

Supporting Information

Encapsulated Guests in the Smallest Spaces: Shrinking Guests by Compression and Investigations under Solvent-Free Conditions

Gebhard Haberhauer*[†], Sascha Woitschetzki[†] and Christof Füten[†]

[†] Institut für Organische Chemie, Universität Duisburg-Essen, Universitätsstr. 7, D-45117 Essen, Germany

1. NMR Spectra of the Container and Complexes	S2
2. Molecular Structures	S11
3. ¹ H NMR and ¹³ C NMR Spectra of the New Compounds	S15
4. Cartesian Coordinates and Absolute Energies of all Calculated Compounds	S23
5. Complete Reference 15	S87

1. NMR Spectra of the Container and Complexes

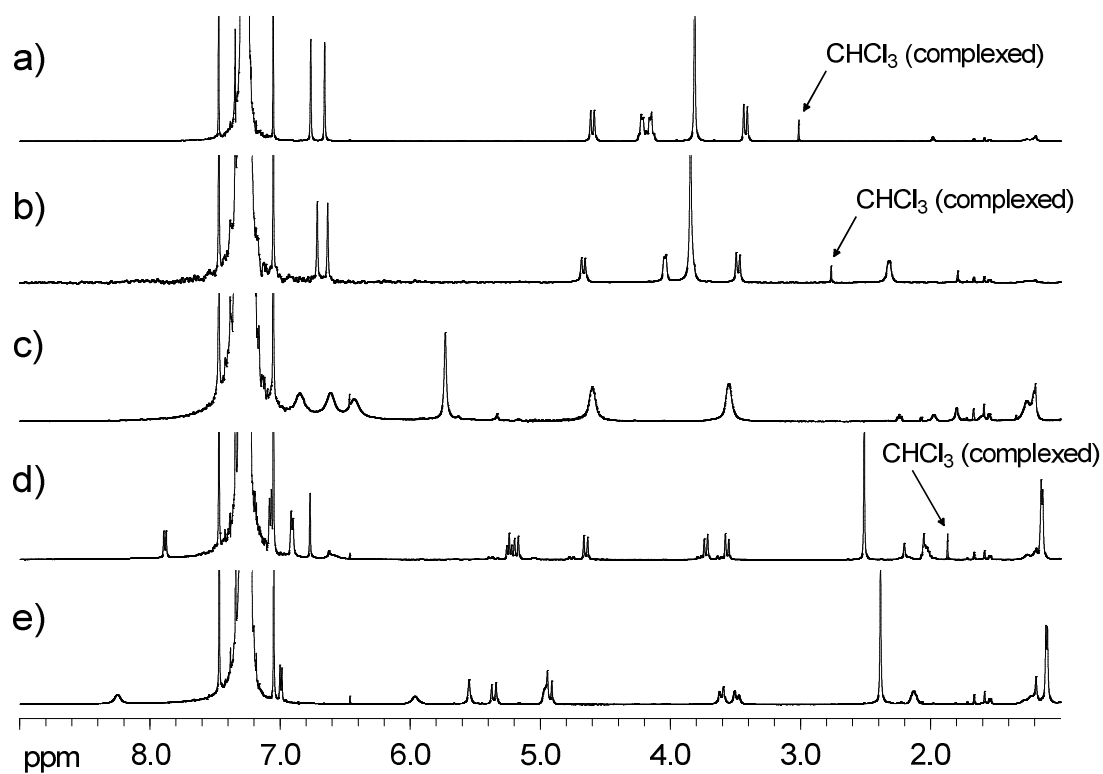


Figure S1. ^1H NMR spectra of cryptophane-A (a), cryptophane-E (b), cryptophane-111 (c), **5** (d) and **6** (e) at 500 MHz in $\text{CHCl}_3/\text{CDCl}_3$ (10/1) at 218 K.

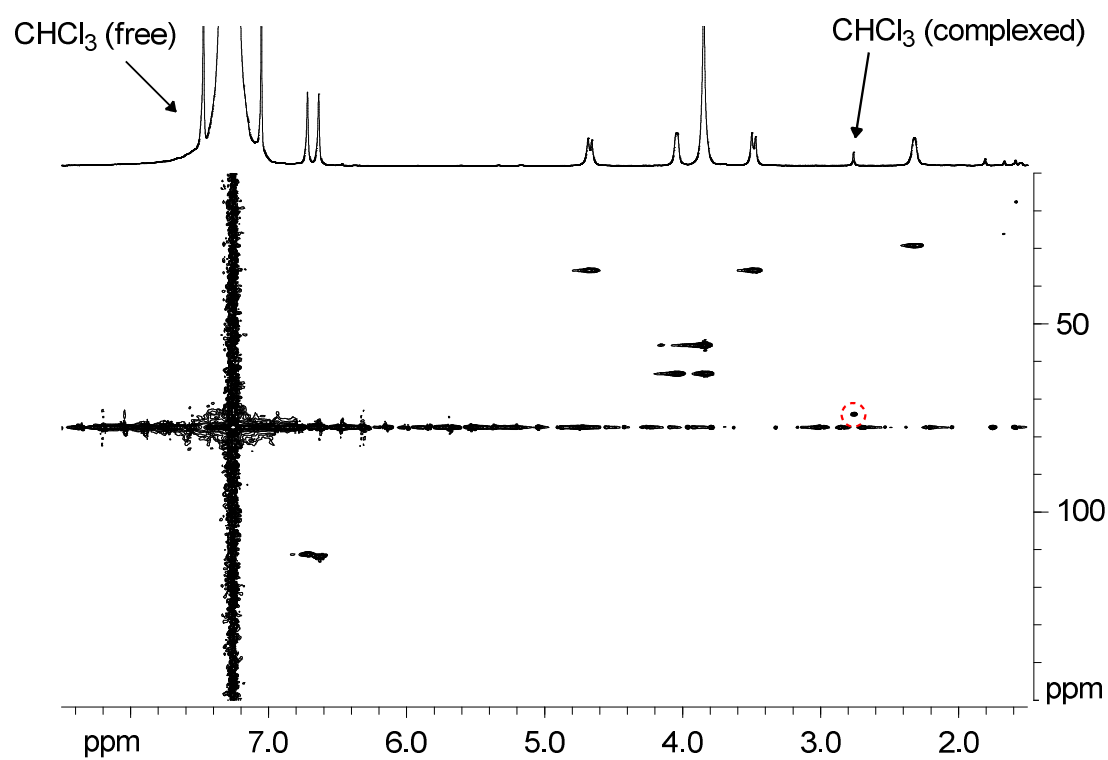


Figure S2. ^1H - ^{13}C COSY NMR spectrum of CHCl_3 @cryptophane-E at 500 MHz in $\text{CHCl}_3/\text{CDCl}_3$ (10/1) at 218 K. The cross peak between the hydrogen of the complexed CHCl_3 and the carbon of the complexed CHCl_3 is highlighted.

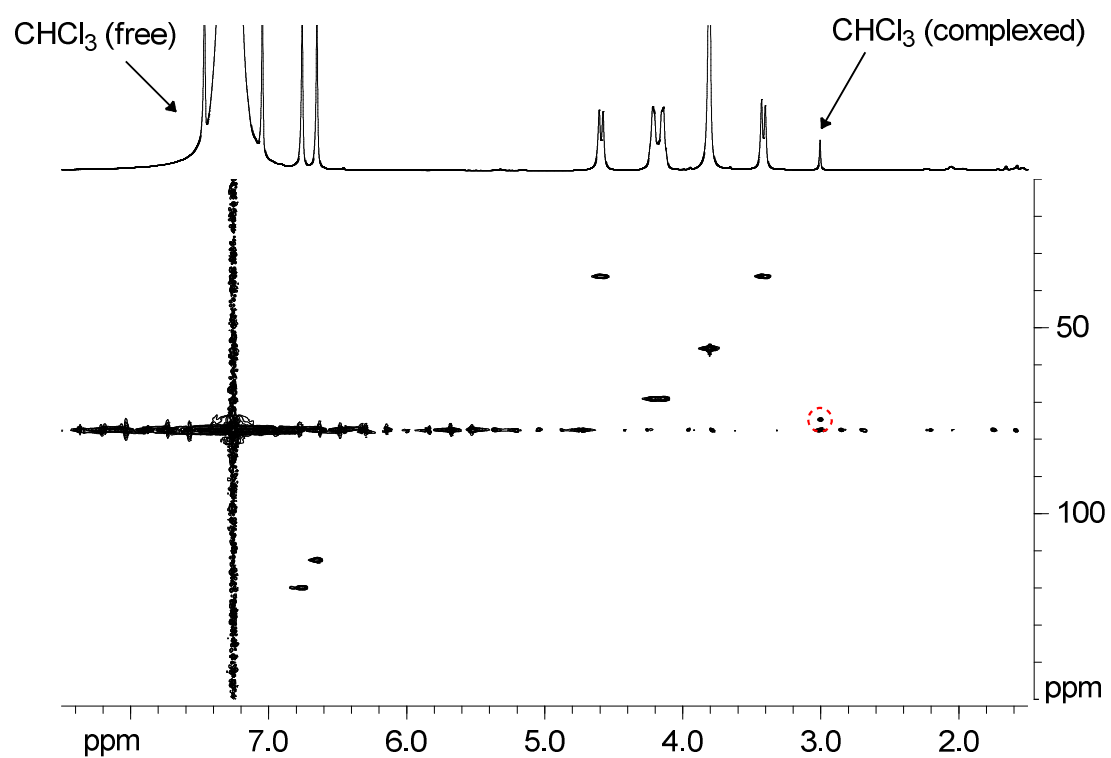


Figure S3. ^1H - ^{13}C COSY NMR spectrum of CHCl_3 @cryptophane-A at 500 MHz in $\text{CHCl}_3/\text{CDCl}_3$ (10/1) at 218 K. The cross peak between the hydrogen of the complexed CHCl_3 and the carbon of the complexed CHCl_3 is highlighted.

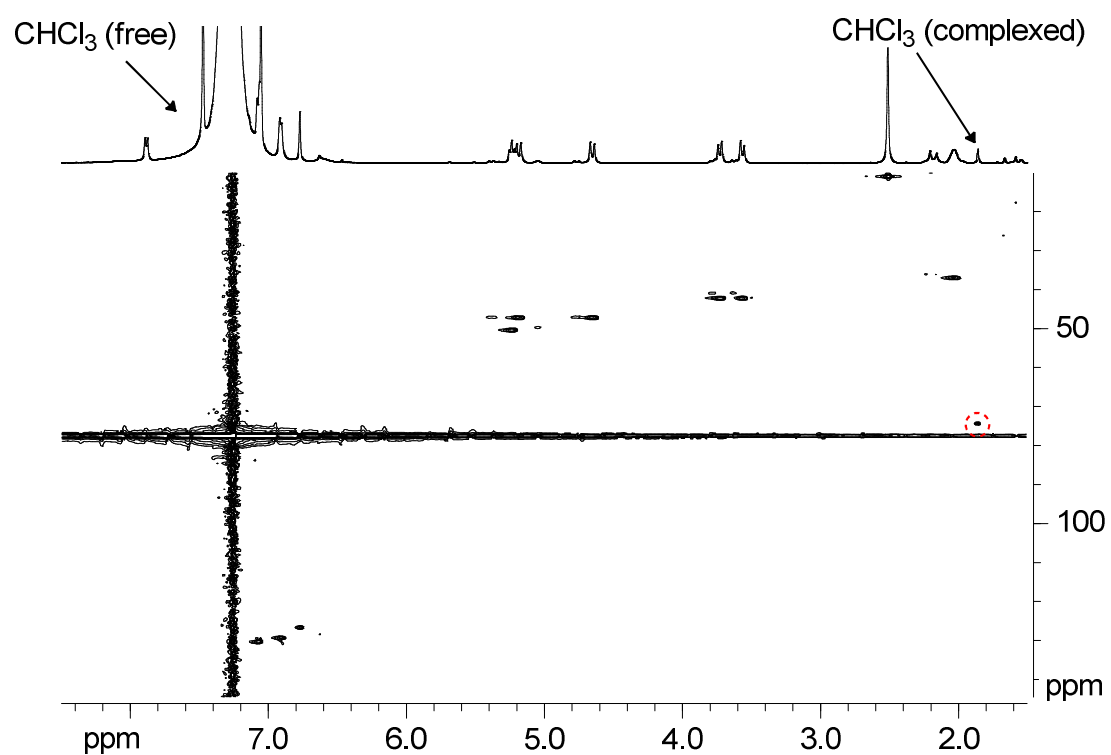


Figure S4. ^1H - ^{13}C COSY NMR spectrum of $\text{CHCl}_3@5$ at 500 MHz in $\text{CHCl}_3/\text{CDCl}_3$ (10/1) at 218 K. The cross peak between the hydrogen of the complexed CHCl_3 and the carbon of the complexed CHCl_3 is highlighted.

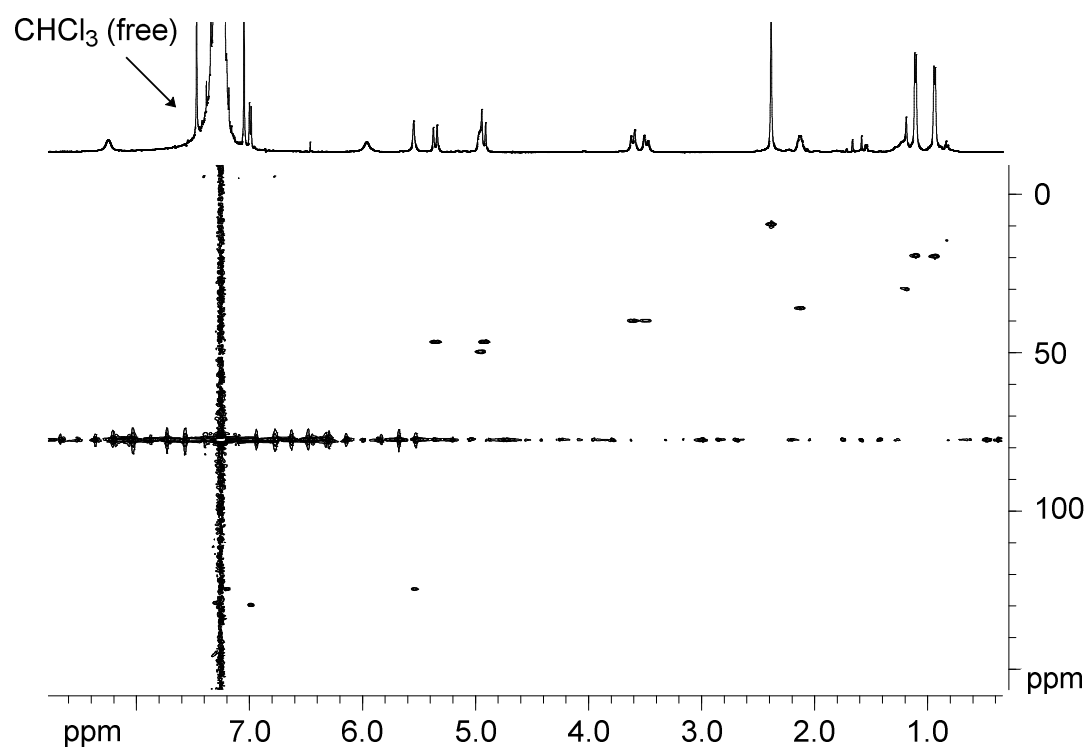


Figure S5. ^1H - ^{13}C COSY NMR spectrum of $\text{CHCl}_3@6$ at 500 MHz in $\text{CHCl}_3/\text{CDCl}_3$ (10/1) at 218 K.

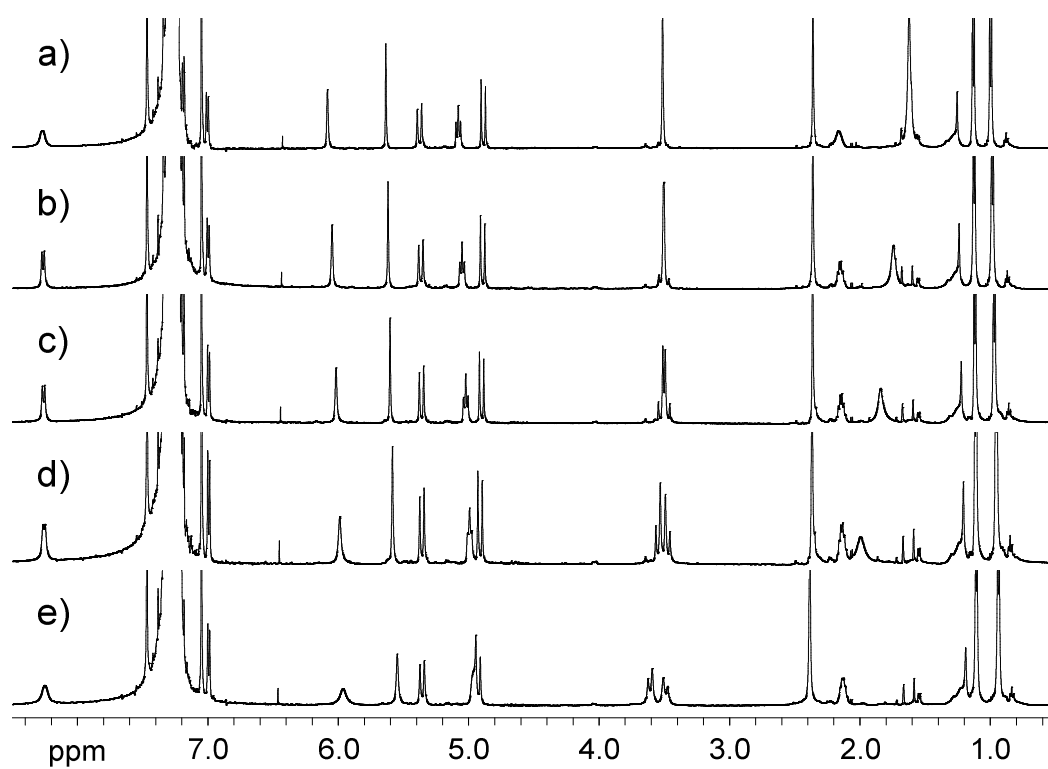


Figure S6. ¹H NMR spectra of **6** at 500 MHz in CHCl₃/CDCl₃ (10/1) at 298 K (a), 278 K (b), 258 K (c), 238 K (d), and 218 K (e).

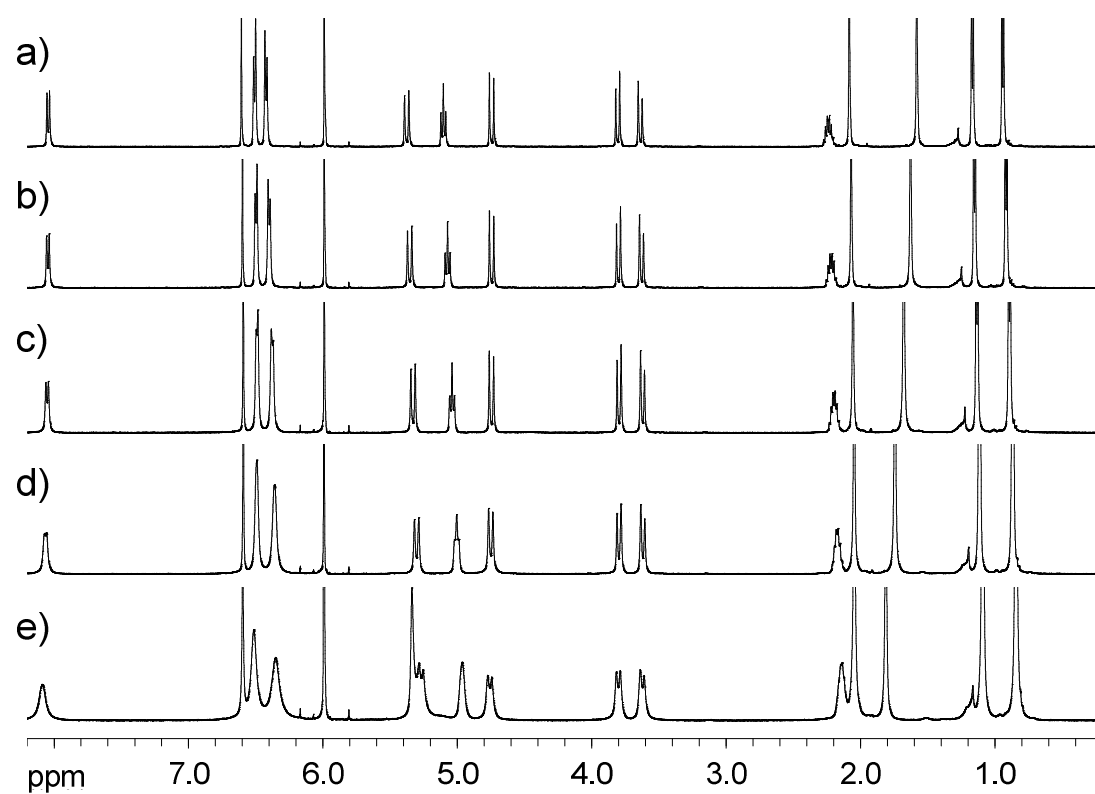


Figure S7. ^1H NMR spectra of **5** at 500 MHz in $\text{C}_2\text{D}_2\text{Cl}_4$ at 318 K (a), 298 K (b), 278 K (c), 258 K (d), and 238 K (e).

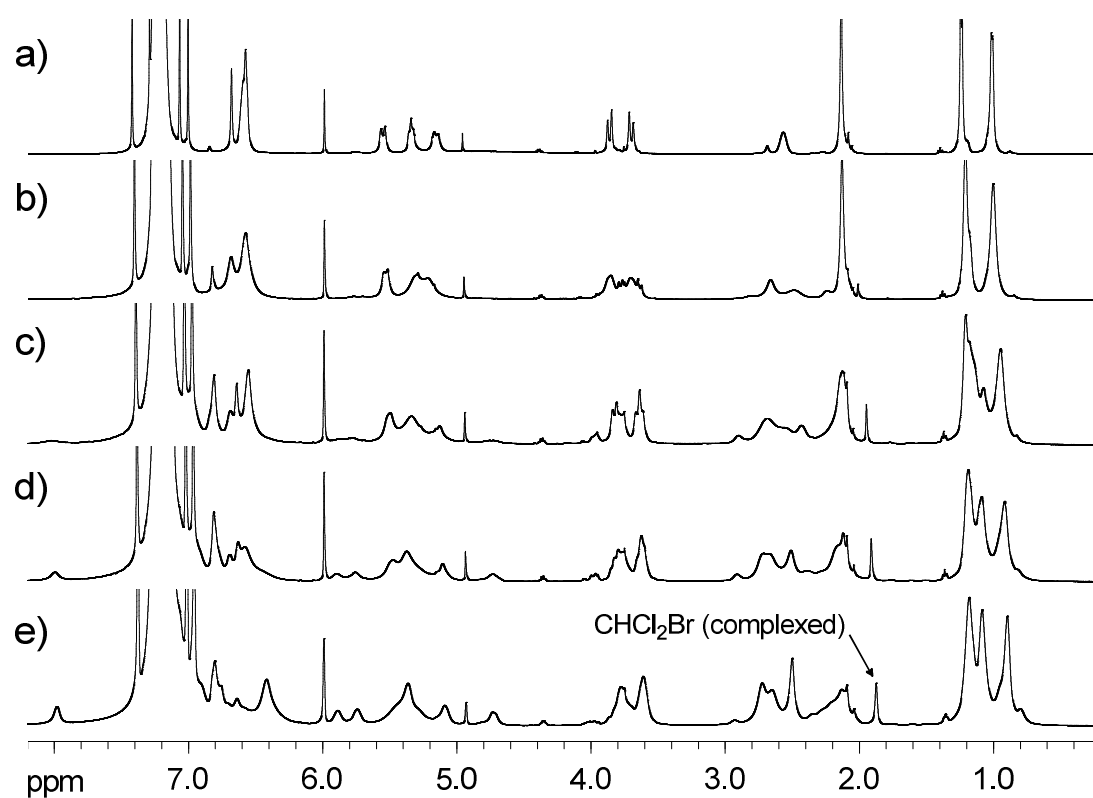


Figure S8. ^1H NMR spectra of **5** at 500 MHz in $\text{CHBrCl}_2/\text{C}_2\text{D}_2\text{Cl}_4$ (5/1) at 298 K (a), 268 K (b), 248 K (c), 238 K (d), and 228 K (e).

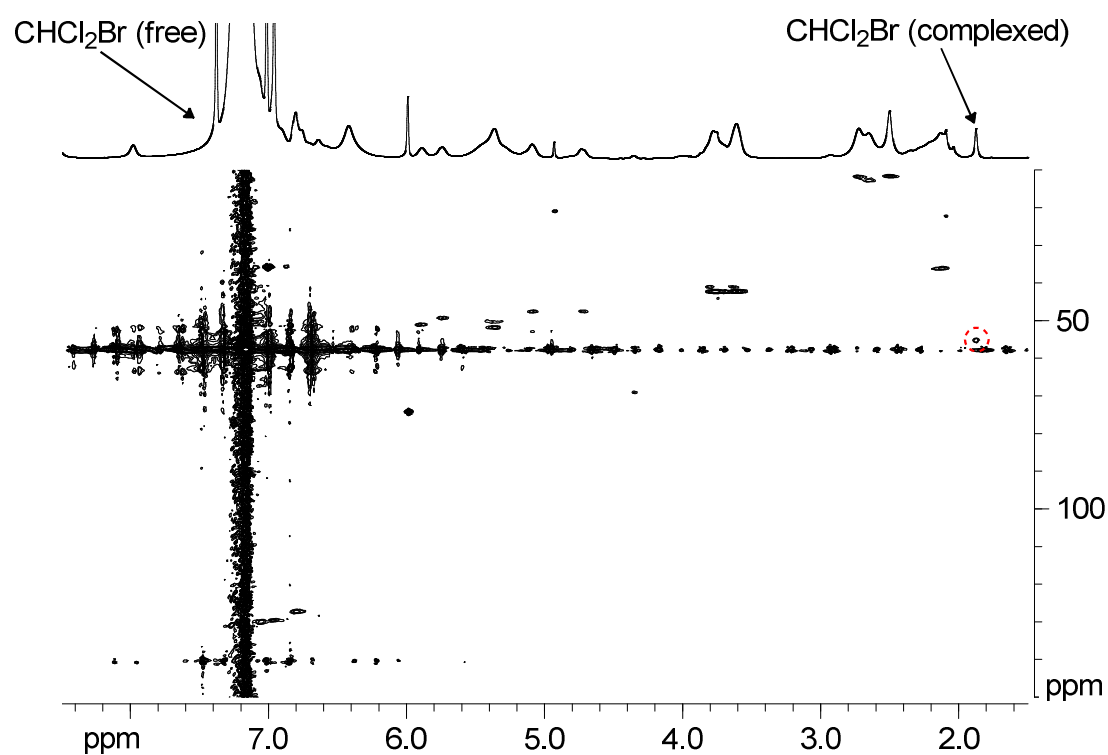


Figure S9. ^1H - ^{13}C COSY NMR spectrum of $\text{CHBrCl}_2@5$ at 500 MHz in $\text{CHBrCl}_2/\text{C}_2\text{D}_2\text{Cl}_4$ (5/1) at 228 K. The cross peak between the hydrogen of the complexed CHBrCl_2 and the carbon of the complexed CHBrCl_2 is highlighted.

2. Molecular Structures

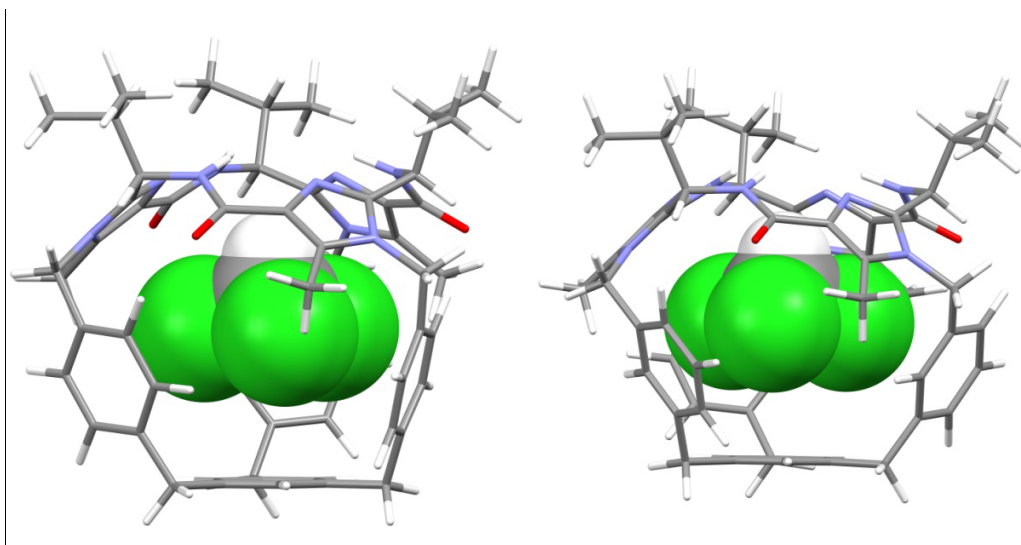


Figure S10. Molecular structures of the complexes $\uparrow\text{CHCl}_3@5$ (left) and $\uparrow\text{CHCl}_3@6$ (right) calculated using B3LYP-D3/def2-TZVP.

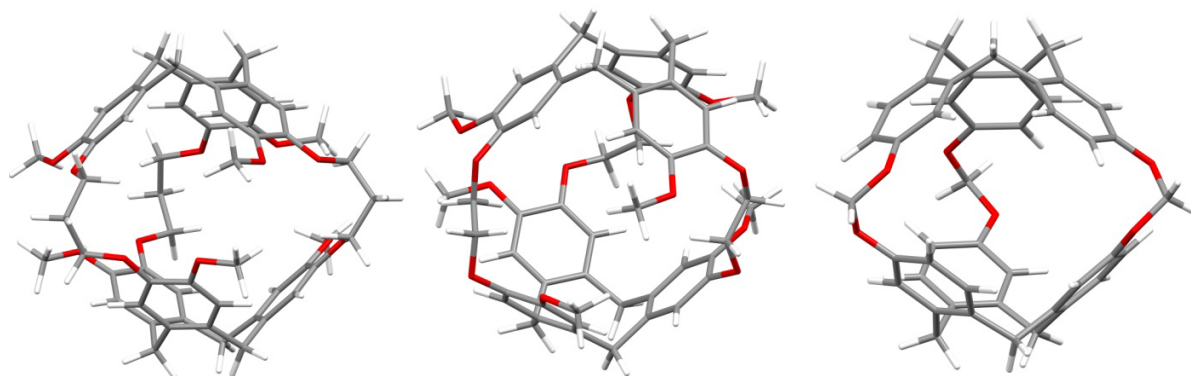


Figure S11. Molecular structures of cryptophane-E (1; left), cryptophane-A (2; middle) and cryptophane-111 (3; right) calculated using B3LYP-D3/def2-TZVP.

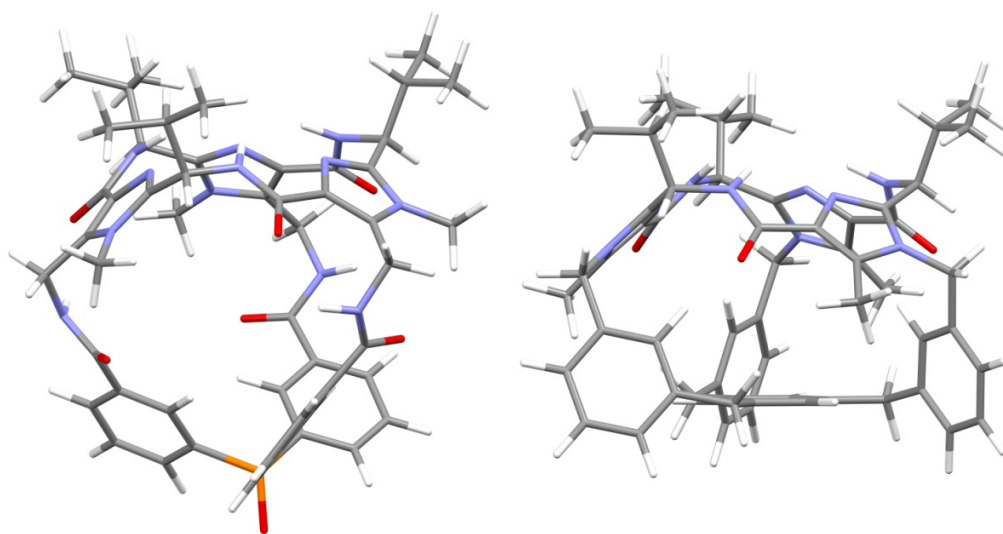


Figure S12. Molecular structures of the imidazole-containing containers **4** (left) and **6** (right) calculated using B3LYP-D3/def2-TZVP.

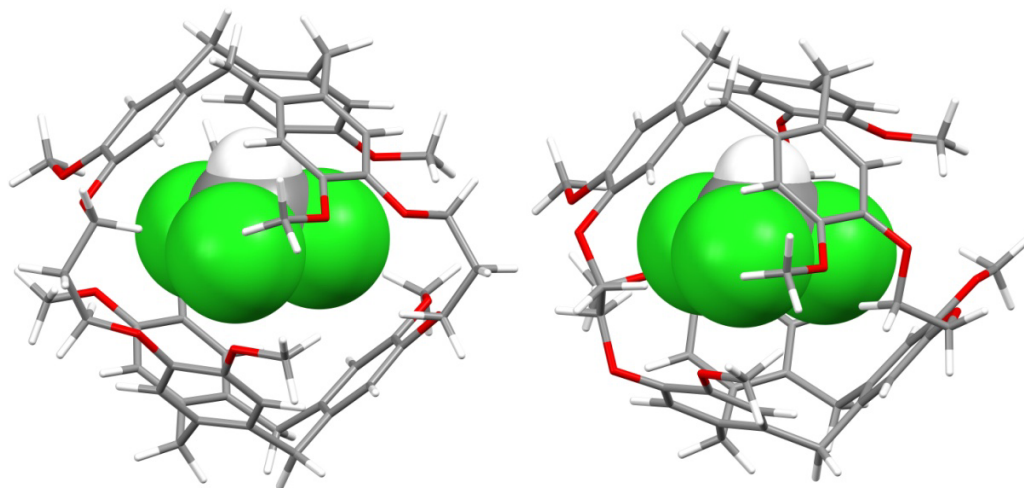


Figure S13. Molecular structures of CHCl_3 @cryptophane-E (left) and CHCl_3 @cryptophane-A (right) calculated using B3LYP-D3/def2-TZVP.

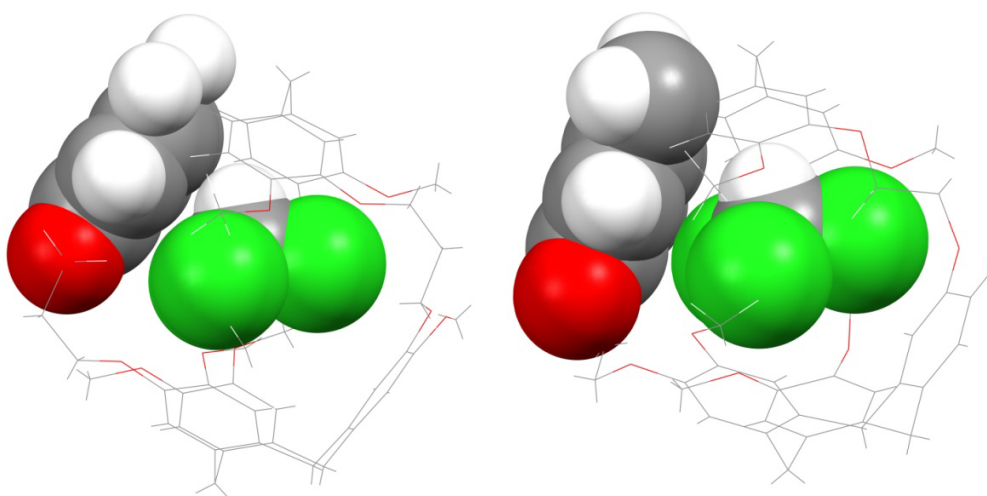


Figure S14. Molecular structures of CHCl₃@cryptophane-E (left) and CHCl₃@cryptophane-A (right) calculated using B3LYP-D3/def2-TZVP.

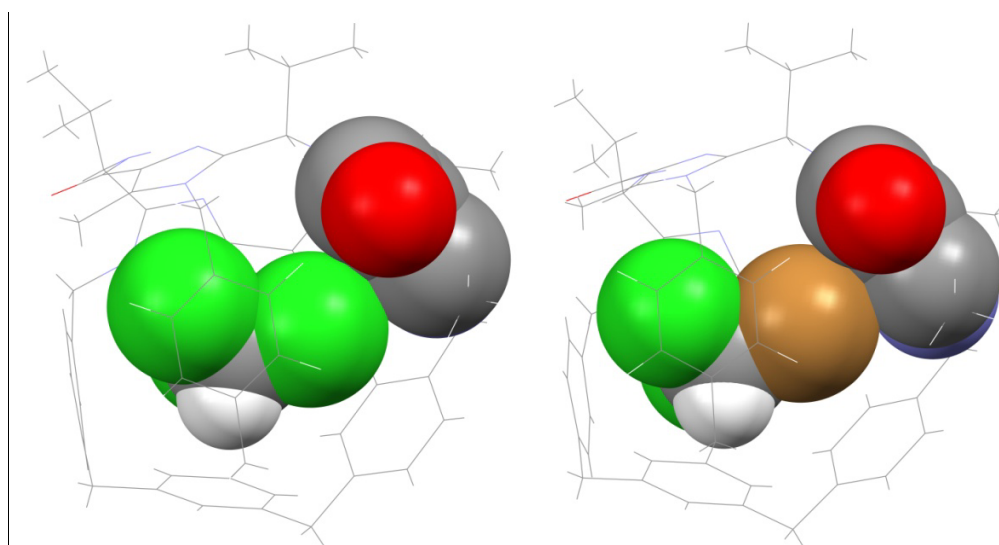


Figure S15. Molecular structures of the complexes ↓CHCl₃@5 (left) and ↓CHBrCl₂@5 (right) calculated using B3LYP-D3/def2-TZVP.

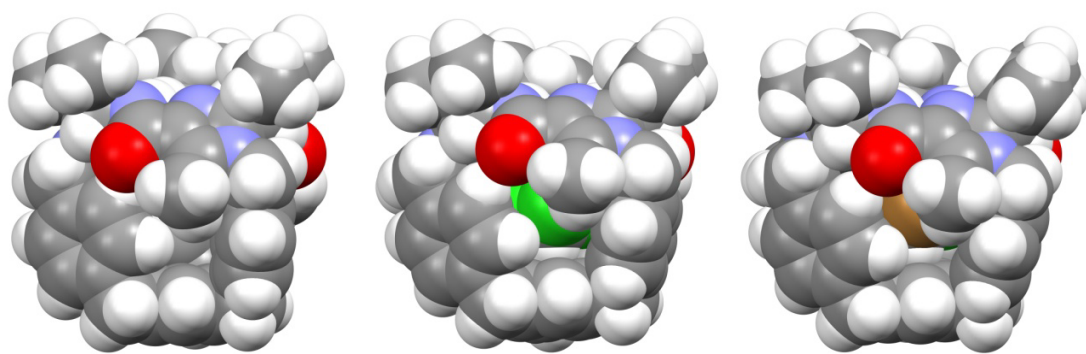
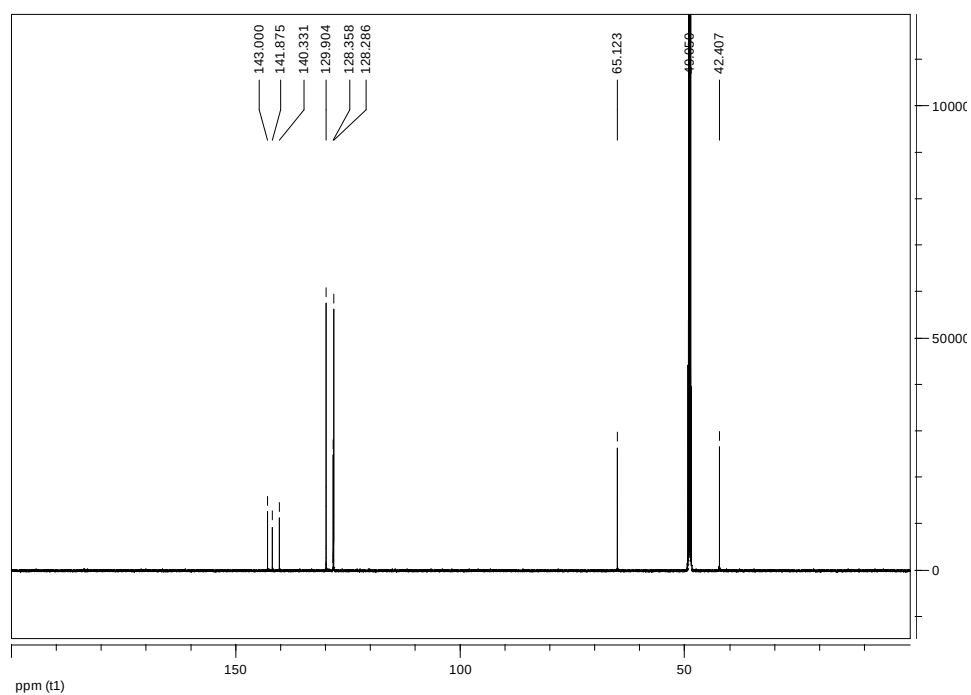
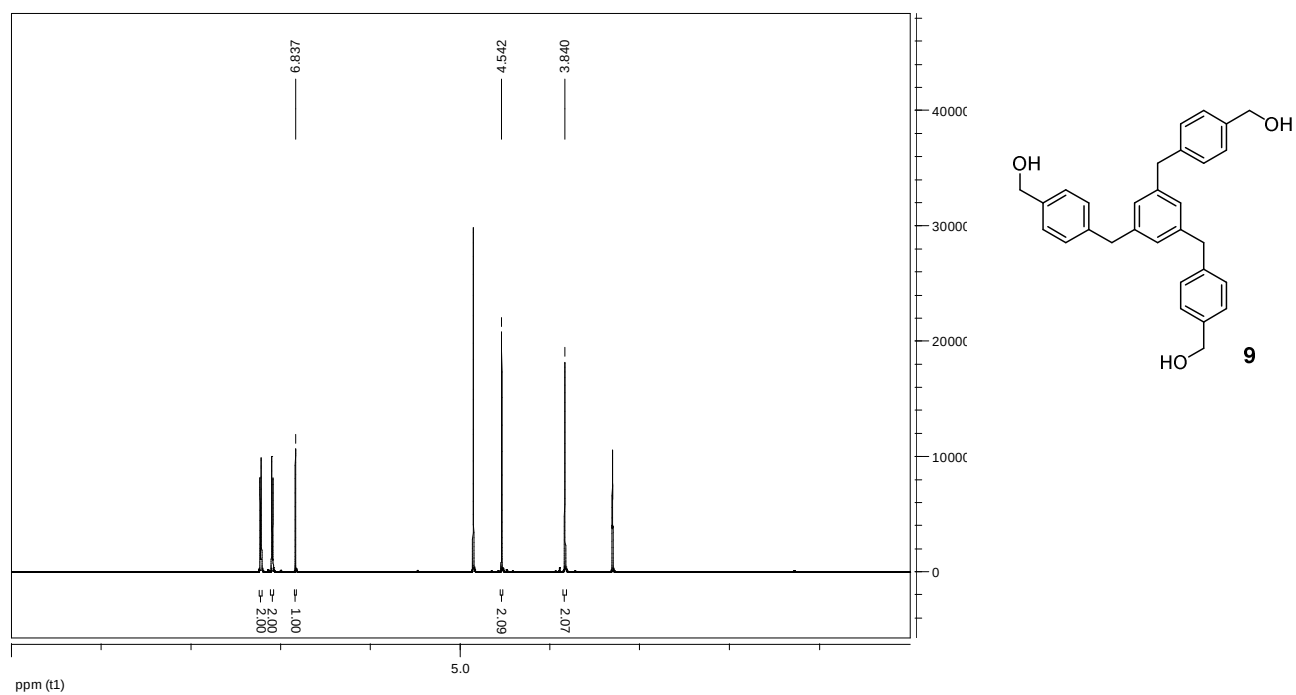
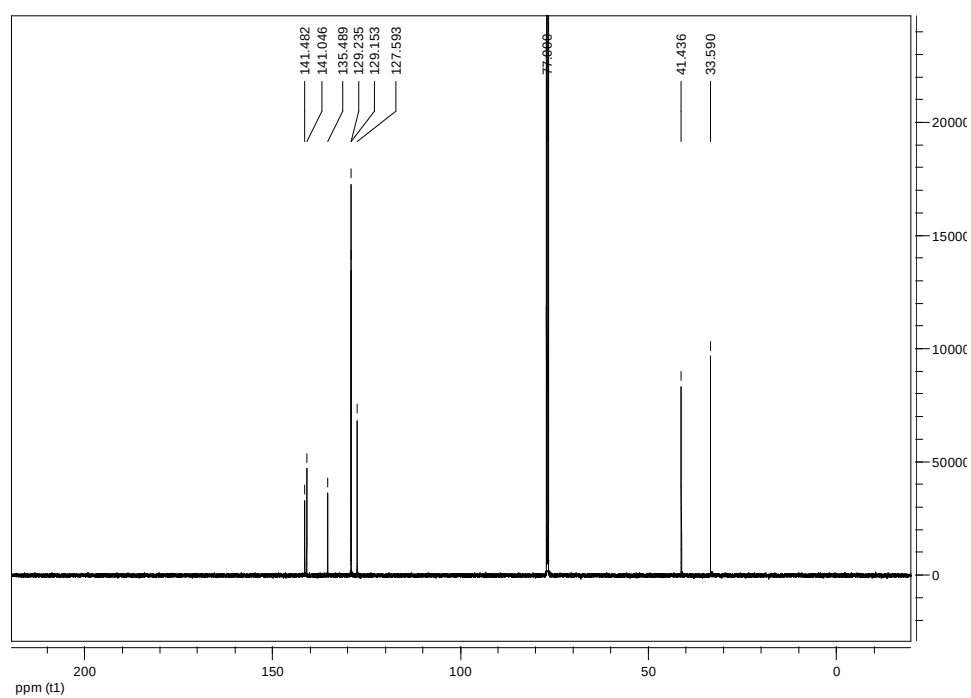
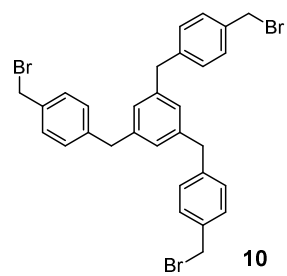
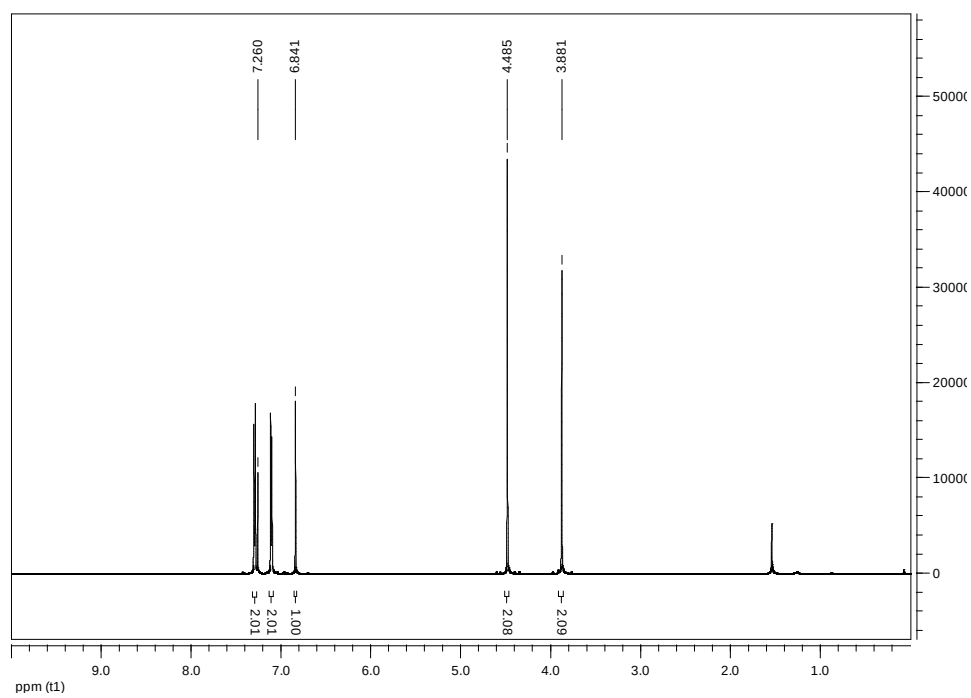
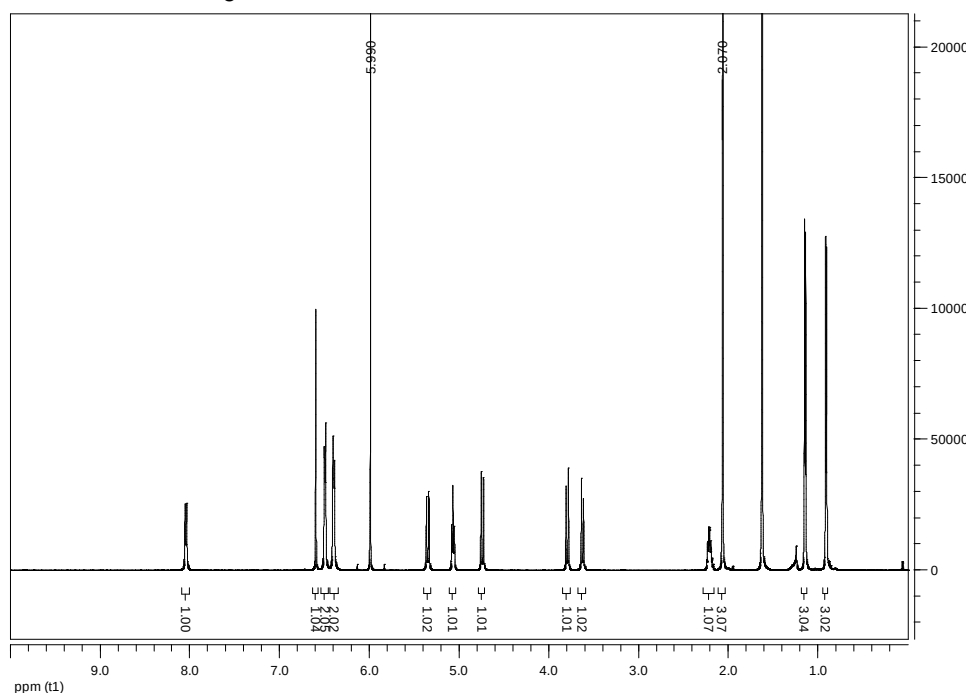
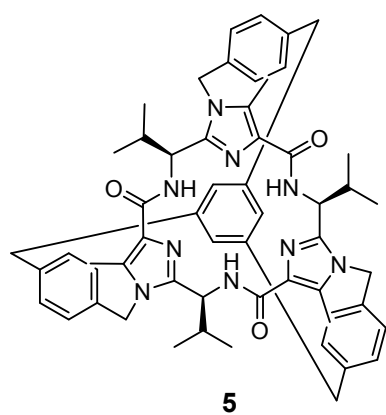


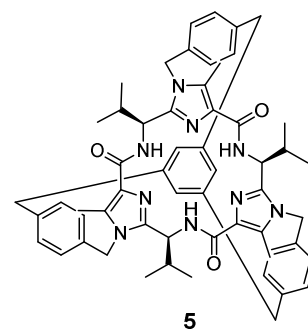
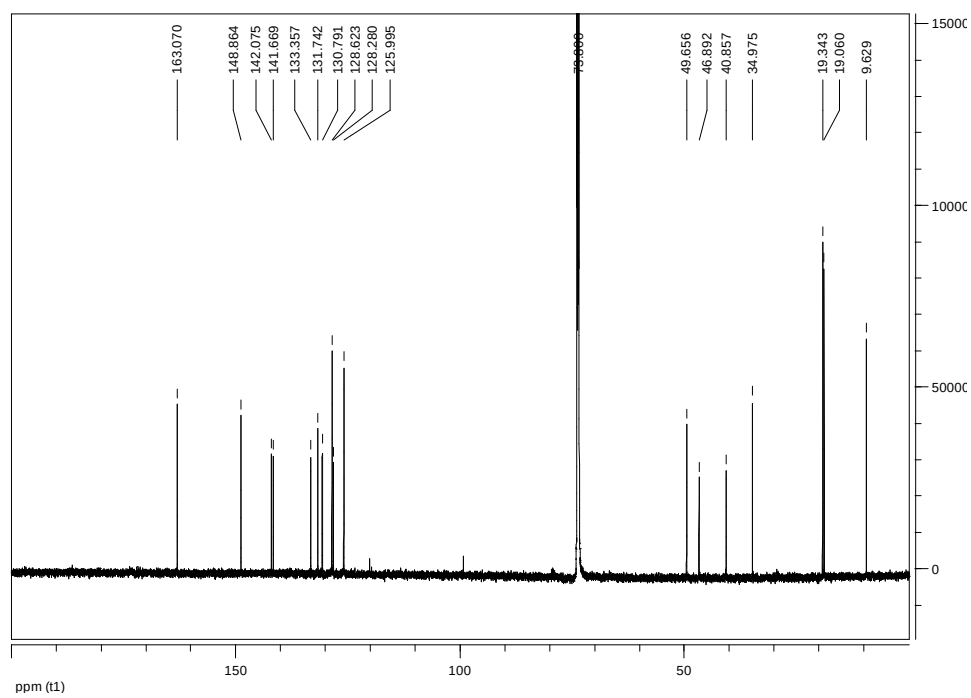
Figure S16. CPK model of container **5** (left) as well as the complexes $\downarrow\text{CHCl}_3@5$ (middle) and $\downarrow\text{CHBrCl}_2@5$ (right) calculated using B3LYP-D3/def2-TZVP.

3. ^1H NMR and ^{13}C NMR Spectra of the New Compounds

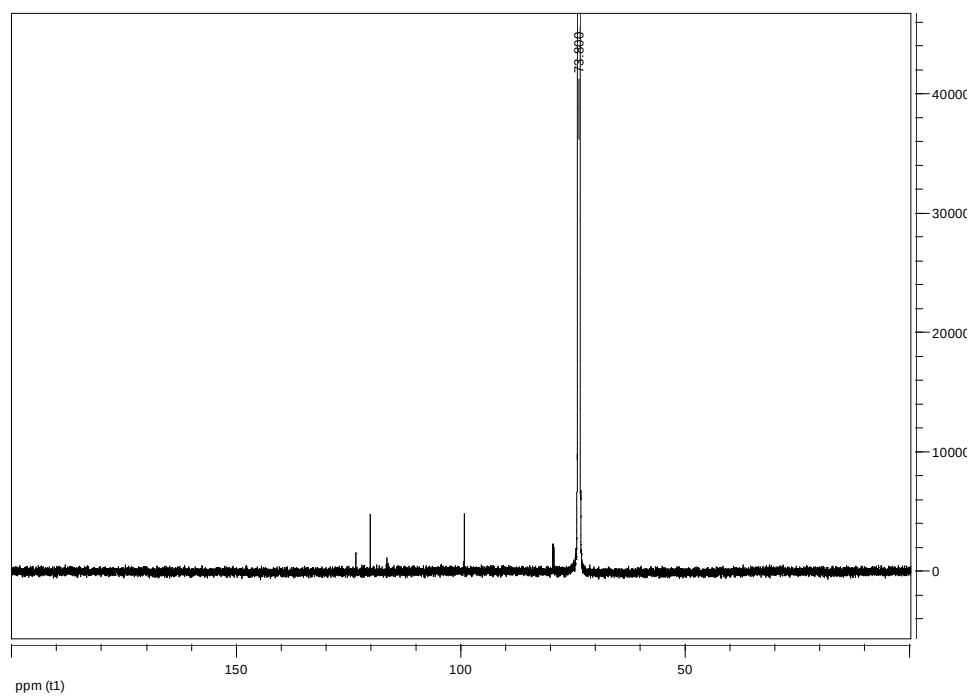


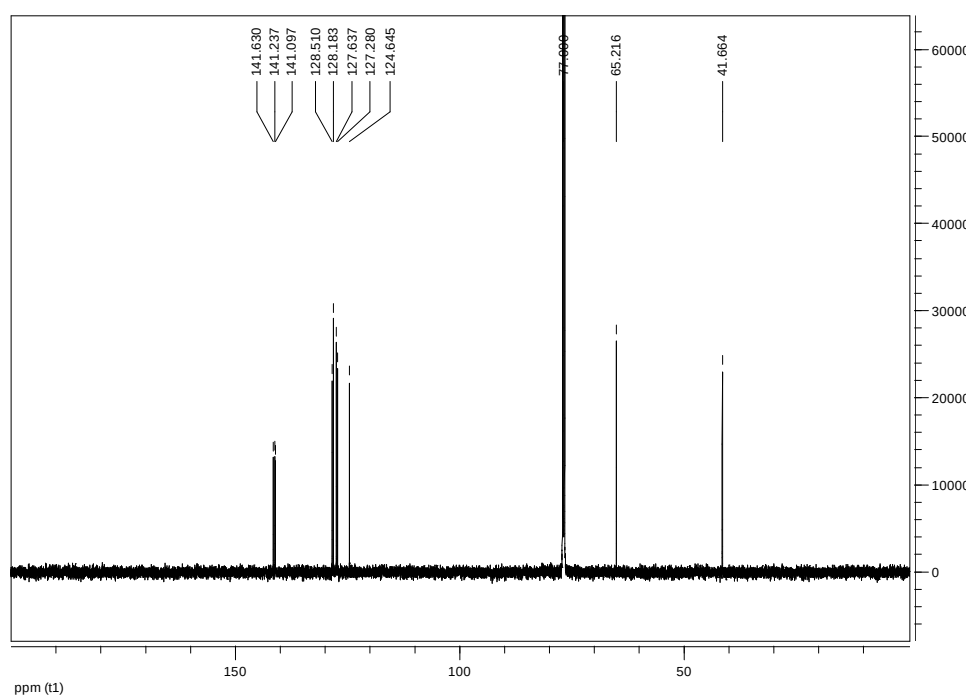
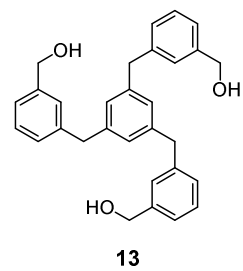
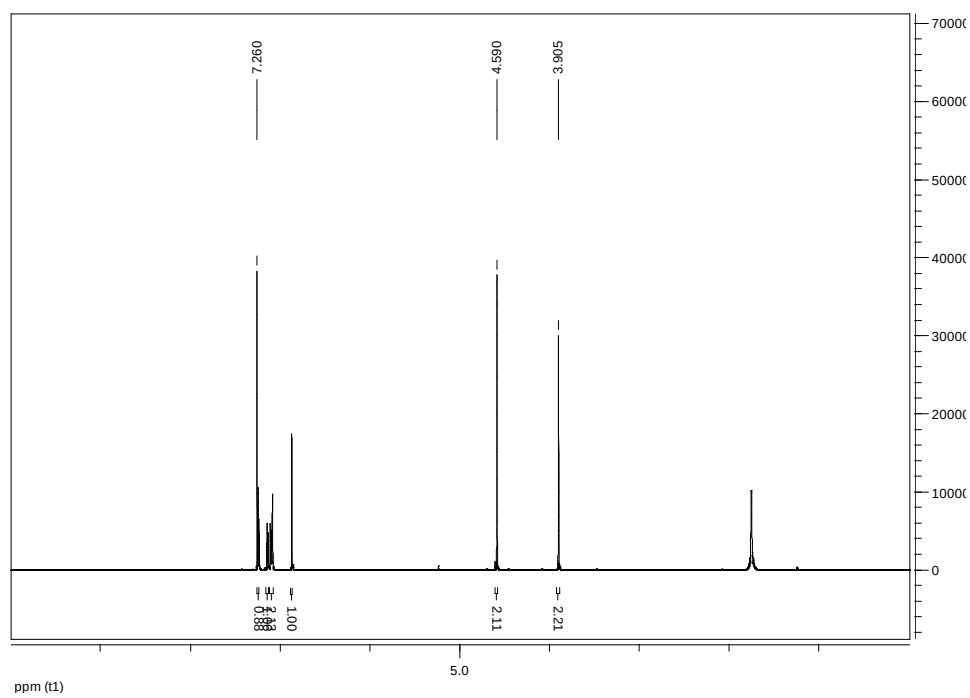


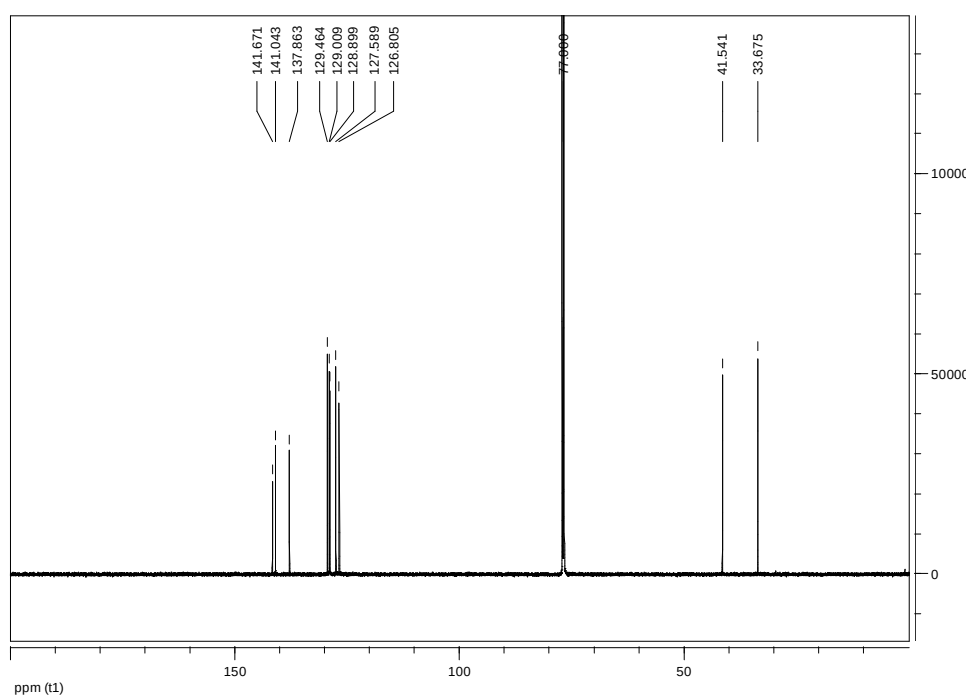
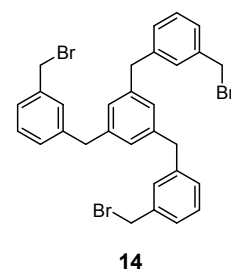
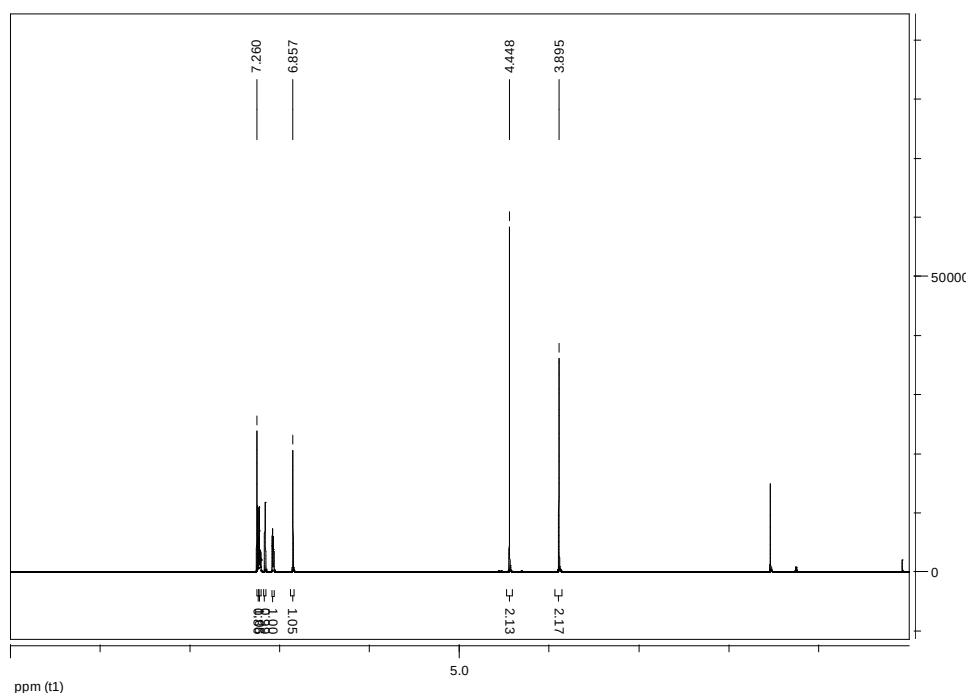


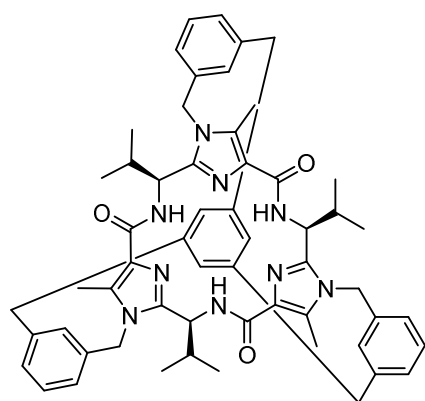


¹³C spectrum of the solvent C₂D₂Cl₄:

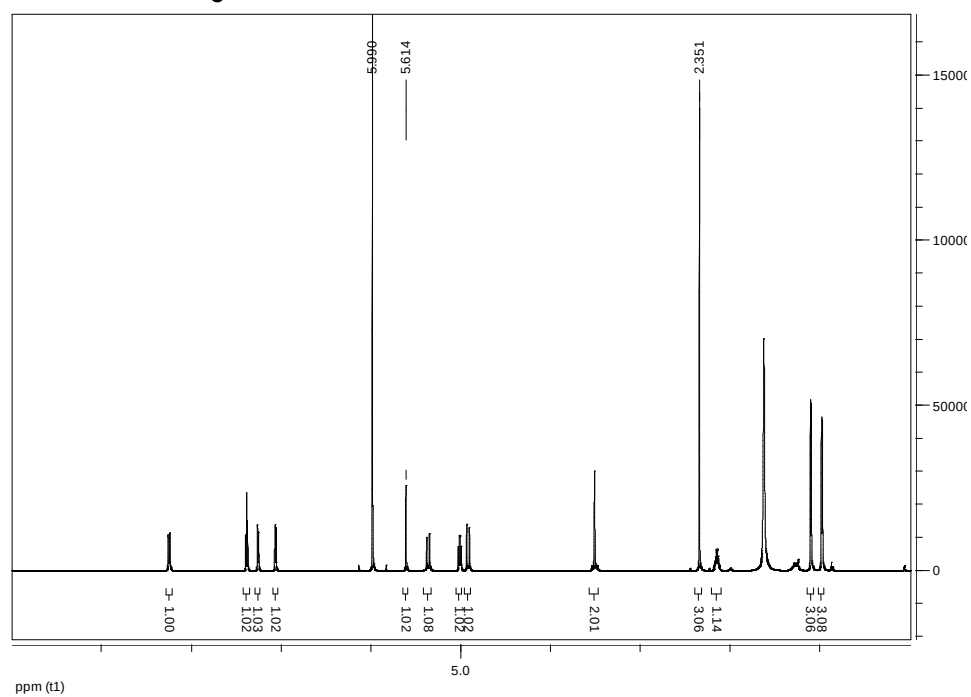


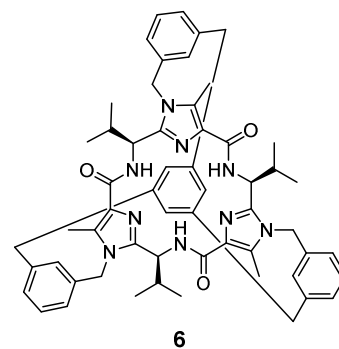
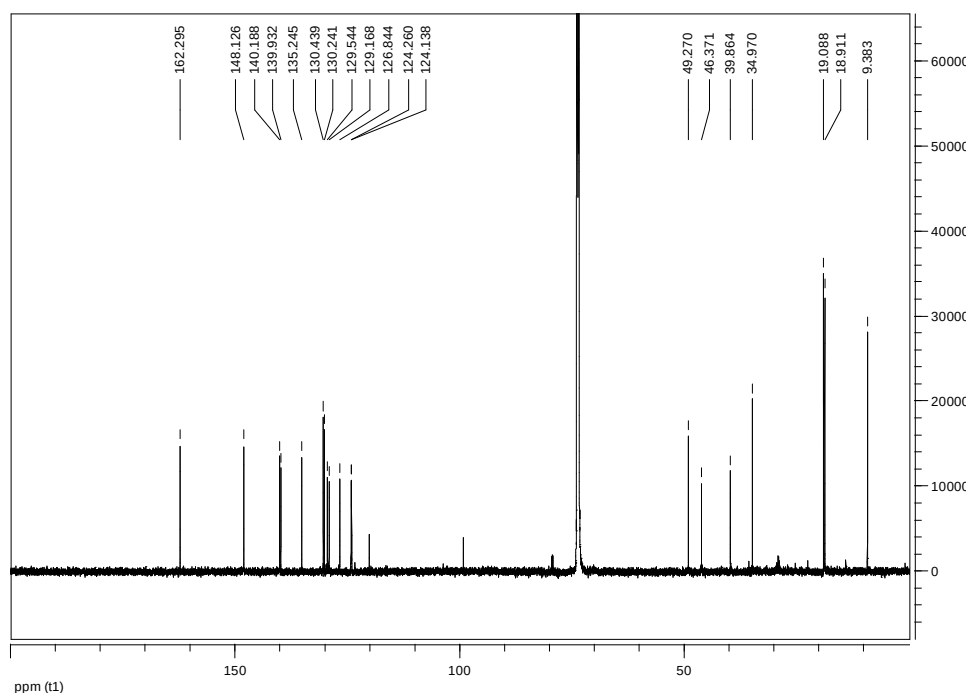




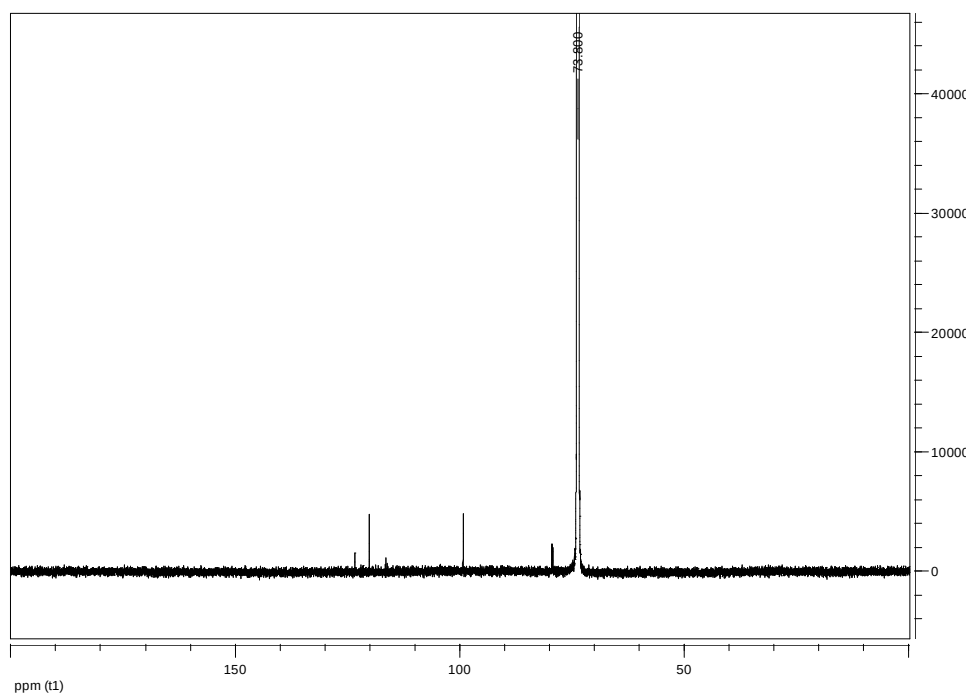


6





¹³C spectrum of the solvent C₂D₂Cl₄:



4. Cartesian Coordinates and Absolute Energies of all Calculated Compounds

Table S1. Absolute energies [au].

Molecule	E^a	E^b
CHCl ₃	-1419.178314	-1419.172204
CHBrCl ₂	-3533.098781	-3533.052813
1	-3109.054627	-3110.271756
CHCl ₃ @ 1	-4528.273462	-4529.480096
2	-2991.172750	-2992.343396
CHCl ₃ @ 2	-4410.393854	-4411.553875
3	-2186.563959	-2187.398764
CHCl ₃ @ 3	-3605.765075	-3606.589514
4	-3501.176209	-3502.423869
↑CHCl ₃ @ 4	-4920.402268	-4921.637198
5	-2926.937950	-2928.051281
↑CHCl ₃ @ 5	-4346.146083	-4347.250454
↓CHCl ₃ @ 5	-4346.148939	-4347.252858
↑CHBrCl ₂ @ 5	-6460.067163	-6461.131007
↓CHBrCl ₂ @ 5	-6460.069805	-6461.133308
6	-2926.941555	-2928.056255
↑CHCl ₃ @ 6	-4346.141459	-4347.245908
↓CHCl ₃ @ 6	-4346.138761	-4347.243451

^a B3LYP-D3/6-31G*, cc-pVTZ

^b B3LYP-D3/def2-TZVP

Table S2. Absolute energies [au] of CHCl₃, **5** and ↓CHCl₃@**5**.

Method	CHCl ₃	5	↓CHCl ₃ @ 5
B3LYP/def2-TZVP	-1419.169896	-2927.856351	-4347.001889
B3LYP-D2/def2-TZVP	-1419.171574	-2928.113440	-4347.311121
B97D/def2-TZVP	-1419.685469	-2927.976132	-4347.665644
B97-D3/def2-TZVP	-1419.405126	-2927.602123	-4347.032302
TPSS/def2-TZVP	-1419.420649	-2930.142596	-4349.540568
TPSS-D2/def2-TZVP	-1419.422248	-2930.387443	-4349.835074
TPSS-D3/def2-TZVP	-1419.422260	-2930.309857	-4349.755527
TPSSH/def2-TZVP	-1419.398023	-2929.838888	-4349.215688
TPSSH-D3/def2-TZVP	-1419.399715	-2930.001845	-4349.425054
PBE0/def2-TZVP	-1418.852385	-2926.257152	-4345.098422
PBE0-D3/def2-TZVP	-1418.853657	-2926.386056	-4345.263539
M05-2X/def2-TZVP	-1419.295689	-2929.305916	-4348.620714
M06-2X/def2-TZVP	-1419.265426	-2928.382921	-4347.679083
M06/def2-TZVP	-1419.238792	-2927.448376	-4346.720784
wB97XD/def2-TZVP	-1419.307344	-2928.660210	-4347.991080
APFD/def2-TZVP	-1418.983341	-2927.245367	-4346.262612
B2PLYPD/def2-TZVP	-1418.851090	-2926.737011	-4345.619100
B3LYP-D3/def2-TZVP(solvent)	-1419.175202	-2928.078600	-4347.279690
M06-2X/def2-TZVP(solvent)	-1419.267666	-2928.403820	-4347.699760
APFD/def2-TZVP(solvent)	-1418.985497	-2927.265427	-4346.282275

Cartesian coordinates of the optimized geometries for CHCl₃ using B3LYP-D3/6-31G*, cc-pVTZ.

C	-0.000008500	0.10837300	0.00000000
H	-0.00218000	1.19421200	0.00000000
Cl	-0.84972100	-0.43576600	1.47305800
Cl	1.70170700	-0.43105300	0.00000000
Cl	-0.84972000	-0.43576600	-1.47305800

Cartesian coordinates of the optimized geometries for CHBrCl₂ using B3LYP-D3/6-31G*,cc-pVTZ.

C	-0.01501900	0.10622200	0.00000000
H	-0.00242100	1.19150600	0.00000000
Cl	-0.86172300	-0.43233400	1.47141300
Cl	-0.86172400	-0.43233400	-1.47141300
Br	1.85978700	-0.47086000	0.00000000

Cartesian coordinates of the optimized geometries for **1** using B3LYP-D3/6-31G*,cc-pVTZ.

C	-2.59859900	1.73299600	-3.16764400
C	-2.46992300	2.84077400	-2.33911900
C	-1.22964400	3.52132300	-2.29934100
C	-0.20189500	3.08910400	-3.12834100
C	-0.33048200	1.96403900	-3.96578200
C	-1.54345300	1.26799200	-3.97589600
C	0.88976500	1.54975100	-4.77931400
C	1.87147200	0.70451500	-3.97740900
C	2.80356700	1.38509100	-3.17065700
C	3.69904500	0.71936600	-2.34302200
C	3.66569000	-0.69481900	-2.30103500
C	2.77641000	-1.36808600	-3.12943700
C	1.86680100	-0.69382100	-3.96693500
C	0.89736000	-1.54357400	-4.77991700
C	-0.32485400	-1.97163300	-3.97768400
C	-0.20117800	-3.11955300	-3.17145700
C	-1.22559700	-3.56233700	-2.34409900
C	-2.43412400	-2.82696200	-2.30239300
C	-2.57313900	-1.71993300	-3.13044700
C	-1.53387800	-1.26869400	-3.96712500
C	-1.78426500	-0.00375200	-4.77939900
O	-3.46735200	3.35471200	-1.55760400
O	-1.15439700	4.58111500	-1.44234000
C	0.10088700	5.23719200	-1.27126900
O	4.64568600	1.32544600	-1.56437000
O	4.54415000	-1.29049100	-1.44280100
C	4.48199500	-2.70559400	-1.27118200
O	-1.17440700	-4.68499000	-1.56518200
O	-3.38883000	-3.29132000	-1.44449700
C	-4.58368300	-2.53118000	-1.27141400
C	0.18036800	3.09037000	3.08857100
C	1.20526600	3.53015700	2.26002200
C	2.45075000	2.85919900	2.30093700
C	2.58710200	1.75219600	3.12927500
C	1.53493900	1.27924500	3.93679600
C	0.31694000	1.96640800	3.92620600
C	1.78459300	0.00917300	4.74014600
C	1.54272500	-1.25750100	3.92792200
C	2.58502400	-1.70166500	3.09124300
C	2.45378100	-2.80991000	2.26356100
C	1.25048900	-3.55379500	2.30570000
C	0.22306400	-3.11800600	3.13303600
C	0.33871300	-1.96897200	3.93884400
C	-0.88638500	-1.54945400	4.74110500
C	-1.86187500	-0.70674400	3.92799600
C	-2.76692100	-1.38743100	3.09074800
C	-3.66117500	-0.72044500	2.26259900
C	-3.70465000	0.69343100	2.30487900
C	-2.81362200	1.36548400	3.13219800
C	-1.87633200	0.69153400	3.93845200
C	-0.90031400	1.54365600	4.73992900
O	1.12244900	4.58901500	1.40259500
C	-0.13733900	5.23649900	1.23174200
O	3.44503900	3.38116000	1.52070400
O	3.41169600	-3.26792100	1.40582200

C	4.60132700	-2.49961600	1.23267900
O	1.20694000	-4.67695800	1.52698900
O	-4.53562200	-1.32219200	1.40452000
C	-4.46343200	-2.73676900	1.23246700
O	-4.65582200	1.29295100	1.52662300
C	-0.02130100	6.09865800	-0.01980600
C	5.28875000	-3.03183200	-0.01950400
C	-5.26766200	-3.06833300	-0.01943700
H	-3.53869100	1.19437000	-3.19203000
H	0.73711000	3.63033600	-3.13335800
H	1.40689100	2.45810600	-5.11428500
H	0.58663600	1.03155900	-5.69182900
H	2.80814400	2.46847500	-3.19554500
H	2.77472600	-2.45185300	-3.13368000
H	0.59864200	-1.02245200	-5.69220000
H	1.42570400	-2.44532500	-5.11520700
H	0.73481200	-3.66517600	-3.19684900
H	-3.51146100	-1.17757500	-3.13510200
H	-2.82945300	-0.00957000	-5.11444100
H	-1.18328400	-0.00578500	-5.69095900
H	0.90502600	4.50310900	-1.13081700
H	0.33084600	5.84537100	-2.15863000
H	3.44352900	-3.03287500	-1.13088300
H	4.89291200	-3.21000000	-2.15831300
H	-4.34870300	-1.46799400	-1.13088400
H	-5.22645200	-2.63470400	-2.15789600
H	-0.76255500	3.62474900	3.09319200
H	3.53113500	1.22051800	3.15414600
H	1.18386000	0.00301800	5.65185400
H	2.82986200	0.01036500	5.07496700
H	3.51944600	-1.15265000	3.09562200
H	-0.70903000	-3.67024200	3.15882200
H	-1.40835500	-2.45479400	5.07669800
H	-0.59135300	-1.02597900	5.65325900
H	-2.75770100	-2.47115800	3.09520700
H	-2.82615800	2.44880600	3.15744700
H	-1.42361800	2.44850100	5.07482600
H	-0.59330700	1.02777200	5.65241800
H	-0.93648400	4.49693100	1.09160100
H	-0.37116200	5.84316100	2.11913600
H	4.35907200	-1.43802700	1.09252200
H	5.24497300	-2.59900000	2.11901000
H	-3.42266400	-3.05666300	1.09227300
H	-4.87102800	-3.24436000	2.11932900
H	0.85987200	6.74557300	0.06547100
H	-0.90702800	6.73929900	-0.10509200
H	5.40692700	-4.11855800	0.06548900
H	6.28712700	-2.58663100	-0.10506400
H	-5.37829100	-4.15584100	-0.10454800
H	-6.26912300	-2.63007500	0.06593600
C	-0.02206500	-5.50570800	-1.68223300
H	-0.24840800	-6.41744500	-1.12701800
H	0.18175100	-5.76939900	-2.72908000
H	0.86084900	-5.02412300	-1.24037900
C	0.06163600	-5.50707700	1.64661200
H	-0.82590400	-5.03331900	1.20555600
H	0.29468600	-6.41758700	1.09212400
H	-0.13849500	-5.77110200	2.69407700
C	-4.75479100	2.76993800	-1.67942100
H	-4.78171300	1.76260400	-1.24151100
H	-5.43141200	3.42043400	-1.12288700
H	-5.08331600	2.72999000	-2.72720800
C	4.73707800	2.80715500	1.64447900
H	4.77323200	1.80023200	1.20621100
H	5.40926900	3.46351000	1.08943000
H	5.06405800	2.76929700	2.69282800

C	4.78220700	2.73305800	-1.68486300
H	3.92444000	3.25923200	-1.24341500
H	5.68603000	2.99317100	-1.13107000
H	4.90851100	3.03903900	-2.73253800
C	-4.80449900	2.69907200	1.64998700
H	-3.95158100	3.23356600	1.20914000
H	-5.71088400	2.95249500	1.09725200
H	-4.93276200	3.00176400	2.69837200

Cartesian coordinates of the optimized geometries for CHCl_3 @1 using B3LYP-D3/6-31G*,cc-pVTZ.

C	-2.60322100	1.68981000	-3.31712300
C	-2.46868400	2.77176700	-2.45762800
C	-1.23416700	3.46044400	-2.41669900
C	-0.21665900	3.06324800	-3.27395000
C	-0.34604400	1.95585500	-4.13459400
C	-1.55317800	1.24992600	-4.14522800
C	0.87459000	1.55746600	-4.95630500
C	1.86205200	0.72229600	-4.15082200
C	2.77002000	1.41421000	-3.32707400
C	3.63946000	0.76011100	-2.46484700
C	3.61590300	-0.65304000	-2.41607400
C	2.76182400	-1.33836300	-3.26993400
C	1.86817900	-0.67583300	-4.13369400
C	0.91276400	-1.53671100	-4.95256700
C	-0.30429300	-1.97415300	-4.14737000
C	-0.16035500	-3.10736700	-3.32447500
C	-1.16384000	-3.53469700	-2.46551400
C	-2.37628700	-2.80806900	-2.41858300
C	-2.54142200	-1.72486700	-3.27179700
C	-1.51872500	-1.28078600	-4.13226500
C	-1.78521900	-0.02244600	-4.95065800
O	-3.44380600	3.23125600	-1.61547300
O	-1.14334300	4.47410500	-1.50547600
C	0.12714500	5.08809400	-1.29647500
O	4.52686000	1.37868600	-1.62745200
O	4.44614600	-1.23567600	-1.50103900
C	4.34319500	-2.64302400	-1.29093800
O	-1.07450700	-4.61412000	-1.62985300
O	-3.29810500	-3.23740900	-1.50625600
C	-4.46382300	-2.44264600	-1.29464700
C	0.19708100	3.04277700	3.17502300
C	1.22234900	3.45110300	2.33049100
C	2.47309300	2.79445600	2.41087100
C	2.60955700	1.72077400	3.28066300
C	1.55128900	1.26369700	4.08881300
C	0.33287000	1.95124800	4.05551100
C	1.78466000	-0.01091900	4.88833600
C	1.52176400	-1.26470400	4.06022600
C	2.53871800	-1.69394900	3.18457200
C	2.38218300	-2.78570400	2.33903900
C	1.18751800	-3.54016700	2.41519000
C	0.18563900	-3.12047100	3.28009700
C	0.31624100	-1.97508300	4.08843200
C	-0.90607100	-1.53949000	4.88462800
C	-1.85902300	-0.68342800	4.05640000
C	-2.73684200	-1.34830600	3.17772300
C	-3.60584800	-0.66665900	2.33439500
C	-3.66656700	0.74450500	2.41656600
C	-2.80344900	1.40127700	3.28367400
C	-1.87428100	0.71544200	4.08885600
C	-0.88510900	1.55613000	4.88456300
O	1.13236300	4.45719200	1.41495600
C	-0.13040200	5.09097500	1.21340900

O	3.46375800	3.27852100	1.60530000
O	3.30154400	-3.21060000	1.42636900
C	4.47614500	-2.42630000	1.22062100
O	1.11529800	-4.64103000	1.61045600
O	-4.43052800	-1.25040400	1.41901100
C	-4.34019500	-2.66068300	1.21711900
O	-4.58591200	1.35867400	1.61498600
C	0.00278300	5.94479500	-0.04187700
C	5.14876500	-2.96401800	-0.03701400
C	-5.14313200	-2.97764400	-0.03912800
H	-3.53652300	1.14019200	-3.33669700
H	0.72131200	3.60577600	-3.26873900
H	1.38190600	2.47152000	-5.29086700
H	0.57427900	1.03685200	-5.86821300
H	2.76271200	2.49712800	-3.35294800
H	2.76053200	-2.42179600	-3.25855900
H	0.61066600	-1.01922000	-5.86562600
H	1.45170300	-2.43326200	-5.28504700
H	0.78157700	-3.64186200	-3.34857400
H	-3.48018700	-1.18377200	-3.26344200
H	-2.83157100	-0.03926100	-5.28174700
H	-1.18670700	-0.02086100	-5.86368300
H	0.90240300	4.32404300	-1.14946700
H	0.39728600	5.70067200	-2.16951200
H	3.29416800	-2.93259000	-1.14319000
H	4.73811000	-3.18351200	-2.16412600
H	-4.18810200	-1.38959300	-1.14809300
H	-5.13060400	-2.51344300	-2.16666400
H	-0.75154100	3.56515300	3.14464200
H	3.55267500	1.18963700	3.32342200
H	1.18405700	-0.01835600	5.79987600
H	2.83023500	-0.02915400	5.22102300
H	3.46676600	-1.13577400	3.15884700
H	-0.74667200	-3.67048400	3.31862500
H	-1.44586800	-2.43565500	5.21594000
H	-0.61337900	-1.01706000	5.79788300
H	-2.71359000	-2.43077700	3.14767200
H	-2.81713800	2.48363700	3.32668000
H	-1.39059700	2.47232600	5.21532700
H	-0.57835400	1.04251100	5.79824300
H	-0.91851600	4.34079400	1.06854300
H	-0.38455400	5.70605000	2.08954200
H	4.21279800	-1.37031200	1.07730600
H	5.13932600	-2.50919700	2.09433400
H	-3.29467700	-2.96218900	1.07400600
H	-4.74426300	-3.19056300	2.09267500
H	0.88818600	6.58474200	0.05206200
H	-0.87594900	6.59377000	-0.13644700
H	5.26299900	-4.05068300	0.05450300
H	6.14921900	-2.52521600	-0.13163100
H	-5.26255800	-4.06369300	-0.13108300
H	-6.14167900	-2.53383100	0.05247500
C	0.12126400	-5.37741000	-1.67910300
H	-0.06487400	-6.26222900	-1.06912400
H	0.35575500	-5.69828700	-2.70322300
H	0.96957200	-4.82102900	-1.25795300
C	-0.04778400	-5.44813600	1.71337500
H	-0.92778900	-4.93835700	1.29859200
H	0.15761300	-6.34393600	1.12565400
H	-0.24418700	-5.74502400	2.75266900
C	-4.70423800	2.57992900	-1.66385600
H	-4.64775200	1.56573300	-1.24564100
H	-5.37482500	3.18325800	-1.05071500
H	-5.10195800	2.54150900	-2.68739500
C	4.74523200	2.67896100	1.71734600
H	4.74773700	1.65892400	1.30971100

H	5.41932800	3.30212900	1.12800500
H	5.09682600	2.66548800	2.75828500
C	4.58745500	2.79599000	-1.67769500
H	3.67943000	3.25099300	-1.25893900
H	5.44515600	3.07935400	-1.06613000
H	4.75038100	3.15923900	-2.70171700
C	-4.71209800	2.76754700	1.73035200
H	-3.83346100	3.28390500	1.31968300
H	-5.59277700	3.03771800	1.14545800
H	-4.87255600	3.07620300	2.77250200
Cl	-1.02579700	1.34329500	0.19123400
Cl	-0.65840200	-1.56369300	0.18395900
Cl	1.67547500	0.20792600	0.18273600
C	-0.00189200	-0.00514600	0.75389300
H	0.00056200	-0.00772000	1.84119700

Cartesian coordinates of the optimized geometries for **2** using B3LYP-D3/6-31G*,cc-pVTZ.

C	3.02031000	1.35310100	3.73240800
H	2.94917700	2.28542200	4.30550100
H	3.84200700	0.79287100	4.18450700
C	3.34589400	1.71099000	2.28713000
C	2.68859600	2.81464500	1.72273200
H	1.97501300	3.39062200	2.30401200
C	2.90257500	3.22563800	0.41479800
O	2.24643800	4.34834800	-0.02215600
C	1.48518400	4.24714800	-1.22847200
C	0.29755800	5.19329500	-1.09932900
H	0.64579300	6.13022800	-0.65536600
H	-0.12306600	5.41851400	-2.08958900
C	3.84028100	2.52983600	-0.37513200
O	4.05813800	3.01169900	-1.64306900
C	5.18271300	2.51047300	-2.34950700
H	6.10892900	2.65843000	-1.77767400
H	5.23261300	3.08076100	-3.27976600
H	5.07480200	1.44370100	-2.58711200
C	2.63941100	1.22426100	-4.35015700
H	2.16092700	1.75221300	-5.18674700
H	3.70591700	1.12242000	-4.55997500
H	2.50799600	1.80555400	-3.42714600
C	4.48514500	1.42250400	0.17049700
H	5.19849400	0.86891000	-0.42937000
C	4.24037700	0.98657700	1.48428900
C	4.90656600	-0.31149800	1.92497300
H	5.89853500	-0.37544600	1.46140400
H	5.08095100	-0.31897500	3.00317100
C	4.08642300	-1.52033300	1.49049000
C	4.26515700	-1.99573200	0.18178000
H	5.02887500	-1.56122000	-0.45808500
C	3.50018300	-3.02129500	-0.35465200
O	3.74730400	-3.47569300	-1.62998900
C	3.13048700	-2.72835400	-2.68786200
H	3.75012100	-2.87470300	-3.57739000
H	3.11125100	-1.65797700	-2.45375000
C	1.72123200	-3.25070600	-2.97213600
H	1.76638100	-4.33208200	-3.13307100
H	1.04828200	-3.05867200	-2.12943400
C	2.50490300	-3.62313600	0.44212200
O	1.76558400	-4.60870700	-0.14902900
C	0.71731400	-5.19511000	0.60501900
H	1.09730200	-5.70720000	1.50027800
H	0.25111900	-5.93028900	-0.05464700
H	-0.03262000	-4.45030300	0.90854600
C	-3.90302100	4.08328000	2.15044600
H	-4.77588600	4.39734400	1.56156200

H	-3.76595500	4.76895500	2.98905600
H	-4.07388100	3.06956600	2.53872000
C	2.34571600	-3.18458300	1.75559200
H	1.59901000	-3.64938000	2.38942300
C	3.11466300	-2.13753400	2.29329000
C	2.82052500	-1.72561500	3.73148900
H	2.62099900	-2.63480800	4.31224000
H	3.70366200	-1.27428800	4.18902600
C	1.61624300	-0.80316700	3.86734700
C	0.34265400	-1.38627500	3.95486700
H	0.22794900	-2.46683300	3.95208800
C	-0.81837200	-0.63396000	4.06179900
O	-2.01802300	-1.28755700	4.18715500
C	-3.01420300	-1.01440400	3.19105400
H	-2.56436100	-0.54834400	2.30623600
H	-3.77133800	-0.33105000	3.59120400
C	-3.62944900	-2.36283600	2.82684600
H	-2.85773400	-3.03518900	2.43790300
H	-4.07203500	-2.82300000	3.71475100
C	-0.72511700	0.77187700	4.11356900
C	-1.81687200	2.86173000	4.46192400
H	-1.14414700	3.12634500	5.28903700
H	-2.82890800	3.18595400	4.71047100
H	-1.49016100	3.36262500	3.54111400
C	-2.90896800	-5.18040600	-0.40463500
H	-3.59278400	-5.47215800	-1.21398900
H	-2.76382200	-6.02863000	0.26824300
H	-1.94208300	-4.89182100	-0.83969400
O	-1.89626400	1.45279500	4.28929400
C	0.53417400	1.36020700	4.01340400
H	0.62377400	2.44010400	4.04502200
C	1.70703300	0.59738000	3.88170600
C	-3.42574000	-1.20294500	-3.59002100
H	-4.08747600	-0.46774200	-4.05267000
H	-3.60479700	-2.14152100	-4.12874800
C	-1.96581500	-0.81442900	-3.78188700
C	-1.01845600	-1.84522900	-3.87727100
H	-1.33731300	-2.88422200	-3.86584900
C	0.34105500	-1.60497500	-4.01884000
O	1.21207900	-2.65689800	-4.17715100
C	0.80054500	-0.27300200	-4.06986800
O	2.14670900	-0.09980800	-4.21824700
C	-0.13437400	0.75938500	-3.98938900
H	0.20031000	1.78951600	-4.04320700
C	-1.51100000	0.51225600	-3.84512300
C	-2.43951500	1.71839900	-3.76832500
H	-2.03762400	2.49982200	-4.42559300
H	-3.42026500	1.46887600	-4.17959400
C	-2.58465400	2.30328300	-2.36924500
C	-1.59881900	3.21298700	-1.94195700
H	-0.80169900	3.45572700	-2.63477700
C	-1.62289700	3.81137900	-0.68605900
O	-0.71451000	4.71792300	-0.21758900
C	-2.69572300	3.50297100	0.18537200
O	-2.70986000	4.15867200	1.38587000
C	-3.66672300	2.60078500	-0.23290600
H	-4.49101700	2.36289900	0.42956200
C	-3.63108000	1.98415500	-1.49776200
C	-4.72649900	0.97527600	-1.81925400
H	-4.94543500	0.96982900	-2.88957900
H	-5.65243900	1.30176700	-1.33037500
C	-4.39354100	-0.42776200	-1.32760600
C	-4.65854000	-0.73293200	0.01740700
H	-5.13538200	-0.00032200	0.66274700
C	-4.34243000	-1.95836500	0.58575500
O	-4.70354600	-2.20518800	1.89083700

O	-3.45755000	-4.14258600	0.39068800
C	-3.73636500	-2.94909400	-0.21756500
C	-3.48193500	-2.66004100	-1.55640400
H	-3.03151100	-3.41405100	-2.19192800
C	-3.79427400	-1.41290500	-2.12597800
H	2.10234300	4.53804900	-2.08832300
H	1.14788100	3.21480800	-1.37965000

Cartesian coordinates of the optimized geometries for $\text{CHCl}_3@2$ using B3LYP-D3/6-31G*,cc-pVTZ.

Cl	1.51754000	-0.06692200	-0.68119200
Cl	-0.85662000	1.05840000	0.60796400
Cl	-0.63823800	-1.83834700	0.25467700
C	0.26518500	-0.31992200	0.55600000
H	0.75694900	-0.41138500	1.51947800
C	3.03941900	1.31354100	3.73077700
H	2.95545500	2.24885800	4.29710200
H	3.87130900	0.77001400	4.18372400
C	3.35487300	1.66795600	2.28222800
C	2.66463900	2.74719700	1.70961200
H	1.92018100	3.29339600	2.28025400
C	2.88809900	3.17608100	0.40977600
O	2.19332200	4.27394600	-0.03143500
C	1.42394600	4.13565200	-1.23117700
C	0.31411600	5.18159700	-1.18307200
H	0.72320300	6.10335300	-0.76044200
H	-0.04697200	5.40301600	-2.19695400
C	3.87427700	2.52664200	-0.36082000
O	4.10166000	3.02653300	-1.61841500
C	5.23323100	2.53963600	-2.32336100
H	6.15682500	2.69651800	-1.74971400
H	5.27860000	3.11191900	-3.25248600
H	5.13744100	1.47177000	-2.56175500
C	2.58984300	1.27572900	-4.22018200
H	2.13064100	1.78080600	-5.08119600
H	3.66215200	1.17723100	-4.39906800
H	2.43009900	1.87522000	-3.31409300
C	4.54579900	1.43614000	0.18880700
H	5.28684500	0.90941600	-0.40173000
C	4.28426700	0.97543700	1.49081700
C	4.96338100	-0.31609900	1.93237500
H	5.95495400	-0.37276200	1.46745200
H	5.13933600	-0.32019200	3.01065600
C	4.15294900	-1.53485000	1.50301200
C	4.33174100	-2.01230700	0.19446300
H	5.08442500	-1.56594100	-0.45032100
C	3.56929100	-3.04063800	-0.34001100
O	3.80549800	-3.49373200	-1.61734900
C	3.16656800	-2.75629000	-2.67019700
H	3.70901200	-3.00420400	-3.58699700
H	3.24911100	-1.67692800	-2.50045300
C	1.70203700	-3.16579600	-2.83232000
H	1.64089300	-4.25584800	-2.90762300
H	1.10173700	-2.84508000	-1.97545500
C	2.58059300	-3.64907000	0.46024000
O	1.84228800	-4.63342700	-0.12937300
C	0.83683900	-5.26947900	0.64410200
H	1.26496000	-5.79343400	1.51036800
H	0.36881700	-5.99945200	-0.02033200
H	0.07906400	-4.55479000	0.99152200
C	-3.94914800	4.25553400	2.07483200
H	-4.82327700	4.58870500	1.49826400
H	-3.78976100	4.93208100	2.91745700
H	-4.13671100	3.24270300	2.45708700

C	2.42433500	-3.21268100	1.77415100
H	1.68208200	-3.68284600	2.40883200
C	3.18857300	-2.16063600	2.30979900
C	2.89419500	-1.76077500	3.75258500
H	2.71561100	-2.67618000	4.32993500
H	3.76928600	-1.29237400	4.20821700
C	1.67208000	-0.86318900	3.89414100
C	0.40538700	-1.46537400	3.97775200
H	0.30631700	-2.54697600	3.97635600
C	-0.77119400	-0.73020800	4.05828400
O	-1.95677900	-1.40526500	4.16263700
C	-2.98551100	-1.08184300	3.21065500
H	-2.55997200	-0.58784900	2.33090400
H	-3.72035700	-0.40906300	3.66434300
C	-3.62651300	-2.40491700	2.80931400
H	-2.87396200	-3.07089600	2.37633200
H	-4.06270000	-2.89622000	3.68377300
C	-0.69738600	0.67870200	4.09594400
C	-1.83665400	2.76638900	4.29512400
H	-1.18109300	3.11483000	5.10469900
H	-2.85922600	3.08078600	4.51007700
H	-1.51470700	3.20343400	3.34077100
C	-2.93080600	-5.14905600	-0.41403500
H	-3.56648700	-5.45955600	-1.25498400
H	-2.78423000	-5.99839200	0.25708500
H	-1.95697300	-4.81946800	-0.80395300
O	-1.87783900	1.34627900	4.23469200
C	0.55349500	1.28423200	4.00243200
H	0.62362400	2.36553400	4.01363800
C	1.73998400	0.53994400	3.89119400
C	-3.47593500	-1.17560200	-3.58774700
H	-4.13545800	-0.44156900	-4.05535000
H	-3.64837500	-2.11461400	-4.12760900
C	-2.01477700	-0.78377900	-3.76164700
C	-1.05989700	-1.81096900	-3.82129800
H	-1.37302900	-2.85123500	-3.79861800
C	0.30074700	-1.56364600	-3.93106900
O	1.18542500	-2.60851300	-4.05353000
C	0.75158300	-0.22958900	-3.98216300
O	2.10269900	-0.04873200	-4.07198600
C	-0.18905200	0.79795200	-3.94316200
H	0.14221600	1.82913200	-3.99199000
C	-1.56705700	0.54397900	-3.83202500
C	-2.50391100	1.74543800	-3.79359500
H	-2.10718300	2.50933100	-4.47420900
H	-3.48343300	1.47784400	-4.19592100
C	-2.65175700	2.37116800	-2.41320300
C	-1.67966800	3.30938100	-2.02168700
H	-0.88633300	3.53688000	-2.72344700
C	-1.69624800	3.93521900	-0.77932500
O	-0.77131900	4.83311200	-0.32860500
C	-2.76344700	3.64335600	0.10461200
O	-2.76421100	4.31579700	1.29711700
C	-3.72662200	2.71637700	-0.28167500
H	-4.54083900	2.48405800	0.39532200
C	-3.68402400	2.05457100	-1.52295100
C	-4.75880200	1.01281600	-1.80763500
H	-4.99728900	0.99187500	-2.87385200
H	-5.68248700	1.32809000	-1.30702600
C	-4.40941800	-0.38793600	-1.31345900
C	-4.65727700	-0.69368700	0.03531400
H	-5.09845800	0.04991200	0.69351600
C	-4.37092100	-1.93329100	0.58977500
O	-4.71298800	-2.18035300	1.90024400
O	-3.55029300	-4.14013900	0.36634700
C	-3.81236300	-2.93678300	-0.23075500

C	-3.56741500	-2.64538000	-1.56991300
H	-3.14306000	-3.40573500	-2.21559300
C	-3.84860200	-1.38522700	-2.12556100
H	2.06002800	4.31268600	-2.10769400
H	1.00858800	3.12270300	-1.29996000

Cartesian coordinates of the optimized geometries for **3** using B3LYP-D3/6-31G*,cc-pVTZ.

O	4.71558800	-3.57787600	7.21883200
O	12.72046300	-2.39137900	8.23049000
O	7.70256300	4.01164900	7.56320900
O	9.37766200	3.98878900	5.88800900
O	4.23752100	-2.32490800	5.26567300
O	12.22006200	-3.65046100	6.28691300
C	6.08230000	-0.61083500	9.84626300
C	6.56332000	-1.93508900	9.90330100
C	6.05054000	-2.88100500	9.01027300
H	6.40506700	-3.90721100	9.03257700
C	5.09392200	-2.54569600	8.05287600
C	4.59548700	-1.24191700	7.99747700
H	3.86752900	-0.94444400	7.25333100
C	5.09344700	-0.30614800	8.90169000
H	4.70660600	0.70910900	8.85595100
C	7.65185600	-2.39554600	10.86840900
H	7.63641000	-1.79700900	11.78184900
H	7.41907700	-3.42058500	11.18105600
C	9.03847100	-2.39085800	10.23527400
C	9.93730800	-1.30819200	10.32810600
C	11.15764800	-1.38098600	9.64925300
H	11.86644500	-0.56004800	9.70305000
C	11.50037900	-2.48410000	8.86850200
C	10.62762100	-3.57148100	8.78351200
H	10.85492300	-4.43415300	8.17037900
C	9.42062500	-3.50479100	9.47655200
H	8.74119700	-4.35088900	9.40748500
C	9.63939400	-0.02958800	11.10544200
H	8.96566100	-0.23403600	11.94049100
H	10.57535500	0.31975700	11.55794000
C	9.09071700	1.08300900	10.22104700
C	7.71450600	1.32492600	10.03203300
C	7.31956300	2.33073300	9.14463800
H	6.26612400	2.53700300	8.98000000
C	8.24733200	3.08440400	8.42728600
C	9.61383100	2.86716800	8.61841300
H	10.35943800	3.42106000	8.06205800
C	10.00512700	1.87829500	9.51851600
H	11.06916400	1.70894500	9.66540600
C	6.61475800	0.52027300	10.71793300
H	6.95774500	0.14146700	11.68307000
H	5.78521900	1.20106100	10.94332100
C	7.93245700	1.06803900	3.25190300
C	9.31311200	1.28560100	3.43799500
C	9.72767000	2.29006900	4.31789000
H	10.78497400	2.47767300	4.48017100
C	8.81485500	3.06597300	5.03075000
C	7.44435500	2.87297700	4.84226100
H	6.70981000	3.44465600	5.39531100
C	7.03375600	1.88527000	3.94952800
H	5.96660400	1.73480200	3.80474800
C	7.36223700	-0.04005800	2.37554700
H	8.03148000	-0.26303900	1.54164900
H	6.43276000	0.32383200	1.92124500
C	7.04064900	-1.30750500	3.16173300
C	7.91928700	-2.40603000	3.26223100
C	7.51672400	-3.50734100	4.02880800

H	8.18049700	-4.36524300	4.10391800
C	6.30861100	-3.54693700	4.72203100
H	6.06533700	-4.40094800	5.34111900
C	5.45597700	-2.44430600	4.62904600
C	5.81910800	-1.35304900	3.84083700
H	5.12559500	-0.51960800	3.78115600
C	9.30524100	-2.44092400	2.62883400
H	9.33113900	-1.84931300	1.71123600
H	9.51888400	-3.47235000	2.32353800
C	10.40277300	-1.99383000	3.59010300
C	10.90905900	-0.67862300	3.63655500
C	11.90441600	-0.38560600	4.57799700
H	12.31072000	0.62234900	4.61546800
C	12.38492400	-1.32363100	5.48932500
H	13.11903800	-1.03432500	6.23063800
C	11.86127500	-2.61791100	5.44468600
C	10.89787100	-2.94234800	4.49034100
H	10.52371300	-3.96169100	4.47625900
C	10.39702100	0.45572800	2.75694400
H	10.04618700	0.07632500	1.79488100
H	11.23886500	1.11937500	2.52582000
C	3.82115500	-3.32591200	6.16279300
H	2.85184100	-2.97483900	6.53509000
H	3.71110200	-4.29330500	5.65891400
C	8.54751300	4.75927000	6.72271300
H	7.86662200	5.38883300	6.13812800
H	9.24071700	5.37981300	7.30247700
C	13.11865800	-3.40684400	7.34138000
H	14.09440700	-3.07655100	6.96683700
H	13.21073400	-4.37213800	7.85277900

Cartesian coordinates of the optimized geometries for CHCl_3 @**3** using B3LYP-D3/6-31G*,cc-pVTZ.

O	0.81694800	4.57867800	-0.50367700
O	0.90147800	-1.80574400	4.22224200
O	1.04653900	-2.70386300	-3.66395600
O	-0.78956400	-3.76633300	-2.60351800
O	-0.99474700	4.09804200	-1.95726700
O	-0.98450400	-0.40114300	4.53194100
C	3.54498500	1.52131600	-1.38758600
C	3.43758600	2.06344500	-0.08932600
C	2.53195500	3.10678200	0.13170700
H	2.40080600	3.51409800	1.12972500
C	1.73865600	3.62472600	-0.89289700
C	1.91488700	3.16734000	-2.19924800
H	1.31631100	3.54542700	-3.01929100
C	2.81665100	2.12701200	-2.41974300
H	2.92288600	1.74191700	-3.43154500
C	4.26785000	1.57253100	1.10041200
H	5.19788500	1.12148300	0.74689700
H	4.56788300	2.45367600	1.68083100
C	3.51367300	0.62481600	2.02263000
C	3.47932500	-0.77426600	1.84396500
C	2.61004900	-1.53295200	2.63537400
H	2.53500900	-2.60656800	2.49008500
C	1.78224600	-0.94587300	3.59318800
C	1.88684800	0.42162700	3.84945900
H	1.25942300	0.91147600	4.58408900
C	2.75279000	1.17802500	3.06077500
H	2.80299400	2.25098800	3.23256800
C	4.35087800	-1.51539000	0.82596500
H	5.25250800	-0.93596900	0.61218800
H	4.69953800	-2.44093200	1.29982200
C	3.61595800	-1.87943600	-0.45637500

C	3.53844600	-1.02790200	-1.57894600
C	2.68698800	-1.37863700	-2.63225300
H	2.57794000	-0.72080700	-3.48915900
C	1.91909500	-2.54358000	-2.60382600
C	2.07034800	-3.44319900	-1.54788600
H	1.49065900	-4.35679800	-1.49237200
C	2.91768200	-3.09340800	-0.49726200
H	3.00302700	-3.77502300	0.34616700
C	4.34506800	0.26766800	-1.71193300
H	5.25026800	0.21007300	-1.10301400
H	4.69068200	0.33662600	-2.75054900
C	-3.52481300	-0.64697800	-1.99467400
C	-3.46231900	-1.75914800	-1.12530500
C	-2.55654500	-2.78720900	-1.40954700
H	-2.46481100	-3.63650300	-0.74011300
C	-1.70235900	-2.73614000	-2.51326500
C	-1.80965000	-1.67837500	-3.41706900
H	-1.15089400	-1.59480100	-4.27255500
C	-2.72379900	-0.66266500	-3.14383500
H	-2.77926000	0.17738400	-3.83171700
C	-4.34382000	0.60621700	-1.70833400
H	-5.25977200	0.36331000	-1.16445300
H	-4.66995300	1.03290400	-2.66422400
C	-3.54918200	1.68067100	-0.96195400
C	-3.62363700	1.87364700	0.43570600
C	-2.87531900	2.91596800	0.99781500
H	-2.94122900	3.08924900	2.06917200
C	-1.99896200	3.70594500	0.25609100
H	-1.37718100	4.43723900	0.75698100
C	-1.87736500	3.45863800	-1.11162000
C	-2.68268900	2.48655900	-1.70905300
H	-2.58253100	2.33668600	-2.77938400
C	-4.39935700	0.95886200	1.37681600
H	-5.29543000	0.56368500	0.89318900
H	-4.75688000	1.55682900	2.22360600
C	-3.54775400	-0.18343100	1.93610500
C	-3.55651300	-1.49281200	1.40553500
C	-2.76018700	-2.46216300	2.02885900
H	-2.77573100	-3.47887600	1.64421600
C	-1.89892200	-2.17082500	3.08497900
H	-1.23865200	-2.93817900	3.46950000
C	-1.84321400	-0.85774200	3.55379800
C	-2.69621600	0.10412700	3.00863400
H	-2.64649200	1.10992200	3.41347600
C	-4.31145200	-1.88861200	0.14208200
H	-5.23719400	-1.31767400	0.04075800
H	-4.61723700	-2.93744800	0.23513100
C	-0.11399200	5.06811200	-1.43874100
H	0.38441200	5.48739700	-2.31939700
H	-0.65842000	5.85335100	-0.90255500
C	0.14074600	-3.78060600	-3.66199900
H	-0.36173900	-3.72193200	-4.63384300
H	0.65855500	-4.74078500	-3.56156900
C	-0.05689500	-1.28883700	5.11337400
H	-0.55669900	-2.17207800	5.52591300
H	0.41254400	-0.71031700	5.91660000
C	-0.50841600	-0.01306900	-0.00504100
H	-1.59308900	-0.04151300	-0.02172400
Cl	0.00781300	1.11923200	1.26222200
Cl	0.09270300	-1.64751600	0.34315400
Cl	0.06616900	0.53334600	-1.59434300

Cartesian coordinates of the optimized geometries for **4** using B3LYP-D3/6-31G*,cc-pVTZ.
N -1.48660800 2.07035400 -2.59777800

N	-1.86492300	3.89740600	-1.38237400
C	-2.67877300	1.93137400	-1.92189800
C	-2.94198900	3.05858100	-1.16795600
C	-4.09983300	3.33278700	-0.24861800
H	-4.09077400	4.36578200	0.10366500
H	-5.03334100	3.15592600	-0.78767400
C	-1.01616900	3.25267500	-2.25653400
C	0.29237600	3.79185200	-2.78402100
H	0.70205200	4.54301700	-2.10265600
H	-4.39619800	1.49650400	0.67913700
C	0.13919500	4.43015100	-4.19183100
H	-0.20435400	3.63035600	-4.86413600
C	-0.91822000	5.54345300	-4.18595600
H	-0.63549700	6.34749800	-3.49345600
H	-1.01301100	5.98647900	-5.18365100
H	-1.90566100	5.17114500	-3.89143500
C	1.48956500	4.95842900	-4.69204000
H	1.86216100	5.75522100	-4.03489700
H	2.24243400	4.16494900	-4.71662200
H	1.39165100	5.37255900	-5.70230900
C	2.32403200	2.65604800	-1.95683500
N	1.25753300	2.70244000	-2.80180700
O	2.69225800	3.61891700	-1.26355400
H	0.94832900	1.81378500	-3.18382400
C	-3.47065200	0.68763700	-1.95391400
N	-2.97980700	-0.25412300	-2.80587400
O	-4.48675700	0.52254900	-1.25852700
H	-2.05554800	-0.07433100	-3.18662500
C	-3.43584800	-1.63598600	-2.79409400
H	-4.29744500	-1.66146900	-2.12052700
C	-2.31521800	-2.49678700	-2.26001200
N	-1.05528200	-2.31293900	-2.59881300
C	-0.34026300	-3.27629600	-1.92213600
N	-2.45085700	-3.55428000	-1.38616700
C	-5.02905800	-1.18805100	-4.71707800
H	-5.91354100	-1.27384300	-4.07221700
H	-4.72598400	-0.13690100	-4.73190400
H	-5.32318300	-1.47703500	-5.73280300
C	-3.89634300	-2.08770700	-4.20709400
H	-3.02579200	-1.97915300	-4.87032000
C	-4.32306200	-3.56262100	-4.20862700
H	-5.16622200	-3.72655900	-3.52421800
H	-4.64821200	-3.86601200	-5.21000400
H	-3.50577200	-4.22771000	-3.90809800
C	-1.18644500	-4.06820500	-1.17015400
C	-0.84720400	-5.21060200	-0.25291100
H	-1.74734400	-5.71661000	0.10017700
H	-0.23096500	-5.93198800	-0.79445600
H	0.89367300	-4.55292900	0.67020900
C	1.13246500	-3.34199000	-1.95116800
N	1.70760900	-2.44495600	-2.79787400
O	1.78001600	-4.14306700	-1.25638200
H	1.09371000	-1.73235500	-3.18071800
C	3.13395300	-2.15618800	-2.78140600
H	3.57866900	-2.88408700	-2.09652200
C	3.76333000	-2.34950000	-4.18811900
H	3.24853500	-1.64924600	-4.86207300
C	3.53591300	-3.78186800	-4.68719700
H	4.03153800	-4.50605800	-4.02747400
H	2.47052700	-4.02880800	-4.71554800
H	3.94637500	-3.90851400	-5.69582300
C	5.25887800	-2.00189300	-4.18094200
H	5.80872900	-2.65402100	-3.48915800
H	5.68953900	-2.14315900	-5.17863100
H	5.43853800	-0.96240600	-3.88494800
C	3.32236500	-0.75138200	-2.25945200

N	2.53125400	0.24566500	-2.60040000
C	3.00694900	1.34946200	-1.92737800
N	4.30687200	-0.33554600	-1.38860400
C	4.11725300	1.01646000	-1.17593000
C	4.93408300	1.88453500	-0.25926500
H	5.82560400	1.36247000	0.09238700
H	5.24513500	2.78140400	-0.80000800
H	3.49108000	3.05695800	0.66862200
C	3.84614100	1.42089000	1.86777900
N	4.16835800	2.33511100	0.90210000
O	4.32875000	0.28618300	1.89373500
C	-3.15067700	2.61883000	1.87497900
N	-4.10688000	2.44335500	0.91223600
O	-2.40732900	3.60241400	1.89861100
C	-0.69659800	-4.03849600	1.87343900
N	-0.07007000	-4.77640200	0.90658200
O	-1.92023300	-3.88639800	1.90193400
C	1.68107700	-2.19882100	4.94192100
C	2.12391000	-3.38968500	4.36780500
C	1.38386000	-3.99756900	3.34968400
C	0.18351200	-3.42087600	2.91818800
C	-0.25747200	-2.22343300	3.49569100
C	0.49094400	-1.59746100	4.49512300
H	2.25582700	-1.72997400	5.73606300
H	3.04511700	-3.84842500	4.71600400
H	1.72252000	-4.93422900	2.91556400
C	1.07592500	2.54911900	4.95089200
C	1.88527300	3.52955800	4.37866500
C	2.77659400	3.19612900	3.35495200
C	2.87315800	1.87047500	2.91615900
C	2.05680600	0.88844000	3.49117300
C	1.14541100	1.22009400	4.49625200
H	0.38720600	2.80922800	5.75027100
H	1.82633500	4.55493600	4.73285700
H	3.41840100	3.95863400	2.92212300
C	-2.73804000	-0.34613400	4.95559700
C	-3.99286800	-0.13460600	4.38603000
C	-4.15144900	0.80495000	3.36337200
C	-3.05206900	1.55104100	2.92249900
C	-1.79213900	1.33395600	3.49467800
C	-1.62238300	0.37824800	4.49899800
H	-2.61740100	-1.07317000	5.75407200
H	-4.85089600	-0.69820000	4.74160700
H	-5.13360900	0.98085500	2.93310900
P	0.00551900	-0.00022200	5.23714900
H	-0.96137400	1.93042500	3.13574200
H	-1.19327000	-1.80485300	3.14365900
H	2.15819100	-0.12961000	3.13318900
C	-3.67626400	-4.03232200	-0.75021800
H	-4.44813600	-3.26757100	-0.83879300
H	-4.03060700	-4.94843100	-1.23385000
H	-3.47062000	-4.20554000	0.30760400
C	-1.66932000	5.19830400	-0.74770400
H	-0.62244100	5.48884600	-0.83900100
H	-2.28925700	5.96065700	-1.23083100
H	-1.91946900	5.10654200	0.31060500
C	5.33885900	-1.15268100	-0.75474300
H	5.06817900	-2.20474700	-0.84340000
H	6.30777000	-0.99651700	-1.24069300
H	5.38690900	-0.88761900	0.30280300
O	0.00662900	-0.00053000	6.72925900

Cartesian coordinates of the optimized geometries for CHCl_3 @ 4 using B3LYP-D3/6-31G*, cc-pVTZ.

N	-1.46692100	2.05352400	-2.62124600
N	-1.82469800	3.87496200	-1.39197900
C	-2.64865100	1.91208700	-1.92443300
C	-2.89529900	3.03380600	-1.15842000
C	-4.03812500	3.30586200	-0.22028600
H	-4.02231200	4.33794400	0.13419800
H	-4.97905000	3.13291700	-0.74816200
C	-0.99218400	3.23691900	-2.28440300
C	0.30052200	3.78703200	-2.83782100
H	0.71139100	4.54690300	-2.16756800
H	-4.30853000	1.46514700	0.70748700
C	0.11404100	4.41378300	-4.24603700
H	-0.22773800	3.60501900	-4.90874100
C	-0.96170700	5.50925600	-4.22854400
H	-0.68196600	6.32060700	-3.54344000
H	-1.07865600	5.94644800	-5.22642300
H	-1.93813800	5.12186400	-3.91761500
C	1.44701700	4.96152700	-4.77154800
H	1.81474500	5.77078000	-4.12693800
H	2.21394300	4.18177000	-4.80079400
H	1.32608400	5.36548700	-5.78338400
C	2.30656500	2.64390700	-1.96996100
N	1.28102100	2.71285500	-2.86506600
O	2.64710800	3.59160100	-1.24450300
H	0.99467800	1.83390700	-3.28432400
C	-3.45005600	0.67648500	-1.96386500
N	-2.99997500	-0.23994400	-2.86661500
O	-4.43834300	0.49369200	-1.23547600
H	-2.09604000	-0.04466500	-3.28539800
C	-3.43561800	-1.62741900	-2.84690800
H	-4.30419300	-1.65721500	-2.18345800
C	-2.31317000	-2.46974900	-2.28935100
N	-1.05084600	-2.29011800	-2.62671600
C	-0.33807300	-3.24271100	-1.92921700
N	-2.45003500	-3.50792000	-1.39490200
C	-5.01108100	-1.22305000	-4.79353900
H	-5.90235700	-1.31687500	-4.15923800
H	-4.72449700	-0.16739100	-4.81436200
H	-5.28777400	-1.52654900	-5.80989600
C	-3.87163700	-2.10033000	-4.25997200
H	-2.99488000	-1.98730900	-4.91439000
C	-4.27689300	-3.58130800	-4.24954700
H	-5.12532900	-3.74963100	-3.57280500
H	-4.58619300	-3.90053300	-5.25098300
H	-3.45360700	-4.23096100	-3.93210000
C	-1.18666900	-4.01574100	-1.16193000
C	-0.85135200	-5.14158200	-0.22347200
H	-1.75341200	-5.64134200	0.13335800
H	-0.23429700	-5.87176000	-0.75260100
H	0.88035300	-4.45637900	0.69881300
C	1.13240300	-3.32101000	-1.96652400
N	1.70627600	-2.47046700	-2.86331500
O	1.78119800	-4.08973800	-1.23930600
H	1.08912600	-1.78292200	-3.28387200
C	3.12733700	-2.16115400	-2.83792000
H	3.57836800	-2.89388100	-2.16320800
C	3.76401700	-2.32203400	-4.24450300
H	3.24182900	-1.61889100	-4.90996100
C	3.56129900	-3.74961400	-4.76735100
H	4.06894300	-4.47574800	-4.11887600
H	2.50037500	-4.01470000	-4.80086000
H	3.97540400	-3.85275300	-5.77707200
C	5.25387300	-1.95102700	-4.22458100
H	5.81019700	-2.60429500	-3.53901300

H	5.69187900	-2.07127300	-5.22176000
H	5.41542900	-0.91321300	-3.91276100
C	3.29895500	-0.76421100	-2.29096600
N	2.51001800	0.23748600	-2.62866900
C	2.97722700	1.33293200	-1.93317600
N	4.26762300	-0.35992500	-1.39913300
C	4.07275500	0.98771600	-1.16725200
C	4.87784100	1.84277600	-0.22863600
H	5.76415500	1.31452100	0.12675500
H	5.19768500	2.74454500	-0.75637600
H	3.41824600	2.99632800	0.69913700
C	3.80609100	1.37493700	1.90981800
N	4.10377600	2.28169500	0.92949700
O	4.29574000	0.24267900	1.93691500
C	-3.09780200	2.61160700	1.91810800
N	-4.03267500	2.41635800	0.93831200
O	-2.36467200	3.60326400	1.94659300
C	-0.71368600	-3.98427400	1.91623500
N	-0.08039300	-4.69347400	0.93270400
O	-1.93925100	-3.84516700	1.94912800
C	1.67499400	-2.19809000	5.00681800
C	2.12011600	-3.37357900	4.40353100
C	1.37396300	-3.96534400	3.38009200
C	0.16394600	-3.39023800	2.97531000
C	-0.28062200	-2.21072200	3.58472200
C	0.47546400	-1.59718900	4.58542100
H	2.25833200	-1.73815200	5.80004400
H	3.04932700	-3.83158500	4.73098700
H	1.71759900	-4.88786900	2.92038400
C	1.08424100	2.54534900	5.01943600
C	1.88499900	3.51731200	4.42127500
C	2.76318400	3.16857500	3.39105900
C	2.85750000	1.83601800	2.97411600
C	2.05275200	0.86254300	3.57790300
C	1.15094300	1.20919900	4.58590100
H	0.40151500	2.81859700	5.81966000
H	1.82821200	4.54850000	4.75864700
H	3.39525500	3.92585400	2.93538800
C	-2.73973300	-0.34389000	5.01408700
C	-3.98204000	-0.14012300	4.41510000
C	-4.12261700	0.80014500	3.39013300
C	-3.01913300	1.55671600	2.97904600
C	-1.77329400	1.35018600	3.58384400
C	-1.61930900	0.39077000	4.58656000
H	-2.63180900	-1.07671400	5.80918700
H	-4.84379600	-0.71238900	4.74714600
H	-5.09472700	0.96586200	2.93382200
P	0.00206000	0.00115200	5.33386000
H	-0.93819000	1.94726800	3.24047700
H	-1.21821900	-1.78907300	3.24559200
H	2.14611400	-0.15798200	3.22959100
C	-3.67323600	-3.95678000	-0.73322300
H	-4.43592600	-3.18344000	-0.82670700
H	-4.04501200	-4.87883800	-1.19156900
H	-3.45426200	-4.10969900	0.32534500
C	-1.60723300	5.16196700	-0.73550000
H	-0.55833200	5.44275900	-0.83363500
H	-2.22606600	5.93957800	-1.19501100
H	-1.84511400	5.05098300	0.32412800
C	5.27494700	-1.18985800	-0.74174200
H	4.99428800	-2.23863300	-0.83817700
H	6.25756700	-1.04271200	-1.20209100
H	5.29809400	-0.92641500	0.31726700
O	0.00193400	0.00211800	6.82612300
C	-0.00341200	0.00085000	-0.06204800
H	-0.00667000	0.00206500	-1.14991200

Cl	-1.54313100	-0.70584800	0.49823300
Cl	0.15695800	1.68858000	0.49589400
Cl	1.38063700	-0.98066200	0.48978900

Cartesian coordinates of the optimized geometries for **5** using B3LYP-D3/6-31G*,cc-pVTZ.

C	2.38508700	2.86124500	-2.92334200
H	3.20464300	3.37903100	-2.42132900
C	1.08946400	3.04468700	-2.16165200
N	-0.05659700	2.59515400	-2.62136300
C	-0.99365800	2.86146900	-1.64276500
C	-0.40357800	3.49078700	-0.56178000
N	0.93978100	3.58835200	-0.89770800
C	2.00008100	4.14858700	-0.04840400
H	1.89151400	5.23937200	-0.01973600
H	2.94956900	3.90891800	-0.53071700
C	-0.99730600	3.99169500	0.71438400
H	-2.08377100	3.94427900	0.63101400
H	-0.68851900	5.02331900	0.92348300
H	-0.68581100	3.38359700	1.57139000
C	-2.37579600	2.36049600	-1.76374500
O	-3.24221100	2.51565300	-0.89326900
N	2.72403100	1.43718500	-2.91439600
H	2.09700100	0.82605200	-3.43094600
C	2.01951700	3.58555600	1.35856500
C	1.98364100	2.20206900	1.58218800
H	1.93721100	1.52363000	0.73820200
C	2.01282600	1.69723900	2.87798100
C	2.09626400	2.55448600	3.98844600
C	2.13931500	3.93197000	3.75868900
H	2.19326900	4.61711400	4.60217400
C	2.09680400	4.44195400	2.45801100
H	2.11213400	5.51913100	2.30336700
C	2.28024500	3.39978400	-4.36787300
H	1.46477100	2.85100100	-4.85927700
C	3.58598500	3.15809000	-5.13708800
H	4.41656600	3.70649200	-4.67262300
H	3.49104100	3.50753900	-6.17177900
H	3.85482500	2.09764800	-5.15239900
C	1.91380900	4.89074200	-4.35885200
H	2.67811900	5.47730200	-3.83080100
H	0.94894700	5.06642400	-3.87208000
H	1.84979200	5.27647500	-5.38264100
C	-3.66677100	0.63505200	-2.92278300
H	-4.52753500	1.08446200	-2.42410200
C	-3.17991000	-0.57831400	-2.15954700
N	-2.21650100	-1.34619400	-2.61664200
C	-1.98341600	-2.29312300	-1.63904600
C	-2.82777700	-2.09800000	-0.56126400
N	-3.58145600	-0.98214300	-0.89793400
C	-4.59627000	-0.34191400	-0.04969000
H	-5.48748200	-0.98008800	-0.02043400
H	-4.86220500	0.60000300	-0.53297800
C	-2.97123300	-2.86465500	0.71315400
H	-2.39040700	-3.78397600	0.62984500
H	-4.02068600	-3.10914500	0.91846600
H	-2.60009600	-2.29438700	1.57218500
C	-0.85945900	-3.24127300	-1.75931000
O	-0.56334800	-4.07158700	-0.89009400
N	-2.60425500	1.64199900	-2.91042400
H	-1.76212700	1.40866200	-3.42981700
C	-4.11811900	-0.04271100	1.35708200
C	-2.89552400	0.60546000	1.58145600
H	-2.27843800	0.89371300	0.73806000
C	-2.47353200	0.88386800	2.87732600

C	-3.26396100	0.54055000	3.98725700
C	-4.48500000	-0.09819500	3.75674600
H	-5.11072700	-0.38421000	4.59963200
C	-4.90516000	-0.39052400	2.45606400
H	-5.85109200	-0.90611800	2.30150900
C	-4.07323500	0.27424600	-4.36913500
H	-3.18752200	-0.15705500	-4.85600700
C	-4.51384900	1.52477000	-5.14118300
H	-4.76439700	1.26723300	-6.17698400
H	-3.73021300	2.28828900	-5.15428300
H	-5.40647000	1.96960400	-4.68138200
C	-5.18008800	-0.78957500	-4.36558200
H	-6.07402500	-0.42090600	-3.84388500
H	-4.85188500	-1.71211400	-3.87571400
H	-5.47550500	-1.03961300	-5.39084900
C	1.28093400	-3.49557600	-2.92024700
H	1.32239700	-4.46362400	-2.41734400
C	2.09162200	-2.46443200	-2.16368100
N	2.27388300	-1.24717200	-2.62465000
C	2.97939400	-0.56944700	-1.65017400
C	3.23496500	-1.39545500	-0.57052700
N	2.64523700	-2.60695700	-0.90306400
C	2.60219200	-3.80358300	-0.05146000
H	3.60201100	-4.25252300	-0.02079600
H	1.92216400	-4.50877100	-0.53289300
C	3.97227700	-1.13315600	0.70188300
H	4.47579600	-0.16935300	0.61602900
H	4.71062300	-1.91782000	0.90728300
H	3.29419000	-1.09774400	1.56230800
C	3.23768600	0.87786100	-1.77111400
O	3.81121200	1.54833800	-0.90267000
N	-0.12179300	-3.07819100	-2.90548500
H	-0.34080300	-2.23140700	-3.42377700
C	2.10309100	-3.53698200	1.35480000
C	0.92289500	-2.81364100	1.57690200
H	0.36020900	-2.43329700	0.73232600
C	0.46816700	-2.58871300	2.87208900
C	1.16600000	-3.09155900	3.98343000
C	2.33831900	-3.81661300	3.75526400
H	2.90272400	-4.20713800	4.59938500
C	2.80387100	-4.03318800	2.45519800
H	3.72919600	-4.58529900	2.30205700
C	1.79243000	-3.67525700	-4.36764400
H	1.72513600	-2.69438500	-4.85847100
C	0.92376500	-4.68256500	-5.13291700
H	1.26905800	-4.77616100	-6.16921800
H	-0.12786100	-4.38169800	-5.14331000
H	0.98233200	-5.67626300	-4.66892400
C	3.26556900	-4.10738600	-4.36616400
H	3.39047100	-5.06462600	-3.84151600
H	3.90472000	-3.36336800	-3.87958000
H	3.62696800	-4.24246300	-5.39199300
C	1.03094100	0.95417500	5.59666700
C	1.32752000	-0.40677100	5.60268000
C	-0.31472400	1.35469000	5.60520000
C	0.30793800	-1.37190900	5.59302300
H	2.36546900	-0.73140100	5.55255900
C	-1.34513800	0.41753700	5.59588600
H	-0.55197100	2.41612700	5.55677500
C	-1.01891900	-0.94805100	5.60112600
H	-1.81924100	-1.68430100	5.54887500
C	-2.78697300	0.84249200	5.40315800
C	2.11935100	1.99091200	5.40445900
C	0.66135000	-2.83261000	5.39814400
H	-0.43455200	-2.00231600	3.02577700
H	1.95544400	0.62245400	3.03306100

H	-1.50929800	1.36200900	3.03228200
H	1.42870000	-3.14333600	6.11836400
H	-0.22223100	-3.45513600	5.59415200
H	3.09957600	1.53820400	5.60572600
H	2.00074100	2.81253100	6.12196900
H	-2.88459500	1.91783200	5.60412300
H	-3.43936700	0.32966500	6.12101700

Cartesian coordinates of the optimized geometries for $\uparrow\text{CHCl}_3@5$ using B3LYP-D3/6-31G*, cc-pVTZ.

C	3.07581000	2.17874100	-2.52776800
H	3.93798100	2.34788500	-1.87803300
C	1.83570600	2.83351100	-1.96718400
N	0.62575200	2.50118300	-2.36269000
C	-0.23988800	3.35082100	-1.70048800
C	0.46229000	4.22059500	-0.89102200
N	1.79642500	3.88030900	-1.06784700
C	2.91587200	4.36868500	-0.24178500
H	2.79743000	5.44988500	-0.12680000
H	3.83504600	4.20408500	-0.80741900
C	-0.02504500	5.27345200	0.04567300
H	-1.07528900	5.46919500	-0.17349600
H	0.54785000	6.20480400	-0.04726200
H	0.04814500	4.94009900	1.08801200
C	-1.70342600	3.16596200	-1.76976200
O	-2.51226100	3.88103700	-1.16232800
N	2.86253100	0.74087400	-2.54420500
H	1.97589800	0.40020600	-2.90020100
C	2.96223100	3.67992000	1.11044800
C	3.46005900	2.37582500	1.23508800
H	3.90476200	1.86218600	0.38634400
C	3.36119800	1.70019900	2.44989600
C	2.76287400	2.29493300	3.56838600
C	2.32972400	3.62095700	3.45596400
H	1.90085100	4.12265300	4.32073200
C	2.43027700	4.30546200	2.24355200
H	2.08242200	5.33354400	2.17884300
C	3.42148700	2.72080600	-3.94334100
H	2.55718300	2.49933000	-4.58581200
C	4.65930900	2.00828700	-4.50283300
H	5.53513300	2.19578400	-3.86834900
H	4.88865800	2.36993400	-5.51222700
H	4.50742700	0.92612200	-4.55053700
C	3.62861400	4.24190300	-3.91706200
H	4.47061300	4.50960200	-3.26354400
H	2.73848700	4.77308900	-3.56231800
H	3.86293000	4.61476400	-4.92053900
C	-3.43095300	1.57070700	-2.53290900
H	-4.01146300	2.23136300	-1.88389100
C	-3.38213800	0.16724500	-1.97788800
N	-2.49357200	-0.71595300	-2.37865700
C	-2.79588000	-1.89022900	-1.71636600
C	-3.89676900	-1.71602100	-0.90229500
N	-4.26689900	-0.38930800	-1.07578000
C	-5.24367700	0.33686900	-0.24339500
H	-6.12084100	-0.30581300	-0.12353800
H	-5.56395700	1.21565900	-0.80695100
C	-4.56541800	-2.66542800	0.03339000
H	-4.20802900	-3.67237100	-0.18544100
H	-5.65831400	-2.63686600	-0.06207500
H	-4.31623000	-2.43543800	1.07652300
C	-1.90312500	-3.06434400	-1.78459300
O	-2.11470700	-4.12018300	-1.17241900
N	-2.07834100	2.10346000	-2.53970600

H	-1.33823200	1.50469100	-2.88978400
C	-4.66182900	0.72094000	1.10515600
C	-3.78327000	1.80616400	1.22511600
H	-3.56775200	2.44978100	0.37570300
C	-3.14268700	2.05978200	2.43640500
C	-3.35065900	1.24399900	3.55603000
C	-4.27967600	0.20280600	3.44840600
H	-4.49392800	-0.42029000	4.31414600
C	-4.92866900	-0.05373500	2.23952900
H	-5.64407000	-0.87040600	2.17898100
C	-4.06655000	1.60470800	-3.95090200
H	-3.44018500	0.96914100	-4.59296500
C	-4.06531700	3.03510100	-4.50480400
H	-4.49066700	3.05667300	-5.51493900
H	-3.05143900	3.44369700	-4.54856200
H	-4.66633600	3.69854900	-3.86933600
C	-5.48781600	1.02387500	-3.93195600
H	-6.14252900	1.61542200	-3.27673500
H	-5.50370600	-0.01435700	-3.58310900
H	-5.92527800	1.04606800	-4.93647000
C	0.34384800	-3.75986200	-2.54109900
H	0.06003700	-4.59261000	-1.89227600
C	1.52932800	-3.01309600	-1.97860600
N	1.84964100	-1.79962900	-2.37335600
C	3.01677200	-1.47657600	-1.70713500
C	3.41519500	-2.52032300	-0.89693600
N	2.45232000	-3.50398600	-1.07658700
C	2.30966900	-4.71483700	-0.24740600
H	3.30273200	-5.15952600	-0.13325400
H	1.70169100	-5.42632300	-0.80966000
C	4.56804400	-2.62726600	0.04273200
H	5.26888600	-1.82187200	-0.17901600
H	5.08147900	-3.59336500	-0.04326500
H	4.24095000	-2.51571900	1.08378000
C	3.58966200	-0.11721800	-1.77096200
O	4.60923900	0.22393600	-1.15599100
N	-0.79709900	-2.85933600	-2.55754500
H	-0.65027600	-1.91915400	-2.90921600
C	1.69446100	-4.40194600	1.10472800
C	0.31822700	-4.16870500	1.23001600
H	-0.35037300	-4.29451800	0.38211000
C	-0.21264400	-3.73877800	2.44475400
C	0.60477400	-3.52281700	3.56200600
C	1.96750700	-3.82075500	3.44847800
H	2.61834000	-3.70283600	4.31196900
C	2.50486600	-4.25775500	2.23643400
H	3.56718200	-4.47943100	2.17055100
C	0.64344500	-4.32852900	-3.95643600
H	0.87732500	-3.46775900	-4.59958500
C	-0.58761000	-5.05326900	-4.51463800
H	-0.38793900	-5.42905800	-5.52505600
H	-1.45461700	-4.38773000	-4.55945700
H	-0.85501300	-5.90923800	-3.88121100
C	1.86368800	-5.26006600	-3.93084100
H	1.68304400	-6.12219900	-3.27388800
H	2.76646300	-4.74813700	-3.58086000
H	2.06827000	-5.65117600	-4.93387900
C	0.01717900	0.01286600	0.67122600
C	1.22355400	0.72024100	4.82937900
C	1.21953700	-0.67401100	4.82831100
C	-0.00640200	1.39670300	4.82340400
C	0.01825700	-1.40063700	4.82568600
H	2.16568500	-1.21126600	4.82274500
C	-1.21604400	0.70340200	4.82040400
H	-0.01424200	2.48469100	4.81368700
C	-1.18716200	-0.69998400	4.81829900

H	-2.12522300	-1.25091800	4.80532000
H	0.03370000	0.02307400	-0.41637200
C	-2.54843100	1.44781000	4.82920400
C	2.53362100	1.50286000	4.84374700
C	0.03868600	-2.92623400	4.83890500
H	-1.27774000	-3.53580600	2.51336200
H	3.72570700	0.67881400	2.51670900
H	-2.44335400	2.88908400	2.50022000
H	0.63552800	-3.26955200	5.69441100
H	-0.98092100	-3.29617300	4.99864100
H	3.36554900	0.80624100	5.00047200
H	2.53237100	2.18892100	5.70158500
H	-2.35978800	2.51735700	4.97929100
H	-3.14201400	1.10979300	5.68926800
Cl	-1.48083600	-0.79517400	1.19258200
Cl	1.44889600	-0.88147100	1.23604200
Cl	0.05781500	1.69894600	1.23976400

Cartesian coordinates of the optimized geometries for $\downarrow\text{CHCl}_3@5$ using B3LYP-D3/6-31G*,cc-pVTZ.

C	3.08084000	2.17802400	-2.55452400
H	3.93651600	2.34180000	-1.89438000
C	1.84059300	2.84478400	-2.00910600
N	0.63347800	2.53833700	-2.42980900
C	-0.23317200	3.36740100	-1.74612300
C	0.46663100	4.20864700	-0.90259200
N	1.80083700	3.86304800	-1.07642800
C	2.91535000	4.33693600	-0.23746900
H	2.81266700	5.42052600	-0.12731200
H	3.83947500	4.15630800	-0.79017500
C	-0.01799300	5.25206100	0.04772300
H	-1.07457400	5.43259200	-0.15355800
H	0.53866400	6.19225700	-0.05863400
H	0.08190500	4.92237000	1.08858200
C	-1.69758800	3.17291200	-1.80740800
O	-2.50605500	3.88614400	-1.19606100
N	2.85843300	0.74046400	-2.57006000
H	1.95951200	0.40590300	-2.90074100
C	2.93812800	3.65584000	1.12007900
C	3.38789200	2.33502400	1.25220500
H	3.80526800	1.79905800	0.40312300
C	3.27979000	1.67668100	2.47555200
C	2.72125400	2.30743900	3.59515100
C	2.32955600	3.64507600	3.47296100
H	1.92829200	4.17096300	4.33676400
C	2.44086600	4.31165400	2.25170200
H	2.12674200	5.35002000	2.17826700
C	3.44816800	2.71710500	-3.96533900
H	2.58709300	2.51075800	-4.61682900
C	4.68064100	1.98803400	-4.51499100
H	5.55146000	2.15455600	-3.86785900
H	4.92892800	2.35351600	-5.51852400
H	4.51018700	0.90913600	-4.57351100
C	3.67741400	4.23486500	-3.92958500
H	4.51639800	4.48685100	-3.26589000
H	2.79125200	4.77675600	-3.58059900
H	3.92690900	4.60999300	-4.92855900
C	-3.42806400	1.57719000	-2.55361600
H	-3.99862400	2.23513300	-1.89273500
C	-3.38626600	0.16853600	-2.01209700
N	-2.51876700	-0.72316100	-2.43641700
C	-2.80248400	-1.88940100	-1.75448200
C	-3.87909900	-1.70514900	-0.90829400
N	-4.24649000	-0.37642900	-1.07869700

C	-5.21259600	0.35005800	-0.23641700
H	-6.09840600	-0.28234700	-0.12416300
H	-5.52192100	1.24015100	-0.78813600
C	-4.53893700	-2.64791800	0.04163100
H	-4.16862800	-3.65328600	-0.16274000
H	-5.63170600	-2.63495900	-0.06180100
H	-4.30026700	-2.39900800	1.08251800
C	-1.90271700	-3.06079900	-1.81923400
O	-2.11591900	-4.11817900	-1.20906700
N	-2.07175400	2.10293700	-2.56535400
H	-1.33199400	1.49161400	-2.89438700
C	-4.63112800	0.71165900	1.11910800
C	-3.71524700	1.76441100	1.24872400
H	-3.46362800	2.39490900	0.39921900
C	-3.08947700	2.00263800	2.47074400
C	-3.35202300	1.20356800	3.59144100
C	-4.31108900	0.19167200	3.47153500
H	-4.56247900	-0.41924000	4.33604300
C	-4.94534700	-0.04763600	2.25145300
H	-5.68479100	-0.84168400	2.17959500
C	-4.07722900	1.62961400	-3.96448800
H	-3.46732600	0.98949400	-4.61755300
C	-4.06229700	3.06325000	-4.50949000
H	-4.50379400	3.09817200	-5.51233400
H	-3.04264200	3.45527500	-4.56759800
H	-4.64138000	3.73242200	-3.85982300
C	-5.50615100	1.06851000	-3.93076100
H	-6.14404900	1.66551800	-3.26387000
H	-5.53154600	0.02869700	-3.58682200
H	-5.95651500	1.10156700	-4.92926500
C	0.34550800	-3.75959500	-2.56185400
H	0.05963100	-4.58266700	-1.90144100
C	1.54157200	-3.01828900	-2.01565000
N	1.88148200	-1.82030100	-2.43676100
C	3.03159100	-1.48449800	-1.75073000
C	3.40760000	-2.51060000	-0.90534500
N	2.44091300	-3.49273600	-1.08051600
C	2.29078600	-4.69346100	-0.24003500
H	3.27933700	-5.14967000	-0.12993500
H	1.66987000	-5.40227800	-0.79144300
C	4.54917500	-2.61164500	0.05022200
H	5.23790800	-1.79081700	-0.15235000
H	5.08188300	-3.56650800	-0.04790700
H	4.20884600	-2.52593500	1.08900500
C	3.59612300	-0.11942700	-1.81091300
O	4.61696100	0.22307900	-1.19741300
N	-0.78945300	-2.84975400	-2.57825100
H	-0.62992800	-1.90284700	-2.90627700
C	1.69090900	-4.36916400	1.11710900
C	0.32287200	-4.09472000	1.24909300
H	-0.35009500	-4.18831200	0.40024800
C	-0.19210800	-3.66907300	2.47223000
C	0.63420800	-3.50126800	3.59166300
C	1.98803700	-3.83345200	3.46923600
H	2.64454600	-3.74882600	4.33250400
C	2.50810300	-4.26653900	2.24840900
H	3.56371900	-4.51624900	2.17481900
C	0.63060700	-4.34788000	-3.97168300
H	0.87598300	-3.49858200	-4.62539000
C	-0.61300500	-5.06010800	-4.51784400
H	-0.42031300	-5.45607300	-5.52195400
H	-1.46774800	-4.37969700	-4.57402300
H	-0.89595200	-5.90006100	-3.86996800
C	1.83645500	-5.29765600	-3.93589600
H	1.64302500	-6.14868000	-3.26801300
H	2.74689700	-4.79482100	-3.59227700

H	2.03502000	-5.70420500	-4.93401300
C	0.00004200	0.00145100	1.56075300
C	1.20724100	0.73711200	4.89232800
C	1.22489900	-0.65895500	4.89093700
C	-0.03472100	1.39506400	4.88794300
C	0.03376400	-1.40550300	4.89215700
H	2.17834000	-1.18257000	4.87731600
C	-1.23504300	0.68192800	4.89040600
H	-0.05800000	2.48253300	4.87071800
C	-1.18408300	-0.72272700	4.88915300
H	-2.11420900	-1.28652500	4.87326700
C	-2.57897500	1.40302200	4.88454800
C	2.50309200	1.54102000	4.88915700
C	0.08065700	-2.92962600	4.88676100
H	-1.25049800	-3.43560100	2.54722800
H	3.60794300	0.64358800	2.55014300
H	-2.36200000	2.80652600	2.54406700
H	0.69854800	-3.27108000	5.72744700
H	-0.92965800	-3.31820500	5.06004700
H	3.34552800	0.86136900	5.06264900
H	2.48824100	2.24577500	5.73110300
H	-2.41081400	2.47311100	5.05327700
H	-3.18205800	1.04188400	5.72797800
Cl	-1.45428900	-0.85031300	0.99012100
Cl	1.47056100	-0.83038300	1.00314400
Cl	-0.00917200	1.69274100	1.00857100
H	-0.00508800	-0.00335800	2.64191200

Cartesian coordinates of the optimized geometries for $\uparrow\text{CHBrCl}_2@5$ using B3LYP-D3/6-31G*,cc-pVTZ.

C	3.03888700	2.15699800	-2.47408400
H	3.90082400	2.31318700	-1.82103600
C	1.79645400	2.79796800	-1.90210000
N	0.58997600	2.43893000	-2.28578800
C	-0.28739800	3.28310200	-1.63324000
C	0.40445500	4.17469400	-0.83764900
N	1.74431900	3.85430900	-1.01525600
C	2.86851800	4.39036000	-0.22287900
H	2.72270900	5.47054800	-0.13165100
H	3.77795200	4.23711600	-0.80679700
C	-0.09624600	5.22934300	0.08937900
H	-1.15145700	5.40199600	-0.12628800
H	0.45722100	6.17075700	-0.01865400
H	-0.00818600	4.90928000	1.13487400
C	-1.75057800	3.09974300	-1.73466900
O	-2.57086200	3.84102600	-1.17488700
N	2.82159600	0.72007100	-2.51810000
H	1.94275400	0.39077400	-2.90387400
C	2.97065000	3.73929100	1.14539300
C	3.53211900	2.46428500	1.29708900
H	3.98434300	1.94598000	0.45483700
C	3.47099100	1.81145700	2.52773600
C	2.84022900	2.39568100	3.63387900
C	2.35588100	3.70222800	3.49714500
H	1.90583900	4.20209100	4.35219700
C	2.42403400	4.36648000	2.27108200
H	2.03171800	5.37710500	2.18812400
C	3.38199100	2.71948100	-3.88241100
H	2.51829600	2.50080000	-4.52675100
C	4.62285900	2.01959100	-4.45127400
H	5.49928800	2.20857100	-3.81793200
H	4.84708400	2.39105100	-5.45822700
H	4.47821600	0.93687500	-4.50710800
C	3.58166500	4.24125800	-3.84246800

H	4.42810200	4.50735200	-3.19420700
H	2.69188400	4.76490000	-3.47599900
H	3.80590700	4.62429000	-4.84441400
C	-3.47897800	1.52652600	-2.55908000
H	-4.06715700	2.16540500	-1.89557500
C	-3.48756400	0.09459300	-2.08196700
N	-2.64408300	-0.80315500	-2.54182500
C	-2.94024800	-1.98012800	-1.88386400
C	-4.00197400	-1.79566500	-1.01889000
N	-4.34660000	-0.45633600	-1.15183000
C	-5.27653600	0.27107100	-0.26805000
H	-6.14985300	-0.36901300	-0.11117600
H	-5.61953200	1.15461000	-0.81089800
C	-4.66639400	-2.75031200	-0.08388600
H	-4.30102600	-3.75404000	-0.30411200
H	-5.75918500	-2.73069300	-0.18696400
H	-4.42615200	-2.52124700	0.96094500
C	-2.02287400	-3.13955700	-1.93027800
O	-2.23109800	-4.20003900	-1.32577000
N	-2.11162900	2.01843700	-2.48252500
H	-1.37076000	1.40930400	-2.81128900
C	-4.63640100	0.64882500	1.05682800
C	-3.77586700	1.75047400	1.14983000
H	-3.60646500	2.40350000	0.29815100
C	-3.10172600	2.01942000	2.33933800
C	-3.26224100	1.20651000	3.46896100
C	-4.16778000	0.14200800	3.38786100
H	-4.34902500	-0.47929600	4.26241200
C	-4.84620800	-0.13256300	2.19913400
H	-5.54948200	-0.96117900	2.16511200
C	-4.06483700	1.65743900	-3.99136800
H	-3.44793900	1.02587600	-4.64613800
C	-3.98665500	3.11081000	-4.47487300
H	-4.39200100	3.20067300	-5.48955300
H	-2.95386100	3.47181100	-4.48448300
H	-4.56479500	3.77225400	-3.81693200
C	-5.50911200	1.13812800	-4.03397500
H	-6.15509700	1.72678500	-3.36737600
H	-5.57610100	0.08681000	-3.73265800
H	-5.91985000	1.22261000	-5.04644200
C	0.26536200	-3.78562800	-2.58107700
H	-0.03369500	-4.61428100	-1.93330300
C	1.42667400	-3.02794900	-1.98280000
N	1.75465300	-1.81014200	-2.35772600
C	2.91534000	-1.49871300	-1.67168300
C	3.30275800	-2.55455500	-0.87247500
N	2.33901400	-3.53166000	-1.07423300
C	2.18264800	-4.74346600	-0.24941300
H	3.16118500	-5.22684600	-0.17219300
H	1.52779200	-5.42716000	-0.79259000
C	4.45499500	-2.68103000	0.06470800
H	5.18087800	-1.90260600	-0.17156300
H	4.93477500	-3.66527200	-0.00501000
H	4.13426500	-2.53825500	1.10361300
C	3.50796200	-0.14765800	-1.71708400
O	4.50931700	0.18078100	-1.06722000
N	-0.88714500	-2.90288000	-2.64960200
H	-0.73965800	-1.95387400	-2.97610400
C	1.62889400	-4.41194200	1.12417200
C	0.27376400	-4.09638600	1.29256200
H	-0.42246400	-4.17658200	0.46009000
C	-0.19193400	-3.64507800	2.52641500
C	0.67247100	-3.48650300	3.61803400
C	2.01066700	-3.86259700	3.46016600
H	2.69543100	-3.78323600	4.30174100
C	2.48127300	-4.32563900	2.23028500

H	3.52661500	-4.60640500	2.12790100
C	0.62171900	-4.36684000	-3.97941400
H	0.86600300	-3.50993300	-4.62384200
C	-0.58115400	-5.11292800	-4.57028500
H	-0.34197300	-5.49974600	-5.56788600
H	-1.45303100	-4.45782400	-4.65450300
H	-0.86131200	-5.96320200	-3.93475800
C	1.85117900	-5.28366200	-3.90491000
H	1.66092100	-6.13884900	-3.24166000
H	2.73799500	-4.75735700	-3.53620200
H	2.08896200	-5.68603500	-4.89615700
C	0.38394400	0.12107400	0.67924000
C	1.31820800	0.79679700	4.88559900
C	1.33550700	-0.59805700	4.91632200
C	0.07783900	1.45049500	4.82331200
C	0.14617200	-1.34369600	4.87571300
H	2.28865100	-1.12178400	4.96105200
C	-1.12015000	0.73804000	4.77706700
H	0.05156500	2.53773500	4.79451300
C	-1.06887500	-0.66378800	4.79702600
H	-1.99598000	-1.23105100	4.75352200
H	0.65347400	0.24180500	-0.36707600
C	-2.46300400	1.46172400	4.73548700
C	2.61435700	1.60609800	4.91327100
C	0.18243600	-2.86798200	4.91636300
H	-1.23881900	-3.37356600	2.63120600
H	3.88151000	0.80945100	2.61242400
H	-2.42391600	2.86785500	2.37960300
H	0.83340300	-3.19126000	5.73888700
H	-0.82280500	-3.24173300	5.14469800
H	3.45779400	0.92682500	5.08351000
H	2.58883700	2.29701700	5.76700500
H	-2.29015500	2.53862300	4.84645400
H	-3.05962700	1.15077100	5.60394400
Cl	1.65762700	-0.82653100	1.47922100
Cl	0.21437000	1.73421800	1.40037100
Br	-1.31825700	-0.82487000	0.71998600

Cartesian coordinates of the optimized geometries for $\downarrow\text{CHBrCl}_2@5$ using B3LYP-D3/6-31G*,cc-pVTZ.

C	3.04606500	2.16399200	-2.50297200
H	3.89940100	2.31759200	-1.83775700
C	1.80324500	2.82317200	-1.95413200
N	0.59927800	2.49530200	-2.36721700
C	-0.27637800	3.32207400	-1.69389400
C	0.41410500	4.18292400	-0.86260000
N	1.75305200	3.85259700	-1.03446200
C	2.87423800	4.37419700	-0.23035400
H	2.73998800	5.45601700	-0.13787700
H	3.78802900	4.21196000	-0.80487800
C	-0.08625800	5.22881000	0.07652700
H	-1.14080100	5.40462400	-0.13967500
H	0.46817000	6.17073300	-0.02447800
H	-0.00078300	4.90371900	1.12042300
C	-1.73917600	3.13063400	-1.78429900
O	-2.55933100	3.85377800	-1.20003900
N	2.81784600	0.72772500	-2.53974600
H	1.91776300	0.40656200	-2.88106600
C	2.95772400	3.72074200	1.13836100
C	3.50806400	2.44139700	1.29226200
H	3.95930100	1.91990800	0.45133900
C	3.43380200	1.78962600	2.52237700
C	2.80056900	2.37962800	3.62388200
C	2.32605200	3.68925900	3.48592500

H	1.87483700	4.19258600	4.33840300
C	2.40886500	4.35259400	2.26083600
H	2.02643700	5.36666700	2.17517700
C	3.41775200	2.71657800	-3.90773800
H	2.55933200	2.51268800	-4.56360400
C	4.65366100	1.99451600	-4.45905200
H	5.52324200	2.16314700	-3.81067900
H	4.90150000	2.36453100	-5.46105900
H	4.48779000	0.91518000	-4.52095600
C	3.64374600	4.23458300	-3.86338700
H	4.48570300	4.48473300	-3.20286900
H	2.75809900	4.77282000	-3.50753300
H	3.88797500	4.61597000	-4.86132900
C	-3.46654700	1.55521000	-2.59250500
H	-4.04562100	2.19871100	-1.92484800
C	-3.46171300	0.12878300	-2.09857100
N	-2.62559000	-0.77323300	-2.56264600
C	-2.89677500	-1.93923300	-1.87389600
C	-3.93904900	-1.74316000	-0.98474000
N	-4.29386400	-0.40885400	-1.13484100
C	-5.21978300	0.32297000	-0.25133800
H	-6.10768000	-0.30152400	-0.11321300
H	-5.53892200	1.21971900	-0.78657700
C	-4.57652500	-2.68105700	-0.01510500
H	-4.22073000	-3.68919700	-0.23023700
H	-5.67169500	-2.65882500	-0.08588900
H	-4.30196100	-2.43217000	1.01649600
C	-1.99014700	-3.10917700	-1.93455600
O	-2.20297600	-4.16380600	-1.32098800
N	-2.10162800	2.05778400	-2.54438000
H	-1.35864200	1.44715500	-2.86694600
C	-4.59405600	0.67330200	1.08844500
C	-3.68429500	1.73329400	1.20024400
H	-3.46097400	2.37065900	0.34847600
C	-3.03784100	1.98072800	2.41000200
C	-3.27463800	1.18510200	3.53914500
C	-4.22127000	0.15913100	3.43525300
H	-4.45443500	-0.45029400	4.30592900
C	-4.87500100	-0.08992100	2.22708300
H	-5.60977200	-0.88970200	2.17272100
C	-4.07857100	1.66635400	-4.01523000
H	-3.47067600	1.03012200	-4.67379700
C	-4.01602600	3.11424300	-4.51687100
H	-4.43792800	3.19001300	-5.52591600
H	-2.98535200	3.48003400	-4.54651300
H	-4.58772000	3.78016700	-3.85763800
C	-5.52094900	1.14005800	-4.02475600
H	-6.15652500	1.73244900	-3.35142600
H	-5.57705400	0.09145000	-3.71179200
H	-5.95192400	1.21235100	-5.02971500
C	0.28387200	-3.78338500	-2.59963000
H	-0.01926700	-4.60347400	-1.94298700
C	1.45266500	-3.02857000	-2.01267900
N	1.79485100	-1.82416000	-2.41361100
C	2.94398200	-1.50028700	-1.71792600
C	3.31699900	-2.54020100	-0.89029600
N	2.34877400	-3.51689900	-1.07957200
C	2.19010300	-4.71832100	-0.24236000
H	3.16784700	-5.20293500	-0.15999800
H	1.53449600	-5.40686600	-0.77886400
C	4.46001500	-2.65909200	0.06112200
H	5.16475500	-1.85359300	-0.14708700
H	4.97130000	-3.62594900	-0.03263000
H	4.12682900	-2.56109700	1.10143300
C	3.52374400	-0.14136400	-1.76041400
O	4.53442000	0.18755100	-1.12324900

N	-0.86317100	-2.89019300	-2.67121000
H	-0.70055200	-1.94145100	-2.99235700
C	1.63597000	-4.38263100	1.13153500
C	0.28530000	-4.04757700	1.29539800
H	-0.40595100	-4.10561700	0.45737700
C	-0.18329600	-3.60706100	2.53227600
C	0.67418600	-3.48433200	3.63419000
C	2.00783400	-3.87794300	3.48004200
H	2.68724400	-3.82500100	4.32809900
C	2.48069100	-4.32648000	2.24565800
H	3.52290200	-4.62004500	2.14641200
C	0.62951600	-4.37970500	-3.99327100
H	0.88088900	-3.53125800	-4.64584200
C	-0.58137400	-5.11995100	-4.57481000
H	-0.34836900	-5.51771400	-5.56960200
H	-1.44736200	-4.45747600	-4.66273100
H	-0.86780300	-5.96208400	-3.93120300
C	1.85060300	-5.30694600	-3.91091700
H	1.65324000	-6.15341600	-3.23847200
H	2.74200400	-4.78424700	-3.54814100
H	2.08414100	-5.72165900	-4.89810200
C	0.13390800	0.00273800	1.61022000
C	1.28523500	0.78007400	4.89767600
C	1.31058600	-0.61617100	4.92359000
C	0.03853000	1.42829600	4.86740400
C	0.12436700	-1.37051300	4.92976500
H	2.26695700	-1.13466500	4.92723700
C	-1.15784900	0.70807400	4.87079200
H	0.00671900	2.51462000	4.82688500
C	-1.09827700	-0.69578000	4.90275700
H	-2.02457400	-1.26623400	4.89301800
C	-2.50658100	1.41856400	4.83084600
C	2.57813700	1.59431100	4.90640800
C	0.17677200	-2.89438200	4.94471600
H	-1.22747800	-3.32220300	2.63109500
H	3.83785400	0.78547300	2.61183200
H	-2.32214800	2.79609500	2.46863600
H	0.83193500	-3.22339400	5.76140100
H	-0.82413600	-3.28257700	5.16760300
H	3.42343900	0.91776000	5.07711500
H	2.55269900	2.28751200	5.75804000
H	-2.34726700	2.49381800	4.97273000
H	-3.11468100	1.07644800	5.67872300
Cl	1.69501600	-0.78955900	1.31164800
Cl	0.19264100	1.73199400	1.21421600
H	-0.10369000	-0.10010300	2.65987000
Br	-1.28478800	-0.87376800	0.60547400

Cartesian coordinates of the optimized geometries for **6** using B3LYP-D3/6-31G*,cc-pVTZ.

C	1.79585100	3.32618000	-2.16992000
H	2.47680600	3.88756800	-1.52254700
C	0.38816200	3.37933400	-1.61939000
N	-0.52984800	2.48643800	-1.91364800
C	-1.63816200	2.80944600	-1.15297500
C	-1.38948600	3.93361900	-0.39024000
N	-0.09323300	4.30350900	-0.71425000
C	0.65353400	5.37498600	-0.05645500
H	0.01477300	6.26321100	-0.01467200
H	1.50045600	5.63035800	-0.69967400
C	-2.22377300	4.67188200	0.60137700
H	-3.18837300	4.16885700	0.68526700
H	-2.39358700	5.71314400	0.29385400
H	-1.74014900	4.69548600	1.58646800
C	-2.85416800	1.96914800	-1.17247200

O	-3.81600000	2.14567300	-0.41452800
N	2.25184600	1.94518400	-2.11929500
H	1.64577700	1.24027900	-2.52759500
C	1.11943500	4.98607200	1.33504700
C	1.55484900	3.68479300	1.58277300
H	1.56309700	2.95154600	0.78405300
C	1.95474500	3.28219000	2.86078500
C	1.94203200	4.22268800	3.89623100
H	2.24129600	3.92247100	4.89803000
C	1.53244000	5.53690300	3.65474200
H	1.52201500	6.25984300	4.46644500
C	1.11003000	5.91749000	2.38023700
H	0.76513100	6.93388800	2.20007800
C	1.88561500	3.89259900	-3.61189100
H	1.22561200	3.27208900	-4.23565900
C	3.31958700	3.79121400	-4.14659500
H	4.00449700	4.39266900	-3.53422700
H	3.37442300	4.16238500	-5.17671200
H	3.67778700	2.75764800	-4.13181200
C	1.38036700	5.34117000	-3.67154500
H	2.01073900	6.00068000	-3.05895800
H	0.34698800	5.43153800	-3.31893400
H	1.41680100	5.71853800	-4.69973600
C	-3.77465500	-0.10904400	-2.15777900
H	-4.59750900	0.19979900	-1.50509700
C	-3.11532000	-1.35605600	-1.61249200
N	-1.88330500	-1.70302700	-1.90949900
C	-1.60774100	-2.82708600	-1.15332200
C	-2.70439000	-3.17648700	-0.39007400
N	-3.67360100	-2.23808900	-0.70949200
C	-4.97565800	-2.13112100	-0.05245400
H	-5.41970200	-3.13077000	-0.00668000
H	-5.62337800	-1.53203300	-0.69836700
C	-2.92417900	-4.27062800	0.59922800
H	-2.00541300	-4.85361300	0.68042900
H	-3.74082400	-4.93836800	0.29182000
H	-3.18564700	-3.86588500	1.58552800
C	-0.27206100	-3.46049900	-1.17841600
O	0.05518000	-4.38930900	-0.42953000
N	-2.80620400	0.97607600	-2.11184500
H	-1.89643000	0.80569000	-2.52937600
C	-4.87739800	-1.52699700	1.33688900
C	-3.96575400	-0.50162100	1.58585400
H	-3.32680300	-0.13546800	0.79054200
C	-3.82497500	0.05311700	2.86176900
C	-4.64391300	-0.41811000	3.89327000
H	-4.54048500	-0.00326100	4.89348700
C	-5.57997100	-1.42740500	3.65009800
H	-6.20907500	-1.79002700	4.45904100
C	-5.69019300	-1.99112700	2.37829500
H	-6.40002200	-2.79557900	2.19686600
C	-4.31744200	-0.31194600	-3.59766300
H	-3.45228300	-0.56904800	-4.22689300
C	-4.95306300	0.98066100	-4.12465800
H	-5.30567000	0.84588300	-5.15396900
H	-4.23981600	1.80975800	-4.10873700
H	-5.81505500	1.26744200	-3.50758700
C	-5.31638200	-1.47627700	-3.65669500
H	-6.20076000	-1.26420700	-3.04015800
H	-4.87426700	-2.41632700	-3.30896100
H	-5.66510500	-1.63042400	-4.68406000
C	1.98790300	-3.21196500	-2.16237800
H	2.13209800	-4.08087400	-1.51294000
C	2.73985000	-2.01904900	-1.61583100
N	2.42732900	-0.77853800	-1.91519200
C	3.26130600	0.02174700	-1.15690200

C	4.10846200	-0.75374400	-0.38985000
N	3.77924000	-2.06216400	-0.70885500
C	4.33384000	-3.24375100	-0.05024500
H	5.42177100	-3.13041800	-0.00188400
H	4.13860900	-4.10379900	-0.69636000
C	5.16432800	-0.39843500	0.60177900
H	5.21027900	0.68851000	0.68454500
H	6.15114500	-0.77168100	0.29487400
H	4.94279500	-0.82814500	1.58725700
C	3.14241300	1.49497900	-1.18373500
O	3.78210700	2.24329000	-0.43410100
N	0.56460500	-2.91311700	-2.11174700
H	0.25814000	-2.03604700	-2.52119900
C	3.75793800	-3.45980000	1.33760200
C	2.41381600	-3.18227300	1.58417500
H	1.77838300	-2.81126600	0.78786500
C	1.86064600	-3.33865300	2.85892400
C	2.67574300	-3.81353500	3.89167800
H	2.26240200	-3.93210200	4.89074900
C	4.01800900	-4.12017000	3.65098200
H	4.64500800	-4.48513900	4.46051900
C	4.56365200	-3.93295300	2.38036900
H	5.61573500	-4.14606400	2.20086200
C	2.43212500	-3.57697100	-3.60402100
H	2.22847300	-2.69506100	-4.22897800
C	1.62231000	-4.76560500	-4.13675000
H	1.91468700	-5.00119000	-5.16689800
H	0.54917400	-4.55470700	-4.12098400
H	1.79764200	-5.65918900	-3.52330500
C	3.93787100	-3.87003500	-3.66274900
H	4.18920300	-4.74680800	-3.04971100
H	4.53626100	-3.02245800	-3.30988900
H	4.24646700	-4.09207000	-4.69047400
C	0.43221600	-2.90518200	3.08843000
H	-0.19810100	-3.33240000	2.29613400
H	0.06248400	-3.31978200	4.03635000
C	2.29504700	1.82868100	3.09075900
C	0.23389000	-1.38838600	3.09783300
C	1.29921800	-0.48890400	3.09916400
C	-1.07630900	-0.88385500	3.09989900
C	1.08098600	0.89823200	3.09811000
H	2.31993400	-0.86045600	3.08781800
H	-1.90811600	-1.58236200	3.08845000
C	-0.23061700	1.37109700	3.09868500
H	-0.41946400	2.44080400	3.08656000
C	-2.73581700	1.07398200	3.09221300
C	-1.32278400	0.48843500	3.09853600
H	2.98181300	1.49702300	2.29978000
H	2.83728200	1.71613200	4.03965600
H	-2.79269200	1.83459500	2.30112100
H	-2.90918200	1.59979600	4.04123100

Cartesian coordinates of the optimized geometries for $\text{†CHCl}_3\text{@6}$ using B3LYP-D3/6-31G*,cc-pVTZ.

C	1.33607900	3.52605600	-2.35936800
H	1.94919800	4.13766800	-1.69621800
C	-0.05311900	3.35587100	-1.79329900
N	-0.89348100	2.44691400	-2.23877000
C	-2.08245300	2.66141600	-1.56664200
C	-1.95637700	3.71939400	-0.69006900
N	-0.64641400	4.15509000	-0.83787000
C	0.02287100	5.16359200	-0.00025900
H	-0.76260900	5.80424200	0.40931200
H	0.63742500	5.78983600	-0.65216700

C	-2.94311000	4.31295400	0.25892900
H	-3.89548500	3.80058100	0.11446100
H	-3.08748700	5.38739000	0.08256500
H	-2.63826700	4.18392400	1.30441900
C	-3.21533600	1.71791900	-1.68390100
O	-4.31500900	1.89718200	-1.14768500
N	1.97592500	2.22178200	-2.40953600
H	1.41469300	1.43718300	-2.72174100
C	0.87021200	4.57138600	1.11513500
C	0.27464700	4.04779100	2.27172600
H	-0.80757800	4.05896000	2.37055200
C	1.04045000	3.49757900	3.30400200
C	2.43596800	3.48235700	3.16376000
H	3.05140200	3.07976000	3.96488400
C	3.04117400	3.98020700	2.01226600
H	4.12065000	3.94376900	1.89880800
C	2.26218500	4.53244900	0.99415900
H	2.75295700	4.91201300	0.10462500
C	1.30328400	4.20673500	-3.75640900
H	0.70162400	3.55921900	-4.40969300
C	2.72199900	4.32070100	-4.32846500
H	3.35604500	4.93561900	-3.67655400
H	2.70119400	4.78724500	-5.32043600
H	3.19297200	3.33771800	-4.41839500
C	0.62841300	5.58410300	-3.68280600
H	1.19310100	6.25981300	-3.02494500
H	-0.39904900	5.52017300	-3.30763200
H	0.59380700	6.04925900	-4.67433500
C	-3.71820700	-0.60564100	-2.35348700
H	-4.55109100	-0.37856400	-1.68702300
C	-2.87654300	-1.72461800	-1.78968100
N	-1.66903000	-1.99816700	-2.23495200
C	-1.26181600	-3.13715500	-1.56471800
C	-2.24214800	-3.55757300	-0.68961700
N	-3.27341500	-2.63967100	-0.83645600
C	-4.48233500	-2.56561400	-0.00053900
H	-4.64460900	-3.56656100	0.40766300
H	-5.33083400	-2.34603600	-0.65316200
C	-2.26463000	-4.70956800	0.25852000
H	-1.34302000	-5.27607600	0.11806800
H	-3.12061200	-5.37341600	0.07801600
H	-2.31117000	-4.38135900	1.30392400
C	0.12154800	-3.64676700	-1.68202800
O	0.51607500	-4.68861800	-1.14534300
N	-2.90792600	0.60001100	-2.40642900
H	-1.94997300	0.50808100	-2.72554500
C	-4.39542200	-1.53708200	1.11645800
C	-3.64220500	-1.78925000	2.27187800
H	-3.10561600	-2.72938000	2.36838200
C	-3.55305000	-0.85217200	3.30578300
C	-4.24356700	0.36075600	3.16799000
H	-4.20454900	1.09400300	3.97023800
C	-4.97924200	0.63445100	2.01728700
H	-5.49310100	1.58486300	1.90627200
C	-5.06379300	-0.31522900	0.99795100
H	-5.63951800	-0.08153700	0.10899400
C	-4.29686100	-0.97389700	-3.74834100
H	-3.43802800	-1.17166600	-4.40551100
C	-5.10640000	0.19798000	-4.31688900
H	-5.50384900	-0.05271000	-5.30753900
H	-4.49091500	1.09742500	-4.40920600
H	-5.95307500	0.43995500	-3.66137200
C	-5.15288200	-2.24638200	-3.67216300
H	-6.01820200	-2.09528600	-3.01156000
H	-4.58358400	-3.10500000	-3.29947700
H	-5.54186500	-2.50812700	-4.66262800

C	2.38472500	-2.91688000	-2.35237300
H	2.60796000	-3.75228400	-1.68821600
C	2.92991200	-1.62757500	-1.78678900
N	2.56401800	-0.44594300	-2.23520500
C	3.34706900	0.47724000	-1.56672500
C	4.20016700	-0.15998500	-0.68946600
N	3.92001600	-1.51218000	-0.83310000
C	4.46151800	-2.59489600	0.00372100
H	5.40751000	-2.23262300	0.41382800
H	4.69895300	-3.43917400	-0.64869800
C	5.20791600	0.39845300	0.25848500
H	5.23867000	1.47963000	0.11488700
H	6.21119800	-0.01136600	0.08039500
H	4.94546800	0.19687500	1.30429900
C	3.09936700	1.93039400	-1.68885800
O	3.80834200	2.79381900	-1.15882600
N	0.93525500	-2.82177800	-2.40566400
H	0.53495800	-1.94638500	-2.72408500
C	3.52620800	-3.03640300	1.11887300
C	3.36848800	-2.26027900	2.27625800
H	3.91540500	-1.32647300	2.37491900
C	2.51112400	-2.65242800	3.30903300
C	1.80423000	-3.85583500	3.16817800
H	1.14940000	-4.19003600	3.96933300
C	1.93497000	-4.62743800	2.01568200
H	1.36711800	-5.54615000	1.90206200
C	2.80081200	-4.22509600	0.99743100
H	2.88550800	-4.83844900	0.10746300
C	2.99309700	-3.22692300	-3.74897100
H	2.72827000	-2.38419300	-4.40326800
C	2.39009800	-4.51626900	-4.32030100
H	2.80182500	-4.72720100	-5.31454700
H	1.30244500	-4.44080500	-4.40589800
H	2.61479500	-5.37164200	-3.67042900
C	4.52395200	-3.32153300	-3.67598000
H	4.83216700	-4.14484200	-3.01636700
H	4.97688300	-2.39602300	-3.30388000
H	4.94458500	-3.52418100	-4.66750400
C	-0.00435500	-0.00286300	0.43129100
C	1.28389600	0.52409700	4.49660700
C	1.11683900	-0.85996000	4.49836000
C	0.18279200	1.39453500	4.49495000
C	-0.18743500	-1.37828600	4.49664600
C	-1.09928200	0.84729500	4.49301300
C	-1.30239600	-0.54145800	4.49510500
H	-0.00553500	-0.00536200	-0.65611600
C	2.32636400	-1.78838600	4.54640100
H	3.22850400	-1.18676400	4.70720200
H	2.23134300	-2.44425600	5.42291700
C	-2.71135700	-1.12482800	4.54196800
H	-2.64118900	-2.20713400	4.70158900
H	-3.23142500	-0.71590300	5.41919900
C	0.38186400	2.90688600	4.54036200
H	-0.59093500	3.38734000	4.69796300
H	0.99492200	3.15391800	5.41785000
H	-1.95893800	1.51277900	4.49235000
H	-0.33458700	-2.45546100	4.49932300
H	2.29004900	0.93605100	4.49960700
Cl	0.22599800	-1.67757500	0.98991100
Cl	1.33304300	1.03436500	0.98226000
Cl	-1.56942500	0.63777200	0.98677800

Cartesian coordinates of the optimized geometries for $\downarrow\text{CHCl}_3@6$ using B3LYP-D3/6-31G*,cc-pVTZ.

C	1.30853300	3.53324100	-2.42948300
H	1.91499200	4.14948000	-1.76419600
C	-0.08020300	3.34881200	-1.86708000
N	-0.93369600	2.48066000	-2.36198300
C	-2.11259300	2.66143400	-1.66558700
C	-1.96980200	3.66481800	-0.72747500
N	-0.65562300	4.09205100	-0.85543100
C	0.02416700	5.05576800	0.02354700
H	-0.75404200	5.68938500	0.45739100
H	0.64480400	5.70107400	-0.60383100
C	-2.94013100	4.20394300	0.26999500
H	-3.90172100	3.71793800	0.09728800
H	-3.07057600	5.29010100	0.17219000
H	-2.62848100	3.99398300	1.30031100
C	-3.23706100	1.70694500	-1.78892900
O	-4.34532000	1.88353400	-1.26669000
N	1.95959700	2.23304500	-2.48375200
H	1.39128800	1.43943000	-2.75974700
C	0.87080800	4.43019500	1.12395800
C	0.28426100	3.94389600	2.30202000
H	-0.79569400	3.98340100	2.41932000
C	1.05935500	3.42302000	3.34439200
C	2.45244900	3.38925000	3.18871800
H	3.07499000	3.01483700	3.99818700
C	3.04655100	3.83751000	2.01209500
H	4.12447900	3.78934000	1.88728300
C	2.26083300	4.36569800	0.98667500
H	2.74725200	4.71107100	0.08145900
C	1.26979900	4.22380600	-3.82059900
H	0.67025600	3.57909600	-4.47809000
C	2.68637400	4.35178100	-4.39450100
H	3.31960000	4.96205200	-3.73752000
H	2.66071000	4.82903800	-5.38128900
H	3.16145000	3.37193800	-4.49695700
C	0.58569900	5.59551100	-3.72779500
H	1.14303300	6.26425200	-3.05648200
H	-0.44242600	5.51744000	-3.35680000
H	0.55052200	6.07643300	-4.71174100
C	-3.70876100	-0.63417500	-2.42186400
H	-4.54056000	-0.41303000	-1.75181900
C	-2.85537500	-1.74618300	-1.86251000
N	-1.67754600	-2.05195100	-2.35884000
C	-1.24558500	-3.16538900	-1.66519100
C	-2.18589000	-3.54424100	-0.72722500
N	-3.21189300	-2.61785600	-0.85255500
C	-4.38852000	-2.51418200	0.02391900
H	-4.54698800	-3.50562800	0.45614200
H	-5.25646800	-2.30055100	-0.60525100
C	-2.16768200	-4.65454500	0.26982700
H	-1.26819300	-5.24662300	0.09474800
H	-3.04510200	-5.30802100	0.17467100
H	-2.13839800	-4.27956800	1.30022700
C	0.14318300	-3.66166800	-1.79065000
O	0.54429900	-4.71254600	-1.27377100
N	-2.90643600	0.57829800	-2.48204400
H	-1.93724500	0.48315800	-2.76576900
C	-4.27584900	-1.46923800	1.12604500
C	-3.55964300	-1.73078600	2.30357000
H	-3.04672700	-2.68215900	2.41886800
C	-3.50198300	-0.79954200	3.34679900
C	-4.17708900	0.41948300	3.19262300
H	-4.16730200	1.14520600	4.00278100
C	-4.86501300	0.70655800	2.01669700
H	-5.36856200	1.66106800	1.89326100

C	-4.92307600	-0.23718400	0.99028200
H	-5.46688400	0.00874000	0.08530100
C	-4.29637800	-1.01370300	-3.80901400
H	-3.44280100	-1.21487600	-4.47142600
C	-5.11469800	0.15026400	-4.38069800
H	-5.52118300	-0.11127900	-5.36488100
H	-4.50168100	1.04974300	-4.48854700
H	-5.95516900	0.39771600	-3.71936200
C	-5.14615600	-2.28876400	-3.70911800
H	-6.00014400	-2.13647400	-3.03385500
H	-4.56601800	-3.14162900	-3.33963000
H	-5.55118400	-2.56035300	-4.69046800
C	2.40584500	-2.89212700	-2.42170500
H	2.63468600	-3.72404600	-1.75481900
C	2.94014000	-1.59670300	-1.86031600
N	2.61717200	-0.42397300	-2.35798500
C	3.36646300	0.50673600	-1.66492600
C	4.16357200	-0.11817600	-0.72605900
N	3.87300500	-1.46968500	-0.85040300
C	4.36908100	-2.54036500	0.02743500
H	5.30544700	-2.18195000	0.46240700
H	4.61970100	-3.39921700	-0.60098900
C	5.11799100	0.45246100	0.26913800
H	5.18010800	1.52774700	0.09434600
H	6.12276400	0.02009000	0.17122400
H	4.78140900	0.28979500	1.30038300
C	3.10523000	1.95813000	-1.79428200
O	3.81678200	2.83101600	-1.28046400
N	0.95448700	-2.80676100	-2.47938800
H	0.55072000	-1.91929300	-2.75892800
C	3.40436000	-2.96509800	1.12681700
C	3.27243600	-2.21549600	2.30549900
H	3.84210900	-1.29736000	2.42337500
C	2.43577800	-2.63155300	3.34764100
C	1.71579600	-3.82460600	3.19086200
H	1.08190500	-4.17978000	3.99998400
C	1.81096300	-4.56187100	2.01353100
H	1.23476100	-5.47398800	1.88809100
C	2.65927400	-4.14042300	0.98848500
H	2.71813400	-4.73300600	0.08298000
C	3.02672500	-3.20388700	-3.81151500
H	2.76775300	-2.36326500	-4.47027800
C	2.43313200	-4.49589700	-4.38612500
H	2.85919400	-4.71005900	-5.37365600
H	1.34682000	-4.42077200	-4.48819900
H	2.64794200	-5.34891700	-3.73000100
C	4.55674200	-3.29386700	-3.71619400
H	4.85781600	-4.10913500	-3.04316200
H	5.00070000	-2.36295400	-3.34652900
H	4.99281100	-3.50472600	-4.69931400
C	1.28838000	0.51246900	4.64821200
C	1.10751900	-0.87194100	4.64572900
C	0.19491600	1.39527600	4.64417400
C	-0.20361700	-1.37756400	4.64715300
C	-1.09450400	0.85987100	4.64557800
C	-1.31201000	-0.52858400	4.64369600
H	-0.00074000	0.00105000	2.53582300
C	2.30485200	-1.81500900	4.62619000
H	3.21931900	-1.23148000	4.78251100
H	2.22558800	-2.50368700	5.47840700
C	-2.72741200	-1.09444000	4.62383400
H	-2.67868500	-2.17838400	4.77934200
H	-3.28362500	-0.68276300	5.47692300
C	0.41380000	2.90416100	4.62211100
H	-0.54918600	3.40509900	4.77445900
H	1.04738800	3.18107200	5.47533700

H	-1.94696900	1.53343000	4.62653900
H	-0.36120100	-2.45262700	4.63010300
H	2.29805000	0.91398600	4.63244800
Cl	-0.02447700	-1.69646200	0.92542700
Cl	1.46449700	0.83002200	0.90920600
Cl	-1.46888500	0.85724400	0.92724400
C	-0.00648200	-0.00135200	1.45825800

Cartesian coordinates of the optimized geometries for CHCl_3 using B3LYP-D3/def2-TZVP.

C	-0.00010900	0.10708200	0.00000100
H	-0.00218900	1.19032800	0.00000000
Cl	-0.84759500	-0.43402900	1.46938300
Cl	1.69748600	-0.42935100	-0.00000100
Cl	-0.84759400	-0.43403000	-1.46938300

Cartesian coordinates of the optimized geometries for CHBrCl_2 using B3LYP-D3/def2-TZVP.

C	-0.01855700	0.10536500	-0.00000100
H	-0.00196700	1.18786700	0.00000000
Cl	-0.85969400	-0.43058500	1.46753400
Cl	-0.85969600	-0.43058500	-1.46753400
Br	1.85881400	-0.46986100	0.00000100

Cartesian coordinates of the optimized geometries for **1** using B3LYP-D3/def2-TZVP.

C	-2.59611700	1.73581500	-3.17444600
C	-2.47248500	2.84174700	-2.35284700
C	-1.23560100	3.51638000	-2.30546700
C	-0.20855900	3.07869000	-3.12314200
C	-0.33309900	1.95693400	-3.95633000
C	-1.54137000	1.26554600	-3.97039600
C	0.88474700	1.54484700	-4.76613900
C	1.86768300	0.70390700	-3.97109000
C	2.80386900	1.38156000	-3.17634800
C	3.69955300	0.72108000	-2.35513000
C	3.66247700	-0.68705300	-2.30521300
C	2.76950100	-1.35717600	-3.12280800
C	1.86152300	-0.68803100	-3.95678300
C	0.89574300	-1.53658000	-4.76702400
C	-0.32366300	-1.96819700	-3.97216500
C	-0.20446700	-3.11833900	-3.17815700
C	-1.22429900	-3.56416800	-2.35711300
C	-2.42546300	-2.82799600	-2.30694700
C	-2.55988300	-1.71889600	-3.12365300
C	-1.52621400	-1.26673500	-3.95735700
C	-1.77734200	-0.00548000	-4.76691100
O	-3.47333100	3.35128500	-1.58048300
O	-1.15851500	4.57314200	-1.45147600
C	0.09373000	5.23025100	-1.27260200
O	4.64417500	1.33196600	-1.58550700
O	4.53659600	-1.28222500	-1.44907400
C	4.48012900	-2.69559100	-1.27208200
O	-1.16811500	-4.68802800	-1.58786200
O	-3.37803400	-3.28870600	-1.45147300
C	-4.57337400	-2.53326300	-1.27266400
C	0.18709500	3.08008400	3.08368100
C	1.21116700	3.52515400	2.26636600
C	2.45302200	2.85980600	2.31442900
C	2.58429700	1.75464400	3.13597800
C	1.53268600	1.27672000	3.93147900
C	0.31948000	1.95937500	3.91711500
C	1.77750200	0.00742900	4.72801500

C	1.53512900	-1.25564800	3.91856200
C	2.57187800	-1.70067500	3.08479700
C	2.44522800	-2.81087400	2.26832000
C	1.24931000	-3.55550900	2.31879700
C	0.22644400	-3.11670700	3.13984900
C	0.33755400	-1.96558200	3.93357400
C	-0.88479400	-1.54247000	4.72840300
C	-1.85653200	-0.70083900	3.91815700
C	-2.75995700	-1.37635800	3.08424000
C	-3.65787500	-0.71264500	2.26700200
C	-3.70526300	0.69518300	2.31722400
C	-2.81387200	1.36198400	3.13815400
C	-1.87260500	0.69104400	3.93240500
C	-0.89536700	1.53890900	4.72709100
O	1.12668300	4.58119400	1.41213600
C	-0.13011600	5.22939500	1.23296600
O	3.45059000	3.37691600	1.54289400
O	3.40096700	-3.26504400	1.41289300
C	4.59099600	-2.50128900	1.23400500
O	1.20085600	-4.67988200	1.54978500
O	-4.52789500	-1.31397500	1.41092400
C	-4.46106100	-2.72683600	1.23342200
O	-4.65468200	1.29939000	1.54832200
C	-0.02105100	6.08174300	-0.01978400
C	5.27425700	-3.02295200	-0.01883800
C	-5.25295700	-3.05964500	-0.01982000
H	-3.53633900	1.20510300	-3.20426000
H	0.72828100	3.61613200	-3.12360700
H	1.39736300	2.45100900	-5.09927300
H	0.58158800	1.02699100	-5.67340600
H	2.81611800	2.46108100	-3.20791100
H	2.76546000	-2.43714700	-3.12270000
H	0.59779500	-1.01513500	-5.67393700
H	1.42489400	-2.43300200	-5.10070100
H	0.72474200	-3.66807200	-3.20946700
H	-3.49373200	-1.17636400	-3.12289700
H	-2.81803200	-0.01453400	-5.10106200
H	-1.17588300	-0.00805600	-5.67275800
H	0.89529100	4.49688800	-1.14419600
H	0.31964800	5.84515000	-2.15171100
H	3.44444900	-3.02411000	-1.14536100
H	4.90089500	-3.19733800	-2.15138500
H	-4.33953800	-1.47227000	-1.14474700
H	-5.21874800	-2.64519100	-2.15159000
H	-0.75365700	3.61069500	3.08368100
H	3.52831200	1.23071700	3.16611700
H	1.17612400	0.00077400	5.63388700
H	2.81822000	0.00554500	5.06219400
H	3.50188500	-1.15157100	3.08380300
H	-0.69885800	-3.67296600	3.17138000
H	-1.40759900	-2.44249400	5.06234100
H	-0.59047900	-1.01882600	5.63524500
H	-2.74814800	-2.45627900	3.08402100
H	-2.83374000	2.44139000	3.16968700
H	-1.41414500	2.44156100	5.06013800
H	-0.58843600	1.02340600	5.63439300
H	-0.92641000	4.49036900	1.10428700
H	-0.36062500	5.84262200	2.11207200
H	4.34975200	-1.44197000	1.10603200
H	5.23716000	-2.60866000	2.11294500
H	-3.42301200	-3.04766800	1.10638800
H	-4.87801800	-3.23196800	2.11263100
H	0.85731800	6.72758500	0.05718600
H	-0.90374600	6.72167200	-0.09665200
H	5.39220900	-4.10674300	0.05829200
H	6.27075800	-2.58057800	-0.09553700

H	-5.36337100	-4.14422500	-0.09697000
H	-6.25250200	-2.62422300	0.05697100
C	-0.03352400	-5.52786300	-1.72724600
H	-0.25775900	-6.42930300	-1.16202700
H	0.13721000	-5.79840800	-2.77399900
H	0.86613900	-5.06035500	-1.31462700
C	0.07305000	-5.52848000	1.69090700
H	-0.83075800	-5.06824800	1.27918700
H	0.30364600	-6.42850700	1.12595600
H	-0.09432500	-5.79967800	2.73803400
C	-4.76757300	2.78936700	-1.72231800
H	-4.81261200	1.77459700	-1.31358000
H	-5.43657900	3.43160200	-1.15468300
H	-5.08701300	2.78069600	-2.76926700
C	4.74919300	2.82566200	1.68669700
H	4.80315900	1.81123100	1.27813700
H	5.41383200	3.47335400	1.12008100
H	5.06704200	2.81966600	2.73416600
C	4.80789000	2.73317900	-1.73038800
H	3.95385100	3.28249200	-1.32078400
H	5.70097800	2.99002700	-1.16561200
H	4.95853300	3.01178700	-2.77817200
C	-4.83001900	2.69895600	1.69533700
H	-3.98082500	3.25600900	1.28607200
H	-5.72560900	2.94926200	1.13155100
H	-4.98218300	2.97472600	2.74366000

Cartesian coordinates of the optimized geometries for CHCl_3 @1 using B3LYP-D3/def2-TZVP.

C	-2.60115800	1.71875000	-3.29193900
C	-2.47279000	2.80956200	-2.45239000
C	-1.23800400	3.48514600	-2.40180000
C	-0.21553500	3.06607600	-3.23302900
C	-0.34036900	1.95285900	-4.07696600
C	-1.54695400	1.25819300	-4.09365100
C	0.87726200	1.54833800	-4.89175600
C	1.86599200	0.71395200	-4.09720700
C	2.79504900	1.39889500	-3.30117700
C	3.67646600	0.74529500	-2.46059100
C	3.63952000	-0.66134700	-2.40037500
C	2.76336100	-1.33987800	-3.22758600
C	1.86263000	-0.67801400	-4.07456500
C	0.90449700	-1.53278400	-4.88820900
C	-0.31374400	-1.97207400	-4.09608400
C	-0.18756300	-3.12059500	-3.30138200
C	-1.19773000	-3.55907400	-2.46572200
C	-2.39736900	-2.82336400	-2.40787800
C	-2.54452700	-1.72379600	-3.23375000
C	-1.51803500	-1.27321600	-4.07641700
C	-1.77727500	-0.01469000	-4.88893300
O	-3.45808900	3.28747400	-1.64006800
O	-1.15002500	4.50974500	-1.50961700
C	0.11628700	5.12614700	-1.29166200
O	4.58768100	1.36282800	-1.65582900
O	4.47998900	-1.24672500	-1.50357300
C	4.37954900	-2.65133200	-1.28303300
O	-1.12241900	-4.65843800	-1.66258900
O	-3.32759900	-3.26041400	-1.51520100
C	-4.49118900	-2.46843400	-1.29111700
C	0.18987100	3.04351700	3.15114300
C	1.21528100	3.46820700	2.32490200
C	2.46338400	2.81923100	2.40635400
C	2.59787000	1.74201200	3.26200400
C	1.54070700	1.27082300	4.05326800
C	0.32401400	1.94834500	4.01787300

C	1.77628500	-0.00140300	4.84647600
C	1.52215100	-1.25545800	4.02429800
C	2.54190400	-1.68716800	3.16278400
C	2.40076300	-2.78830500	2.33692500
C	1.21562700	-3.54659700	2.41583500
C	0.21049400	-3.12336100	3.26523100
C	0.32690100	-1.97062200	4.05520400
C	-0.89539800	-1.53706200	4.84283900
C	-1.85199500	-0.68872300	4.01950600
C	-2.73260500	-1.35454400	3.15389900
C	-3.61662300	-0.68126700	2.32965100
C	-3.68461000	0.72349600	2.41430500
C	-2.81775300	1.38099300	3.26694500
C	-1.87568400	0.70364100	4.05406600
C	-0.88942500	1.54624900	4.84179900
O	1.12214000	4.47921300	1.42152200
C	-0.14026600	5.10880800	1.21308900
O	3.45477300	3.30532500	1.61034600
O	3.32652400	-3.21220800	1.43694500
C	4.49571400	-2.42405100	1.22307000
O	1.14728400	-4.65039000	1.62228900
O	-4.44294600	-1.26994300	1.42543600
C	-4.34728300	-2.67732800	1.21532500
O	-4.60924300	1.33591400	1.62508800
C	-0.00696600	5.96709000	-0.03275100
C	5.17171000	-2.96486100	-0.02513900
C	-5.15517500	-2.99660500	-0.03075000
H	-3.53804200	1.18277100	-3.32056200
H	0.72299000	3.60040600	-3.22313300
H	1.38315800	2.45771200	-5.22609400
H	0.57392100	1.02868000	-5.79785200
H	2.80072300	2.47808100	-3.33544100
H	2.75375600	-2.41963300	-3.21123700
H	0.60604500	-1.01267700	-5.79566800
H	1.44078300	-2.42547200	-5.22020900
H	0.74410900	-3.66546000	-3.33339400
H	-3.47584000	-1.17721300	-3.22035500
H	-2.81848700	-0.03066600	-5.22086000
H	-1.17716400	-0.01626700	-5.79565800
H	0.89037700	4.36452700	-1.15532800
H	0.38288300	5.74636400	-2.15539200
H	3.33290600	-2.93967100	-1.14491500
H	4.78120800	-3.19406800	-2.14675500
H	-4.21482900	-1.41830600	-1.15460400
H	-5.16450900	-2.54350200	-2.15270300
H	-0.75911700	3.55736000	3.11591000
H	3.54271800	1.22185400	3.30904300
H	1.17519800	-0.01154500	5.75242300
H	2.81731800	-0.01555400	5.17846900
H	3.46221900	-1.12359100	3.13243500
H	-0.71246600	-3.68174900	3.30875600
H	-1.43022200	-2.43097000	5.17338000
H	-0.60605700	-1.01267400	5.75075700
H	-2.70058000	-2.43304200	3.11914900
H	-2.84300200	2.45936800	3.31526400
H	-1.39618000	2.45690200	5.17056900
H	-0.57954300	1.03522300	5.75059200
H	-0.91898800	4.35505300	1.06300600
H	-0.40153400	5.71728800	2.08693300
H	4.22235800	-1.37506900	1.07409300
H	5.15712700	-2.49544000	2.09424600
H	-3.30312300	-2.96756500	1.06553400
H	-4.74000400	-3.21147600	2.08863500
H	0.87549400	6.60457600	0.06391800
H	-0.88231600	6.61557100	-0.11985900
H	5.28437000	-4.04773000	0.07024000

H	6.17039500	-2.52975600	-0.11345000
H	-5.27374100	-4.07954500	-0.11665600
H	-6.15093900	-2.55630200	0.06550500
C	0.04943400	-5.45322500	-1.73938300
H	-0.14977600	-6.33814300	-1.14029500
H	0.25780400	-5.76273300	-2.76824100
H	0.91719300	-4.92806100	-1.32769800
C	-0.00112900	-5.47498000	1.73473100
H	-0.89218900	-4.97620500	1.34037100
H	0.20606900	-6.35964500	1.13817300
H	-0.17652400	-5.77997700	2.77114400
C	-4.73327800	2.67195000	-1.71685900
H	-4.71206800	1.65459900	-1.31310500
H	-5.39701900	3.28287300	-1.11043100
H	-5.10997700	2.65524400	-2.74451400
C	4.74275600	2.72410000	1.73059200
H	4.75770600	1.70036600	1.34299500
H	5.40737800	3.34193600	1.13229900
H	5.09180000	2.73195800	2.76806700
C	4.68881100	2.77498000	-1.73760000
H	3.79706100	3.26418900	-1.33256200
H	5.55138900	3.04838800	-1.13517400
H	4.85845600	3.10668300	-2.76683700
C	-4.75791000	2.74054700	1.75141700
H	-3.88427800	3.27219200	1.36024400
H	-5.63114700	3.00409200	1.15991100
H	-4.93423700	3.03391200	2.79109900
Cl	-1.01046200	1.35092900	0.18284000
Cl	-0.66826100	-1.55252900	0.17628800
Cl	1.67466400	0.19547100	0.17741300
C	-0.00107400	-0.00288300	0.74074800
H	0.00010100	-0.00497800	1.82585100

Cartesian coordinates of the optimized geometries for **2** using B3LYP-D3/def2-TZVP.

C	3.01395500	1.34515700	3.71708500
H	2.94384700	2.27475700	4.28617600
H	3.83273400	0.78626100	4.16489600
C	3.33766500	1.70058700	2.27594300
C	2.68407400	2.79831200	1.71145300
H	1.96990100	3.36998500	2.28976500
C	2.90371900	3.21178800	0.41217100
O	2.24768400	4.33125500	-0.02647600
C	1.47556500	4.22290200	-1.22448100
C	0.29877600	5.17357600	-1.10959300
H	0.64704000	6.10869200	-0.67034000
H	-0.10941500	5.39359800	-2.10196100
C	3.84799800	2.52700200	-0.36929800
O	4.08171100	3.01447400	-1.62646800
C	5.21254300	2.52450400	-2.32891500
H	6.12856500	2.65898800	-1.74537400
H	5.27602700	3.11053100	-3.24365000
H	5.10378000	1.46681300	-2.58811400
C	2.62363200	1.25031800	-4.37417100
H	2.14943900	1.76010500	-5.21907800
H	3.68828700	1.15231200	-4.57361800
H	2.48164100	1.84015900	-3.46325400
C	4.48524000	1.42193600	0.17518600
H	5.20250300	0.87496200	-0.41937800
C	4.23214500	0.98186900	1.47941500
C	4.88808200	-0.31543300	1.91781100
H	5.87634600	-0.38444300	1.45780500
H	5.05565600	-0.32413500	2.99222600
C	4.06586800	-1.51633800	1.48291300
C	4.23967800	-1.98843000	0.17915700

H	4.99736000	-1.55228100	-0.46078400
C	3.48128200	-3.01227200	-0.35299900
O	3.73073200	-3.46775200	-1.62423500
C	3.12920300	-2.72070000	-2.68853300
H	3.75968100	-2.86113600	-3.56683500
H	3.10412100	-1.65502100	-2.44973300
C	1.72921700	-3.24280600	-2.98741500
H	1.77667200	-4.31740200	-3.16718100
H	1.05699400	-3.06655000	-2.14497000
C	2.49773300	-3.61901200	0.44386900
O	1.76898700	-4.61259600	-0.13520900
C	0.75691000	-5.23998500	0.63351100
H	1.17044600	-5.73624800	1.51754100
H	0.30943400	-5.98773300	-0.01796600
H	-0.01193000	-4.52583400	0.94779300
C	-3.91702100	4.09715400	2.12961800
H	-4.78693800	4.40744200	1.54186600
H	-3.77866900	4.78719300	2.95919000
H	-4.08780100	3.09043000	2.52495400
C	2.33965600	-3.17851600	1.75101600
H	1.59910000	-3.64548300	2.38395200
C	3.10290400	-2.13355700	2.28489200
C	2.81499000	-1.72095300	3.71836400
H	2.61897500	-2.62544000	4.29918500
H	3.69588000	-1.26824800	4.16742500
C	1.61528400	-0.80155400	3.85783500
C	0.34724300	-1.38150000	3.94931200
H	0.23440500	-2.45866600	3.94944900
C	-0.80950700	-0.63390000	4.05487500
O	-2.00492600	-1.28884200	4.18272000
C	-3.00837700	-1.01416800	3.19684000
H	-2.56090200	-0.54914900	2.31452400
H	-3.75625400	-0.33066200	3.60435100
C	-3.63154700	-2.35284300	2.83235900
H	-2.86643400	-3.03036800	2.44921700
H	-4.08310300	-2.80757200	3.71393000
C	-0.71681600	0.76625000	4.10659300
C	-1.80762400	2.85245400	4.49332300
H	-1.15203000	3.09143400	5.33655200
H	-2.82024500	3.17005900	4.73047900
H	-1.46472100	3.37699600	3.59629700
C	-2.95584800	-5.18613900	-0.40436900
H	-3.64908400	-5.45041400	-1.20942300
H	-2.84130800	-6.03600000	0.26551800
H	-1.98199100	-4.93322400	-0.83642300
O	-1.88234800	1.44978600	4.28051000
C	0.53750700	1.35125800	4.00620300
H	0.62490600	2.42750500	4.04166500
C	1.70591000	0.59257800	3.87194700
C	-3.40680900	-1.20049100	-3.57209800
H	-4.06726300	-0.46975000	-4.03275200
H	-3.58175100	-2.13743100	-4.10587500
C	-1.95352400	-0.80836300	-3.76640200
C	-1.00535900	-1.82969200	-3.86461300
H	-1.31866300	-2.86661600	-3.85139700
C	0.34660200	-1.58504000	-4.01115600
O	1.21866500	-2.63033500	-4.17979400
C	0.79758300	-0.25708000	-4.06872800
O	2.13693500	-0.07289100	-4.22554800
C	-0.13908400	0.76594800	-3.98671300
H	0.19009600	1.79315000	-4.05027300
C	-1.50808700	0.51455700	-3.83668200
C	-2.44034100	1.71100100	-3.76251200
H	-2.04543900	2.48919200	-4.42025500
H	-3.41618700	1.45313600	-4.16799500
C	-2.58808500	2.29989900	-2.37102000

C	-1.60804600	3.20822000	-1.94625100
H	-0.80962200	3.44620200	-2.63314900
C	-1.63585900	3.81155000	-0.69978400
O	-0.72611500	4.71292600	-0.23682200
C	-2.70797500	3.51055700	0.16571800
O	-2.72739100	4.16527500	1.36111400
C	-3.67300000	2.60987400	-0.24993100
H	-4.49670200	2.37808800	0.40940800
C	-3.63142200	1.98554600	-1.50453300
C	-4.71495200	0.97028700	-1.82076100
H	-4.92926000	0.95685500	-2.88719200
H	-5.63972800	1.29083400	-1.33588800
C	-4.37587400	-0.42425100	-1.32353800
C	-4.64240700	-0.72535100	0.01561200
H	-5.11959600	0.00707300	0.65501600
C	-4.33027700	-1.94340800	0.58664800
O	-4.69524500	-2.18462900	1.88845200
O	-3.46597400	-4.12990000	0.39129500
C	-3.73044900	-2.93478300	-0.21017200
C	-3.46888200	-2.64734900	-1.54193400
H	-3.01993400	-3.40214900	-2.17112800
C	-3.77600500	-1.40661300	-2.11351000
H	2.08820000	4.49691600	-2.08889500
H	1.13413300	3.19276200	-1.35529900

Cartesian coordinates of the optimized geometries for $\text{CHCl}_3@2$ using B3LYP-D3/def2-TZVP.

Cl	1.50926300	-0.07951300	-0.67202300
Cl	-0.85206700	1.06257900	0.60856200
Cl	-0.64794200	-1.83469300	0.27353500
C	0.25600200	-0.32020900	0.56034200
H	0.74795900	-0.41049200	1.52115900
C	3.04516200	1.30782400	3.71969100
H	2.96006100	2.24014100	4.28203400
H	3.87660500	0.76831600	4.16716200
C	3.35676100	1.66137800	2.27520900
C	2.66659200	2.73223500	1.70254300
H	1.91789000	3.27023300	2.26915000
C	2.89158800	3.16213500	0.41041100
O	2.18907100	4.25133200	-0.03423400
C	1.41213900	4.09966700	-1.22683200
C	0.31546300	5.14997100	-1.20284500
H	0.72388700	6.07174900	-0.78857900
H	-0.03134300	5.35993500	-2.21975500
C	3.88711000	2.52818600	-0.35025400
O	4.12907800	3.03474700	-1.59711100
C	5.27876000	2.57583100	-2.28983700
H	6.18640000	2.74151200	-1.70122300
H	5.32976600	3.15832400	-3.20742800
H	5.20495900	1.51350800	-2.54255100
C	2.56347500	1.28989900	-4.20058000
H	2.12005400	1.79027600	-5.06736300
H	3.63581900	1.19792600	-4.35638000
H	2.38160400	1.88489500	-3.30038300
C	4.55496500	1.44257000	0.19815800
H	5.30175400	0.92578900	-0.38688300
C	4.28731500	0.97650600	1.49031500
C	4.96364600	-0.31098400	1.92986900
H	5.95072800	-0.36695500	1.46624600
H	5.13588200	-0.31451800	3.00405000
C	4.15747600	-1.52702300	1.50209700
C	4.33282000	-2.00236700	0.19894300
H	5.07923800	-1.55465600	-0.44634100
C	3.57595200	-3.02790300	-0.33146200
O	3.80660500	-3.47526000	-1.60896600

C	3.16589000	-2.73831200	-2.65902000
H	3.70477400	-2.98348600	-3.57433200
H	3.25026200	-1.66354700	-2.48497300
C	1.70491700	-3.14495900	-2.81366500
H	1.64101600	-4.23138000	-2.88532700
H	1.11254500	-2.82047400	-1.95705200
C	2.59870200	-3.64024900	0.46867300
O	1.86326000	-4.62591500	-0.11041600
C	0.87041000	-5.27289100	0.66806000
H	1.30949000	-5.79492700	1.52463300
H	0.40253100	-5.99993800	0.00757100
H	0.11477700	-4.56582700	1.02317600
C	-3.95593000	4.25144700	2.05022000
H	-4.82727200	4.58406700	1.47719000
H	-3.79342400	4.92675500	2.88767700
H	-4.14286700	3.24301400	2.43330000
C	2.44478700	-3.20334500	1.77621000
H	1.70846400	-3.67509200	2.41010700
C	3.20226400	-2.15309800	2.30781400
C	2.90975000	-1.75268500	3.74498200
H	2.73597500	-2.66382000	4.32172700
H	3.77973400	-1.27975400	4.19426600
C	1.68836900	-0.86273600	3.88701700
C	0.42844500	-1.46468100	3.97047300
H	0.33371600	-2.54316900	3.96719300
C	-0.74542000	-0.73707700	4.04907500
O	-1.92732500	-1.41525100	4.14694000
C	-2.96427200	-1.08345000	3.20864000
H	-2.54477500	-0.57688500	2.33747100
H	-3.69294500	-0.42044600	3.67779500
C	-3.60972100	-2.39444300	2.79367800
H	-2.86456000	-3.05375700	2.34693500
H	-4.04015800	-2.89630400	3.66046100
C	-0.67444500	0.66587000	4.09336100
C	-1.81210800	2.75225600	4.31374100
H	-1.17299200	3.08899700	5.13598900
H	-2.83478100	3.06251000	4.51235900
H	-1.47333800	3.19826900	3.37387600
C	-3.03886900	-5.16897400	-0.43768100
H	-3.70238900	-5.45697500	-1.25955400
H	-2.90839800	-6.01698600	0.23153000
H	-2.06591300	-4.87679700	-0.84749200
O	-1.84967300	1.33412900	4.23343900
C	0.56991500	1.27086800	4.00163100
H	0.63667700	2.34840600	4.02032500
C	1.75297800	0.53403700	3.88580800
C	-3.47758200	-1.17439300	-3.58236100
H	-4.13193100	-0.44162200	-4.04860100
H	-3.64778000	-2.11035700	-4.11907600
C	-2.02061400	-0.78303100	-3.75541100
C	-1.06548300	-1.80294300	-3.80820800
H	-1.37505500	-2.84051800	-3.77933200
C	0.28894800	-1.55364100	-3.91454200
O	1.17683600	-2.59286800	-4.03031900
C	0.73344300	-0.22436100	-3.97630900
O	2.07902800	-0.03452200	-4.05889300
C	-0.20710600	0.79506400	-3.94475200
H	0.12076400	1.82273800	-4.00269000
C	-1.57870200	0.53978600	-3.83461000
C	-2.51394900	1.73572400	-3.79908900
H	-2.11910000	2.49505800	-4.47851900
H	-3.48955000	1.46569200	-4.19658000
C	-2.66075000	2.36404400	-2.42509300
C	-1.69219100	3.29843500	-2.03634100
H	-0.90011000	3.52362400	-2.73440700
C	-1.70912400	3.92695500	-0.80248300

O	-0.78099800	4.81811700	-0.35776100
C	-2.77341200	3.64207500	0.07716700
O	-2.77555400	4.30859300	1.26726700
C	-3.73181700	2.71791100	-0.30553000
H	-4.54323900	2.48991600	0.37015500
C	-3.68865400	2.05255700	-1.53818400
C	-4.75613800	1.00991600	-1.81771500
H	-4.99077200	0.98314100	-2.87993800
H	-5.67699600	1.32284200	-1.32041900
C	-4.40728900	-0.38425200	-1.31977700
C	-4.65079100	-0.68351900	0.02485100
H	-5.08466900	0.06226100	0.67986200
C	-4.36996000	-1.91640300	0.58102300
O	-4.69833400	-2.15298100	1.89376600
O	-3.60387200	-4.13506200	0.34959000
C	-3.83764600	-2.92643900	-0.23826200
C	-3.59132100	-2.63935300	-1.57167600
H	-3.18111900	-3.40495000	-2.21397400
C	-3.85532200	-1.38182300	-2.12654200
H	2.04539500	4.25004400	-2.10597400
H	0.98854800	3.09206400	-1.26839100

Cartesian coordinates of the optimized geometries for **3** using B3LYP-D3/def2-TZVP.

O	4.72737500	-3.56269900	7.22242300
O	12.70065000	-2.38800800	8.22895300
O	7.70871100	3.99302200	7.56536800
O	9.37079100	3.97012600	5.88628800
O	4.25735900	-2.32186500	5.26702900
O	12.20880900	-3.63539300	6.28310600
C	6.08917000	-0.60883600	9.84214800
C	6.57001500	-1.92655400	9.89624400
C	6.06121200	-2.86719700	9.00528000
H	6.41947500	-3.88824300	9.02443900
C	5.10308200	-2.53627900	8.05772000
C	4.60299000	-1.23950600	8.00716300
H	3.86968200	-0.94415200	7.27242200
C	5.10109100	-0.30677800	8.90523500
H	4.71255900	0.70360200	8.86046000
C	7.65249800	-2.38637700	10.85986200
H	7.63876800	-1.78563900	11.76622900
H	7.41710700	-3.40572300	11.17314400
C	9.03451600	-2.38674500	10.23006500
C	9.92840500	-1.30785600	10.31916200
C	11.14211100	-1.37971400	9.64125400
H	11.84553300	-0.55876700	9.69096400
C	11.48706700	-2.48050000	8.87024900
C	10.62017200	-3.56507200	8.79107300
H	10.84982700	-4.42959600	8.18757800
C	9.41690000	-3.49778900	9.47878700
H	8.74221300	-4.34275400	9.41183200
C	9.63294600	-0.03445200	11.09543800
H	8.95823100	-0.23920500	11.92334000
H	10.56522500	0.31056600	11.54768000
C	9.08939500	1.07644000	10.21544300
C	7.71953900	1.31597900	10.02455700
C	7.32657500	2.31577100	9.13952500
H	6.27634000	2.51721100	8.97254600
C	8.24935600	3.07122500	8.43085900
C	9.60967100	2.85815700	8.62609400
H	10.35400200	3.41653500	8.07926100
C	9.99960700	1.87158100	9.51994400
H	11.06002500	1.70607100	9.66806700
C	6.62394600	0.51629900	10.71026700
H	6.96911300	0.13562100	11.66850600

H	5.80027600	1.19629700	10.93705000
C	7.93370100	1.06165100	3.25744100
C	9.30794100	1.27679800	3.44570800
C	9.72030100	2.27520000	4.32340100
H	10.77427100	2.45808900	4.48819900
C	8.81233200	3.05272500	5.02739800
C	7.44814700	2.86390700	4.83446200
H	6.71489400	3.44001300	5.37789200
C	7.03902600	1.87865000	3.94782900
H	5.97561100	1.73206600	3.80149800
C	7.36877500	-0.04490500	2.38555300
H	8.03903800	-0.26821700	1.55884800
H	6.44290000	0.31454500	1.93146900
C	7.04972900	-1.30716500	3.17071700
C	7.92340700	-2.40200100	3.26732100
C	7.52050400	-3.50050700	4.02630100
H	8.17947500	-4.35731100	4.09918600
C	6.31605300	-3.54087000	4.71413900
H	6.07033900	-4.39686200	5.32343000
C	5.46938100	-2.44095200	4.62719000
C	5.83486400	-1.35186300	3.84903200
H	5.14678000	-0.51838500	3.79375800
C	9.30489100	-2.43196900	2.63721300
H	9.32915600	-1.83816200	1.72661500
H	9.52114900	-3.45782100	2.33139400
C	10.39644100	-1.98542800	3.59695300
C	10.90216900	-0.67665800	3.64078300
C	11.89652600	-0.38628600	4.57476800
H	12.30432900	0.61678500	4.61142200
C	12.37729000	-1.32134200	5.47986000
H	13.11649800	-1.03426500	6.21197500
C	11.85246400	-2.60867100	5.43970300
C	10.88785600	-2.92871000	4.49493200
H	10.51037300	-3.94291200	4.48376200
C	10.38779300	0.45191500	2.76484900
H	10.03479200	0.07077400	1.80966300
H	11.22380900	1.11484100	2.53238600
C	3.83617600	-3.31695000	6.16494600
H	2.86906900	-2.96555500	6.53297400
H	3.72622600	-4.28300700	5.66574900
C	8.54714600	4.74146900	6.72280900
H	7.86660500	5.36934700	6.14228700
H	9.23991200	5.36050700	7.29838400
C	13.10390300	-3.39775700	7.33918200
H	14.07748900	-3.06708000	6.96901200
H	13.19582900	-4.36167500	7.84605200

Cartesian coordinates of the optimized geometries for CHCl₃@3 using B3LYP-D3/def2-TZVP.

O	0.81620400	4.54577600	-0.49867300
O	0.89920600	-1.79295600	4.19082800
O	1.04445800	-2.68450700	-3.63943500
O	-0.79086400	-3.74462900	-2.59303100
O	-0.99568600	4.07713900	-1.94342500
O	-0.98574500	-0.40185600	4.50778400
C	3.55065200	1.51693100	-1.38345900
C	3.44033600	2.05386400	-0.08998000
C	2.53383800	3.08800200	0.13147700
H	2.39662900	3.48647800	1.12832400
C	1.74771600	3.60730500	-0.88852900
C	1.92969800	3.15848100	-2.19047900
H	1.34074800	3.54221600	-3.01010100
C	2.82933700	2.12438000	-2.41148200
H	2.94118300	1.74821200	-3.42180600
C	4.26987800	1.56601900	1.09511600

H	5.19380600	1.11420000	0.74101700
H	4.56878400	2.44489000	1.67065500
C	3.51958600	0.62359100	2.01686700
C	3.48096300	-0.76894200	1.83577200
C	2.61058900	-1.52317400	2.61904400
H	2.52897100	-2.59172600	2.46676900
C	1.79037600	-0.94002200	3.57579600
C	1.90221400	0.41959500	3.83749200
H	1.28532200	0.90688000	4.57748700
C	2.76646200	1.17293300	3.05462900
H	2.82298300	2.24045900	3.23365000
C	4.35151100	-1.50788700	0.82293100
H	5.24736300	-0.92854800	0.60880000
H	4.69814200	-2.42837300	1.29736400
C	3.62060500	-1.87350500	-0.45487200
C	3.53985800	-1.02389700	-1.57095600
C	2.68735500	-1.36974200	-2.61673300
H	2.57232500	-0.70898000	-3.46599200
C	1.92636000	-2.53134300	-2.59110900
C	2.08330400	-3.43037300	-1.54379300
H	1.51340400	-4.34639200	-1.49268400
C	2.92897300	-3.08447900	-0.49858800
H	3.02019000	-3.76896900	0.33681700
C	4.34633700	0.26612200	-1.70441400
H	5.24563300	0.20798700	-1.09517000
H	4.69033900	0.33227300	-2.73877100
C	-3.52666200	-0.64652800	-1.99115000
C	-3.45674900	-1.74958400	-1.12099200
C	-2.55105900	-2.76992900	-1.40161200
H	-2.44971200	-3.60887800	-0.72644600
C	-1.71157200	-2.72610000	-2.50809200
C	-1.83232400	-1.68196700	-3.41656200
H	-1.19114100	-1.60733400	-4.28205000
C	-2.74200800	-0.67025800	-3.14383500
H	-2.80829200	0.15902400	-3.83785600
C	-4.33908100	0.60338300	-1.70117200
H	-5.24957300	0.36154600	-1.15717800
H	-4.66319200	1.03214300	-2.65147200
C	-3.54473200	1.67221700	-0.95639700
C	-3.62626500	1.86926900	0.43408500
C	-2.89427400	2.91746800	0.99123200
H	-2.97089400	3.09995400	2.05638800
C	-2.02277400	3.70535800	0.25285300
H	-1.41900400	4.44854000	0.75095800
C	-1.88760000	3.44855600	-1.10575000
C	-2.67851900	2.47173000	-1.69832800
H	-2.56814300	2.31202800	-2.76277800
C	-4.39496500	0.95294700	1.37028400
H	-5.28517900	0.55672300	0.88728200
H	-4.75069900	1.54519300	2.21572000
C	-3.54325300	-0.18426500	1.92631500
C	-3.55836500	-1.48956800	1.40299700
C	-2.77827800	-2.45809900	2.03425900
H	-2.80357900	-3.47451800	1.66030200
C	-1.92221400	-2.16818100	3.08676200
H	-1.27942800	-2.93977300	3.48316200
C	-1.85336100	-0.85778900	3.54263000
C	-2.69215400	0.10278400	2.99064900
H	-2.63247000	1.10872600	3.38389300
C	-4.30602900	-1.88006800	0.14052500
H	-5.22602700	-1.30903200	0.03784000
H	-4.61002700	-2.92489900	0.22899900
C	-0.11141100	5.04349400	-1.42927500
H	0.38657100	5.46033500	-2.30707500
H	-0.65018500	5.82860300	-0.89426800
C	0.14224700	-3.76138100	-3.64637000

H	-0.35493800	-3.70355600	-4.61711900
H	0.65915100	-4.71808400	-3.54531800
C	-0.05475100	-1.28387800	5.08758300
H	-0.54885600	-2.16567200	5.50095700
H	0.41488600	-0.70664900	5.88692100
C	-0.51071600	-0.01199900	-0.00196200
H	-1.59265000	-0.04060700	-0.01732400
Cl	0.00019300	1.11732700	1.26187700
Cl	0.08587800	-1.64229500	0.34424500
Cl	0.05713500	0.53310600	-1.58767200

Cartesian coordinates of the optimized geometries for **4** using B3LYP-D3/def2-TZVP.

N	-1.49931100	2.06769900	-2.63954200
N	-1.84149600	3.86701800	-1.39511300
C	-2.67498400	1.91943000	-1.94642300
C	-2.91561400	3.03262400	-1.17397100
C	-4.04977000	3.30018500	-0.23101400
H	-4.03582800	4.33085700	0.11723700
H	-4.98946400	3.12586900	-0.75220000
C	-1.01697400	3.23633900	-2.29355900
C	0.28053900	3.77761700	-2.83417700
H	0.67550700	4.54445300	-2.16787200
H	-4.36455800	1.47892200	0.73628900
C	0.12114800	4.38978900	-4.24728900
H	-0.18574400	3.57311900	-4.91079800
C	-0.97014200	5.46244500	-4.26929100
H	-0.72300800	6.28343700	-3.59004500
H	-1.07001300	5.88414900	-5.27114600
H	-1.94344800	5.06214300	-3.97942300
C	1.45401400	4.95561600	-4.73921300
H	1.79161300	5.76865300	-4.09004200
H	2.23284400	4.19281100	-4.74983600
H	1.35272300	5.35305400	-5.75125800
C	2.30126700	2.65390000	-1.97403500
N	1.25688700	2.70323200	-2.83449700
O	2.64548300	3.60157700	-1.26087100
H	0.98314300	1.82439500	-3.25401500
C	-3.45815700	0.67231900	-1.97658300
N	-2.97737700	-0.25532600	-2.83791000
O	-4.45247500	0.49674500	-1.26544600
H	-2.07733600	-0.05197900	-3.25287100
C	-3.41514800	-1.63908300	-2.83824300
H	-4.27920700	-1.68349300	-2.17508600
C	-2.29617500	-2.48845100	-2.29424400
N	-1.04246800	-2.31932800	-2.63808900
C	-0.32602500	-3.26353200	-1.94538300
N	-2.42985100	-3.51894700	-1.39700700
C	-5.02139400	-1.22241100	-4.74620300
H	-5.89606000	-1.34608900	-4.10131200
H	-4.75868700	-0.16433300	-4.75171700
H	-5.30805800	-1.50801400	-5.76039500
C	-3.85993700	-2.08618800	-4.25227800
H	-2.99895700	-1.93779300	-4.91391500
C	-4.23339600	-3.57004800	-4.27508400
H	-5.06912900	-3.77197100	-3.59870200
H	-4.54310800	-3.87020300	-5.27778800
H	-3.39705100	-4.20751200	-3.98188900
C	-1.16983000	-4.03105500	-1.17539100
C	-0.83334100	-5.14953200	-0.23543400
H	-1.73235800	-5.65459000	0.11132400
H	-0.21181900	-5.87386200	-0.75894200
H	0.89918400	-4.50920900	0.73239000
C	1.14539400	-3.31971100	-1.97354300
N	1.71199800	-2.44187700	-2.83442200

O	1.79159700	-4.09403500	-1.26080300
H	1.08860000	-1.76330300	-3.25191900
C	3.13091900	-2.13561400	-2.83348400
H	3.59549800	-2.85904300	-2.16340200
C	3.74357500	-2.30970300	-4.24440600
H	3.19575100	-1.63355600	-4.91063700
C	3.56035500	-3.74666400	-4.73487900
H	4.08660200	-4.44776300	-4.08084600
H	2.50857800	-4.03275000	-4.75214200
H	3.96132100	-3.86219700	-5.74402900
C	5.22080400	-1.91025800	-4.26241000
H	5.80254200	-2.53718600	-3.58025200
H	5.63841800	-2.03883800	-5.26274900
H	5.36732400	-0.86757600	-3.97396300
C	3.31060900	-0.73989600	-2.29626800
N	2.53504900	0.25995000	-2.63914400
C	2.99266200	1.35358800	-1.94693900
N	4.27089700	-0.33766000	-1.40118200
C	4.08079600	1.00866900	-1.17848600
C	4.87797300	1.85907600	-0.23611800
H	5.76529300	1.33437300	0.11164300
H	5.19334400	2.76150100	-0.75702700
H	3.45544200	3.03699100	0.73225800
C	3.80487000	1.38220100	1.89504000
N	4.10427500	2.28463600	0.92407100
O	4.28553100	0.25360700	1.91287300
C	-3.10340100	2.60545400	1.89995300
N	-4.03480500	2.41610300	0.92866200
O	-2.36539400	3.58492400	1.91848500
C	-0.70765500	-3.99434600	1.90186200
N	-0.07635100	-4.69721200	0.92523000
O	-1.92592100	-3.85225400	1.92489100
C	1.61842200	-2.23488900	5.03605100
C	2.04449700	-3.42852800	4.47180600
C	1.32353300	-4.00816700	3.43165900
C	0.15862600	-3.40040000	2.96815000
C	-0.26340900	-2.19827500	3.53503600
C	0.46544700	-1.60197100	4.55787600
H	2.17615400	-1.78699900	5.84924200
H	2.93779800	-3.91336700	4.84498900
H	1.65050000	-4.94894100	3.00660900
C	1.13436300	2.51141400	5.04481400
C	1.95702500	3.47661900	4.48248800
C	2.81192500	3.14407800	3.43565700
C	2.85940000	1.83410300	2.96400400
C	2.02644900	0.86850200	3.52789700
C	1.15275900	1.19959800	4.55760900
H	0.47498200	2.76821000	5.86488200
H	1.93864700	4.49013200	4.86310700
H	3.46548300	3.89667400	3.01214600
C	-2.74566800	-0.27612400	5.04588300
C	-3.99319500	-0.04484600	4.48475400
C	-4.13342300	0.86374300	3.43956000
C	-3.02242700	1.55958200	2.96755300
C	-1.76921300	1.31924800	3.52997900
C	-1.61882900	0.39562700	4.55836100
H	-2.63784000	-0.97714800	5.86443100
H	-4.86160900	-0.56782000	4.86525300
H	-5.11228300	1.05505300	3.01751500
P	-0.00051700	-0.00251700	5.29154400
H	-0.92464900	1.87491100	3.14775700
H	-1.17246000	-1.75036000	3.15932800
H	2.08589400	-0.14063300	3.14524700
C	-3.65915100	-3.98023100	-0.76398400
H	-4.39995000	-3.18609000	-0.79960500
H	-4.05376400	-4.85652700	-1.28016100

H	-3.45389900	-4.20858800	0.27939100
C	-1.62651100	5.16250400	-0.76307500
H	-0.56967600	5.41162100	-0.80616700
H	-2.19455900	5.94031200	-1.27550600
H	-1.91940400	5.09774600	0.28212300
C	5.29220000	-1.16617800	-0.77259600
H	4.99543100	-2.20920200	-0.83390100
H	6.25217800	-1.04198900	-1.27610000
H	5.37081900	-0.89267400	0.27711300
O	-0.00090400	-0.00195100	6.77593100

Cartesian coordinates of the optimized geometries for $\uparrow\text{CHCl}_3@4$ using B3LYP-D3/def2-TZVP.

N	-1.48333900	2.05695100	-2.65791000
N	-1.80886400	3.85019300	-1.40182300
C	-2.64996100	1.90555800	-1.94726500
C	-2.87602900	3.01264600	-1.16360800
C	-3.99457800	3.27723900	-0.20152700
H	-3.97189300	4.30575700	0.15205900
H	-4.94133800	3.10798500	-0.71197300
C	-0.99828500	3.22704300	-2.31575800
C	0.28775700	3.77422100	-2.87619700
H	0.68567000	4.54828200	-2.22047900
H	-4.27182500	1.44596500	0.75925300
C	0.10401500	4.37539700	-4.29042700
H	-0.20465400	3.55221400	-4.94528600
C	-0.99702500	5.43804100	-4.30336500
H	-0.74714400	6.26544900	-3.63291100
H	-1.11437200	5.85236800	-5.30631200
H	-1.96247300	5.03131400	-3.99702100
C	1.42496800	4.95039200	-4.80328800
H	1.76149500	5.77259900	-4.16515800
H	2.21171700	4.19583100	-4.81675500
H	1.30726300	5.33828300	-5.81718500
C	2.29138300	2.64420100	-1.99011800
N	1.27239600	2.70861700	-2.88116100
O	2.62307300	3.58305400	-1.26200800
H	1.01423600	1.83810500	-3.32621600
C	-3.44450400	0.66770200	-1.98677400
N	-2.99217000	-0.24181700	-2.88385800
O	-4.42169400	0.48197300	-1.25715200
H	-2.10970900	-0.02592300	-3.32821000
C	-3.41642100	-1.62894600	-2.88405300
H	-4.28964900	-1.67747600	-2.23406600
C	-2.29874200	-2.46563100	-2.31985600
N	-1.04284600	-2.30130800	-2.66244600
C	-0.32911200	-3.23658500	-1.95207800
N	-2.43368100	-3.47820700	-1.40492200
C	-4.99682900	-1.24204200	-4.81970300
H	-5.88138800	-1.37530600	-4.19039300
H	-4.74827000	-0.18057700	-4.82463700
H	-5.26143900	-1.53538400	-5.83766600
C	-3.83355500	-2.08898100	-4.30165600
H	-2.96393400	-1.93568300	-4.95089900
C	-4.18960400	-3.57704600	-4.31930500
H	-5.03330300	-3.78312100	-3.65402400
H	-4.48079200	-3.88744500	-5.32434300
H	-3.35067700	-4.20276100	-4.00875200
C	-1.17524300	-3.98538400	-1.16805900
C	-0.84482000	-5.08769300	-0.20742000
H	-1.74673000	-5.58178600	0.14681600
H	-0.22638300	-5.82262800	-0.72013700
H	0.87998000	-4.41037400	0.74972700
C	1.13982000	-3.30930300	-1.99008900

N	1.70640300	-2.46111800	-2.88214200
O	1.78501700	-4.06707900	-1.26134100
H	1.08167300	-1.80213000	-3.32729900
C	3.12180900	-2.14263100	-2.87710500
H	3.59139600	-2.87072900	-2.21613900
C	3.73774200	-2.29350300	-4.28861900
H	3.18788800	-1.61163200	-4.94749200
C	3.56481100	-3.72485300	-4.79870900
H	4.09761500	-4.43057400	-4.15501000
H	2.51542200	-4.01949900	-4.81889900
H	3.96588500	-3.82326600	-5.80957300
C	5.21258900	-1.88523500	-4.29635600
H	5.79571300	-2.51992200	-3.62245900
H	5.63363900	-1.99606600	-5.29730700
H	5.35251300	-0.84643400	-3.99122700
C	3.29098800	-0.75286900	-2.32212100
N	2.51733600	0.25073800	-2.66334800
C	2.96787200	1.33802200	-1.95373500
N	4.23654400	-0.35956900	-1.40963700
C	4.04185600	0.98298800	-1.17189200
C	4.82829200	1.82235500	-0.21088700
H	5.70989500	1.29201400	0.14228300
H	5.15085400	2.72808500	-0.72191600
H	3.37872400	2.97341000	0.75097100
C	3.79097500	1.35467500	1.94533700
N	4.04583000	2.23826100	0.94499300
O	4.30147000	0.23967300	1.98363300
C	-3.07089900	2.60827000	1.95247000
N	-3.96617200	2.39044200	0.95381600
O	-2.35854500	3.60620400	1.98977000
C	-0.72428900	-3.96400600	1.95198500
N	-0.08942200	-4.62183300	0.94698200
O	-1.94527800	-3.85274700	1.99669100
C	1.63375500	-2.22278200	5.07213700
C	2.06433200	-3.40229500	4.48262800
C	1.33057800	-3.97744300	3.44860700
C	0.14650400	-3.38212300	3.02030400
C	-0.28123000	-2.19613800	3.61458600
C	0.46171500	-1.60029700	4.62690300
H	2.20600700	-1.77490100	5.87521300
H	2.97283700	-3.87841400	4.82950800
H	1.66585300	-4.90444800	3.00035500
C	1.11990900	2.51896300	5.08219100
C	1.92851500	3.48137300	4.49557700
C	2.78695900	3.13552300	3.45553900
C	2.85470500	1.81514400	3.01807100
C	2.03815000	0.85229600	3.60837300
C	1.15752300	1.19558200	4.62745200
H	0.45255400	2.78799600	5.89179200
H	1.89463700	4.50397600	4.85000700
H	3.42484500	3.88854200	3.00947200
C	-2.73976800	-0.29558900	5.08068800
C	-3.97837000	-0.07495500	4.49635400
C	-4.10995100	0.84539500	3.45994000
C	-3.00078200	1.56589700	3.02331500
C	-1.75773800	1.33905400	3.61175000
C	-1.61339200	0.40130200	4.62756100
H	-2.63763000	-1.01184200	5.88666800
H	-4.84617200	-0.61765600	4.84961700
H	-5.08174600	1.02277800	3.01607900
P	0.00164100	-0.00139400	5.36725900
H	-0.91457900	1.90631200	3.24838000
H	-1.19837400	-1.75360400	3.25690300
H	2.10566400	-0.16096300	3.24311800
C	-3.65790800	-3.90863400	-0.74106500
H	-4.40622100	-3.12623500	-0.82947200

H	-4.04308600	-4.82164400	-1.19678400
H	-3.44804200	-4.06918700	0.31469800
C	-1.57470400	5.12923100	-0.74339400
H	-0.52670400	5.39701500	-0.84317100
H	-2.18469900	5.91241400	-1.19559900
H	-1.80736200	5.02823400	0.31480900
C	5.23117500	-1.19844000	-0.75241000
H	4.94185200	-2.24060500	-0.85045600
H	6.21292800	-1.05971700	-1.20747600
H	5.26207000	-0.94475600	0.30526800
O	0.00090400	-0.00097500	6.85179500
C	-0.00289100	-0.00564200	-0.05581700
H	-0.00534900	-0.00534100	-1.14143800
Cl	-1.53018200	-0.72852500	0.50061300
Cl	0.13619000	1.67905000	0.49873900
Cl	1.38823800	-0.96714700	0.49539000

Cartesian coordinates of the optimized geometries for **5** using B3LYP-D3/def2-TZVP.

C	2.46278100	2.84982900	-2.62830900
H	3.26096100	3.23883300	-1.99632700
C	1.11699800	3.15440100	-2.02170900
N	0.00806700	2.61092600	-2.45192000
C	-1.00317200	3.10464600	-1.65649000
C	-0.49205300	3.97784300	-0.72436800
N	0.86928600	4.00204300	-0.96530800
C	1.84469900	4.67465600	-0.10652700
H	1.54486700	5.71728600	0.00761100
H	2.80031000	4.67214100	-0.62758500
C	-1.14613600	4.75883700	0.35943900
H	-2.22341900	4.65839000	0.26324300
H	-0.88142200	5.81893400	0.30224900
H	-0.84346100	4.40003800	1.34640700
C	-2.38548100	2.60074600	-1.75660300
O	-3.30634800	3.02224800	-1.05795300
N	2.64068500	1.40641100	-2.64651200
H	1.90173900	0.85120700	-3.05693000
C	1.97072100	4.01083100	1.24850800
C	2.28565900	2.65397400	1.33840000
H	2.49717300	2.08910700	0.44122800
C	2.34550000	2.02561800	2.57027700
C	2.09916300	2.73078300	3.75173800
C	1.81147900	4.08918600	3.65967900
H	1.62166500	4.65939900	4.56195800
C	1.74507100	4.72226200	2.42069200
H	1.49668700	5.77672000	2.37116500
C	2.61436500	3.46486800	-4.03730000
H	1.84685100	3.00533300	-4.67001300
C	3.99393800	3.14818200	-4.61545300
H	4.78197400	3.58631300	-3.99606700
H	4.09102900	3.55822100	-5.62296700
H	4.16940200	2.07340000	-4.66582500
C	2.36753100	4.97485500	-3.99880300
H	3.08473100	5.46772700	-3.33439800
H	1.36140300	5.21662700	-3.65163200
H	2.48984800	5.40931100	-4.99279100
C	-3.69940500	0.71307300	-2.63660400
H	-4.43877700	1.21311300	-2.01100900
C	-3.29260700	-0.60201000	-2.02147000
N	-2.26768100	-1.29346300	-2.44729400
C	-2.19561200	-2.41630200	-1.65157400
C	-3.21163400	-2.40813100	-0.72421100
N	-3.90827300	-1.23853800	-0.96698900
C	-4.97234900	-0.72412300	-0.10433900
H	-5.73167600	-1.49911200	0.00966700

H	-5.44159600	0.11058600	-0.62174800
C	-3.57386900	-3.36848500	0.35297500
H	-2.93664500	-4.24423300	0.27062400
H	-4.61910900	-3.68139000	0.27118700
H	-3.44283000	-2.92562600	1.34307400
C	-1.06838300	-3.36228900	-1.74718700
O	-0.98047500	-4.37589200	-1.05504000
N	-2.53905400	1.58955100	-2.65526900
H	-1.68947500	1.22784900	-3.06761600
C	-4.45487100	-0.29164000	1.25127200
C	-3.42490900	0.64583000	1.34494500
H	-3.03024100	1.10308100	0.44826600
C	-2.91173400	1.00635100	2.57895500
C	-3.41192200	0.44757900	3.75850400
C	-4.45419100	-0.46927400	3.66241400
H	-4.86122100	-0.91451600	4.56328600
C	-4.96849600	-0.83710600	2.42136000
H	-5.76519400	-1.57110400	2.36852400
C	-4.30242900	0.52592800	-4.04726000
H	-3.52072600	0.07794700	-4.67073300
C	-4.70607700	1.87450900	-4.64466200
H	-5.10903400	1.74317000	-5.65128900
H	-3.85709900	2.55581700	-4.70288200
H	-5.47665000	2.35268500	-4.03295800
C	-5.49361000	-0.43419700	-4.00324800
H	-6.28253600	-0.04327100	-3.35258400
H	-5.20948700	-1.42214300	-3.63634800
H	-5.92183100	-0.55945500	-4.99943000
C	1.22945300	-3.55346500	-2.61708300
H	1.16759400	-4.44017700	-1.98655700
C	2.16828800	-2.54132600	-2.01160500
N	2.25146800	-1.30936100	-2.44203800
C	3.18933600	-0.68159900	-1.65130900
C	3.69404300	-1.56191800	-0.72227600
N	3.03082900	-2.75186100	-0.95932600
C	3.12630800	-3.93346900	-0.10084800
H	4.17912400	-4.19555600	0.01129200
H	2.64519000	-4.75876300	-0.62198100
C	4.71049200	-1.39003700	0.35012200
H	5.13561400	-0.39359500	0.27242900
H	5.51403400	-2.12697700	0.25695700
H	4.26882700	-1.51129800	1.34209700
C	3.44405500	0.76751900	-1.75256600
O	4.27333900	1.35412800	-1.05835100
N	-0.10817000	-2.98320100	-2.63371300
H	-0.21672400	-2.06449600	-3.04204900
C	2.49047800	-3.71382100	1.25577200
C	1.15083700	-3.33261100	1.35068500
H	0.54956900	-3.24843300	0.45619000
C	0.57890400	-3.07427700	2.58483600
C	1.32260200	-3.19293900	3.76246300
C	2.64993200	-3.60001400	3.66562400
H	3.24540500	-3.70526400	4.56555900
C	3.22890200	-3.85555000	2.42473400
H	4.27125500	-4.14935500	2.37049700
C	1.68402400	-3.99057600	-4.02793600
H	1.67170400	-3.09408400	-4.65738700
C	0.71687400	-5.02258100	-4.60957200
H	1.02258100	-5.30847700	-5.61824300
H	-0.30057200	-4.63386700	-4.65828500
H	0.69999000	-5.92625000	-3.99362100
C	3.11393100	-4.53537800	-3.99149700
H	3.17980400	-5.40727200	-3.33287300
H	3.82676200	-3.78819200	-3.63778400
H	3.42987800	-4.85186600	-4.98724500
C	1.02248400	0.95705000	5.16349200

C	1.33257500	-0.39489700	5.16640600
C	-0.32319400	1.33927400	5.16759200
C	0.32906000	-1.36948000	5.16942500
H	2.37152500	-0.70576600	5.14116100
C	-1.33904800	0.39485400	5.16988300
H	-0.57279000	2.39472800	5.14318200
C	-0.99679800	-0.96172500	5.17284900
H	-1.78578100	-1.70615800	5.15149700
C	-2.79424400	0.80770900	5.09421100
C	2.10748300	2.01063700	5.08461500
C	0.69880200	-2.83679800	5.09629800
H	-0.45712000	-2.75875000	2.63577400
H	2.57165800	0.96630400	2.61612100
H	-2.09779000	1.72078200	2.62921100
H	1.39631400	-3.08443500	5.90030600
H	-0.19685400	-3.44249100	5.25584600
H	3.08062300	1.53774200	5.23908500
H	1.97786600	2.73805000	5.88989300
H	-2.87206600	1.88608300	5.25525000
H	-3.35964800	0.32644500	5.89607200

Cartesian coordinates of the optimized geometries for $\text{CHCl}_3@5$ using B3LYP-D3/def2-TZVP.

C	3.06801300	2.16872000	-2.51448300
H	3.92242000	2.34340700	-1.86151600
C	1.83220100	2.83259400	-1.96729300
N	0.62684700	2.51539100	-2.36584300
C	-0.23554700	3.36789000	-1.71307100
C	0.46797400	4.22930100	-0.90564800
N	1.79540300	3.87501100	-1.07066500
C	2.91209200	4.35684300	-0.24495800
H	2.81283300	5.43665600	-0.13860500
H	3.83113700	4.17236000	-0.79630400
C	-0.01194300	5.28503700	0.02442300
H	-1.01905200	5.57357800	-0.26279500
H	0.63450400	6.16531800	0.01068500
H	-0.05025800	4.91594900	1.05285000
C	-1.69576200	3.17869600	-1.77437600
O	-2.49593500	3.89443100	-1.17197000
N	2.85149700	0.73550100	-2.51911800
H	1.98095400	0.38838400	-2.89675900
C	2.94278500	3.68027400	1.10885400
C	3.43705900	2.38304900	1.24267500
H	3.88563400	1.86950100	0.40020800
C	3.33141900	1.71392600	2.45323900
C	2.73223100	2.31074300	3.56214700
C	2.29896600	3.62955100	3.44013500
H	1.86503300	4.13325500	4.29642400
C	2.40390100	4.30602300	2.23054400
H	2.05106600	5.32784100	2.15937200
C	3.42627200	2.69575600	-3.92744100
H	2.57762200	2.45359100	-4.57694100
C	4.67693700	1.99426900	-4.45958700
H	5.53752900	2.19562200	-3.81603000
H	4.91556800	2.34886900	-5.46452200
H	4.54050700	0.91371800	-4.50342700
C	3.61089200	4.21491300	-3.91930000
H	4.43160600	4.50283200	-3.25472800
H	2.70907800	4.73638800	-3.59359600
H	3.86020600	4.57565100	-4.91898500
C	-3.41736000	1.57605400	-2.52319700
H	-4.00053000	2.22808700	-1.87349700
C	-3.37417500	0.17410400	-1.97582000
N	-2.49815700	-0.71178800	-2.37562400

C	-2.80471700	-1.88434700	-1.72177700
C	-3.90163700	-1.70537000	-0.91350700
N	-4.25772700	-0.37827400	-1.07766000
C	-5.22788100	0.34839000	-0.24572100
H	-6.11373400	-0.27683500	-0.13562900
H	-5.53036000	1.23752300	-0.79448000
C	-4.57729800	-2.65053200	0.01399100
H	-4.33016100	-3.66666900	-0.28003600
H	-5.66221100	-2.52520300	0.00591600
H	-4.23314000	-2.50802100	1.04211600
C	-1.91269400	-3.05567300	-1.78209900
O	-2.13107300	-4.10247800	-1.17223900
N	-2.06945300	2.10883500	-2.52147500
H	-1.32990900	1.52977700	-2.89382900
C	-4.64946400	0.71059100	1.10543400
C	-3.77326900	1.78769100	1.23749200
H	-3.55736300	2.43555900	0.39557400
C	-3.13634400	2.02907400	2.44610700
C	-3.34924000	1.21023500	3.55462900
C	-4.27309100	0.17381100	3.43405800
H	-4.48868500	-0.45609300	4.28963600
C	-4.91564400	-0.07198600	2.22636600
H	-5.62297700	-0.88975700	2.15611300
C	-4.04710900	1.61967100	-3.93846500
H	-3.40979000	1.00536900	-4.58406500
C	-4.06488700	3.05251600	-4.47310100
H	-4.49239700	3.07943100	-5.47742400
H	-3.06096700	3.47494000	-4.51913000
H	-4.66872600	3.69902400	-3.83032000
C	-5.45449500	1.01833200	-3.93408200
H	-6.11612000	1.58299000	-3.26953400
H	-5.45492200	-0.02371600	-3.60998800
H	-5.88992900	1.05488600	-4.93441900
C	0.33416000	-3.75033600	-2.52831700
H	0.05819600	-4.58013400	-1.87824600
C	1.52190700	-3.00925600	-1.97464300
N	1.84886200	-1.80535600	-2.36974400
C	3.01708300	-1.48496900	-1.71401500
C	3.41162600	-2.52642300	-0.90911900
N	2.44239400	-3.49953000	-1.07749000
C	2.29957100	-4.70656400	-0.25044600
H	3.28307600	-5.16459500	-0.14707600
H	1.67557000	-5.40843200	-0.79865500
C	4.56548700	-2.63916700	0.02119200
H	5.32626100	-1.92225200	-0.27411000
H	4.99413900	-3.64371600	0.01962100
H	4.26775700	-2.40534600	1.04703400
C	3.58556300	-0.12674400	-1.77077700
O	4.60356300	0.20442700	-1.16323200
N	-0.80283500	-2.85142700	-2.53655400
H	-0.67001900	-1.92258300	-2.91171400
C	1.70432600	-4.39007500	1.10476300
C	0.33480700	-4.16574400	1.24292300
H	-0.33769100	-4.29924000	0.40341900
C	-0.18597900	-3.73406200	2.45423300
C	0.63559800	-3.50898400	3.55863600
C	1.99375800	-3.79525000	3.43215400
H	2.65096500	-3.66703500	4.28448700
C	2.52067000	-4.23217300	2.22236700
H	3.58135300	-4.43930100	2.14728100
C	0.62186000	-4.31937800	-3.94094600
H	0.83165900	-3.46018300	-4.58804300
C	-0.60191100	-5.06158000	-4.47931500
H	-0.40770600	-5.43953800	-5.48525900
H	-1.47612000	-4.41187800	-4.52287500
H	-0.85152900	-5.91289300	-3.83988600

C	1.85279100	-5.22847400	-3.93040400
H	1.69855400	-6.08454400	-3.26611700
H	2.75047200	-4.70128500	-3.60347800
H	2.04465200	-5.62304400	-4.92997400
C	0.01021700	-0.01237600	0.64734400
C	1.20952800	0.73150800	4.82256500
C	1.22310700	-0.65655500	4.82086900
C	-0.02421300	1.38852600	4.81619500
C	0.03714900	-1.39671000	4.82141800
H	2.17313800	-1.17899500	4.81645500
C	-1.21948600	0.68284200	4.81779100
H	-0.04641800	2.47247900	4.80771200
C	-1.17153800	-0.71420800	4.81642700
H	-2.09924200	-1.27506000	4.80941300
H	0.02024500	-0.02093300	-0.43791400
C	-2.55622900	1.40793000	4.82865400
C	2.50545200	1.52688100	4.83687100
C	0.07567000	-2.91679400	4.83456800
H	-1.24746600	-3.53508800	2.52882900
H	3.69150000	0.69528800	2.52345100
H	-2.43477500	2.85102400	2.51542200
H	0.68083900	-3.25046800	5.68213100
H	-0.93512600	-3.29532800	4.99936200
H	3.34100900	0.84299200	4.99888000
H	2.49133600	2.21554100	5.68651000
H	-2.38072500	2.47372200	4.98801100
H	-3.14626700	1.05405700	5.67878200
Cl	-1.47286400	-0.82261300	1.19157100
Cl	1.45023000	-0.87927200	1.21807000
Cl	0.03758200	1.67839000	1.18672400

Cartesian coordinates of the optimized geometries for CHCl_3 @5 using B3LYP-D3/def2-TZVP.

C	3.07061500	2.17124600	-2.54078000
H	3.92212800	2.34478200	-1.88327600
C	1.83452700	2.84039300	-2.00103300
N	0.63194900	2.54489600	-2.42092000
C	-0.23287400	3.37333600	-1.74327000
C	0.46790100	4.20668200	-0.90216500
N	1.79612500	3.85260700	-1.06978900
C	2.91056300	4.32689700	-0.23816700
H	2.81894300	5.40778700	-0.13267400
H	3.83142800	4.13605500	-0.78442600
C	-0.00754200	5.24644500	0.04927600
H	-1.03437500	5.50081500	-0.19725400
H	0.60784900	6.14829700	0.00340600
H	0.01456600	4.88197000	1.07928900
C	-1.69444500	3.17635500	-1.80345600
O	-2.49627100	3.89137200	-1.20111500
N	2.85181600	0.73698600	-2.54457100
H	1.96902900	0.39198800	-2.89564300
C	2.93200900	3.65456000	1.11845000
C	3.37499600	2.33873900	1.25120600
H	3.78866100	1.80476500	0.40352500
C	3.26464300	1.68173600	2.46774200
C	2.71023400	2.31012200	3.58294700
C	2.32603600	3.64378000	3.46057500
H	1.92619900	4.16932200	4.32035600
C	2.43838000	4.30787900	2.24481100
H	2.12418700	5.34216000	2.17127100
C	3.43818100	2.70122700	-3.94948100
H	2.58498800	2.48209600	-4.60092500
C	4.67493400	1.98233300	-4.48992400
H	5.53703200	2.15046400	-3.83888800

H	4.92563000	2.35200800	-5.48651200
H	4.51341100	0.90644500	-4.55572600
C	3.65205100	4.21643200	-3.92408600
H	4.48006600	4.48042400	-3.25838200
H	2.76115400	4.75056300	-3.58846800
H	3.90497500	4.58418600	-4.92028300
C	-3.41642000	1.57217400	-2.54158100
H	-3.99353700	2.22188500	-1.88389600
C	-3.37782400	0.16621900	-2.00431900
N	-2.52151000	-0.72719600	-2.42619700
C	-2.80629500	-1.89126600	-1.75022900
C	-3.87772600	-1.70186500	-0.90794000
N	-4.23454800	-0.37396700	-1.07277700
C	-5.20172000	0.35282200	-0.23856500
H	-6.09090800	-0.26870100	-0.13192600
H	-5.49996500	1.24510800	-0.78446500
C	-4.54035600	-2.63520000	0.04172200
H	-4.24359300	-3.65078400	-0.20428500
H	-5.62931900	-2.55685500	-0.00631000
H	-4.23881700	-2.43333800	1.07277200
C	-1.90519700	-3.05888100	-1.81165000
O	-2.12285700	-4.11024800	-1.20814300
N	-2.06548400	2.10110900	-2.54237100
H	-1.32431800	1.51014500	-2.89324400
C	-4.62868900	0.70950600	1.11682600
C	-3.71769500	1.75721700	1.24884300
H	-3.46816600	2.38615200	0.40188300
C	-3.09221500	1.99267000	2.46427600
C	-3.35040300	1.19496800	3.57906100
C	-4.30723000	0.18914400	3.45786000
H	-4.55662700	-0.42261400	4.31745800
C	-4.93979600	-0.04800300	2.24318100
H	-5.67394500	-0.84165600	2.17035400
C	-4.05881200	1.62746500	-3.94989800
H	-3.44254400	0.99958400	-4.60255500
C	-4.05587500	3.05915900	-4.48716900
H	-4.50742200	3.09350400	-5.48077300
H	-3.04340600	3.45676900	-4.55821500
H	-4.62781200	3.72132500	-3.83129900
C	-5.47800500	1.05472900	-3.92416800
H	-6.11841000	1.63495100	-3.25200900
H	-5.49442500	0.01388200	-3.59610000
H	-5.92656700	1.09708500	-4.91844500
C	0.34490200	-3.74872800	-2.54904100
H	0.07029500	-4.57325600	-1.89139200
C	1.54167600	-3.01204500	-2.00963600
N	1.88851800	-1.82380000	-2.43081400
C	3.03696100	-1.48829800	-1.75090700
C	3.40567100	-2.51036300	-0.90704100
N	2.43524000	-3.48358500	-1.07539900
C	2.28802200	-4.68474800	-0.24209800
H	3.26965500	-5.14735500	-0.13778200
H	1.66049800	-5.38643800	-0.78654200
C	4.53923200	-2.61573300	0.05006400
H	5.27860500	-1.86048900	-0.20009400
H	5.00700000	-3.60279600	0.01700500
H	4.20836700	-2.44023300	1.07692300
C	3.59754600	-0.12415600	-1.80854500
O	4.61771000	0.21065300	-1.20525100
N	-0.78937400	-2.84391000	-2.55239800
H	-0.64817600	-1.90663900	-2.90359800
C	1.69662600	-4.36491500	1.11450300
C	0.33519500	-4.09314600	1.24731200
H	-0.33436600	-4.18907800	0.40051000
C	-0.17875300	-3.66681000	2.46339000
C	0.64324500	-3.49417500	3.57745900

C	1.99125300	-3.82603000	3.45513500
H	2.64688100	-3.73830800	4.31390000
C	2.50982300	-4.25864300	2.24013400
H	3.56296100	-4.50195700	2.16630400
C	0.62206200	-4.33188500	-3.95704000
H	0.85234100	-3.48276500	-4.61012400
C	-0.61391500	-5.05361800	-4.49473900
H	-0.41816700	-5.45267900	-5.49225200
H	-1.47135100	-4.38357500	-4.55767400
H	-0.89034000	-5.88764300	-3.84371800
C	1.83341800	-5.26683600	-3.93170700
H	1.65670100	-6.11311000	-3.26019500
H	2.74010400	-4.75567200	-3.60377100
H	2.02233100	-5.67454600	-4.92656200
C	-0.00116400	-0.00233800	1.55025700
C	1.19851800	0.74054900	4.87213200
C	1.22138800	-0.64937900	4.86866000
C	-0.04156700	1.38958400	4.86833000
C	0.03914800	-1.39918000	4.86897100
H	2.17433800	-1.16592600	4.85558900
C	-1.23373100	0.67477500	4.86928500
H	-0.07054600	2.47311400	4.85388800
C	-1.17587600	-0.72384200	4.86631000
H	-2.09985500	-1.29029200	4.85135300
C	-2.57522100	1.39020600	4.86586600
C	2.48851900	1.54465100	4.87115800
C	0.09009600	-2.91848400	4.86532800
H	-1.23307400	-3.43165500	2.53469700
H	3.58410900	0.64962100	2.53829100
H	-2.36397500	2.79103300	2.53447000
H	0.70509800	-3.25581400	5.70403200
H	-0.91662100	-3.30535700	5.03511900
H	3.32739000	0.86723700	5.04221700
H	2.47187200	2.24615700	5.70998000
H	-2.40740700	2.45596800	5.03310100
H	-3.17392000	1.02793300	5.70611700
Cl	-1.45152400	-0.86077400	0.99535800
Cl	1.46885700	-0.82248600	0.98917600
Cl	-0.02505500	1.68697600	1.00799700
H	0.00074300	-0.00952000	2.62885500

Cartesian coordinates of the optimized geometries for $\text{†CHBrCl}_2@5$ using B3LYP-D3/def2-TZVP.

C	3.03859800	2.16273700	-2.47300400
H	3.88878500	2.32692000	-1.81196200
C	1.80245600	2.82946800	-1.93054100
N	0.59879600	2.49987000	-2.32381900
C	-0.26936500	3.35035100	-1.67683200
C	0.42955700	4.22322500	-0.87751800
N	1.76036900	3.87809300	-1.04194100
C	2.88173200	4.38703100	-0.23645400
H	2.76647700	5.46668100	-0.14425500
H	3.79514100	4.20975900	-0.79919000
C	-0.05762100	5.28238900	0.04425700
H	-1.07519600	5.54405100	-0.23174300
H	0.56884700	6.17652800	0.00663500
H	-0.07097600	4.92759500	1.07822500
C	-1.73000800	3.16016000	-1.75548800
O	-2.53879900	3.88824600	-1.17933600
N	2.80899800	0.73142900	-2.48604900
H	1.93914200	0.39401100	-2.87384500
C	2.94630900	3.73216400	1.12749700
C	3.48596700	2.45496500	1.28111400
H	3.94749300	1.94126800	0.44540400

C	3.39990700	1.79915700	2.50133200
C	2.77168100	2.38668200	3.59909400
C	2.30113700	3.69124500	3.45971000
H	1.84739000	4.19177900	4.30746800
C	2.38996300	4.35576100	2.24214200
H	2.00697900	5.36566400	2.15825100
C	3.41277800	2.68992800	-3.88185200
H	2.57080700	2.44832100	-4.54033100
C	4.66816500	1.98537500	-4.39855300
H	5.52154600	2.18866100	-3.74605200
H	4.91825900	2.33569300	-5.40214500
H	4.53153400	0.90479800	-4.43950100
C	3.60117200	4.20853500	-3.87567400
H	4.41458500	4.49657600	-3.20229600
H	2.69679700	4.73399500	-3.56367100
H	3.86438200	4.56490700	-4.87334900
C	-3.44849000	1.57082000	-2.55091000
H	-4.04232200	2.21358400	-1.90175200
C	-3.44562000	0.15358000	-2.04452300
N	-2.59785000	-0.74584300	-2.47286800
C	-2.92367500	-1.92226800	-1.83716400
C	-4.00963400	-1.73304900	-1.01544900
N	-4.33338100	-0.39322700	-1.14707900
C	-5.26526500	0.34389700	-0.28030900
H	-6.15964400	-0.26568300	-0.15340100
H	-5.56525700	1.24505400	-0.81058100
C	-4.69809600	-2.68271200	-0.10105600
H	-4.49512600	-3.69733200	-0.43147100
H	-5.77765200	-2.51853100	-0.07930500
H	-4.32622600	-2.58884400	0.92277900
C	-2.01853900	-3.08759100	-1.86485300
O	-2.24933500	-4.13694200	-1.26492200
N	-2.09236500	2.07982300	-2.49086100
H	-1.34996000	1.49811300	-2.85241700
C	-4.64788200	0.68245100	1.06081900
C	-3.78870700	1.77261000	1.19675900
H	-3.60835700	2.44532000	0.36617700
C	-3.12402300	1.99810100	2.39405000
C	-3.29667800	1.15380400	3.49072200
C	-4.19909200	0.09920500	3.36629300
H	-4.38284300	-0.55282900	4.21283500
C	-4.86572100	-0.13301200	2.16929300
H	-5.55972800	-0.96178800	2.09957800
C	-4.03250200	1.66439900	-3.98282300
H	-3.38235500	1.06162000	-4.62645900
C	-4.01819300	3.11237900	-4.47439000
H	-4.40896800	3.17396400	-5.49213800
H	-3.00943900	3.52590600	-4.47268500
H	-4.63803400	3.74559400	-3.83380300
C	-5.44555500	1.07968000	-4.03685500
H	-6.11758800	1.62648300	-3.36761600
H	-5.46430700	0.02635400	-3.75187400
H	-5.85549000	1.15819200	-5.04560700
C	0.26502300	-3.75699500	-2.51693500
H	-0.02062400	-4.57882300	-1.86024100
C	1.44510800	-3.01073500	-1.95341600
N	1.76940400	-1.80070500	-2.33291300
C	2.94774500	-1.49322300	-1.68652900
C	3.35079900	-2.54865200	-0.90516900
N	2.37647600	-3.51598400	-1.07435100
C	2.23842300	-4.72767100	-0.25290200
H	3.21613100	-5.20451100	-0.18385200
H	1.58437200	-5.41396500	-0.78531700
C	4.52292200	-2.68012500	-0.00128400
H	5.28700800	-1.97318500	-0.31158100
H	4.93608600	-3.69091500	-0.01401500

H	4.25118000	-2.44281500	1.03072800
C	3.53009300	-0.14053800	-1.73619000
O	4.54829100	0.17911900	-1.12323100
N	-0.87422400	-2.86309500	-2.55983300
H	-0.73499400	-1.93095000	-2.92404100
C	1.69300200	-4.40834800	1.12272800
C	0.33457800	-4.15066500	1.30599200
H	-0.36506700	-4.25630100	0.48365400
C	-0.13551300	-3.71790200	2.53815800
C	0.72792100	-3.51265600	3.61389100
C	2.07357700	-3.83027500	3.44183500
H	2.76289900	-3.71599600	4.27064700
C	2.54823300	-4.27818200	2.21463900
H	3.60031800	-4.51101900	2.10371400
C	0.57700700	-4.34482900	-3.91857800
H	0.77748500	-3.49201000	-4.57700400
C	-0.63118900	-5.11379400	-4.45382900
H	-0.42648100	-5.49890100	-5.45498400
H	-1.51631900	-4.48009700	-4.50745900
H	-0.86813200	-5.96222500	-3.80597300
C	1.82129800	-5.23474100	-3.88807700
H	1.67925200	-6.07930800	-3.20666100
H	2.71128800	-4.68815200	-3.57258800
H	2.01910700	-5.64713700	-4.87928400
C	0.22692000	0.02554100	0.66182600
C	1.27298700	0.77318400	4.84793300
C	1.31986900	-0.61461600	4.87788000
C	0.02391600	1.39773100	4.79678000
C	0.15225200	-1.38362300	4.85786100
H	2.28159700	-1.11465500	4.91234400
C	-1.15411700	0.66335300	4.77672200
H	-0.02515400	2.48048400	4.77018100
C	-1.07246300	-0.73166800	4.79907200
H	-1.98574300	-1.31507900	4.77753000
H	0.36814200	0.05248800	-0.41335000
C	-2.50600300	1.35946300	4.76535100
C	2.54707300	1.60500900	4.87667700
C	0.22559200	-2.90191200	4.90556500
H	-1.18796900	-3.49276100	2.65111200
H	3.79214200	0.79366700	2.58611800
H	-2.43863700	2.83369500	2.46543400
H	0.88349700	-3.20229700	5.72535200
H	-0.76639700	-3.29652100	5.13446900
H	3.39836900	0.94577900	5.05738800
H	2.49928000	2.29947600	5.72049900
H	-2.35303600	2.42836200	4.92759800
H	-3.09514700	0.99464200	5.61163200
Cl	1.58510100	-0.85540100	1.38045400
Cl	0.14418500	1.69008400	1.25759800
Br	-1.45842400	-0.90152000	0.98386100

Cartesian coordinates of the optimized geometries for CHBrCl_2 @5 using B3LYP-D3/def2-TZVP.

C	3.03896600	2.15746300	-2.49811100
H	3.88703800	2.31892000	-1.83334300
C	1.80199900	2.82644800	-1.95976900
N	0.60086800	2.51406200	-2.37110800
C	-0.26900200	3.34484200	-1.70431300
C	0.42638900	4.19709000	-0.87795200
N	1.75807000	3.85132800	-1.04251500
C	2.87912200	4.35891100	-0.23692400
H	2.76875500	5.43970400	-0.14915300
H	3.79248800	4.17506600	-0.79736000
C	-0.06100900	5.25129000	0.05158200

H	-1.07270100	5.52650600	-0.23322200
H	0.57421400	6.13981400	0.02644400
H	-0.08773600	4.89165200	1.08346600
C	-1.72985600	3.15158300	-1.78454500
O	-2.53963500	3.87727400	-1.20547000
N	2.80825200	0.72546400	-2.51709400
H	1.92535100	0.39400100	-2.88067100
C	2.94171300	3.71187800	1.13115600
C	3.48378200	2.43719200	1.29226300
H	3.94390500	1.91898400	0.45834400
C	3.39606100	1.78794100	2.51583900
C	2.76220700	2.38055000	3.60758400
C	2.29065600	3.68387000	3.46162600
H	1.83263400	4.18740100	4.30525300
C	2.38279100	4.34160600	2.24133800
H	1.99874100	5.35042800	2.15057700
C	3.41879000	2.69209200	-3.90235300
H	2.57331100	2.46896600	-4.56258000
C	4.66438300	1.97775400	-4.42890200
H	5.52012000	2.15794600	-3.77257800
H	4.92053000	2.34065000	-5.42658300
H	4.51160600	0.90022200	-4.48724600
C	3.62679800	4.20805300	-3.87758500
H	4.45273300	4.47605500	-3.21103500
H	2.73324300	4.73933200	-3.54462900
H	3.88027000	4.57631700	-4.87346200
C	-3.45058400	1.56637400	-2.57979300
H	-4.03848300	2.20500100	-1.92073500
C	-3.44764000	0.14522800	-2.08339900
N	-2.62070700	-0.75946500	-2.53952200
C	-2.90214400	-1.92363600	-1.86177700
C	-3.94619400	-1.72241100	-0.98552300
N	-4.28504000	-0.38748400	-1.12964000
C	-5.21014200	0.34687800	-0.25413700
H	-6.10652200	-0.26050500	-0.12854300
H	-5.50866900	1.25160800	-0.77893800
C	-4.59749000	-2.65397400	-0.02586900
H	-4.33768600	-3.67271700	-0.29818200
H	-5.68471900	-2.54552300	-0.03139100
H	-4.25027900	-2.47718500	0.99498100
C	-1.99800800	-3.09276400	-1.91403900
O	-2.22045500	-4.13986400	-1.30640800
N	-2.09175700	2.07168000	-2.52069700
H	-1.34817000	1.47930300	-2.86325300
C	-4.59527000	0.67769500	1.09036900
C	-3.68814000	1.72910000	1.21892300
H	-3.46186500	2.37247100	0.37657300
C	-3.04422900	1.95775300	2.42656700
C	-3.28271400	1.15089400	3.53963800
C	-4.22677400	0.13270600	3.41941900
H	-4.45941500	-0.48912900	4.27651400
C	-4.87562000	-0.09810200	2.21223300
H	-5.60411300	-0.89721000	2.14482500
C	-4.04801300	1.67327600	-4.00426500
H	-3.42045100	1.05654800	-4.65659800
C	-4.01025700	3.12032200	-4.49714900
H	-4.42205700	3.19024200	-5.50608200
H	-2.99222900	3.50961000	-4.51809000
H	-4.60018400	3.76866100	-3.84353900
C	-5.47426900	1.11922100	-4.03500900
H	-6.12592200	1.68959900	-3.36507300
H	-5.51259600	0.07037600	-3.73479400
H	-5.89444200	1.19262200	-5.03989300
C	0.27608300	-3.76756800	-2.57567200
H	-0.01574900	-4.58827900	-1.92007400
C	1.45069500	-3.02020900	-2.00115300

N	1.79749400	-1.82524600	-2.40370400
C	2.95055800	-1.50313300	-1.72286800
C	3.32200600	-2.53976000	-0.90011500
N	2.34703700	-3.50642600	-1.07505900
C	2.19441400	-4.70777200	-0.24342000
H	3.16512900	-5.19901000	-0.17170300
H	1.52894000	-5.38851400	-0.76885900
C	4.46817000	-2.66439100	0.03972300
H	5.22476900	-1.93445600	-0.23294900
H	4.90560800	-3.66536300	0.01444700
H	4.16309400	-2.46418400	1.07015500
C	3.52591600	-0.14538700	-1.76474100
O	4.53820700	0.17605200	-1.14108000
N	-0.86693400	-2.87458400	-2.63046100
H	-0.71821400	-1.93606900	-2.97533500
C	1.65625300	-4.37713300	1.13321700
C	0.30840900	-4.06680500	1.31033600
H	-0.38607600	-4.13642800	0.48034400
C	-0.15433000	-3.63254900	2.54460900
C	0.70784400	-3.48729100	3.63159700
C	2.04118500	-3.85501900	3.46494800
H	2.72758100	-3.78368400	4.30107600
C	2.50739800	-4.29834800	2.23299800
H	3.55096100	-4.56785600	2.12439500
C	0.60457700	-4.35917300	-3.97044500
H	0.82285000	-3.50989600	-4.62751100
C	-0.59791200	-5.12342400	-4.52546500
H	-0.37606700	-5.51455200	-5.52062100
H	-1.47792500	-4.48464000	-4.59927000
H	-0.85255900	-5.96756000	-3.87853700
C	1.84258400	-5.25689500	-3.91205500
H	1.68218700	-6.09624100	-3.22803300
H	2.72922100	-4.71355800	-3.58181700
H	2.05713400	-5.67600300	-4.89697500
C	0.11211500	-0.00127000	1.60687800
C	1.26368300	0.77919000	4.88371300
C	1.30863800	-0.61022900	4.90599400
C	0.01268800	1.40599700	4.85838000
C	0.13942800	-1.37960400	4.91519300
H	2.26964000	-1.11189900	4.90824000
C	-1.16792800	0.67182000	4.86305900
H	-0.03556800	2.48813000	4.82414700
C	-1.08732200	-0.72531800	4.89161000
H	-2.00186500	-1.30738300	4.88499600
C	-2.52014900	1.36440800	4.83198300
C	2.54136000	1.60591000	4.89064600
C	0.21421200	-2.89748100	4.93754000
H	-1.19837300	-3.36568000	2.65143100
H	3.79012500	0.78391200	2.60691700
H	-2.32485700	2.76430300	2.49356200
H	0.87828100	-3.21017000	5.74731100
H	-0.77620500	-3.29583000	5.16718000
H	3.38978500	0.94222200	5.06717100
H	2.50478400	2.30381900	5.73210700
H	-2.37176800	2.43406300	4.99230100
H	-3.12416700	1.00007900	5.66754000
Cl	1.65315800	-0.80710300	1.27785800
Cl	0.15715400	1.70717400	1.14762600
H	-0.08314000	-0.06331100	2.66551800
Br	-1.35344600	-0.91205500	0.70250300

Cartesian coordinates of the optimized geometries for **6** using B3LYP-D3/def2-TZVP.

C	1.81641300	3.30293800	-2.23303500
H	2.50079600	3.86757200	-1.59846500

C	0.42206200	3.35514000	-1.66100700
N	-0.51197100	2.49569800	-1.97371900
C	-1.61022800	2.81432100	-1.20428800
C	-1.33569900	3.90640500	-0.41443900
N	-0.03426500	4.25304700	-0.72529000
C	0.72053100	5.31173000	-0.06525900
H	0.11377400	6.21863700	-0.06137000
H	1.59642100	5.52493600	-0.67689100
C	-2.14991600	4.63487500	0.59389200
H	-3.12943800	4.16851400	0.65811300
H	-2.27843000	5.68698300	0.32097700
H	-1.67463800	4.60917800	1.57818100
C	-2.83346000	1.98965500	-1.23645300
O	-3.78433500	2.16433600	-0.47647000
N	2.27752200	1.92708300	-2.18767000
H	1.69196300	1.22383000	-2.61872400
C	1.13226800	4.95188700	1.34608100
C	1.55058100	3.66209300	1.64489000
H	1.59437400	2.91334700	0.86476300
C	1.90244700	3.29599900	2.94181100
C	1.85851600	4.26261400	3.94402300
H	2.12320100	3.99210300	4.95973500
C	1.46407600	5.56465900	3.65279600
H	1.43066600	6.30878100	4.43925800
C	1.09062900	5.90740000	2.35946400
H	0.75653900	6.91538000	2.13962600
C	1.88372700	3.87500700	-3.66848900
H	1.23846200	3.24434600	-4.29076500
C	3.31260000	3.81235100	-4.20943600
H	3.98419400	4.41738600	-3.59339700
H	3.35365000	4.19778900	-5.23040100
H	3.69525500	2.79163300	-4.21443500
C	1.34473200	5.30658200	-3.71309700
H	1.95403700	5.97000600	-3.09130500
H	0.31221200	5.36663900	-3.36418700
H	1.37433300	5.69651400	-4.73224900
C	-3.76205900	-0.07544400	-2.21789300
H	-4.58695900	0.23684200	-1.57545400
C	-3.10870100	-1.31092400	-1.65186400
N	-1.89744100	-1.68851200	-1.96667100
C	-1.62442100	-2.80324500	-1.20337100
C	-2.70742400	-3.11499700	-0.41458100
N	-3.65827100	-2.15955700	-0.72040800
C	-4.95462000	-2.03971500	-0.06297600
H	-5.43132500	-3.02114200	-0.05806000
H	-5.57878100	-1.39275400	-0.67762300
C	-2.93042500	-4.18714700	0.59092100
H	-2.03524100	-4.79988800	0.65547800
H	-3.77523400	-4.82577300	0.31536000
H	-3.14873100	-3.76477700	1.57561200
C	-0.29919700	-3.45250300	-1.24152500
O	0.02025100	-4.37683600	-0.49605600
N	-2.79921800	1.01020600	-2.18095200
H	-1.90193100	0.85520900	-2.62159300
C	-4.85636000	-1.50000700	1.34794900
C	-3.95226900	-0.49030600	1.65011100
H	-3.32232600	-0.07724300	0.87349200
C	-3.81824300	-0.00068200	2.94740500
C	-4.63669000	-0.52299700	3.94630600
H	-4.53982400	-0.15800900	4.96229600
C	-5.56467900	-1.51720100	3.65120200
H	-6.19523300	-1.91859700	4.43514900
C	-5.66816500	-2.01352700	2.35789800
H	-6.37186600	-2.80788500	2.13544200
C	-4.30433300	-0.29925500	-3.64925700
H	-3.44087500	-0.53896000	-4.28099400

C	-4.97060600	0.97137900	-4.17786100
H	-5.33392600	0.81992700	-5.19656600
H	-4.27856000	1.81338900	-4.18377900
H	-5.82509800	1.24623500	-3.55246300
C	-5.27351600	-1.48259400	-3.69168000
H	-6.15005300	-1.28953100	-3.06548100
H	-4.80657500	-2.40726100	-3.34793400
H	-5.63090900	-1.64843700	-4.70973200
C	1.95754400	-3.21426000	-2.21383400
H	2.09949700	-4.08382200	-1.57080000
C	2.70300700	-2.03013200	-1.65168700
N	2.42420900	-0.79303700	-1.96818700
C	3.25385700	0.00202600	-1.20699500
C	4.06652700	-0.77872900	-0.41821900
N	3.71423900	-2.08025700	-0.72198400
C	4.25534800	-3.26158000	-0.06133800
H	5.34344600	-3.18074200	-0.04569300
H	4.01585300	-4.12553800	-0.67935300
C	5.10939600	-0.43479000	0.58405600
H	5.18949300	0.64694000	0.65114000
H	6.08532100	-0.84261400	0.30263300
H	4.85862500	-0.83841900	1.56879100
C	3.15123000	1.47384900	-1.24764400
O	3.78515100	2.21486300	-0.49827100
N	0.53646000	-2.91948800	-2.17446100
H	0.22578900	-2.05736100	-2.60278800
C	3.72511000	-3.45050000	1.34387700
C	2.39751800	-3.16726300	1.63625700
H	1.73350800	-2.81772800	0.85675800
C	1.89385100	-3.30538500	2.92774300
C	2.74348700	-3.76733100	3.93038000
H	2.36888700	-3.87420200	4.94179700
C	4.06959800	-4.07783000	3.64503800
H	4.72322400	-4.43442800	4.43176100
C	4.56382000	-3.91013400	2.35774700
H	5.60457800	-4.12625000	2.14261700
C	2.42051300	-3.57525300	-3.64526500
H	2.19918900	-2.70767500	-4.27752000
C	1.64937000	-4.78568400	-4.17289300
H	1.96010400	-5.02425700	-5.19235900
H	0.57461400	-4.60492300	-4.17678800
H	1.83829100	-5.66375600	-3.54876600
C	3.92900000	-3.82848000	-3.68733500
H	4.19614200	-4.68556200	-3.06108400
H	4.49949400	-2.96369300	-3.34297800
H	4.25190100	-4.05611300	-4.70492100
C	0.47590000	-2.88660200	3.21216800
H	-0.18123600	-3.32311800	2.45377600
H	0.15424900	-3.29883700	4.17338400
C	2.24755300	1.85965000	3.23189500
C	0.25218300	-1.37974400	3.22715500
C	1.29655400	-0.46607100	3.23027300
C	-1.06161000	-0.89966600	3.23392300
C	1.05514000	0.91188500	3.23522200
H	2.32040500	-0.81798700	3.20702300
H	-1.87814600	-1.61072700	3.21325800
C	-0.25837500	1.35974600	3.24097200
H	-0.46506700	2.42279000	3.22531700
C	-2.74885600	1.01833300	3.24009500
C	-1.33116000	0.46156800	3.23922200
H	2.96272500	1.50835200	2.48199100
H	2.75468600	1.78919900	4.19898100
H	-2.80491600	1.81600500	2.49306100
H	-2.94078200	1.48938900	4.20913700

Cartesian coordinates of the optimized geometries for $\uparrow\text{CHCl}_3@6$ using B3LYP-D3/def2-TZVP.

C	1.33449600	3.51898500	-2.37710300
H	1.94132100	4.13112300	-1.71320800
C	-0.05232600	3.34882900	-1.81511400
N	-0.89949200	2.46201500	-2.27192000
C	-2.08105300	2.66471500	-1.59161400
C	-1.94113500	3.69805700	-0.69661800
N	-0.63195700	4.12329200	-0.83804000
C	0.03723700	5.12327700	0.00334900
H	-0.74037800	5.77034300	0.40681200
H	0.66249400	5.74089100	-0.63928400
C	-2.90962500	4.27575600	0.27317000
H	-3.87764200	3.81115700	0.10671100
H	-3.01261400	5.35748000	0.14819100
H	-2.61248800	4.08605500	1.30699900
C	-3.21076900	1.72215000	-1.71009400
O	-4.30110800	1.90087100	-1.17126000
N	1.97546700	2.21823300	-2.42257800
H	1.43023400	1.43720500	-2.75912100
C	0.87243200	4.53599800	1.12513800
C	0.27554800	4.01858700	2.27713600
H	-0.80329400	4.02455000	2.36987300
C	1.03394800	3.48616500	3.31626000
C	2.42450900	3.48220900	3.18753200
H	3.03602600	3.09344300	3.99314800
C	3.03083900	3.97281200	2.04142200
H	4.10811700	3.94655900	1.93844600
C	2.25912700	4.50552600	1.01602900
H	2.75293800	4.87729300	0.12900700
C	1.30849000	4.19822100	-3.76927500
H	0.73859400	3.53730000	-4.43133400
C	2.72935700	4.34926200	-4.31470400
H	3.33337900	4.97723200	-3.65395800
H	2.71274800	4.81474300	-5.30243800
H	3.22795300	3.38396800	-4.40020600
C	0.59852900	5.55264500	-3.70908400
H	1.12986500	6.24064300	-3.04366200
H	-0.43067400	5.46216100	-3.35659300
H	0.57110300	6.01451700	-4.69768900
C	-3.71512900	-0.59733000	-2.37761300
H	-4.54573500	-0.37574400	-1.71097100
C	-2.87631400	-1.71527600	-1.81748500
N	-1.68384400	-2.00598200	-2.27186600
C	-1.27155700	-3.13259200	-1.59255300
C	-2.23943100	-3.52946600	-0.70147500
N	-3.26071700	-2.60670300	-0.84376500
C	-4.46196700	-2.52659900	-0.00389400
H	-4.63752900	-3.52460300	0.39517000
H	-5.30758300	-2.28814900	-0.64646400
C	-2.26029000	-4.66057100	0.26422400
H	-1.37135100	-5.26348300	0.10214500
H	-3.14332400	-5.29159300	0.12996600
H	-2.25384700	-4.31243500	1.29955500
C	0.11015400	-3.63907400	-1.70615700
O	0.49960000	-4.67229300	-1.16577100
N	-2.90761400	0.60703500	-2.42495600
H	-1.96015200	0.52594300	-2.76563500
C	-4.36951300	-1.51431100	1.12238600
C	-3.61838300	-1.77370400	2.27097500
H	-3.07986300	-2.70908400	2.35849000
C	-3.53572800	-0.85323500	3.31246700
C	-4.23218800	0.35092900	3.19019000
H	-4.19993000	1.07223700	3.99820300
C	-4.96534400	0.63194600	2.04755900

H	-5.48505000	1.57656900	1.94960400
C	-5.04045500	-0.29974200	1.01950600
H	-5.61266600	-0.05683600	0.13485600
C	-4.29446000	-0.95751500	-3.76843700
H	-3.43949300	-1.11621400	-4.43488900
C	-5.14031500	0.19668400	-4.30716100
H	-5.53485000	-0.04662200	-5.29599700
H	-4.55748300	1.11412400	-4.38840200
H	-5.98598300	0.39941400	-3.64436400
C	-5.10876100	-2.25185700	-3.70955300
H	-5.96643200	-2.14209800	-3.03811500
H	-4.51127500	-3.09831600	-3.36585400
H	-5.50091300	-2.50211500	-4.69703800
C	2.37252700	-2.91229000	-2.36508500
H	2.59586000	-3.74022500	-1.69604900
C	2.91733900	-1.62469800	-1.80531400
N	2.57105600	-0.44785600	-2.26142900
C	3.34260100	0.47435600	-1.58696600
C	4.17222000	-0.16305800	-0.69611100
N	3.88367200	-1.50932900	-0.83411800
C	4.42019800	-2.58808000	0.00432300
H	5.36948600	-2.23612000	0.40484200
H	4.64236800	-3.43768200	-0.63922700
C	5.16457600	0.38681700	0.26555900
H	5.24061400	1.45810100	0.10154000
H	6.15294300	-0.06100400	0.12821100
H	4.86414000	0.21931100	1.30247100
C	3.09382500	1.92413800	-1.70875900
O	3.79676600	2.77935700	-1.17429300
N	0.92592300	-2.81746800	-2.41739500
H	0.52229200	-1.95759100	-2.76085800
C	3.49980600	-3.02157600	1.13015800
C	3.34504200	-2.24271000	2.27954400
H	3.87786000	-1.30406900	2.36535700
C	2.51248400	-2.63851100	3.32342200
C	1.82620500	-3.84882900	3.20143200
H	1.18987000	-4.18726700	4.01041800
C	1.95304700	-4.62285700	2.05787200
H	1.40083400	-5.54887200	1.96067400
C	2.79248300	-4.21558900	1.02797600
H	2.87158900	-4.83112100	0.14282300
C	2.97861000	-3.23323900	-3.75478400
H	2.69016900	-2.41244000	-4.42067300
C	2.40320400	-4.54213400	-4.29737400
H	2.81105100	-4.75879800	-5.28717700
H	1.31741900	-4.49637600	-4.37791500
H	2.65192800	-5.37752000	-3.63745100
C	4.50665500	-3.29106600	-3.69280600
H	4.83839900	-4.09127800	-3.02358700
H	4.93988800	-2.35164700	-3.34486400
H	4.92163700	-3.50213700	-4.68030300
C	0.00277000	-0.01477700	0.44877100
C	1.27983300	0.52765000	4.50552300
C	1.12019500	-0.85083700	4.50508700
C	0.18007300	1.39036000	4.50311500
C	-0.17664600	-1.37209000	4.49711000
C	-1.09369300	0.83958300	4.49644100
C	-1.29058300	-0.54437200	4.49708700
H	0.01004800	-0.01623900	-0.63612100
C	2.33109700	-1.76927300	4.55158500
H	3.22669500	-1.16285500	4.69991200
H	2.24436800	-2.41662900	5.42961400
C	-2.69156200	-1.13470200	4.53872500
H	-2.61378700	-2.21412100	4.68225800
H	-3.20862600	-0.74018300	5.41872500
C	0.37091100	2.89872000	4.54551200

H	-0.60209800	3.37216000	4.69093600
H	0.97387900	3.14915900	5.42347200
H	-1.95248100	1.49971500	4.49323900
H	-0.31906900	-2.44607600	4.49384600
H	2.28088700	0.94158200	4.51026600
Cl	0.18960100	-1.69043100	1.00484100
Cl	1.35549300	0.98992400	1.00736300
Cl	-1.54817400	0.65967900	0.98879800

5. Complete Reference 15

- [15] Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, Revision A.02, Gaussien, Inc., 2009.