# **Supplementary information**

## A rule to distinguish diastereomeric bianthrones by <sup>1</sup>H NMR

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**Figure S1.** Relationship between relative free energy ( $\Delta G$ ) and dihedral angle ( $\angle$ 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 <sup>1</sup>H NMR shifts for chrysophanol bianthrone (1).



**Figure S3.** Differences of the calculated <sup>1</sup>H NMR data for *cis* (*meso*) and *trans* chrysophanol bianthrone (1).



Figure S4. Experimental and calculated differences of <sup>1</sup>H NMR shifts for emodin bianthrone (2).

1,1'	2,2'	3,3'	5,5'	6,6'	7,7'	8,8'	I/°	II/°	III/°	IV/°
OH	Н	Н	Н	Н	Н	OH		71	.9	
$OCH_3$	Н	$CH_3$	Н	OH	Н	OH	76.5	76.5	70.8	69.3
$OCH_3$	Н	$\mathrm{CH}_3$	Cl	OH	Н	OH	73.0	73.0	55.3	69.3
OAc	Η	$CH_3$	Н	OCH <sub>3</sub>	Н	$OCH_3$	72.5	72.5	79.0	68.3
OH	СООН	$CH_3$	Н	OH	Н	OH	71.7	71.7	71.2	70.1
OH	Н	$CH_3$	Н	Н	Н	OH	71.6	71.6	70.8	72.0
OH	Н	$CH_3$	Cl	Н	Н	OH	71.5	71.5	54.6	72.6
OH	Н	$CH_3$	Н	OH	Н	OH	71.2	71.2	71.0	71.6
OH	Н	$CH_3$	Н	OH	$CH_3$	OH	71.3	71.3	70.9	71.3
OH	Н	$CH_3$	Н	OCH <sub>3</sub>	Н	OH	71.4	71.4	70.7	72.1
OH	Н	$CH_3$	Н	OCH <sub>3</sub>	Н	OCH <sub>3</sub>	73.6	73.6	78.1	71.6
OH	Н	$\mathrm{CH}_3$	Н	Н	$CH_3$	OH	71.7	71.7	71.1	71.3
OH	Н	$CH_3$	Н	Н	OCH <sub>3</sub>	OH	71.1	71.1	70.7	70.4
OH	Н	СООН	Н	Н	Н	OH	71.7	71.7	70.4	69.7
OH	Н	$\mathrm{CH}_3$	Cl,H	Н	Н	OH	69.6	74.8	70.0	74.5
OH	Н	$\mathrm{CH}_3$	Н	Н,ОН	Н	OH	71.8	71.5	72.0	71.9
OH	Н	$\mathrm{CH}_3$	Н	H,OCH <sub>3</sub>	Н	OH	72.0	72.2	72.1	71.8
OH	Н	$CH_3$	Н	OH,OCH <sub>3</sub>	Н	OH	72.3	71.9	71.9	72.6
OH	Н	CH <sub>3</sub>	Н	Н	H,OCH <sub>3</sub>	OH	70.7	72.0	71.5	71.8

**Table S1.** Calculated degrees for the dihedral angles  $\angle$ H-10–C-10–C-10'–H-10' at the gas-phase B3LYP/6-31G(d) level<sup>*a*</sup>

<sup>*a*</sup>Without groups at 4/4' and 10/10' positions.

pos.	$\delta_{\mathrm{I}}$	$\delta_{\mathrm{II}}$	$\delta_{ m III}$	$\delta_{\mathrm{IV}}$
OH-1	12.21	12.34	12.02	12.47
2	6.83	7.19	6.88	7.20
CH <sub>3</sub> -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 <sub>3</sub> -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

**Table S2.** Calculated <sup>1</sup>H NMR data for the conformers of *cis* (*meso*) and *trans* chrysophanol bianthrone (1)















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

atom	Х	Y	Z
С	2.8502	0.6031	0.2596
С	1.9048	1.6533	0.2902
С	2.2872	2.9366	-0.0903
С	3. 5989	3. 1857	-0. 5141
С	4.5361	2.1650	-0.5740
С	4.1756	0.8639	-0.1932
С	2.4888	-0.7306	0.7430
С	1.2196	-0.9159	1.4409
С	0.2750	0.1398	1. 5095
С	0.4646	1.3805	0.6661
С	0.9773	-2.1223	2.1592
С	-0.1725	-2.2386	2.9552
С	-1.0594	-1.1783	3.0415
С	-0.8445	0.0079	2.3239
С	-1.9049	1.6532	-0.2901
С	-2.8502	0.6030	-0.2597
С	-4.1757	0.8638	0.1930
С	-4.5363	2.1648	0. 5738
С	-3.5991	3.1856	0.5141
С	-2.2874	2.9365	0.0904
С	-0.4646	1.3805	-0.6659
С	-0.2750	0.1398	-1.5093
С	-1.2196	-0.9160	-1.4409
С	-2. 4889	-0.7307	-0.7431
С	0.8447	0.0079	-2.3237
С	1.0597	-1.1782	-3.0412
С	0.1727	-2.2386	-2.9551
С	-0.9772	-2.1223	-2.1592
0	3.3082	-1.6881	0.6337
0	-3.3082	-1.6882	-0.6339
Н	-0. 0989	2.2420	-1.2341
Н	0.0988	2.2420	1.2343
0	1.8175	-3. 1660	2.1267
0	5.1132	-0.0912	-0. 2703
0	-1.8173	-3. 1660	-2.1267
0	-5. 1133	-0.0914	0.2700
Н	2.5705	-2.9136	1.5338
Н	4.6857	-0.9374	0.0225
Н	-2.5705	-2.9137	-1.5340
Н	-4.6857	-0.9375	-0.0228
Н	1.5663	3.7494	-0.0557
Н	3.8877	4.1937	-0.8002
Н	5.5540	2.3400	-0.9062
Н	-0. 3298	-3.1646	3. 4981
Н	-1.9387	-1.2670	3.6740
Н	-1.5552	0.8231	2.4045
Н	-5.5542	2.3398	0.9060
Н	-3.8879	4.1936	0.8002
Н	-1.5665	3.7493	0.0558
Н	1.5554	0.8232	-2.4041
Н	1.9390	-1.2669	-3.6736
Н	0.3301	-3.1646	-3.4980

atom	Х	Y	Z
С	-1.2199	-0.9160	1.4406
С	-0.2751	0.1395	1.5092
С	0.8444	0.0073	2.3235
С	1.0592	-1.1790	3.0409
С	0.1721	-2.2392	2.9546
С	-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 1759	0.9642	-0.1022
C	-4 5261	2 1655	-0.5720
C	-4. 5501	2.1000	-0.5739
C	-3. 5987	3. 1801	-0. 5140
C	-2.2871	2.9366	-0.0903
C	0.2751	0. 1395	-1.5092
<u> </u>	1.2199	-0.9161	-1. 4406
С	0.9778	-2. 1226	-2.1587
С	-0.1721	-2.2392	-2.9545
С	-1.0592	-1.1791	-3.0409
С	-0.8444	0.0072	-2.3235
С	0.4647	1.3803	-0.6660
С	1.9048	1.6533	-0.2901
С	2.8504	0.6032	-0.2595
С	2.4892	-0.7306	-0.7428
С	2.2871	2.9366	0.0903
С	3. 5987	3. 1861	0.5140
С	4.5361	2.1655	0. 5739
С	4.1758	0.8643	0.1932
0	-3.3085	-1.6881	0.6335
0	3. 3085	-1.6881	-0.6335
Н	0.0989	2,2417	-1.2343
Н	-0.0989	2.2418	1, 2343
0	-5 1138	-0.0905	-0.2706
0	-1 8183	-3 1659	2 1260
0	5 1138	-0.0905	0.2706
0	1 8183	-3 1659	-2 1260
н	-4 6866	-0 9370	0.0216
Ц	-9 5712	_2 0128	1 5339
П	4 6867		-0.0216
11	1.000/ 0.5710	-9 0199	
П	2.0/13	-2. 9128	-1. 2000
Н	1.0005	0.8224	2. 404Z
H	1.9385	-1.2679	3.0732
H	0.3293	-3. 1653	3. 4973
H	-5.5540	2. 3406	-0.9062
H	-3.8873	4. 1941	-0.8001
Н	-1.5661	3. 7493	-0.0556
Н	-0. 3293	-3.1654	-3. 4972
Н	-1.9386	-1.2680	-3.6732
Н	-1.5553	0.8224	-2.4042
Н	1.5661	3.7493	0.0556
Н	3. 8873	4. 1941	0.8001
Н	5. 5540	2. 3406	0.9062

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

atom	Х	Y	Z
С	-2.5640	1.2555	-0.1157
С	-1.2967	1.2509	-0.7528
С	-0.8305	2.4064	-1.3639
С	-1.6002	3. 5798	-1.3301
С	-2.8196	3.6199	-0.6734
С	-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
0	-0 4494	-0.0001	-0.6811
<u> </u>	-3 3162	-2,4613	-0.0538
<u> </u>	-2 8198	-3 6100	-0.6732
<u> </u>	-1 6004	-3 5799	-1 3300
<u> </u>	-0. 8207	-2 4065	-1.3300
C	-0.8307	-2.4005	-1. 3039
<u> </u>	1. 2967	1.2509	0. 7528
<u> </u>	2. 5640	1. 2555	0.1157
<u> </u>	3.3161	2.4614	0.0539
C	2.8196	3.6199	0.6734
C	1.6002	3. 5797	1. 3302
С	0.8305	2.4064	1.3640
С	0. 4494	-0.0001	0.6811
С	1.2968	-1.2510	0.7527
С	2.5641	-1.2555	0.1157
С	3. 1632	0.0000	-0. 3353
С	0.8307	-2. 4065	1.3639
С	1.6004	-3.5799	1.3300
С	2.8198	-3.6199	0.6732
С	3. 3162	-2.4613	0.0538
0	-4.2430	0.0001	0.9943
0	4.2430	0.0001	-0.9944
Н	-0.2696	-0.0001	1.5064
Н	0.2696	-0.0001	-1.5064
0	-4.5069	-2.5392	0.5584
0	-4.5067	2.5393	0.5583
0	4.5069	-2.5393	-0.5584
0	4.5067	2.5394	-0.5583
Н	-4. 7067	-1.6377	0.9187
Н	-4. 7064	1.6377	0. 9186
н	4, 7066	-1.6377	-0, 9187
H	4, 7065	1.6378	-0.9186
Н	0 1382	2 4078	-1 8537
Н	-1 2277	4 4756	-1 8197
н	-3 4186	4 5235	-0 6296
 Ц	-3 /180	-1 5924	-0 6294
Ц	_1 9980	-4 $4757$	-1 8106
п	-1.2200		-1.0190
<u>П</u>	0.100	-2. 4080	-1.0000
<u>H</u>	J. 4180	4. 5235	0.0290
<u>H</u>	1.2277	4.4/50	1.0198
<u>H</u>	-0.1382	2.4078	1.8538
H	-0.1380	-2.4080	1.8537
Н	1.2280	-4. 4757	1.8196
Н	3. 4188	-4.5235	0. 6294

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

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

atom	Х	Y	Z
С	-1.4192	-0.9390	1.3367
C	-0.3468	-0.0108	1 3793
C	0.8222	-0.3427	2 0481
C	0.0222	1 6007	2.0401
C C	0.9913	-1.0097	2.0447
U C	-0.0408	-2.5360	2.5745
C	-1.2485	-2.2190	1. 9352
С	-2.7159	-0. 5537	0.7971
С	-2.9518	0.8462	0.4350
С	-1.8850	1.7734	0.4354
С	-0.4605	1.3080	0.6486
C	-4. 2705	1, 2930	0.1338
C	-4 5007	2 6514	-0.1302
C	2 4491	2.0014	0.1014
C	-3. 4431	J. 0400	-0.1014
L C	-2.1393	3.1170	0.1741
С	1.8289	1.3632	-0.5163
С	2.6148	0. 1931	-0. 6225
С	3. 9878	0.2473	-0.2540
С	4.5495	1.4607	0.1657
С	3.7798	2.6180	0.2346
С	2, 4138	2, 5526	-0.0998
C	0.3381	1.3040	-0.7678
C	-0.0861	0 1652	-1 6671
C	0.0001	-1 0070	-1 7457
C	0.7071	1.0079	
C C	2.0379	-1.0432	-1. 1440
U .	-1.2736	0.2406	-2.3868
С	-1.7021	-0.8510	-3.1567
С	-0. 9636	-2.0216	-3. 2146
С	0. 2483	-2.1162	-2.5135
0	-3.6573	-1.3965	0.7180
0	2.7209	-2.1093	-1.1542
Н	0.0364	2.2462	-1.2365
Н	0.0585	2.0744	1.2336
С	2, 2955	-1,9461	3, 3249
C	4.3989	3,9324	0.6440
0	-5 3223	0.4625	0.0938
0	-2 2102	-3 1526	1 0286
0	0.0200	2 2609	2 6161
0	0. 9300	-3.2008	-2.0101
0	4. 7852	-0.8319	-0. 2868
H	-4.9767	-0. 4463	0. 2941
H	-2.9851	-2.7639	1. 4473
Н	1.7589	-3. 1530	-2.0697
Н	4.2279	-1.5884	-0.6065
Н	1.6315	0.3785	2.1049
Н	0.0555	-3. 5225	3.0174
Н	-5.5152	2.9679	-0.3485
Н	-3, 6300	4,6015	-0.2956
Н	-1 3233	3 8350	0.1864
Н	5.6024	1 4687	0.4310
Ц	1 2071	2 4521	_0.0280
11	1.0071	1 1449	-0.0289
Н	-1.8724	1. 1443	-2.3512
H	-2.6318	-0.7776	-3.7146
Н	-1.2873	-2.8764	-3. 7990
Н	2.2608	-2.9305	3.8001
Н	3.1206	-1.9470	2.6013
Н	2.5437	-1.2036	4.0929
Н	5.3621	3.7853	1.1414
Н	3.7430	4. 4888	1.3229
Н	4. 5721	4. 5707	-0. 2323

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

atom	Х	Y	Z
С	-2.6149	0.1931	-0.6224
С	-1 8290	1 3631	-0.5162
C	-2.4138	2 5526	-0.0997
C	-3 7798	2.6020	0.2347
C	-1 5496	1 4608	0.1658
C	-4. 5490	1.4000	0.1050
U C	-3. 9879	0. 2473	-0. 2539
C	-2.0381	-1.0432	-1.1446
С	-0. 7073	-1.0080	-1.7457
С	0.0860	0. 1651	-1.6671
С	-0.3382	1.3039	-0. 7678
С	-0.2485	-2.1163	-2.5136
С	0.9634	-2.0217	-3.2146
С	1,7020	-0.8511	-3.1568
C	1 2735	0.2405	-2.3868
C	0.3469	-0.0109	1 3793
C	1 4104	-0.0200	1.2267
C	1. 4194	-0. 9390	1.007
U C	1.2487	-2. 2190	1. 9352
C	0.0411	-2.5361	2.5746
С	-0.9912	-1.6097	2.6448
С	-0.8221	-0.3428	2.0482
С	0.4605	1.3079	0.6486
С	1.8850	1.7734	0. 4353
С	2.9518	0.8462	0. 4349
С	2,7159	-0.5537	0.7971
С	2, 1393	3, 1171	0.1741
C	3 4430	3 5486	-0.1015
C	4 5006	2 6515	-0.1204
C	4. 0000	2.0010	0.1226
C O	4.2705	1. 2931	0.1550
0	-2.7211	-2.1092	-1.1543
0	3.6575	-1.3964	0.7179
Н	-0.0585	2.0743	1.2336
Н	-0.0365	2.2461	-1.2365
С	-4. 3989	3.9324	0.6442
С	-2.2952	-1.9463	3. 3251
0	-0.9390	-3.2608	-2.6161
0	-4, 7853	-0.8318	-0.2867
0	5 3223	0 4626	0.0935
0	2 2105	-3 1526	1 9286
U	_1 7501	-2 1520	-2 0608
II		-3. 1330	-2.0098
Н	-4. 2281	-1. 5884	-0.0005
H	4.9767	-0.4462	0. 2939
H	2.9853	-2.7638	1. 4473
Н	-1.8070	3. 4531	-0. 0288
Н	-5.6024	1.4688	0.4311
Н	1.2871	-2.8765	-3. 7991
Н	2.6317	-0.7777	-3.7146
Н	1.8723	1.1442	-2.3512
Н	-0.0551	-3 5226	3 0175
Н	-1.6314	0.3783	2 1050
Ц	1 2020	2 9250	0.1864
II	1. 3232	3. 0330	0.1004
Н	J. 0298	4.0015	-0.2957
H	5.5151	2.9680	-0.3488
Н	-4. 5721	4. 5708	-0.2321
Н	-5.3620	3. 7854	1.1416
Н	$-3.74\overline{29}$	4. 4888	1.3231
Н	-3.1204	-1.9470	2.6016
Н	-2.2605	-2.9307	3.8002
Н	-2.5433	-1.2039	4. 0933
**		2. 2000	

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

atom	Х	Ŷ	L
С	0.8968	-0.8205	-1.6019
с С	0.0259	0.2552	1 50010
0	-0.0238	0.2000	-1. 0202
L	-1.2713	0.1345	-2.1260
C	-1.6639	-1.0602	-2.7657
С	-0.7791	-2.1298	-2.8086
С	0. 4994	-2.0284	-2.2402
C	2 2663	-0.6581	-1 1350
C	2.2003	0.0301	1.1330
l	2.7333	0.6744	-0.7433
C	1.8195	1.7473	-0. 6378
С	0.3314	1.4965	-0.7437
С	4.1190	0.9071	-0.5132
ſ	4 5672	2 2047	-0.2253
C	2.6560	2.2011	0.1560
C	5.0000	5. 2494	-0.1505
C	2.2880	3. 0271	-0.3534
С	0.0258	0.2555	1.5281
С	-0.8968	-0.8203	1.6020
ſ	-0 4994	-2 0282	2 2404
C	0.7701	2.0202	2.2101
C	0.7791	-2.1293	2.0000
C	1.6639	-1.0598	2.7658
С	1.2713	0.1348	2.1259
С	-0.3314	1.4966	0.7435
С	-1.8195	1,7474	0.6376
C	-2 7334	0.6745	0 7/32
C	2.1004	0.6590	1 1250
C	-2.2003	-0.0360	1.1500
C	-2.2880	3. 0271	0.3531
С	-3.6569	3.2495	0.1559
С	-4.5673	2.2048	0.2251
С	-4, 1190	0.9072	0.5131
0	3 0723	-1 6347	-1 1461
0	-2 0722	-1 6246	1.1/62
0	-3.0723	-1.0340	1. 1403
Н	0.1261	2.3636	1.2308
Н	-0.1261	2.3635	-1.2311
С	-3.0436	-1.1666	-3.3666
С	3.0436	-1.1662	3, 3668
0	5 0323	-0.0753	-0.5572
0	1 2025	2,0025	0.0012
0	1. 5065	-3. 0923	-2. 3307
0	-5. 0323	-0.0752	0.5573
0	-1. 3085	-3. 0922	2. 3391
Н	4.5419	-0.9107	-0.7754
Н	2.1592	-2.8498	-1.8913
Н	-4 5419	-0.9106	0 7755
Ц	-2 1502	-2 8495	1 8017
11	2.1352	2.0490	1.0917
H	-1.9665	0.9678	-2.0926
H	-1.0492	-3.0661	-3. 2870
Н	5.6292	2.3586	-0.0650
Н	4.0120	4.2544	0.0563
Н	1 5888	3 8565	-0.2837
Ц	1.0000	-2.0657	2 2001
11	1.0492	0.0001	0.0004
H	1.9005	0.9681	2.0924
Н	-1.5888	3.8565	0.2832
Н	-4.0120	4.2544	-0.0568
Н	-5. 6293	2.3586	0.0648
Н	-3.8115	-1.1112	-2.5844
U II	_3 1779	_2 1007	_3 0057
П	-0.1110	-2.1087	-3. 9037
H	-3.2362	-0.3423	-4.0638
Н	3. 2360	-0.3420	4.0641
Н	3.8115	-1. 1104	2.5846
Н	3.1779	-2.1084	3.9056

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

atom	Х	Y	Z
С	2 8371	0 2915	0 3809
C C	1 0000	1 2420	0.2602
C	1.0922	1. 3420	0.0000
C	2.2878	2.6225	-0.0008
С	3.6163	2.898	-0.3765
С	4.5437	1.8612	-0.3924
C	4 1755	0 5605	-0.0212
C	9.4610	1 0200	0.0212
L .	2.4019	-1.0389	0.8529
C	1.1632	-1.2257	1. 4959
С	0.2138	-0.1725	1.5192
С	0.4371	1.0689	0.684
C	0.893	-2 4305	2 2061
C	0.000	2. 1000	2.2001
L .	-0. 2913	-2. 5492	2.9493
C	-1. 1849	-1. 4917	2.9923
С	-0.9412	-0.3066	2.2826
С	-1.8922	1.3428	-0.3682
ſ	-2 8371	0.2915	-0.3808
C	4 1755	0. 2010	0.0010
C	-4.1755	0. 5005	0.0212
C	-4. 5438	1.8611	0.3924
С	-3.6164	2.8979	0.3766
С	-2.2878	2,6225	0,0008
C	-0.4371	1 069	-0.6839
C	0.9197	0.1794	1 E101
U C	-0.2137	-0.1724	-1. 5191
C	-1.1632	-1.2256	-1.4959
С	-2.4618	-1.0389	-0.8529
С	0.9412	-0.3065	-2.2826
С	1 1849	-1 4915	-2 9924
C	0.2014	-2 540	-2.0405
C C	0.2914	-2. 349	-2. 9495
C	-0.893	-2. 4304	-2.2062
0	3. 2889	-1.9945	0.784
0	-3.2888	-1.9946	-0.784
Н	-0.0478	1, 9298	-1.2371
Н	0.0478	1 0208	1 2372
	0.0470	1. 3230	0.7071
L C	4.020	4.3054	-0.7371
С	-4. 0261	4. 3053	0. 7371
0	1.7383	-3.471	2.2142
0	5.1208	-0.3897	-0.0599
0	-1 7382	-3 4709	-2 2143
0	E 1202	0.2000	0.0500
0	-5.1208	-0.3898	0.0599
H	2.5156	-3. 2159	1.654
Н	4. 6859	-1.2365	0.2206
Н	-2.5155	-3.2158	-1.6541
Н	-4.6859	-1.2366	-0.2206
Н	1,5595	3, 431	0.0015
Ц	5.5746	2 0227	-0.6969
	0.0740	2.0321	-0.0000
H	-0.4701	-3. 4745	3. 4867
H	-2.0922	-1.582	3. 5837
Н	-1.6582	0.506	2.3278
Н	-5.5746	2,0326	0.6868
Н	-1 5595	3 4311	-0.0014
II	1.6500	0.5061	0.0011
П	1.0002		-2. 3210
Н	2.0922	-1.5818	-3. 5838
Н	0.4701	-3.4743	-3.4869
Н	3.2912	4.778	-1.3987
Н	4 999	4 3253	-1 2364
Ц	1 1006	/ 0200	0 1619
11	4.1000	4. 0000	0.1012
Н	-4. 1002	4. 9322	-0.1611
Н	-4.9994	4. 3253	1.236
Н	$-3.29\overline{15}$	4.7777	1.3993

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

atom	Х	Y	Z
С	2.8533	-0. 1155	0.0526
С	1.7276	-0.6818	-0.6001
С	1,7922	-1.9768	-1.0845
С	2,9536	-2.7614	-0.9177
C	4 043	-2, 2287	-0.2398
C	4 0114	-0.9143	0.2523
C	2 8810	1 2074	0.2020
<u> </u>	1 9520	2 1607	0.0112
C	1. 6329	2.1097	-0.2127
C	0.1214	1.0971	-0.030
C C	0.4488	0. 1221	-0.0712
<u> </u>	2.0545	3.5766	-0.2659
C	1. 1658	4. 3766	-1.0024
С	0.0989	3. 7894	-1.6647
C	-0. 1327	2.4074	-1.5871
С	-1.7279	0.682	0. 5997
С	-2.8536	0.1153	-0.0526
С	-4.0119	0.9138	-0.2521
С	-4.0438	2.2283	0.2395
С	-2.9543	2.7614	0.9171
С	-1.7927	1.9771	1.0839
С	-0. 4489	-0.1216	0.6708
С	-0.7271	-1.5967	0.8578
С	-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	1.0040
C	-2 0537	-3 5766	0.2663
0	2.0007	1 2025	1 0242
0	-2 8200	-1 2042	-1 0225
<u> </u>	-3. 6399	-1. 6042	-1.0333
П	0.1034	0.2403	1. 5027
H	-0.1636	-0. 2396	-1.5032
<u> </u>	2.988	-4.169	-1.4592
C	-2.989	4. 1691	1.4584
0	3. 0834	4. 1823	0. 3457
0	5.103	-0. 4544	0.8811
0	-3. 0827	-4. 1826	-0. 3449
0	-5. 1036	0. 4535	-0.8806
Н	3. 611	3. 4724	0. 7938
Н	4. 9121	0. 4842	1.1386
Н	-3. 6106	-3. 4728	-0. 7929
H	-4. 9126	-0. 4851	-1.138
Н	0.9274	-2.4086	-1.581
Н	4.9479	-2.8082	-0.0842
Н	1.3506	5.4449	-1.0458
Н	-0.575	4.4112	-2.2482
Н	-0.9947	1.9736	-2.0842
Н	-4.9488	2.8076	0.084
Н	-0.9278	2.4092	1.58
Н	0.9956	-1.9726	2.0835
Н	0.5765	-4.4102	2.2479
Н	-1.3492	-5. 4446	1.0463
H	2.8467	-4.1751	-2.5471
H	3, 938	-4.6639	-1, 2385
Н	2 179	-4 7717	-1 0284
Н	-2 8502	4 1751	2 5467
Н	-2.0302	4 6646	1 9255
и П	_9 170£	4 7719	1.2000
п	-2.1/80	4.1114	1.0290

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

atom	Х	Ŷ	L
С	2, 5349	0.9411	0.0924
C C	1 2812	0.8977	0.7544
<u> </u>	0.7076	2 020	1 3801
C	1 5170	2.025	1. 3659
U C	1. 5179	3. 2423	1. 3008
<u> </u>	2.7234	3. 3052	0.6778
C	3. 2452	2.1705	0. 0367
С	3.1581	-0.2883	-0.3857
С	2.5937	-1.5663	0.0507
С	1.3366	-1.6029	0.7068
С	0.4604	-0.3699	0.6737
С	3, 3716	-2.753	-0.046
C	2 9107	-3 9346	0.5571
C	1 701	-3 9354	1 2331
C	0.0050	-2 7807	1.200
C	0.9009	-2.1001	1. 502
<u> </u>	-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
С	-1.5179	3.2423	-1.3668
С	-0.7976	2.0289	-1.3891
С	-0. 4603	-0.3699	-0.6737
С	-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 C	-1 701	-3.0354	-1 2331
C	2.0107	2 0246	0 5571
C	-2.9107	-3. 9340	-0. 3371
<u> </u>	-3. 3710	-2.755	0.040
0	4. 2302	-0.2512	-1.0582
0	-4. 2302	-0.2512	1.0582
Н	0. 2444	-0. 4004	-1.5106
Н	-0.2444	-0. 4004	1.5106
С	0.9658	4. 4522	2.0797
С	-0.9658	4.4522	-2.0797
0	4.5546	-2.7905	-0.6769
0	4.423	2.2932	-0. 5933
0	-4.5546	-2.7905	0.6769
0	-4, 423	2, 2932	0, 5933
Н	4 7269	-1 8764	-1 0203
Н	4 6442	1 4012	-0.9655
Н	-1 7269	-1.8764	1 0203
Ц	-4.6442	1.0104	0.0656
II	4.0442	1.4012	1 002
11	-0.1045	1. 9919	1.095
H	3. 2984	4.225	0. 6313
<u>H</u>	3. 529	-4.8234	0. 4863
Н	1. 3566	-4.8491	1.7102
H	-0.054	-2.8129	1.8076
Н	-3.2984	4.225	-0.6313
Н	0.1645	1.9918	-1.893
Н	0.054	$-2.81\overline{29}$	-1.8076
Н	-1.3566	-4.8491	-1.7102
Н	-3.529	-4.8234	-0. 4863
Н	0.911	4.2774	3. 1616
Н	1.5856	5.3377	1.9128
H	-0.0528	4, 6758	1.7404
Н	0.0528	4 6757	-1 7405
Ц	_1 5856	5 2277	_1 0190
П		0.0011	-1.3120
П	-0.911	4.2//4	-3. 1010

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

atom	Х	Y	Z
С	-0.9462	-1.1108	1.6021
C	_0_0007	-0.049	1 5137
C	1,0004	0.045	0.1044
L	1.2384	-0. 1825	2.1044
С	1.6222	-1.3798	2.7434
С	0.7232	-2.4369	2.7993
С	-0.5604	-2.3189	2 2457
C	0.0001	0.0202	1 1527
U.	-2. 3218	-0. 9282	1.1557
С	-2. 7652	0. 3979	0. 7449
С	-1.8395	1.4595	0.6097
С	-0.3526	1 1962	0 7267
C C	-4.1509	0.6574	0.5208
C	4. 1303	0.0374	0.0250
L	-4. 582	1.9501	0.2156
С	-3.6515	2.9802	0. 1113
С	-2.2805	2.7382	0.3019
С	1.8164	1,4566	-0.6226
С С	2 7204	0.2826	-0.7167
C	2.1294	0.3820	-0.7107
C	4.1066	0.6224	-0.4576
С	4.5435	1.9198	-0.1568
С	3.6452	2.9814	-0.1009
C	2 278	2 7333	-0.3259
C	0 290	1 2014	-0 7492
C	0.329	1.2044	-0.7465
U	-0.0128	-0.0334	-1.54/5
С	0. 9142	-1.1074	-1.6096
С	2.272	-0.947	-1.1197
С	-1.2444	-0.139	-2.1718
C	-1 5926	-1 3280	-2 8385
C	0.7010	1. 5205	2.0303
U C	-0.7216	-2.4125	-2.8788
C	0. 5337	-2.3122	-2.2708
0	-3.1457	-1.8921	1.1965
0	3.0819	-1.9237	-1.1212
Н	-0.123	2 0716	-1 2398
Ц	0 1020	2 0587	1 2230
	0.1025	2.0307	1.2233
L .	3.0076	-1.5026	3. 3284
C	4. 1266	4. 3848	0. 1776
0	-5.0808	-0.3016	0.6233
0	-1.3858	-3.3697	2.3621
0	1 3488	-3 3713	-2 3535
0	5.0246	-0.3573	_0 4925
0	J. 0240	0.0070	0.4000
H	-4. 5972	-1. 1439	0.8382
H	-2.2408	-3. 1102	1. 931
Н	2.1879	-3.1226	-1.8827
Н	4.5405	-1.1923	-0.7182
0	-4.0113	4.2586	-0.1796
Н	-5 6442	2 191	0.0632
0	0.0172	1 2502	2 4000
0	-2.8155	-1. 3503	-3. 4288
H	-0. 9826	-3. 339	-3. 3827
Н	-4.9754	4.3039	-0.2819
Н	-2.9528	-2.2238	-3.8417
Н	1.9433	0.6421	2,0637
Ц	0.0840	-3 3748	3 2703
II	1 5004	0.0140	0.0050
Н	-1. 3884	5. 5091	0.2053
Н	5.6032	2.0697	0.0266
Н	1.5716	3. 5587	-0.2643
Н	-1.9604	0.6744	-2.1561
Н	3. 2172	-0.6825	4. 0257
Ц	3 7660	_1 /521	2 5275
11	0.1000	0.4475	2.0010
H	3.1377	-2.4475	3. 8636
Н	4. 1746	4. 9715	-0. 7492
Н	5.1268	4.3859	0.6209
Н	3. 4488	4.9127	0.8577

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

atom	Х	Y	Z
С	-2.7295	0. 3825	-0.7168
C	-1.8164	1 4565	-0.6226
C C	-1.0104	1.4000	-0.0220
L	-2.2781	2.7332	-0.326
С	-3.6453	2.9813	-0. 1011
С	-4.5436	1.9197	-0.1569
C	-4 1066	0 6223	-0 4577
C	0.0710	0.0471	1 1107
U	-2. 2719	-0.9471	-1. 1197
С	-0. 9141	-1.1074	-1.6096
С	0.0128	-0.0333	-1.5475
С	-0.329	1.2044	-0.7484
C	-0.5334	-2 3121	-2 2707
C	0.001	2.0121	2.2101
U	0.7219	-2.4124	-2.8788
С	1. 5928	-1.3286	-2.8385
С	1.2445	-0.1388	-2.1719
С	0.0096	-0.0491	1.5137
C	0.946	-1 1108	1 602
C	0. 540	1.1100	1.002
L .	0.5604	-2.319	2.2456
С	-0. 7231	-2. 4369	2.7994
С	-1.6222	-1.3798	2.7435
С	-1.2385	-0.1826	2, 1045
C	0.3525	1 1962	0 7267
C	1 0204	1. 1502	0.1201
U C	1.8394	1. 4595	0.0098
C	2.7651	0.398	0.745
С	2.3217	-0. 9283	1.1535
С	2.2804	2.7383	0.3022
С	3.6514	2,9804	0.1116
C	1 5819	1 9502	0.2158
C	4 1500	0.0574	0.2100
U O	4. 1508	0.0574	0. 5299
0	-3. 0818	-1.9238	-1.1215
0	3.1455	-1.8922	1.1961
Н	-0.1031	2.0586	1.2239
Н	0.1229	2.0717	-1,2398
C	-4 1268	4 3847	0 1772
C	2.0075	1.5017	2 2000
U O	-5.0075	-1. 3027	3. 3200
0	-1.3484	-3. 3714	-2.3535
0	-5.0247	-0.3574	-0. 4835
0	5.0806	-0.3015	0.6232
0	1, 3859	-3, 3696	2, 362
Ц	-2 1874	-3 1228	-1 8825
II	4 5407	1 1025	0.7175
П	-4. 5407	-1. 1923	-0.7175
Н	4. 597	-1.1439	0.838
Н	2.2408	-3.1099	1.9308
0	2.8155	-1.356	-3.4288
Н	0, 983	-3, 3388	-3.3827
0	4 0112	4 2588	-0.1792
0	T. 0112	1.2000	0. 1152
Н	5. 0441	2.1211	0.0034
Н	2.953	-2.2236	-3.8416
Н	4.9753	4. 3039	-0.2815
Н	-1.5717	3. 5586	-0.2644
Н	-5, 6033	2,0695	0.0264
Н	1 9603	0.6747	-2 1562
II	1. 5005	0.0141	2.1502
H	-0. 9847	-3. 3749	3.2795
Н	-1.9434	0.6421	2.0638
Н	1.5883	3.5692	0.2057
Н	-4.1758	4.971	-0.7498
Н	-5.1266	4.3857	0.6214
Ц	_2 //95	/ 012	0.9566
11	0. 1100	1. 313	0.0000
H	-3.7669	-1.4538	2.5379
Н	-3. 1372	-2. 4474	3.8645
Н	-3.2172	-0.6822	4.0256

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

atom	Х	Y	L
C	0 0005	_1 0067	_1 G14
U	0.0900	-1.0907	-1.014
С	-0.0279	-0.026	-1.5287
С	-1.2775	-0.1495	-2.118
C	-1 6604	_1 2427	_2 7507
<u> </u>	1.0034	1. 3427	2.1391
C	-0. 7796	-2.4077	-2.8144
С	0.5029	-2.3025	-2.2556
C	2 2727	-0.928	-1 1576
C	0.7000	0.020	0.7001
C	2.7303	0.3973	-0.7601
С	1.8171	1.4714	-0.6428
С	0.328	1.2168	-0.7439
C	4 1161	0.6401	_0 521
U .	4.1101	0.0401	-0.001
С	4.5624	1. 9318	-0.2348
С	3.6449	2.9768	-0.1582
C	2 272	2 7493	-0.3523
C	0.0077		1 5000
L	0.0277	-0.0253	1. 5288
С	-0.8985	-1.0962	1.6143
С	-0.5025	-2.3017	2, 2564
C C	0.79	2.0011	2.2001
U	0.78	-2.4062	2.8194
С	1.6695	-1.341	2.7605
С	1.2773	-0.1482	2.1183
ſ	-0 3283	1 9171	0 7435
0	0.0200	1. 2111	0.7400
C	-1.8173	1.4715	0.6423
С	-2.7305	0.3974	0.7598
С	-2.2727	-0.9278	1, 1575
C	0.0700	0.0210	0.2515
U	-2.2122	2. 7494	0. 3515
С	-3.6451	2.9768	0.1574
С	-4.5626	1,9318	0.2341
C	-4 1163	0.6402	0.5306
C .	-4.1103	0.0402	0.000
0	3. 0852	-1.902	-1.185
0	-3.0851	-1.9019	1.1848
Н	0 1311	2 083	1 2307
II	0.1011	2.000	1.001
П	-0.1314	2.0825	-1.2315
С	-3.0534	-1.4536	-3.3506
С	3.0534	-1.4513	3.3517
0	5 0311	-0.3379	-0.5857
0	1.0170	0.0010	0.0007
0	1.3176	-3.3618	-2.3665
0	-5.0315	-0.3376	0.5853
0	-1.3165	-3.3616	2.3678
U U	4 5270	_1 1722	_0. 8126
11	4.0019	1.1140	1.0005
Н	2.1712	-3.1139	-1.9265
Н	-4.5386	-1.1722	0.8121
Н	-2.1701	-3.1151	1.9277
<u> </u>	4 0202	4 2540	0 119
0	4.0203	4. 2049	0.112
Н	5.6254	2.091	-0.075
0	-4. 0206	4.2549	-0.1131
Н	-5 6255	2 0909	0 0742
TT	4 0040	4 9007	0.0114
П	4.9849	4. 2907	0.2131
Н	-4. 9852	4.2906	-0.2142
Н	-1.9756	0.6811	-2.0762
Н	-1 0486	-3 343	-3 2955
11	1.0100	0.010	0.2000
Н	1.5894	3. 5894	-0.2701
Н	1.0492	-3.3413	3.2968
Н	1.9752	0.6826	2.0762
II	_1 5006	2 5005	0.2601
П	-1. 0090	J. JOYD	0.2091
<u> </u>	-3. 2567	-0.6262	-4.0411
Н	-3.1859	-2.393	-3.8949
Ц	_2 Q156	_1 /096	-2 5621
11	0.0100	1. 1000	2.0021
Н	3.1863	-2.3907	3.8958
Н	3.8158	-1.4057	2.5634
Н	3, 256	-0.6239	4. 0424
**	3. 200		

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

atom	X	Y	Z
С	-2.77	0.3839	-0.6942
C	-1 8406	1 4425	-0.5822
C	0.0007	0 7010	0.0022
C	-2.2031	2.7213	-0.2073
C	-3.648	2.9882	-0.0449
С	-4. 5635	1.9443	-0.1291
С	-4.1466	0.6445	-0.4494
С	-2.3319	-0.9474	-1.1111
<u> </u>	-0.974	-1 1245	_1 5067
C	0.014	0.0625	1.5007
U C	-0.0334	-0.0625	-1. 5322
C	-0.3564	1. 1782	-0. 7291
С	-0.6101	-2.3306	-2.2653
С	0.6428	-2.4447	-2.8757
С	1 5266	-1 3714	-2.8346
<u> </u>	1 1042	_0_18	-2 1620
<u> </u>	1. 1942	1 4490	2.1025
L .	1.8406	1.4420	0. 5823
С	2.77	0. 384	0. 6942
С	4.1466	0.6446	0.4494
С	4.5635	1.9444	0.1292
C	3 648	2 9882	0.045
C	0.010	2.3002	0.010
<u> </u>	2.2031	2.7213	0.2074
C	0.3564	1. 1782	0. 7292
С	0. 0334	-0.0626	1.5323
С	0.974	-1.1246	1.5967
С	2.3319	-0.9474	1.1109
C	-1 1942	-0.1801	2 163
C	1. 10 12	1. 2715	2.100
C C	-1. 5200	-1. 5715	2.0340
C	-0.6427	-2. 4448	2.8757
С	0.6102	-2.3306	2.2654
0	-3.1564	-1.9115	-1.1279
0	3.1564	-1.9115	1.1275
Н	-0.0906	2 041	1 233
П Ц	0.0006	2.011	_1.200
11	0.0900	2.041	-1. 2329
C	-4.1067	4. 394	0.2589
С	4. 1066	4. 3941	-0. 2589
0	-1.4396	-3.3783	-2.3529
0	-5.0841	-0.3121	-0.5169
0	1 4397	-3 3784	2 3529
0	5 084	-0.3121	0.5169
0	0.0770	0.0121	1.0071
H	-2.2779	-3.1163	-1.8871
H	-4.6122	-1.1573	-0.7364
Н	2.2781	-3. 1163	1.8873
Н	4.612	-1.1572	0.7367
0	2.7465	-1.4105	-3. 4297
Н	0.8906	-3 3718	-3 385
0	2 7465	1 4106	2 4207
0	-2.7403	-1.4100	3.4297
H	-0.8905	-3.372	3.385
Н	2.8732	-2.2783	-3.8455
Н	-2.8733	-2.2785	3.8454
Н	-1.5652	3. 5351	-0.192
Н	-5 6222	2 1089	0 0467
Н	1 0104	0.6249	-2 1/81
11	I. JIJ4	0.0249	
H	5. 6222	2.109	-0.0466
Н	1.5651	3. 5352	0.1922
Н	-1.9194	0.6248	2.1482
Н	-4.1152	5.0074	-0.6517
Н	-5.1186	4, 4051	0.6744
Ц	_2 /27/	/ 2271	0 0720
11	0.4014	4.00/1	0. 9149
H	3.4386	4.8863	-0.9748
Н	5.1193	4. 4053	-0.6724
Н	4.1128	5.0082	0.6512

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

atom	Х	Y	
C	9 0701	0 5202	0 0000
C	-2.8781	0.5382	-0.8890
С	-1.8507	1.5082	-0.8818
<u> </u>	0 1740	0.0507	0.0000
C	-2.1748	2.8587	-0.8288
С	-3 5142	3 2866	-0.7674
0	4 5000	0.2000	0.7070
C	-4. 5280	2.3337	-0.7379
С	-4 2310	0 9650	-0 7945
0	1. 2010	0.0000	0.1510
C	-2.5586	-0.8817	-1.0411
C	-1 2003	-1 2661	-1 3773
0	1.2003	1.2001	1.0110
C	-0.1556	-0.3025	-1.4019
C	-0 3989	1 0804	-0.8381
C .	0.0000	1.0004	0.0001
С	-0.9185	-2.5955	-1.8017
C	0 3567	-2 0386	-2 2608
U.	0.3307	-2.9380	-2.2098
С	1.3491	-1.9639	-2.3238
C	1 0022	-0.6450	_1 9960
U	1.0922	-0.0439	-1.8809
С	-0.3606	0.1884	1.6121
C	0 4272	0.0251	1 0492
U	0.4373	-0. 9351	1. 9405
С	-0.1300	-1.9719	2.7395
C C	1 4526	1 9691	2 1010
U	-1.4330	-1.8021	5. 1910
С	-2.2174	-0.7418	2,8902
<u> </u>	1 6596	0.0055	9 1050
U	-1. 6536	0.2855	2.1059
С	$0 \ 1777$	1 2436	0 6709
- C	1 (000	1.2100	0.0100
C	1.6898	1.3267	0.6420
C	2 4739	0 2104	1 0232
0	1.0500	0.2101	1.0202
C	1.8522	-0.9750	1.5962
C	2 2998	2 4800	0 1791
<u> </u>	2.2330	2.4000	0.1131
C	3.7036	2.5505	0.0721
C	1 1970	1 /589	0 /185
<u> </u>	4.4310	1.4303	0.4105
C	3.8893	0.2882	0.8910
0	-3 1799	-1 7514	-0.9637
0	5. 1155	1.1014	0.0001
0	2.5526	-1.9996	1.8617
Ц	-0.2056	2 2100	0 9878
11	0.2000	2.2190	0. 9010
Н	0.1851	1.8011	-1.4192
C	2 9402	1 7606	0 7522
U	-3. 8403	4.7000	-0.7552
С	-3.6456	-0.6223	3.3625
0	_1 9472	-2 5600	_1 7019
0	-1.0473	-3. 0009	-1. 7912
0	-5.2568	0, 0993	-0.7514
0	4 0000	0,7220	1 0100
0	4. 6936	-0. 7339	1.2133
0	0.5580	-3.0680	3.0926
U U		2 1407	1 4440
Н	-2.6826	-3. 1487	-1.4448
Н	-4.8609	-0.8101	-0.8093
II	4 1015	1 4720	
Н	4. 1015	-1.4739	1. 5150
Н	1.4646	-2.9735	2.7004
0		0 1707	0.7700
0	2.0004	-2.1797	-2.1180
Н	0.5194	-3.9605	-2.5873
0	4 1000	2 7201	0.2042
0	4.1000	3.7321	-0. 3843
Н	5, 5768	1.4715	0.3436
C	2 0597	2 4077	2 9159
U	2. 9001	-3.4077	-3. 2132
С	5.5968	3.8853	-0.5152
Ц	2 2/10	-3 8030	-4 0654
П	2. 3410	-3. 8039	-4.0004
Н	6.0120	3.1637	-1.2294
Ц	-1 2709	3 6010	-0.8332
11	1. 3190	5.0010	0.0000
Н	-5.5722	2.6250	-0.6754
Ц	1 0004	0 0746	-1 0339
11	1. 5004	0.0140	1. 3334
Н	-1.8553	-2.6746	3. 7886
Ц	-2 2524	1 1509	1 8790
П	-2.2004	1.1090	1.0129
Н	1.7197	3.3516	-0.1086
Ц	_2 7296	5 1091	_1 7577
11	5. (500	J. 1941	1.1011
Н	-4.8659	4.9421	-0. 4183
U	_2 1610	5 2140	-0.0051
П	-3. 1010	0.0140	-0.0901
Н	-4.3372	-0.6431	2.5106
II	_2 0171	_1 /205	4 0201
п	-3. 9171	-1. 4385	4.0381
Н	-3.8115	0. 3263	3.8871
II	4 0026	_2 4945	_2 5057
П	4.0020	-3. 4245	-3. 5257
Н	2.862 $\overline{0}$	$-4.21\overline{78}$	$-2.40\overline{26}$
II	E 7500	4 0000	0 0001
<u>н</u>	J. 1908	4. 8983	-0.8901
Н	6. $1020$	3. $7722$	0.4519

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

atom	Х	Ŷ	Z
C	0 4979		1 0401
U	-0.4372	-0. 9355	1.9481
ſ	0 3607	0 1881	1 6122
0	0.0001	0.1001	1.0122
C	1.6537	0.2850	2.1060
C	9 9175	-0.7426	2 8800
U	2.2115	0.1420	2.0033
С	1.4536	-1.8630	3. 1904
C	0 1200	1 0795	2 7200
U	0.1300	-1.9725	2.7390
C	-1 8522	-0.9751	1 5961
C .	1.0022	0.0101	1.0001
C	-2.4738	0.2104	1.0234
C	-1 6906	1 2267	0 6422
U U	1.0890	1. 3207	0.0423
С	-0.1775	1.2436	0.6713
C C	2,0000	0.0001	0.0010
U	-3.8892	0.2881	0.8912
C	-4 4969	1 4588	0 4188
0	1. 1303	1.4500	0. 1100
C	-3. 7035	2.5505	0.0726
C	_2 2007	2 4800	0 1705
U	-2. 2991	2.4800	0.1795
С	1.8509	1.5083	-0.8815
C	0.0700	0 5202	0,0000
U	2.0102	0. 5383	-0. 8889
C	4 2311	0 9649	-0 7945
0	1. 2011	0.0010	0.1310
C	4. 5282	2.3336	-0. 7378
C	2 5145	2 2267	-0.7670
U	0.0140	3.2001	0.1010
С	2.1750	2.8588	-0. 8283
C	0 2000	1 0006	_0 0270
L	0. 3990	1.0000	-0.0378
С	0.1556	-0.3021	-1.4019
Č Č	1 0000	1 0050	1 0775
<u> </u>	1.2002	-1.2658	<u>-1.377</u> 5
C	2 5585	-0.8816	-1 0411
0	2.0000	0.0010	1.0111
C	-1.0923	-0.6453	-1.8869
C	-1 3494	-1 9631	-2 3241
C	1.0404	1. 5051	2.0241
С	-0.3571	-2.9380	-2.2703
C	0 0191	-2 5051	_1 0021
U. U.	0. 9181	-2. 5951	-1. 8021
0	-2.5526	-1.9997	1.8615
<u> </u>	2,4700	1 7515	0.0027
0	3.4790	-1.7515	-0.9637
Н	-0 1849	1 8015	-1 4187
11	0.1015	1.0010	1. 1101
Н	0.2058	2.2189	0. 9883
C	3 6458	-0.6235	3 3620
<u> </u>	5.0450	0.0233	5. 5020
С	3.8406	4. 7606	-0.7522
0	-4 6022	_0 7241	1 9125
0	-4.0933	-0.7341	1.2155
0	-0.5581	-3.0687	3. 0918
0	1.0400		1 7010
0	1.8408	-3. 5607	-1. 7919
0	5 2569	0 0993	-0 7518
U U	4 1000	1 4700	1 5100
Н	-4.1008	-1.4739	1.5160
Н	-1 4648	-2 9738	2 6998
11	1. 1010	2.3100	2.0550
Н	2.6821	-3.1490	-1.4455
Н	4 8612	-0.8101	-0.8099
	1.0012	0.0101	0.0000
0	-4.1879	3. 7322	-0.3837
Ц	-5 5767	1 4715	0 3440
	0.0101	1. 1/10	0.0110
0	-2.6068	-2.1786	-2.7789
Ц	-0.5100	-3 0508	-2 5880
11	0.0100	0.0000	2.0000
C C	-5. 5967	3.8853	-0.5149
C	-2 0502	-2 1866	-2 9159
<u> </u>	2. 3030	3.4000	0.4100
Н	-6.0116	3. 1639	-1.2294
Ц	_9 2490	-3 0030	_1 06E7
Н	-2.3428	-3.8030	-4.0657
Н	2.2536	1.1593	1.8734
II	1 0550	9 6757	2 7070
Н	1. 8553	-2.0757	3. 1818
Н	-1,7196	3.3517	-0.1080
11	5.5704	0.0011	0.0754
Н	5.5724	2.6249	-0.6754
Н	1 3801	3 6020	-0.8329
11	1.0001	0.0020	0.0025
Н	-1.9004	0.0754	-1.9330
Н	3 8129	0 3264	3 8830
11	0.0123	0.0201	0.0000
Н	4. 3373	-0.6475	2.5100
Ц	3 0164	-1 /389	4 0308
11	0.0104	1.4302	т. 0390
Н	3. 7339	5. 1936	-1.7555
Ц	1 9677	4 0/17	_0 4919
П	4.00//	4. 9417	-0.4218
Н	3. 1644	5. 3129	-0.0900
TT	6 1001	2 7700	0 4510
Н	-0.1021	3. 1120	0.4519
Н	$-5, \overline{7506}$	4.8983	-0.8897
TT	0.0004	4 0107	0.4007
Н	-2.8624	-4.2167	-2.4027
Ц	-4 0034	-3 4933	-3 5253
	T. UUUT	0. 1400	0.0400

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

atom	Х	Ŷ	
C	0.9660	1 2509	1 6250
U	-0.8000	-1. 5562	1.0559
С	0.0567	-0.2862	1.5296
C	1 9177	0 4060	2,0054
U	1. 5177	-0.4000	2.0934
С	1.7238	-1.5963	2.7332
ſ	0.8368	-2 6624	2 8088
Ŭ	0.0308	2.0024	2.0000
С	-0.4561	-2.5611	2.2739
ſ	-2 2401	-1 1942	1 2038
C	2.2451	1.1342	1.2030
C	-2.7161	0. 1281	0.8103
ſ	-1 8070	1 2054	0 6737
0	1.0010	1.2004	0.0131
C	-0.3155	0.9545	0.7482
C	-4 1033	0 3699	0 6044
<u> </u>	1. 1000	1.0507	0.0011
C	-4.5654	1.6597	0.3114
С	-3.6527	2, 7085	0.2153
Č	0.0021	2.1000	0.2100
U	-2. 2729	2.4774	0. 3883
С	-0.0566	-0.2869	-1.5298
C	0.8662	_1 2590	-1 6259
U	0.0002	-1. 5569	-1.0308
С	0.4561	-2.5622	-2.2731
ſ	-0.8370	-2 6639	-2 8074
0	0.0010	2.0000	2.0014
C	-1.7240	-1.5977	-2.7322
C	-1 3177	-0 4070	-2.0952
	0.0150		0.7401
0	0.3156	0.9542	-0.7491
С	1.8071	1.2051	$-0.67\overline{45}$
C C	9 7169	0 1070	0.0100
L L	2. (102	0.1278	-0.8108
С	2.2494	-1.1945	-1.2042
ſ	9 9790	9 4779	-0 3803
<u> </u>	2.2123	2.4112	0.3093
С	3.6526	2.7084	-0.2160
ſ	4 5654	1 6595	-0.3117
<u> </u>	4.1004	1.0000	0.0117
C	4.1034	0.3697	-0.6045
0	-3.0585	-2.1705	1.2491
0	2.0501	2.1706	1.2101
0	3.0591	-2.1706	-1. 2499
Н	-0.1509	1.8212	-1.2276
U U	0.1510	1 9919	1 2264
11	0.1510	1.0210	1.2204
С	3. 1195	-1.7034	3.2969
ſ	-3 1198	-1 7052	-3 2956
<u> </u>	5.1150	1.7052	5.2550
0	-5.0169	-0.6091	0.6776
0	-1 2669	-3 6217	2 4036
0	1.2005	0.0005	2.4030
0	5.0169	-0.6095	-0.6772
0	1.2667	-3.6229	-2.4023
U U	4 5100	1 4495	0.0070
Н	-4. 5192	-1. 4425	0. 8979
Н	-2.1287	-3. 3762	1.9782
Ц	4 5101	-1 $4497$	-0.8976
11	4.0101	1. 1127	0.0570
Н	2. 1288	-3. 3772	-1.9777
0	-3, 9928	3, 9941	-0.0501
<u> </u>	E 6204	1 7055	0.1720
H	-5. 6304	1. 7955	0.1739
0	3. 9927	3.9939	0.0492
Н	5 6304	1 7953	-0 1739
11	5.0004	4.0110	0.1103
U	-5.3682	4.3119	-0.2310
С	5.3681	4.3117	0.2306
U U	_5 7027	2 7750	_1 0000
H	-5. 7927	3.7750	-1. 0882
Н	5.7922	3.7749	1.0881
Н	2 0139	0 4251	2 0360
11	2.0105	0.4201	2.0500
Н	1.1165	-3. 5958	3.2876
Н	-1,5956	3, 3203	0. 2895
II	1 1160	2 5075	2 2005
П	-1.1108	-3. 09/0	-3. 2000
H	-2.0140	0. 4240	-2.0362
Н	1 5956	3 3201	-0.2908
11	1.0000	0.0201	0.2000
H	3. 3355	-0.8733	3.9802
Н	3,2637	-2.6407	3,8419
II	2 0650	1 6605	9 1091
Н	J. 8098	-1.0005	2.4934
Н	-3.2645	-2.6432	-3.8392
Ц	-3 8660	-1 6602	-2 1020
11	5.0000	1.0000	2. HUZU
H	-3. 3356	-0.8760	-3.9801
Н	-5 9525	4 0816	0 6682
TT	F 4010	E 90FC	0.0002
Н	-5.4012	<u>Ე. ᲙᲐᲔᲮ</u>	-0.4219
Н	5.9527	4.0812	-0.6683
II	E 4010	E 20E4	0 4010
П	0.4010	J. 3894	0.4212

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

atom	X	Ŷ	
C	0 0000		1 1401
U	-2.6206	0.5425	-1.1401
С	-1.7183	1.5982	-0.8781
C C	2,0007	2.0001	0 6426
U	-2.2027	2.8794	-0. 6436
С	-3.5838	3.1517	-0.6507
ſ	-1 1768	2 1108	-0.8829
C	4. 4700	2.1100	0.0029
С	-4.0175	0.8087	-1.1264
ſ	-2 1253	-0.7922	-1 4764
0	2.1255	0.1522	1. 1704
С	-0. 7078	-0.9749	-1.7314
ſ	0 2144	0 0849	-1 5153
0	0.2111	0.0045	1.0100
C	-0.2309	1. 3290	-0.7779
С	-0.2396	-2.1821	-2.3241
C C	1 0002	9, 2102	2,7102
U	1.0985	-2. 3102	-2. 7192
С	1.9691	-1.2395	-2.5368
C	1 5258	-0.0422	-1 0225
C	1. 5256	0.0423	1. 5555
С	1.7184	1.5984	0.8777
C	2 6207	0 5427	1 1400
0	2.0201	0.0121	1.1100
C	4. 0175	0.8090	1.1266
С	4, 4768	2.1111	0.8828
	2,5000	0 1510	0.0500
U	3. 5839	3. 1519	0. 6502
С	2.2028	2.8795	0.6431
C	0 2200	1 2202	0 7776
U C	0.2309	1. 3292	0.1110
С	-0.2143	0.0852	1.5152
ſ	0 7070	-0.9746	1 7314
	0.1013	0. 3140	1.1014
U C	2.1254	-0.7919	1.4765
С	-1.5257	-0.0418	1.9335
C C	1.0600	1 0200	9 5279
U. U.	-1.9690	-1. 2389	2.0312
С	-1.0982	-2.3095	2.7198
ſ	0 2397	-2 1816	2 3244
0	0.2551	2.1010	2. 3244
0	-2.9407	-1.7534	-1.6263
0	2 9407	-1 7531	1 6265
U	0.0050	0,1000	1.0200
Н	-0. 2958	2. 1896	1.2024
Н	0.2959	2.1894	-1.2029
C .	-1.0806	4 5507	-0.4271
U C	4.0000	4. 5557	0.4271
С	4.0806	4. 5598	0.4258
0	-1 0465	-3 2290	-2 5441
0	1.0100	0.1450	1.0450
0	-4.9345	-0.1458	-1.3450
0	1.0465	-3.2285	2.5447
0	4 0245	0 1454	1 2456
0	4. 9345	-0.1454	1. 3430
Н	-1.9493	-2.9631	-2.2242
Н	-1 1311	-0.9924	-1 4824
11	1. 1011	0. 5524	1. 1021
Н	1. 9492	-2.9628	2.2243
Н	4, 4343	-0.9920	1, 4833
0	2 9720	1 2460	2 0022
0	5.2130	-1.2400	-2. 9022
Н	1.4044	-3.2455	-3.1699
0	-3 2729	-1 2451	2 9025
0	1 40 40	1.2101	2.3020
Н	-1.4042	-3.2447	3.1708
С	3.8094	$-2.42\overline{43}$	$-3.49\overline{34}$
<u> </u>	_3 0101	_2 /921	3 /027
U U	-3. 0101	-2.4231	J. 4931
H	3.2997	-2.6657	-4. 4343
Н	-3 3030	-2 6630	4 4363
11	1, 5000	2.0050	4. 1000
Н	-1.5032	3.6907	-0.4519
Н	-5.5493	2,2796	-0.8853
II	2 2420	0 7591	1 7006
П	2.2439	0.7561	-1. 7990
Н	5. 5494	2.2800	0.8855
Н	1 5033	3 6908	0 4511
11	0.0407	0.0000	1 7005
<u>H</u>	-2.2437	0.7586	1.7995
Н	-5.1557	4.5789	-0.2262
 U	-3 2060	5 1945	_1 2100
п	-3. 0900	0.1040	-1. 5106
H	-3. 5662	5.0352	0.4159
Н	5 1571	4 5797	0 2329
11	0.1011		0.4000
Н	3.5721	5.0317	-0.4229
Н	3.8882	5.1874	1.3057
Ц	1 8580	-0 0000	-2 6021
11	4.0009	2.2033	2.0221
H	3.7387	-3.2793	-2.8104
Н	-4 8603	-2 2025	3 6902
11	1.0000	2.2020	0.0004
I H	-3.7370	-3.2789	2.8118

Cartesian coordinates of 4-1 optimized at the gas-phase DSL11/0-510(d) leve	Cartesian	coordinates of	` <b>4-</b> I (	optimized	at the	gas-phase	B3LYP/6-	31G(d)	) level
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atom	λ	Ϋ́	L
C	1 3647	-1 1751	-1 2286
0	1. 5041	1.1101	1.2200
C	0. 3299	-0.2260	-1.3944
С	-0.8734	-0.5881	-1.9984
	1 1040	1.0007	0.0001
U	-1.1240	-1. 9087	-2.3804
С	-0.1218	-2.8618	-2.1976
C	1 1100	-2 5156	-1 6441
U.	1.1160	-2. 5150	-1.0441
С	2.6862	-0. 7393	-0.7170
C	2 0357	0 7051	-0 5937
<u> </u>	2.3331	0.1001	0.0001
С	1.8988	1.6499	-0.7283
C	0 4693	1 1805	-0.8568
0	0. 1000	1.1000	0.0000
U	4.2639	1.1724	-0.3644
С	4. 5266	2.5463	-0.3192
<u> </u>	2,4947	2.0100	0 4920
L L	3.4847	5. 4549	-0.4830
С	2.1680	3.0124	-0.6797
C	-1 7968	1 5410	0.3105
U .	1.1508	1. 5410	0.3135
С	-2.6910	0. 4712	0.5112
C	-4 0710	0 6849	0.2216
<u> </u>	4.0110	0.0045	0.2210
C	-4.5037	1. 9313	-0.2413
C	-3 6053	2 9891	-0 4255
C	0.0000	0.7774	0.1444
U	-2.2569	2.1114	-0.1444
С	-0.3096	1.3764	0.5558
	0.0204	0.2040	1 5525
U	0.0204	0.2940	1. 0000
С	-0.8566	-0.8089	1.6786
C	-2 1771	-0.8188	1 0437
<u> </u>	2.1111	0.0100	1.0431
С	1. 2013	0. 3442	2.2782
С	1 5450	-0.7284	3 1202
<u> </u>	0.7976	1 0407	2 0047
L	0.7276	-1.8497	3. 2247
С	-0.4681	-1.9057	2.5003
0	2 5090	1 5507	0 4642
0	5. 5969	-1. 5507	-0.4045
0	-2.8645	-1.8602	1.0197
Н	0.0711	2 3307	0 9330
11	0.0111	2.0007	1 5007
Н	-0.0491	1.8627	-1. 5387
С	-2,4769	-2.3022	-2.9188
C C	4 1046	4 2224	0 0002
U.	-4.1040	4. 3334	-0. 8985
0	5.2916	0. 3332	-0.1920
0	2 1138	-3 4168	-1 4903
0	2.1130	3.4108	1.4903
0	-1.2264	-3. 0036	2.6237
0	-4 9215	-0.3490	0 4234
<u> </u>	1.0210	0.0100	0. 1201
Н	4.8951	-0.5861	-0. 2223
Н	-2.0069	-2.8628	2.0163
U U	_1 6422	0 1629	_9 1454
11	1.0432	0.1028	2.1434
Н	-0.3157	-3.8856	-2. 4939
Н	5 5494	2 8737	-0 1520
II	1 2001	2.0101	0. 7027
H	1. 3801	3.7506	-0. 7937
Н	-5.5530	2.0949	-0.4581
Ц	-1 5487	3 5021	-0.2788
11	1.0407	5.5521	0.2100
Н	1.8797	1. 1858	2.2008
Н	0 9931	-2 6930	3 8566
TT	0 1110	2.0000	9 4410
Н	-2.4440	-3.2035	-3. 4412
Н	-3.1934	-2.3917	-2.0915
Ц	-2 8678	-1 5478	-3 6106
11	2.0010	1. 5476	5.0100
Н	-4. 7385	4. 2336	-1.7873
Н	-3 2761	5 0035	-1 1464
II	4 7007	4.0040	0 1051
Н	-4.7097	4.8240	-0.1251
С	-6.3105	-0.1549	0.2067
Ц	-6 7793	-1 1077	0 4579
11	0.1190	1.10//	0.4019
H	-6.7156	0.6331	0.8547
Н	-6 5268	0 0909	-0.8413
	1.0050	4.7500	1 0000
U	1.9058	-4. /596	-1.9006
Н	1.6944	-4.8276	-2.9757
U	2 0/15	-5 9766	_1 6000
11	2.0410	J. 2100	1.0022
H	1.0898	-5.2320	-1.3388
0	3 6841	4 8027	-0 4557
11	4 0000	4.0704	0.0100
Н	4.6286	4. 9784	-0.3190
0	2.7106	$-0.61\overline{16}$	3.8110
II	2 0507	_1 4000	/ 2010
П	4.0091	-1.4230	4.3410
#### Cartesian coordinates of 4-II optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	Z
C	2 6010	0 4711	0 5112
L	2.0910	0.4711	0. 3112
С	1.7969	1.5409	0. 3194
C	2 2570	9 7774	-0 1445
C	2.2010	2.1114	0.145
C	3.6054	2.9890	-0. 4256
C	4 5038	1 9312	-0.2415
0	1.0000	1. 5012	0.2110
C	4.0710	0.6847	0.2214
C	2 1771	-0.8188	1 0438
C		0.0100	1.0100
U	0.8566	-0.8089	1.0/8/
С	-0.0203	0.2941	1.5535
C C	0.2007	1 2764	0 5557
U	0. 3097	1. 3704	0. 5557
С	0.4681	-1.9056	2.5005
C	-0.7275	-1 8496	3 2249
0	1.5440	1.0100	0.2215
Ľ	-1.5449	-0.7282	3. 1202
С	-1.2012	0.3443	2,2783
C C	0.2200	0.0061	1 2042
L L	-0. 3299	-0.2201	-1. 3943
С	-1.3648	-1.1751	-1.2285
C	_1 1199	-2 5156	-1 6441
Ŭ	-1.1162	-2. 5150	-1.0441
С	0. 1216	-2.8619	-2.1976
C	1 1238	-1 9089	-2 3803
	1.1230	1. 3003	1.0000
U	0.8734	-0.5883	-1.9983
С	-0.4692	1, 1804	-0.8568
Č	_1 0000	1 6/00	_0 7994
U	-1. 0900	1.0499	-0.7284
С	-2.9356	0.7051	-0.5937
- C	-2 6262	-0 7303	-0 7168
C	2.0002	0.1555	0.7100
С	-2.1679	3. 0124	-0.6798
С	-3,4846	3, 4549	-0.4831
<u>C</u>	4 5965		0.2102
U	-4. 5265	2. 5464	-0. 3192
С	-4.2638	1.1725	-0.3644
0	2 8645	-1 8602	1 0199
0	2.5010	1.5502	0 4629
0	-3. 5969	-1. 5507	-0.4038
Н	0.0492	1.8626	-1.5388
Н	-0.0710	2 3307	0 9329
	4 1047	4 2224	0.0004
U U	4.1047	4. 3334	-0. 8984
С	2.4768	-2.3025	-2.9186
0	1 2265	-3 0035	2 6239
0	1.2200	0.0000	2.0200
0	4. 9214	-0. 3492	0. 4230
0	-5, 2916	0.3333	-0. 1919
0	0 1149	2 4167	1 4004
0	-2.1142	-3.4107	-1.4904
Н	2.0070	-2.8626	2.0166
Ц	-4 8951	-0 5859	-0.2221
11	4.0551	0.0000	0.2221
H	1.5489	3. 5921	-0.2788
Н	5, 5531	2,0946	-0.4585
II II	0.0020	2 6020	2 9560
П	-0.9930	-2.0928	5. 6509
Н	-1.8797	1. 1859	2.2008
Н	0 3154	-3 8858	-2 4939
11	1 6490	0.1000	0.1454
H	1.6432	0. 1626	-2.1454
Н	-1.3800	3.7506	-0.7939
 	-5 5402	2 9729	_0_1521
11	0.0490	4.0130	0.1021
H	4. 7102	4.8238	-0.1254
Н	4 7382	4 2336	-1 7877
11	2.0700	T. 2000	1 1401
H	3.2702	5.0036	-1.1401
Н	3. 1932	-2.3919	-2.0913
Ц	2 8678	-1 5481	-3 6105
11	2.0010	1. 5461	5.0105
Н	2.4438	-3.2639	-3.4409
С	-1.9063	-4.7594	-1.9009
		-5.2762	-1 6927
11	-2.0422	-5.2705	-1.0827
Н	-1.6948	-4.8273	-2.9760
Н	-1.0906	-5.2321	-1.3392
C	6 3105	-0 1550	0.2066
U	0.0100	0.1000	0.2000
H	b.7154	0.6330	0.8547
Н	6.7793	-1.1077	0.4579
	6 5271	0 0007	_0 \$/12
11	0.02/1	0.0301	0.0410
0	-2.7105	-0.6114	3.8111
Н	-2.8597	-1.4229	4.3218
0	_2 6840	1 8027	-0 4550
0	-3.0840	4.0027	-0.4009
1 11	-4 6285	4 9785	-0 3194

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

atom	X	Ĭ	L
C	-4 5574	2 1466	0 2017
0	1.0011	2.1100	0.2011
L L	-3.6613	3. 2126	0.1712
С	-2.2883	3.0062	0.3762
C	-1 8176	1 7263	0 6416
C	2, 7051	0,6249	0.7224
U	-2.7051	0.0342	0.7224
С	-4.0891	0.8540	0.4629
C	-0.3312	1 4814	0 7420
C	0.0075		1 5274
Ľ	0.0275	0.2462	1.5374
С	-0.8655	-0.8474	1.6220
C	-2 2381	-0.7140	1 0801
0	1.0700	0.1005	0.1470
Ľ	1. 2792	0. 1865	2.1472
С	1.7095	-0.9679	2.8076
C	0 8456	-2.0609	2 8817
C	0.0100	2.0005	2.0011
U	-0.4331	-2.0166	2. 3104
С	0. 3313	1.4814	-0.7420
С	1.8176	1.7263	-0.6417
<u> </u>	2,7052	0,6241	0.7225
U	2.7052	0.0341	-0. 7225
С	2.2381	-0.7140	-1.0801
C	0 8655	-0.8475	-1 6220
C C	0.0275	0.2462	1 5274
U	-0.0273	0.2402	-1. 5574
C	0. 4330	-2.0166	-2.3103
С	-0.8457	-2.0610	-2.8815
C C	_1 7006	-0.0620	-2 8075
C	-1.7090	-0.9080	-2.8075
U	-1.2792	U. 1865	-2.1472
С	2.2884	3.0062	-0.3763
C	3 6614	3 2125	-0.1712
C	5.0014	0.1405	0.1112
C	4. 5575	2.1465	-0.2018
С	4.0891	0.8539	-0.4630
0	-3 0160	-1 6855	0 9909
0	2,0100	1.0000	0.0000
0	3.0160	-1. 6856	-0. 9909
С	3.0992	-1.0361	3. 3920
C	-3 0993	-1 0361	-3 3918
0	0.0335 4.076E	0 1502	0.4525
0	-4.9705	-0.1502	0.4555
0	-1.2986	-3.0526	2.3978
0	4,9765	-0.1503	-0.4537
0	1 2085	-2 0527	-2 2077
0	1. 2900	-3. 0527	-2.3911
H	-4. 4438	-0.9782	0.6409
С	-0.9156	-4.2181	3. 1115
Н	4 4439	-0.9783	-0.6412
 	4. 4455	0.0100	0.0112
t	0.9155	-4. 2182	-3.1115
Н	0. 1273	2.3489	1.2275
Н	-0.1273	2.3489	-1.2276
 Ц	1 1704	-2 0555	2 2025
II	1.1794	-2.9555	3. 3933
Н	-1.1795	-2.9556	-3. 3933
Н	0.0460	-4.7063	-2.6528
Н	-0.0461	-4 7062	2 6529
TT	5.0101 E 0000	0,000	0.0007
Н	-a. b∠00	2. 2005	0.0227
Н	-1.6170	3.8577	0.3209
Н	1.9402	1.0459	2.0915
 Ц	_1 0402	1 0450	-2.0014
11	-1. 9402	1.0439	-2.0914
H	1.6171	3.8577	-0.3209
Н	5.6201	2.2883	-0.0228
Н	3 3262	-0 1426	3 9849
11	0.0402	1 0000	0.0010
Н	3. 8483	-1.0909	2. 5915
Н	3.2277	-1.9137	4.0329
Н	-3 8484	-1 0909	-2 5913
TT	0.0101	1 0107	1 0007
Н	-3.2219	-1.9137	-4. 0327
Н	-3. 3263	-0.1426	-3.9848
Н	-0 6939	-3 9954	4 1634
II	1 7701	1 0000	2 0565
П	-1. ((01	-4. 0009	3. 0000
Н	0.6937	-3.9954	-4.1633
Н	1.7759	-4.8870	-3.0565
<u> </u>	_1 0606	1 4010	_0_0607
0	-4.0020	4. 4919	-0.0087
Н	-5.0263	4.5053	-0.1812
0	4.0627	4. 4918	0.0688
11	E 0964	1. 1010	0.1010
П	<b>D.</b> U204	4.0001	U. 1812

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

atom	Х	Ŷ	
C	0 6979	2 4950	2 9070
U	0.0278	-2.4230	-2. 0919
С	1. 4896	-1.3335	-2.9033
С	1, 1619	-0.1479	-2,2234
C C		0.0574	1 5420
U	-0.0445	-0.0374	-1. 5456
С	-0.9638	-1.1311	-1.5628
С	-0.5976	-2.3374	-2.2274
C C	-0.2658	1 1667	_0 7222
U	-0. 3038	1.1007	-0. 7232
С	-1.8511	1. 4123	-0.5557
С	-2.7824	0.3607	-0.6399
C C	2 2125	1 0025	1 0010
U	-2. 5125	-1.0035	-1.0010
С	-2.2716	2.7129	-0.2603
С	-3.6152	3,0066	-0.0364
C C	4 5502	1 0691	0 1117
U	-4. 5502	1.9001	-0.1117
С	-4.1588	0.6597	-0.4136
С	0.3658	1.1667	0.7232
- C	0.0443	-0.0574	1 5438
Ŭ	0.0443	-0.0374	1. 5456
С	0.9638	-1.1311	1.5628
С	2.3125	-1.0035	1,0009
C C	9 7094	0.2607	0,6200
U C	2.1024	0.3007	0.0399
С	1.8511	1.4123	0.5558
С	4, 1588	0.6597	0.4137
Č	4 5502	1 0691	0 1119
	4.0002	1. 3001	0.1110
С	3.6152	3. 0066	0.0364
С	2,2716	2,7129	0.2603
C	_1 1610	-0.1470	9 9924
U C	-1.1019	-0.1479	2.2234
C	-1.4895	-1. 3335	2.9033
С	-0.6278	-2,4251	2,8979
Č	0.5976	-2 3375	2 2274
U	0.3970	-2. 3373	2.2214
0	-3.0559	-1.9998	-0.9085
0	3.0559	-1.9999	0.9085
C	-4.0701	4 4158	0.2507
<u> </u>	-4.0701	4.4158	0.2397
C	4. 0701	4. 4158	-0. 2597
0	-1.4021	-3.4072	-2.2530
0	-5.0460	-0.3554	-0.5171
0	5.0400	0.3334	0.5171
0	1.4021	-3. 4072	2.2530
0	5.0460	-0.3554	0.5171
Ц	-2 2038	-3 1559	-1 7110
11	2.2030	5.1555	1. 7110
C	-6.4260	-0.0933	-0.3176
Н	2.2038	-3.1559	1.7110
C	6 4260	-0.0933	0 3176
U	0.0579	0.0300	1 9961
Н	0.0578	2.0425	-1.2201
Н	-0.0578	2.0425	1.2261
Н	-5,5959	2, 1944	0,0616
Ц	5 5959	2 1944	-0.0615
11	0.0000	2.1344	0.0015
H	6.6252	0.2739	-0.6975
Н	-6.6252	0.2739	0.6975
Н	0.8767	-3, 3530	-3,4057
и	1 9716	0.6711	_2 2220
П	1.0/10	0.0/11	-2.2330
Н	-1.5349	3. 5119	-0.2097
Н	1.5349	3.5119	0.2097
Ц	-1.8716	0.6711	2 2330
11	1.0710	0.0711	2.2330
Н	-0.8767	-3.3531	3.4056
Н	-3.2214	5.0769	0. 4594
Н	-4 7353	4 4452	1 1307
II	4 6995	4 0279	0 5961
п	-4.0200	4.03/2	-0.0001
Н	4. 7348	4. 4452	-1.1310
Н	4.6290	4.8370	0.5859
Ц	3 2214	5 0771	-0 /588
11	J. 2214	0.0111	0. 1000
H	-b. 8119	0.6300	-1.0479
Н	-6.9264	-1.0525	-0.4591
Н	6 8119	0 6300	1 0480
TT	6 0004		0 4501
Н	0.9264	-1.0525	0.4591
0	2.6848	-1.3540	-3.5547
Н	2,8134	-2,2315	-3, 9485
<u> </u>	_9 6040	_1 95/1	2 5547
U	-2.0848	-1.3541	3. 3347
н н	-2.8134	-2 2316	3 9485

Г

Cartesian coordi	nates of 5-I optimi	ized at the gas-pha	se B3LYP/6-31G	(d) level
a <b>t</b> a m	V	V	7	

atom	Λ	1	L
C	-1 1719	1 4634	0 1043
U C	4.4715	1.4034	0.1043
C	-3.6870	2.5489	-0. 2962
C	-2 2007	2 5140	_0 1244
C	2.3001	2. 5140	0.1244
C	-1.6904	1.4014	0.4453
C	-2 4533	0 2875	0.8627
0	2.1000	0.2010	0.0021
C	-3.8649	0. 3399	0.6822
C	-0 1789	1 4076	0 5572
<u>C</u>	0.1105	1.4010	0.0012
C	0.3539	0.4778	1.6188
C	-0 3943	-0.6674	1 9738
0	0.0040	0.0014	1.5150
C	-1.7770	-0.8613	1.5101
C	1 6006	0 6997	2 1891
0	1.0000	0.0001	2,1001
C	2.1691	-0.2316	3.0799
C	1 4563	-1 3794	3 4046
0	1. 1000	1.0101	0.1010
C	0. 1834	-1.6143	2.8635
C	0 4950	1 1486	-0.8964
0	0.4550	1. 1400	0.0304
C	1.8996	1.7026	-0.9214
C	2 9923	0 8339	-0 7388
<u>C</u>	0.0110	0.0000	0.0004
C	2.8119	-0.6310	-0.6884
С	1 5082	-1 1761	-1 1188
<u>C</u>	1.0002	0.0000	1.1100
C	0.4114	-0.3009	-1.3203
С	1 3289	-2 5526	-1 4350
Č	0 1100	2 0146	1 0575
L L	0.1128	-3.0140	-1.95/5
С	-0.9337	-2.1168	-2.1789
Č	0 7014	0 7600	1 0600
L U	-0. (814	-0.7023	-1.8008
C	2.1057	3.0740	-1.0363
Č	2 2001	2 6001	_0 0620
U	5. 3984	3. 6221	-0.9630
С	4. 4798	2,7730	-0.7441
C	1 2063	1 3885	-0.6101
U C	4.2903	1. 3003	0.0191
0	-2.3682	-1.9379	1.7262
0	3 7714	-1 3606	-0.3690
0	5.7714	1. 5000	0.0000
C	3.5561	0.0056	3.6252
0	-4 5906	-0.7208	1 1013
0	4.000	0.1200	1.1015
0	-0.4531	-2.7404	3. 2209
0	5 3765	0 6275	-0.3829
0	0.0100	0.0210	0.0025
0	2.3742	-3. 3833	-1.2311
С	-6,0032	-0.6936	0.9802
<u> </u>	0.1007	0.0000	0.0010
Н	0.1267	2.4303	0.8012
Н	-0.1182	1 7426	-1 5818
II	E 1000	2 1607	0 6604
П	5.4909	3. 1007	-0.0604
Н	-6.3187	-0.6206	-0.0690
II	5.0101	1 4000	0.0000
П	-5. 5439	1.4909	-0. 0228
Н	-1.7182	3. 3749	-0. 4378
Ц	2 1605	1 5010	1 0250
11	2.1005	1. 5919	1.9209
H	1.8672	-2.1252	4.0786
Ц	-0.0079	-4 0609	-2 1953
	0.0015	1.0005	2.1500
Н	-1.6157	-0.0927	-2.0343
Н	1 2538	3 7350	-1 1852
TT	2 6500	1 01 / 1	4 0447
П	3. 0529	1.0141	4.0447
Ĥ	4.3011	-0.0834	2.8240
Ü	2 8197	_0 7169	1 1057
11	3.0124	0.7100	4.4007
Н	-6.3480	-1.6422	1.3946
Н	-6 4440	0 1340	1 5515
	4 1050	0.1010	0.0505
0	-4. 1852	3.0831	-0. 8565
С	-5, 5884	3. 7944	-1.0475
л. П	-5 0652	2 0179	_1 7940
П	-0.9002	3.0172	-1. (240
H	-6.1294	3. 7401	-0.0941
Н	-5 7400	4 7749	-1 4986
			1.1000
L C	3.6076	5.1076	-1.1366
Н	2 8215	5 6839	-0.6356
11 TT	4 5740	5.0000	0.0000
Н	4.5/42	<b>b.</b> 4263	<u>-0</u> .7346
Н	3 5842	5 3854	-2 1987
C	0.0012	4 7015	1 5400
L	2.2452	-4. (015	-1.5420
Н	3.2094	-5.2061	-1.2912
U U	1 4501	_5 0205	-0.0427
П	1.4091	-0. 2000	-0.9427
H	2.0386	-4. 9194	-2.6089
C	-2 3866	-3 8308	-2 0052
	2.0000	0.0020	2.3352
H	-3. 4087	-3.8734	-3.3754
Н	-1 6997	-4 2120	-3 7630
11 TT	0.0007		0.1000
<u>H</u>	-2.3087	-4.4550	-2.0949
0	-2.1374	-2.4652	-2.7024
т	_1 9159	_0 7007	9 710
<u>н</u>	-1.3152	-2. (331	2. (185
H	5 0338	-0.3081	-0.3041
**	5.0000	0.0001	J. UUII

Cartesian coordi	nates of 5-II optim	nized at the gas-ph	ase B3LYP/6-31C	d(d) level
a <b>t</b> a m	V	V	7	

atom	Х	Ŷ	L
C	_1 0220	-2 2860	1 0526
U C	1. 5235	2.2800	1. 9000
С	-2.5432	-1.5225	0.9595
C	-1 0672	_0 2221	0 5255
<u>C</u>	1. 5075	0. 3221	0.000
С	-0.7753	0. 1232	1.0973
C	-0 1232	-0.6226	2 1051
<u></u>	0.1232	0.0220	2.1051
С	-0.7243	-1.8427	2.5271
C	-0 1789	1 4076	0 5572
0	0.1105	1.4070	0.3312
С	0.7601	2.0913	1.5196
C	1 4526	1 9160	9 4770
U	1.4350	1. 5106	2.4770
С	1. 1197	-0.0958	2.7166
Ē	1 0012	2 4554	1 4202
U	1.0012	5.4004	1.4202
С	1.9754	4.0821	2.2215
Ē	2 6802	2 2204	2 1200
U	2.0092	5. 5204	5.1500
С	2, 4459	1, 9457	3. 2781
Č	0.4050	1 1406	0.9064
U	0.4950	1. 1400	-0. 8904
С	1. 5263	0.0497	-0.8000
- C	1 1901	_1 2566	_1 2022
U	1. 1891	-1.2300	-1.2023
С	-0.0942	-1.5494	-1.8720
Č	0 0061	0.4046	2 2662
U	-0.8801	-0.4040	-2.3003
С	-0.5373	0, 9130	-1.9764
Č	1 0422	0 5622	2 2065
U	-1.9455	-0. 3033	-3. 3005
С	-2.5935	0.5544	-3.8481
Č	_9 1076	1 0200	_2 1607
	-2. 1970	1.0390	-3. 4097
C	-1.1700	2.0150	-2.5358
Č	9 7719	0 2101	-0 3323
U	4. 1114	0. 3101	-0.2333
C	3.7109	-0.7182	$-0.04\overline{48}$
Č	3 2600	_2 0101	-0 4040
U	5. 3090	-2.0191	-0.4049
С	2.1192	-2.3070	-0.9700
0	1 8307	-0.7018	3 4686
0	1.0307	-0. 7918	5.4000
0	-0.4300	-2.7335	-2.0722
- C	2 2626	5 5591	9 0279
U	2.2020	0.0021	2.0372
0	-0.1055	-2.5413	3.5050
Ő	2 1679	1 9600	4 1950
0	3. 1072	1.2088	4. 1850
0	1.8419	-3, 5853	-1.2710
Ő	9 9770	1 0015	2 6661
0	-2.2119	-1. 8215	-3.0001
С	-0.6909	-3.7401	3.9859
Ū	-1 0004	2 0850	0 2250
П	-1.0094	2.0639	0. 5559
Н	1, 0153	2.0862	-1.1175
ÎÎ	4 0605	2 9426	0.9527
П	4.0005	-2.8430	-0. 2337
Н	-0.7662	-4. 4994	3.1963
II	9 9704	9 9119	0 0060
П	-2.3704	-3. 2113	2.2003
Н	-2.4753	0.2531	-0.2325
II	0.4500	1 0469	0.6055
П	0.4500	4.0408	0.0955
Н	3. 4558	3.7665	3. 7653
Ц	-2 3018	0 /188	-4 5623
11	5. 5510	0.4100	4.0020
H	-0.8931	3. 0244	-2.2547
Ц	3 0236	1 3256	0 0646
11	5.0250	1. 5250	0.0040
Н	1. 3401	b.144b	2.0583
Н	2 7372	5 7287	1 0634
11	2.1012	<u> </u>	
Н	<u>∠. 9</u> 330	<b>b. 9</b> 332	<u>2. 8</u> 131
Н	-0.0182	-4.0982	4.7667
<del></del>		_2 5600	1 1169
11	1.0002	3. 0023	4.4100
0	-3.7104	-1.8656	0.3523
C	_1 2602	-2 0662	0 7//2
U	4. 3002		0. (443
H H		0.0000	0 5511
Ц	-3. 7320	-3. 9454	0.0011
11	-3.7320 -4.6393	-3.9454 -3.0443	1 8056
TT	-3.7320 -4.6393	-3.9454 -3.0443	1.8056
Н	$\begin{array}{r} -3.7320 \\ -4.6393 \\ -5.2634 \end{array}$	$\begin{array}{r} -3.9454 \\ -3.0443 \\ -3.1278 \end{array}$	$     \begin{array}{r}       0.3311 \\       1.8056 \\       0.1350 \\     \end{array} $
H C	$\begin{array}{r} -3.7320 \\ -4.6393 \\ -5.2634 \\ 5.0743 \end{array}$	$\begin{array}{r} -3.9454 \\ -3.0443 \\ -3.1278 \\ -0.4089 \end{array}$	$ \begin{array}{r} 0.3311 \\ 1.8056 \\ 0.1350 \\ 0.5263 \\ \end{array} $
H C	$\begin{array}{r} -3.7320 \\ -4.6393 \\ -5.2634 \\ 5.0743 \\ \hline 5.0743 \\ \hline \end{array}$	$\begin{array}{r} -3.9454 \\ -3.0443 \\ -3.1278 \\ -0.4089 \\ 0.2002 \end{array}$	$\begin{array}{c} 0.5311 \\ 1.8056 \\ 0.1350 \\ 0.5263 \\ 1.2240 \end{array}$
H C H	$\begin{array}{r} -3.7320 \\ -4.6393 \\ -5.2634 \\ \hline 5.0743 \\ \hline 5.0120 \end{array}$	$\begin{array}{r} -3.9454 \\ -3.0443 \\ -3.1278 \\ -0.4089 \\ 0.3292 \end{array}$	$\begin{array}{r} 0.3311 \\ \hline 1.8056 \\ \hline 0.1350 \\ \hline 0.5263 \\ \hline 1.3340 \end{array}$
Н С Н Н	$\begin{array}{r} -3.\ 7320 \\ -4.\ 6393 \\ -5.\ 2634 \\ 5.\ 0743 \\ 5.\ 0120 \\ 5.\ 5573 \end{array}$	$\begin{array}{r} -3.9454 \\ -3.0443 \\ -3.1278 \\ -0.4089 \\ 0.3292 \\ -1.3080 \end{array}$	$\begin{array}{r} 0.3311 \\ \hline 1.8056 \\ \hline 0.1350 \\ \hline 0.5263 \\ \hline 1.3340 \\ \hline 0.9211 \end{array}$
H C H H	$\begin{array}{r} -3.7320 \\ -4.6393 \\ -5.2634 \\ 5.0743 \\ 5.0120 \\ 5.5573 \\ 5.720 \end{array}$	$\begin{array}{r} -3.9454 \\ -3.0443 \\ -3.1278 \\ -0.4089 \\ 0.3292 \\ -1.3080 \\ \end{array}$	$\begin{array}{r} 0.5311 \\ \hline 1.8056 \\ \hline 0.1350 \\ \hline 0.5263 \\ \hline 1.3340 \\ \hline 0.9211 \\ \hline 0.9241 \end{array}$
H C H H H	$\begin{array}{r} -3.7320 \\ -4.6393 \\ -5.2634 \\ 5.0743 \\ 5.0120 \\ 5.5573 \\ 5.7359 \end{array}$	$\begin{array}{r} -3.9454 \\ -3.0443 \\ -3.1278 \\ -0.4089 \\ 0.3292 \\ -1.3080 \\ 0.0102 \end{array}$	$\begin{array}{r} 0.3311 \\ 1.8056 \\ 0.1350 \\ 0.5263 \\ 1.3340 \\ 0.9211 \\ -0.2434 \end{array}$
H C H H H C	$\begin{array}{r} -3.\ 7320 \\ -4.\ 6393 \\ -5.\ 2634 \\ 5.\ 0743 \\ 5.\ 0120 \\ 5.\ 5573 \\ 5.\ 7359 \\ -3.\ 3182 \end{array}$	$\begin{array}{r} -3.9454 \\ -3.0443 \\ -3.1278 \\ -0.4089 \\ 0.3292 \\ -1.3080 \\ 0.0102 \\ -2.0279 \end{array}$	$\begin{array}{r} 0.3311 \\ \hline 1.8056 \\ \hline 0.1350 \\ \hline 0.5263 \\ \hline 1.3340 \\ \hline 0.9211 \\ \hline -0.2434 \\ \hline -4.6083 \end{array}$
H C H H H C C	$\begin{array}{r} -3.7320 \\ -4.6393 \\ -5.2634 \\ 5.0743 \\ 5.0120 \\ 5.5573 \\ 5.7359 \\ -3.3182 \\ 2.2021 \end{array}$	$\begin{array}{r} -3.9454 \\ -3.0443 \\ -3.1278 \\ -0.4089 \\ 0.3292 \\ -1.3080 \\ 0.0102 \\ -2.0279 \\ 2.101 \end{array}$	$\begin{array}{r} 0.3311 \\ \hline 1.8056 \\ 0.1350 \\ \hline 0.5263 \\ \hline 1.3340 \\ \hline 0.9211 \\ \hline -0.2434 \\ \hline -4.6083 \\ \hline 4.7959 \\ \hline \end{array}$
H C H H H C H	$\begin{array}{r} -3.7320 \\ -4.6393 \\ -5.2634 \\ 5.0743 \\ 5.0120 \\ 5.5573 \\ 5.7359 \\ -3.3182 \\ -3.3921 \end{array}$	$\begin{array}{r} -3.9454 \\ -3.0443 \\ -3.1278 \\ -0.4089 \\ 0.3292 \\ -1.3080 \\ 0.0102 \\ -2.0279 \\ -3.1101 \end{array}$	$\begin{array}{r} 0.3311\\ 1.8056\\ 0.1350\\ 0.5263\\ 1.3340\\ 0.9211\\ -0.2434\\ -4.6083\\ -4.7252\end{array}$
Н С Н Н Н С Н Н	$\begin{array}{r} -3.\ 7320 \\ -4.\ 6393 \\ -5.\ 2634 \\ 5.\ 0743 \\ 5.\ 0120 \\ 5.\ 5573 \\ 5.\ 7359 \\ -3.\ 3182 \\ -3.\ 3921 \\ -4.\ 2765 \end{array}$	$\begin{array}{r} -3.9454 \\ -3.0443 \\ -3.1278 \\ -0.4089 \\ 0.3292 \\ -1.3080 \\ 0.0102 \\ -2.0279 \\ -3.1101 \\ -1.6363 \end{array}$	$\begin{array}{r} 0.3311\\ \hline 1.8056\\ \hline 0.1350\\ \hline 0.5263\\ \hline 1.3340\\ \hline 0.9211\\ \hline -0.2434\\ \hline -4.6083\\ \hline -4.7252\\ \hline -4.2436\end{array}$
H C H H C C H H H	$\begin{array}{r} -3.7320 \\ -4.6393 \\ -5.2634 \\ 5.0743 \\ 5.0120 \\ 5.5573 \\ 5.7359 \\ -3.3182 \\ -3.3921 \\ -4.2765 \\ 2.0826 \end{array}$	$\begin{array}{r} -3.9454 \\ -3.0443 \\ -3.1278 \\ -0.4089 \\ 0.3292 \\ -1.3080 \\ 0.0102 \\ -2.0279 \\ -3.1101 \\ -1.6363 \\ 1.5797 \end{array}$	$\begin{array}{c} 0.5311\\ 1.8056\\ 0.1350\\ 0.5263\\ 1.3340\\ 0.9211\\ -0.2434\\ -4.6083\\ -4.7252\\ -4.2436\\ -5.5705\end{array}$
H C H H H C H H H	$\begin{array}{r} -3.\ 7320\\ -4.\ 6393\\ -5.\ 2634\\ 5.\ 0743\\ 5.\ 0743\\ 5.\ 5573\\ 5.\ 7359\\ -3.\ 3182\\ -3.\ 3921\\ -4.\ 2765\\ -3.\ 0826\\ \end{array}$	$\begin{array}{r} -3.9454 \\ -3.0443 \\ -3.1278 \\ -0.4089 \\ 0.3292 \\ -1.3080 \\ 0.0102 \\ -2.0279 \\ -3.1101 \\ -1.6363 \\ -1.5727 \\ -\end{array}$	$\begin{array}{c} 0.5311\\ \hline 1.8056\\ \hline 0.1350\\ \hline 0.5263\\ \hline 1.3340\\ \hline 0.9211\\ \hline -0.2434\\ \hline -4.6083\\ \hline -4.7252\\ \hline -4.2436\\ \hline -5.5795\\ \hline \end{array}$
H C H H H C H H C	$\begin{array}{r} -3.\ 7320\\ -4.\ 6393\\ -5.\ 2634\\ 5.\ 0743\\ 5.\ 0120\\ 5.\ 5573\\ 5.\ 7359\\ -3.\ 3182\\ -3.\ 3921\\ -4.\ 2765\\ -3.\ 0826\\ -3.\ 8384\end{array}$	$\begin{array}{r} -3.9454 \\ -3.0443 \\ -3.1278 \\ -0.4089 \\ 0.3292 \\ -1.3080 \\ 0.0102 \\ -2.0279 \\ -3.1101 \\ -1.6363 \\ -1.5727 \\ 2.8804 \end{array}$	$\begin{array}{r} 0.5311\\ \hline 1.8056\\ \hline 0.1350\\ \hline 0.5263\\ \hline 1.3340\\ \hline 0.9211\\ \hline -0.2434\\ \hline -4.6083\\ \hline -4.7252\\ \hline -4.2436\\ \hline -5.5795\\ \hline -4.8644 \end{array}$
H C H H C H C H H H C C U	$\begin{array}{r} -3.\ 7320\\ -4.\ 6393\\ -5.\ 2634\\ 5.\ 0743\\ 5.\ 0120\\ 5.\ 5573\\ 5.\ 7359\\ -3.\ 3182\\ -3.\ 3921\\ -4.\ 2765\\ -3.\ 0826\\ -3.\ 8384\\ -4.\ 1275\end{array}$	$\begin{array}{r} -3.9454 \\ -3.0443 \\ -3.1278 \\ -0.4089 \\ 0.3292 \\ -1.3080 \\ 0.0102 \\ -2.0279 \\ -3.1101 \\ -1.6363 \\ -1.5727 \\ 2.8804 \\ 3.0071 \\ \end{array}$	$\begin{array}{r} 0.5311\\ 1.8056\\ 0.1350\\ 0.5263\\ 1.3340\\ 0.9211\\ -0.2434\\ -4.6083\\ -4.7252\\ -4.2436\\ -5.5795\\ -4.8644\\ -5.6044\\ -5.0050\end{array}$
H C H H C H H H C H H C H	$\begin{array}{r} -3.\ 7320\\ -4.\ 6393\\ -5.\ 2634\\ 5.\ 0743\\ 5.\ 0120\\ 5.\ 5573\\ 5.\ 7359\\ -3.\ 3182\\ -3.\ 3921\\ -4.\ 2765\\ -3.\ 0826\\ -3.\ 8384\\ -4.\ 1275\end{array}$	$\begin{array}{r} -3.9454 \\ -3.0443 \\ -3.1278 \\ -0.4089 \\ 0.3292 \\ -1.3080 \\ 0.0102 \\ -2.0279 \\ -3.1101 \\ -1.6363 \\ -1.5727 \\ 2.8804 \\ 3.9071 \\ \end{array}$	$\begin{array}{c} 0.3311\\ 1.8056\\ 0.1350\\ 0.5263\\ 1.3340\\ 0.9211\\ -0.2434\\ -4.6083\\ -4.7252\\ -4.2436\\ -5.5795\\ -4.8644\\ -5.0950\\ \end{array}$
H C H H C H H H C H H C H H H	$\begin{array}{r} -3.\ 7320\\ -4.\ 6393\\ -5.\ 2634\\ 5.\ 0743\\ 5.\ 0120\\ 5.\ 5573\\ 5.\ 7359\\ -3.\ 3182\\ -3.\ 3921\\ -4.\ 2765\\ -3.\ 0826\\ -3.\ 8384\\ -4.\ 1275\\ -3.\ 5446\end{array}$	$\begin{array}{c} -3.9454 \\ -3.0443 \\ -3.1278 \\ -0.4089 \\ 0.3292 \\ -1.3080 \\ 0.0102 \\ -2.0279 \\ -3.1101 \\ -1.6363 \\ -1.5727 \\ 2.8804 \\ 3.9071 \\ 2.3706 \end{array}$	$\begin{array}{c} 0.3311\\ \hline 1.8056\\ \hline 0.1350\\ \hline 0.5263\\ \hline 1.3340\\ \hline 0.9211\\ \hline -0.2434\\ \hline -4.6083\\ \hline -4.7252\\ \hline -4.7252\\ \hline -4.2436\\ \hline -5.5795\\ \hline -4.8644\\ \hline -5.0950\\ \hline -5.7912\\ \end{array}$
Н С Н Н Н С Н Н С Н Н С Н Н Н Н	$\begin{array}{r} -3.\ 7320\\ -4.\ 6393\\ -5.\ 2634\\ 5.\ 0743\\ 5.\ 0743\\ 5.\ 0120\\ 5.\ 5573\\ 5.\ 7359\\ -3.\ 3182\\ -3.\ 3921\\ -4.\ 2765\\ -3.\ 0826\\ -3.\ 8384\\ -4.\ 1275\\ -3.\ 5446\\ -4.\ 6895\end{array}$	$\begin{array}{c} -3.9454 \\ -3.0443 \\ -3.1278 \\ -0.4089 \\ 0.3292 \\ -1.3080 \\ 0.0102 \\ -2.0279 \\ -3.1101 \\ -1.6363 \\ -1.5727 \\ 2.8804 \\ 3.9071 \\ 2.3706 \\ 2.3560 \end{array}$	$\begin{array}{c} 0.5311\\ 1.8056\\ 0.1350\\ 0.5263\\ 1.3340\\ 0.9211\\ -0.2434\\ -4.6083\\ -4.7252\\ -4.2436\\ -5.5795\\ -4.8644\\ -5.0950\\ -5.7912\\ -4.4122\end{array}$
H C H H H C H H H C H H H H H H	$\begin{array}{r} -3.\ 7320\\ -4.\ 6393\\ -5.\ 2634\\ 5.\ 0743\\ 5.\ 0120\\ 5.\ 5573\\ 5.\ 7359\\ -3.\ 3182\\ -3.\ 3921\\ -4.\ 2765\\ -3.\ 0826\\ -3.\ 8384\\ -4.\ 1275\\ -3.\ 5446\\ -4.\ 6895\end{array}$	$\begin{array}{r} -3.9454 \\ -3.0443 \\ -3.1278 \\ -0.4089 \\ 0.3292 \\ -1.3080 \\ 0.0102 \\ -2.0279 \\ -3.1101 \\ -1.6363 \\ -1.5727 \\ 2.8804 \\ 3.9071 \\ 2.3706 \\ 2.3560 \\ 2.3560 \end{array}$	$\begin{array}{c} 0.3311\\ \hline 1.8056\\ \hline 0.1350\\ \hline 0.5263\\ \hline 1.3340\\ \hline 0.9211\\ \hline -0.2434\\ \hline -4.6083\\ \hline -4.7252\\ \hline -4.2436\\ \hline -5.5795\\ \hline -4.8644\\ \hline -5.0950\\ \hline -5.7912\\ \hline -4.4122\\ \hline \end{array}$
H C H H C H C H H C H H H H H O	$\begin{array}{r} -3.\ 7320\\ -4.\ 6393\\ -5.\ 2634\\ 5.\ 0743\\ 5.\ 0120\\ 5.\ 5573\\ 5.\ 7359\\ -3.\ 3182\\ -3.\ 3921\\ -4.\ 2765\\ -3.\ 0826\\ -3.\ 0826\\ -3.\ 8384\\ -4.\ 1275\\ -3.\ 5446\\ -4.\ 6895\\ -2.\ 7502\\ \end{array}$	$\begin{array}{r} -3.9454 \\ -3.0443 \\ -3.1278 \\ -0.4089 \\ 0.3292 \\ -1.3080 \\ 0.0102 \\ -2.0279 \\ -3.1101 \\ -1.6363 \\ -1.5727 \\ 2.8804 \\ 3.9071 \\ 2.3706 \\ 2.3560 \\ 2.9800 \end{array}$	$\begin{array}{c} 0.3311\\ 1.8056\\ 0.1350\\ 0.5263\\ 1.3340\\ 0.9211\\ -0.2434\\ -4.6083\\ -4.7252\\ -4.2436\\ -5.5795\\ -4.8644\\ -5.0950\\ -5.7912\\ -4.4122\\ -3.9567\\ \end{array}$
Н С Н Н Н С Н Н С Н Н С Н Н Н Н С Н Н Н С Н Н Н С Н Н Н С Н Н Н С Н Н Н С Н Н Н Н С Н Н Н С Н Н Н С Н Н Н С Н Н Н С Н Н Н С С Н Н Н С С Н Н Н С С Н Н Н С С Н Н С С Н С Н С С Н С Н С С С Н С С С Н С С Н С С Н С С Н С С Н С С С С С С С С С С С С С С С С С С Н С	$\begin{array}{r} -3.\ 7320\\ -4.\ 6393\\ -5.\ 2634\\ 5.\ 0743\\ 5.\ 0743\\ 5.\ 05573\\ 5.\ 7359\\ -3.\ 3182\\ -3.\ 3921\\ -4.\ 2765\\ -3.\ 0826\\ -3.\ 8384\\ -4.\ 1275\\ -3.\ 5446\\ -4.\ 6895\\ -2.\ 7502\\ 2.\ 8676\end{array}$	$\begin{array}{r} -3.9454 \\ -3.0443 \\ -3.1278 \\ -0.4089 \\ 0.3292 \\ -1.3080 \\ 0.0102 \\ -2.0279 \\ -3.1101 \\ -1.6363 \\ -1.5727 \\ 2.8804 \\ 3.9071 \\ 2.3706 \\ 2.3560 \\ 2.9800 \\ 0.3197 \end{array}$	$\begin{array}{c} 0.5311\\ 1.8056\\ 0.1350\\ 0.5263\\ 1.3340\\ 0.9211\\ -0.2434\\ -4.6083\\ -4.7252\\ -4.2436\\ -5.5795\\ -4.8644\\ -5.0950\\ -5.7912\\ -4.4122\\ -3.9567\\ 4.1136\end{array}$
H C H H H C H H H C H H H H H H H H H H	$\begin{array}{r} -3.\ 7320\\ -4.\ 6393\\ -5.\ 2634\\ 5.\ 0743\\ 5.\ 0120\\ 5.\ 5573\\ 5.\ 7359\\ -3.\ 3182\\ -3.\ 3921\\ -4.\ 2765\\ -3.\ 0826\\ -3.\ 8384\\ -4.\ 1275\\ -3.\ 5446\\ -4.\ 6895\\ -2.\ 7502\\ 2.\ 8676\\ -3.\ 8676$	$\begin{array}{r} -3.9454 \\ -3.0443 \\ -3.1278 \\ -0.4089 \\ 0.3292 \\ -1.3080 \\ 0.0102 \\ -2.0279 \\ -3.1101 \\ -1.6363 \\ -1.5727 \\ 2.8804 \\ 3.9071 \\ 2.3706 \\ 2.3560 \\ 2.9800 \\ 0.3197 \\ 0.556 \\ 0.3197 \\ 0.556 \\ 0.55$	$\begin{array}{c} 0.3311\\ \hline 1.8056\\ \hline 0.1350\\ \hline 0.5263\\ \hline 1.3340\\ \hline 0.9211\\ \hline -0.2434\\ \hline -4.6083\\ \hline -4.7252\\ \hline -4.2436\\ \hline -5.5795\\ \hline -4.8644\\ \hline -5.0950\\ \hline -5.7912\\ \hline -4.4122\\ \hline -3.9567\\ \hline 4.1136\\ \hline -5.6956\\ \hline -5.6956\\ \hline -5.6956\\ \hline -5.7912\\ \hline $

Cartesian coordi	nates of 5-III optir	nized at the gas-pl	hase B3LYP/6-310	G(d) level
atom	Y	V	7	

atom	X	V V	7
C	4 5040	1 0228	-0 1368
C C	9,4020	1. 5556	0.1300
Ľ	3. 4930	2. 8990	-0.1300
C	2. 1631	2. 5255	-0.3400
С	1.8343	1. 1919	-0.5595
С	2.8309	0.1906	-0. 5776
С	4, 1807	0, 5883	-0.3601
Č	0 3689	0.8428	-0.7241
- C	0.1345	-0.4389	-1 4831
C	0.1343	0.4303	1.4031
<u> </u>	1.1178	-1.4524	-1. 4439
C	2.4511	-1.2122	-0.8697
С	-1.0702	-0.6600	-2.1380
С	-1.3593	-1.9075	-2.7243
С	-0.4100	-2,9205	-2,6630
Č	0.8240	-2 7151	-2,0275
Č	-0.3680	0 9499	0.7941
<u> </u>	0.3003	1 1010	0.7241
<u> </u>	-1. 8343	1. 1919	0. 5595
C	-2.8309	0. 1906	0.5776
С	-2.4511	-1.2121	0.8696
С	-1.1178	-1.4523	1.4439
С	-0 1345	-0 4389	1 4831
Č	-0.82/0	-9 7151	2 0275
C	0.0240	_2.1101	2.0210
	0.4039	-2.9200	2.0030
L	1.3592	-1.9075	2. 7244
С	1.0702	-0.6600	2.1381
С	-2.1631	2.5255	0.3400
С	-3. 4929	2.8996	0.1300
Ċ	-4, 5040	1, 9338	0.1368
Č	-4 1807	0.5883	0.3600
0	2 2475	-2 1579	-0.7074
0	3. 2473	-2.1070	
0	-3.2475	-2.1578	0.7073
C	-2.7104	-2.1464	-3.3522
С	2.7103	-2.1464	3. 3523
0	5.1302	-0.3740	-0.3910
0	1 6949	-3 7345	-2,0036
0	-5 1302	-0.3740	0.3010
0	-1 6040	-2 7245	2 0026
0	-1.0949	-3.7343	2.0030
Ľ	6. 4942	-0.0174	-0.2348
С	-6. 4942	-0.0173	0.2348
Н	-0.1056	1.6670	-1.2660
Н	0.1056	1.6670	1.2660
Н	-6.6865	0.4301	-0.7493
Ĥ	-5 5327	2 2215	-0.0223
Ц	6 6965	0 4201	0.7402
	0.0803	0.4301	0. 7493
H	5. 5327	2.2214	0.0223
H	1.4011	3. 2988	-0.3353
Н	-1.8143	0. 1303	-2.1765
Н	-0.6021	-3.8985	-3.0939
Н	0.6021	-3. 8985	3.0940
Н	1.8142	0.1303	2.1766
Ĥ	-1 4011	3 2988	0 3353
Ц	-2 01/7	-1 2017	_2 QQ1/
11 U	_2 /795	_9 9694	_9 5705
П	-3.4723	-2.2034	-2.0700
H	-2. (166	-3.0522	-3.9661
Н	3. 4724	-2.2634	2.5706
Н	2.7165	-3.0522	3.9662
Н	3.0146	-1.3017	3.9815
Н	7.0496	-0.9526	-0.3192
Ĥ	6 8253	0.6746	-1.0204
 Ц	-7.0406	-0.0526	0 2101
11	1.0490 6.0050	0. 3020	1 0000
П	-0.0203	0.0740	1.0203
0	-3.7094	4.2272	-0.0687
0	3.7094	4.2272	0.0687
С	5.0392	4.6823	0.2740
Н	5, 4823	4, 2385	1, 1749
Н	5 6776	4 4630	-0 5915
<u>Ш</u>	1 0664	5 7629	0.0010
П	4. 3004	0.1000	0.4037
U U	-5.0392	4.6823	-0.2740
Н	-5. 4822	4.2386	-1.1749
Ĥ	-5.6775	4.4630	0.5915
Н	-4.9663	5.7634	-0.4037
H	-2.4761	-3. 4128	1.4741
Ц	2.1101	_2 /120	_1 /7/9
11	2. 1101	0.4140	1. 4144

Cartesian coordi	nates of 5-IV optin	nized at the gas-pl	hase B3LYP/6-310	G(d) level
			1	1

atom	Х	Y	Z
C	1 2609	-1 9870	-9 7499
<u></u>	1.2005	1. 5010	2. 1422
C	2.0890	-0.8804	-2.5402
C	1 5868	0 2759	-1 9319
C	1.0000	0.2100	1.5515
U	0.2628	0.3303	-1.5178
С	-0.6157	-0.7608	-1.7390
- C	_0_021	-1 0217	_2 2404
<u>U</u>	-0.0031	-1.9317	-2. 3494
С	-0.2101	1. 5658	-0. 7832
C	-1 691/	1 8218	-0 9300
C	1.0314	1.0210	0.3300
C	-2.5645	0.7440	-1.1719
C	-2,0550	-0.6154	-1 4404
č	2.0000	2 1060	0 7400
U	-2. 1962	5. 1000	-0. 7488
С	-3.5791	3.3553	-0.7956
C	-4 4504	2 2894	-1 0017
<u>U</u>	4.4304	2.2094	1.0017
C	-3.9664	0. 9857	-1.1807
C	0 2098	1 5657	0 7834
č	0.2000	0.2201	1 5170
U	-0.2629	0. 3301	1.5179
С	0.6158	-0.7610	1.7388
- C	2 0550	-0.6154	1 4401
<u>U</u>	2.0550	-0.0134	1.4401
С	2.5644	0.7441	1. 1718
C	1 6912	1 8219	0 9301
<u>C</u>	2.0002	0.0050	1 1005
U	3. 9002	0.9899	1.1805
C	4.4501	2.2897	1.0017
<u> </u>	2 5788	3 3556	0 7959
	3. 3100	0.000	0.1330
C	2. 1958	3.1061	0.7491
С	-1.5868	0.2756	1.9322
Č	1.0000	0 0000	2 5405
L L	-2.0888	-0.8809	2. 5405
С	-1.2606	-1.9874	2.7422
C	0 0833	-1 9319	2 3492
0	0.0000	1. 5015	1 4005
0	-2.8494	-1.5757	-1. 4885
0	2.8496	-1.5756	1.4879
Č	-4 1060	1 7628	-0.6458
<u>U</u>	4.1000	4. 7020	0.0438
C	4. 1055	4. 7631	0.6462
0	-0.9233	-2.9722	-2.5494
Ŏ	4 9504	0.0011	1 2500
0	-4. 8594	0.0011	-1. 3598
0	0. 9236	-2.9724	2.5490
0	4 8593	0.0013	1 3595
C	1.0000	4 1900	2,0010
U	-0.4486	-4. 1389	-3.2016
С	0. 4491	-4.1392	3.2011
Н	0 3266	2 4293	-1 1892
	0.0200	2. 1255	1.1005
Н	-0.3269	2.4292	1. 1895
Н	-0.3523	-4.6255	2.6297
Û	-1 6507	_2 9916	2 2051
11	1.0307	2.0010	3.2031
Н	0.3528	-4.6252	-2.6301
Н	1.6512	-2.8811	-3,2052
Û	2 2502	1 1196	_1 7709
	2.2000	1.1120	-1. 7798
Н	-1.5109	3. 9322	-0.5689
Н	-5, 5258	2, 4392	-1.0252
Ü.	5 5255	2 4205	1 0252
11	0.0200	2.4395	1.0232
H	1.5105	3. 9323	0.5693
Н	-2.2584	1.1123	1.7803
Ŭ.	_4 0255	5 2106	-1 5050
11	4.0000	5. 5100	1.0900
Н	-3. 5319	5.3288	0.0963
Н	-5.1572	4. 7672	-0.3415
<u> </u>	2 5214	5 2201	
П	3. 3314	0.0291	-0.0909
H	5.1567	4. 7676	0.3418
Н	4 0350	5 3107	1 5955
<u> </u>	_1 2001	_1 0007	-2 2507
П	-1. 3001	-4.0007	-3.2001
Н	-0.0909	-3.9201	-4.2164
Н	1.3086	-4.8090	3. 2580
U II	0.0015	-2 0205	1 9150
П	0.0910	-3. 9203	4. 2109
0	-3. 3955	-0.8320	2.9023
0	3 3958	-0.8314	-2 9018
Č	2 0064	1 0076	2.2010
	5. 9904	-1.90/0	-3.4084
Н	3.9512	-2.8400	-2.7791
Н	3 5235	-2 2611	-4 4206
11	5.0200 E 000E	1 7001	2.6407
Н	5. 0395	-1. (221	-3. 0407
С	-3.9960	-1.9883	3.4688
Ĥ	-3 9508	-2 8405	2 7794
11	0.000		4 4000
Н		/ / DIM	4.4709
	-3. 5229	2.2013	1.1200
Н	-3.5229 -5.0391	-1.7229	3. 6474
<u>Н</u> Н	-3.5229 -5.0391 4.3229	-1.7229 -0.8390	3.6474 1 4220
H H T	-3.5229 -5.0391 4.3229	$ \begin{array}{r} -2.2019 \\ -1.7229 \\ -0.8390 \\ 0.8390 \end{array} $	$     \begin{array}{r}       3.6474 \\       1.4220 \\       1.4220     \end{array} $

# Cartesian coordinates of 1,1'-acetylated 5-I optimized at the gas-phase B3LYP/6-31G(d) level $\frac{1}{2}$

atom	Λ	1	L
C	4.5841	2.0550	0.2043
C	2 7157	2 1/56	0 0803
	0.1101	0.1400	0.0033
C	2.3766	2.9452	-0.2550
C	1.8991	1.6581	$-0.\overline{4844}$
C	2 7444	0 5368	-0.3678
C		0.7571	0.0010
L	4.1052	0. (5/1	-0.0212
С	0.4315	1.4859	-0.8148
C	0 1434	0 2359	-1 6114
C	0.0760	0.2000	1.0114
t	0.9769	-0. 8929	-1.4779
С	2.2077	-0.8281	-0.6261
C	-0 9864	0 1865	-2 4301
0	1.0000	0.1000	2. 1001
U	-1.3600	-0. 9863	-3. 0930
С	-0. 5369	-2.1067	-2.9612
C	0 6097	-2 0581	-2 1780
<u>C</u>	0.4719	1 6052	0.5214
U	-0.4718	1.6055	0. 5214
С	-1.8946	1.9788	0.1694
C	-2 8934	0 9929	0 1153
C	2.0001	0.4250	0.4425
U.	-2. 0007	-0.4550	0.4425
С	-1.3666	-0.6329	1.3044
С	-0.3878	0.3825	1,4063
Č	_1 1000	-1 8041	2 0012
C C	1.1990	1.0041	2.0512
С	-0. 1037	-1.9323	2.9562
С	0, 8333	-0.9001	3,0484
	0.6884	0.2574	2 2757
	0.0004	0.2014	4.4101
C	-2.1901	3.3070	-0.1580
С	-3.4728	3.6985	-0.5429
C .	-4 4695	2 7162	-0.6006
C	T. 1020	1 9050	0.0000
L	-4.1862	1.3958	-0.2812
0	2.7494	-1.8425	-0.1997
0	-3 2630	-1 3568	0 0415
0	0.2000	1.0000	0.0110
t	-2.6464	-1.0480	-3.8773
0	4.9114	-0.3261	0.0562
0	1 3260	-3 2433	-2.0724
0	F 9950	0.4016	0.4472
0	-5. 2259	0.4916	-0.4473
0	-2.1475	-2.7629	1.9909
С	6, 2943	-0.1477	0.3115
	0 1273	2 3516	-1 /122
П	0.1275	2.3310	-1.4155
Н	-0. 0302	2.4491	1.0618
Н	-5, 4849	2,9679	-0.8928
Н	6 4702	0.3000	1 2088
ll	0.4702	0.3000	1.2900
Н	5.6217	2.2107	0.4603
Н	1.7289	3.8117	-0.3478
Н	-1 6067	1 0723	-2 5321
11	1.0007	1.0723	2.0021
Н	-0.7771	-3. 0382	-3.4648
Н	0.0102	-2.8252	3.5526
Н	1 4371	1 0364	2 3612
11	1.4571	1.0504	2.3012
H	-1. 3998	4.0535	-0.1056
Н	-2.8187	-0.1245	-4. 4411
Н	-3, 4931	-1.1763	-3, 1902
II	9.6520	1 0060	4 5904
H	-2.6530	-1. 8868	-4. 5804
Н	6.7260	-1.1496	0.2900
Н	6, 7731	0.4706	-0,4593
C .	2 5000	-3 3002	-2 5841
	2.000	4 5002	0 1101
L	3.2770	-4. 5605	-2.1181
Н	3.5509	-4.4198	-1.0670
Н	2.6012	-5. 4180	-2. 1802
<u></u> Ц	1 1751	-4 7350	-2 7110
	1.1101	1. 1000	4. (113
0	3.0726	-2.4514	-3.2962
0	4.0883	4.4396	0.2874
C	5 4376	4 7184	0 6308
<u> </u>	5.1010	A 9490	1 5700
П	0. (10)	4.2420	1.0190
Н	<u>6. 1</u> 293	4.3944	-0.1576
Н	5.4986	5.8025	0.7403
	-2 70/19	5 1370	-0.8650
U	3. 1342	5.1313	0.0009
<u> </u>	-2.8866	5.7460	-0.9303
Н	-4.3284	5. 2233	-1.8194
Н	-4 4381	5 5814	-0.0958
C	0 0510	2.0011	9 7000
L	-2.0512	-3.9244	2. 1982
Н	-2.9270	-4.5255	2.5485
Н	-1.1426	-4.4984	2.5736
II	_2 0725	_2 £700	2 0602
п	-2.0120	-3.0(88	3.0083
C	2.1732	-2.1015	4.6235
Н	3.0973	-1.9069	5.1706
	1 2662	-9 3057	5 3305
11	1.0002	2.3037	0.0000
<u> </u>	2.3130	-2.9729	3.9717
0	1.9166	-0.9270	3.8680
C	-5 7134	-0 1698	0 6571
0	0.110H	0.1000	1 7000
0	-5.4450	0.1409	1. (893
С	-6.6044	-1.3004	0.2209
Н	-7 1910	-1 6543	1 0697
11	7 9600	0.0024	0 5007
H	-1.2600	-0.9934	-0. 5987
Н	-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	Λ	I	L
C	0 1037	-1 9323	2 9561
C C	. 1031	_0_0001	2.JJUI 9 0409
U	-0.8334	-0.9001	3.0483
C	-0.6884	0.2574	2.2757
С	0.3877	0.3825	1.4063
С	1.3665	-0.6329	1.3044
С	1, 1990	-1.8040	2,0912
<u> </u>	0.4718	1 6053	0.5215
<u> </u>	1,0046	1.0000	0. 3213
L L	1.8946	1.9788	0.1695
C	2.8934	0.9929	0.1154
С	2.5587	-0.4350	0.4425
С	2.1901	3. 3070	-0. 1579
C	3 4729	3 6985	-0 5429
C C	4 4605	2 7162	-0.6005
C	4,1969	1 2059	0.0003
Ľ	4.1802	1. 3938	-0.2811
C	-0.4314	1.4861	-0.8148
С	-0.1434	0.2360	-1.6114
С	-0.9768	-0.8927	-1.4779
С	-2.2075	-0.8281	-0.6261
C	-2 7443	0 5367	-0.3677
<u> </u>	_1 8001	1 6582	-0.4844
C	1.0391	0.7560	0.4044
U	-4.1051	0.7569	-0.0211
C	-4. 5841	2.0548	0.2043
С	-3.7158	3.1455	0.0893
С	-2.3767	2.9452	-0.2550
С	0, 9863	0.1868	-2, 4302
r r	1 3600	-0 9859	-3 0033
C C	0 5360	-9 1064	-9 0615
	0.0009	-2.1004	2. 9010
C	-0.6096	-2.0579	-2.1782
0	3.2628	-1.3568	0.0414
0	-2.7492	-1.8425	-0.1998
С	3.7943	5.1379	-0.8657
0	2 1475	-2.7628	1 9909
0	5 2259	0.4916	-0 4471
0	1 2255	2 9491	0.1111
0	-1. 5257	-3.2431	-2.0723
0	-4.9113	-0. 3263	0.0565
C	2.0513	-3.9244	2.7982
Н	0.0302	2.4491	1.0619
Н	-0.1273	2.3518	-1.4132
Н	0.7771	-3.0378	-3, 4652
Н	1 1428	-4 4984	2 5737
11	0.0102	1, 1001	2.5151
П	-0.0103	-2.0232	3. 3320
H	-1.4371	1.0364	2.3611
Н	1.3998	4.0535	-0.1055
Н	5.4850	2.9678	-0. 8928
Н	-5.6218	2.2104	0.4604
Н	-1.7290	3.8118	-0.3479
Н	1 6067	1 0726	-2 5322
11	2 0060	5 7450	0.0206
П	2.0000	5.7459	-0.9300
H	4. 3291	5.2234	-1.8189
H	4. 4378	5.5814	-0.0952
Н	2.9271	-4.5254	2.5486
Н	2.0726	-3. 6787	3.8683
С	5.7132	-0.1701	0.6573
С	6 6041	-1 3007	0 2211
Ŭ H	5 9588	-2 1072	-0 1436
 Ц	7 2500	_0.0037	-0.5084
11	7 1004	U. 3331	1 0600
П	1.1904	-1.0049	1.0099
0	5.4447	0.1406	1.7894
0	-1.9167	-0. 9270	3.8680
С	-2.1734	-2. 1016	4.6232
Н	-2, 3131	-2.9730	3, 9713
Н	-1.3666	-2, 3060	5, 3393
Н	-3.0976	-1 9071	5 1701
11 C	0.0010	_1. 5071	_2 0776
U	2.0403	-1.04/0	0.0110
H	2.8186	-0.1239	-4.4413
Н	3.4931	-1.1759	-3.1906
Н	2.6529	-1.8862	-4.5808
С	-6. 2943	-0. 1480	0.3107
Н	-6, 7260	-1.1498	0.2888
H	-6 4710	0 2996	1 2980
и	-6 7795	0.4705	-0 /603
	5 4977	4 7101	0. 1000
U	-5.43//	4. (101	0.0315
H	-5.4986	5.8022	0. (414
Н	-6.1298	4. 3943	-0.1566
Н	$-5.71\overline{82}$	4.2414	1.5797
0	-4.0885	4. 4395	0.2873
С	-2, 5988	-3.3002	-2.5841
0 0	-3 0726	-2 4513	-3 2960
С С	_3 9767	_1 5605	_9 1101
U 11	J. 2101 4 174E	4.0000	2.1101
П	-4.1/45	-4. (303	-2. (123
H	-2.6006	-5. 4178	-2.1795
11	2 5519	4 4105	1 0671

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

atom	Λ	1	L
C	-4 4877	2 4165	-0 5475
C	2 4042	2,1100	0.0017
U .	-3. 4945	3.3002	-0.3647
C	-2.2064	3.0185	0.0112
С	-1.9049	1,6804	0.2481
	-2 8796	0.6758	0.0838
0	4 1957	1.0672	0.0000
L L	-4. 1857	1.0073	-0.3181
С	-0.4875	1.3233	0.6458
C	-0 4010	0 0447	1 4461
C	1 2659	0.0695	1. 1101
U	-1. 3052	-0.9685	1.2047
С	-2.5305	-0.7465	0.3510
С	0,6772	-0.1533	2,3096
C	0.8685	_1 2677	2 0760
0	0.0005	1.3011	2.5700
C	-0.0855	-2.3722	2.7995
С	-1.1812	-2.1743	1.9679
C	0 4875	1 3234	-0 6459
<u>C</u>	1.0040	1.0201	0.0105
L	1.9049	1.6804	-0.2481
С	2.8795	0.6758	-0. 0838
С	2, 5304	-0.7464	-0.3511
C .	1 2652	-0.0685	_1 2648
0	1.3032	0.3003	1.2040
С	0.4010	0.0447	-1.4462
С	1.1812	-2.1743	-1.9680
C	0.0856	-9 3791	-2 7006
0	0.0000	1.0070	2.1550
L	-0.8685	-1.30/6	-2.9761
C	-0.6771	-0.1532	-2. 3097
C	2 2063	3 0185	-0 0111
<u> </u>	2 1012	2 2000	0.0010
U	3.4343	3.3004	0.3048
<u> </u>	4.4877	2.4165	0.5476
С	4.1856	1.0673	0.3181
0	-3 1681	-1 6819	-0 1233
0	9 1600	1 2010	0.1400
0	3. 1080	-1.0819	0.1233
С	2.1029	-1.5972	3.8107
С	-2.1029	-1.5971	-3.8109
0	-5 1169	0.0030	-0.4442
0	5.1109	0.0939	0.4442
0	-2. 0357	-3.2581	1.8193
0	5.1168	0.0939	0.4442
0	2 0357	-3 2580	-1 8194
0	2.0551	0.1101	0.7001
U	-6.4600	0.4484	-0.7291
С	6.4600	0.4484	0.7292
Н	-0 1087	2 1429	1 2654
Ш	0.1007	2 1420	1 2654
H	0.1087	2.1429	-1.2054
Н	6. 5539	0.9266	1.7134
Н	5, 4863	2,7029	0.8432
Ц	-6 5539	0.9266	-1 7134
11	0.3339	0.9200	1. (154
Н	-5.4863	2.7029	-0.8431
Н	-1.4598	3.7960	0.1413
Н	1 4022	0 6444	2 4437
11	0.0114	2, 2000	2.1101
H	0.0114	-3. 3290	3. 3035
Н	-0.0114	-3. 3289	-3. 3037
Н	-1.4021	0.6445	-2.4438
Н	1 4598	3 7960	-0 1413
	2 2450	0.7190	4 4105
П	2. 5459	-0.7189	4.4195
Н	2.9610	-1.7905	3.1536
Н	1.9872	-2.4567	4.4783
Н	-2.9610	-1 7903	-3 1538
	_1 0071	_9 4566	_1 1705
П	1. 30/1	2.4000	4.4100
Н	-2.3458	-0.7188	-4. 4197
Н	-7.0145	-0.4913	-0.7327
Н	-6 8755	1 1131	0 0396
II	7 0145	_0 /019	0 7220
П	1.0140	0.4913	0.1328
<u> </u>	6.8754	1.1131	-0.0395
С	3.3330	-3.1520	-2.2579
C	-3 3330	-3 1521	2 2579
	A 1964	_1 9101	_1 7500
	4.1304	-4. 3191	-1. 7509
Н	4.3316	-4.1495	-0. 6865
Н	3.5774	-5.2541	-1.8469
Н	5 0809	-4 3786	-2 2933
C	_/ 1969	_4 2104	1 7519
U	4. 1000	4. 0134	1.1012
Н	-4.3324	-4.1494	0.6869
Н	-3.5770	-5.2542	1.8463
Н	-5.0804	-4.3793	2. 2942
0	2 7252	_9 9464	_2 0425
0	3. (303	2.2404	2. 9430
0	<u>-3.735</u> 3	-2.2465	2.9435
0	3.6931	4.7196	0.5826
0	-3 6931	4 7196	-0 5825
	_1 0051	E 1705	_0 0620
U	4. 9001	0.1700	0. 9020
<u> </u>	-5.2921	4.7478	-1.9274
Н	-5.7371	4.9239	-0.2015
Н	-4 9064	6 2552	-1 0529
	4.0050	E 1705	0.0000
Ļ.	4.9850	0.1(05	0.9622
Н	5.2921	4.7477	1.9276
Н	5, 7370	4, 9239	0.2017
H	4 9064	6 2552	1 0531
	1. 0001	0.2002	1.0001

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

atom	Λ	I	L
C	-0 4364	-1 7789	3 0632
0	0.4304	1. 1103	0.0004
C	-1.2576	-0.6505	<u>3. 1265</u>
C	-0.9524	0 4885	2 3737
C	0.10021	0. 1000	1 5507
L	0.1668	0.4991	1.5507
С	1.0307	-0.6175	1.4789
C	0 7023	-1 7671	2 2462
0	0.1023	1.1011	2.2402
C	0.4250	1.7120	0.6864
С	1.8947	1,9314	0.4066
Č	0 7000	0.9499	0 2005
C	2.1022	0.0433	0.3895
С	2.2778	-0.5430	0.6769
С	2 3490	3 2227	0 1163
<u>C</u>	2.0100	0.1201	0.1000
U	3.0837	3.4700	-0.1936
С	4.5727	2.3930	-0.2088
C	4 1313	1 1083	0 0747
C	0 4950	1.7190	0.0111
U	-0.4250	1.7120	-0. 6866
С	-0. 1668	0.4990	-1.5507
C	-1 0308	-0.6175	-1 4789
C	2 9779	0.5420	0.6760
t	-2.2110	-0. 3430	-0.0709
С	-2.7822	0.8433	-0. 3895
C	-1 8947	1 9315	-0 4067
C	4 1919	1 1000	0. 0747
t	-4.1515	1.1065	-0.0747
С	-4.5726	2.3930	0.2088
C	-3 6856	3 4766	0 1935
C	0.0000	2,0000	0.1355
L	-2. 3489	3. 2228	-0.1105
С	0.9524	0.4884	-2.3738
ſ	1 2576	-0 6506	-3 1266
<u> </u>	0.4000	1 7701	0.1400
L	0.4363	-1. ( (91	-3.0632
С	$-0.70\overline{23}$	-1.7672	-2.2461
0	2 8961	-1 5330	0 2994
0	2.0301	1.0000	0.4334
0	-2.8961	-1.5330	-0. 2993
С	4.1769	4.8749	-0. 4806
C	-4 1768	4 8750	0 4804
C	4.1700	4.0150	0.4004
0	1.5427	-2.8253	2.1766
0	5.0778	0.0997	-0.0367
0	-1 5428	-2 8254	-2 1765
0	1. 5420	2.0234	2.1705
0	-5.0777	0.0998	0.0369
С	1.2987	-3.9608	2.9895
C	-1 2088	-3 9609	-2 0803
0	1.2300	5. 5005	2. 3033
Н	0.0528	2.5932	1.2204
Н	-0.0527	2.5931	-1.2206
Н	-0.3457	-4 4435	-2 7355
	0.6742	0 6570	2.1000
H	0.0743	-2.0078	-3. 6440
Н	0.3457	-4.4434	2.7357
Н	-0.6744	-2 6577	3 6441
	1 6120	1 2440	0.0111
H	-1.6139	1. 3448	2.4382
Н	1.6422	4.0503	0.1393
Н	5 6246	2 5358	-0 4388
II	5. 6246	2.5555	0.4299
H	-5.6246	2. 5559	0.4388
Н	-1.6421	4.0503	-0. 1396
Н	1.6139	1.3447	-2,4384
Ŭ	2 2461	5 5933	-0 5554
11	5.5401	0.0000	1 4100
Н	4. 7412	4.9145	-1.4198
Н	4.8473	5.2296	0.3125
Н	-4 7408	4 9147	1 4198
11	4.0475	5,0000	0.0105
H	-4.8475	5.2296	-0.3125
Н	-3. 3460	5.5834	0.5548
Н	2.1178	-4.6506	2.7794
Ц	1 30/17	-3 7040	4 0572
11	0 1170	4 0507	0.7700
Н	-2.1179	-4. 0507	-2. (192
Н	-1.3047	-3. 7051	-4.0571
C	-5 4212	-0.6163	-1 0857
Č	E 4010	0.6169	1 0050
L	<b>D.</b> 4212	-0.0103	1.0859
C	-6. 2169	-1.8302	-0.6900
Н	-5, 5169	-2,5602	-0.2692
	_6 05/5	_1 5950	0.0702
П	0.9040	1, 0000	0.0192
Н	-6.7048	-2.2528	-1.5693
С	0.01 51	_1 9201	0.6902
Н	6.2171	1.0301	
	<u>6.2171</u> 5.5177	-2 5592	0 2671
11	6.2171 5.5177	-2. 5592	0.2671
H	6.2171 5.5177 6.9564	-2. 5592 -1. 5842	0.2671 -0.0772
H H	6.2171 5.5177 6.9564 6.7031	-2. 5592 -1. 5842 -2. 2539	0.2671 -0.0772 1.5700
H H 0	$\begin{array}{r} 6.2171 \\ \hline 5.5177 \\ \hline 6.9564 \\ \hline 6.7031 \\ \hline -5.1142 \end{array}$	$ \begin{array}{r}     1.6301 \\     -2.5592 \\     -1.5842 \\     -2.2539 \\     -0.2902 \end{array} $	$\begin{array}{r} 0.2671 \\ -0.0772 \\ 1.5700 \\ -2.2039 \end{array}$
H H 0	$\begin{array}{r} 6.2171 \\ 5.5177 \\ 6.9564 \\ 6.7031 \\ -5.1142 \\ \end{array}$	-2. 5592 -1. 5842 -2. 2539 -0. 2902	0. 2671 -0. 0772 1. 5700 -2. 2039
H H 0 0	$\begin{array}{r} 6.2171 \\ \overline{5.5177} \\ 6.9564 \\ \overline{6.7031} \\ -\overline{5.1142} \\ \overline{5.1142} \end{array}$	$\begin{array}{r} -2.5592 \\ -1.5842 \\ -2.2539 \\ -0.2902 \\ -0.2901 \end{array}$	$\begin{array}{r} 0.\ 2671 \\ -0.\ 0772 \\ 1.\ 5700 \\ -2.\ 2039 \\ 2.\ 2041 \end{array}$
H H 0 0 0	$\begin{array}{r} 6.2171 \\ \overline{5.5177} \\ 6.9564 \\ \overline{6.7031} \\ -\overline{5.1142} \\ \overline{5.1142} \\ 2.3724 \end{array}$	$\begin{array}{r} 1.3301 \\ -2.5592 \\ -1.5842 \\ -2.2539 \\ -0.2902 \\ -0.2901 \\ -0.5636 \end{array}$	0.2671 -0.0772 1.5700 -2.2039 2.2041 -3.8982
H H 0 0 0 0	$\begin{array}{r} 6.2171 \\ \overline{5.5177} \\ 6.9564 \\ \overline{6.7031} \\ -\overline{5.1142} \\ \overline{5.1142} \\ 2.3724 \\ -2.3725 \end{array}$	$\begin{array}{r} 1.3301 \\ -2.5592 \\ -1.5842 \\ -2.2539 \\ -0.2902 \\ -0.2901 \\ -0.5636 \\ -0.5634 \end{array}$	0.2671 -0.0772 1.5700 -2.2039 2.2041 -3.8982 3.8981
H H 0 0 0 0 0 0	$\begin{array}{r} 6.2171 \\ \overline{5.5177} \\ 6.9564 \\ 6.7031 \\ -\overline{5.1142} \\ \overline{5.1142} \\ 2.3724 \\ -\overline{2.3725} \\ -\overline{2.3725} \\ -\overline{2.3725} \end{array}$	$\begin{array}{r} 1.3301 \\ -2.5592 \\ -1.5842 \\ -2.2539 \\ -0.2902 \\ -0.2901 \\ -0.5636 \\ -0.5634 \\ -1.5634 \end{array}$	0. 2671 -0. 0772 1. 5700 -2. 2039 2. 2041 -3. 8982 3. 8981 4. 6205
H H 0 0 0 0 0 C	$\begin{array}{r} 6.2171 \\ \overline{5.5177} \\ 6.9564 \\ \overline{6.7031} \\ -\overline{5.1142} \\ \overline{5.1142} \\ 2.3724 \\ -\overline{2.3725} \\ -\overline{2.7879} \\ -\overline{2.7879} \\ -\overline{2.7879} \\ \end{array}$	$\begin{array}{c} -2.5592 \\ -1.5842 \\ -2.2539 \\ -0.2902 \\ -0.2901 \\ -0.5636 \\ -0.5634 \\ -1.7066 \\ -1.7066 \end{array}$	$\begin{array}{r} 0.2671 \\ -0.0772 \\ 1.5700 \\ -2.2039 \\ 2.2041 \\ -3.8982 \\ 3.8981 \\ 4.6305 \\ 6.655 \end{array}$
H H 0 0 0 0 C H	$\begin{array}{r} 6.2171 \\ \overline{5.5177} \\ 6.9564 \\ 6.7031 \\ -5.1142 \\ \overline{5.1142} \\ 2.3724 \\ -2.3725 \\ -2.7879 \\ -2.9869 \end{array}$	$\begin{array}{r} 1.3301 \\ -2.5592 \\ -1.5842 \\ -2.2539 \\ -0.2902 \\ -0.2901 \\ -0.5636 \\ -0.5634 \\ -1.7066 \\ -2.5564 \end{array}$	$\begin{array}{r} 0.2671 \\ -0.0772 \\ 1.5700 \\ -2.2039 \\ 2.2041 \\ -3.8982 \\ 3.8981 \\ 4.6305 \\ 3.9656 \end{array}$
н Н О О О С Н Н	$\begin{array}{r} 6.2171 \\ \overline{5.5177} \\ 6.9564 \\ 6.7031 \\ -5.1142 \\ \overline{5.1142} \\ 2.3724 \\ -2.3725 \\ -2.7879 \\ -2.9869 \\ -2.0421 \end{array}$	$\begin{array}{r} 1.3301 \\ -2.5592 \\ -1.5842 \\ -2.2539 \\ -0.2902 \\ -0.2901 \\ -0.5636 \\ -0.5634 \\ -1.7066 \\ -2.5564 \\ -1.9971 \end{array}$	$\begin{array}{r} 0.2671 \\ -0.0772 \\ 1.5700 \\ -2.2039 \\ 2.2041 \\ -3.8982 \\ 3.8981 \\ 4.6305 \\ 3.9656 \\ 5.3822 \end{array}$
H H O O O C H H H	$\begin{array}{r} 6.2171\\ \overline{5.5177}\\ 6.9564\\ \overline{6.7031}\\ -5.1142\\ \overline{5.1142}\\ 2.3724\\ -2.3725\\ -2.7879\\ -2.9869\\ -2.0421\\ 2.7117\end{array}$	$\begin{array}{r} 1.3301 \\ -2.5592 \\ -1.5842 \\ -2.2539 \\ -0.2902 \\ -0.2901 \\ -0.5636 \\ -0.5634 \\ -1.7066 \\ -2.5564 \\ -1.9971 \\ 1.4170 \end{array}$	$\begin{array}{r} 0.2671 \\ -0.0772 \\ 1.5700 \\ -2.2039 \\ 2.2041 \\ -3.8982 \\ 3.8981 \\ 4.6305 \\ 3.9656 \\ 5.3822 \\ 5.1241 \end{array}$
н H 0 0 0 0 0 С H H H H	$\begin{array}{r} 6.2171 \\ \overline{5.5177} \\ 6.9564 \\ 6.7031 \\ \hline -5.1142 \\ \overline{5.1142} \\ 2.3724 \\ \hline -2.3725 \\ \hline -2.7879 \\ \hline -2.9869 \\ \hline -2.0421 \\ \hline -3.7117 \\$	$\begin{array}{r} 1.3301 \\ -2.5592 \\ -1.5842 \\ -2.2539 \\ -0.2902 \\ -0.2901 \\ -0.5636 \\ -0.5634 \\ -1.7066 \\ -2.5564 \\ -1.9971 \\ -1.4170 \\ -1.4170 \\ \end{array}$	$\begin{array}{r} 0.2671 \\ -0.0772 \\ 1.5700 \\ -2.2039 \\ 2.2041 \\ -3.8982 \\ 3.8981 \\ 4.6305 \\ 3.9656 \\ 5.3822 \\ 5.1341 \\ 5.1341 \end{array}$
н H 0 0 0 0 С H H H H C	$\begin{array}{r} 6.2171\\ \overline{5.5177}\\ 6.9564\\ 6.7031\\ -5.1142\\ \overline{5.1142}\\ 2.3724\\ -2.3725\\ -2.7879\\ -2.9869\\ -2.0421\\ -3.7117\\ 2.7878\\ \end{array}$	$\begin{array}{c} -2.5592 \\ -1.5842 \\ -2.2539 \\ -0.2902 \\ -0.2901 \\ -0.5636 \\ -0.5634 \\ -1.7066 \\ -2.5564 \\ -1.9971 \\ -1.4170 \\ -1.7068 \end{array}$	$\begin{array}{r} 0.2671 \\ -0.0772 \\ 1.5700 \\ -2.2039 \\ 2.2041 \\ -3.8982 \\ 3.8981 \\ 4.6305 \\ 3.9656 \\ 5.3822 \\ 5.1341 \\ -4.6305 \end{array}$
н H 0 0 0 0 С H H H H H H H H H H	$\begin{array}{r} 6.2171\\ \overline{5.5177}\\ 6.9564\\ 6.7031\\ -5.1142\\ \overline{5.1142}\\ 2.3724\\ -2.3725\\ -2.7879\\ -2.9869\\ -2.0421\\ -3.7117\\ 2.7878\\ 2.9869\end{array}$	$\begin{array}{r} 1.3301 \\ -2.5592 \\ -1.5842 \\ -2.2539 \\ -0.2902 \\ -0.2901 \\ -0.5636 \\ -0.5634 \\ -1.7066 \\ -2.5564 \\ -1.9971 \\ -1.4170 \\ -1.7068 \\ -2.5566 \end{array}$	$\begin{array}{r} 0.2671 \\ -0.0772 \\ 1.5700 \\ -2.2039 \\ 2.2041 \\ -3.8982 \\ 3.8981 \\ 4.6305 \\ 3.9656 \\ 5.3822 \\ 5.1341 \\ -4.6305 \\ -3.9656 \end{array}$
н H 0 0 0 0 С H H H C H H H	$\begin{array}{r} 6.2171 \\ \overline{5.5177} \\ 6.9564 \\ \overline{6.7031} \\ -5.1142 \\ \overline{5.1142} \\ 2.3724 \\ -2.3725 \\ -2.7879 \\ -2.9869 \\ -2.0421 \\ -3.7117 \\ 2.7878 \\ 2.9869 \\ -2.0421 \\ \end{array}$	$\begin{array}{c} 1.3301 \\ -2.5592 \\ -1.5842 \\ -2.2539 \\ -0.2902 \\ -0.2901 \\ -0.5636 \\ -0.5634 \\ -1.7066 \\ -2.5564 \\ -1.9971 \\ -1.4170 \\ -1.7068 \\ -2.5566 \\ 1.0074 \end{array}$	$\begin{array}{r} 0.2671 \\ -0.0772 \\ 1.5700 \\ -2.2039 \\ 2.2041 \\ -3.8982 \\ 3.8981 \\ 4.6305 \\ 3.9656 \\ 5.3822 \\ 5.1341 \\ -4.6305 \\ -3.9656 \\ -3.9656 \\ -3.9656 \\ -3.9656 \\ -3.9656 \\ -3.9656 \\ -3.9656 \\ -3.9656 \\ -3.9656 \\ -5.3922 \\ -3.9656 \\ -3.9656 \\ -5.3922 \\ -5.3922 \\ -5.392 \\ -5.3922 $
н H 0 0 0 0 0 0 0 0 0 0 0 0 0	$\begin{array}{r} 6.2171\\ \overline{5.5177}\\ 6.9564\\ \overline{6.7031}\\ -5.1142\\ \overline{5.1142}\\ 2.3724\\ -2.3725\\ -2.7879\\ -2.9869\\ -2.0421\\ -3.7117\\ 2.7878\\ 2.9869\\ 2.0420\\ \overline{5.555}\\ -5.55\\ -5.5$	$\begin{array}{c} 1.3301 \\ -2.5592 \\ -1.5842 \\ -2.2539 \\ -0.2902 \\ -0.2901 \\ -0.5636 \\ -0.5634 \\ -1.7066 \\ -2.5564 \\ -1.9971 \\ -1.4170 \\ -1.7068 \\ -2.5566 \\ -1.9974 \\ -1.9974 \\ -1.975 \end{array}$	$\begin{array}{r} 0.2671 \\ -0.0772 \\ 1.5700 \\ -2.2039 \\ 2.2041 \\ -3.8982 \\ 3.8981 \\ 4.6305 \\ 3.9656 \\ 5.3822 \\ 5.1341 \\ -4.6305 \\ -3.9656 \\ -5.3822 \\ -5.3822 \\ -5.1341 \\ -4.6305 \\ -5.3822 \\ -5.382 \\ -5.3$

Cartesian coordin	nates of 3,3'-dicar	boxyl-1,1',8,8'-ter	trahydroxybianthr	one-I optimized at the gas-phase
B3LYP/6-31	G(d) level			
	17	77	7	

atom	X	Y	Z
С	-0.3147	-0.6705	2.2275
С	0.4865	-0.0042	1.2716
С	1.6211	-0. 6269	0.7701
С	1.9690	-1.9188	1.1981
С	1.1821	-2.5997	2.1204
С	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 7426	0.2692	-0.7084
C	1.6205	1.0662	-0.7084
C	-1.0293	1.0544	-1.1043
C	-2.7330	-1.9344	-1.0225
C	-3. 9328	-1.4874	-0.4015
C	-4. 0299	-0. 1089	-0. 0424
C	-2.9430	0.7082	-0. 1574
C C	-0.5513	1. 1982	-0. 7485
<u> </u>	0.4873	0.8178	-1.7782
<u> </u>	0.6078	-0.5302	-2. 1996
C	-0.4079	-1.5179	-1.8264
<u> </u>	1.3556	1.7750	-2.2846
C	2. 3763	1. 4055	-3. 1779
C	2. 5399	0.0817	-3.5671
C O	1.6581	-0.8982	-3.0868
0	-2.2313	-0. 6160	3. 0152
0	-0.2079	-2. 7303	-2. 1539
П	-0. 9105	2.2037	-0. 9802
П	0.9938	1. 9338	0.0707
0	-3. 3731	1. 3923	4. 2938
0	-0. 6909	-2.0832	3. 3273
0	1. 8440	-2.1000	-3. 5105
0	-2.0001	-3. 2300	-1.4102
Н	-3. 1995	0.0177	4. 2017
П	-1.4062	-2.1195	3.1121
П	1. 1394	-2.7107	-3. 0904
11	2, 2600	0 1226	
<u>П</u>	1 4224	-2 5008	2 4500
 Ц	_2 2110	<i>J. JJJ</i>	2.4303
Ш	-1. 2021	5 2140	2 2514
П	-1.0021 -0.2207	0. 5149	2. 5514
 Ц	-0.2307	-2 1707	-0.2727
 Ц	-2 0297	1 7261	0.1922
<u>П</u>	1 2656	2 9194	-2 0072
 Ц	2 2070	_0 2165	_1 2478
	2 2050	-0.2105	-4.2470
0	2 0227	-2.0220	-0.10214
0	3. 2441	-2 7624	1 0075
<u>U</u>	J. 4032 1 9005	-3. (034	1.0970
П	4. 2000 2. 0710	-4.0000	<u> </u>
	3.2/12	2.4894	-3.0800
U 11	4. 2312	2. U38U	-4. 5218
П	4. (522	2.8210	-4. 1119
U	3. 10/8	J. 0000	-3. 3//3
П	-4.9041	0.1093	0.3010

Cartesian coordinates of 3,3'	-dicarboxyl-1,1',8,8	-tetrahydroxybian	throne-II optim	mized at the g	as-phase
B3LYP/6-31G(d) level	-		-	-	-

atom	Х	Y	Z
С	2.1231	-0.1090	1.1339
С	1.5748	1.1175	0.6925
С	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	0.9901
C	1.9704	-0.3462	1 7010
C	1.2704		1. 7910
C	-0.0875	-0.7333	2.1758
<u> </u>	-0.6371	0.5102	1.7691
C	0.0809	1. 3535	0.7405
С	-0. 8223	-1.5690	3.0660
С	-2.0620	-1.1362	3. 5618
С	-2.5592	0. 1002	3. 1848
С	-1.8577	0.9238	2.2909
С	-1.8760	1.9243	-0.8249
С	-3. 0933	1.2047	-0.7796
С	-4. 3288	1.9146	-0.7493
С	-4.3249	3. 3165	-0.7961
С	-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	-2 0801	-0.2558	-0. 8106
C	-3.0691	-0.2008	-0.8190
C	0. 5258		-1.0047
C	0.4841	-2.2506	-1.9932
<u> </u>	-0.6927	-2.9800	-1.8753
C	-1.8647	-2.3430	-1.4404
0	1.7414	-2. 2368	2.0975
0	-4.1665	-0. 9030	-0.6892
H	0.1608	1. 7292	-1.3881
Н	-0. 0836	2.4084	0.9816
0	-0.3722	-2.7623	3.4759
0	4.1012	-1.4926	1.3687
0	-2.9775	-3.0851	-1.3661
0	-5.5160	1.2961	-0.6814
Н	0.5085	-2.9054	3.0448
Н	3. 3825	-2.0838	1.7095
Н	-3. 7049	-2.4871	-1.0569
Н	-5.3343	0.3225	-0.6444
Н	2,0139	3, 0435	-0, 1822
Н	5, 4020	0. 4488	0. 3436
Н	-2.5974	-1 7866	4 2453
Н	-3 5109	0.4382	3 5856
Н	-2 2708	1 8856	2 0068
Ш	_5 2782	2 9242	_0 7814
	0.0650	2 9705	0.0204
П	-0.9039	0.2575	-0.9204
П	1.4001		-1.7000
H	-0.7351	-4.0331	-2.1247
C	4.6197	2.9468	-0. 5493
0	4. 1845	4.0156	-0. 9283
0	5.9346	2.6325	-0. 6189
Н	6. 3749	3. 4077	-1.0142
С	1.7514	-2.8747	-2.4752
0	1.6189	$-4.19\overline{14}$	$-2.76\overline{29}$
Н	2. 4989	-4. 4903	-3.0586
0	2.8034	-2.2823	-2.6029
Н	-3.1248	5.0865	-0. 9099

Г

atom	Λ	Ĭ	L
С	0.3511	1.8389	-0.6971
С	-0.4938	1,4577	0.3753
<u>C</u>	-1 8643	1 6541	0.2718
<u> </u>	-2 4175	2 1894	-0.9043
<u> </u>	1 6102	2.1034	1 0042
<u> </u>	-1.0102	2. 3203	-1.9043
<u> </u>	-0. 2204	2.3587	-1.8923
<u> </u>	1.8082	1.8192	-0.5373
С	2.3747	1. 5737	0. 7858
С	1.5429	1.1614	1.8543
С	0.0931	0.8067	1.6064
С	3.7614	1.8044	1.0227
С	4.2793	1.6505	2.3174
С	3. 4419	1.2672	3.3531
С	2.0805	1.0183	3. 1285
С	0.4938	-1.4577	0.3751
C	-0.3511	-1 8388	-0.6973
<u> </u>	0.3011	-2 3585	-1 8925
<u> </u>	1 6102	2.5360	1.0925
<u> </u>	1.0102	-2. 3200	-1. 9645
<u> </u>	2.4175	-2. 1892	-0.9045
<u> </u>	1.8643	-1.6540	0.2717
С	-0.0932	-0. 8069	1.6063
С	-1.5430	-1.1616	1.8542
С	-2.3747	-1.5739	0.7856
С	-1.8082	-1.8192	-0. 5375
С	-2.0806	-1.0187	3.1284
С	-3, 4420	-1.2676	3, 3530
C	-4 2793	-1 6508	2 3172
<u> </u>	-3 7614	-1.8047	1 0225
0	2 5597	2,0006	-1.5147
0	2. 3367	2.0990	1.5147
0	-2. 5587	-2.0996	-1. 5149
H	0.4868	-1.1314	2.4762
H	-0. 4869	1. 1312	2.4763
0	4.6066	2. 1804	0.0545
0	0. 5151	2.7215	-2.9518
0	-4.6066	-2. 1806	0.0542
0	-0.5150	-2.7213	-2.9521
Н	4.0852	2.2235	-0.7867
Н	1.4634	2.5523	-2.7177
Н	-4.0852	-2.2236	-0. 7869
Н	-1.4633	-2.5521	-2.7180
Н	-2, 5306	1, 4036	1.0884
H	-2, 0256	2, 9321	-2,8985
н Н	5 3364	1 8365	2 4734
 Ц	2 2/72	1 1568	4 3551
11 U	J. 0410 1 //9/	0 7121	2 0546
<u>П</u>	1.4434	0. (131	J. 7040
H	2.0256	-2. 9318	-2. 8987
H	2.5306	-1.4036	1.0883
H	-1.4435	-0. 7134	3.9545
Н	-3.8479	-1.1573	4. 3549
Н	-5.3365	-1.8369	2.4731
С	-3.8975	2.3771	-0.9417
С	3.8976	-2.3768	-0.9419
0	-4.6466	2. 1218	-0.0210
0	4, 6466	-2, 1215	-0.0212
0	-4 3402	2 8701	-2 1230
<u> </u>	-5 2004	2.0101	-2 02/2
0	1 2402	2. 3404 _9 0607	
U 11	4. 3403	-2.0091	-2.1233
Н	5.3084	-2.9460	-2.0345

Cartesian	coordinates	of	3,3'-0	licarboxyl-1,1',8,	8'-tetrahydroxybia	inthrone-III	optimized	at	the	gas-phase
B3LY	P/6-31G(d) 1	evel		·						
1		V		V	7					

atom	X	Y	Z
С	-2.7887	-0.2082	-0.5690
С	-1,8649	0.8594	-0.4973
C C	-2.3075	2 1328	-0.1635
C	-3 6653	2.1020	0.1100
C	J. 0033	2.3009	0.1129
C C	-4. 5803	1. 3189	0.0693
C	-4. 1594	0.0261	-0.2660
C	-2.3501	-1.5375	-1.0098
С	-1.0139	-1.6928	-1.5728
С	-0.0885	-0.6171	-1.5401
С	-0.3879	0.6128	-0.7141
С	-0.6769	-2.8898	-2.2694
С	0.5480	-2.9774	-2.9486
С	1.4164	-1.8986	-2.9406
C	1 1080	-0.7222	-2,2400
C	1 8649	0.8594	0.4974
C	1.0045	0.0004	0. 5600
C	2.1001	-0.2062	0.0090
	4. 1594	0.0201	0.2000
C	4. 5863	1.3190	-0.0693
C	3.6652	2.3610	-0.1129
С	2.3075	2.1328	0.1635
С	0.3879	0.6127	0.7141
С	0.0885	-0.6172	1.5401
С	1.0139	-1.6928	1.5728
С	2.3501	-1.5375	1.0098
С	-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	2.0100
0	-3 1576	-2 5092	-0.9823
0	2 1576	2.5092	0. 9023
0	3. 1370	-2. 3092	0.9023
П	-0.0240	1.4000	1. 2303
H	0.0240	1. 4858	-1.2303
0	-1.4944	-3. 9494	-2.3250
0	-5. 0835	-0. 9443	-0.2889
0	1. 4944	-3.9495	2.3249
0	5.0835	-0.9443	0.2889
Н	-2.3076	-3.7181	-1.8087
Н	-4. 6139	-1.7841	-0. 5290
Н	2.3077	-3.7181	1.8086
Н	4.6139	-1.7841	0.5290
Н	-1.6212	2.9721	-0.1131
Н	-5, 6349	1, 4810	0. 2868
Н	0 7779	-3 8956	-3 4780
Ц	2 3550	-1 06/1	-3 4949
П	1 0070	-1.3041	-0.4044 -0.9465
П	1.0070	0.1072	-2.2400
H	5.6348	1. 4810	-0.2868
H	1.6211	2.9722	0.1131
Н	-1.8070	0.1071	2.2466
Н	-2.3550	-1.9641	3. 4842
Н	-0.7772	-3.8956	3.4788
С	-4. 0729	3.7551	0.4559
С	4.0728	3.7552	-0. 4558
0	-3.3110	4.6982	0.5193
0	3.3110	4. 6982	-0.5194
0	-5 4003	3 8755	0 6975
Н	-5 5495	4 8160	0 9079
0	5 /009	3 8755	-0 6075
U 11	5.5404	J. 0100 A Q161	
П	0.0494	4.0101	-0. 9060

Cartesian	coordinates	of	3,3'-d	icarboxyl-1,1',8,8	3'-tetrahydroxybia	inthrone-IV	optimized	at	the	gas-phase
B3LYI	P/6-31G(d) le	evel								
a <b>t</b> a m		v		V	7					

Cartesian coordi	nates of 9-I optimi	ized at the gas-pha	se B3LYP/6-31G	(d) level
	V	V	7	

atom	λ	Ĭ	L
C	0 5984	0.3656	1 0726
0	0. 3364	0.3030	1. 5720
С	-0.2619	-0.6633	1.5081
C	-1 5202	_0 9121	2 0722
U	-1. 5202	-0. 8131	2.0122
С	-1.9884	0.0707	3.0667
C	1 1655	1 1007	2 4000
U	-1. 1655	1.1027	3. 4988
С	0 1244	1 2624	2 9713
0	0.1211	1.2024	2.5115
С	1. 9818	0.4417	1. 5229
C	2 5202	-0.6402	0 7119
L L	2. 3292	-0.0492	0.7112
С	1.6715	-1.6631	0.2144
C	0 1710	1 5440	0.0505
U	0.1712	-1.5440	0.3585
ſ	3 9247	-0.7141	0 4777
0	0.0211	0.1111	0. 1111
С	4.4641	-1.8180	-0. 2338
C	2 6105	_9 9149	-0.6010
L L	5.0105	-2.0142	-0. 0919
С	2,2259	-2.7317	-0.4723
 	1 0571	1 4411	1 0700
U	-1.9571	-1.4411	-1.0762
ſ	-2 9369	-0.4510	-0.8347
0	2.0000	0.4510	0.0011
С	-4. 3003	-0.8418	-0.7202
C	4 6570	2 1960	0 0001
U	-4.0370	-2. 1800	-0. 8921
С	-3 6929	-3 1512	-1 1678
<u>C</u>	0.0020	0.1012	1.1010
C	-2.3415	-2.7659	-1.2458
C	-0.4886	-1 0788	-1 0547
0	0.4000	1.0100	1.0517
С	-0.2170	0.3715	-1.3758
C	_1 9064	1 2500	_1 1110
U	-1.2004	1. 5569	-1.1119
С	-2.5642	0.9596	-0.7483
0	1,0000	0.7700	1 0707
C	1.0090	0.7736	-1.8787
С	1 2939	2 1334	-2,0945
0	1.2000	2.1001	1.0010
С	0.3570	3.1153	-1.8040
C	-0.0170	9 7391	-1 3083
U	0. 5115	2.1321	1. 3003
0	2.7287	1, 3934	1, 8973
0	2 4246	1 0000	0 4456
0	-3. 4340	1. 8282	-0. 4450
Н	0 0252	-1 7030	-1 7930
11	0.0202	1.1000	1.1000
Н	-0.2364	-2.5481	0.5166
C	-3 3800	-0.1016	3 6240
0	5.0000	0.1010	5.0240
С	-4.0880	-4.5895	-1.4002
0	1 7057	0.9109	0.0014
0	4. 7657	0.2198	0.9014
0	0.8704	2. 2668	3, 4530
0	1 7070	2.2000	1,0000
0	-1. 7978	3.7114	-1.0689
0	-5 2801	0 0339	-0 4460
0	5.2001	0.0000	0.1100
H	4.2401	0.9084	1.3644
Ц	1 7308	2 2210	2 0774
11	1.1330	2.2319	2. 5114
H	-2.6217	3.2716	-0. 7355
II	1 0100	0.0250	0 2644
11	4.0490	0. 9230	0.3044
Н	-2.1675	-1.6159	1.7328
II	1 4041	1 9065	4 9572
Н	-1. 4941	1.8005	4.2373
Н	4,0095	-3,6699	-1.2250
TT	1 5050		0.0510
П	1. 2020	-3. 5245	-0.8516
Н	-5.7074	-2.4478	-0.8079
TT	1 5040	2. 110	1 4405
<u>H</u>	-1. 5843	-3. 5227	-1.4405
Н	1 7714	0 0360	-2 1060
77	0.0055	0.0000	2.1000
Н	2.2657	2.4087	-2.4885
Н	-3 5851	0 6141	4 4251
11	5.0004	0.0141	4.4201
H	-4. 1325	0.0422	2.8384
Ц	-3 5231	-1 1130	4 0236
11	5.5251	1.1130	4.0230
Н	-5.0812	-4.8038	-0.9947
TI	_9 9794	_E 9004	_0_0409
п	-3. 3724	-0.2804	-0. 9408
Н	-4.1131	-4.8175	$-2.47\overline{40}$
		4 4500	1 0004
0	0. 5353	4.4533	-1.9624
C	1 7953	4 9022	-2 4338
	0.0000	1. 5022	2.1000
Н	2.0096	4. 5192	-3. 4408
Н	1 7988	5 9908	-2 4685
	1.1200	0.0000	2. 1000
H	2.6072	4.6079	-1. 7554
0	5 8141	-1 7024	-0 4001
0	J. 0141	1. 1934	0.4001
C	6. 4161	-2.8716	-1.0961
II	7 1051	_9 6544	_1 1196
п	(.4004	-2.0344	-1.1130
H	6 2483	-3 8282	-0.5830
H	6.2483	-3.8282	-0.5830

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

C	~	Ŷ	
	2 0260	0 4510	0 9246
0	2.9309	-0.4310	-0. 8340
С	1.9571	-1.4411	-1.0762
C	2 3/15	-2 7650	-1 2458
<u> </u>	2. 3413	2.1035	1.2450
С	3. 6929	-3. 1512	-1.1677
C	4 6570	-2 1860	-0.8921
- C	1.0010	0.0410	0.7000
U	4.3003	-0.8419	-0.7202
С	2.5642	0, 9596	-0.7483
C .	1 2064	1 2500	1 1110
U	1.2004	1. 3369	-1.1119
С	0.2170	0.3715	-1.3758
ſ	0 4886	-1 0789	-1 0546
0	0.4000	1.0105	1.0010
C	0.9180	2.7321	-1.3084
С	-0.3570	3, 1153	-1.8040
C C	1 2020	9 1994	2,0045
U	-1. 2939	2.1334	-2.0943
С	-1.0089	0.7736	-1.8786
ſ	0.2619	-0.6633	1 5081
0	0.2013	0.0000	1.0700
C	-0. 5984	0.3656	1.9726
С	-0 1244	1 2624	2 9713
<u> </u>	1 1655	1 1027	2.0110
U	1.1055	1. 1027	3. 4988
С	1.9884	0.0708	3.0667
<u> </u>	1 5202	-0.8130	2 0722
<u> </u>	1. 5262	0.0130	2.0122
С	-0.1712	-1.5440	0.3586
C	-1 6715	-1 6631	0 2144
- C	1.0110	0.0400	0.7110
C	-2. 5292	-0.6492	0.7112
С	-1.9818	0.4417	1.5229
C C	2 2250	9 7917	0 4799
U C	-2.2239	-2.1311	-0.4723
C	-3.6105	-2.8141	-0.6920
С	-4, 4641	-1.8180	-0.2338
Č	-2,0247	-0.7141	0 4777
<u> </u>	5. 5241	0.7141	0.4777
0	3. 4346	1.8281	-0. 4457
0	-2.7288	1.3935	1.8973
U	0.2264	-2 5480	0 5166
	0.2304	2. 5460	0. 5100
Н	-0. 0252	-1.7030	-1.7930
С	4.0879	-4.5895	-1.4002
ſ	3 3700	-0.1016	3 6240
<u> </u>	1.7070	0.1010	3.0240
0	1. 7978	3.7114	-1.0689
0	5.2801	0.0339	-0.4460
0	-4 7857	0.2100	0.9014
0	4.1001	0.2133	0. 5014
0	-0.8704	2.2668	3.4530
Н	2.6218	3.2716	-0.7355
Ц	1 8108	0.0240	-0.3644
11	4.0430	0. 5245	0.3044
Н	-4. 2401	0.9084	1.3644
Н	-1,7398	2, 2320	2.9774
II	1 5049	2 5997	1 4404
11	1. 3843	-3. 5221	-1.4404
Н	5.7074	-9 4479	
		2. 1113	-0.8079
Н	-2.2656	2.4087	-0.8079 -2.4885
H	-2.2656	2.4087	-0.8079 -2.4885 -2.1060
H H	-2.2656 -1.7714	2. 4087 0. 0360	-0.8079 -2.4885 -2.1060
H H H	$\begin{array}{r} -2.\ 2656 \\ -1.\ 7714 \\ 1.\ 4941 \end{array}$	2. 4087 2. 4087 0. 0360 1. 8065	$ \begin{array}{r} -0.\ 8079 \\ -2.\ 4885 \\ -2.\ 1060 \\ 4.\ 2573 \end{array} $
H H H H	$\begin{array}{r} -2.\ 2656 \\ -1.\ 7714 \\ 1.\ 4941 \\ 2.\ 1675 \end{array}$	$\begin{array}{r} 2.4087 \\ \hline 0.0360 \\ \hline 1.8065 \\ \hline -1.6158 \end{array}$	$\begin{array}{r} -0.8079 \\ -2.4885 \\ -2.1060 \\ 4.2573 \\ 1.7328 \end{array}$
H H H H	$\begin{array}{r} -2.\ 2656 \\ -1.\ 7714 \\ 1.\ 4941 \\ 2.\ 1675 \\ 1.\ 5858 \end{array}$	$\begin{array}{r} 2.4087 \\ \hline 0.0360 \\ \hline 1.8065 \\ \hline -1.6158 \\ 2.5244 \end{array}$	$\begin{array}{r} -0.8079 \\ -2.4885 \\ -2.1060 \\ 4.2573 \\ 1.7328 \\ 0.8516 \end{array}$
H H H H H	$\begin{array}{r} -2.\ 2656 \\ -1.\ 7714 \\ 1.\ 4941 \\ 2.\ 1675 \\ -1.\ 5858 \\ \end{array}$	$\begin{array}{r} 2.4087 \\ \hline 0.0360 \\ \hline 1.8065 \\ \hline -1.6158 \\ \hline -3.5244 \\ \hline 0.0202 \\ \hline \end{array}$	$\begin{array}{r} -0.8079 \\ -2.4885 \\ -2.1060 \\ 4.2573 \\ 1.7328 \\ -0.8516 \\ -0.8516 \end{array}$
H H H H H H	$\begin{array}{r} -2.\ 2656 \\ -1.\ 7714 \\ 1.\ 4941 \\ 2.\ 1675 \\ -1.\ 5858 \\ -4.\ 0095 \end{array}$	$\begin{array}{r} 2.4087 \\ \hline 0.0360 \\ \hline 1.8065 \\ \hline -1.6158 \\ \hline -3.5244 \\ \hline -3.6699 \end{array}$	$\begin{array}{r} -0.\ 8079 \\ -2.\ 4885 \\ -2.\ 1060 \\ 4.\ 2573 \\ 1.\ 7328 \\ -0.\ 8516 \\ -1.\ 2250 \end{array}$
H H H H H H H	$\begin{array}{r} -2.\ 2656 \\ -1.\ 7714 \\ 1.\ 4941 \\ 2.\ 1675 \\ -1.\ 5858 \\ -4.\ 0095 \\ 4.\ 1131 \end{array}$	$\begin{array}{r} 2.4087 \\ \hline 2.4087 \\ \hline 0.0360 \\ \hline 1.8065 \\ \hline -1.6158 \\ \hline -3.5244 \\ \hline -3.6699 \\ \hline -4.8175 \end{array}$	$\begin{array}{r} -0.\ 8079 \\ -2.\ 4885 \\ -2.\ 1060 \\ 4.\ 2573 \\ 1.\ 7328 \\ -0.\ 8516 \\ -1.\ 2250 \\ -2.\ 4740 \end{array}$
H H H H H H H	$\begin{array}{r} -2.\ 2656 \\ -1.\ 7714 \\ 1.\ 4941 \\ 2.\ 1675 \\ -1.\ 5858 \\ -4.\ 0095 \\ 4.\ 1131 \\ 5.\ 0812 \end{array}$	$\begin{array}{c} 2.4087\\ \hline 0.0360\\ \hline 1.8065\\ \hline -1.6158\\ \hline -3.5244\\ \hline -3.6699\\ \hline -4.8175\\ \hline -4.8039\end{array}$	$\begin{array}{r} -0.8079 \\ -2.4885 \\ -2.1060 \\ 4.2573 \\ 1.7328 \\ -0.8516 \\ -1.2250 \\ -2.4740 \\ -0.9946 \end{array}$
H H H H H H H H	$\begin{array}{r} -2.\ 2656 \\ -1.\ 7714 \\ 1.\ 4941 \\ 2.\ 1675 \\ -1.\ 5858 \\ -4.\ 0095 \\ 4.\ 1131 \\ 5.\ 0812 \\ 2.\ 2702 \end{array}$	$\begin{array}{r} 2.4087\\ \hline 0.0360\\ \hline 1.8065\\ \hline -1.6158\\ \hline -3.5244\\ \hline -3.6699\\ \hline -4.8175\\ \hline -4.8039\\ \hline 5.8004\end{array}$	$\begin{array}{r} -0.\ 8079 \\ -2.\ 4885 \\ -2.\ 1060 \\ 4.\ 2573 \\ 1.\ 7328 \\ -0.\ 8516 \\ -1.\ 2250 \\ -2.\ 4740 \\ -0.\ 9946 \\ 0.\ 9400 \end{array}$
H H H H H H H H H	$\begin{array}{r} -2.\ 2656 \\ -1.\ 7714 \\ 1.\ 4941 \\ 2.\ 1675 \\ -1.\ 5858 \\ -4.\ 0095 \\ 4.\ 1131 \\ 5.\ 0812 \\ 3.\ 3723 \end{array}$	$\begin{array}{r} 2.4087\\ \hline 2.4087\\ \hline 0.0360\\ \hline 1.8065\\ \hline -1.6158\\ \hline -3.5244\\ \hline -3.6699\\ \hline -4.8175\\ \hline -4.8039\\ \hline -5.2804 \end{array}$	$\begin{array}{r} -0.\ 8079 \\ -2.\ 4885 \\ -2.\ 1060 \\ 4.\ 2573 \\ 1.\ 7328 \\ -0.\ 8516 \\ -1.\ 2250 \\ -2.\ 4740 \\ -0.\ 9946 \\ -0.\ 9408 \end{array}$
H H H H H H H H H H H	$\begin{array}{r} -2.\ 2656 \\ -1.\ 7714 \\ 1.\ 4941 \\ 2.\ 1675 \\ -1.\ 5858 \\ -4.\ 0095 \\ 4.\ 1131 \\ 5.\ 0812 \\ 3.\ 3723 \\ 4.\ 1325 \end{array}$	$\begin{array}{r} 2.4087\\ \hline 2.4087\\ \hline 0.0360\\ \hline 1.8065\\ \hline -1.6158\\ \hline -3.5244\\ \hline -3.6699\\ \hline -4.8175\\ \hline -4.8039\\ \hline -5.2804\\ \hline 0.0423\\ \end{array}$	$\begin{array}{r} -0.\ 8079 \\ -2.\ 4885 \\ -2.\ 1060 \\ 4.\ 2573 \\ 1.\ 7328 \\ -0.\ 8516 \\ -1.\ 2250 \\ -2.\ 4740 \\ -0.\ 9946 \\ -0.\ 9408 \\ 2.\ 8384 \end{array}$
H H H H H H H H H H	$\begin{array}{r} -2.\ 2656 \\ -1.\ 7714 \\ 1.\ 4941 \\ 2.\ 1675 \\ -1.\ 5858 \\ -4.\ 0095 \\ 4.\ 1131 \\ 5.\ 0812 \\ 3.\ 3723 \\ 4.\ 1325 \\ 3.\ 5854 \end{array}$	$\begin{array}{c} 2.4087\\ \hline 2.4087\\ \hline 0.0360\\ \hline 1.8065\\ \hline -1.6158\\ \hline -3.5244\\ \hline -3.6699\\ \hline -4.8175\\ \hline -4.8039\\ \hline -5.2804\\ \hline 0.0423\\ \hline 0.6141\\ \end{array}$	$\begin{array}{r} -0.\ 8079 \\ -2.\ 4885 \\ -2.\ 1060 \\ 4.\ 2573 \\ 1.\ 7328 \\ -0.\ 8516 \\ -1.\ 2250 \\ -2.\ 4740 \\ -0.\ 9946 \\ -0.\ 9408 \\ 2.\ 8384 \\ 4.\ 4251 \end{array}$
H H H H H H H H H H	$\begin{array}{r} -2.\ 2656 \\ -1.\ 7714 \\ 1.\ 4941 \\ 2.\ 1675 \\ -1.\ 5858 \\ -4.\ 0095 \\ 4.\ 1131 \\ 5.\ 0812 \\ 3.\ 3723 \\ 4.\ 1325 \\ 3.\ 5854 \\ 2.\ 5824 \end{array}$	$\begin{array}{c} 2.4087\\ \hline 0.0360\\ \hline 1.8065\\ \hline -1.6158\\ \hline -3.5244\\ \hline -3.6699\\ \hline -4.8175\\ \hline -4.8039\\ \hline -5.2804\\ \hline 0.0423\\ \hline 0.6141\\ \hline 1.190\\ \end{array}$	$\begin{array}{r} -0.\ 8079 \\ -2.\ 4885 \\ -2.\ 1060 \\ 4.\ 2573 \\ 1.\ 7328 \\ -0.\ 8516 \\ -1.\ 2250 \\ -2.\ 4740 \\ -0.\ 9946 \\ -0.\ 9408 \\ 2.\ 8384 \\ 4.\ 4251 \\ 4.\ 0226 \end{array}$
H H H H H H H H H H H H H	$\begin{array}{r} -2.\ 2656 \\ -1.\ 7714 \\ 1.\ 4941 \\ 2.\ 1675 \\ -1.\ 5858 \\ -4.\ 0095 \\ 4.\ 1131 \\ 5.\ 0812 \\ 3.\ 3723 \\ 4.\ 1325 \\ 3.\ 5854 \\ 3.\ 5231 \\ \end{array}$	$\begin{array}{c} 2.4087\\ \hline 2.4087\\ \hline 0.0360\\ \hline 1.8065\\ \hline -1.6158\\ \hline -3.5244\\ \hline -3.6699\\ \hline -4.8175\\ \hline -4.8039\\ \hline -5.2804\\ \hline 0.0423\\ \hline 0.6141\\ \hline -1.1129\\ \hline -1.129\\ \hline \end{array}$	$\begin{array}{r} -0.\ 8079 \\ -2.\ 4885 \\ -2.\ 1060 \\ 4.\ 2573 \\ 1.\ 7328 \\ -0.\ 8516 \\ -1.\ 2250 \\ -2.\ 4740 \\ -0.\ 9946 \\ -0.\ 9408 \\ 2.\ 8384 \\ 4.\ 4251 \\ 4.\ 0236 \\ 4.\ 0236 \end{array}$
H H H H H H H H H H H O	$\begin{array}{r} -2.\ 2656 \\ -1.\ 7714 \\ 1.\ 4941 \\ 2.\ 1675 \\ -1.\ 5858 \\ -4.\ 0095 \\ 4.\ 1131 \\ 5.\ 0812 \\ 3.\ 3723 \\ 4.\ 1325 \\ 3.\ 5854 \\ 3.\ 5231 \\ -5.\ 8141 \end{array}$	$\begin{array}{c} 2.4087\\ \hline 2.4087\\ \hline 0.0360\\ \hline 1.8065\\ \hline -1.6158\\ \hline -3.5244\\ \hline -3.6699\\ \hline -4.8175\\ \hline -4.8039\\ \hline -5.2804\\ \hline 0.0423\\ \hline 0.6141\\ \hline -1.1129\\ \hline -1.7934\\ \end{array}$	$\begin{array}{r} -0.\ 8079 \\ -2.\ 4885 \\ -2.\ 1060 \\ 4.\ 2573 \\ 1.\ 7328 \\ -0.\ 8516 \\ -1.\ 2250 \\ -2.\ 4740 \\ -0.\ 9946 \\ -0.\ 9408 \\ 2.\ 8384 \\ 4.\ 4251 \\ 4.\ 0236 \\ -0.\ 4002 \end{array}$
H H H H H H H H H H H C	$\begin{array}{r} -2.\ 2656 \\ -1.\ 7714 \\ 1.\ 4941 \\ 2.\ 1675 \\ -1.\ 5858 \\ -4.\ 0095 \\ 4.\ 1131 \\ 5.\ 0812 \\ 3.\ 3723 \\ 4.\ 1325 \\ 3.\ 5854 \\ 3.\ 5231 \\ -5.\ 8141 \\ -6.\ 4161 \end{array}$	$\begin{array}{r} 2.4087\\ \hline 0.0360\\ \hline 1.8065\\ \hline -1.6158\\ \hline -3.5244\\ \hline -3.6699\\ \hline -4.8175\\ \hline -4.8039\\ \hline -5.2804\\ \hline 0.0423\\ \hline 0.6141\\ \hline -1.1129\\ \hline -1.7934\\ \hline -2.8715\\ \end{array}$	$\begin{array}{r} -0.\ 8079 \\ -2.\ 4885 \\ -2.\ 1060 \\ 4.\ 2573 \\ 1.\ 7328 \\ -0.\ 8516 \\ -1.\ 2250 \\ -2.\ 4740 \\ -0.\ 9946 \\ -0.\ 9946 \\ -0.\ 9408 \\ 2.\ 8384 \\ 4.\ 4251 \\ 4.\ 0236 \\ -0.\ 4002 \\ -1.\ 0961 \\ \end{array}$
H H H H H H H H H H C	$\begin{array}{r} -2.\ 2656 \\ -1.\ 7714 \\ 1.\ 4941 \\ 2.\ 1675 \\ -1.\ 5858 \\ -4.\ 0095 \\ 4.\ 1131 \\ 5.\ 0812 \\ 3.\ 3723 \\ 4.\ 1325 \\ 3.\ 5854 \\ 3.\ 5231 \\ -5.\ 8141 \\ -6.\ 8161 \\ -6.\ 2482 \end{array}$	$\begin{array}{c} 2.4087\\ \hline 0.0360\\ \hline 1.8065\\ \hline -1.6158\\ \hline -3.5244\\ \hline -3.6699\\ \hline -4.8175\\ \hline -4.8039\\ \hline -5.2804\\ \hline 0.0423\\ \hline 0.6141\\ \hline -1.1129\\ \hline -1.7934\\ \hline -2.8715\\ \hline -2.8715\\ \hline -2.8222\end{array}$	$\begin{array}{r} -0.\ 8079 \\ -2.\ 4885 \\ -2.\ 1060 \\ 4.\ 2573 \\ 1.\ 7328 \\ -0.\ 8516 \\ -1.\ 2250 \\ -2.\ 4740 \\ -0.\ 9946 \\ -0.\ 9408 \\ 2.\ 8384 \\ 4.\ 4251 \\ 4.\ 0236 \\ -0.\ 4002 \\ -1.\ 0961 \\ -0.\ 520 \end{array}$
H H H H H H H H H H H C C H H	$\begin{array}{r} -2.\ 2656\\ -1.\ 7714\\ 1.\ 4941\\ 2.\ 1675\\ -1.\ 5858\\ -4.\ 0095\\ 4.\ 1131\\ 5.\ 0812\\ 3.\ 3723\\ 4.\ 1325\\ 3.\ 5854\\ 3.\ 5231\\ -5.\ 8141\\ -6.\ 4161\\ -6.\ 2483\\ -6.\ 2483\\ -6.\ 265\\ -$	$\begin{array}{c} 2.4087\\ \hline 2.4087\\ \hline 0.0360\\ \hline 1.8065\\ \hline -1.6158\\ \hline -3.5244\\ \hline -3.6699\\ \hline -4.8175\\ \hline -4.8039\\ \hline -5.2804\\ \hline 0.0423\\ \hline 0.6141\\ \hline -1.1129\\ \hline -1.7934\\ \hline -2.8715\\ \hline -3.8282\\ \hline 0.0254\\ \hline$	$\begin{array}{r} -0.8079 \\ -2.4885 \\ -2.1060 \\ 4.2573 \\ 1.7328 \\ -0.8516 \\ -1.2250 \\ -2.4740 \\ -0.9946 \\ -0.9408 \\ 2.8384 \\ 4.4251 \\ 4.0236 \\ -0.4002 \\ -1.0961 \\ -0.5830 \\ -0.5830 \\ -0.4002 \end{array}$
H H H H H H H H H H O C H H	$\begin{array}{r} -2.\ 2656\\ -1.\ 7714\\ 1.\ 4941\\ 2.\ 1675\\ -1.\ 5858\\ -4.\ 0095\\ 4.\ 1131\\ 5.\ 0812\\ 3.\ 3723\\ 4.\ 1325\\ 3.\ 5854\\ 3.\ 5231\\ -5.\ 8141\\ -6.\ 4161\\ -6.\ 2483\\ -7.\ 4854\end{array}$	$\begin{array}{c} 2.4087\\ \hline 2.4087\\ \hline 0.0360\\ \hline 1.8065\\ \hline -1.6158\\ \hline -3.5244\\ \hline -3.6699\\ \hline -4.8175\\ \hline -4.8039\\ \hline -5.2804\\ \hline 0.0423\\ \hline 0.6141\\ \hline -1.1129\\ \hline -1.7934\\ \hline -2.8715\\ \hline -3.8282\\ \hline -2.6544\\ \end{array}$	$\begin{array}{r} -0.\ 8079 \\ -2.\ 4885 \\ -2.\ 1060 \\ 4.\ 2573 \\ 1.\ 7328 \\ -0.\ 8516 \\ -1.\ 2250 \\ -2.\ 4740 \\ -0.\ 9946 \\ -0.\ 9408 \\ 2.\ 8384 \\ 4.\ 4251 \\ 4.\ 0236 \\ -0.\ 4002 \\ -1.\ 0961 \\ -0.\ 5830 \\ -1.\ 1136 \end{array}$
Н Н Н Н Н Н Н Н Н Н Н О С С Н Н Н	$\begin{array}{r} -2.\ 2656\\ -1.\ 7714\\ 1.\ 4941\\ 2.\ 1675\\ -1.\ 5858\\ -4.\ 0095\\ 4.\ 1131\\ 5.\ 0812\\ 3.\ 3723\\ 4.\ 1325\\ 3.\ 5854\\ 3.\ 5231\\ -5.\ 8141\\ -6.\ 4161\\ -6.\ 2483\\ -7.\ 4854\\ -6.\ 0436\end{array}$	$\begin{array}{r} 2.4087\\ \hline 2.4087\\ \hline 0.0360\\ \hline 1.8065\\ \hline -1.6158\\ \hline -3.5244\\ \hline -3.6699\\ \hline -4.8175\\ \hline -4.8039\\ \hline -5.2804\\ \hline 0.0423\\ \hline 0.6141\\ \hline -1.1129\\ \hline -1.7934\\ \hline -2.8715\\ \hline -3.8282\\ \hline -2.6544\\ \hline -2.9458\end{array}$	$\begin{array}{r} -0.\ 8079 \\ -2.\ 4885 \\ -2.\ 1060 \\ 4.\ 2573 \\ 1.\ 7328 \\ -0.\ 8516 \\ -1.\ 2250 \\ -2.\ 4740 \\ -0.\ 9946 \\ -0.\ 9408 \\ 2.\ 8384 \\ 4.\ 4251 \\ 4.\ 0236 \\ -0.\ 4002 \\ -1.\ 0961 \\ -0.\ 5830 \\ -1.\ 1136 \\ -2.\ 1270 \end{array}$
H H H H H H H H H H H H H H H H H	$\begin{array}{r} -2.\ 2656 \\ -1.\ 7714 \\ 1.\ 4941 \\ 2.\ 1675 \\ -1.\ 5858 \\ -4.\ 0095 \\ 4.\ 1131 \\ 5.\ 0812 \\ 3.\ 3723 \\ 4.\ 1325 \\ 3.\ 5854 \\ 3.\ 5854 \\ 3.\ 5231 \\ -5.\ 8141 \\ -6.\ 4161 \\ -6.\ 2483 \\ -7.\ 4854 \\ -6.\ 0436 \\ -0.\ 5252 \end{array}$	$\begin{array}{c} 2.4087\\ \hline 0.0360\\ \hline 1.8065\\ \hline -1.6158\\ \hline -3.5244\\ \hline -3.6699\\ \hline -4.8175\\ \hline -4.8039\\ \hline -5.2804\\ \hline 0.0423\\ \hline 0.6141\\ \hline -1.1129\\ \hline -1.7934\\ \hline -2.8715\\ \hline -3.8282\\ \hline -2.6544\\ \hline -2.9458\\ \hline 4.4522\end{array}$	$\begin{array}{r} -0.\ 8079 \\ -2.\ 4885 \\ -2.\ 1060 \\ 4.\ 2573 \\ 1.\ 7328 \\ -0.\ 8516 \\ -1.\ 2250 \\ -2.\ 4740 \\ -0.\ 9946 \\ -0.\ 9946 \\ -0.\ 9408 \\ 2.\ 8384 \\ 4.\ 4251 \\ 4.\ 0236 \\ -0.\ 4002 \\ -1.\ 0961 \\ -0.\ 5830 \\ -1.\ 1136 \\ -2.\ 1270 \\ -1.\ 0624 \end{array}$
H H H H H H H H H H H H H H H H O C H H H H	$\begin{array}{r} -2.\ 2656\\ -1.\ 7714\\ 1.\ 4941\\ 2.\ 1675\\ -1.\ 5858\\ -4.\ 0095\\ 4.\ 1131\\ 5.\ 0812\\ 3.\ 3723\\ 4.\ 1325\\ 3.\ 5854\\ 3.\ 5231\\ -5.\ 8141\\ -6.\ 4161\\ -6.\ 2483\\ -7.\ 4854\\ -6.\ 0436\\ -0.\ 5352\\ 1.\ 5252\\ -1.\ 5252\\ -2$	$\begin{array}{c} 2.4087\\ \hline 2.4087\\ \hline 0.0360\\ \hline 1.8065\\ \hline -1.6158\\ \hline -3.5244\\ \hline -3.6699\\ \hline -4.8175\\ \hline -4.8039\\ \hline -5.2804\\ \hline 0.0423\\ \hline 0.6141\\ \hline -1.1129\\ \hline -1.7934\\ \hline -2.8715\\ \hline -3.8282\\ \hline -2.6544\\ \hline -2.9458\\ \hline 4.4533\\ \hline 4.4533\\ \hline 4.6262\end{array}$	$\begin{array}{r} -0.\ 8079 \\ -2.\ 4885 \\ -2.\ 1060 \\ 4.\ 2573 \\ 1.\ 7328 \\ -0.\ 8516 \\ -1.\ 2250 \\ -2.\ 4740 \\ -0.\ 9946 \\ -0.\ 9408 \\ 2.\ 8384 \\ 4.\ 4251 \\ 4.\ 0236 \\ -0.\ 4002 \\ -1.\ 0961 \\ -0.\ 5830 \\ -1.\ 1136 \\ -2.\ 1270 \\ -1.\ 9624 \\ -0.\ 9624 \\ -0.\ 9624 \\ -0.\ 9624 \\ -0.\ 9628 \\ -0.\$
H H H H H H H H H H H C C H H H H O C	$\begin{array}{r} -2.\ 2656\\ -1.\ 7714\\ 1.\ 4941\\ 2.\ 1675\\ -1.\ 5858\\ -4.\ 0095\\ 4.\ 1131\\ 5.\ 0812\\ 3.\ 3723\\ 4.\ 1325\\ 3.\ 5854\\ 3.\ 5231\\ -5.\ 8141\\ -6.\ 4161\\ -6.\ 2483\\ -7.\ 4854\\ -6.\ 0436\\ -0.\ 5352\\ -1.\ 7953\\ \end{array}$	$\begin{array}{c} 2.4087\\ \hline 0.0360\\ \hline 1.8065\\ \hline -1.6158\\ \hline -3.5244\\ \hline -3.6699\\ \hline -4.8175\\ \hline -4.8039\\ \hline -5.2804\\ \hline 0.0423\\ \hline 0.6141\\ \hline -1.1129\\ \hline -1.7934\\ \hline -2.8715\\ \hline -3.8282\\ \hline -2.6544\\ \hline -2.9458\\ \hline 4.4533\\ \hline 4.9022\\ \hline \end{array}$	$\begin{array}{r} -0.\ 8079 \\ -2.\ 4885 \\ -2.\ 1060 \\ 4.\ 2573 \\ 1.\ 7328 \\ -0.\ 8516 \\ -1.\ 2250 \\ -2.\ 4740 \\ -0.\ 9946 \\ -0.\ 9946 \\ -0.\ 9408 \\ 2.\ 8384 \\ 4.\ 4251 \\ 4.\ 0236 \\ -0.\ 4002 \\ -1.\ 0961 \\ -0.\ 5830 \\ -1.\ 1136 \\ -2.\ 1270 \\ -1.\ 9624 \\ -2.\ 4338 \\ \end{array}$
Н Н Н Н Н Н Н Н Н Н Н Н Н Н	$\begin{array}{r} -2.\ 2656\\ -1.\ 7714\\ 1.\ 4941\\ 2.\ 1675\\ -1.\ 5858\\ -4.\ 0095\\ 4.\ 1131\\ 5.\ 0812\\ 3.\ 3723\\ 4.\ 1325\\ 3.\ 5854\\ 3.\ 5231\\ -5.\ 8141\\ -6.\ 4161\\ -6.\ 2483\\ -7.\ 4854\\ -6.\ 0436\\ -0.\ 5352\\ -1.\ 7953\\ -1.\ 7288\end{array}$	$\begin{array}{c} 2.\ 4087\\ \hline 0.\ 0360\\ \hline 1.\ 8065\\ \hline -1.\ 6158\\ \hline -3.\ 5244\\ \hline -3.\ 6699\\ \hline -4.\ 8175\\ \hline -4.\ 8039\\ \hline -5.\ 2804\\ \hline 0.\ 0423\\ \hline 0.\ 6141\\ \hline -1.\ 1129\\ \hline -1.\ 7934\\ \hline -2.\ 8715\\ \hline -3.\ 8282\\ \hline -2.\ 6544\\ \hline -2.\ 9458\\ \hline 4.\ 4533\\ \hline 4.\ 9022\\ \hline 5.\ 9908\\ \end{array}$	$\begin{array}{r} -0.\ 8079 \\ -2.\ 4885 \\ -2.\ 1060 \\ 4.\ 2573 \\ 1.\ 7328 \\ -0.\ 8516 \\ -1.\ 2250 \\ -2.\ 4740 \\ -0.\ 9946 \\ -0.\ 9946 \\ -0.\ 9408 \\ 2.\ 8384 \\ 4.\ 4251 \\ 4.\ 0236 \\ -0.\ 4002 \\ -1.\ 0961 \\ -0.\ 5830 \\ -1.\ 1136 \\ -2.\ 1270 \\ -1.\ 9624 \\ -2.\ 4338 \\ -2.\ 4685 \end{array}$
Н Н Н Н Н Н Н Н Н Н Н Н Н Н	$\begin{array}{r} -2.\ 2656\\ -1.\ 7714\\ 1.\ 4941\\ 2.\ 1675\\ -1.\ 5858\\ -4.\ 0095\\ 4.\ 1131\\ 5.\ 0812\\ 3.\ 3723\\ 4.\ 1325\\ 3.\ 5854\\ 3.\ 5231\\ -5.\ 8141\\ -6.\ 4161\\ -6.\ 2483\\ -7.\ 4854\\ -6.\ 0436\\ -0.\ 5352\\ -1.\ 7953\\ -1.\ 7288\\ -2.\ 0096\\ \end{array}$	$\begin{array}{c} 2.\ 4087\\ \hline 0.\ 0360\\ \hline 1.\ 8065\\ \hline -1.\ 6158\\ \hline -3.\ 5244\\ \hline -3.\ 6699\\ \hline -4.\ 8175\\ \hline -4.\ 8039\\ \hline -5.\ 2804\\ \hline 0.\ 0423\\ \hline 0.\ 6141\\ \hline -1.\ 1129\\ \hline -1.\ 7934\\ \hline -2.\ 8715\\ \hline -3.\ 8282\\ \hline -2.\ 6544\\ \hline -2.\ 9458\\ \hline 4.\ 4533\\ \hline 4.\ 9022\\ \hline 5.\ 9908\\ \hline 4.\ 5192\\ \end{array}$	$\begin{array}{r} -0.\ 8079 \\ -2.\ 4885 \\ -2.\ 1060 \\ 4.\ 2573 \\ 1.\ 7328 \\ -0.\ 8516 \\ -1.\ 2250 \\ -2.\ 4740 \\ -0.\ 9946 \\ -0.\ 9946 \\ -0.\ 9408 \\ 2.\ 8384 \\ 4.\ 4251 \\ 4.\ 0236 \\ -0.\ 4002 \\ -1.\ 0961 \\ -0.\ 5830 \\ -1.\ 1136 \\ -2.\ 1270 \\ -1.\ 9624 \\ -2.\ 4338 \\ -2.\ 4685 \\ -2.\ 4685 \\ -3.\ 4408 \end{array}$
H H H H H H H H H H H O C H H H H H H H	$\begin{array}{r} -2.\ 2656\\ -1.\ 7714\\ 1.\ 4941\\ 2.\ 1675\\ -1.\ 5858\\ -4.\ 0095\\ 4.\ 1131\\ 5.\ 0812\\ 3.\ 3723\\ 4.\ 1325\\ 3.\ 5854\\ 3.\ 5231\\ -5.\ 8141\\ -6.\ 4161\\ -6.\ 2483\\ -7.\ 4854\\ -6.\ 0436\\ -0.\ 5352\\ -1.\ 7953\\ -1.\ 7288\\ -2.\ 0096\\ -2.\ 5052\end{array}$	$\begin{array}{c} 2.4087\\ \hline 2.4087\\ \hline 0.0360\\ \hline 1.8065\\ \hline -1.6158\\ \hline -3.5244\\ \hline -3.6699\\ \hline -4.8175\\ \hline -4.8039\\ \hline -5.2804\\ \hline 0.0423\\ \hline 0.6141\\ \hline -1.1129\\ \hline -1.7934\\ \hline -2.8715\\ \hline -3.8282\\ \hline -2.6544\\ \hline -2.9458\\ \hline 4.4533\\ \hline 4.9022\\ \hline 5.9908\\ \hline 4.5192\\ \hline 4.2022\\ \hline 5.9908\\ \hline 5.9908\\ \hline 4.5192\\ \hline 5.9908\\ \hline 5.9008\\ \hline 5.9008\\$	$\begin{array}{r} -0.\ 8079 \\ -2.\ 4885 \\ -2.\ 1060 \\ 4.\ 2573 \\ 1.\ 7328 \\ -0.\ 8516 \\ -1.\ 2250 \\ -2.\ 4740 \\ -0.\ 9946 \\ -0.\ 9946 \\ -0.\ 9408 \\ 2.\ 8384 \\ 4.\ 4251 \\ 4.\ 0236 \\ -0.\ 4002 \\ -1.\ 0961 \\ -0.\ 5830 \\ -1.\ 1136 \\ -2.\ 1270 \\ -1.\ 9624 \\ -2.\ 4338 \\ -2.\ 4685 \\ -3.\ 4408 \\ -3.\$

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

atom	Х	Y	L
C	0 9602	1 1602	1 6165
L	-0. 8095	-1. 1002	1.0105
С	0.0479	-0.0804	1.5282
C C	1 2024	0 1070	2,1061
U	1.3034	-0. 1970	2.1061
С	1.7114	-1.3897	2,7391
- C	0.0010		2.7070
U	0.8313	-2.4020	2. 1910
С	-0.4561	-2.3666	2,2486
- C	0.0400	1 0070	1 1000
U	-2.2462	-1.0078	1. 1000
С	-2 7269	0 3218	0 7790
0	1.0140	0.0210	0.1100
C	-1.8140	1.4009	0.6665
C	-0 3244	1 1583	0 7470
0	0.0211	1.1000	0.1110
C	-4.1115	0. 5309	0.5692
ſ	-4 5861	1 8385	0 2854
U C	4. 5001	1.0000	0.2004
С	-3.6796	2.8892	0.2100
ſ	-2 3048	2 6675	0 3924
0	2.0040	2.0010	0.0024
С	-0.0480	-0.0804	-1.5282
ſ	0 8693	-1 1602	-1 6165
U	0.0093	1.1002	1.0105
С	0.4561	-2.3666	-2.2486
C	_0 9212	-2 1626	_2 7071
U	-0.8313	-2.4020	-2.1911
С	-1.7114	-1.3897	-2.7391
Č	1 2024	0 1070	2 1061
L U	-1. 5034	-0.1970	-2.1001
С	0. 3243	1.1583	-0.7470
Č	1 0140	1 4000	0 6665
L L	1.8140	1.4009	-0. 0005
С	2.7269	0.3218	-0.7789
č	0.0400	1 0070	1 1005
L	2.2462	-1.0078	-1.1005
С	2.3048	2.6676	-0.3924
Č	2.0010	2,0000	0.0100
U	3. 6796	2.8892	-0.2100
С	4, 5861	1.8385	-0.2854
Č	4 1115	0 5200	0 5602
U	4.1115	0. 5309	-0. 5692
0	-3 0435	-1 9916	1 1884
0	0.0100	1.0010	1,1001
0	3.0436	-1.9916	-1.1885
Н	-0 1395	2 0266	-1 2265
11	0.1005	2.0200	1.0005
Н	0.1395	2.0266	1.2265
C	3 1024	-1 4918	3 3146
<u>C</u>	0.1024	1. 4010	0.0140
С	-3. 1023	-1.4918	-3. 3146
0	-5 0202	-0.4522	0 6243
0	5.0202	0.4522	0.0245
0	-1.2582	-3. 4351	2.3597
0	5 0202	-0.4522	-0 6242
0	5.0202	0.4322	0.0242
0	1.2582	-3. 4351	-2.3597
Ц	-1 5164	_1 9919	0 8260
11	-4. 5104	-1.2010	0.8300
Н	-2.1158	-3.1971	1.9228
Ц	4 5164	_1 9919	_0 8250
11	4. 5104	1.2010	0.0333
Н	2.1158	-3. 1971	-1.9227
Ц	1 0052	0 6384	2 0586
11	1. 3302	0.0304	2.0000
Н	1.1129	-3. 3981	3.2705
Ц	-1 0200	3 8050	0 0060
11	1.0290	0.0004	0.0009
H H	-1.6212	3. 5090	0.3118
Ц	_1 1199	_3 2001	_3 9706
11	1.1120	0.0001	3.2700
Н	-1.9952	0.6385	-2.0587
Ц	1 6911	3 5000	-0.2110
11	1.0211	5.5050	0.0119
I H	4. 0290	3.8952	-0.0069
Ц	3 3064	-0.6653	4 0059
11	5. 5004	-0.0000	4.0039
Н	3.8554	-1.4368	2.5180
Ц	2 2494	_9 4299	2 9525
11	5.2404	2.4322	5.0555
Н	-3. 3063	-0.6652	-4.0059
Ц	-3 8554	-1 /260	-2 5121
11	5.0004	1.4309	2. 5161
Н	-3.2484	-2.4321	-3. 8536
0	5 031/	1 0388	-0 1107
	J. 3314	1. 3300	0.1107
0	-5.9315	1.9388	0.1107
C C	6 4710	3 0000	0 1656
L U	0.4/10	3. 2202	0.1030
Н	6.0714	3.6342	1. 1016
Ц	7 5477	3 0749	0.2665
П	1.0411	3.0742	0.2000
Н	6.2753	3. 9263	-0.6528
C C	_6 4710	2 0000	_0 1656
L U		$1 \qquad 0. \ 4404$	-0.1000
I II	-0.4710	0.2202	2
Н	-6.0715	3.6342	-1.1016
H	-6.0715 -7.5477	3.6342	-1.1016
H H	$\begin{array}{r} -6.\ 4710 \\ -6.\ 0715 \\ -7.\ 5477 \end{array}$	3. 6342 3. 0741	-1.1016 -0.2664

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

atom	Λ	ĭ	L
С	2,6974	0.7156	0.8770
C C	1 7001	1 7960	0.7160
U	1. 7891	1. 7809	0.7160
С	2.2676	3.0627	0. 4430
C	3 6461	3 2151	0.3120
C	5.0401	3.3131	0.3120
С	4. 5424	2.2586	0.4408
C	4 0904	0 9614	0 7191
0	1.0304	0.0014	1.0550
C	2.2221	-0.6136	1.2552
С	0 8299	-0.7789	1 6679
C	0.0200	0, 2005	1 5200
U	-0.0872	0.3005	1. 5380
С	0.2976	1.5343	0.7566
C C	0.4271	-1 0705	2 2004
U .	0.4371	-1. 9795	2.3094
С	-0.8700	-2.0861	2.8553
C	-1 7358	-1 0060	2 7550
0	1.1000	1.0000	2.1000
C	-1.3472	0.1752	2.0992
С	-1.7892	1.7869	-0.7159
C C	-2 6075	0.7156	-0.8770
U	-2.0915	0.7150	-0.0110
С	-4.0905	0.9613	-0. 7191
ſ	-4 5426	2 2584	-0 4407
0	1. 0120	2.2001	0.1101
C	-3.6463	3. 3149	-0.3116
С	-2.2678	3.0627	-0.4427
Č Č	0.2079	1 5945	0.7565
L	-0.2978	1. 5345	-0. (000
C	0.0872	0.3008	-1.5380
ſ	-0 8200	-0 7788	-1 6678
	0.0233	0.1100	1.0070
C	-2.2221	-0.6136	-1.2552
С	1.3471	0.1756	-2,0993
Č	1 7259	-1 0056	_2 7552
U	1.7336	-1.0050	-2.1002
С	0.8702	-2.0857	-2.8554
С	-0. 4369	-1.9794	-2.3094
0	2 0222	_1 5952	1 2002
0	3.0322	1.0000	1. 3032
0	-3.0321	-1.5852	-1.3094
Н	0, 1783	2.4042	-1.2214
Ц	-0.1785	2 4039	1 9917
	0.1100	2.4035	1. 2211
l	4. 1402	4. (185	0.0566
С	-4.1406	4.7182	-0.0561
0	1 2457	-3 0356	2 4553
	T. 2101	0.0007	2.1000
0	5. 0107	-0.0087	0.8287
0	-1.2454	-3.0356	-2.4552
0	-5.0106	-0.0089	-0.8289
0	0.1070	0.0005	0.0205
Н	2. 1070	-2. 7888	2.0297
Н	4.5165	-0.8490	1.0154
Н	-2 1067	-2 7887	-2 0298
11	4.5104	2.1001	1.0150
Н	-4. 5164	-0. 8492	-1.0156
Н	1.5646	3.8853	0.3287
Н	5 6121	2 4110	0 3340
11	0.7000	1.0050	0.0010
Н	-2.7309	-1.0652	3. 1811
Н	-2,0557	0, 9942	2,0325
Ц	-5 6192	2 /116	-0 2216
11	0.0120	2. 1110	0.001
H	-1.5648	3.8854	-0.3284
Н	2,0555	0.9947	-2.0327
Ц	2 7310	-1 0647	_2 1019
11	2.1310	1.0047	5. 1012
H	4.1142	5.3144	0.9784
Н	3. 5133	5.2354	-0.6786
Н	5 1712	4 7212	-0.3094
TI II	4 1147		0.0770
П	-4.1147	5. 3143	-0. 9779
Н	-5.1715	4.7209	0.3100
Н	-3 5137	5 2352	0.6791
0	1 1/00	2.2002	9 AEEC
U	1.1490	-3. 2128	-3.4556
0	-1.1487	-3.2732	3.4556
C	2 4433	-3 4481	-4 0080
11	0 6005	0. 101	1.0000
П	2.0395	-2.1211	-4.0137
H	3.2245	-3.3545	-3.2418
Н	2.4569	-4, 4596	-4.4172
C III	_9 //91	_2 //00	1 0074
	-2.4431	-3. 4400	4.0074
H	-2.6398	-2.7286	4.8133
II			
Н	-3.2241	-3.3550	3. 2410
<u>Н</u> U	-3.2241	-3.3550	3. 2410

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

atom	Å	Y	L
C	-1 0283	-0.6305	1 7145
U	1.0205	0.0303	1.7145
С	-0.0580	0.3749	1.4680
C	1 1605	0 2200	9 1905
U	1.1005	0. 3308	2.1290
С	1.4820	-0.7275	3.0048
C	0 5515	-1 7360	3 9107
U .	0.0010	1.7300	5.2157
С	-0. 7033	-1.7014	2.5938
C	-2 3766	-0 5132	1 1751
U	2.3700	0.0152	1.1751
С	-2.7713	0.7265	0.5022
C	-1 8046	1 7179	0 2137
<u> </u>	1.0040	1.1112	0.2157
С	-0.3332	1.4521	0.4435
C	-4 1379	0 9638	0 1890
0	4. 1010	0.000	0.1030
C	-4.5463	2. 1882	-0.3815
С	-3 5688	3 1457	-0.6311
0	0.0000	0.0010	0.0011
U	-2.2159	2.9213	-0. 3459
С	1.8918	1.4129	-0.8395
- C		0.0000	0.0000
U	2. 7850	0.3282	-0. 6889
С	4 1579	0 5959	-0 4265
C C	4 6107	1 0200	0.2652
L L	4. 6107	1. 9208	-0. 3653
С	3, 7332	2.9847	-0.5516
C C	2 2600	2 7160	0.7774
L L	2. 3099	2.7100	-0.7774
С	0.4065	1.1598	-0.9750
C C	0.0702	0.2042	1 5915
L L	0.0703	-0.2042	-1. 5515
С	0.9708	-1.2862	-1.3559
	2 2176	-1.0475	-0.8442
U. U.	2.3170	-1.0475	-0. 8442
С	-1.1401	-0. 4316	-2.1725
C	-1 4810	-1 7217	-2 6052
0	1.4010	1. 7217	2.0052
С	-0.6456	-2.8150	-2.4137
C	0 5969	-2 5901	-1 7822
0	0.0000	2.0001	1.1022
0	-3. 2252	-1.4354	1.3594
0	3 1047	-2 0145	-0.6201
<u> </u>	0.0004	1,0000	1.0407
Н	-0.0084	1. 9209	-1.6437
Н	0.1274	2.3842	0.7869
	0.1211	0.7609	2,6706
L L	2. 8300	-0.7608	3.0700
С	4. 2331	4,4089	-0.5302
0	5 0061	0.0512	0 4220
0	-5.0961	0.0512	0.4220
0	-1.5609	-2.6945	2.8695
0	1 4001	-2 6550	-1 6252
0	1.4001	3.0330	1.0252
0	5.0567	-0.3811	-0.2266
Н	-4 6443	-0.7432	0 8114
11	1.0110	0.1102	0.0111
Н	-2.3888	-2.5090	2.3559
Н	2, 2232	-3,3309	-1, 1759
II	4 5050	1 9400	0.2007
П	4. 5059	-1.2400	-0. 3097
Н	1.8905	1.1166	1.9618
U U	0.7654	-2 5601	2 8820
11	0.7034	-2. 3091	3.8820
Н	-3.8694	4. 0987	-1.0608
Н	-1 4854	3 6968	-0 5627
11	1.4004	5.0500	0.0021
Н	5.6659	2.0889	-0.1726
Н	1 6792	3 5472	-0.9040
11	1.0152	0.001	0.0010
Н	-1.8307	0.3891	-2.3352
Н	-2,4349	-1.8755	-3.1045
II	2,0102	1 5049	4 2720
H	2. 9192	-1. 5942	4.3738
Н	3.6323	-0.8656	2.9232
Ц	3 0208	0 1696	1 9177
11	5.0298	0.1090	4.2177
Н	5.2230	4. 4804	-0.0703
Н	3 5408	5 0641	0 0216
11		0.0011	0.0210
Н	4.3111	4.8096	-1.5495
C	-6 0034	2 4127	-0 6898
	C C170	0.0040	0.0100
Н	-0.01/9	<i>2.32</i> 40	0.2139
Н	$-6, \overline{1632}$	3,4049	-1.1224
11	_6 200E	1 6610	_1 20/1
п	-0. 3809	1.0019	-1. 3941
С	-1.0094	-4.2068	-2.8593
Ц	-1 0028	-4 2186	-3 3388
11	1. 3320	7.2100	0.0000
H	-0.2721	-4.6030	-3.5673
Н	-1 0202	-1 9009	-2 0100
11	1.0434	1. 0000	2.0103

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

atom	λ	Y	L
C	-2 7856	0 3282	-0.6889
U. U.	-2. 1850	0. 3282	-0. 0889
С	-1.8918	1.4129	-0.8396
с С	2,000	0.7100	0.7774
U	-2.3699	2.7160	-0.7774
C	-3 7332	2 9847	-0.5516
0	0.1008	1.0007	0.0010
C	-4.6107	1. 9207	-0.3654
C	-4 1570	0 5058	-0 4265
U	-4. 1579	0. 3938	-0.4203
С	-2 3176	-1 0476	-0.8442
0	2.0110	1.0110	1.0550
C	-0.9708	-1.2862	-1.3559
C	0.0702	0.2042	1 5215
U	-0.0703	-0.2042	-1.0510
С	-0 4065	1 1598	-0.9750
0	0. 1000	1.1000	0.0100
C	-0. 5969	-2.5901	-1.7822
C	0 6457	_2 9150	-9 4127
U	0.0437	-2.8130	-2.4157
С	1 4810	-1 7217	-2 6052
0	1, 1401	0,4010	0,1705
C	1.1401	-0.4316	-2.1725
C	0.0580	0 3740	1 4680
U. U.	0.0380	0.3749	1.4080
С	1.0283	-0.6305	1.7145
0	2.0200	1 5010	0 5000
C	0.7033	-1.7013	2. 5938
C	-0 5516	-1 7350	3 2107
U. U.	0. 0010	1.7339	5.2151
С	-1,4820	-0.7274	3.0048
0	1. 1020	0.1211	0.0010
	<u>–</u> 1. 1605	<u>0</u> . 3308	Z. 1295
C	0 3330	1 4591	0 4434
U	0.0004	1.4041	0.4404
C C	1.8046	1.7172	0.2137
<u> </u>	0.7710	0.7000	0 5000
L	2.7713	0.7266	0.5022
C	2 3766	-0.5132	1 1751
0	2.0100	0.0102	1.1101
С	2.2159	2.9213	-0.3459
C	2 5600	2 1457	0 6211
U	5. 5000	5. 1457	-0.0311
С	4 5463	2 1882	-0.3815
0	1.0100	2.1002	0.0010
C	4. 1379	0.9638	0. 1890
0	-2 1046	-2 0146	-0.6200
0	-3. 1040	-2.0140	-0.0200
0	3. 2252	-1,4354	1, 3594
	0 1075	0,0040	0.7000
Н	-0.1275	2.3843	0.7869
Н	0 0084	1 9209	-1 6437
	0.0001	1. 5205	1.0101
С	-4.2331	4.4089	-0. 5303
C	0 0255	0 7609	2 6706
U	-2. 8300	-0.7008	5.0700
0	-1 4001	-3 6550	-1 6252
0	1. 1001	0.0000	1.0202
0	-5.0567	-0.3811	-0. 2267
0	5 0061	0.0512	0 4220
0	5.0501	0.0312	0.4220
0	1.5609	-2.6944	2.8695
II	0 0000	2 2200	1 1750
П	-2.2232	-3. 3309	-1.1759
Н	-4 5659	-1 2400	-0.3097
11	1.0000	0.7400	0.0114
Н	4.0443	-0.7432	0.8114
Н	2 3887	-2 5090	2 3560
11	2.0001	2.0000	2.0000
H	-1.6792	3. 5472	-0.9041
Ц	-5 6650	2 0000	-0 1796
11	5.0059	2.0000	0.1720
Н	2.4350	-1.8754	-3.1045
II	1 0007	0.2001	0 0050
п	1.0307	0. 3091	-2. 3352
Н	-0.7655	-2.5691	3.8820
11 TT	1 0005	1 1107	1 0010
Н	-1.8905	1.1167	1.9618
Н	1 1851	3 6062	-0 5628
11	1. 1004	5.0300	0. 0020
H H	3.8694	4. 0987	-1.0608
II	_1 9111	1 2006	_1 5405
П	-4. 3111	4.0090	-1. 0490
Н	$-5, 22\overline{31}$	4, 4804	$-0.07\overline{04}$
11 TT	0.5400	E 0041	
Н	-3. 5498	5.0641	0.0216
Ц	-3 6393	-0 8653	2 0252
11	5.0525	0.0000	4. 3434
H H	-2.9193	-1.5943	4. 3737
II	2 0007	0 1606	4 9170
п	-3. 0297	0.1090	4.21/8
C	1.0095	-4.2068	-2.8592
	0.0701	1. 2000	0.5050
Н	0.2721	-4.6030	-3.5672
Ц	1 0028	-1 9186	-3 3388
11	1. 3340	4.2100	0.000
Н	1.0293	-4.9009	-2.0108
<u> </u>	6 0024	9 4197	0 6000
<u> </u>	0.0034	2.4121	-0.0898
Н	6.1632	3. 4049	-1, 1225
11	0.1002	0.0017	0.0100
I Н	6.6179	2.3247	0.2139
-	-		
Ц	6 2005	1 6619	-1 20/1

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

atom	Λ	ľ	L
C	0 9063	-0.9659	-1 6023
- C	0.0001	0.1007	1.0020
C	-0.0201	0.1067	-1.5263
C	-1 2667	-0.0185	-2 1212
0	1.2001	0.0100	0.7500
C	-1.6569	-1.2144	-2.7596
С	-0 7683	-2 2808	-2 8053
<u>C</u>	0.1000	2.2000	2.0000
C	0.5112	-2.1750	-2.2401
С	2 2765	-0.8002	-1 1367
0	2.2100	0.0002	1.1001
C	2.7403	0. 5321	-0.7422
C	1 8210	1 6009	-0.6357
0	1.0210	1.0000	0.0001
C	0. 3339	1. 3490	-0.7423
С	4 1232	0 7672	-0.5116
<u>C</u>	1. 1202	0.1012	0.0100
C	4.5960	2.0636	-0.2169
С	3.6641	3. 0944	-0.1500
- C	0.0011	0.0011	0.2477
U	2.2948	2.8794	-0.3477
С	0.0201	0.1065	1.5264
C .	0,0062	0.0661	1 6021
U	-0. 9063	-0.9661	1.0021
С	-0.5112	-2.1754	2.2398
Č.	0 7699	9 9919	2 9050
U	0.7082	-2.2013	2.8030
С	1.6568	-1.2148	2.7596
<u> </u>	1 2666	-0.0180	9 1914
U	1.2000	0.0109	2.1214
С	-0. 3339	1.3489	0.7426
C	-1 8200	1 6008	0 6360
U	1.0209	1.0008	0.0300
С	-2.7403	0. 5320	0.7422
ſ	-2 2765	-0.8004	1 1366
C .	2.2105	0.0004	1.1500
С	-2.2947	2.8754	0.3482
ſ	-3 6640	3 0944	0 1504
0	5.0010	5.0511	0.1504
С	-4.5959	2.0636	0.2171
C	-4 1231	0 7672	0 5116
0	1.1201	1.7765	1 1510
0	3.0839	-1.7765	-1.1512
0	-3.0839	-1.7767	1, 1510
<u>_</u>	0.1040	0.0140	1 0015
H	0. 1246	2.2146	1.2315
Н	-0.1246	2.2148	-1.2311
C	2 0204	1 2964	2 2556
L	-3. 0384	-1.3264	-3. 3556
С	3, 0383	-1.3269	3, 3556
0	E 02E0	0,0100	0 5610
0	5.0359	-0.2189	-0. 5610
0	1. 3234	-3.2367	-2.3413
0	5 0250	0.2120	0 5607
0	-0.0009	-0.2169	0. 3007
0	-1.3235	-3.2371	2.3408
Ц	4 5419	-1 0526	-0.7811
	4. 5415	1.0520	0.7011
Н	2.1741	-2.9911	-1.8953
Н	-4 5419	-1 0527	0 7808
11	0.1741	1.0021	0.1000
Н	-2.1741	-2.9914	1.8948
С	6,0691	2.2827	0.0085
C C	6 0600	0.0007	0,0094
U	-0.0090	2.2821	-0.0084
Н	-1.9644	0.8125	-2.0854
Ц	-1 0363	-3 9189	-3 2830
11	1.0000	J. 2102	0.2000
H	4.0146	4.1013	0.0657
Н	1 6005	3 7088	-0 2736
11	1.0000	0.1000	0.2100
Н	1.0362	-3.2187	3.2826
Н	1 9644	0 8122	2 0857
11	1.0011	0.0122	0.0749
Н	-1.6005	3.7088	0.2743
Н	-4.0145	4.1013	-0.0652
II	_9 0905	_0 5007	_1 0400
П	-3. 2385	-0. 0007	-4.0490
Н	-3.8033	-1.2783	-2.5699
Ц	-2 1606	-9 9679	-2 8075
11	5.1090	2.2013	5.0915
H	3.2384	-0.5013	4.0491
Н	3 8032	-1 2789	2 5699
11	0.0004	1.2103	2.0000
Н	3.1694	-2.2679	3.8974
Н	6.6543	1.9759	-0.8663
TT	6 0005	2,0,00	0.0140
Н	0.2805	J. JJ02	U. 2149
Н	6.4355	1.6839	0.8508
<u></u>	-6 6549	1 0750	0 9669
П	-0.0042	1.9100	0.0003
Н	-6.2804	3. 3363	-0.2146
U	-6 1252	1 6949	-0.8508
11	0.4000	1.0042	0.0000

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

atom	Λ	1	L
C	-2 8160	0 5287	-0 4764
0	1.0700	1.5004	0. 1101
C	-1.8792	1.5864	-0.4321
С	-2 2952	2 8632	-0.0750
0	2.2002	2.0002	0.0100
C	-3.6369	3. 1295	0.2577
С	-4.5572	2.0863	0.2429
0	4 1004	0.7000	0 1171
C	-4.1684	0.7886	=0.1171
С	-2.4171	-0.7991	-0.9378
C	1 0070	0.0760	1 5205
t	-1.0979	-0.9709	-1. 5595
С	-0.1568	0.0844	-1.5289
C	_0_4120	1 2010	-0.6002
C	-0.4130	1. 5210	-0.0992
С	-0.7984	-2.1768	-2.2418
C	0 4098	-2 3123	-2 9591
0	0.4050	2.0120	2. 3031
C	1.2858	-1.2342	-2.9593
C	1 0179	-0.0500	-2 2573
0	1.0700	1 5004	0 4001
C	1.8792	1.5864	0.4321
С	2.8160	0.5287	0.4764
C	4 1004	0.7000	0 1171
U	4.1084	0.7880	0.1171
С	4.5572	2.0863	-0.2429
C	2 6260	2 1205	0.2577
	5.0509	0.1290	0.2011
l C	2.2952	2.8632	0.0750
C	0 4130	1 3217	0 6992
0	0.1500	1.0411	1 5000
U	0.1568	0.0844	1.5289
C	1.0979	-0.9769	1.5395
Č	9 4171	0.7001	0.0270
L	2.4171	-0. 7991	0. 9378
С	-1.0179	-0.0500	2.2573
C	-1 2858	-1 2342	2 9593
0	1.2000	0.0100	2.0000
C	-0.4098	-2.3123	2.9591
С	0.7984	-2.1768	2.2418
0	-3 2416	-1 7595	-0.8948
0	3.2410	1.7555	0.0340
0	3.2416	-1.7595	0.8948
Н	0.0094	2.1866	1.2360
Ч	-0.0094	2 1866	-1 2360
11	0.0034	2.1000	1.2300
C	-4.0680	4. 5338	0.6053
С	4,0680	4, 5338	-0.6053
0	_1 6421	-2,2207	-2 2741
0	-1.0431	-3.2207	-2.2741
0	-5.1086	-0.1679	-0.1097
0	1.6431	-3.2207	2.2741
ů.	5 1096	0 1670	0 1007
0	5.1060	-0.1079	0.1097
Н	-2.4382	-2.9638	-1.7386
Н	-4 6586	-1 0114	-0.3760
TT TT	0.4000		1 7290
Н	2.4382	-2.9638	1.7380
Н	4.6586	-1.0114	0. 3760
С	0 6938	-3 5935	-3 6979
Č	0 6020	2 5025	2 6070
0	-0.0330	-3. 3933	2.0212
Н	-1.5723	3.6763	-0.0529
Н	-5, 5981	2.2505	0.5041
11	0 0100	1 9159	2 5017
11	4.4100	-1.3132	-3. 3217
Н	1.7373	0.7616	-2.2826
Н	5.5982	2.2505	-0.5041
II	1 5700	2.2000	0.0590
Н	1.5723	3.0703	0.0529
Н	-1.7373	0.7616	2.2826
Н	-9 9139	-1 3152	3 5217
11	4 1070	1.0102 E 1500	0.0050
П	-4.1270	5.1580	-0.2959
Н	-3.3535	5.0147	1.2829
Н	-5 0528	4 5455	1 0814
11	4 1071		1.0017
Н	4.1271	5.1581	0.2959
Н	5.0530	4.5456	-1.0810
Н	3 3537	5 01/6	-1 2833
11	0.0001	0.0110	1.4000
Н	-0.0861	-3.8059	-4.4386
Н	1.6576	-3.5415	-4.2130
Ц	0.7124	-1 1101	-3 0130
11	0.1124	1.1134	0.0100
Н	-1.6576	-3.5415	4.2130
Н	0.0861	-3.8059	4.4386
II	0.7194	4 4404	2 0120
11	-0.7124	-4.4494	9.0190

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

atom	λ	Y	L
C	0 6402	0 7019	1 0272
U	-0. 6492	-0.7018	1.9275
C	0 2176	0 3654	1 5787
	1 4705	0.4400	0 1500
C	1.4795	0.4420	2.1500
C	1 9459	-0 5544	3 0319
0	1.0100	1 0004	0.0010
C	1.1159	-1.6224	3. 3475
ſ	-0 1789	-1 7089	2 81/19
0	0.1105	1.1005	2.0145
С	-2.0384	-0. 7096	1. 4815
ſ	-2 5734	0 4602	0 7070
U	2.0734	0.4002	0.1919
С	-1.7169	1.5163	0. 4103
C	_0_2154	1 2014	0 5450
U	0.2134	1. 3014	0. 5455
С	-3.9756	0. 5776	0. 5603
ſ	-4 5175	1 7331	-0.0285
<u> </u>	4.0110	1.7551	0.0200
С	-3.6332	2.7634	-0.3706
C	-2 2493	2 6599	-0 1629
0	1.0171	1 4000	0.1025
C	1.9171	1.4803	-0.8841
C	2 9034	0 4738	-0 7817
<u> </u>	4.0047	0.0554	0.0001
C	4.2647	0.8554	-0.6284
С	4.6118	2.2134	-0.6248
	0 0401	2,0001	0.7010
U	3.6401	3.2001	-0.7613
С	2.2904	2.8189	-0.8794
C C	0 4501	1 1005	_0_0102
U	0.4001	1.1000	-0.9103
С	0.1881	-0.2941	-1.4101
ſ	1 10/6	$-1 \ 90.47$	-1 9795
	1.1040	-1.2941	-1.2720
C	2.5359	-0. 9397	-0.8763
ſ	-1 0425	-0.6221	-1 9505
<u> </u>	1.0423	0.0221	1. 5505
C	-1.3154	-1.9499	-2.3221
C	-0.3820	-2 9796	-2 1612
0	0.0020	2.5150	1 0007
C	0.8768	-2.6397	-1.6367
0	-2.7933	-1.6920	1,7595
0	2,1000	1.0020	0.6045
0	3. 4183	-1. 8345	-0. 6945
Н	-0.0666	1.8143	-1.5685
II	0 1951	2 2506	0.9214
11	0.1651	2.3390	0.0314
С	3.3421	-0. 4591	3.5962
C	4 0220	4 6598	-0.8022
<u> </u>	4.0225	4.0330	0.0022
0	-4. 8261	-0.4059	0.8951
0	-0 9334	-2 7543	3 1862
0	0.001	2.1010	5.1002
0	1. 7807	-3.6241	-1.5072
0	5 2522	-0 0424	-0 4797
U U	4.0725	1 1401	1 0700
Н	-4.2735	-1.1401	1.2793
Н	-1.8080	-2.6503	2,7295
II	2 6045	2 2006	1 1945
П	2.0045	-3.2080	-1.1345
Н	4.8256	-0.9388	-0. 5093
Н	2 1303	1 2757	1 9054
11	2.1505	1.2101	1.0004
Н	1. 4419	-2.4102	4.0196
Н	-1.6194	3, 4931	-0.4596
II	5 6615	9 4601	_0 E1E0
П	0.0010	4091	-0.0100
H	1.5269	3.5892	-0.9683
Н	-1 8191	0 1911	-2 0881
11		1.0570	4.01001
Н	3. 5418	-1.2573	4.3168
Н	4, 0891	-0.5299	2, 7954
TT	0 E011	0 5000	4 0000
Н	ა. 5011	U. 9UZ8	4.0980
Н	5.0360	4.8206	-0. 4218
Ц	3 3306	5 2708	-0 2008
11	0.0020	0.2100	0.2090
H	3.9905	5.0426	-1.8308
C	-6 0008	1 8616	-0.2772
U U	C 4450	0.0010	0.0005
H	-b. 4458	2.6856	0.2995
Н	-6.2244	2.0361	-1.3396
II	6 E100	0.0459	0.0170
Н	-0.0130	0.9493	0.0172
С	-0.7097	-4.4006	-2.5505
Ŭ	_0 0215		-2 6955
П	-0. 9210	-4.4900	-3. 0200
H	0.1314	-5.0575	-2.3261
Н	-1 5810	-4 7847	-2 0008
	0.5405	0 1010	0.0450
0	-2. 5485	-2.1812	-2.8453
Н	-2.6386	-3.1245	-3.0535
0	_/ 0799	3 0.024	-0 0203
U	-4.0723	J. 94J4	-0. 2000
Н	-5.0380	3.8925	-1.0178

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

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$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	8838
C         2.         13.1         0.         13.1           C         -4.         6.115         2.         2.141         -0.         6.243           C         -4.         2.644         0.         8560         -0.         6273           C         -2.         5359         -0.         9392         -0.         8762           C         -1.         1846         -1.         2943         -1.         7126           C         -0.         1800         -0.2938         -1.         6110           C         -0.         8770         -2.         6392         -1.         6371           C         0.         3818         -2.         9791         -2.         1615           C         1.         0426         -0.         6218         -1.         9505           C         1.0426         -0.         6556         3.0307         C         -1.         1165         -1.         6231         -1.         971           C         0.         1717         1.         5162         3.0307         C         -1.         1497           C         0.         2.1656         13814         0.5463 <th><math display="block">\begin{array}{c ccccccccccccccccccccccccccccccccccc</math></th> <th>8701</th>	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	8701
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	0191
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	7609
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	6949
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	C         -4. 2644         0. 8560         -0.           C         -2. 5359         -0. 9392         -0.	0243
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	C         -2.5359         -0.9392         -0.	6278
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	0210
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $		8762
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	C = 1 1846 = 1 9943 = -1	2726
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	$\begin{array}{c} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 $	2120
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	C $-0.1880$ $-0.2938$ $-1.$	4100
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $		0101
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	-0.4500 1.1088 $-0.$	9101
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	-0.8770 $-2.6392$ $-1.$	6371
C         0.3183         -2.9731         -2.1015           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         0.6491         -0.7023         1.9271           C         0.1785         -1.7098         2.8140           C         -1.4797         0.4414         2.1497           C         0.2156         1.3814         0.5463           C         1.7171         1.5162         0.4108           C         2.45735         0.4601         0.7983           C         2.495         2.6599         -0.1622           C         3.9334         2.7633         -0.3700           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         -0.1849         2.3595         0.8320           H         -0.1		1015
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	0.3818 -2.9791 -2.	1015
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	(1 3153 -1 9495 -2)	3222
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $		0222
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	C 1. 0426 $-0.6218$ $-1.$	9505
C         0. 2110         0. 3030         1. 3131           C         0. 6491         -0. 7023         1. 9271           C         0. 1785         -1. 7098         2. 8140           C         -1. 1465         -1. 6237         3. 3461           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. 6599         -0. 1622           C         3. 6334         2. 7633         -0. 3700           C         3. 6334         2. 7633         -0. 0702           C         3. 6334         2. 7633         -0. 0700           C         3. 9757         0. 5774         0. 5607           O         -3. 4183         -1. 8340         -0. 6946           O         2. 7932         -1. 6924         1. 7592           H         -0. 0869         1. 8147         -1. 5680           C         -3. 3430         -0. 4607         -3. 5942           O         -1. 7809         -3. 6235         -3. 1853		5787
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $		5101
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	C 0. 6491 -0. 7023 1. 9	9271
C         0.         1.185         -1.093         2.8440           C         -1.1655         -1.6237         3.3461           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         2.6599         -0.1622           C         3.6334         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           0         -3.4183         -1.8340         -0.6946           0         2.7932         -1.6924         1.7592           H         -0.1849         2.3595         0.8320           H         0.0669         1.8147         -1.5680           C         -3.4330         -0.4607         3.5942           O         -1.7809         -3.6235         -1.5077           0         -5.2520         -0.0417         -0.4789           0         4.8262<		2140
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	0.1785 -1.7098 2.8	3140
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	-1.1165 $-1.6237$ $3.3$	3461
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		0005
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	-1.9464 $-0.5556$ $3.0$	J307
C         1.112         2.1111         2.1131           C         1.3156         1.3814         0.5463           C         1.7171         1.5162         0.4108           C         2.0385         -0.7099         1.4818           C         2.0385         -0.7099         1.4818           C         2.4495         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         2.3595         0.8320           H         -0.0669         1.8147         -1.5680           C         -4.0222         4.6605         -0.8012           C         -3.4330         -0.4607         3.5942           O         -1.7809         -3.6235         -1.5077           O         -5.2520         -0.0417         -0.4789           O         4.8262         -0.0417         -0.4789           O         4.8265         -0.9381         -0.5089           H         -2.66047 <t< th=""><th>C = -1.4797 = 0.4414 = 2.7</th><th>1497</th></t<>	C = -1.4797 = 0.4414 = 2.7	1497
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		- 100
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	U U U. 2156   1. 3814   0. 5	5463
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	C 1 7171 1 5169 0 /	4108
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		1100
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	C 2. 5735 0. 4601 0. 7	7983
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	C 2 0385 $-0.7000$ 1 /	1818
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		1010
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	C $2.2495$ $2.6599$ $-0.$	1622
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	0 3 6334 2 7633 -0	3700
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	0 3.0334 2.1033 0.	5100
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	C 4. 5177 1. 7329 $-0$ .	0280
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	0 3 9757 0 5774 0 5	5607
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	0.0114	1001
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	0 -3.4183 -1.8340 -0.	6946
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		7502
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	0 2. 1952 $-1.0924$ 1.	1092
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	H = -0.1849 2.3595 0.8	3320
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		EGOD
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Н 0.0009 1.8147 -1.	0000
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	C $-4.0222$ $4.6605$ $-0.$	8012
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		-049
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	-3.3430 $-0.4007$ $3.3$	)94 <i>2</i>
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	0 $-1,7809$ $-3,6235$ $-1.$	5077
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		4700
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	0 -5.2520 -0.0417 -0.	4789
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	0 4 8262 -0 4061 0 8	3953
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		1050
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	0 $0.9330$ $-2.7553$ $3.1$	1853
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	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 $-2.1303$ $1.2753$ $1.9053$ H $-2.0389$ $4.8202$ $-0.4588$ H $-5.0389$ $4.8202$ $-0.4299$ H $-3.3376$ $5.2696$ $-0.2001$ H $-3.5977$ $5.0465$ $-1.8281$ 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 $0$		1001
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	H $-4.8255$ $-0.9381$ $-0.$	5089
HHHHHHH1. 21311. 14031. 2131H1. 8078-2. 65082. 7293H-1. 52653. 5896-0. 9681H-5. 66112. 4698-0. 5152H1. 81920. 1214-2. 0880H-1. 4427-2. 41194. 0177H-2. 13031. 27531. 9053H1. 61963. 4931-0. 4588H-5. 03894. 8202-0. 4299H-3. 33765. 2696-0. 2001H-3. 97975. 0465-1. 8281H-3. 5423-1. 25824. 3158H-4. 0895-0. 53342. 7931H-3. 50330. 50174. 0951C0. 7093-4. 4001-2. 5511H0. 9223-4. 4940-3. 6259H1. 5799-4. 7849-2. 0006H-0. 1323-5. 0567-2. 3279C6. 00101. 8614-0. 2766H6. 51390. 94560. 0190H6. 22482. 0345-1. 3392O4. 07263. 9232-0. 9296H5. 03823. 8922-1. 0175O2. 5484-2. 1809-2. 8454	H $4.2737$ $-1.1403$ $1.6$	2707
H1.8078 $-2.6508$ $2.7293$ 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 $-3.3376$ $5.2696$ $-0.2001$ H $-3.5423$ $-1.2582$ $4.3158$ H $-3.5423$ $-1.2582$ $4.3158$ 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 $0.9223$ $-4.4940$ $-3.6259$ H $0.9223$ $-2.0367$ $-2.3279$ C $6.0010$ $1.8614$ $-0.2766$ H $6.5139$ $0.9456$ $0.0190$ H $6.2248$ $2.0345$ $-1.3392$ $0$ $4.0726$ $3.9232$ $-0.9296$ H $5.0382$ $3.8922$ $-1.0175$ $0$ $2.5484$ $-2.1809$ $-2.8454$		2131
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	H = 1.8078 = -2.6508 = 2.7	7293
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		9681
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Н _1.5265 3.5896 _0	5001
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Н -1.5265 3.5896 -0.	5152
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	H -1. 5265 3. 5896 -0. H -5. 6611 2. 4698 -0.	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	H -1.5265 3.5896 -0. H -5.6611 2.4698 -0. H 1.8192 0.1214 -2	0880
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	H         -1.5265         3.5896         -0.           H         -5.6611         2.4698         -0.           H         1.8192         0.1214         -2.	0880
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	0880 0177
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	0880 0177 0053
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	H         -1.5265         3.5896         -0.           H         -5.6611         2.4698         -0.           H         1.8192         0.1214         -2.           H         -1.4427         -2.4119         4.0           H         -2.1303         1.2753         1.9	0880 0177 9053
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	0880 0177 9053 4588
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	0880 0177 9053 4588 4299
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	0880 0177 9053 4588 4299
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	0880 0177 0053 4588 4299 2001
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	0880 0177 0053 4588 4299 2001 8281
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	0880 0177 9053 4588 4299 2001 8281
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	0880 0177 0053 4588 4299 2001 8281 3158
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	0880 0177 0053 4588 4299 2001 8281 3158 7021
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	0880 0177 9053 4588 4299 2001 8281 3158 7931
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	0880 0177 9053 4588 4299 2001 8281 3158 7931 9951
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	0880 0177 9053 4588 4299 2001 8281 3158 7931 0951 5511
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	0880 0177 9053 4588 4299 2001 8281 3158 7931 9951 5511
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	0880 0177 9053 4588 4299 2001 8281 3158 7931 9951 5511 6259
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	0880 0177 9053 4588 4299 2001 8281 3158 7931 0951 5511 6259 0006
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	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	0880 0177 9053 4588 4299 2001 8281 3158 7931 9951 5511 6259 0006
C         0.0010         1.8014         -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	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	0880 0177 9053 4588 4299 2001 8281 3158 7931 9951 5511 6259 0006 3279
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	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	0880           0177           9053           4588           4299           2001           8281           3158           7931           0951           5511           6259           0006           3279           2766
H         6. 5139         0. 9456         0. 0190           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	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	0880           0177           9053           4588           4299           2001           8281           3158           7931           9951           5511           6259           0006           3279           2766
H         b. 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	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	0880 0177 9053 4588 4299 2001 8281 3158 7931 9951 5511 6259 0006 3279 2766 2991
H         6. 2248         2. 0345         -1. 3392           0         4. 0726         3. 9232         -0. 9296           H         5. 0382         3. 8922         -1. 0175           0         2. 5484         -2. 1809         -2. 8454	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	0880 0177 9053 4588 4299 2001 8281 3158 7931 0951 5511 6259 0006 3279 2766 2991
0         4.0726         3.9232         -0.9296           H         5.0382         3.8922         -1.0175           0         2.5484         -2.1809         -2.8454	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	0880           0177           9053           4588           4299           2001           8281           3158           7931           9951           5511           6259           0006           3279           2766           2991           0190
0         4.0726         3.9232         -0.9296           H         5.0382         3.8922         -1.0175           0         2.5484         -2.1809         -2.8454	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	0880           0177           9053           4588           4299           2001           8281           3158           7931           9951           5511           6259           0006           3279           2766           2991           0190           3392
H         5. 0382         3. 8922         -1. 0175           0         2. 5484         -2. 1809         -2. 8454	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	0880           0177           9053           4588           4299           2001           8281           3158           7931           9951           5511           6259           0006           3279           2766           2991           1190           3392
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	0880           0177           9053           4588           4299           2001           8281           3158           7931           9951           5511           6259           0006           3279           2766           2991           0190           3392           9296
0 2.5484 -2.1809 -2.8454	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	0880           0177           9053           4588           4299           2001           8281           3158           7931           9951           5511           6259           0006           3279           2766           2991           9190           3392           9296           0175
	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	0880 0177 9053 4588 4299 2001 8281 3158 7931 0951 5511 6259 0006 3279 2766 2991 0190 3392 9296 0175
H $2.6384$ $-3.1242$ $-3.0536$	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	0880           0177           9053           4588           4299           2001           8281           3158           7931           9951           5511           6259           0006           3279           2766           2991           9190           3392           9296           0175           8454

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

atom	Λ	Ĭ	L
C	0 9079	_1 9196	-1 6162
U	0. 8978	-1.2180	-1.0102
С	-0.0300	-0.1495	-1.5282
C	-1 2816	-0.2742	-9 1131
0	-1.2810	-0.2742	-2.1131
С	-1.6746	-1.4677	-2.7529
ſ	-0 7833	-2 5313	-2 8111
0	0.1000	2.0010	2.0111
С	0.5009	-2. 4248	-2.2567
ſ	2 2731	-1 0/96	-1 1610
0	2.2101	1.0450	1.1010
С	2.7329	0.2749	-0.7632
C	1 8164	1 3449	-0.6463
0	1.0101	1.0115	0.0100
U	0.3277	1. 0927	-0.7444
С	4, 1195	0.5171	-0.5331
C	4 5010	1 9060	0.2244
U	4. 5910	1.0009	-0.2344
С	3. 6496	2.8419	-0.1628
C	2 2776	2 6187	-0.3553
Ū.	2.2110	2.0107	0.0000
С	0.0300	-0. 1492	1. 5279
ſ	-0.8978	-1 2184	1 6162
0	0.0010	1.2101	1.0102
C	-0.5007	-2.4245	2.2569
С	0. 7837	-2.5309	2.8109
<u>C</u>	1 6740	1 4070	0.7505
L	1.6749	-1.4673	2. 7525
С	1.2817	-0.2739	2.1126
C	_0 2278	1 0028	0.7440
U	-0. 3278	1.0928	0.7440
C	-1.8164	1. 3449	0.6459
ſ	-2 7320	0 2750	0 7634
	4.1043		1 1010
C	-2.2732	-1.0495	1.1613
C	-2 2778	2 6187	0 3545
<u>C</u>	2.2110	2.0101	0.1692
U	-3. 6499	2. 8417	0.1623
С	-4.5912	1.8066	0.2343
<u> </u>	_4 1196	0.5171	0.5336
C	4.1190	0.0171	0.000
0	3. 0822	-2.0276	-1.1901
0	-3.0826	-2.0271	1, 1908
U U	0 1224	1 0502	1 2200
П	0.1324	1.9392	1. 2299
Н	-0.1325	1.9590	-1.2304
С	-3.0614	-1.5813	-3, 3368
C C	2,0619	1 5010	2,2261
U	5.0018	-1. 5807	3. 3301
0	5.0214	-0.4776	-0.5911
0	1 3154	-3 $4844$	-2 3709
0	1.0104	0.4770	2.5105
0	-5. 0213	-0.4778	0. 5927
0	-1.3150	-3. 4842	2.3713
Ц	4 5145	-1 3053	-0.8182
11	4. 5145	1. 3033	0.0102
Н	2.1695	-3. 2369	-1.9319
Н	-4 5141	-1 3054	0.8196
11	0, 1000	1.0001	1 0204
H	-2. 1692	-3. 2368	1. 9324
С	6.0600	2.0684	-0.0054
C C	-6.0602	2 0680	0,0056
<u> </u>	0.0003	2.0080	0.0030
Н	-1.9804	0. 5556	-2.0677
Н	-1 0528	-3 4672	-3 2908
II	1.0020	2,4000	0.2700
Н	1.0003	3.4029	-0.2702
Н	1.0533	-3.4668	3.2907
Ц	1 0204	0 5560	2 0670
11	1. 5004	0.000	2.0010
H	-1.6005	3. 4629	0.2690
Н	-3 2714	-0.7521	-4 0232
11	0.2111	1 5410	0.5400
Н	-3. 8192	-1.5419	-2.5438
Н	-3.1937	-2.5192	-3.8837
Ц	3 2710	-0.7516	4 0225
11	3.2113	0.7510	4.0223
Н	3.8194	-1.5412	2.5429
Н	3 1944	-2 5186	3 8829
II	6 4715	0 7750	0 7400
Н	0.4/15	2.1100	-0.7403
Н	6.2543	2.4762	0.9971
Ц	6 6270	1 1/19	-0 0060
11	0.0270	1.1412	0.0900
H	-6.4734	2.7695	0.7450
Н	-6 2539	2 4827	-0 9942
TT	6 0000	1 1005	0.0000
Н	-0.0202	1.1395	0.0888
0	-4. 0192	4.1229	-0.1078
Н	4 0001	4 1659	-0.2083
1 11	-4. 98.31	4. 10.09	
0	-4.9831	4.1000	0.1075
0	-4. 9831 4. 0187	4. 1035	0. 1075

# Cartesian coordinates of 7,7'-methylated **2**-IV optimized at the gas-phase B3LYP/6-31G(d) level $\frac{1}{2}$

atom	Λ	1	L
ſ	2 7148	0 6005	0 8585
<u> </u>	2.1110	0.0000	0.0000
C	1.8011	1.6659	0.6944
C	2.2700	2.9430	0.4119
C	3 6468	3 2023	0.2748
<u> </u>	5.0400	0.1500	0.2140
U	4. 5488	2. 1522	0.4105
С	4. 1053	0.8537	0.6986
ſ	2 2441	-0.7300	1 2430
<u> </u>		0.1500	1.2100
L	0.8601	-0. 9009	1.6511
С	-0.0638	0.1695	1.5325
ſ	0.3102	1 4080	0 7500
<u> </u>	0.0102	0,1000	0.1000
L	0.4504	-2.1069	2.2946
С	-0.8367	-2.2360	2.8438
C	-1 6961	-1 1366	2 7430
<u> </u>	1.0001	1.1500	2.1450
U	-1. 3232	0.0528	2.0935
С	-1.8010	1.6659	-0.6944
C	-2 7148	0 6006	-0.8585
<u>C</u>	4 1052		0.0005
U. U.	-4. 1053	0.8537	-0. 6985
С	-4.5487	2.1523	-0.4105
C	-3 6467	3 2024	-0.2748
C C	2,2600	2 0420	0.4110
U. U.	-2.2099	2.9430	-0.4119
С	-0.3101	1.4080	-0.7501
С	0,0638	0, 1695	-1.5326
C C	_0 9601	_0_000	_1 6511
<u> </u>	-0.8001	-0. 9009	-1.0311
С	-2.2441	-0. 7299	-1.2429
С	1. 3232	0.0528	-2.0935
Č	1 6961	-1 1366	-2.7431
<u> </u>	1.0901	-1.1300	-2. 7431
С	0.8367	-2.2360	-2.8438
C	-0.4505	-2.1069	-2.2946
0	3 0634	-1 6983	1 2998
0	2.0034	1.0000	1.2007
0	-3.0634	-1.6983	-1. 2997
Н	0. 1647	2.2730	-1.2242
Н	-0 1647	2 2730	1 2241
	4 1215	4 6064	0,0050
U C	4.1313	4.0004	0.0050
С	-4. 1314	4.6064	-0.0051
0	1.2836	-3.1532	2.4143
0	5 0324	-0.1085	0.8182
0	3.0324	0.1005	0.0102
0	-1.2836	-3. 1532	-2. 4143
0	-5.0323	-0.1084	-0.8181
Н	2 1441	-2 8810	1 9941
11	4 5490	0.0510	1.0000
Н	4. 5429	-0. 9519	1.0028
Н	-2.1441	-2.8810	-1.9941
Н	-4.5429	-0.9519	-1.0027
	-1 2683	-3 5065	3 5350
<u> </u>	1.2005	5.5005	3. 3330
U U	1.2682	-3.5066	-3. 5350
Н	1.5618	3. 7611	0.2958
Н	5.6173	2.3106	0.3005
II	_2 0466	0 0500	2 0400
П	-2.0400	0.0000	4.0409
H	<u>-5.61</u> 72	2.3107	-0.3005
Н	-1.5617	3.7611	-0.2958
Ц	2 0466	0.8580	-2 0/10
	2.0400	0.0000	2.0410
Н	4.0775	5.2196	0.9141
Н	3. 5165	5.1022	-0.7545
Н	5 1703	4 6136	-0.3379
11	4 0779	T. 0100	0.0010
П	-4.0772	3.2197	-0.9141
H	-5.1703	4.6137	0.3377
Н	-3.5165	5.1022	0.7546
Ц	-1 5088	-3 3360	1 5016
11	1. JU00	0.0000	T. JJHU
Н	-2.1519	-3. 9538	3.0573
Н	$-0.46\overline{87}$	$-4.24\overline{71}$	3. 4980
Н	2 1521	-3 9536	-3 0576
II	1 5000	0.000	1 EQ4C
Н	1. 5083	-3.3371	-4. 5946
Н	0.4688	-4.2474	-3.4975
0	2.9489	-1.1608	-3.2691
й	3 1111	_2 0250	_2 6779
П	J. 1111	-2.0209	-3.0112
0	-2.9490	-1.1608	3.2690
Н	$-3.11\overline{12}$	-2.0259	3.6771

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

atom	Х	Y	
C	1 6600	1 1745	0 0252
U	-1.6609	1.1745	-0. 9352
С	-0.5521	0.3481	-1.2057
C C	0,6240	0.0202	1 6961
U	0. 6349	0. 9322	-1.6261
С	0.7974	2.3228	-1.7447
C .	0.2054	2 1700	1 4944
U	-0.2034	5.1700	-1.4244
С	-1.5092	2.5839	-1.0338
C .	2 0790	0 5995	0 6002
U	-2.9789	0. 0000	-0.0883
С	-3.1656	-0.8390	-0.8701
C	-2 0558	-1 6990	_1 1028
U	-2.0338	-1.0889	-1.1028
С	-0.6453	-1.1464	-1.0052
C	_1 1792	-1 4010	-0.8794
U	-4.4703	-1.4010	-0.0724
С	-4.6568	-2.7638	-1.1277
C	-3 5403	-3 5700	-1 3756
U	-3. 3493	-3. 5700	-1.3750
С	-2.2473	-3. 0366	-1.3574
C	1 5466	-1 5630	0 2633
Ŭ	1. 5400	1.0000	0.2033
С	2.2756	-0.5294	0.8739
C	3 6771	-0.4505	0 6514
<u> </u>	5.0771	0.4303	0.0314
С	4. 3622	-1.3995	-0.1463
C	3 6062	-2 4520	-0.7250
<u> </u>	3.0002	2.4320	0.7230
С	2.2210	-2.5000	-0.5090
C	0.0406	-1 6205	0.3841
<u> </u>	0.0400	1.0255	0.3041
С	-0.5068	-0.8999	1.5906
C	0 2342	0 1602	2 1648
Ŭ	0.2342	0.1092	2.1040
С	1.6055	0. 4180	1.7700
C	-1 7447	-1 2440	2 1036
<u> </u>	1. 7447	1.2440	2.1030
С	-2.2918	-0.5072	3. 1728
ſ	-1 6103	0 5717	3 7251
<u> </u>	1.0103	0.0111	3.7231
С	-0.3467	0.9156	3. 2346
0	-3 9679	1 3336	-0.4024
0	5. 5015	1.0000	0.4024
0	2.2523	1. 3974	2.2560
Н	-0 2429	-26842	0 4576
11	0.2423	1.0012	1.7700
Н	-0.0428	-1.6359	-1.7768
C	2 1442	2 8145	-2 2148
<u> </u>	4,0000	2.0110	1 5750
C	4. 2029	-3.5469	-1.5756
0	-5 5738	-0.6679	-0 6433
<u> </u>	0.5641	2,2002	0.7550
0	-2.5641	3. 3803	-0.7558
0	0.2792	1.9431	3, 8181
0	4.0741	0 5570	1 0174
0	4.3741	0. 5578	1.2174
Н	-5.2713	0.2606	-0.4710
II	2 2425	0 704E	0 5242
Н	-3. 3435	2. 7845	-0. 5343
Н	1.1588	2.0432	3.3717
Ц	2 7920	1 1977	1 7292
11	5.7230	1.1277	1. 7525
Н	1. 4766	0.2957	-1.8774
Н	-5 6671	-3 1629	-1 1302
11	0.0011	5.1025	1.1502
Н	-1.4123	-3. 7028	-1.5505
Н	1 6590	-3 3115	-0.9646
	0.0101	0.0110	1 7015
H	-2.3161	-2.0721	1.7015
Н	-2.0234	1, 1523	4, 5451
II	9 7749	1 0642	_9 4090
Н	2.1142	1.9043	-2. 4929
Н	2.0528	3.4908	-3. 0683
Ц	2 6472	2 2025	-1 4256
11	2.0473	0.0000	1.4330
Н	3. 4211	-4.2524	-1.8737
Н	1 9896	-4 0863	-1 0421
11	4. 3030	4.0003	1.0421
H	4.6828	-3. 1422	-2. 4703
ſ	-0 1060	4 6805	-1 5126
	5. 1000	1.0000	0.0040
<u> </u>	<b>5.</b> 8552	-1.3249	-0.3948
0	0.9806	5 1919	-1.6857
<u> </u>	6 4000	0 1107	1 1100
0	0.4303	-2.1167	-1.1128
0	$-1.\overline{1948}$	5.4622	$-1.\overline{4092}$
II .	1 0000	4 0242	1 0101
П	-1. 9090	4. 9243	-1.2131
0	6.5573	-0.3492	0.2046
Ц	5 0702	0 2260	0 7374
<u> </u>	0. 3100	0.2200	0.1314
0	-3.6576	-4.8952	-1.6409
Н	-4 5938	-5 1519	-1 6370
	1.0000	0.1010	1.0010
0	-3. 5076	-0.9073	3.6189
Ц	-3 2003	-0 3343	1 2/00
11	0.1000	0.0010	T. JTJJ

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

atom	Х	Ŷ	L
C	0 6240	0 6520	_2 2405
U	0.0340	0.0030	-2.2493
С	0.3746	-0.7149	-2.0329
ſ	1 09/13	-1 6580	-2 7536
0	1.0545	1.0000	2.1550
C	2.1125	-1.3093	-3.6569
С	2 4312	0 0577	-3 8509
<u> </u>	1 0717	1 0000	0.0000
C	1.6/17	1.0230	-3.1470
С	-0.2364	1,6738	-1.6649
C C	1 4512	1.0640	0.0040
U	-1.4515	1.2049	-0. 9848
С	-1.7073	-0.1042	-0. 7238
C	-0.6453	-1 1464	-1 0052
C	0.0433	1.1404	1.0052
С	-2.4342	2.2336	-0.6177
C	-3 6375	1 8249	-0.0353
0	0.0010	0.4700	0.0000
C	-3.8709	0.4709	0. 1883
С	-2,9050	-0.4953	-0.1490
C C	0.6420	0 4411	1 0006
U	0.0429	-0.4411	1.0990
С	0.0112	0. 1246	2.2192
C	0 5602	1 2002	2 7000
U C	0.3002	1.3003	2.1990
С	1.7400	1.9013	2.2961
C	2 3758	1 2906	1 1839
<u> </u>	1.0004	0.1401	0.0144
L	1.8064	0.1421	0.0144
С	0.0406	-1.6295	0.3841
Č	-0.8060	-2 4492	1 9444
U	-0.8900	-2.4402	1. 2444
C	-1.5531	-1.8396	2.3487
ſ	-1 1641	-0 5228	2 8102
0	1.1041	0. 5220	2.0102
C	-1.1452	-3.7719	0. 9286
С	-2.0834	-4.5087	1,6785
<u> </u>	2,0001	2,0270	2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2
U	-2.1140	-3. 9270	2. (300
С	-2.5148	-2.5977	3. 0833
0	0 0245	2 9071	-1 8263
0	1 7707	2.3011	1.0200
0	-1. 7787	0.0345	3. 1122
Н	0.8623	-2.2734	0.0548
Н	-1 1471	-2 0464	-1 3743
	2,0005	2.0101	1.0110
L L	2.8085	-2. 4419	-4.3706
С	3.6501	1.8032	0.5577
0	-2 2587	3 5452	-0.8150
0	1,0000	0,0102	0.0100
0	1. 9369	2.3330	-3. 3421
0	-3.1851	-2.0936	4.1247
0	-0.0612	1 8589	3 8595
0	1.0007	1.0000	1 0104
Н	-1.3607	3.6606	-1.2194
Н	1, 2812	2,8602	-2.7912
II	9.9754	1 1600	4 2405
П	-2.0734	-1.1000	4. 2495
Н	-0.8757	1.3032	4.0637
Н	0 8663	-2 7103	-2 6214
11	0.0003	2.1103	2.0214
Н	-4.3701	2.5828	0.2274
Н	-3.1266	-1.5395	0.0481
II	2 2061	0.2002	0.2207
11	2.3001	0.3062	0.2091
Н	-0.6366	-4. 2661	0.1094
Н	-3 5052	-4 4815	3 3177
11	0.0002	1. 1010	1 1000
Н	2.3186	-3.3901	-4. 1299
Н	2,8070	-2,2993	-5,4540
II	2 9692	2 5004	4 0950
П	3. 0023	-2. 3004	-4.0830
Н	3.9530	1.1423	-0.2604
Н	4 4602	1 8650	1 2887
11	1. 1002	1.0000	1.2001
Н	3. 5268	2.8188	0.1732
С	3, 5536	0. 4398	-4.7939
C .	0 2220	2 1560	2 0022
<u> </u>	2.3330	3.1303	2. 5022
0	4. 3079	-0.3843	-5.2674
0	3.3215	3.6911	2.4415
Ο	3 7006	1 7359	-5 1991
U 11	0.1000	0.0017	J. 1441
Н	3.0670	2.2917	-4.6247
0	1 7428	3.6877	3.9853
	1.1120	-	
Н	0.9509	3 1703	4 2303
H	0. 9509	3. 1703	4.2393
H 0	0. 9509	3. 1703 0. 0110	4. 2393 0. 7385
Н О Н	$\begin{array}{r} 1.120 \\ 0.9509 \\ -5.0215 \\ -5.6149 \end{array}$	3. 1703 0. 0110 0. 7571	4. 2393 0. 7385 0. 9219
H 0 H	$\begin{array}{r} 1.120\\ 0.9509\\ -5.0215\\ -5.6149\\ -2.2702 \end{array}$	3. 1703 0. 0110 0. 7571 -5. 7088	4. 2393 0. 7385 0. 9219 1. 3071
H 0 H 0	0. 9509 -5. 0215 -5. 6149 -2. 2703	$\begin{array}{r} 3.1703 \\ 0.0110 \\ 0.7571 \\ -5.7988 \\ \end{array}$	4. 2393 0. 7385 0. 9219 1. 3071

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

atom	Λ	Ĩ	L
ſ	0 5340	-0.5160	-1 8173
U G	0.0040	0.0100	1.0175
С	-0.3430	0. 5386	-1.4955
ſ	-1 6901	0 4105	-1 8045
C	1.0301	0.4105	1.0045
C	-2.2300	-0.7497	-2.3839
С	-1.3786	-1.8458	-2.6688
	0,0001	1.0100	2.0000
U	0.0021	-1.7044	-2.3871
С	1, 9817	-0.3412	-1.6908
C C	9 5110	0.0712	1 2605
U	2. 3116	0.9715	-1. 5095
С	1.6455	2.0336	-1.0106
C	0 1601	1 7751	-0.7935
U	0.1051	1. 7751	0.1933
С	3. 9135	1.2265	-1.4679
C	4 4095	2 5133	-1 2373
Č	2 5210	2.0100	0.0117
L	3. 5312	3. 5431	-0.9117
С	2.1497	3. 3049	-0.7917
C	0.3428	0 5390	1 /053
C	0.0420	0.000	1.4555
С	-0.5340	-0.5157	1.8175
ſ	-0.0017	-1 7038	2 3876
<u> </u>	0.0011	1.7030	2.3010
C	1. 3790	-1.8449	2.6690
С	2, 2303	-0.7487	2, 3836
C C	1 6000	0 4119	1 9040
U	1. 0900	0.4112	1. 8040
С	-0.1696	1.7752	0. 7930
ſ	-1 6461	2 0335	1 0102
C	1.0401	2.0555	1.0102
С	-2.5121	0.9711	1.3695
C	-1 9817	-0.3412	1 6911
<u> </u>	0.1505	0.0112	0.7010
L	-2.1505	3.3046	0.7910
С	-3.5321	3.5425	0.9111
C	4 4101	2 5126	1 9971
U C	-4.4101	2. 5120	1.2371
C	-3.9138	1.2260	1.4679
0	2,7679	-1.3064	-1.9420
0	-2 7677	-1 3064	1 9/26
0	2.1011	1.0004	1. 5120
H	0. 3825	2.6402	1. 1739
Н	-0.3832	2.6399	-1.1746
ſ	-3 7125	-0 7424	-2 6668
<u> </u>	2,7190	0.7411	2.0000
L	3. 7128	-0.7411	2.0002
0	4. 7974	0.2732	-1.7824
0	0.8361	-2 7257	-2 6777
0	0.0301	2.1251	1.7000
0	-4. 7974	0.2725	1. 7828
0	-0.8355	-2.7252	2.6786
Н	4 2882	-0 5694	-1 9023
11	4.2002	0.3034	1. 5025
Н	1. 7691	-2.4356	-2.4400
Н	-4.2880	-0.5699	1,9029
II	1 7696	2 4252	2, 4,12
П	-1.7080	-2.4352	2.4412
0	3. 9486	4.8140	-0.6903
Н	5 4793	2 6798	-1 3258
 	0.4100	2.0130	1.0200
0	-3.9499	4. 8133	0.6894
Н	-5.4800	2.6789	1.3257
Ц	/ 9108	1 8654	-0.8097
11	1.0100	1.0001	0.0001
Н	-4.9120	4. 8045	0.8089
Н	-2.3603	1.2370	-1.5940
Ц	1 5022	4 1360	-0.5301
11	1.0044	4.1000	0.0001
Н	2.3600	1. 2378	1. 5932
Н	-1.5032	4.1357	0. 5291
Ц	-4 1292	0.2426	-2 /351
11	1.1252	0.2420	2.4001
Н	-3. 9262	-0. 9891	-3.7097
Н	-4.2328	-1.4997	-2.0744
Н	3 9268	-0.9878	3 7090
II	4 0001	1 4004	0.1000
Н	4. 2331	-1.4984	2.0131
Н	4.1292	0.2440	2.4345
C	1 9608	-3 1105	3 2650
C	1 0500	0.1100	0.2000 0.0C47
	-1. 9999	-3.1117	-3. 2047
0	-3.1561	-3.2792	-3.3823
0	3. 1571	-3.2780	3.3819
	1 1166	_1 0666	3 6076
0	1.1100	-4.0000	0.0070
Н	0. 1892	-3.8236	3.4880
0			
0	-1.1154	-4.0679	-3, 6862
U U	-1.1154	-4.0679	-3.6862

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

atom	Λ	I	L
C	2 7385	0 0698	0 7566
0	2.1000	0.0000	0.1000
С	1.8228	1. 1269	0.6258
C	2 2962	2 3970	0 3228
C	2.2902	2.3910	0. 3220
С	3.6571	2.6728	0. 1222
C	4 6002	1 6166	0 9199
U	4.0002	1.0100	0.2183
С	4, 1194	0. 3236	0, 5380
0	0.0701	1 0000	1,1000
U	2.2781	-1.2602	1.1660
C	0 9134	-1 4265	1 6203
0	0.0100	1. 1200	1.0200
С	-0.0169	-0.3543	1.5375
C	0 2252	0 9911	0 7200
U. U.	0.0000	0.8811	0.1399
С	0.5229	-2.6298	2.2828
C	0.7490	9,7000	0.0000
U	-0.7426	-2.7299	2.8080
C	-1 6139	-1 6475	2 8111
0	1.0105	1.0110	2.0111
С	-1.2556	-0.4588	2.1439
C	_1 0000	1 1960	-0.6258
C	1.0220	1.1209	0.0238
С	-2.7386	0.0698	-0.7566
- -	4 1104	0.0007	0 5000
U	-4.1194	0.3237	-0. 5380
C	-4 6002	1 6166	-0.2183
0	1.0002	1.0100	0.2100
С	-3.6571	2.6728	-0.1221
C	-2 2961	2 3970	-0.3228
U. U.	2.2901	2.3510	0. 3228
С	-0.3353	0.8811	-0.7399
C .	0.0160	0.2542	1 5975
U	0.0109	-0. 5545	-1. 5575
С	-0 9134	-1 4265	-1 6204
C	0.0700	1.000	1.0201
U	-2.2782	-1.2602	-1.1661
C	1 2556	-0.4588	-2 1439
<u> </u>	1.2000	0.4000	2.1100
C	1.6139	-1.6475	-2.8111
C	0 7496	-2 7200	_2 2626
U	0.7420	-2.7299	-2. 8080
С	-0.5229	-2.6298	-2.2828
0	2,0001	0,0000	1 1000
0	3. 0901	-2.2328	1. 1998
0	-3.0961	-2,2328	-1.1997
0	0.1107	1.2020	1. 1001
Н	0.1137	1.7517	-1.2284
Н	-0 1137	1 7516	1 2284
11	0.1101	1.1010	1.2204
С	4. 0270	4. 1029	-0. 1871
C	-4 0270	4 1020	0 1979
U	-4.0270	4.1030	0.1872
0	1.3349	-3.6878	2.3883
0	1 0067	0 6079	0 6202
0	4.9907	-0.6978	0. 6393
0	-1 3349	-3 6878	-2 3884
0	1.0010	0.0077	2.0001
0	-4.9968	-0.6977	-0.6394
Н	2 1879	-3 4462	1 9445
11	2.1015	5. 1102	1. 5115
Н	4.4714	-1.5282	0.8586
Н	-2 1879	-3 4461	-1 9446
11	2.1015	5. 4401	1. 5440
Н	-4.4716	-1.5281	-0.8588
0	-2 8430	-1 6607	3 3783
0	2.0400	1.0037	5.5705
Н	-1.0091	-3.6542	3. 3733
0	2 9420	1 6606	2 2702
<u> </u>	2.0439	1.0090	3. 3103
Н	1.0091	-3.6542	-3. 3732
 I I	_9 0007	_9 5964	2 0116
п	-2. 9001	-2. 3204	5.0110
Н	2,9888	-2.5264	-3.8115
11	1 5007	2 0100	0.9401
Н	1. 3887	3. 2183	0.2401
Н	-1.9706	0.3552	2.1215
11 TT	1.5100	0.0002	0.0400
Н	<u>–</u> 1. 5886	3.2183	-0.2400
Н	1 9706	0 3552	-2 1214
11	1.0100	4.5002	
H H	3. 1318	4.7320	-0.1602
Ц	4 7607	4 4019	0 5238
11	1.1001	T. TJ14	0.0200
Н	4. 4986	4. 1897	-1.1693
Ц	-1 7606	/ /012	-0 5227
11	4.7000	4.4910	0.0201
Н	-4. 4986	4. 1897	1.1694
Ц	_2 1217	4 7290	0 1604
П	-3. 1317	4. 1320	0.1004
С	-6,0691	1.8988	0.0236
<u> </u>	6 0001	1 0000	0.0000
	0.0091	1.8988	-0.0236
0	6 4687	2 9905	-0.3724
	0.1001	2.0000	0.0723
0	-6.4689	2.9905	0.3722
0	-6 9520	0 9033	-0 1632
	0.0020	0.0000	0.1002
H H	-6. 4934	0.0743	-0.4113
0	6 9521	0 0034	0 1633
<u> </u>	0.3321	0.0034	0.1033
I H	6. 4937	0.0744	0.4115

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

atom	Х	Y	1.
C	0 7050	1 0005	1 2270
U	0.7053	-1.0325	-1.3372
C	-0.0721	-0.4622	-1 4807
0	0.0121	0.1022	1. 1001
C	-1.3295	-0.5177	-2.0788
C	-1 8840	-1 7354	-2 4848
0	1.0040	1.1554	2.4040
С	-1.1336	-2.9012	-2.3305
C	0 1529	_2 9695	_1 7774
U	0.1556	-2.8085	-1.7774
С	2,0890	-1.5213	-0.8254
C	9 0074	0 1000	0.7070
C	2.6974	-0. 1800	-0. 7879
С	1 9162	0.9872	-0.9376
0	0.4110	0.0000	0.0011
C	0.4118	0.8600	-0.9311
C	4 1100	-0.0669	-0.6635
0	4.1100	0.0005	0.0000
С	4.7177	1. 1880	-0.7642
C	3 0486	2 3200	-0.0501
C .	5. 5400	2. 3230	0.0001
С	2.5445	2.2264	-1.0348
C	-1 6470	1 5904	0 4210
U	1.0470	1. 5054	0.4219
С	-2.6738	0.6390	0.5787
C	4 0100	1 0500	0.0720
U	-4. 0199	1.0566	0.3739
С	-4,2932	2.3864	0. 0368
0	0.0014	0.0010	0.1004
C	-3.2644	3. 3240	-0.1084
C	-1 9449	2 9097	0 0782
0	0 1010	1 1070	0.5102
C	<u>-0</u> . 1918	1. 1879	<u>0</u> . 5510
ſ	0 0062	0 0631	1 5389
<u> </u>	0.0002	0.0001	1.0000
C	-0.9948	-0. 9379	1.6076
C	-2 3175	-0 7395	0 0033
0	4.0110	0.1000	0.000
С	1.1411	-0.0499	2.3384
C	1 3365	-1 1954	3 1448
C	1.0000	1.1554	5.140
С	0. 3987	-2.2201	3.1430
C	-0.7706	-2 1056	2 3855
C .	0.1100	2.1000	2.0000
0	2.7682	-2.5210	-0.5201
0	-3 1282	-1 6840	0 9220
0	5.1202	1.0040	0. 3220
Н	0. 3702	2.0630	0.8814
Н	-0.0023	1 6586	-1 5505
11	0.0023	1.0000	1.0000
C	-3. 2932	-1.7889	-3.0193
C	-3 5880	4 7631	-0.4307
0	5.0000	1,1001	0.4500
0	4.8993	-1. 1289	-0.4700
0	0 9157	-3 9777	-1 6520
0	0.0101	0.0111	1.0020
0	-1.6539	-3.1098	2.4423
0	-4 9943	0 1283	0 5261
<u> </u>	1. 00 10	0.1200	0.0201
Н	4.2821	-1.9133	-0.3950
Н	-2 4048	-2 8450	1 8380
11	2.1010	2.0100	1.0000
Н	-1.9013	0.3962	-2.2059
Н	-1 5633	-3 8439	-2.6473
II	F 7007	1.0405	
П	5.7997	1. 2495	-0. 6829
Н	-5.3174	2.7079	-0.1133
II	1 1000	2.000	0,0000
Н	-1. 1338	3.6228	-0. 0399
Н	0.5473	-3.1165	3, 7388
II	2 4001	9 7000	2 5007
Н	-3.4821	-2.7093	-3. 3807
Н	-4.0062	-1.7505	-2.1850
II	_2 5064	_0 0262	_2 6725
11	5. 5004	0. 9303	3.0133
Н	-4.4157	4.8383	-1.1447
Ц	_9 7990	5 2822	-0 8538
11	4.1440	0.2022	0.0000
Н	-3.8893	5. 3086	0.4733
C	-6 3521	0 5253	0 4067
C .	0.0021	0.0200	0.4007
Н	-6.9362	-0.3752	0.6032
Н	-6 6143	1 2978	1 1411
11	0.0143	1.2510	1. 1411
Н	-6.5800	0.8924	-0.6025
C	0 4067	-5 2246	-2 1015
	0.1007	5. <u>22</u> 10	0.1700
Н	0.1837	-5.2080	-3.1762
Н	1 2003	-5 9478	-1 9071
11	0 40 40	5. 5110 E E100	1 5400
<u>H</u>	-0.4942	-9. 9100	-1.5469
0	4. $5012$	3.5624	$-1.07\overline{26}$
	5 4659	2 1700	_0_0000
Н	<b>5.</b> 4052	১. ৭/১১	-0. 9988
0	2.4606	-1.2481	3.8985
ц Ц	2 1710	_2 0008	1 3705
П	2. 4/40	-2.0906	4.0190
C1	1.6321	3.7172	-1.2450
<u>C1</u>	9 9456	1 0016	9 4490
U1	2.0400	1. 4410	4.4400

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

atom	Å	Ŷ	L
ſ	2 6738	0.6389	0 5787
0	1.6460	1 5000	0.0101
C	1.6469	1. 5893	0. 4222
С	1 9449	2 9097	0.0788
- C	2.0042	2.0001	0.1000
U	3.2043	3.3240	-0.1080
С	4.2931	2.3864	0.0368
C	4 0109	1 0565	0.2726
L L	4. 0198	1.0505	0. 3730
С	2.3176	-0. 7396	0.9935
C	0.0040	_0.0291	1 6079
C	0. 9949	-0. 9381	1.0078
С	-0.0062	0.0629	1.5390
ſ	0 1918	1 1877	0 5513
0	0.1510	1.1011	0.0010
C	0.7708	-2.1058	2. 3857
С	-0.3985	-2 2204	3 1432
- C	1 2205	1 1050	2 1440
C	-1.3365	-1. 1958	3. 1449
С	-1.1412	-0.0503	2, 3384
C	0.0721	0.4621	1 4906
C	0.0721	-0.4021	-1.4800
С	-0.7055	-1.6325	-1.3374
C	-0 1540	-2 8684	-1 7775
U C	0.1540	2.0004	1.1115
C	1. 1335	-2.9012	-2.3306
C	1 8840	-1 7355	-2 4848
0	1.0010	0 5177	2.1010
C	1. 3296	-0.5177	-2.0787
С	-0.4117	0, 8600	-0.9310
Č	_1 0161	0.0974	-0.0276
U	-1.9101	0.9014	-0.9310
С	-2.6975	-0.1797	-0.7880
ſ	-2 0892	-1 5211	-0.8258
C	2.0092	1. J211	0.0200
С	-2.5443	2.2266	-1.0346
С	-3 9484	2 3294	-0 9590
<u> </u>	4 7170	1 1005	0.7040
L L	-4. /1/6	1. 1885	-0.7642
С	-4.1101	-0.0666	-0.6636
0	2 1994	-1 6840	0 0225
0	3.1204	-1.0840	0.9223
0	-2.7686	-2. 5208	-0.5208
Н	0.0025	1.6587	-1.5501
II	0.2702	2,0629	0.0017
11	-0.3703	2.0028	0.0017
С	3. 5881	4. 7629	-0.4309
С	3 2932	-1 7889	-3 0192
0	1 6549	2 1000	2 4496
0	1.0342	-3. 1099	2.4420
0	4.9944	0. 1281	0. 5251
0	-4 8994	-1 1284	-0 4701
0	0.0150	2,0776	1 (500
0	-0.9158	-3.9770	-1.6522
Н	2.4051	-2.8449	1.8382
Н	-1 2823	-1 9128	-0.3950
11	4.2023	1. 5120	0.0000
Н	1. 1337	3. 6229	-0.0388
Н	5, 3173	2,7079	-0.1134
II	0 5471	2 1160	2 7200
П	-0. 3471	-3.1108	5.7590
Н	1.5632	-3.8440	-2.6473
Н	1 9015	0 3961	-2 2057
TT	F 7005	1 0001	0 0000
Н	-5. (995	1.2501	-0.0829
Н	3.9057	5.3046	0.4699
Ц	4 4040	4 8272	-1 1575
11		T. 0014	1, 1010
Н	2.7184	5.2864	-0.8392
Н	3, 4823	-2.7097	-3.5799
TT	4 0061	1 7400	9 10/0
п	4.0001	-1. (498	-2.1849
Н	3.5061	-0.9367	-3.6740
ſ	-0.4071	-5 2244	-2 1025
U		J. 2211	1. 0000
H	-1.2008	-5.9475	-1.9086
Н	-0.1840	-5.2070	-3.1772
II	0.1010	5. 2010 E E1CO	1 5400
Н	0.4938	-9. 9103	-1. 5480
С	6.3521	0. 5257	0.4066
Н	6 6136	1 2980	1 1413
TT	6.0200	0.0747	0 6001
Н	0. 9303	-0.3(4)	0.0031
H	6.5804	0.8931	-0.6024
0	-2.4606	-1.2486	3.8985
U U	_9 4740	_9_0014	4 9704
П	-2.4148	-2.0914	4. 3/94
0	-4.5009	3. 5629	-1.0724
Н	-5.4648	3.4793	-0.9988
C1	-2 3450	1 9910	2 1/20
	-2. 3439	1.2210	2.4430
61	- 0010	1 9 717E	1 9447

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

atom	Λ	1	L
С	-4.5622	1, 1514	0.8246
0	1.0022		0.0210
C	-3.8845	2.3625	0.7553
С	-2,4726	2.3849	0.7628
C	1 7444	1 2010	0.9796
L L	-1. 7444	1.2019	0.8786
С	-2.4335	-0.0261	1.0094
C	-2 8520	-0.0491	0.0267
U	-3. 8529	-0.0401	0.9307
С	-0.2346	1. 1695	0. 7825
C	0.3710	0.0350	1 5784
C	0.5115	0.0550	1.5704
C	-0.3111	-1. 1916	1.7225
C	-1 7145	-1 2882	1 2678
0	1.1110	1.2002	1.2010
C	1.6416	0.2046	2.1287
С	2,2866	-0.8408	2, 7941
C .	1 6207	2 0675	2 0105
U.	1.0307	-2.0075	2.9195
С	0.3458	-2.2595	2.3979
C	0 2345	1 1694	-0 7827
	1 7440	1.1001	0.1021
C	1.7442	1.2020	-0.8787
С	2 4334	-0.0260	-1 0094
Č	1 7146	1 0000	1 9676
L L	1.7140	-1.2882	-1.2070
С	0.3112	-1.1918	-1.7224
<u> </u>	-0.2710	0.0248	_1 5794
C	0.3715	0.0348	1. 5764
С	-0.3456	-2.2598	-2.3977
C	-1 6305	-2.0679	-2 9194
	1.0000	0.0410	0.7041
C	-2.2866	-0.8412	-2.7941
С	-1.6417	0. 2043	-2.1288
C C	0 4794	0, 2040	0.7020
U	2.4724	2. 3849	-0.7630
С	3.8843	2.3626	-0.7554
ſ	4 5621	1 1515	-0.8247
<u> </u>	4. 5021	1.1313	0.0247
C	3.8528	-0.0480	-0.9367
0	-2.3202	-2.3751	1, 1948
0	2 2205	2 2750	1 1045
0	2. 3203	-2.3730	-1. 1945
С	3. 6880	-0. 6639	3. 3259
C	-3 6879	-0.6645	-3 3260
0	5.0015	0.0045	5. 5200
0	-4. 5558	-1.1870	0.9751
0	-0.3236	-3 4265	2 5264
0		1 1070	0.0759
0	4. 5550	-1. 1870	-0.9752
0	0.3239	-3.4267	-2.5261
U	-2 9740	_1 0200	1 0211
Î	-3. 8749	-1. 9200	1.0311
С	0.3001	-4. 5130	3. 1945
Н	3 8746	-1 9199	-1 0314
	0.0110	1.5155	2 1040
L L	-0. 2998	-4. 5133	-3. 1942
Н	0.1647	2.1110	1.1666
Ц	-0.1649	2 1109	-1 1668
11	0.1045	2.1109	1.1008
Н	2.1334	-2.8775	3. 4343
Н	-2 1332	-2.8780	-3 4341
II	1 0011	4 0000	
Н	-1.2211	-4. 8228	-2.6850
Н	1.2215	-4.8225	2.6853
Ц	-5 6470	1 1122	0 7036
11	0.0473	1.1100	0.1300
Н	2.1462	1.1605	2.0206
Н	-2 1463	1 1601	-2.0208
II	<b>E</b> C 470	1 1104	0.7020
Н	5.0478	1.1134	-0. 7936
Н	3.8565	0.3601	3.6752
Ц	4 4947	-0.8653	2 5368
11	1.1211	0.0000	2.000
Н	3.8965	-1.3486	4. 1543
Н	-4 4246	-0.8655	-2 5368
11	1. 12 10	1.0405	4 1541
Н	-3.8965	-1. 3495	-4.1541
Н	-3.8564	0.3594	-3.6757
Ц	0 5253	_1 2707	1 9/12
11	0.0200	1.2101	т. 4410
Н	-0. 4242	-5.3282	3.1600
Н	-0. 5249	-4, 2711	-4.2410
TT	0.0210	E 200E	9 1505
Н	0.4246	-9. 3789	-3. 1995
0	-4.5340	3. 5493	0.6633
Ц	-5 /000	3 3 2 2 1 1	0 6801
11	0.4000	0.5044	0.0034
0	4. 5339	3. 5494	-0.6635
Н	5 4898	3, 3845	-0.6895
	0, 70.00		
C1	_1 6000	2 0506	0 6969
C1	-1. 6903	3.9506	0. 6363

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

atom	Λ	I	L
C	-0.9004	-25770	2 7504
C .	0. 5004	2.0110	2.1504
C	-1.7060	-1.4534	2.8808
C	-1 3237	-0.2309	2 2815
0	1.0201	0.2303	2.2010
C	-0.1379	-0.1434	1.5553
С	0 7286	-1 2619	1 5028
<u>C</u>	0.1200	0.4074	1.0020
C	0.3197	-2.4974	2.0709
С	0 2619	1 0847	0 7724
<u>C</u>	1 7504	1 0100	0.0145
C	1.7564	1.3196	0.8145
С	2.6492	0. 2328	0.8457
C C	9 1022	1 1200	0.0051
U	2.1035	-1.1382	0. 9851
С	2.2295	2.6314	0.7754
C	2 5070	2 0014	0 7526
U.	5. 5919	2. 9014	0.7550
С	4. 4964	1.8293	0.7715
C	4 0462	0 5052	0.8143
C	4.0402	0.0002	0.0145
C	-0.2619	1.0848	-0.7723
C	0 1379	-0 1433	-1 5553
0	0.1015	0.1400	1.0000
C	-0.7286	-1.2618	-1.5029
С	-2,1033	-1.1382	-0.9853
<u>C</u>	0.0400	0,0000	0.0457
U	-2.6493	0. 2328	-0.8457
С	-1.7564	1, 3196	-0.8144
C	_1 0469	0 5050	_0 01/9
U	-4.0402	0.0002	-0. 8143
С	-4.4964	1.8294	-0.7714
ſ	-3 5000	2 0015	-0.7524
	5. 5960	2. 3013	0.7004
С	-2.2295	2.6315	-0.7751
C	1 3237	-0.2306	-2 2816
<u> </u>	1. 7000	1 4500	2.2010
C	1.7060	-1.4530	-2.8810
С	0, 9005	-2.5768	-2.7506
Č	0.2106	2 4072	2 0711
L	-0.3190	-2.4972	-2.0711
0	2.7927	-2.1564	0.7862
0	-2 7927	-2 1563	-0.7864
0	2.1521	2.1000	0.1004
С	4. 1110	4. 3201	0.6932
C	-4 1111	4 3202	-0.6928
0	1.0710	1.0202	0.0020
0	1.0712	-3.6020	2.0013
0	4.8895	-0.5509	0.8563
0	1.0700	2,6010	2,0015
0	-1.0709	-3. 6019	-2.0015
0	-4.8895	-0.5508	-0.8564
U	1 9902	_2 2479	1 4792
Î	1.0003	-3. 3472	1.4723
С	6. 2897	-0.3192	0.8464
Н	-1 8799	-3 3474	-1 4722
	1.0100 C. 0007	0.0101	0.0405
Ľ	-6.2897	-0.3191	-0.8465
Н	-0.2299	1.9590	1.2045
U	0.2208	1 0501	_1 2042
11	0.2230	1. 5551	1.2043
Н	5. 5595	2.0392	0.7585
Н	-5 5596	2 0392	-0.7584
11	0.0000	0.1004	0.1001
H	-0.0008	0. 1934	0.0707
Н	6.6067	0. 1935	-0.0707
Ц	_1 1096	-3 2000	3 19/0
11	1.1920	J. J <u>4</u> 74	J. 1049
H	1.5191	3. 4549	0.7619
Н	-1 5192	3 4549	-0.7616
11	1 1000	0.1010	0.1010
H	1. 1928	-3. 5288	-3. 1851
Н	3. 3325	5.0389	0.9665
Ц	4 4510	4 5700	_0_2100
11	4.4515	4. 5705	0.3133
H	4.9629	4. 4681	1.3665
Н	-4 4517	4 5709	0 3204
11	1. 1011	1.0100	1 2050
H	-4.9631	4.4082	-1. 3058
Н	-3.3326	5.0390	-0.9662
U U	6 6105	0.2614	1 7102
11	0.0100	0.2044	1.1190
H	6.7479	-1.3086	0.8844
Н	-6 6105	0 2645	-1 7193
11	0.0100	0.2010	1. 1133
H	-6.7479	-1.3086	-0.8846
0	-2.8725	-1.4782	3.5701
11	2,0100	0.0704	2 0000
П	-3. 0193	-2.3794	১. ৬৬৬৬
0	2.8725	-1.4778	-3. 5703
Ц	2 0102	-2 3780	-3 8000
11	5.0135	2.0100	0.5500
C1	-2.3672	1.1556	2.5502
C1	2 3671	1 1559	-2 5501
01	2. 0011	1. 1000	<b>2.</b> 0001

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

atom	Å	Ŷ	L
С	-1.2350	-0.7417	1,6085
C	-0.1464	0 1614	1 4077
<u> </u>	0.1404	0.1014	1.4311
L	1.0598	-0.1373	2.1138
С	1.2493	-1.3536	2.8025
С	0.1998	-2.2599	2.8805
С	-1.0441	-1.9703	2, 3007
C C	-2 5599	-0.3721	1 1297
C	2.0000	0.0721	0.6671
U C	-2. 7959	0.9975	0.0071
C	-1.7136	1.8925	0.5060
С	-0.2866	1.4106	0.6574
С	-4.1248	1.4525	0.4302
С	-4 3472	2 7894	0.0675
C	-3 2726	3 6561	-0.0648
C	1 0601	2.0147	0.1471
C	-1.9601	3. 2147	0.1471
C	1.9131	1.2966	-0.6638
С	2.6645	0.1008	-0. 7016
С	4.0601	0.1540	-0. 4348
С	4 6746	1 3875	-0 1791
C	3 9361	2 5670	-0.1774
C	0.5301	2. 5010	0.1114
L .	2. 5494	2.5060	-0.4112
C	0. 4065	1.2543	-0.8041
С	-0.1018	0.0439	-1.5553
С	0.6632	-1.1526	-1.5597
С	2,0262	-1, 1661	-1.0585
C C	_1 3310	0.0873	-2 1000
<u> </u>	1.0010	1 0606	2.1500
C C	-1.0420	-1.0090	-2.0009
<u> </u>	-1.1350	-2.2670	-2. 7907
С	0.1183	-2. 3192	-2. 1726
0	-3.5192	-1.1968	1.1887
0	2.6889	-2.2469	-1.0094
Н	0, 0896	2, 1545	-1.3401
Н	0.2903	2 2130	1 1288
	0.2303	1 6617	2 4160
C	2. 5928	-1.0017	3.4100
L .	4.6101	3.8982	0.0518
0	-5. 1933	0. 6513	0. 5461
0	-2.0203	-2.8788	2.4400
0	0.7742	-3. 4862	-2.1996
0	4,8306	-0.9455	-0.4113
H	-4 8513	-0.2478	0 7898
II	9,0010	0.2410	1.0050
Н	-2.8212	-2. 5115	1. 9850
H	1.0380	-3.3390	-1.7309
Н	4.2357	-1.7132	-0. 6188
Н	-5.3691	3.1132	-0.0999
0	-3.0526	-0.9485	-3. 4125
Н	-1.5225	-3.1686	-3.2571
Н	-3 3109	-1 8048	-3 7896
II	1 0020	0.5677	2 0522
H	1.8830	0. 5077	2.0532
H	0.3104	-3. 2075	3.3985
Н	-1.1311	3. 9087	0.0341
Н	5.7434	1.3928	0.0121
Н	1,9672	3, 4252	-0.3920
Н	-1 9244	0 9942	-2 2186
Ц	2 0150	-0 8565	4 0879
11	2. 3100	1.7500	1.0014
H	3.3603	-1. (563	2.6372
Н	2.5724	-2. 5946	3.9863
Н	4.7514	4. 4319	-0.8973
Н	5.5954	3.7758	0.5112
Н	4.0076	4.5457	0.6986
Н	-3 4594	4 6929	-0 3366
11	J. 1041	1. 0040	0.0000
### Cartesian coordinates of **14**-II optimized at the gas-phase B3LYP/6-31G(d) level

atom	Λ	I	L
С	2.6743	0. 4941	0.6179
C	1 71/19	1 52/1	0.4886
C	2 1075	1. J241 9. 7097	0.4000
C C	2.1073	2.1031	0.0550
C	3. 4482	3.0569	-0.2785
С	4. 3894	2.0358	-0.1888
С	4.0231	0.7564	0.2507
С	2.2966	-0.8066	1.1656
С	0.9751	-0.9669	1.7672
С	0.0068	0.0637	1.6587
C	0.2502	1 2327	0.7311
C	0.6034	-2 1150	2 5611
C	0.0334	2.1150	2.3011
U C	-0. 5211	-2. 1962	3. 2392 9. 1700
L C	-1.4356	-1. 1592	3.1709
С	-1. 1816	-0. 0330	2. 3741
С	-0. 1850	-0. 2338	-1. 3829
С	-1.0919	-1.3225	-1.3221
С	-0.7072	-2.5725	-1.8812
С	0.5456	-2.7064	-2.4983
С	1.4142	-1.6265	-2.5874
C	1 0313	-0.3878	-2.0324
C	-0.5196	1 0692	-0.6912
C	-2 0020	1.0052	-0.5012
C	-2.0039	1. 3017	-0.3018
C C	-2.9020	0.2086	-0. 4855
C	-2. 4434	-1.1367	-0.8075
С	-2.4660	2.5910	-0. 2798
С	-3. 8297	2.8132	-0.0255
С	-4.7316	1.7535	0.0214
С	-4.2795	0.4497	-0.2058
0	3.1384	-1.7517	1.1978
0	-3.2393	-2.1204	-0.7189
Н	-0.1249	1.8941	-1, 2931
Н	-0.2045	2 1259	1 1714
C II	3 8551	4 4452	-0 7090
C	2 7660	-1 7658	-3 2412
0	2.7009 1 EEEE	2 1226	2, 6012
0	1.0000	-3.1330	2.0912
0	4. 9791	-0. 1846	0.3029
0	-5. 1815	-0. 5387	-0.1533
0	-1.5053	-3. 6497	-1.8575
Н	2. 3494	-2. 9116	2.1408
Н	4. 5453	-1.0126	0.6371
Н	-4.6859	-1.3830	-0.3316
Н	-2.3413	-3.3766	-1.3987
Н	-0. 7083	-3.0770	3.8643
0	-4.2120	4.1027	0.1732
Н	-5 7877	1 9094	0 2242
Н	-5.1702	4 1325	0.3246
Н	1 3669	3 5760	-0.03/3
II	1. 3003 E 4202	2 2047	0.0545
П	0.4292	2.2047	-0.4010
H	-1.9107	0.7626	2.3139
H	0.8075	-3.6761	-2.9103
Н	1.7113	0. 4552	-2.1058
Н	-1.7958	3. 4448	-0. 3010
Н	3.8985	5.1232	0.1534
Н	4.8419	4. 4468	-1.1811
Н	3.1350	4.8712	-1.4168
Н	3, 5686	-1.6298	-2.5041
Н	2 8939	-2,7500	-3 7009
Ц	2.0000	-1 0049	-4 0160
11	4. J144 0. 0600	1.0042	2 7050
н	-2. 3083	-1.2207	J. 12DJ

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

atom	Λ	I	L
С	0, 6697	-1, 1326	-1.5689
C	0.1065	0.0542	1.5000
C	-0.1005	0.0342	-1. 3312
C	-1.3581	0.0770	-2.1291
С	-1.9023	-1.0760	-2.7327
С	-1.1625	-2.2513	-2.7390
С С	0 11020	_2 2075	_2 1715
C C	0.1196	-2.2970	-2.1710
C	2.0506	-1.1331	-1.1020
С	2.6772	0.1315	-0. 7383
С	1.9143	1.3206	-0.6658
C	0.4061	1 2666	-0.7863
C	4.0015	0.1060	0. 1005
U	4.0815	0. 1960	-0. 5015
C	4. 6933	1. 4255	-0. 2378
С	3.9223	2.5847	-0.2029
С	2,5331	2,5351	-0.4073
C	-0 1186	0 1636	1 5162
C	1 2007	0. 7496	1.6160
C	-1.2007	-0.7480	1.0108
С	-1.0034	-1.9803	2.3015
С	0.2392	-2.2618	2.8881
С	1.2825	-1.3478	2.8184
C C	1 0886	-0.1308	2 1310
C	0.0070	1, 4170	2.1013
<u> </u>	-0.2078	1.4178	0.6854
C	-1.6972	1.8942	0. 5463
С	-2.7710	0.9855	0.6828
С	-2.5244	-0.3881	1.1293
C	-1 9541	3 2197	0.2071
<u> </u>	2 2600	2 6402	0.0125
C	-3. 2009	5. 0495	-0.0135
C	-4. 3348	2.7668	0.0864
С	-4.1009	1.4270	0. 4294
0	2.7266	-2.2067	-1.0892
0	-3,4759	-1.2230	1, 1676
U U	0.2114	2 2102	1.1554
	0.0701	2.2192	1.1004
H	0.0781	2.1007	-1.3160
C	-3. 2833	-1.0216	-3. 3381
С	2.6233	-1.6479	3.4418
0	4.8597	-0.8950	-0.5188
0	0.7859	-3 4594	-2 2371
0	E 1607	0.6057	0 E02E
0	-5. 1597	0.0007	0. 5035
0	-1.9719	-2.8985	2. 4289
Н	4.2628	-1.6641	-0.7259
Н	1.6633	-3.3123	-1.7990
Н	-4.8102	-0.2879	0.7584
Ц	-2 7715	-2 5398	1 9655
0	4.4015	2.0007	1. 3033
0	4. 4015	3.8097	0.0340
H	5.7667	1. 4470	-0.0708
Н	-5.3579	3.0813	-0.0911
Н	-1.9393	0, 9939	-2.1238
Н	-1 5510	-3 1597	-3 1891
Ц	1.0679	2 4607	-0.3505
II	1. 9078	5.4007	-0.3395
H	0.3542	-3.2105	3. 4032
Н	1.9073	0.5801	2.0759
Н	-1.1314	3. 9238	0. 1132
Н	-3.3573	-0.2197	-4.0826
Н	-3 5478	-1 96/15	-3 82/18
11	4 0007	0.0141	0.0240
H	-4.0367	-0.8141	-2.50/6
Н	2.6042	-2. 5815	4. 0112
Н	3. 3979	-1.7375	2.6695
Н	2.9348	-0.8414	4.1165
Ц	5 4916	3 7911	0 1/52
11	0. 1410	4 0000	0.0000
Н	-3.4579	4. 6888	-0.2688

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

atom	Λ	1	L
С	-2,8998	0.1932	-0. 4394
C C	-2.0011	1 2827	-0.4807
C	2.0011	1.2021	0.4007
L .	-2.4008	2.5722	-0.2534
C	-3. 8229	2.8205	0. 0305
С	-4.7064	1.7480	0.0993
С	-4.2667	0.4367	-0.1305
С	-2.4448	-1.1580	-0.7661
C	-1 1124	-1 3416	-1 3149
C	_0.2028	-0.2520	_1 2008
C	0.2030	0.2009	1. 3330
<u> </u>	-0. 5208	1.0479	-0.6971
C	-0.7480	-2. 5933	-1.8938
C	0. 4735	-2.7297	-2.5609
С	1.3251	-1.6350	-2.6647
С	0.9919	-0.3966	-2.0847
С	1.7366	1.5088	0.4471
С	2,7128	0.4969	0.5959
C C	4 0618	0.7806	0.2427
C	4. 4075	2,0502	0.2121
C	4.4075	2.0593	-0.2100
C	3. 4481	5.0594	-0. 3340
C	2.1103	2.7675	-0.0064
С	0.2764	1.2071	0. 7087
С	0.0507	0. 0382	1.6417
С	1.0325	-0.9789	1.7551
С	2.3546	-0.8025	1.1580
С	-1.1346	-0.0689	2.3614
C	-1.3740	-1.1944	3, 1635
C	-0 4469	-2 2197	3 2552
<u> </u>	0.7664	-2 1258	2 5567
0	2 2200	2.1250	2. 5501
0	-3. 2309	-2.1403	-0.0309
0	3. 2115	-1.7331	1.2067
Н	-0.1742	2.0981	1.1580
H	-0.1350	1.8715	-1.3063
С	-4.3092	4.2351	0.2345
С	3.8323	4.4468	-0.7884
0	-1.5476	-3.6659	-1.8410
0	-5.1733	-0.5486	-0.0498
0	1,6428	-3, 1314	2, 6936
0	5 0382	-0.1335	0.3349
H	-2 3662	-3 3870	-1 3509
Ц	_1 6995	-1 2060	-0.2217
II	9 4279	2 2065	0.2317
П	2.4372	-2. 6903	2.1400
Н	4.0152	-0.9718	U. 000U
0	2. 5128	-1.6964	-3. 3199
H	0. 7222	-3.6929	-2.9980
H	-0.6220	-3. 0996	3.8652
Н	-1.7721	3. 4088	-0.2969
Н	-5.7575	1.8986	0.3262
Н	1.6904	0.4256	-2.1834
Н	5, 4466	2, 2433	-0.4714
Н	1 3571	3 5462	-0.1093
Н	-1 8791	0.7175	2 3002
II	4. 2026	4.7619	2. 3002 0. 72E6
П	-4. 3920	4. (012	-0.7200
H	-5. 2943	4.2500	0.7098
H	-3.6151	4.8106	0.8574
Н	3.1084	4.8468	-1.5074
Н	4.8211	4.4570	-1.2562
Н	3.8600	5.1413	0.0616
Н	-2.3050	-1.2642	3.7198
Н	2.6434	-2.5945	-3.6640

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

atom	Х	Y	Z
C	0.0000	0 0441	1 0220
U	-0. 9896	-0.0441	1. 9329
С	0.1392	0.6858	1.4785
<u>C</u>	1 0700	0.4004	
C	1.3790	0.4664	2.0602
С	1 5573	-0 5153	3 0572
		1.0007	0.0012
C	0.4637	-1.2607	3.4788
С	-0.8108	-1 0353	2 9383
<u>C</u>	0.0100	0.0014	1 4000
U	-2.3284	0.2914	1.4083
С	-2.5197	1, 4847	0.6407
<u>C</u>	1 4000	0, 1000	0 1414
U	-1.4029	2. 1929	0. 1414
С	-0.0023	1,6486	0.3216
C	2 0222	1 0609	0.2702
U	-3. 8333	1.9692	0. 3783
С	-4.0035	3. 1574	-0.3477
C C	2,0020	2 9490	0.0106
U	-2. 8932	3. 8460	-0.8100
С	-1.5977	3. 3709	-0.5745
C	2 0449	0.0624	-1 0714
U	2.0440	0.9024	-1.0714
С	2.7133	-0.2539	-0.8065
C	1 1996	0.2490	0.6725
U .	4.1200	-0.2409	-0.0723
С	4.8411	0.9456	-0.8460
C	4 1813	2 1345	-1 1425
<u>C</u>	0.7770	0 1010	1.0410
U	2.1113	2.1311	-1.2418
С	0.5318	1.0149	-1.0768
C C	0 1915	0 2121	1 2022
U. U.	-0.1213	-0.3121	-1. 3922
С	0.5640	-1.5214	-1.0944
C	1 9650	-1 5083	-0 7163
0	1. 5050	1.0000	0.1100
С	-1.3994	-0.3515	-1.9169
С	-2.0468	-1.5895	-2.1255
C	1 4150	2,0000	1 0000
<u> </u>	-1.4150	-2. 7870	-1.8022
С	-0.1114	-2.7596	-1.2896
0	-3 3290	-0.3900	1 8/03
0	0.5250	0.000	0.0000
0	2. 5614	-2.5813	-0. 3938
Н	0.2198	1.7447	-1.8305
U U	0.6694	2 4074	0,4000
П	0.0004	2.4974	0.4909
С	2.9335	-0.7604	3.6246
C	4 9565	3 4090	-1 3744
0	1.0000	1, 2254	0.0055
0	-4. 9351	1. 3354	0.8055
0	-1.8253	-1.7724	3. 4130
0	0 4638	-3 0370	-1 0153
0	0.4030	5.5515	1.0100
0	4.8271	-1.3571	-0.3767
Н	-4.6289	0.5197	1, 2805
II	9 6419	1 4709	2 0222
11	-2.0418	-1. 4798	2.9322
H	1.3764	-3.7377	-0.6770
Н	4 1668	-2,0953	-0 2991
II	E 0120	2.5007	0 5274
П	-5.0138	5. 3097	-0. 3274
0	-3.2935	-1.5006	-2.6458
Н	-1 8828	-3 7533	-1 9397
11	0.0050	1.0404	1 7001
Н	2.2359	1.0464	1.7321
Н	0.5639	-2.0278	4.2404
U	-0.7404	2 0242	_0_0402
11	0.7404	3. 5243	0. 5452
Н	5. 9219	0.9120	-0.7463
Н	2 2581	3 0633	-1 4552
II	1,0260	0 5547	9 1711
H	-1. 9369	0. 5547	-2.1711
Н	3. 3761	0. 1682	4.0048
Н	3 6080	-1 1427	2 8477
11		1.1741	
<u>H</u>	2.9104	-1.4877	4. 4410
Н	5,0306	3.6305	-2.4473
U	5 07/0	3 2260	_0 0014
П	5. 9149	3. 3300	-0. 9014
H	4.4661	4.2674	-0.9018
C	-4 0.0277	-2 6997	-2.8686
11	4 0000		2.0000
Н	-4.9890	-2.3855	-3.2115
Н	-3.5178	-3.3510	-3.5889
Ц	-1 1809	-3 2468	-1 0210
11	т. 1034	J. 2400	1. 3313
і Н	-3.0316	4.7730	-1.3641

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

atom	Х	Y	Z
C	2 7229	0 9173	0 6174
<u>C</u>	1 5700	1 7205	0.0111
C	1.5788	1. 7325	0.4623
С	1.7177	3. 0380	0.0076
ſ	2 9805	3 5685	-0.3177
0	2.3000	0.7501	0.011
C	4. 1058	2.7581	-0.2010
С	3, 9968	1, 4384	0.2577
C .	2 6061	-0.4252	1 1917
0	2.0001	0.4232	1. 1017
L	1. 3359	-0. 8394	1.7723
С	0. 1834	-0.0234	1.6423
C	0 1988	1 1604	0 7019
C	1 2702	2 0116	2 5700
Û	1.2795	-2.0110	2.3790
C	0.0978	-2. 3247	3.2680
С	-1.0033	-1.4911	3.1589
	-0.9695	-0.3458	2 3/00
C	0. 0000	0.0400	1, 2050
L	0.0649	-0.3973	-1. 3858
С	-0.6210	-1.6362	-1.3059
C	-0.0036	-2 8018	-1 8375
C	1.0560	2.0010	2 4470
U U	1.2005	-2. 7090	-2.4479
С	1.9062	-1.4865	-2.5571
С	1.2934	-0.3318	-2.0277
C	-0.5144	0.9221	-0.7214
<u>C</u>	-0. 5144	0.0321	-0. 7214
C	-2.0181	0. 7848	-0.5461
С	-2.6942	-0.4591	-0.5099
C	-1 9881	-1 6993	-0.8006
<u>C</u>	0.7101	1.0000	0.0000
U	-2. 7191	1.9637	-0.3570
С	-4.1077	1.9370	-0.1162
С	-4, 7926	0.7254	-0.0496
Č	-4 0927	-0.4729	-0.2438
0	4. 0921	0.4729	0.2430
0	3.6194	-1. 1822	1. 2367
0	-2.5841	-2.8141	-0.6941
Н	-0.2761	1, 7053	-1.3373
U II	-0.4266	1.0500	1 1999
11	-0.4200	1. 9509	1.1200
C	3. 1073	5.0033	-0.7689
С	3.2642	-1.3810	-3.2065
0	2 3253	-2 8368	2 7303
0	E 1906	0.7094	0.2255
0	5.1206	0.7084	0. 3355
0	-4. 7946	-1.6120	-0.1722
0	-0.5842	-4.0098	-1.7943
Н	3 0656	-2 4669	2 1849
11	<b>3.0000</b>	0 1040	0.0701
Н	4. 8001	-0. 1849	0.0781
Н	-4.1484	-2.3524	-0.3280
Н	-1.4604	-3.8902	-1.3445
Н	0.0827	-3 2185	3 8828
0	4 6006	0.2100	0.0414
0	-4. 0880	3. 1521	0.0414
Н	-5.8563	0.6631	0. 1411
Н	0.8351	3,6651	-0.1013
Н	5 09/1	3 1271	-0.4579
11	1.0464	0,0000	0.4373
H	-1.8464	0.2882	2.2131
Н	1.6988	-3.6199	-2.8393
Н	1,8034	0.6226	-2.1150
Ц	-2 2241	2 0204	-0.3033
11	2.2241	5. 0000	0.0010
H	3. 0231	5.6886	0.0848
Н	4.0724	5.1901	-1.2488
Н	2.3142	5.2715	-1.4759
Ц	4 0220	_1 0829	_9 /715
П	4.0230	-1.0032	-2.4/10
H	3. 5757	-2.3322	-3.6472
Н	3. 2673	-0. 6202	-3. 9963
C	-6.0920	3 2112	0 2712
U 11	C 0044	4 9710	0.2112
Н	-0.3344	4.2/19	0.3010
Н	-6.6512	2.7694	-0. 5625
Н	-6.3655	2.7020	1.2035
Ц	_1 0110	-1 7305	3 7067
11	1. JIIU	1.1000	0.1001

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

atom	Х	Ŷ	
C	0.0000	1 0007	1 5500
C	0.2690	-1.3237	-1.5598
C	-0.3105	-0.0292	-1 5359
0	0.0100	0.0252	1.0000
С	-1.5479	0. 1817	-2.1267
C	-2 2703	-0.8794	-2 7114
0	2.2103	0.0154	2.7114
С	-1.7228	-2.1557	-2.7078
C	-0.4500	_2 2051	_2 1452
0	0.4333	2.3331	2.1400
С	1.6350	-1.5352	-1.0950
C	2 4554	-0.3803	-0.7571
L	2.4004	-0. 3802	-0.7371
С	1,8904	0.9176	-0.7052
C	0.2011	1 0070	0.0100
U	0. 3911	1.0970	-0. 8102
С	3.8510	-0.5314	-0.5238
C	4 6507	0 5000	0.9977
U	4.0587	0. 5888	-0. 2877
С	4, 0830	1.8580	-0.2758
C	0,000	0.0100	0 4750
U	2.0908	2.0192	-0.4758
С	-0.2694	0.1004	1.5057
<u>C</u>	1 4770		1 0001
C	-1.4778	-0.6339	1.6251
C	-1 4641	-1 8782	2 3152
<u>C</u>	0.0710	1.0102	0.0004
C	-0.2718	-2.3466	2.8864
ſ	0 8995	-1 6054	2 7972
0	0.0057	1.0001	2.1912
C	0.8857	-0.3745	2.1085
ſ	-0.2344	1 3586	0 6687
	0.2011	1.0000	0.0001
С	-1.5752	2.0478	0. 5407
C	-2 7736	1 3138	0 6911
0	2.1150	1.0100	0.0311
C	-2.7355	-0.0782	1.1467
C	-1 6304	3 3955	0 1958
<u> </u>	1.0304	5.5555	0.1556
С	-2.8663	4.0189	-0.0178
C	-4 0531	3 3001	0 0950
<u> </u>	4.0331	5. 5051	0.0550
С	-4.0228	1.9511	0.4447
0	9 1317	-2 7026	-1 0641
0	2.1317	2. 1020	1.0041
0	-3.8033	-0.7571	1.2004
Ц	0 4672	2 0640	1 1257
11	0.4072	2.0040	1.1201
H	0. 1979	2.0326	-1.3445
C	-3 6326	-0.6180	-3 3055
0	5.0520	0.0100	5.5055
С	2.1878	-2.1111	3.3977
0	4 4479	-1 7326	-0 5178
0	4.4472	1.7320	0.0178
0	0.0162	-3.6477	-2.1978
0	-5 1036	1 3006	0 5313
0	0.1000	1. 5000	0.0010
0	-2.5611	-2.6350	2.4603
Н	3 7353	-2 4012	-0 7094
11	0.1000	2.4012	0.1034
Н	0.9068	-3.6337	-1.7614
Н	-4 9812	0 3659	0 7905
11	1. 5012	0.0000	0.1500
Н	-3. 3007	-2.1603	2.0016
0	4 7733	3 0069	-0.0721
		0.4005	0.1000
Н	5.7162	0. 4235	-0.1266
Н	-5.0180	3.7746	-0.0769
11	1.0700	1 1700	0.0100
Н	-1.9789	1. 1782	-2.1299
Н	-2 2517	-2 9972	-3 1445
11	2.2011	2:0014	0.1110
Н	2.2878	3. 0244	-0.4432
Н	-0.2975	-3 3006	3 4038
11	1 0001	0.0000	0. 1000
Н	1.8031	0.2018	2.0380
Н	-0 7107	3 9654	0 0918
11	2, 5040	0.1055	4 0200
Н	-3. 5949	0.1955	-4.0399
Н	-4.0345	-1.5067	-3,8003
TT	4 9490	0 0100	
<u>н</u>	-4. 3430	-0.3138	-2. 5262
H	2.0305	-3.0212	3.9836
II	2 0170	0 0070	9 6100
Н	2.9179	-2.3313	2.0100
н	2.6435	-1.3571	4.0506
C	6 1907	2 0206	0 1965
L	0.1807	2.9300	0.1205
Н	6. 6826	2.4888	-0.7428
U	6 5179	3 0601	0.2574
п	0.0172	5. 9001	0.2014
Н	6. 4263	2.3489	1.0235
TT	0.0071	E 0707	0 0700
П	-2.09/1	0.0131	-0.2182

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Cartesian coordi	nates of 15-IV opt	imized at the gas-	phase B3LYP/6-3	G(d) level
a <b>t</b> a m	V	V	7	

atom	λ	Ĭ	L
C	-2 9689	-0.0728	-0 5423
0	2.5005	1.0707	0.0120
C	-2.1700	1. 0787	-0.7226
C	-2 7645	2 3347	-0.7561
0	2.1045	2.0011	0.1001
C	-4. 1547	2.4901	-0.6009
C	-4 9420	1 3616	-0.3952
0	1. 5120	1. 5010	0.0002
C	-4.3714	0.0813	-0.3632
C	-2 3727	-1 4078	-0 5978
0	2.0121	1. 1010	0.0010
C	-0.9917	-1.5469	-1.0233
C	-0.1782	-0.4024	-1 2450
0	0.1102	0. 1021	1.2100
C	-0.6622	0.9611	-0.8028
С	-0 4727	-2 8320	-1 3507
<u>0</u>	0.0044	2.0020	1.0110
C	0.8044	-2.9633	-1.9119
С	1.5623	-1.8222	-2.1581
C	1 0709	-0.5410	_1 9210
U.	1.0702	-0. 5419	-1. 8219
С	1.4501	1.8285	0. 3791
C	2 1911	0 9548	0 7594
0	2.1311	0.0010	0.1034
С	3.8375	1.3038	0. 4442
С	4 1079	2 5153	-0.2070
<u>C</u>	2,0707	2.0100	0.5500
Ľ	3.0787	3. 3836	-0.5560
С	1.7493	3.0231	-0. 2636
<u> </u>	0.0052	1 1949	0 5000
L L	0.0002	1.4040	0. 0999
C	-0. 1901	0.4219	1.7064
C	0.8625	-0.4636	2 0513
<u> </u>	0.0020	0.4000	2.0010
C	2.2060	-0.2621	1.5136
С	-1, 4121	0. 3243	2,3635
C C	_1 6152	-0.6700	2 2219
U.	-1.0152	-0.0700	3. 3310
С	-0.6147	-1.5727	3.6531
С	0 6350	-1 4809	3 0218
0	0.0000	1. 1000	0.0210
0	-3.0843	-2. 4309	-0. 3599
0	3. 1329	-1.0845	1.7737
Ц	-0.5542	2 2204	0.8577
11	0.0042	2.3394	0.0011
Н	-0.3041	1.7045	-1.5223
C	-4 7789	3 8626	-0.6792
<u>C</u>	1.1105	1.7055	1 0011
C	3. 3769	4.7055	-1.2211
0	-1.1750	-3.9563	-1.1585
0	-5 1007	-0.0620	-0.1627
0	-5. 1907	-0.9020	-0.1037
0	1.5804	-2.3609	3.3824
0	4 8776	0 5153	0 7517
U U	0.0510	0.0100	0.7700
H	-2.0510	-3. 6831	-0.7763
Н	-4.6199	-1.7749	-0.1645
Ц	2 2011	-2 1441	2 8542
11	2.3311	2.1441	2.0042
Н	4. 5025	-0.2934	1. 1872
0	2.7953	-1.8307	-2.7177
U U	1 1500	2,0600	2, 1402
П	1.1009	-3. 9009	-2.1493
H	-0.7604	-2.3517	4.3941
Н	-2 1455	3 2171	-0.9062
TT	C 0105	1 4400	0.0010
H	-6.0165	1.4420	-0.2610
Н	1.7011	0.3159	-2.0226
Ц	5 1441	2 7536	-0.4267
11	0.0400	2.1550	0.4201
Н	0.9430	3.6965	-0.5473
Н	-2.2127	1.0156	2, 1239
II	4 0200	4 2040	1 7206
П	-4. 0390	4.2049	-1.7200
Н	-5. 7935	3.8661	-0.2703
Н	-4 1857	4 6033	-0 1311
TT	0.0750	4.0000	0.0070
H	2.6750	4.9086	-2.0378
Н	4.3921	4.7308	-1.6276
<u></u>	3 2055	5 5222	_0 5044
11	J. 2000	0.0044	0.0044
C	3. 3780	-3.0819	-3.0661
Н	2.7754	-3.6068	-3.8175
II	4 9574	0.0000	2 1012
П	4. 30/4	-2.0403	-3. 4843
Н	3. 5010	-3.7222	-2.1843
Ц	-2 5757	-0 7346	3 8360
11	I	0.1010	0.0000

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

atom	Х	Y	Z
C	1 0019	-0.4291	1 9202
L	1. 0918	-0.4381	1. 6295
С	-0.0888	-1.0356	1.3165
C	-1 2008	-0.8678	1 0883
0	1.2300	0.0010	1. 3003
C	-1.3771	-0.0691	3.1476
С	-0.2319	0, 5490	3, 6330
C C	1 0049	0 2722	2,0051
U	1.0048	0. 3732	2.9951
С	2.3916	-0.7426	1.2479
C	2 /903	-1 7927	0 2308
0	2.4505	1.1321	0.2500
C	1. 3209	-2.3695	-0.3144
С	-0.0412	-1.7987	0.0131
<u>C</u>	2 7670	2, 2702	0 1717
U	3.7070	-2.2792	-0.1717
С	3.8500	-3. 3431	-1.0820
C	2 6891	-3 9102	-1 5877
0	2.0031	5. 5102	1.0077
C	1. 4289	-3. 4271	-1.2137
С	-2.0855	-0.7708	-1.1504
<u>C</u>	2.6565	0 4222	0.6756
L L	-2.0505	0. 4323	-0.0750
С	-4.0637	0. 4963	-0.4742
	-1.8642	-0.6104	-0.7884
0	4.0042	0.0104	0.1004
С	-4.3009	-1.7802	-1.2890
С	-2.9048	-1.8507	-1,4553
<u> </u>	0 5000	0.0150	1 0/15
L	-0. 5823	-0.9198	-1.2415
С	0.1460	0. 3993	-1.3896
C	-0 4330	1 5976	-0.8874
<u> </u>	0.4330	1. 3970	0.0074
C	-1.8230	1.6090	-0.4371
С	1.4028	0.4569	-1.9680
<u>C</u>	9 1101	1 6650	2 0209
L	2.1101	1.0059	-2.0308
С	1.5890	2.8372	-1.5073
C	0 2916	2 8143	-0.9282
0	0.2510		1. 0701
0	3.4386	-0.1710	1.6731
0	-2.3291	2.6519	0.0723
Ц	-0.2552	-1 5404	_9 1117
11	0.3333	1. 5404	2.1117
Н	-0.7511	-2.6305	0. 0705
С	-2 7110	0 1207	3 8269
<u> </u>	5 1700	2 0540	1 6601
U	-5.1709	-2.9540	-1.0081
0	4.9149	-1.7607	0.2899
0	2 0724	0 9796	3 5335
0	2.0124	0.0700	0.4000
0	-0. 1882	3.9736	-0.4636
0	-4.6724	1.5877	0.0155
U	1 6666	_1_0246	0.0080
11	4.0000	1.0240	0.000
Н	2.8517	0.7457	2.9670
Н	-1.0925	3, 7792	-0.1058
II	2,0616	2 2621	0.1751
11	-3.9010	2.2021	0.1751
H	-2.1884	-1.3474	1.6100
Н	-0.2615	1 1752	4 5192
II	4 0000	9 7016	1 9650
П	4. 8339	-3. 7010	-1. 3059
Н	2.7599	-4.7420	-2.2838
Н	0 5311	-3 8813	-1 6254
11	C. 0011	0.0010	0.0001
Н	-5. 9352	-0. 5238	-0.6320
Н	-2.4609	-2.7714	-1.8288
Ц	1 8540	-0.4409	-2 3770
11	1.0540	0.4403	2.3110
Н	3. 0988	1.6709	-2.4925
Н	-2.6158	0.7045	4.7468
II	2.0100	0.010	2 1044
П	-3. 4128	0.0430	3. 1044
H	-3. 1669	-0.8443	4.0795
Н	-6 1684	-2 8745	-1 2259
11	4 7004	2.0110	1.0447
H	-4. /264	-3.9020	-1.3447
Н	$-5.29\overline{48}$	-3.0111	-2.7575
0	2 1009	1 0512	_1 5024
0	2.1992	4.0010	1. 0004
C	3.5061	4.1387	-2.0475
Н	3, 5177	3, 8785	-3.1147
II	2 0000	5 1001	_1 0960
П	3. 8088	D. 1801	-1.9209
Н	4.2103	3. 4898	-1.5099

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

atom	Х	Ŷ	Z
C	2 8765	0 7315	0 6422
C	1 0070	1 6652	0.4021
C	1.0273	1.0000	0.4631
С	2.1092	2.9516	0. 0396
С	3. 4244	3. 3463	-0.2707
C	4 4556	2 4196	-0 1497
C	4 2022	1 1161	0.0000
Ū	4. 2023	1.1101	0.2983
С	2.6117	-0. 5939	1. 1966
С	1.2990	-0.8736	1.7727
ſ	0.2416	0.0622	1 6384
C	0.2410	1.9420	0.7070
<u> </u>	0.3922	1.2430	0.1010
	1.1091	-2.0394	2.5683
С	-0.1071	-2.2308	3.2416
С	-1.1118	-1.2836	3.1287
C	-0.9470	-0 1417	2 3309
C	0.1126	-0.2604	_1 2070
C	0.1120	-0.2094	-1. 3979
C	-0.6929	-1. 4358	-1.3260
С	-0.1899	-2.6551	-1.8613
С	1,0731	-2.6828	-2.4713
C C	1 8396	-1 529/	-2 5727
C	1.0000	0.2220	2.0121
L .	1. 3428	-0. 3229	-2.0300
С	-0.3444	1.0047	-0. 7236
С	-1.8449	1.1043	-0.5623
С	-2.6500	-0.0625	-0.5298
- C	-2.0577	-1 3714	-0.8202
C	2.0011	0.0000	0.0202
(	-2.4466	2.3388	-0.3770
С	-3.8282	2.4463	-0. 1489
С	-4.6302	1.3131	-0.0926
С	-4.0412	0.0348	-0.2817
0	3 5370	-1 4553	1 2552
0	0.0019	1.4000	0.7190
0	-2.7540	-2.4234	-0.7129
H	-0.0118	1.8556	-1. 3273
Н	-0.1487	2.0935	1.1343
С	3, 7081	4, 7622	-0.7101
Č	3,2016	-1 5533	-3 2215
0	2.0506	1.0000	0.7001
0	2.0596	-2.9723	2.7231
0	5. 2413	0.2704	0.3820
0	-4.8542	-1.0268	-0.2216
0	-0.8836	-3.8013	-1.8227
Н	2 8415	-2 6788	2 1891
II	4 0000	0.5017	0.7169
	4.0000		0.7102
H	-4. 2805	-1.8240	-0.3675
H	-1.7425	-3.6020	-1.3688
Н	1.2993	3.6697	-0.0717
Н	5.4802	2,6829	-0.3945
Н	-0.2243	-3 1228	3 8478
U	-2.0461	-1 4204	2 6642
	-2.0401	-1.4294	0.0043
H	-1.7509	0.5822	2.2518
Н	1.4249	-3.6306	-2.8669
Н	1.9461	0.5762	-2.1156
Н	-1.8474	3, 2454	-0.4081
Ц	-1 2660	3 4296	-0.0185
II	2, 6000	5. 4230 E. 4471	0.0100
H	3. 0908	5.4471	0. 1479
H	4.6918	4.8475	-1.1810
Н	2.9546	5.1185	-1.4215
Н	3.9837	-1.3149	-2.4895
Н	3, 4273	-2, 5335	-3,6508
Ц	3 9791	-0.8053	-4 0206
	J. 2121	1 2004	T. 0200
0	-5. 9/18	1.3024	0.1291
С	-6.6243	2.5480	0.3092
Н	$-6.\overline{5240}$	3. 1884	-0.5775
Н	-7.6779	2.3118	0.4666
Ц	-6 2272	3 08/1	1 1865
11	0.4014	0.0011	1. 1000

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

atom	Х	Ŷ	
C	1 4554	0 6902	1 6265
U	-1.4004	-0.0893	1.0205
С	-0.3394	0. 1800	1.5142
ſ	0 8638	-0 1657	2 1113
0	1.0107	1 2027	2.1110
U	1.0197	-1. 3937	2. 1818
С	-0.0583	-2.2658	2.8688
C	-1 2073	-1 0212	2 3030
<u>C</u>	-1. 2973	-1. 9313	2.3030
С	-2.7696	-0.2758	1.1567
C	-2.9671	1 1072	0 7143
C	1 9509	1 0722	0 5676
U	-1. 8598	1.9732	0. 5676
С	-0.4492	1.4408	0.6882
C	-4 2814	1 6006	0 4758
C	4 4000	1.0000	0.1275
U	-4.4668	2.9490	0.1375
С	-3.3683	3. 7894	0.0273
ſ	-2 0691	3 3087	0 2331
0	2.0031	0.0050	0.2001
C	-0. 3797	0.0859	-1.5359
С	0. 3287	-1.1435	-1.5754
C	0.2905	2 2764	9 1759
<u>C</u>	-0.2893	-2.2704	-2.1735
С	-1.5676	-2.1572	-2.7413
С	-2 2398	-0.9420	-2 7321
C	1 6200	0.1791	2,1021
U U	-1.0300	0.1761	-2.1291
С	0. 2039	1.2657	-0.7922
C	1 7121	1 2366	-0.6932
<u> </u>	0 4150	0.0070	0.7507
U. L	2.4152	0.0072	-0. 7567
С	1.7061	-1.2266	-1.1087
C	2 4209	2 4029	-0 4536
C	2.1205	2.1023	0. 2506
U	3. 8118	2. 3799	-0.2596
С	4. 5142	1. 1812	-0.2888
С	3, 8134	-0.0287	-0.5361
0	2 7521	1 0794	1, 2062
0	-3.7331	-1.0724	1.2002
0	2.3125	-2.3382	-1.0862
Н	-0.0866	2.1841	-1.3129
Ц	0 1682	2 9174	1 1510
11	0.1082	2.2174	1.1510
0	2.3578	-1.7517	3. 3859
С	-3.6176	-0.8099	-3. 3327
0	-5 3703	0.8206	0 5594
0	0.0100	0.0200	0.0004
0	-2. 2999	-2.8107	2. 4405
0	4. 5308	-1.1601	-0.5485
0	0 3070	-3 4751	-2 2400
0	0.0010	0.0004	2.2400
H	-5. 0523	-0.0864	0.8091
Н	-3.0908	-2.4185	1.9896
Н	3 8880	-1 8927	-0 7397
II	1 1907	2 2016	1 7094
П	1. 1097	-3. 3810	-1. 7964
Н	1.7096	0.5117	2.0457
Н	0.0265	-3.2215	3, 3767
Н	-3 5196	1 8359	-0.2246
11	5.5150	4.0000	0.2240
H	-1.2205	3. 9804	0. 1312
Н	-2.0082	-3.0421	-3.1900
Н	-2 1599	1 1257	-2 1193
11	1 0007	2, 2500	0 4110
Н	1. 8997	3. 3560	-0.4110
Н	4. 3351	3. 3130	-0.0844
Н	2.7172	-0.9593	4, 0534
U U	2 1120	_1 9749	2 5001
11	5.1150	-1.0740	2. 3991
H	2.3091	-2.6834	3.9565
Н	$-3.64\overline{95}$	$-0.00\overline{26}$	-4.0744
Ц	-4 3558	-0 5636	-2 5580
11	T. JUJU	1 7050	
Н	-3.9354	-1.7353	-3.8213
0	5.8539	1.0431	-0.1006
ſ	6 6151	2 2142	0 1429
	0.0101	0.7007	1.0004
Н	0.2905	2.1231	1.0004
Н	7.6466	1.8788	0.2621
Н	6 5570	2 9169	-0 6993
TT	E 4700	2.0100	0.0000
Н	-5.4/89	J. JUJJ	-0.0286

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

atom	Х	Ŷ	
0	0 5014	1 1000	0 5140
C	-2.5944	-1.1292	0.5149
C	-1 5235	-1 9683	0 1314
0	1.0200	1. 5005	0.1514
С	-1.7763	-3.1102	-0.6191
C	-2 0925	-2 4470	_1 0202
U	5.0825	5.4475	1.0202
С	-4.1364	-2.6095	-0.6698
C	2 0126	1 4541	0.0019
U	-3.9136	-1.4541	0.0912
С	-2,3601	0 0239	1 3805
0	1.0510	0.0200	1.0000
C	-1.0510	0. 1886	2.0071
C	0.0281	-0.6602	1 6513
U	0.0281	0.0002	1.0313
С	-0.0975	-1.5860	0.4626
C	0 9966	1 1994	2 0649
U	-0. 8800	1.1204	5.0040
С	0.3273	1, 1800	3.7666
0	1 0540	1,1000	0,1005
C	1.3542	0.3138	3. 4285
C	1 2136	-0.6032	2 3765
0	1.2150	0.0002	2.0100
C	2.1370	-1.1216	-0.7193
C	2 0206	0.0154	-0.4167
Ľ	2.9200	0.0154	-0.4107
С	4.3150	-0.1498	-0.1814
Č	4 0020	1 4000	0.0047
U	4. 8938	-1.4220	-0.2847
C	4 1229	-2 5333	-0 6114
0	1. 1225	2.0000	0.0170
C	2.7404	-2.3697	-0.8176
ſ	0.6350	-1 0000	-0.8648
U	0.0330	1.0000	0.0040
С	0.1691	0.3904	-1.2295
C	0.0579	1 5997	0 0077
L	0. 9378	1. 3237	-0.0077
С	2.3232	1.3489	-0.3961
Č	1 0479	0 5000	1 0000
C	-1.0473	0. 5906	-1.8608
С	-1 5224	1 8866	-2 1279
0	1.0221	1.0000	2.1213
C	-0. 7883	3.0060	-1.7620
ſ	0 4759	2 8325	-1 1371
U	0.4155	2.0323	1.1371
0	-3.3085	0.8174	1.6526
0	3 0130	2 3476	-0.0385
0	5.0155	2.3410	0.0303
Н	0. 3197	-1.6895	-1.6548
II.	0.4557	0.5050	0.0007
H	0.4557	-2.5053	0.6807
C	-3 3326	-4 7148	-1 8021
0	0.0020	1.1110	1.0021
С	4. 7594	-3. 8932	-0.7674
0	-1 9505	1 0704	2 1192
0	1.0090	1. 5704	5.4425
0	-4.9750	-0.6914	0. 3936
0	1 1607	2 0407	0 0207
0	1.1007	5. 9407	-0. 8327
0	5, 1186	0.8751	0.1385
U U	0 0077	1 7000	0.0541
Н	-2.6377	1. 7936	2.8541
Н	-4.6321	0.0755	0.9223
TT TT	0.0110	0.0100	0.4100
H	2.0110	3.6400	-0.4199
Н	4 5458	1 6846	0 1788
TT TT	0.0500	2, 2500	0.0007
Н	-0.9502	-3. (388	-0.9037
Н	-5.1558	-2.8311	-0.9710
11	0.0000	0.0400	2,0110
Н	2.2866	0.3469	<u> 3. 9</u> 858
Н	2 0341	-1 2669	2 1262
11	2.0011	1.2005	2.1202
Н	5.9612	-1.5101	-0.1059
Н	2 1330	-3 2401	-1 0601
11	2.1000	5.2401	1.0001
Н	-1.6536	-0.2598	-2.1540
Ц	-2 4705	2 0010	_9 6927
11	-2.4195	2.0019	-2.0237
Н	-3.2840	-5. 5937	-1.1460
II	_9 5705	_1 0560	_9 E9E6
Н	-2. 3193	-4. 8900	-2. 3830
Н	-4.3199	-4. 7081	-2.2731
TT T	4 0200	4 1000	1 0070
H	4.9306	-4.123b	-1.82/3
Н	5 7268	-3 9444	-0.2591
11	4 1151	4 2011	0.0051
Н	4.1171	-4.6844	-0.3651
0	-1 1502	4 2981	-1 9603
	1.1034	1. 2001	1. 5005
I C	-2.4195	4. 5418	-2.5632
Ц	-9 1671	1 1200	-3 2005
П	-2.4074	4.1302	-3. 3003
Н	-3.2400	4. 1232	-1.9652
II	_9 5910	5 6979	_9 6094
Н	-2. 5219	5.0213	-2.0084
Н	0.4249	1.8995	4.5727
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### Cartesian coordinates of 17-I optimized at the gas-phase B3LYP/6-31G(d) level

atom	X	Y	L
C	-0.6492	-0.7018	1 0273
U	-0.0492	-0.7018	1. 9275
С	0.2176	0.3654	1.5787
C .	1 4705	0.4420	2 1500
U	1.4795	0.4420	2.1500
С	1,9459	-0.5544	3, 0319
C	1 1150	1 (004	2 2475
U	1.1159	-1.6224	3.3475
C	-0 1789	-1 7089	2 8149
C	0.1105	1.1005	2.0145
С	-2.0384	-0. 7096	1. 4815
C	9 5794	0 4602	0 7070
U	-2.3734	0.4002	0. 1919
С	-1.7169	1.5163	0.4103
Č	0.0154	1 0014	0. 5450
C	-0.2154	1. 3814	0. 5459
ſ	-3 9756	0 5776	0 5603
0	0.0100	0.0110	0.0000
С	-4.5175	1.7331	-0.0285
C	2 6220	9 7624	0.2706
U	-3. 0332	2.7034	-0. 3700
С	-2,2493	2,6599	-0.1629
Č	1 0171	1 4000	0.0041
C	1.9171	1.4803	-0.8841
ſ	2 9034	0 4738	-0.7817
C	2.3034	0.4150	0.1011
С	4.2647	0.8554	-0.6284
C	4 6119	9 9194	0 6249
U	4.0118	2.2134	-0.0248
С	3 6401	3 2001	-0 7613
0	0.0101	0.2001	0.1010
C	2.2904	2.8189	-0.8794
ſ	0 4501	1 1085	-0.0103
Ŭ	0.4301	1.1005	0. 5105
I C	0.1881	-0.2941	-1.4101
C	1 1016	_1 9047	_1 9795
U	1.1840	-1.2947	-1.2723
С	2.5359	-0.9397	-0.8763
Č	1 0405	0, 0001	1 0505
C	-1.0425	-0.6221	-1.9505
С	-1 3154	-1 9499	-2 3221
0	1.0101	1.0100	2.0221
С	-0.3820	-2.9796	-2.1612
ſ	0.8768	-2 6307	-1 6367
U	0.8708	2.0391	1.0307
0	-2.7933	-1.6920	1, 7595
0	2 4102	1 0245	0.6045
0	3. 4183	-1. 8345	-0. 6945
Н	-0.0666	1 8143	-1 5685
11	0.0000	1.0110	1.0000
Н	0.1851	2.3596	0.8314
ſ	3 3/21	-0 4591	3 5962
0	5.5421	0.4001	5. 5562
С	4.0229	4.6598	-0.8022
0	1 0961	0 4050	0.9051
0	-4.0201	-0.4039	0.8931
0	-0.9334	-2.7543	3, 1862
Ő	1 7007	2.0010	1 5070
0	1.7807	-3.6241	-1.5072
0	5 2522	-0 0424	-0 4797
0	0.2022	0.0121	0. 1101
Н	-4.2735	-1.1401	1. 2793
Ц	-1 8080	-2 6503	2 7205
11	1.0000	2.0303	2.1255
Н	2.6045	-3. 2086	-1.1345
Ц	4 9256	_0 0200	-0 5003
11	4.0230	0. 9366	0.0095
Н	2. 1303	1.2757	1.9054
II	1 4410	_9 /109	4 0106
п	1.4419	-2.4102	4.0190
Н	-1.6194	3, 4931	-0.4596
II		9 4601	0 E1E0
Н	5.0015	2.4091	-0. 5158
Н	1.5269	3.5892	-0.9683
11	1 0101	0 1011	0.0001
Н	-1. 8191	0.1211	-2.0881
Н	3.5418	-1.2573	4.3168
11	4 0001	1.2010	0.7054
Н	4.0891	-0. 5299	2.7954
Н	3 5011	0 5028	4 0986
11	5. 5011	0.0020	1.0500
Н	5.0360	4.8206	-0. 4218
Ц	3 3396	5 2708	-0.2008
11	0.0020	0.2100	0.2030
H H	3. 9905	5.0426	-1.8308
C	-6 0009	1 8616	_0 9779
<u> </u>	0.0000	1.0010	0.2112
Н	-6.4458	2.6856	0.2995
II	-6 2244	9 0961	_1 2206
п	-0. 2244	2.0301	-1. 2280
Н	-6.5136	0.9453	0.0172
<u> </u>	0.7007	4 4000	
<u> </u>	-0.7097	-4.4000	-2. 0000
Н	-0.9215	$-4, \overline{4950}$	-3,6255
TT	0 1014		0 0001
Н	0.1314	- <u>ə. U5</u> 75	-2.3261
Н	-1 5810	-4 7847	-2.0008
	1.0010		2.0000
0	-2.5485	-2.1812	-2.8453
Н	-2 6386	-3 1245	-3 0535
	2.0000	0.0001	0.0000
0	-4.0723	3. 9234	-0. 9303
II	_E 0200	2 0005	_1 0170
п П	-0.0000	J. 092J	-1.01/0

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

atom	Å	Y	L
C	-2 0032	0 4743	-0.7814
U	-2.9032	0.4745	-0.7814
С	-1.9168	1.4808	-0.8838
C	2 2001	2 9104	0.9701
U	-2.2901	2. 8194	-0.8791
С	-3.6397	3.2007	-0.7609
C	4 6115	9 9141	0 6242
U	-4.0115	2.2141	-0.0245
С	-4.2644	0.8560	-0.6278
C		0,0000	0.0700
U	-2. 5359	-0.9392	-0.8762
С	-1.1846	-1,2943	-1.2726
- C	0 1000	0,0000	1 4100
C	-0.1880	-0. 2938	-1.4100
С	-0 4500	1 1088	-0.9101
0	0. 1000	1.1000	1.0071
C	-0.8770	-2.6392	-1.6371
C	0 3818	-2 9791	-2 1615
0	0.0010	2.0101	2.1010
C	1. 3153	-1.9495	-2.3222
ſ	1 0426	-0.6218	-1 9505
0	1.0120	0.0210	1. 5505
С	-0.2176	0.3650	1. 5787
C	0 6491	-0.7023	1 0271
C	0.0451	0.1025	1. 3211
С	0. 1785	-1.7098	2.8140
ſ	-1 1165	-1 6237	3 3461
C	1.1105	1.0251	5.5401
С	-1.9464	-0.5556	3.0307
C	_1 4707	0 4414	9 1407
U	-1.4/9/	0.4414	2.1497
С	0.2156	1.3814	0. 5463
Č.	1 7171	1 5169	0 4109
U	1. (1(1	1. 5162	0.4108
С	2.5735	0.4601	0.7983
C C	2,0295	0.7000	1 4010
C	2.0385	-0. 7099	1.4818
C	2 2495	2 6599	-0.1622
C C	2.2100	0.7000	0. 2700
C	3.0334	2.7033	-0.3700
С	4 5177	1 7329	-0.0280
C C	2.0757	0.5774	0.0200
C	3.9757	0.5774	0. 5607
0	-3 4183	-1 8340	-0 6946
0	0.7000	1.0010	1 7500
0	2. 7932	-1.6924	1. 7592
Н	-0 1849	2 3595	0.8320
11	0.1045	2.0000	0.0520
Н	0.0669	1.8147	-1.5680
ſ	-4 0222	4 6605	-0.8012
0	4.0222	4.0003	0.0012
С	-3. 3430	-0.4607	3.5942
0	-1 7809	-3 6235	-1 5077
0	1.1005	5.0255	1. 0011
0	-5.2520	-0.0417	-0. 4789
0	4 8262	-0.4061	0.8953
0	4. 8202	-0.4001	0.8955
0	0. 9330	-2.7553	3. 1853
II	2 6047	2 2000	1 1951
П	-2.0047	-3.2080	-1.1551
Н	-4.8255	-0.9381	-0.5089
Ц	4 9797	-1 1402	1 9707
11	4.2131	-1.1403	1.2191
Н	1.8078	-2.6508	2.7293
Ц	-1 5265	2 5906	_0_0691
11	-1. 5205	5. 5690	-0. 9081
Н	-5.6611	2.4698	-0.5152
Ц	1 9109	0 1914	-2 0000
11	1.0152	0.1214	2.0880
Н	-1.4427	-2.4119	4.0177
Ц	_9 1202	1 9759	1 0052
11	-2.1303	1.2700	1.9055
Н	1.6196	3. 4931	-0.4588
Ц	-5 0380	4 8202	-0 4200
11	0.0003	1.0202	0. 1433
Н	-3. 3376	5.2696	-0.2001
Ц	-3 0707	5 0465	-1 8281
11	5. 9191	5.0405	1.0201
Н	-3. 5423	-1.2582	4.3158
Ц	-4 0895	-0 5334	2 7031
11	4.0055	0.0004	2.1331
Н	-3. 5033	0.5017	4.0951
ſ	0 7093	-4 4001	-2 5511
C	0.1033	4.4001	2.0011
Н	0.9223	-4.4940	-3. 6259
Ц	1 5700	-1 7810	-2 0006
11	1.0199	4. 1049	2.0000
Н	-0.1323	-5.0567	-2.3279
C	6 0010	1 9614	_0 2766
U	0.0010	1.0014	-0.2700
Н	6.4456	2.6862	0.2991
II	6 5120	0.0456	0.0100
Н	0. 5139	0.9450	0.0190
Н	6. 2248	2.0345	$-1.33\overline{92}$
	4 0790	2,0010	0.0000
0	4.0720	<b>3.</b> 9232	-0.9296
Н	5.0382	3.8922	$-1.01\overline{75}$
 	9 5404	0 1000	
0	2.5484	-2.1809	-2.8454
Н	2.6384	$-3.12\overline{42}$	$-3.05\overline{36}$
			2. 0000

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

atom	Λ	I	L
C	0 8078	-1 2186	-1 6162
Ľ	0. 8978	-1.2180	-1.0102
С	-0.0300	-0.1495	-1.5282
C	-1 2816	-0.2742	-9 1131
U	-1.2810	-0.2742	-2.1131
С	-1.6746	-1.4677	-2.7529
ſ	-0.7833	-2 5313	-2 8111
C	0.1000	2.0010	2.0111
С	0.5009	-2. 4248	-2.2567
C	2 2731	-1 0496	-1 1610
0	2.2101	1.0450	1. 1010
C	2.7329	0.2749	-0.7632
C	1 8164	1 3449	-0.6463
0	1.0101	1.0115	0.0100
C	0.3277	1. 0927	-0.7444
C	4 1195	0 5171	-0 5331
	4 5010	1 0000	0.0001
L	4. 5910	1.8069	-0.2344
С	3. 6496	2.8419	-0.1628
C .	9 9776	9 6107	0.2552
U	2.2110	2.0107	-0. 3333
С	0.0300	-0.1492	1.5279
ſ	-0.8978	-1 2184	1 6162
C	0.0310	1.2104	1.0102
С	-0.5007	-2.4245	2.2569
ſ	0 7837	-2 5309	2 8109
0	0.1001	2.0000	2.0105
C	1.6749	-1.4673	2.7525
С	1.2817	-0.2739	2, 1126
	0.0070	1,0000	0.7440
U	-0. 3278	1. 0928	0.7440
С	-1.8164	1, 3449	0.6459
C C	0 7000	0.9750	0 7694
L	-2. 7329	0.2750	0.7634
С	-2.2732	-1.0495	1.1613
C	_9 9778	9 6197	0.2545
U	-2.2110	2.0107	0.3345
С	-3. 6499	2.8417	0.1623
ſ	-4 5912	1 8066	0 2343
<u> </u>	4.1100	1.0000	0.2343
C	-4.1196	0.5171	0. 5336
0	3 0822	-2 0276	-1 1901
0	2,0026	2.0210	1 1000
0	-3. 0826	-2.0271	1. 1908
Н	0.1324	1.9592	1.2299
U U	_0_1225	1.0500	_1 2204
11	-0.1323	1. 9590	-1.2304
С	-3.0614	-1.5813	-3. 3368
ſ	3 0618	-1 5807	3 3361
0	5.0010	1.0001	0.0001
0	5.0214	-0.4776	-0.5911
0	1 3154	-3 4844	-2 3709
0	<u> </u>	0. 4770	2.0105
0	-5. 0213	-0.4778	0. 5927
0	-1.3150	-3.4842	2.3713
Ü	4 5145	_1 2052	_0 9199
11	4. 5145	-1. 3033	-0.0102
Н	2.1695	-3.2369	-1.9319
Н	-4 5141	-1 3054	0.8196
11	0, 1000	1.0001	1 0204
Н	-2.1692	-3.2368	1.9324
С	6.0600	2.0684	-0.0054
C .	-6.0602	2 0680	0,0056
U	-0.0003	2.0080	0.0050
Н	-1.9804	0. 5556	-2.0677
Н	-1 0528	-3 4672	-3 2908
II	1.0020	2,4000	0.0700
Н	1.0003	5.4629	-0.2702
Н	1.0533	-3.4668	3.2907
Ц	1 0204	0 5560	2 0670
11	1. 3004	0.0000	2.0010
H	-1.6005	3.4629	0.2690
Н	-3 2714	-0 7521	-4 0232
TT	0.0100	1 5/10	0 5400
Н	-3. 8192	-1. 5419	-2. 3438
Н	-3.1937	-2.5192	-3.8837
Ц	3 9710	-0 7516	4 0225
11	0.2119	0.7510	т. 0220
H	3.8194	-1.5412	2.5429
Н	3, 1944	-2.5186	3.8829
TT	C 1715	0.7750	0.7400
Н	0.4/15	2.1150	-0.7403
Н	6.2543	2.4762	0.9971
<u>и</u>	6 6270	1 1/10	_0_0060
П	0.0210	1.1412	-0.0900
H	-6.4734	2.7695	0.7450
Н	-6 2539	2 4827	-0 9949
11	0.4000		0.0000
H	<u>-b.62</u> 62	1.1395	0.0888
0	-4.0192	4.1229	-0.1078
U U	_1 0001	1 1650	_0 0000
п	-4. 9031	4.1009	-0.2083
0	4.0187	4.1231	$0.\ 1075$
U	1 0997	1 1669	0 2002
1 11	7. 3041	4.1002	0.2000

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

atom	λ	Ĭ	L
ſ	2 7148	0 6005	0 8585
0	2.1140	0.0000	0.0000
С	1.8011	1.6659	0.6944
C	2 2700	2 9430	0 4119
0	2.2100	2. 5450	0.4115
C	3.6468	3. 2023	0.2748
С	4 5488	2 1522	0 4105
<u>C</u>	1.0100	0.0507	0. 1100
C	4. 1053	0.8537	0.6986
C	2 2441	-0.7300	1 2430
0	2.2111	0.1000	1.2100
C	0.8601	-0.9009	1.6511
C	-0.0638	0 1695	1 5325
0	0.0000	0.1000	1.0020
C	0. 3102	1.4080	0.7500
ſ	0 4504	-2 1069	2 2946
0	0.4504	2.1003	2.2340
C	-0.8367	-2.2360	2.8438
ſ	-1 6961	-1 1366	2 7430
0	1.0001	1.1500	2.1430
C	-1.3232	0.0528	2.0935
C	-1 8010	1 6659	-0 6944
0	1.0010	1.0003	0.0511
С	-2.7148	0.6006	-0.8585
C	-4 1053	0 8537	-0 6985
<u> </u>	4. 1000	0.0001	0.0505
С	-4. 5487	2.1523	-0.4105
C	-3 6467	3 2024	-0.2748
<u> </u>	3.0407	3.2024	0.2740
С	-2.2699	2.9430	-0.4119
ſ	-0.3101	1 4080	-0.7501
U .	0.3101	1.4000	0.7501
С	0.0638	0.1695	-1.5326
C	_0_9601	_0_000	_1 6511
U.	-0.8001	-0.9009	-1.0511
С	-2.2441	-0. 7299	-1.2429
C	1 2020	0.0528	-2 0935
<u> </u>	1. 3232	0.0528	2.0933
С	1.6961	-1.1366	-2.7431
ſ	0 8367	-2 2360	-2 8/138
<u> </u>	0.0307	2.2300	2.0430
С	-0.4505	-2.1069	-2.2946
0	3 0634	-1 6983	1 2008
0	5.0034	1.0903	1.2330
0	-3.0634	-1.6983	-1.2997
Н	0 1647	2 2730	-1 2242
11	0.1047	2.2130	1. 2242
Н	-0. 1647	2.2730	1.2241
ſ	/ 1315	4 6064	0.0050
<u> </u>	4.1010	1.0004	0.0000
С	-4. 1314	4.6064	-0.0051
0	1 2836	-3 1532	2 4143
0	1.2000	0.1002	2.1113
0	5.0324	-0.1085	0.8182
0	-1 2836	-3 1532	-2 $4143$
0	1.2000	0.1002	2.1110
0	-5. 0323	-0.1084	-0.8181
Н	2 1441	-2 8810	1 9941
11	2.1111	2:0010	1.0000
Н	4. 5429	-0.9519	1.0028
Н	-2.1441	-2.8810	-1 9941
II	4 5490		1 0007
П	-4. 5429	-0. 9519	-1.0027
С	-1.2683	-3.5065	3. 5350
C .	1 9699	2 5066	2 5250
U	1.2062	-3. 3000	-3. 3350
Н	1.5618	3. 7611	0.2958
Ц	5 6173	2 2106	0 3005
11	0.0110	2.0100	0.0000
Н	-2.0466	0.8580	2.0409
Н	-5 6172	2 3107	-0.3005
TT	1 5017	0.7011	0.0050
Н	-1.5017	3. (011	-0.2958
Н	2.0466	0.8580	-2.0410
11	4.0775	5. 0000 F. 0100	0.0141
Н	4.0775	5.2196	0.9141
Н	3, 5165	5, 1022	-0.7545
II	E 1702	4 0120	0, 2270
Н	5.1703	4.0130	-0.3379
Н	-4.0772	5.2197	-0.9141
II	E 1702	4 6197	0.2277
Н	-5.1703	4.0137	0.3377
Н	-3.5165	5. 1022	0.7546
II	_1 E000	_9 9960	1 5046
П	-1. 0088	-3. 3309	4. 0940
Н	-2.1519	-3.9538	3.0573
II	_0 4607	_1 9471	2 1000
п	-0.4087	-4.24/1	J. 4960
Н	2.1521	-3.9536	-3.0576
Ц	1 5082	_2 2271	-1 5016
11	1.0000	0.00/1	4.0940
Н	0.4688	-4.2474	-3.4975
0	2 0/80	-1 1609	-2 2601
0	2. 3403	1.1000	3.2091
Н	3. 1111	-2.0259	-3. 6772
0	-2 0/00	-1 1608	3 2600
0	2. 3430	1.1000	5.2030
i U	-3 1119	-2 0259	1 3 6771

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

atom	Å	Ŷ	L
С	1, 1496	-1.2524	-1.3799
C	0.2131	-0.1878	-1 3864
C	-0.9863	-0.3328	-2.0664
C	1 2200	1 5499	2.0004
C	-1. 5209	-1. 0420	-2.7100
U C	-0. 4222	-2.6014	-2.6780
С	0.8134	-2.4750	-2. 0267
С	2. 4763	-1.0621	-0.8211
С	2.9035	0.2874	-0. 4249
С	1.9654	1.3510	-0.4004
С	0.4927	1.0678	-0.5945
С	4.2750	0. 5292	-0.1364
С	4.7038	1.8369	0.1379
С	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	-2.0213	0.1001	0.0130
C	-3. 9902	0.3009	0.0000
C C	-4.4720	1. 5810	-0.0092
U C	-3.6197	2.6815	-0.0259
С	-2.2575	2. 4997	0. 2823
С	-0.2724	1.0651	0.8453
С	0.0734	-0.1441	1.6836
С	-0.8039	-1.2578	1.7159
С	-2.1388	-1.1654	1.1280
С	1.2658	-0. 1903	2.3979
С	1.6162	-1.3446	3.1144
С	0.7940	-2.4593	3. 1231
C	-0, 4247	-2, 4314	2, 4274
0	3 2955	-2.0248	-0 7594
0	-2 8959	-2 1794	1 0896
Ц	0.1086	1 958/	1.3479
Ц	0.1000	1.0160	_1 1200
	0.0493	1. 5105	2 2050
C	-2.0304		-3. 3930
C O	-4. 1439	4.0384	-0. 3539
0	5. 1976	-0. 4407	-0.1179
0	1.6412	-3. 5284	-2.0544
0	-1.1970	-3. 5257	2. 4815
0	-4.8692	-0. 7113	0. 3152
Н	4. 7244	-1.2895	-0. 3266
Н	2.4548	-3. 2707	-1.5516
Н	-2.0094	-3. 3319	1.9471
Н	-4.3656	-1.5219	0.5873
Н	-1.6929	0. 4911	-2.0910
Н	-0.6486	-3. 5482	-3.1585
Н	5, 7550	2.0049	0.3462
Н	4, 1230	3, 8943	0. 3255
Н	-5, 5242	1,6810	-0.2580
Н	-1 5844	3 3525	0.2479
Ц	2 5504	-1 3648	3 6603
11	2. 5504	2 2610	3.0093 2.6659
П	1.0009	-3. 3019	3.0002 2.0250
Н	-2. (428	-2.0248	-3. 9350
H	-3.4731	-1.6313	-2.6609
H	-2.8223	-0.8602	-4.1075
Н	-5.1265	4.0115	-0.8325
Н	-3. 4612	4. 5968	-1.0207
Н	-4.2469	4.6625	0.5570
C1	1.3601	4.0353	$-0.\ \overline{1270}$
Н	1.9290	0.6685	2.4022

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

atom	Λ	Ĭ	L
С	2,6645	0.3931	0. 4948
C	1 8166	1 4949	0.2446
C	2 3470	2 6752	-0.2584
C	2. 5410	2.0132	0.5204
C	3.7230	2.7903	-0. 0521
C	4. 5572	1.7020	-0.3190
С	4. 0475	0. 4970	0. 1829
С	2.1278	-0.8215	1.0966
С	0.7860	-0.7883	1.6862
С	-0.0485	0.3482	1.4904
С	0.3214	1.3445	0. 4151
С	0.3981	-1.8236	2.5786
C	-0.7916	-1 6915	3 3125
C	-1 5568	-0.5493	3 1830
C	1 1000	0. 3433	2 2042
C C	-1. 1880	0.4000	2.2842
C	-0.1144	-0. 4389	-1.4563
C	-1.1340	-1.4011	-1.2396
С	-0.8607	-2.7696	-1. 5109
С	0.3964	-3.1456	-2.0100
С	1.3760	-2.1942	-2.2605
С	1.1031	-0.8364	-1.9886
С	-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	-2.1274	2 7441	-1.2427
C	2.1374	2.1441	-1.2437 1.2070
C	-3.4011	J. 1300 0. 0100	-1.2079
U C	-4. 4919	2.2132	-0.9960
L Ô	-4.1738	0.8563	-0.8342
0	2.8526	-1.8525	1.2104
0	-3. 3747	-1.8454	-0. 6151
Н	0.2085	1.6498	-1.7227
Н	-0.0984	2.3197	0.6710
С	4.2830	4.1047	-1.0350
С	2.7360	-2.5911	-2.7789
0	1.1299	-2.9261	2.7805
0	4.9007	-0.5271	0.3459
0	-5, 1835	-0.0045	-0.6408
0	-1 7679	-3,7376	-1 3203
U U U U U U U U U U U U U U U U U U U	1 9370	-2 8464	2 2090
Ц	1.3370	-1 2862	0.7024
П	-4. 5725	-0.0051	-0.5474
11	-4. 1101	-0.9001	
Н	-2. 3875	-3. 2988	-0.9740
H	1.6907	3. 5226	-0. 4444
Н	5.6197	1.7541	-0. 5360
H	-1.0722	-2.4873	3. 9939
Н	-2.4557	-0. 4237	3. 7773
Н	0.5723	-4.1997	-2.2010
Н	1.8718	-0.0953	-2.1847
Н	-3.7364	4.1859	-1.3461
Н	-5.5364	2.5044	-0.9571
Н	4.3532	4.8364	-0.2196
Н	5, 2853	3,9789	-1. 4546
Н	3 6300	4 5434	-1 8063
Ц	3 5064	-9 2049	_9 0992
П	0. 0004 0. 7760	-2. 3942	-2.0223
Н	2. (109	-3.0333	-3.0350
H	3.0056	-2.0124	-3.6705
<u>C1</u>	-2. 1941	1.9113	2.2690
Н	-1.3579	3. 4861	-1.3961

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

atom	Λ	I	L
С	4.3959	2.3959	-0.4612
С	3. 3824	3, 3434	-0.4752
C	2 0427	2 9664	-0.6374
<u> </u>	1 7095	1 6253	-0.8045
C	2 7204	0.6450	0.0040
C C	2.7294	0.0459	-0. 8260
C	4.0837	1.0391	-0.6302
C	0.2549	1.2133	-0.8714
С	0.0279	-0. 1213	-1.5424
С	1.0573	-1.0975	-1.5377
С	2.4035	-0. 7553	-1.0992
С	-1.1992	-0. 4199	-2.1159
С	-1.4677	-1.6978	-2.6501
С	-0.4757	-2.6691	-2.6152
С	0.7872	-2.3880	-2.0720
С	-0.3904	1, 2692	0, 6265
C	-1. 8983	1, 3231	0.5343
C	-2 6608	0 1404	0.7105
C	-2.0006	-1 0014	1 1704
C	-0.6404	-1 0322	1.6583
C	0.0404	0.1524	1.0000
C	0. 1233	0.1024	1. 0000
C C	-0.0845	-2.1257	2.3799
L C	1. 1920	-2.0071	2.9488
C	1.9213	-0.8315	2.8226
С	1. 3705	0.2491	2.1010
С	-2.5775	2.4949	0.2001
С	-3.9660	2. 5131	0.0176
С	-4. 7043	1.3508	0.1501
С	-4.0655	0.1496	0.4924
0	3. 3053	-1.6422	-1.0367
0	-2.6733	-2.1671	1.2491
С	-2.8319	-1.9973	-3.2206
С	3.3024	-0. 7056	3. 4158
0	5.0937	0.1552	-0.5956
0	1.7033	-3.3660	-2.0936
0	-4.8254	-0.9496	0.5964
0	-0 7395	-3,2814	2 5565
Н	4 6930	-0.7415	-0.7393
Н	2 5253	-2 9995	-1.6774
Н	-4 2177	-1 6933	0.8532
Н	-1 6090	-3 1959	2 0002
Ц	-0.2020	1 0831	-1 4233
П Ц	-0.0254	2 2212	1.4233
	1 7919	4.0220	0.0012
	-1.7218	4.0289	-0.0013
H	5.4305	2.0713	-0.3250
H	3.6319	4. 3943	-0.3546
H	-1.9760	0.3382	-2.1459
Н	-0.6473	-3.6648	-3.0121
H	1.5874	-2.8600	3. 4915
Н	1.9451	1.1646	1.9994
Н	-4. 4564	3. 4480	-0. 2325
Н	-5.7786	1.3429	0.0005
Н	-3.1208	-1.2500	-3.9692
Н	-2.8653	-2.9839	-3.6911
Н	-3.5942	-1.9727	-2.4312
Н	4.0566	-0.6278	2.6221
Н	3. 5551	-1.5683	4. 0385
Н	3, 3887	0. 1988	4. 0297
Н	1. 2605	3. 7197	-0. 6297
			5. 5201

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Cartesian coordi	nates of 5-chlorina	ated 1-IV optimize	d at the gas-phase	B3LYP/6-31G(d) level
a <b>t</b> a m	V	V	7	

atom	V	V	7
atom	Λ 0.0050	1	
С	0.6853	-2.8593	-2.7690
С	1, 5208	-1.7634	-2.9056
C C	1 1026	_0 5261	_2 2207
C	1.1550	0. 3201	2.3231
C	0.0117	-0.3795	-1.6116
С	-0.8813	-1.4752	-1.5018
ſ	-0.5261	-2 7304	-2 0700
<u> </u>	0.0201	0.0010	2.0100
t	-0.3108	0. 9219	-0.9125
С	-1.7960	1.1652	-0.7622
С	-2.6855	0.0686	-0.6740
C	-2 2160	-1 9877	_0_0315
C	2.2100	1.2011	0. 9313
С	-2.2815	2.4603	-0.6626
С	-3.6508	2.7113	-0.4469
C	-4 5248	1 6375	-0.3217
C	1.0210	0.2179	0.0211
t	-4.0035	0.3172	-0.4272
С	0.4493	1.0836	0.5252
С	0.2795	-0.1168	1.4294
C	1 2388	-1 1663	1 3630
C	1.2300	1.1003	1.3030
C	2. 5243	-0.9426	0.6933
С	2.8772	0.4088	0.2758
C	1 9007	1 4298	0 2752
C	4.0100	0.7070	0.0000
t	4. 2138	0.1212	-0.0906
С	4. 5498	2.0505	-0. 4082
С	3, 5899	3.0575	-0.3813
C	2 2606	2 7311	-0.0477
C	2.2000	2. (311	0.0477
C	-0. 7905	-0.2674	2.3099
С	-0.9766	-1.4556	3.0349
С	-0.0929	-2.5086	2,9043
C	1,0266	_2 2759	2 0000
C	1.0300	2.3130	2.0000
0	-2.9883	-2.2771	-0.7653
0	3.3620	-1.8837	0.5856
С	-4.1510	4, 1319	-0.3468
C	2 0641	1 1010	_0.6972
C	5. 9041	4.4075	-0.0872
0	-1.3144	-3.8111	-1.9853
0	-4.9627	-0.6702	-0.3078
0	1 8910	-3 4049	2 0333
0	E 10E0	0.1062	0.1447
0	5. 1650	-0. 1905	-0. 1447
H	-2. 1210	-3. 5393	-1. 4755
Н	-4.4670	-1.5229	-0.4107
Н	2 6372	-3 1340	1 4375
II	4 7690	1.0652	0.0961
П	4.7000	-1.0000	0.0001
H	0.1060	1.7444	-1.5019
Н	-0.0362	1.9474	0.9850
C1	-1.9294	1.0386	2.6315
Ц	0.0201	-3 8245	_3 2002
11	0. 5251	J. 024J	3.2002
H	2.4472	-1.8635	-3.4647
Н	-1.5938	3.2996	-0.7452
Н	-5 5851	1 7926	-0 1476
II	E E000	2 2626	0.6727
11	5. 5606	2.2030	-0.0737
H	1. 5059	3. 5147	-0. 0407
Н	-1.8280	-1.5363	3.7024
Н	-0 2317	-3 4359	3 4494
TT	2 7000	1 6479	0. 5110
Н	-3.7026	4.04/3	0.0119
Н	-3.8846	4.7079	-1.2415
Н	-5.2379	4.1688	-0.2316
Н	3 0033	5 0873	0 2317
11	4 0400	4 5501	1 1070
H	4. 9493	4. 5531	-1.15/9
Н	3.2325	4.9570	-1.3545
Н	1.8663	0.3172	-2.4433