
C	1.7366	1.5088	0.4471
C	2.7128	0.4969	0.5959
C	4.0618	0.7806	0.2427
C	4.4075	2.0593	-0.2160
C	3.4481	3.0594	-0.3346
C	2.1103	2.7675	-0.0064
C	0.2764	1.2071	0.7087
C	0.0507	0.0382	1.6417
C	1.0325	-0.9789	1.7551
C	2.3546	-0.8025	1.1580
C	-1.1346	-0.0689	2.3614
C	-1.3740	-1.1944	3.1635
C	-0.4469	-2.2197	3.2552
C	0.7664	-2.1258	2.5567
O	-3.2389	-2.1405	-0.6509
O	3.2115	-1.7331	1.2067
H	-0.1742	2.0981	1.1580
H	-0.1350	1.8715	-1.3063
C	-4.3092	4.2351	0.2345
C	3.8323	4.4468	-0.7884
O	-1.5476	-3.6659	-1.8410
O	-5.1733	-0.5486	-0.0498
O	1.6428	-3.1314	2.6936
O	5.0382	-0.1335	0.3349
H	-2.3662	-3.3870	-1.3509
H	-4.6885	-1.3960	-0.2317
H	2.4372	-2.8965	2.1485
H	4.6152	-0.9718	0.6550
O	2.5128	-1.6964	-3.3199
H	0.7222	-3.6929	-2.9980
H	-0.6220	-3.0996	3.8652
H	-1.7721	3.4088	-0.2969
H	-5.7575	1.8986	0.3262
H	1.6904	0.4256	-2.1834
H	5.4466	2.2433	-0.4714
H	1.3571	3.5462	-0.1093
H	-1.8791	0.7175	2.3002
H	-4.3926	4.7612	-0.7256
H	-5.2943	4.2566	0.7098
H	-3.6151	4.8106	0.8574
H	3.1084	4.8468	-1.5074
H	4.8211	4.4570	-1.2562
H	3.8600	5.1413	0.0616
H	-2.3050	-1.2642	3.7198
H	2.6434	-2.5945	-3.6640

Cartesian coordinates of **15**-I optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	-0.9896	-0.0441	1.9329
C	0.1392	0.6858	1.4785
C	1.3790	0.4664	2.0602
C	1.5573	-0.5153	3.0572
C	0.4637	-1.2607	3.4788
C	-0.8108	-1.0353	2.9383
C	-2.3284	0.2914	1.4683
C	-2.5197	1.4847	0.6407
C	-1.4029	2.1929	0.1414
C	-0.0023	1.6486	0.3216
C	-3.8333	1.9692	0.3783
C	-4.0035	3.1574	-0.3477
C	-2.8932	3.8480	-0.8106
C	-1.5977	3.3709	-0.5745
C	2.0448	0.9624	-1.0714
C	2.7133	-0.2539	-0.8065
C	4.1286	-0.2489	-0.6725
C	4.8411	0.9456	-0.8460
C	4.1813	2.1345	-1.1425
C	2.7773	2.1311	-1.2418
C	0.5318	1.0149	-1.0768
C	-0.1215	-0.3121	-1.3922
C	0.5640	-1.5214	-1.0944
C	1.9650	-1.5083	-0.7163
C	-1.3994	-0.3515	-1.9169
C	-2.0468	-1.5895	-2.1255
C	-1.4150	-2.7870	-1.8022
C	-0.1114	-2.7596	-1.2896
O	-3.3290	-0.3900	1.8403
O	2.5614	-2.5813	-0.3938
H	0.2198	1.7447	-1.8305
H	0.6684	2.4974	0.4909
C	2.9335	-0.7604	3.6246
C	4.9565	3.4090	-1.3744
O	-4.9351	1.3354	0.8055
O	-1.8253	-1.7724	3.4130
O	0.4638	-3.9379	-1.0153
O	4.8271	-1.3571	-0.3767
H	-4.6289	0.5197	1.2805
H	-2.6418	-1.4798	2.9322
H	1.3764	-3.7377	-0.6770
H	4.1668	-2.0953	-0.2991
H	-5.0138	3.5097	-0.5274
O	-3.2935	-1.5006	-2.6458
H	-1.8828	-3.7533	-1.9397
H	2.2359	1.0464	1.7321
H	0.5639	-2.0278	4.2404
H	-0.7404	3.9243	-0.9492
H	5.9219	0.9120	-0.7463
H	2.2581	3.0633	-1.4552
H	-1.9369	0.5547	-2.1711
H	3.3761	0.1682	4.0048
H	3.6080	-1.1427	2.8477
H	2.9104	-1.4877	4.4410
H	5.0306	3.6305	-2.4473
H	5.9749	3.3368	-0.9814
H	4.4661	4.2674	-0.9018
C	-4.0277	-2.6997	-2.8686
H	-4.9890	-2.3855	-3.2775
H	-3.5178	-3.3510	-3.5889
H	-4.1892	-3.2468	-1.9319
H	-3.0316	4.7730	-1.3641

Cartesian coordinates of **15**-II optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	2.7229	0.9173	0.6174
C	1.5788	1.7325	0.4623
C	1.7177	3.0380	0.0076
C	2.9805	3.5685	-0.3177
C	4.1058	2.7581	-0.2010
C	3.9968	1.4384	0.2577
C	2.6061	-0.4252	1.1817
C	1.3359	-0.8394	1.7723
C	0.1834	-0.0234	1.6423
C	0.1988	1.1604	0.7019
C	1.2793	-2.0116	2.5790
C	0.0978	-2.3247	3.2680
C	-1.0033	-1.4911	3.1589
C	-0.9695	-0.3458	2.3499
C	0.0649	-0.3973	-1.3858
C	-0.6210	-1.6362	-1.3059
C	-0.0036	-2.8018	-1.8375
C	1.2563	-2.7090	-2.4479
C	1.9062	-1.4865	-2.5571
C	1.2934	-0.3318	-2.0277
C	-0.5144	0.8321	-0.7214
C	-2.0181	0.7848	-0.5461
C	-2.6942	-0.4591	-0.5099
C	-1.9881	-1.6993	-0.8006
C	-2.7191	1.9637	-0.3570
C	-4.1077	1.9370	-0.1162
C	-4.7926	0.7254	-0.0496
C	-4.0927	-0.4729	-0.2438
O	3.6194	-1.1822	1.2367
O	-2.5841	-2.8141	-0.6941
H	-0.2761	1.7053	-1.3373
H	-0.4266	1.9509	1.1288
C	3.1073	5.0033	-0.7689
C	3.2642	-1.3810	-3.2065
O	2.3253	-2.8368	2.7303
O	5.1206	0.7084	0.3355
O	-4.7946	-1.6120	-0.1722
O	-0.5842	-4.0098	-1.7943
H	3.0656	-2.4669	2.1849
H	4.8561	-0.1849	0.6781
H	-4.1484	-2.3524	-0.3280
H	-1.4604	-3.8902	-1.3445
H	0.0827	-3.2185	3.8828
O	-4.6886	3.1521	0.0414
H	-5.8563	0.6631	0.1411
H	0.8351	3.6651	-0.1013
H	5.0941	3.1271	-0.4579
H	-1.8464	0.2882	2.2737
H	1.6988	-3.6199	-2.8393
H	1.8034	0.6226	-2.1150
H	-2.2241	2.9294	-0.3933
H	3.0231	5.6886	0.0848
H	4.0724	5.1901	-1.2488
H	2.3142	5.2715	-1.4759
H	4.0230	-1.0832	-2.4715
H	3.5757	-2.3322	-3.6472
H	3.2673	-0.6202	-3.9963
C	-6.0920	3.2112	0.2712
H	-6.3344	4.2719	0.3515
H	-6.6512	2.7694	-0.5625
H	-6.3655	2.7020	1.2035
H	-1.9110	-1.7305	3.7067

Cartesian coordinates of **15**-III optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	0.2690	-1.3237	-1.5598
C	-0.3105	-0.0292	-1.5359
C	-1.5479	0.1817	-2.1267
C	-2.2703	-0.8794	-2.7114
C	-1.7228	-2.1557	-2.7078
C	-0.4599	-2.3951	-2.1453
C	1.6350	-1.5352	-1.0950
C	2.4554	-0.3802	-0.7571
C	1.8904	0.9176	-0.7052
C	0.3911	1.0970	-0.8102
C	3.8510	-0.5314	-0.5238
C	4.6587	0.5888	-0.2877
C	4.0830	1.8580	-0.2758
C	2.6968	2.0192	-0.4758
C	-0.2694	0.1004	1.5057
C	-1.4778	-0.6339	1.6251
C	-1.4641	-1.8782	2.3152
C	-0.2718	-2.3466	2.8864
C	0.8995	-1.6054	2.7972
C	0.8857	-0.3745	2.1085
C	-0.2344	1.3586	0.6687
C	-1.5752	2.0478	0.5407
C	-2.7736	1.3138	0.6911
C	-2.7355	-0.0782	1.1467
C	-1.6304	3.3955	0.1958
C	-2.8663	4.0189	-0.0178
C	-4.0531	3.3091	0.0950
C	-4.0228	1.9511	0.4447
O	2.1317	-2.7026	-1.0641
O	-3.8033	-0.7571	1.2004
H	0.4672	2.0640	1.1257
H	0.1979	2.0326	-1.3445
C	-3.6326	-0.6180	-3.3055
C	2.1878	-2.1111	3.3977
O	4.4472	-1.7326	-0.5178
O	0.0162	-3.6477	-2.1978
O	-5.1936	1.3006	0.5313
O	-2.5611	-2.6350	2.4603
H	3.7353	-2.4012	-0.7094
H	0.9068	-3.6337	-1.7614
H	-4.9812	0.3659	0.7905
H	-3.3007	-2.1603	2.0016
O	4.7733	3.0069	-0.0721
H	5.7162	0.4235	-0.1266
H	-5.0180	3.7746	-0.0769
H	-1.9789	1.1782	-2.1299
H	-2.2517	-2.9972	-3.1445
H	2.2878	3.0244	-0.4432
H	-0.2975	-3.3006	3.4038
H	1.8031	0.2018	2.0380
H	-0.7107	3.9654	0.0918
H	-3.5949	0.1955	-4.0399
H	-4.0345	-1.5067	-3.8003
H	-4.3430	-0.3138	-2.5262
H	2.0305	-3.0212	3.9836
H	2.9179	-2.3373	2.6100
H	2.6435	-1.3571	4.0506
C	6.1807	2.9306	0.1265
H	6.6826	2.4888	-0.7428
H	6.5172	3.9601	0.2574
H	6.4263	2.3489	1.0235
H	-2.8971	5.0737	-0.2782

Cartesian coordinates of **15**-IV optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	-2.9689	-0.0728	-0.5423
C	-2.1700	1.0787	-0.7226
C	-2.7645	2.3347	-0.7561
C	-4.1547	2.4901	-0.6009
C	-4.9420	1.3616	-0.3952
C	-4.3714	0.0813	-0.3632
C	-2.3727	-1.4078	-0.5978
C	-0.9917	-1.5469	-1.0233
C	-0.1782	-0.4024	-1.2450
C	-0.6622	0.9611	-0.8028
C	-0.4727	-2.8320	-1.3507
C	0.8044	-2.9633	-1.9119
C	1.5623	-1.8222	-2.1581
C	1.0702	-0.5419	-1.8219
C	1.4501	1.8285	0.3791
C	2.4944	0.9548	0.7594
C	3.8375	1.3038	0.4442
C	4.1079	2.5153	-0.2070
C	3.0787	3.3836	-0.5560
C	1.7493	3.0231	-0.2636
C	0.0052	1.4343	0.5999
C	-0.1901	0.4219	1.7064
C	0.8625	-0.4636	2.0513
C	2.2060	-0.2621	1.5136
C	-1.4121	0.3243	2.3635
C	-1.6152	-0.6700	3.3318
C	-0.6147	-1.5727	3.6531
C	0.6350	-1.4809	3.0218
O	-3.0843	-2.4309	-0.3599
O	3.1329	-1.0845	1.7737
H	-0.5542	2.3394	0.8577
H	-0.3041	1.7045	-1.5223
C	-4.7789	3.8626	-0.6792
C	3.3769	4.7055	-1.2211
O	-1.1750	-3.9563	-1.1585
O	-5.1907	-0.9620	-0.1637
O	1.5804	-2.3609	3.3824
O	4.8776	0.5153	0.7517
H	-2.0510	-3.6831	-0.7763
H	-4.6199	-1.7749	-0.1645
H	2.3911	-2.1441	2.8542
H	4.5025	-0.2934	1.1872
O	2.7953	-1.8307	-2.7177
H	1.1509	-3.9609	-2.1493
H	-0.7604	-2.3517	4.3941
H	-2.1455	3.2171	-0.9062
H	-6.0165	1.4420	-0.2610
H	1.7011	0.3159	-2.0226
H	5.1441	2.7536	-0.4267
H	0.9430	3.6965	-0.5473
H	-2.2127	1.0156	2.1239
H	-4.8398	4.2049	-1.7206
H	-5.7935	3.8661	-0.2703
H	-4.1857	4.6033	-0.1311
H	2.6750	4.9086	-2.0378
H	4.3921	4.7308	-1.6276
H	3.2855	5.5322	-0.5044
C	3.3780	-3.0819	-3.0661
H	2.7754	-3.6068	-3.8175
H	4.3574	-2.8453	-3.4843
H	3.5010	-3.7222	-2.1843
H	-2.5757	-0.7346	3.8360

Cartesian coordinates of **16**-I optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	1.0918	-0.4381	1.8293
C	-0.0888	-1.0356	1.3165
C	-1.2908	-0.8678	1.9883
C	-1.3771	-0.0691	3.1476
C	-0.2319	0.5490	3.6330
C	1.0048	0.3732	2.9951
C	2.3916	-0.7426	1.2479
C	2.4903	-1.7927	0.2308
C	1.3209	-2.3695	-0.3144
C	-0.0412	-1.7987	0.0131
C	3.7670	-2.2792	-0.1717
C	3.8500	-3.3431	-1.0820
C	2.6891	-3.9102	-1.5877
C	1.4289	-3.4271	-1.2137
C	-2.0855	-0.7708	-1.1504
C	-2.6565	0.4323	-0.6756
C	-4.0637	0.4963	-0.4742
C	-4.8642	-0.6104	-0.7884
C	-4.3009	-1.7802	-1.2890
C	-2.9048	-1.8507	-1.4553
C	-0.5823	-0.9158	-1.2415
C	0.1460	0.3993	-1.3896
C	-0.4330	1.5976	-0.8874
C	-1.8230	1.6090	-0.4371
C	1.4028	0.4569	-1.9680
C	2.1181	1.6659	-2.0308
C	1.5890	2.8372	-1.5073
C	0.2916	2.8143	-0.9282
O	3.4386	-0.1710	1.6731
O	-2.3291	2.6519	0.0723
H	-0.3553	-1.5404	-2.1117
H	-0.7511	-2.6305	0.0705
C	-2.7110	0.1207	3.8269
C	-5.1709	-2.9540	-1.6681
O	4.9149	-1.7607	0.2899
O	2.0724	0.9796	3.5335
O	-0.1882	3.9736	-0.4636
O	-4.6724	1.5877	0.0155
H	4.6666	-1.0246	0.9080
H	2.8517	0.7457	2.9670
H	-1.0925	3.7792	-0.1058
H	-3.9616	2.2621	0.1751
H	-2.1884	-1.3474	1.6100
H	-0.2615	1.1752	4.5192
H	4.8339	-3.7016	-1.3659
H	2.7599	-4.7420	-2.2838
H	0.5311	-3.8813	-1.6254
H	-5.9352	-0.5238	-0.6320
H	-2.4609	-2.7714	-1.8288
H	1.8540	-0.4409	-2.3770
H	3.0988	1.6709	-2.4925
H	-2.6158	0.7045	4.7468
H	-3.4128	0.6430	3.1644
H	-3.1669	-0.8443	4.0795
H	-6.1684	-2.8745	-1.2259
H	-4.7264	-3.9020	-1.3447
H	-5.2948	-3.0111	-2.7575
O	2.1992	4.0513	-1.5034
C	3.5061	4.1387	-2.0475
H	3.5177	3.8785	-3.1147
H	3.8088	5.1801	-1.9269
H	4.2103	3.4898	-1.5099

Cartesian coordinates of **16**-II optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	2.8765	0.7315	0.6422
C	1.8273	1.6653	0.4831
C	2.1092	2.9516	0.0396
C	3.4244	3.3463	-0.2707
C	4.4556	2.4196	-0.1497
C	4.2023	1.1161	0.2983
C	2.6117	-0.5939	1.1966
C	1.2990	-0.8736	1.7727
C	0.2416	0.0622	1.6384
C	0.3922	1.2430	0.7070
C	1.1091	-2.0394	2.5683
C	-0.1071	-2.2308	3.2416
C	-1.1118	-1.2836	3.1287
C	-0.9470	-0.1417	2.3309
C	0.1126	-0.2694	-1.3979
C	-0.6929	-1.4358	-1.3260
C	-0.1899	-2.6551	-1.8613
C	1.0731	-2.6828	-2.4713
C	1.8396	-1.5294	-2.5727
C	1.3428	-0.3229	-2.0366
C	-0.3444	1.0047	-0.7236
C	-1.8449	1.1043	-0.5623
C	-2.6500	-0.0625	-0.5298
C	-2.0577	-1.3714	-0.8202
C	-2.4466	2.3388	-0.3770
C	-3.8282	2.4463	-0.1489
C	-4.6302	1.3131	-0.0926
C	-4.0412	0.0348	-0.2817
O	3.5379	-1.4553	1.2552
O	-2.7540	-2.4234	-0.7129
H	-0.0118	1.8556	-1.3273
H	-0.1487	2.0935	1.1343
C	3.7081	4.7622	-0.7101
C	3.2016	-1.5533	-3.2215
O	2.0596	-2.9723	2.7231
O	5.2413	0.2704	0.3820
O	-4.8542	-1.0268	-0.2216
O	-0.8836	-3.8013	-1.8227
H	2.8415	-2.6788	2.1891
H	4.8800	-0.5917	0.7162
H	-4.2805	-1.8240	-0.3675
H	-1.7425	-3.6020	-1.3688
H	1.2993	3.6697	-0.0717
H	5.4802	2.6829	-0.3945
H	-0.2243	-3.1228	3.8478
H	-2.0461	-1.4294	3.6643
H	-1.7509	0.5822	2.2518
H	1.4249	-3.6306	-2.8669
H	1.9461	0.5762	-2.1156
H	-1.8474	3.2454	-0.4081
H	-4.2660	3.4296	-0.0185
H	3.6908	5.4471	0.1479
H	4.6918	4.8475	-1.1810
H	2.9546	5.1185	-1.4215
H	3.9837	-1.3149	-2.4895
H	3.4273	-2.5335	-3.6508
H	3.2721	-0.8053	-4.0206
O	-5.9718	1.3024	0.1291
C	-6.6243	2.5480	0.3092
H	-6.5240	3.1884	-0.5775
H	-7.6779	2.3118	0.4666
H	-6.2372	3.0841	1.1865

Cartesian coordinates of **16**-III optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	−1.4554	−0.6893	1.6265
C	−0.3394	0.1800	1.5142
C	0.8638	−0.1657	2.1113
C	1.0197	−1.3937	2.7878
C	−0.0583	−2.2658	2.8688
C	−1.2973	−1.9313	2.3030
C	−2.7696	−0.2758	1.1567
C	−2.9671	1.1072	0.7143
C	−1.8598	1.9732	0.5676
C	−0.4492	1.4408	0.6882
C	−4.2814	1.6006	0.4758
C	−4.4668	2.9490	0.1375
C	−3.3683	3.7894	0.0273
C	−2.0691	3.3087	0.2331
C	−0.3797	0.0859	−1.5359
C	0.3287	−1.1435	−1.5754
C	−0.2895	−2.2764	−2.1753
C	−1.5676	−2.1572	−2.7413
C	−2.2398	−0.9420	−2.7321
C	−1.6300	0.1781	−2.1291
C	0.2039	1.2657	−0.7922
C	1.7121	1.2366	−0.6932
C	2.4152	0.0072	−0.7567
C	1.7061	−1.2266	−1.1087
C	2.4209	2.4029	−0.4536
C	3.8118	2.3799	−0.2596
C	4.5142	1.1812	−0.2888
C	3.8134	−0.0287	−0.5361
O	−3.7531	−1.0724	1.2062
O	2.3125	−2.3382	−1.0862
H	−0.0866	2.1841	−1.3129
H	0.1682	2.2174	1.1510
C	2.3578	−1.7517	3.3859
C	−3.6176	−0.8099	−3.3327
O	−5.3703	0.8206	0.5594
O	−2.2999	−2.8107	2.4405
O	4.5308	−1.1601	−0.5485
O	0.3070	−3.4751	−2.2400
H	−5.0523	−0.0864	0.8091
H	−3.0908	−2.4185	1.9896
H	3.8880	−1.8927	−0.7397
H	1.1897	−3.3816	−1.7984
H	1.7096	0.5117	2.0457
H	0.0265	−3.2215	3.3767
H	−3.5196	4.8359	−0.2246
H	−1.2205	3.9804	0.1312
H	−2.0082	−3.0421	−3.1900
H	−2.1599	1.1257	−2.1193
H	1.8997	3.3560	−0.4110
H	4.3351	3.3130	−0.0844
H	2.7172	−0.9593	4.0534
H	3.1130	−1.8748	2.5991
H	2.3091	−2.6834	3.9565
H	−3.6495	−0.0026	−4.0744
H	−4.3558	−0.5636	−2.5589
H	−3.9354	−1.7353	−3.8213
O	5.8539	1.0431	−0.1006
C	6.6151	2.2142	0.1429
H	6.2905	2.7237	1.0604
H	7.6466	1.8788	0.2621
H	6.5570	2.9169	−0.6993
H	−5.4789	3.3033	−0.0286

Cartesian coordinates of **16**-IV optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	-2.5944	-1.1292	0.5149
C	-1.5235	-1.9683	0.1314
C	-1.7763	-3.1102	-0.6191
C	-3.0825	-3.4479	-1.0202
C	-4.1364	-2.6095	-0.6698
C	-3.9136	-1.4541	0.0912
C	-2.3601	0.0239	1.3805
C	-1.0510	0.1886	2.0071
C	0.0281	-0.6602	1.6513
C	-0.0975	-1.5860	0.4626
C	-0.8866	1.1284	3.0648
C	0.3273	1.1800	3.7666
C	1.3542	0.3138	3.4285
C	1.2136	-0.6032	2.3765
C	2.1370	-1.1216	-0.7193
C	2.9206	0.0154	-0.4167
C	4.3150	-0.1498	-0.1814
C	4.8938	-1.4220	-0.2847
C	4.1229	-2.5333	-0.6114
C	2.7404	-2.3697	-0.8176
C	0.6350	-1.0000	-0.8648
C	0.1691	0.3904	-1.2295
C	0.9578	1.5237	-0.8877
C	2.3232	1.3489	-0.3961
C	-1.0473	0.5906	-1.8608
C	-1.5224	1.8866	-2.1279
C	-0.7883	3.0060	-1.7620
C	0.4759	2.8325	-1.1371
O	-3.3085	0.8174	1.6526
O	3.0139	2.3476	-0.0385
H	0.3197	-1.6895	-1.6548
H	0.4557	-2.5053	0.6807
C	-3.3326	-4.7148	-1.8021
C	4.7594	-3.8932	-0.7674
O	-1.8595	1.9704	3.4423
O	-4.9750	-0.6914	0.3936
O	1.1607	3.9407	-0.8327
O	5.1186	0.8751	0.1385
H	-2.6377	1.7936	2.8541
H	-4.6321	0.0755	0.9223
H	2.0110	3.6400	-0.4199
H	4.5458	1.6846	0.1788
H	-0.9502	-3.7588	-0.9037
H	-5.1558	-2.8311	-0.9710
H	2.2866	0.3469	3.9858
H	2.0341	-1.2669	2.1262
H	5.9612	-1.5101	-0.1059
H	2.1339	-3.2401	-1.0601
H	-1.6536	-0.2598	-2.1540
H	-2.4795	2.0019	-2.6237
H	-3.2840	-5.5937	-1.1460
H	-2.5795	-4.8560	-2.5856
H	-4.3199	-4.7081	-2.2731
H	4.9306	-4.1236	-1.8273
H	5.7268	-3.9444	-0.2591
H	4.1171	-4.6844	-0.3651
O	-1.1592	4.2981	-1.9603
C	-2.4195	4.5418	-2.5632
H	-2.4674	4.1302	-3.5805
H	-3.2400	4.1232	-1.9652
H	-2.5219	5.6273	-2.6084
H	0.4249	1.8995	4.5727

Cartesian coordinates of **17**-I optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	−0.6492	−0.7018	1.9273
C	0.2176	0.3654	1.5787
C	1.4795	0.4420	2.1500
C	1.9459	−0.5544	3.0319
C	1.1159	−1.6224	3.3475
C	−0.1789	−1.7089	2.8149
C	−2.0384	−0.7096	1.4815
C	−2.5734	0.4602	0.7979
C	−1.7169	1.5163	0.4103
C	−0.2154	1.3814	0.5459
C	−3.9756	0.5776	0.5603
C	−4.5175	1.7331	−0.0285
C	−3.6332	2.7634	−0.3706
C	−2.2493	2.6599	−0.1629
C	1.9171	1.4803	−0.8841
C	2.9034	0.4738	−0.7817
C	4.2647	0.8554	−0.6284
C	4.6118	2.2134	−0.6248
C	3.6401	3.2001	−0.7613
C	2.2904	2.8189	−0.8794
C	0.4501	1.1085	−0.9103
C	0.1881	−0.2941	−1.4101
C	1.1846	−1.2947	−1.2725
C	2.5359	−0.9397	−0.8763
C	−1.0425	−0.6221	−1.9505
C	−1.3154	−1.9499	−2.3221
C	−0.3820	−2.9796	−2.1612
C	0.8768	−2.6397	−1.6367
O	−2.7933	−1.6920	1.7595
O	3.4183	−1.8345	−0.6945
H	−0.0666	1.8143	−1.5685
H	0.1851	2.3596	0.8314
C	3.3421	−0.4591	3.5962
C	4.0229	4.6598	−0.8022
O	−4.8261	−0.4059	0.8951
O	−0.9334	−2.7543	3.1862
O	1.7807	−3.6241	−1.5072
O	5.2522	−0.0424	−0.4797
H	−4.2735	−1.1401	1.2793
H	−1.8080	−2.6503	2.7295
H	2.6045	−3.2086	−1.1345
H	4.8256	−0.9388	−0.5093
H	2.1303	1.2757	1.9054
H	1.4419	−2.4102	4.0196
H	−1.6194	3.4931	−0.4596
H	5.6615	2.4691	−0.5158
H	1.5269	3.5892	−0.9683
H	−1.8191	0.1211	−2.0881
H	3.5418	−1.2573	4.3168
H	4.0891	−0.5299	2.7954
H	3.5011	0.5028	4.0986
H	5.0360	4.8206	−0.4218
H	3.3326	5.2708	−0.2098
H	3.9905	5.0426	−1.8308
C	−6.0008	1.8616	−0.2772
H	−6.4458	2.6856	0.2995
H	−6.2244	2.0361	−1.3396
H	−6.5136	0.9453	0.0172
C	−0.7097	−4.4006	−2.5505
H	−0.9215	−4.4950	−3.6255
H	0.1314	−5.0575	−2.3261
H	−1.5810	−4.7847	−2.0008
O	−2.5485	−2.1812	−2.8453
H	−2.6386	−3.1245	−3.0535
O	−4.0723	3.9234	−0.9303
H	−5.0380	3.8925	−1.0178

Cartesian coordinates of **17**-II optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	-2.9032	0.4743	-0.7814
C	-1.9168	1.4808	-0.8838
C	-2.2901	2.8194	-0.8791
C	-3.6397	3.2007	-0.7609
C	-4.6115	2.2141	-0.6243
C	-4.2644	0.8560	-0.6278
C	-2.5359	-0.9392	-0.8762
C	-1.1846	-1.2943	-1.2726
C	-0.1880	-0.2938	-1.4100
C	-0.4500	1.1088	-0.9101
C	-0.8770	-2.6392	-1.6371
C	0.3818	-2.9791	-2.1615
C	1.3153	-1.9495	-2.3222
C	1.0426	-0.6218	-1.9505
C	-0.2176	0.3650	1.5787
C	0.6491	-0.7023	1.9271
C	0.1785	-1.7098	2.8140
C	-1.1165	-1.6237	3.3461
C	-1.9464	-0.5556	3.0307
C	-1.4797	0.4414	2.1497
C	0.2156	1.3814	0.5463
C	1.7171	1.5162	0.4108
C	2.5735	0.4601	0.7983
C	2.0385	-0.7099	1.4818
C	2.2495	2.6599	-0.1622
C	3.6334	2.7633	-0.3700
C	4.5177	1.7329	-0.0280
C	3.9757	0.5774	0.5607
O	-3.4183	-1.8340	-0.6946
O	2.7932	-1.6924	1.7592
H	-0.1849	2.3595	0.8320
H	0.0669	1.8147	-1.5680
C	-4.0222	4.6605	-0.8012
C	-3.3430	-0.4607	3.5942
O	-1.7809	-3.6235	-1.5077
O	-5.2520	-0.0417	-0.4789
O	4.8262	-0.4061	0.8953
O	0.9330	-2.7553	3.1853
H	-2.6047	-3.2080	-1.1351
H	-4.8255	-0.9381	-0.5089
H	4.2737	-1.1403	1.2797
H	1.8078	-2.6508	2.7293
H	-1.5265	3.5896	-0.9681
H	-5.6611	2.4698	-0.5152
H	1.8192	0.1214	-2.0880
H	-1.4427	-2.4119	4.0177
H	-2.1303	1.2753	1.9053
H	1.6196	3.4931	-0.4588
H	-5.0389	4.8202	-0.4299
H	-3.3376	5.2696	-0.2001
H	-3.9797	5.0465	-1.8281
H	-3.5423	-1.2582	4.3158
H	-4.0895	-0.5334	2.7931
H	-3.5033	0.5017	4.0951
C	0.7093	-4.4001	-2.5511
H	0.9223	-4.4940	-3.6259
H	1.5799	-4.7849	-2.0006
H	-0.1323	-5.0567	-2.3279
C	6.0010	1.8614	-0.2766
H	6.4456	2.6862	0.2991
H	6.5139	0.9456	0.0190
H	6.2248	2.0345	-1.3392
O	4.0726	3.9232	-0.9296
H	5.0382	3.8922	-1.0175
O	2.5484	-2.1809	-2.8454
H	2.6384	-3.1242	-3.0536

Cartesian coordinates of **17**-III optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	0.8978	-1.2186	-1.6162
C	-0.0300	-0.1495	-1.5282
C	-1.2816	-0.2742	-2.1131
C	-1.6746	-1.4677	-2.7529
C	-0.7833	-2.5313	-2.8111
C	0.5009	-2.4248	-2.2567
C	2.2731	-1.0496	-1.1610
C	2.7329	0.2749	-0.7632
C	1.8164	1.3449	-0.6463
C	0.3277	1.0927	-0.7444
C	4.1195	0.5171	-0.5331
C	4.5910	1.8069	-0.2344
C	3.6496	2.8419	-0.1628
C	2.2776	2.6187	-0.3553
C	0.0300	-0.1492	1.5279
C	-0.8978	-1.2184	1.6162
C	-0.5007	-2.4245	2.2569
C	0.7837	-2.5309	2.8109
C	1.6749	-1.4673	2.7525
C	1.2817	-0.2739	2.1126
C	-0.3278	1.0928	0.7440
C	-1.8164	1.3449	0.6459
C	-2.7329	0.2750	0.7634
C	-2.2732	-1.0495	1.1613
C	-2.2778	2.6187	0.3545
C	-3.6499	2.8417	0.1623
C	-4.5912	1.8066	0.2343
C	-4.1196	0.5171	0.5336
O	3.0822	-2.0276	-1.1901
O	-3.0826	-2.0271	1.1908
H	0.1324	1.9592	1.2299
H	-0.1325	1.9590	-1.2304
C	-3.0614	-1.5813	-3.3368
C	3.0618	-1.5807	3.3361
O	5.0214	-0.4776	-0.5911
O	1.3154	-3.4844	-2.3709
O	-5.0213	-0.4778	0.5927
O	-1.3150	-3.4842	2.3713
H	4.5145	-1.3053	-0.8182
H	2.1695	-3.2369	-1.9319
H	-4.5141	-1.3054	0.8196
H	-2.1692	-3.2368	1.9324
C	6.0600	2.0684	-0.0054
C	-6.0603	2.0680	0.0056
H	-1.9804	0.5556	-2.0677
H	-1.0528	-3.4672	-3.2908
H	1.6003	3.4629	-0.2702
H	1.0533	-3.4668	3.2907
H	1.9804	0.5560	2.0670
H	-1.6005	3.4629	0.2690
H	-3.2714	-0.7521	-4.0232
H	-3.8192	-1.5419	-2.5438
H	-3.1937	-2.5192	-3.8837
H	3.2719	-0.7516	4.0225
H	3.8194	-1.5412	2.5429
H	3.1944	-2.5186	3.8829
H	6.4715	2.7756	-0.7403
H	6.2543	2.4762	0.9971
H	6.6270	1.1412	-0.0960
H	-6.4734	2.7695	0.7450
H	-6.2539	2.4827	-0.9942
H	-6.6262	1.1395	0.0888
O	-4.0192	4.1229	-0.1078
H	-4.9831	4.1659	-0.2083
O	4.0187	4.1231	0.1075
H	4.9827	4.1662	0.2083

Cartesian coordinates of **17**-IV optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	2.7148	0.6005	0.8585
C	1.8011	1.6659	0.6944
C	2.2700	2.9430	0.4119
C	3.6468	3.2023	0.2748
C	4.5488	2.1522	0.4105
C	4.1053	0.8537	0.6986
C	2.2441	-0.7300	1.2430
C	0.8601	-0.9009	1.6511
C	-0.0638	0.1695	1.5325
C	0.3102	1.4080	0.7500
C	0.4504	-2.1069	2.2946
C	-0.8367	-2.2360	2.8438
C	-1.6961	-1.1366	2.7430
C	-1.3232	0.0528	2.0935
C	-1.8010	1.6659	-0.6944
C	-2.7148	0.6006	-0.8585
C	-4.1053	0.8537	-0.6985
C	-4.5487	2.1523	-0.4105
C	-3.6467	3.2024	-0.2748
C	-2.2699	2.9430	-0.4119
C	-0.3101	1.4080	-0.7501
C	0.0638	0.1695	-1.5326
C	-0.8601	-0.9009	-1.6511
C	-2.2441	-0.7299	-1.2429
C	1.3232	0.0528	-2.0935
C	1.6961	-1.1366	-2.7431
C	0.8367	-2.2360	-2.8438
C	-0.4505	-2.1069	-2.2946
O	3.0634	-1.6983	1.2998
O	-3.0634	-1.6983	-1.2997
H	0.1647	2.2730	-1.2242
H	-0.1647	2.2730	1.2241
C	4.1315	4.6064	0.0050
C	-4.1314	4.6064	-0.0051
O	1.2836	-3.1532	2.4143
O	5.0324	-0.1085	0.8182
O	-1.2836	-3.1532	-2.4143
O	-5.0323	-0.1084	-0.8181
H	2.1441	-2.8810	1.9941
H	4.5429	-0.9519	1.0028
H	-2.1441	-2.8810	-1.9941
H	-4.5429	-0.9519	-1.0027
C	-1.2683	-3.5065	3.5350
C	1.2682	-3.5066	-3.5350
H	1.5618	3.7611	0.2958
H	5.6173	2.3106	0.3005
H	-2.0466	0.8580	2.0409
H	-5.6172	2.3107	-0.3005
H	-1.5617	3.7611	-0.2958
H	2.0466	0.8580	-2.0410
H	4.0775	5.2196	0.9141
H	3.5165	5.1022	-0.7545
H	5.1703	4.6136	-0.3379
H	-4.0772	5.2197	-0.9141
H	-5.1703	4.6137	0.3377
H	-3.5165	5.1022	0.7546
H	-1.5088	-3.3369	4.5946
H	-2.1519	-3.9538	3.0573
H	-0.4687	-4.2471	3.4980
H	2.1521	-3.9536	-3.0576
H	1.5083	-3.3371	-4.5946
H	0.4688	-4.2474	-3.4975
O	2.9489	-1.1608	-3.2691
H	3.1111	-2.0259	-3.6772
O	-2.9490	-1.1608	3.2690
H	-3.1112	-2.0259	3.6771

Cartesian coordinates of 5-chlorinated **1**-I optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	1.1496	-1.2524	-1.3799
C	0.2131	-0.1878	-1.3864
C	-0.9863	-0.3328	-2.0664
C	-1.3209	-1.5428	-2.7106
C	-0.4222	-2.6014	-2.6780
C	0.8134	-2.4750	-2.0267
C	2.4763	-1.0621	-0.8211
C	2.9035	0.2874	-0.4249
C	1.9654	1.3510	-0.4004
C	0.4927	1.0678	-0.5945
C	4.2750	0.5292	-0.1364
C	4.7038	1.8369	0.1379
C	3.7947	2.8790	0.1292
C	2.4405	2.6350	-0.1324
C	-1.7584	1.2495	0.6245
C	-2.6275	0.1351	0.6798
C	-3.9962	0.3089	0.3338
C	-4.4720	1.5816	-0.0092
C	-3.6197	2.6815	-0.0259
C	-2.2575	2.4997	0.2823
C	-0.2724	1.0651	0.8453
C	0.0734	-0.1441	1.6836
C	-0.8039	-1.2578	1.7159
C	-2.1388	-1.1654	1.1280
C	1.2658	-0.1903	2.3979
C	1.6162	-1.3446	3.1144
C	0.7940	-2.4593	3.1231
C	-0.4247	-2.4314	2.4274
O	3.2955	-2.0248	-0.7594
O	-2.8959	-2.1794	1.0896
H	0.1086	1.9584	1.3479
H	0.0493	1.9169	-1.1200
C	-2.6584	-1.6775	-3.3950
C	-4.1439	4.0584	-0.3539
O	5.1976	-0.4407	-0.1179
O	1.6412	-3.5284	-2.0544
O	-1.1970	-3.5257	2.4815
O	-4.8692	-0.7113	0.3152
H	4.7244	-1.2895	-0.3266
H	2.4548	-3.2707	-1.5516
H	-2.0094	-3.3319	1.9471
H	-4.3656	-1.5219	0.5873
H	-1.6929	0.4911	-2.0910
H	-0.6486	-3.5482	-3.1585
H	5.7550	2.0049	0.3462
H	4.1230	3.8943	0.3255
H	-5.5242	1.6810	-0.2580
H	-1.5844	3.3525	0.2479
H	2.5504	-1.3648	3.6693
H	1.0559	-3.3619	3.6652
H	-2.7428	-2.6248	-3.9350
H	-3.4731	-1.6313	-2.6609
H	-2.8223	-0.8602	-4.1075
H	-5.1265	4.0115	-0.8325
H	-3.4612	4.5968	-1.0207
H	-4.2469	4.6625	0.5570
Cl	1.3601	4.0353	-0.1270
H	1.9290	0.6685	2.4022

Cartesian coordinates of 5-chlorinated **1**-II optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	2.6645	0.3931	0.4948
C	1.8166	1.4949	0.2446
C	2.3470	2.6752	-0.2584
C	3.7236	2.7963	-0.5321
C	4.5572	1.7020	-0.3190
C	4.0475	0.4970	0.1829
C	2.1278	-0.8215	1.0966
C	0.7860	-0.7883	1.6862
C	-0.0485	0.3482	1.4904
C	0.3214	1.3445	0.4151
C	0.3981	-1.8236	2.5786
C	-0.7916	-1.6915	3.3125
C	-1.5568	-0.5493	3.1830
C	-1.1880	0.4650	2.2842
C	-0.1144	-0.4389	-1.4563
C	-1.1340	-1.4011	-1.2396
C	-0.8607	-2.7696	-1.5109
C	0.3964	-3.1456	-2.0100
C	1.3760	-2.1942	-2.2605
C	1.1031	-0.8364	-1.9886
C	-0.3423	0.9955	-1.0399
C	-1.7976	1.4063	-1.0768
C	-2.8141	0.4396	-0.8971
C	-2.4810	-0.9843	-0.8662
C	-2.1374	2.7441	-1.2437
C	-3.4811	3.1385	-1.2079
C	-4.4919	2.2132	-0.9960
C	-4.1738	0.8563	-0.8342
O	2.8526	-1.8525	1.2104
O	-3.3747	-1.8454	-0.6151
H	0.2085	1.6498	-1.7227
H	-0.0984	2.3197	0.6710
C	4.2830	4.1047	-1.0350
C	2.7360	-2.5911	-2.7789
O	1.1299	-2.9261	2.7805
O	4.9007	-0.5271	0.3459
O	-5.1835	-0.0045	-0.6408
O	-1.7679	-3.7376	-1.3203
H	1.9370	-2.8464	2.2090
H	4.3723	-1.2862	0.7024
H	-4.7787	-0.9051	-0.5474
H	-2.5875	-3.2988	-0.9740
H	1.6907	3.5226	-0.4444
H	5.6197	1.7541	-0.5360
H	-1.0722	-2.4873	3.9939
H	-2.4557	-0.4237	3.7773
H	0.5723	-4.1997	-2.2010
H	1.8718	-0.0953	-2.1847
H	-3.7364	4.1859	-1.3461
H	-5.5364	2.5044	-0.9571
H	4.3532	4.8364	-0.2196
H	5.2853	3.9789	-1.4546
H	3.6399	4.5434	-1.8063
H	3.5064	-2.3942	-2.0223
H	2.7769	-3.6535	-3.0350
H	3.0056	-2.0124	-3.6705
Cl	-2.1941	1.9113	2.2690
H	-1.3579	3.4861	-1.3961

Cartesian coordinates of 5-chlorinated **1**-III optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	4.3959	2.3959	-0.4612
C	3.3824	3.3434	-0.4752
C	2.0427	2.9664	-0.6374
C	1.7095	1.6253	-0.8045
C	2.7294	0.6459	-0.8260
C	4.0837	1.0391	-0.6302
C	0.2549	1.2133	-0.8714
C	0.0279	-0.1213	-1.5424
C	1.0573	-1.0975	-1.5377
C	2.4035	-0.7553	-1.0992
C	-1.1992	-0.4199	-2.1159
C	-1.4677	-1.6978	-2.6501
C	-0.4757	-2.6691	-2.6152
C	0.7872	-2.3880	-2.0720
C	-0.3904	1.2692	0.6265
C	-1.8983	1.3231	0.5343
C	-2.6608	0.1404	0.7105
C	-2.0096	-1.0914	1.1794
C	-0.6404	-1.0322	1.6583
C	0.1233	0.1524	1.5038
C	-0.0845	-2.1257	2.3799
C	1.1920	-2.0071	2.9488
C	1.9213	-0.8315	2.8226
C	1.3705	0.2491	2.1010
C	-2.5775	2.4949	0.2001
C	-3.9660	2.5131	0.0176
C	-4.7043	1.3508	0.1501
C	-4.0655	0.1496	0.4924
O	3.3053	-1.6422	-1.0367
O	-2.6733	-2.1671	1.2491
C	-2.8319	-1.9973	-3.2206
C	3.3024	-0.7056	3.4158
O	5.0937	0.1552	-0.5956
O	1.7033	-3.3660	-2.0936
O	-4.8254	-0.9496	0.5964
O	-0.7395	-3.2814	2.5565
H	4.6930	-0.7415	-0.7393
H	2.5253	-2.9995	-1.6774
H	-4.2177	-1.6933	0.8532
H	-1.6090	-3.1959	2.0902
H	-0.2920	1.9831	-1.4233
H	-0.0354	2.2212	1.0277
Cl	-1.7218	4.0289	-0.0013
H	5.4365	2.6713	-0.3250
H	3.6319	4.3943	-0.3546
H	-1.9760	0.3382	-2.1459
H	-0.6473	-3.6648	-3.0121
H	1.5874	-2.8600	3.4915
H	1.9451	1.1646	1.9994
H	-4.4564	3.4480	-0.2325
H	-5.7786	1.3429	0.0005
H	-3.1208	-1.2500	-3.9692
H	-2.8653	-2.9839	-3.6911
H	-3.5942	-1.9727	-2.4312
H	4.0566	-0.6278	2.6221
H	3.5551	-1.5683	4.0385
H	3.3887	0.1988	4.0297
H	1.2605	3.7197	-0.6297

Cartesian coordinates of 5-chlorinated **1**-IV optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	0.6853	-2.8593	-2.7690
C	1.5208	-1.7634	-2.9056
C	1.1936	-0.5261	-2.3297
C	0.0117	-0.3795	-1.6116
C	-0.8813	-1.4752	-1.5018
C	-0.5261	-2.7304	-2.0700
C	-0.3108	0.9219	-0.9125
C	-1.7960	1.1652	-0.7622
C	-2.6855	0.0686	-0.6740
C	-2.2160	-1.2877	-0.9315
C	-2.2815	2.4603	-0.6626
C	-3.6508	2.7113	-0.4469
C	-4.5248	1.6375	-0.3217
C	-4.0635	0.3172	-0.4272
C	0.4493	1.0836	0.5252
C	0.2795	-0.1168	1.4294
C	1.2388	-1.1663	1.3630
C	2.5243	-0.9426	0.6933
C	2.8772	0.4088	0.2758
C	1.9007	1.4298	0.2752
C	4.2138	0.7272	-0.0906
C	4.5498	2.0505	-0.4082
C	3.5899	3.0575	-0.3813
C	2.2606	2.7311	-0.0477
C	-0.7905	-0.2674	2.3099
C	-0.9766	-1.4556	3.0349
C	-0.0929	-2.5086	2.9043
C	1.0366	-2.3758	2.0808
O	-2.9883	-2.2771	-0.7653
O	3.3620	-1.8837	0.5856
C	-4.1510	4.1319	-0.3468
C	3.9641	4.4873	-0.6872
O	-1.3144	-3.8111	-1.9853
O	-4.9627	-0.6702	-0.3078
O	1.8910	-3.4049	2.0333
O	5.1850	-0.1963	-0.1447
H	-2.1210	-3.5393	-1.4755
H	-4.4670	-1.5229	-0.4107
H	2.6372	-3.1340	1.4375
H	4.7680	-1.0653	0.0861
H	0.1060	1.7444	-1.5019
H	-0.0362	1.9474	0.9850
Cl	-1.9294	1.0386	2.6315
H	0.9291	-3.8245	-3.2002
H	2.4472	-1.8635	-3.4647
H	-1.5938	3.2996	-0.7452
H	-5.5851	1.7926	-0.1476
H	5.5808	2.2636	-0.6737
H	1.5059	3.5147	-0.0407
H	-1.8280	-1.5363	3.7024
H	-0.2317	-3.4359	3.4494
H	-3.7026	4.6473	0.5119
H	-3.8846	4.7079	-1.2415
H	-5.2379	4.1688	-0.2316
H	3.9933	5.0873	0.2317
H	4.9493	4.5531	-1.1579
H	3.2325	4.9570	-1.3545
H	1.8663	0.3172	-2.4433