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Supporting Information

Chlorinated Derivatives of C_{78}-fullerene Isomers Showing Unusually Short Intermolecular Halogen- Halogen Contacts

Kalin S. Simeonov, Konstantin Yu. Amsharov, Martin Jansen*

Max Planck Institute for Solid State Research, Heisenbergstrasse 1, Stuttgart 70469, Germany

M.Jansen@fkf.mpg.de

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Figure S1. Three different orientation of the $C_{78}(2)Cl_{18}$ molecule (left, top) and $C_{78}(3)Cl_{18}$ molecule (right, top) and superimposure of all three orientations for both molecules (bottom).

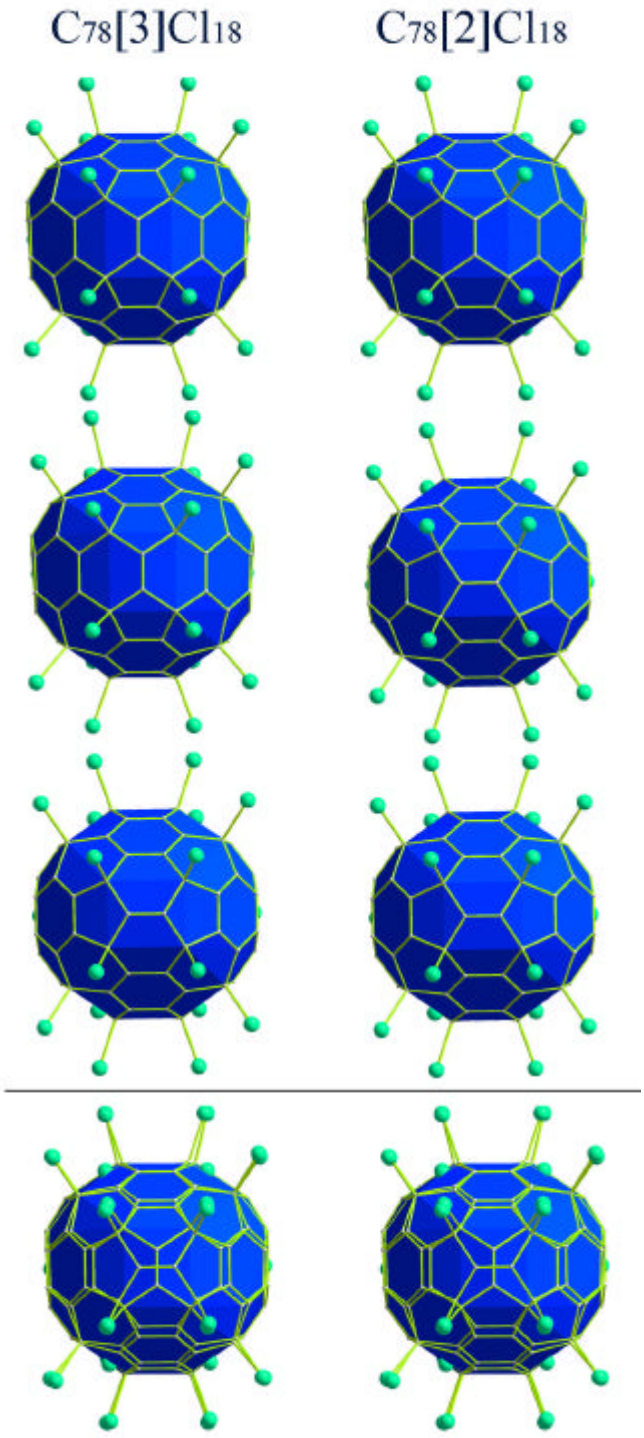


Figure S2. ORTEP projections of $C_{78}(2)Cl_{18}$ (left, top and bottom) and $C_{78}(3)Cl_{18}$ (right, top and bottom). Thermal ellipsoids are drown at 50% probability level.

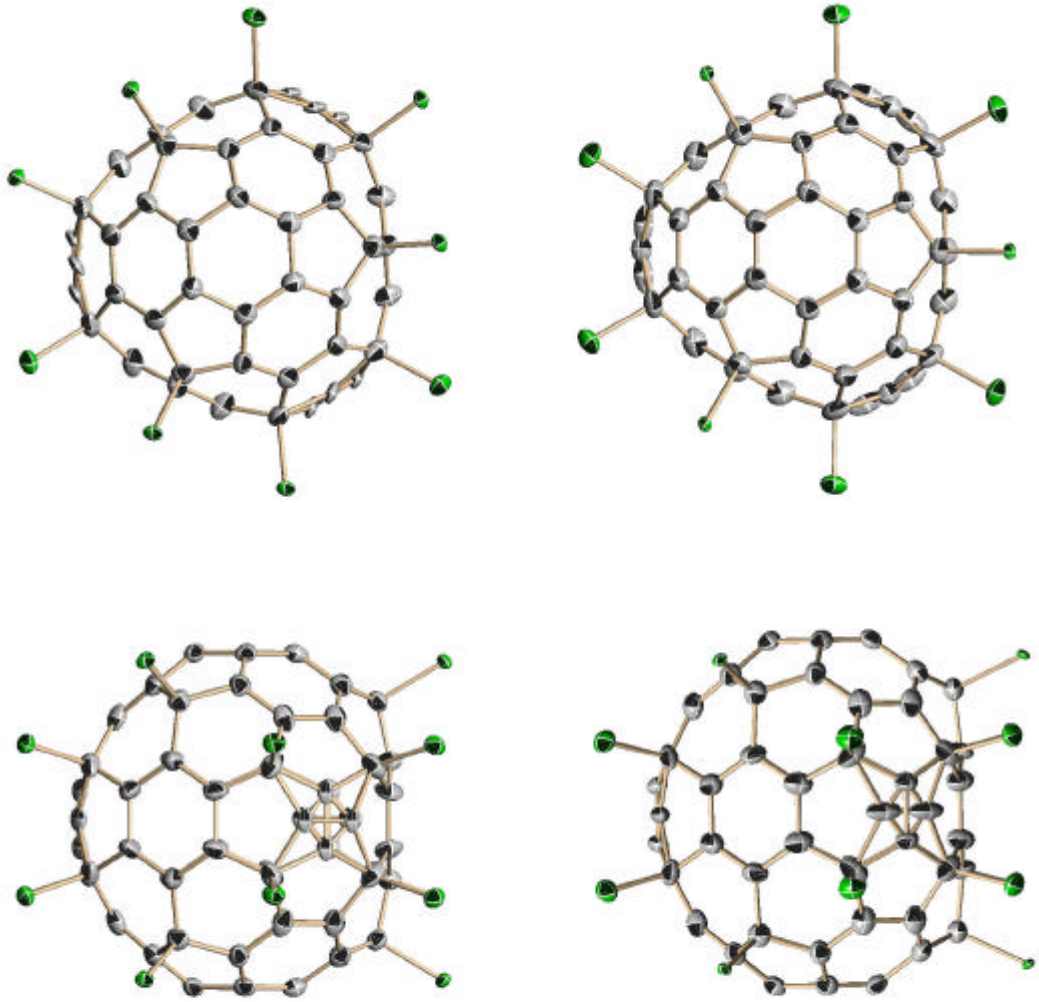


Figure S3. Electron density map calculated from observed structure factor (F(obs), structure **II**). Only one orientation of Br_2 molecule is presented for clarity.

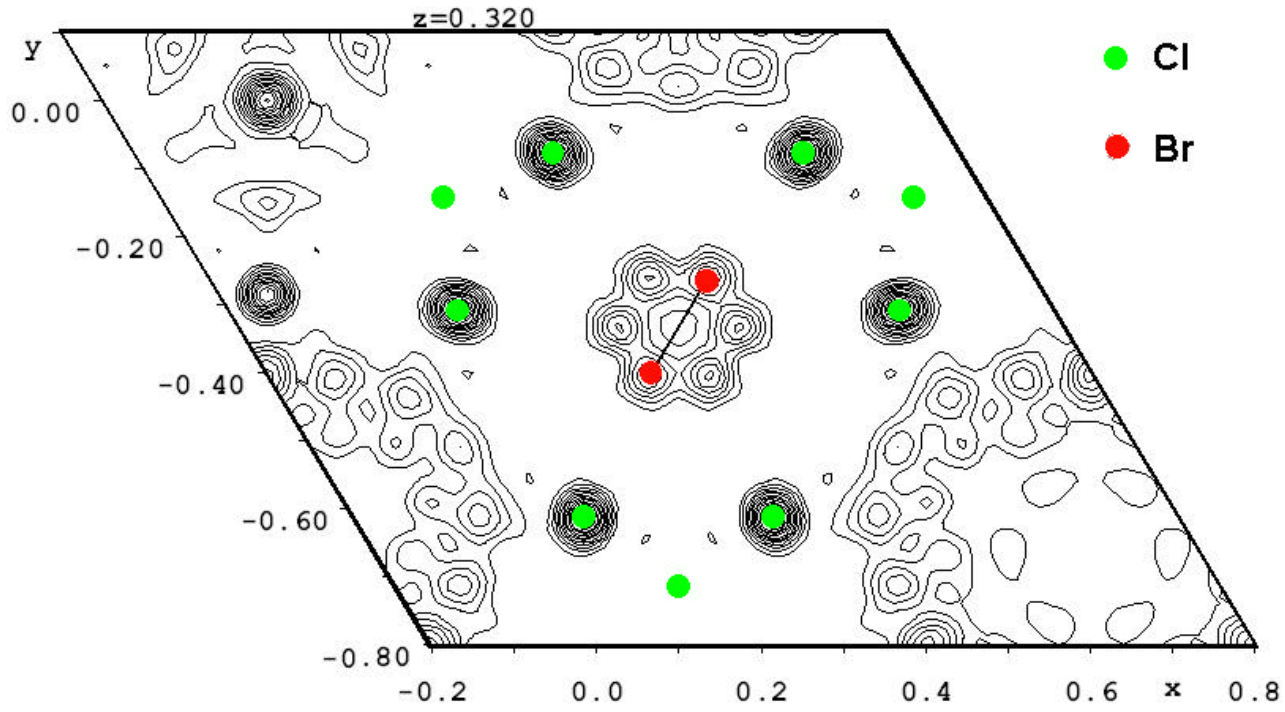
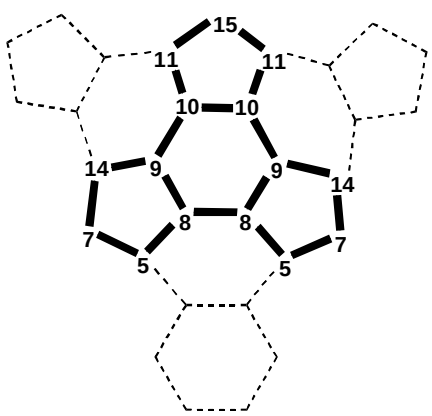
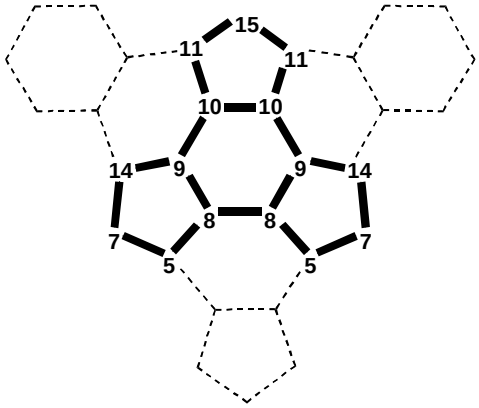


Figure S4. Trindane fragments (bold) in the $C_{78}(2)Cl_{18}$ and $C_{78}(3)Cl_{18}$ which superpose under rotation of the fullerene molecule at 120^{o}.



C_{78}:2



C_{78}:3

Table S1. The C-C distances in trindane fragment of $C_{78}(2)Cl_{18}$.

Bonding*	DFT	DFT avarage	X-Ray	Deviation Å
8-9 10-10	1.460 1.455	1.456	1.446	0.010
8-8 9-10	1.395 1.401	1.398	1.372	0.026
8-5 9-14 10-11	1.416 1.417 1.421	1.418	1.426	-0.008
5-7 7-14 11-15	1.536 1.516 1.520	1.524	1.520	0.004

Tabele S2. The C-C distances in trindane fragment of $C_{78}(3)Cl_{18}$.

Bonding*	DFT	DFT avarage	X-Ray	Deviation Å
8-9 10-10	1.457 1.461	1.459	1.444	0.005
8-8 9-10	1.400 1.393	1.397	1.400	-0.003
8-5 9-14 10-11	1.418 1.417 1.414	1.416	1.411	0.005
5-7 7-14 11-15	1.516 1.537 1.532	1.528	1.523	0.005

* Numbering of carbon atoms according to Colt, J.; Scuseria, G.E. *Chem. Phys. Lett.* **1992**, *199*, 505.

Table S3. Cartesian Coordinates for Optimized Structure for $C_{78}(2)Cl_{18}$ by B3LYP/6-31G.

Atom	X	Y	Z
C	-3.44020	0.66350	-1.99170
C	-3.89100	1.45780	-0.79040
C	-2.54900	1.45020	-2.92040
C	-3.44020	-0.66350	-1.99170
C	3.44020	0.66350	-1.99170
C	2.54900	1.45020	-2.92040
C	3.89100	1.45780	-0.79040
C	3.44020	-0.66350	-1.99170
C	0.00000	2.95320	-3.08970
C	1.17770	3.44090	-2.26220
C	-1.17770	3.44090	-2.26220
C	0.00000	1.42210	-3.22190
C	-2.78060	2.90670	1.58440
C	-1.40510	3.22140	2.19120
C	-2.62010	3.41780	0.16600
C	-3.06450	1.42120	1.61940
C	2.78060	2.90670	1.58440
C	2.62010	3.41780	0.16600
C	1.40510	3.22140	2.19120

C	3.06450	1.42120	1.61940
C	0.72740	4.21410	-1.15880
C	1.43120	4.18080	0.05190
C	-0.72740	4.21410	-1.15880
C	0.69730	4.07380	1.30930
C	-0.69730	4.07380	1.30930
C	-1.43120	4.18080	0.05190
C	2.33550	2.71170	-2.14360
C	3.07420	2.70850	-0.92490
C	-0.71690	2.38550	3.06960
C	-3.07420	2.70850	-0.92490
C	0.71690	2.38550	3.06960
C	-1.49040	1.23970	3.66810
C	1.49040	1.23970	3.66810
C	-2.33550	2.71170	-2.14360
C	-1.22740	0.70820	-3.19080
C	1.22740	0.70820	-3.19080
C	3.59460	0.71090	0.51270
C	2.51210	0.69770	2.68210
C	-2.51210	0.69770	2.68210
C	-3.59460	0.71090	0.51270
C	0.66920	0.00000	3.93360

C	-0.66920	0.00000	3.93360
C	-1.22740	-0.70820	-3.19080
C	1.22740	-0.70820	-3.19080
C	3.59460	-0.71090	0.51270
C	2.51210	-0.69770	2.68210
C	-2.51210	-0.69770	2.68210
C	-3.59460	-0.71090	0.51270
C	-2.54900	-1.45020	-2.92040
C	-3.89100	-1.45780	-0.79040
C	3.89100	-1.45780	-0.79040
C	2.54900	-1.45020	-2.92040
C	-2.78060	-2.90670	1.58440
C	-1.40510	-3.22140	2.19120
C	-2.62010	-3.41780	0.16600
C	-3.06450	-1.42120	1.61940
C	0.00000	-2.95320	-3.08970
C	1.17770	-3.44090	-2.26220
C	-1.17770	-3.44090	-2.26220
C	0.00000	-1.42210	-3.22190
C	2.78060	-2.90670	1.58440
C	1.40510	-3.22140	2.19120
C	2.62010	-3.41780	0.16600

C	3.06450	-1.42120	1.61940
C	-1.43120	-4.18080	0.05190
C	-0.69730	-4.07380	1.30930
C	-0.72740	-4.21410	-1.15880
C	0.69730	-4.07380	1.30930
C	1.43120	-4.18080	0.05190
C	0.72740	-4.21410	-1.15880
C	-0.71690	-2.38550	3.06960
C	0.71690	-2.38550	3.06960
C	-1.49040	-1.23970	3.66810
C	1.49040	-1.23970	3.66810
C	2.33550	-2.71170	-2.14360
C	-2.33550	-2.71170	-2.14360
C	3.07420	-2.70850	-0.92490
C	-3.07420	-2.70850	-0.92490
Cl	-2.34010	1.84620	5.28770
Cl	-2.34010	-1.84620	5.28770
Cl	2.34010	1.84620	5.28770
Cl	2.34010	-1.84620	5.28770
Cl	5.76640	1.87950	-0.88110
Cl	4.17700	3.85490	2.49720
Cl	3.42920	1.83710	-4.58550

Cl	0.00000	3.74080	-4.83630
Cl	-4.17700	3.85490	2.49720
Cl	-5.76640	1.87950	-0.88110
Cl	-5.76640	-1.87950	-0.88110
Cl	-4.17700	-3.85490	2.49720
Cl	-3.42920	-1.83710	-4.58550
Cl	0.00000	-3.74080	-4.83630
Cl	5.76640	-1.87950	-0.88110
Cl	4.17700	-3.85490	2.49720
Cl	-3.42920	1.83710	-4.58550
Cl	3.42920	-1.83710	-4.58550

Table S4. Cartesian Coordinates for Optimized Structure for $C_{78}(3)Cl_{18}$ by B3LYP/6-31G.

Atom	X	Y	Z
C	0.00000	0.66470	4.02210
C	1.25750	1.46090	3.76820
C	-1.25750	1.46090	3.76820
C	0.00000	-0.66470	4.02210
C	-2.72720	2.90270	1.59300
C	-2.56530	3.20370	0.09480
C	-1.41210	3.40010	2.16080
C	-2.91200	1.42010	1.83020
C	2.72720	2.90270	1.59300
C	2.56530	3.20370	0.09480
C	1.41210	3.40010	2.16080
C	2.91200	1.42010	1.83020
C	0.00000	2.85440	-3.26500
C	-1.18960	3.17780	-2.35570
C	1.18960	3.17780	-2.35570
C	0.00000	1.42120	-3.68420
C	-0.69990	4.12900	1.17490
C	-1.42380	4.02350	-0.08570

C	0.69990	4.12900	1.17490
C	-0.73050	3.98980	-1.29290
C	0.73050	3.98980	-1.29290
C	1.42380	4.02350	-0.08570
C	-3.01040	2.37760	-0.93560
C	-2.31790	2.37150	-2.19420
C	-3.92170	1.24070	-0.54900
C	-2.52300	1.24430	-3.17880
C	3.01040	2.37760	-0.93560
C	0.71320	2.70210	3.12190
C	2.31790	2.37150	-2.19420
C	3.92170	1.24070	-0.54900
C	2.52300	1.24430	-3.17880
C	-0.71320	2.70210	3.12190
C	-2.22390	0.71080	2.84770
C	-3.56330	0.69770	0.82480
C	-1.20050	0.70130	-3.68320
C	1.20050	0.70130	-3.68320
C	3.56330	0.69770	0.82480
C	2.22390	0.71080	2.84770
C	-3.76360	0.00000	-1.39480
C	-3.13560	0.00000	-2.57590

C	3.13560	0.00000	-2.57590
C	3.76360	0.00000	-1.39480
C	-2.22390	-0.71080	2.84770
C	-3.56330	-0.69770	0.82480
C	-1.20050	-0.70130	-3.68320
C	1.20050	-0.70130	-3.68320
C	3.56330	-0.69770	0.82480
C	2.22390	-0.71080	2.84770
C	-1.25750	-1.46090	3.76820
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C	2.72720	-2.90270	1.59300
C	2.56530	-3.20370	0.09480
C	1.41210	-3.40010	2.16080
C	2.91200	-1.42010	1.83020
C	-2.72720	-2.90270	1.59300
C	-2.56530	-3.20370	0.09480
C	-1.41210	-3.40010	2.16080
C	-2.91200	-1.42010	1.83020
C	0.00000	-2.85440	-3.26500
C	1.18960	-3.17780	-2.35570
C	-1.18960	-3.17780	-2.35570
C	0.00000	-1.42120	-3.68420

C	0.69990	-4.12900	1.17490
C	1.42380	-4.02350	-0.08570
C	-0.69990	-4.12900	1.17490
C	0.73050	-3.98980	-1.29290
C	-0.73050	-3.98980	-1.29290
C	-1.42380	-4.02350	-0.08570
C	3.01040	-2.37760	-0.93560
C	2.31790	-2.37150	-2.19420
C	3.92170	-1.24070	-0.54900
C	2.52300	-1.24430	-3.17880
C	-3.01040	-2.37760	-0.93560
C	-0.71320	-2.70210	3.12190
C	-2.31790	-2.37150	-2.19420
C	-3.92170	-1.24070	-0.54900
C	-2.52300	-1.24430	-3.17880
C	0.71320	-2.70210	3.12190
Cl	5.74680	1.85670	-0.59790
Cl	5.74680	-1.85670	-0.59790
Cl	3.59870	1.88940	-4.64360
Cl	3.59870	-1.88940	-4.64360
Cl	-3.59870	1.88940	-4.64360
Cl	0.00000	3.99700	-4.80940

Cl	-5.74680	1.85670	-0.59790
Cl	-4.20330	3.87280	2.34150
Cl	4.20330	3.87280	2.34150
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Cl	2.15470	-1.90180	5.41320
Cl	4.20330	-3.87280	2.34150
Cl	-2.15470	-1.90180	5.41320
Cl	-4.20330	-3.87280	2.34150
Cl	-3.59870	-1.88940	-4.64360
Cl	0.00000	-3.99700	-4.80940
Cl	-2.15470	1.90180	5.41320
Cl	-5.74680	-1.85670	-0.59790

(20) M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, *Gaussian 03*, revision C 02; Gaussian, Inc.: Wallingford, CT, 2004.