7 Anhang

Abkürzungen

Abb	Abbildung
AFM	atomic force microscopy
BOC	*tert*-Butoxycarbonyl
CD	zirkularer Dichroismus
d	Dublett (NMR)
dd	Dublett von Dubletts (NMR)
DABCO	1,4-Diazabicyclo[2.2.2]octan
DBU	1,8-Diazabicyclo[5.4.0]undec-7-en
DCC	Dicyclohexylcarbodiimid
DCM	Dichlormethan
DMAP	4-(N, N'-Dimethylamino)pyridin
DMF	Dimethylformamid
DPTS	4-(N, N'-Dimethylamino)pyridinium tosylate
EI	electron ionization (MS)
ESI	electron spray ionization (MS)
FAB	fast atom bombardment
g	Gramm
GC	Gaschromatography
GPC	gel permeation chromatography
HOBt	1-Hydroxybenzoetriazol
HPLC	high-performance liquid chromatography
HRMS	high resolution mass spectroscopy
J	Kopplungskonstante (NMR)
LAH	Lithiumaluminiumhydrid
m	Multiplett (NMR)
M	molar
m/z	Masse/ Ladungsverhältnis (MS)
mL	Milliliter
µL	Mikroliter
mmol	Millimol
M_n	number average molecular weight (GPC)
*m*PE, O*m*PE, P*m*PE	*meta*-Phenylenethinylen, oligo(*m*PE), poly(*m*PE)
MS	Massenspektrometrie
M_w	weight average mlecular weight (GPC)
NMR	nuclear magnetic resonance
Nr	Nummer
P_n	Anzahl der Wiederholungseinheiten (GPC)
PDI	Polydispersitätsindex (GPC)
q	Quartett (NMR)
RCM	ring-closing metathesis
s	Singulett (NMR)
STM	scanning tunnel microscopy
t	Triplett (NMR)
TBAI	Tetrabutylammoniumiodid
TEA	Triethylamin
TFE	1,1,1-Trifluorethanol
Tg	Triglyme (Triethylenglykolmonomethylether)
THF	Tetrahydrofuran
TMS	Trimethylsilyl
TMSA	Trimethylsilylacetylen
TrCl	Tritylchlorid (Triphenylchlormethan)
UV	Ultraviolett

Kristallographische Daten[1]

*A_2-Monomer **37***

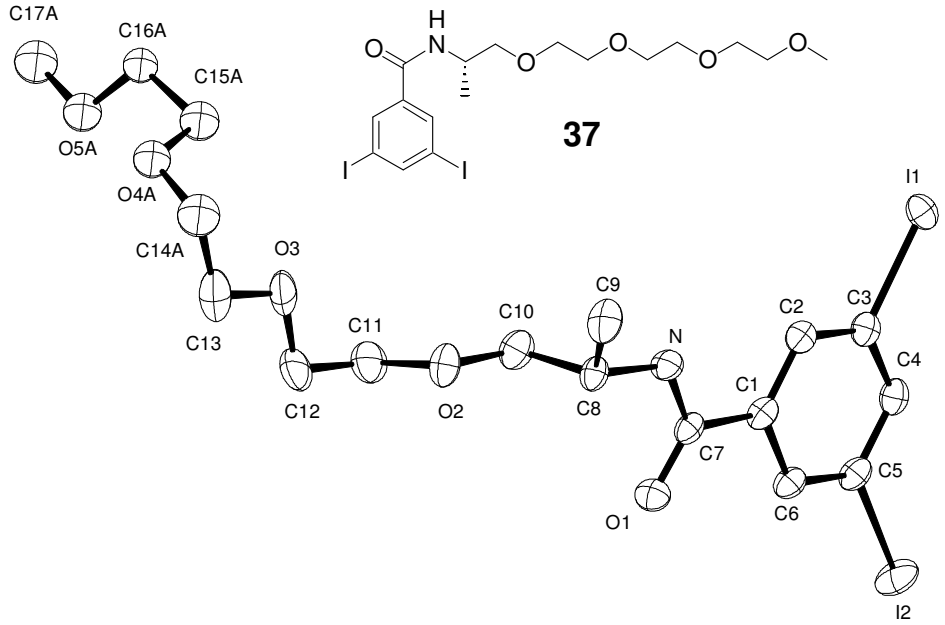

Table 1. Crystal data and structure refinement.

Identification code	5460	
Empirical formula	$C_{17}H_{25}I_2NO_5$	
Color	colourless	
Formula weight	577.18 g · mol^{-1}	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	**$P2_12_12_1$, (no. 19)**	
Unit cell dimensions	a = 10.3890(5) Å	α= 90°.
	b = 13.4407(5) Å	β= 90°.
	c = 15.7105(8) Å	γ = 90°.
Volume	2193.74(17) $Å^3$	
Z	4	
Density (calculated)	1.748 Mg · m^{-3}	
Absorption coefficient	2.891 mm^{-1}	
F(000)	1120 e	
Crystal size	0.20 x 0.18 x 0.06 mm^3	
θ range for data collection	3.00 to 31.38°.	
Index ranges	$-15 \le h \le 15$, $-19 \le k \le 19$, $-23 \le l \le 23$	
Reflections collected	20860	
Independent reflections	7125 [R_{int} = 0.0432]	
Reflections with I>2σ(I)	6842	
Completeness to θ = 31.38°	98.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.0 and 0.7723	

[1] Die Kristallstrukturen wurden von der Röntgenstruktur-Abteilung am MPI für Kohleforschung in Mülheim (Ruhr) gemessen.

Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7125 / 0 / 221	
Goodness-of-fit on F^2	1.063	
Final R indices [I>2σ(I)]	R_1 = 0.0425	wR^2 = 0.0966
R indices (all data)	R_1 = 0.0446	wR^2 = 0.0978
Absolute structure parameter	0.12(3)	
Largest diff. peak and hole	2.164 and -1.589 e·Å^{-3}	

Table 2. Atomic coordinates and equivalent isotropic displacement parameters (Å^2).

U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
C(1)	0.3324(4)	0.5675(3)	0.3280(3)	0.024(1)
C(2)	0.2867(4)	0.5396(3)	0.2490(3)	0.024(1)
C(3)	0.1876(4)	0.5931(3)	0.2115(3)	0.025(1)
C(4)	0.1309(4)	0.6750(3)	0.2509(3)	0.028(1)
C(5)	0.1771(5)	0.7013(3)	0.3314(3)	0.028(1)
C(6)	0.2773(5)	0.6502(3)	0.3696(3)	0.026(1)
C(7)	0.4434(4)	0.5185(3)	0.3729(3)	0.023(1)
C(8)	0.6014(4)	0.3839(3)	0.3766(3)	0.026(1)
C(9)	0.5966(5)	0.2733(4)	0.3602(4)	0.037(1)
C(10)	0.7227(5)	0.4322(4)	0.3411(4)	0.035(1)
C(11)	0.9460(6)	0.4475(5)	0.3677(4)	0.043(1)
C(12)	1.0582(5)	0.3935(5)	0.4061(5)	0.047(1)
C(13)	1.1973(7)	0.2548(7)	0.3877(6)	0.069(2)
C(14A)	1.2383(14)	0.1649(11)	0.3359(9)	0.048(3)
C(14B)	1.2522(16)	0.2165(12)	0.3031(11)	0.055(3)
C(15A)	1.2498(12)	0.2414(9)	0.2009(8)	0.041(2)
C(15B)	1.3663(17)	0.2362(13)	0.1707(12)	0.062(4)
C(16A)	1.3482(10)	0.2705(8)	0.1352(7)	0.032(2)
C(16B)	1.4206(16)	0.3179(13)	0.1095(11)	0.062(4)
C(17A)	1.5050(13)	0.3904(10)	0.0977(10)	0.049(3)
C(17B)	1.5578(19)	0.4546(15)	0.1052(14)	0.077(5)
I(1)	0.1213(1)	0.5505(1)	0.0901(1)	0.029(1)
I(2)	0.0936(1)	0.8225(1)	0.3941(1)	0.041(1)
N	0.4901(4)	0.4337(3)	0.3387(3)	0.028(1)
O(1)	0.4878(3)	0.5540(3)	0.4379(2)	0.029(1)
O(2)	0.8312(3)	0.3909(3)	0.3834(3)	0.036(1)
O(3)	1.0921(4)	0.3123(4)	0.3542(3)	0.056(1)
O(4A)	1.3178(8)	0.1937(6)	0.2680(5)	0.037(2)
O(4B)	1.3068(9)	0.2833(6)	0.2453(5)	0.039(2)
O(5A)	1.4273(9)	0.3484(6)	0.1643(6)	0.039(2)
O(5B)	1.5074(10)	0.3765(8)	0.1588(7)	0.052(2)

Table 3. Bond lengths [Å] and angles [°].

C(1)-C(2)	1.381(7)	C(1)-C(6)	1.410(6)
C(1)-C(7)	1.503(6)	C(2)-C(3)	1.387(6)
C(3)-C(4)	1.393(7)	C(3)-I(1)	2.107(5)
C(4)-C(5)	1.397(7)	C(5)-C(6)	1.385(6)
C(5)-I(2)	2.092(4)	C(7)-O(1)	1.218(6)
C(7)-N	1.350(6)	C(8)-N	1.462(6)
C(8)-C(9)	1.510(6)	C(8)-C(10)	1.523(7)

C(10)-O(2)	1.421(7)	C(11)-O(2)	1.435(6)
C(11)-C(12)	1.500(9)	C(12)-O(3)	1.407(8)
C(13)-O(3)	1.438(9)	C(13)-C(14A)	1.518(16)
C(13)-C(14B)	1.535(19)	C(14A)-O(4A)	1.403(16)
C(14B)-O(4B)	1.397(18)	C(15A)-O(4A)	1.422(15)
C(15A)-C(16A)	1.505(17)	C(15B)-O(4B)	1.470(19)
C(15B)-C(16B)	1.56(2)	C(16A)-O(5A)	1.407(13)
C(16B)-O(5B)	1.43(2)	C(17A)-O(5A)	1.437(17)
C(17B)-O(5B)	1.44(2)		

C(2)-C(1)-C(6)	119.4(4)	C(2)-C(1)-C(7)	124.5(4)
C(6)-C(1)-C(7)	116.0(4)	C(1)-C(2)-C(3)	119.7(4)
C(2)-C(3)-C(4)	122.3(5)	C(2)-C(3)-I(1)	119.1(3)
C(4)-C(3)-I(1)	118.6(3)	C(3)-C(4)-C(5)	117.2(4)
C(6)-C(5)-C(4)	121.7(4)	C(6)-C(5)-I(2)	119.6(4)
C(4)-C(5)-I(2)	118.8(3)	C(5)-C(6)-C(1)	119.7(5)
O(1)-C(7)-N	121.8(4)	O(1)-C(7)-C(1)	120.8(4)
N-C(7)-C(1)	117.4(4)	N-C(8)-C(9)	110.8(4)
N-C(8)-C(10)	108.1(4)	C(9)-C(8)-C(10)	112.6(4)
O(2)-C(10)-C(8)	108.6(4)	O(2)-C(11)-C(12)	108.7(5)
O(3)-C(12)-C(11)	109.7(5)	O(3)-C(13)-C(14A)	116.5(8)
O(3)-C(13)-C(14B)	98.4(9)	C(14A)-C(13)-C(14B)	33.4(7)
O(4A)-C(14A)-C(13)	110.7(11)	O(4B)-C(14B)-C(13)	119.8(12)
O(4A)-C(15A)-C(16A)	106.7(10)	O(4B)-C(15B)-C(16B)	109.8(13)
O(5A)-C(16A)-C(15A)	111.6(10)	O(5B)-C(16B)-C(15B)	106.4(14)
C(7)-N-C(8)	120.6(4)	C(10)-O(2)-C(11)	111.9(4)
C(12)-O(3)-C(13)	113.3(6)	C(14A)-O(4A)-C(15A)	113.3(10)
C(14B)-O(4B)-C(15B)	114.4(11)	C(16A)-O(5A)-C(17A)	112.6(10)
C(16B)-O(5B)-C(17B)	108.3(13)		

Table 4. Anisotropic displacement parameters (Å^2).

The anisotropic displacement factor exponent takes the form:

$-2\pi^2[\, h^2\, a^{*2} U_{11} + ... + 2\, h\, k\, a^*\, b^*\, U_{12}\,]$.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(1)	0.025(2)	0.018(2)	0.030(2)	0.003(2)	0.005(2)	0.002(2)
C(2)	0.025(2)	0.018(2)	0.031(2)	0.000(2)	0.004(2)	-0.002(2)
C(3)	0.024(2)	0.021(2)	0.031(2)	0.004(2)	0.003(2)	-0.004(2)
C(4)	0.022(2)	0.027(2)	0.034(2)	0.005(2)	0.000(2)	0.003(2)
C(5)	0.027(2)	0.022(2)	0.034(2)	-0.001(2)	0.005(2)	0.008(2)
C(6)	0.027(2)	0.020(2)	0.030(2)	-0.001(2)	0.004(2)	0.004(2)
C(7)	0.022(2)	0.019(2)	0.029(2)	0.001(2)	0.007(2)	-0.001(1)
C(8)	0.021(2)	0.022(2)	0.034(2)	0.001(2)	0.001(2)	0.004(2)
C(9)	0.031(2)	0.020(2)	0.060(3)	0.002(2)	0.001(2)	0.007(2)
C(10)	0.032(2)	0.032(3)	0.041(3)	0.005(2)	0.005(2)	0.002(2)
C(11)	0.037(3)	0.045(3)	0.047(3)	-0.002(3)	0.001(2)	-0.014(3)
C(12)	0.031(2)	0.062(4)	0.048(3)	-0.006(3)	-0.004(3)	-0.021(2)
C(13)	0.028(3)	0.094(6)	0.084(6)	-0.017(5)	-0.004(4)	-0.008(3)
I(1)	0.029(1)	0.025(1)	0.032(1)	0.002(1)	-0.004(1)	-0.006(1)
I(2)	0.046(1)	0.033(1)	0.043(1)	-0.003(1)	0.008(1)	0.020(1)
N	0.028(2)	0.026(2)	0.028(2)	-0.003(2)	-0.001(2)	0.008(2)
O(1)	0.034(2)	0.023(1)	0.031(2)	-0.001(1)	-0.001(1)	0.003(1)
O(2)	0.025(2)	0.036(2)	0.049(2)	0.007(2)	0.003(2)	-0.003(1)
O(3)	0.020(2)	0.072(3)	0.074(3)	-0.026(3)	-0.004(2)	-0.007(2)

A_2 Monomer **38**

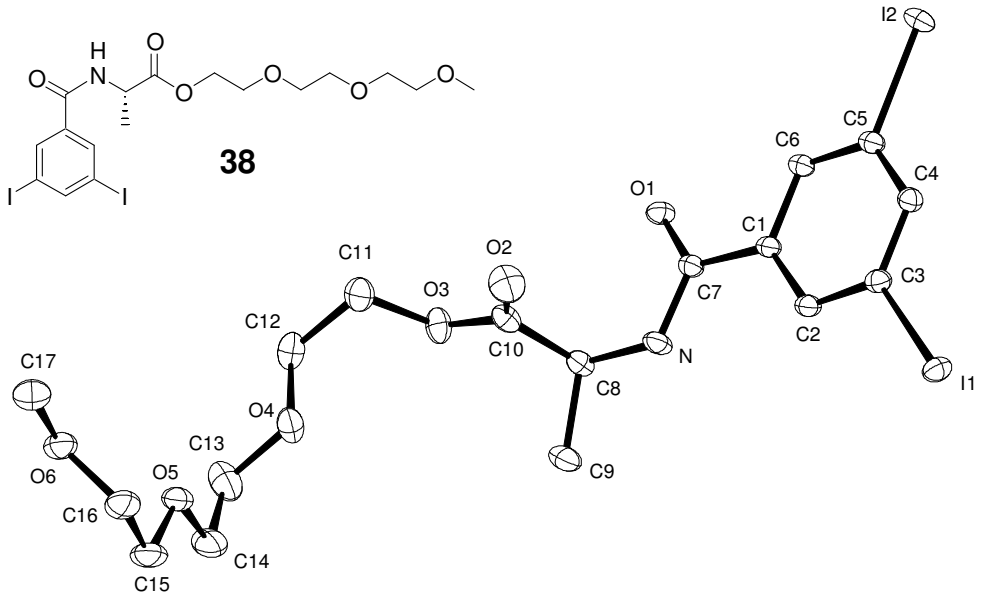

Table 1. Crystal data and structure refinement.

Identification code	5284	
Empirical formula	$C_{17}H_{23}I_2NO_6$	
Color	colourless	
Formula weight	591.16 g · mol^{-1}	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	**$P2_12_12_1$, (no. 19)**	
Unit cell dimensions	a = 9.4462(1) Å	α= 90°.
	b = 14.3234(2) Å	β= 90°.
	c = 16.0490(2) Å	γ = 90°.
Volume	2171.46(5) $Å^3$	
Z	4	
Density (calculated)	1.808 Mg · m^{-3}	
Absorption coefficient	2.926 mm^{-1}	
F(000)	1144 e	
Crystal size	0.56 x 0.44 x 0.24 mm^3	
θ range for data collection	3.11 to 33.15°.	
Index ranges	$-14 \le h \le 14$, $-22 \le k \le 22$, $-24 \le l \le 24$	
Reflections collected	58608	
Independent reflections	8197 [R_{int} = 0.0372]	
Reflections with I>2σ(I)	8158	
Completeness to θ = 33.15°	98.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00 and 0.66	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8197 / 0 / 239	
Goodness-of-fit on F^2	1.169	
Final R indices [I>2σ(I)]	R_1 = 0.0173	wR^2 = 0.0427
R indices (all data)	R_1 = 0.0174	wR^2 = 0.0428
Absolute structure parameter	0.038(11)	

Largest diff. peak and hole 0.671 and -0.647 e · Å^{-3}

Table 2. Atomic coordinates and equivalent isotropic displacement parameters (Å^2).
U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
C(1)	0.1544(2)	0.0562(1)	0.6405(1)	0.015(1)
C(2)	0.2107(2)	0.0302(1)	0.7179(1)	0.017(1)
C(3)	0.3182(2)	0.0844(1)	0.7528(1)	0.017(1)
C(4)	0.3714(2)	0.1629(1)	0.7127(1)	0.017(1)
C(5)	0.3169(2)	0.1865(1)	0.6346(1)	0.016(1)
C(6)	0.2094(2)	0.1336(1)	0.5982(1)	0.016(1)
C(7)	0.0351(2)	0.0052(1)	0.5992(1)	0.016(1)
C(8)	-0.1417(2)	-0.1163(1)	0.6053(1)	0.019(1)
C(9)	-0.1655(2)	-0.2093(1)	0.6503(1)	0.029(1)
C(10)	-0.2750(2)	-0.0562(1)	0.6122(1)	0.021(1)
C(11)	-0.5176(2)	-0.0538(2)	0.5703(2)	0.028(1)
C(12)	-0.6245(2)	-0.1309(2)	0.5632(1)	0.027(1)
C(13)	-0.7369(2)	-0.2491(2)	0.6405(2)	0.035(1)
C(14)	-0.7766(3)	-0.2726(2)	0.7286(2)	0.037(1)
C(15)	-0.9046(3)	-0.2173(2)	0.8434(2)	0.035(1)
C(16)	-0.9646(2)	-0.1305(2)	0.8808(1)	0.031(1)
C(17)	-1.1271(3)	-0.0081(2)	0.8552(1)	0.031(1)
I(1)	0.4025(1)	0.0452(1)	0.8687(1)	0.020(1)
I(2)	0.3962(1)	0.3040(1)	0.5728(1)	0.020(1)
N	-0.0213(2)	-0.0680(1)	0.6400(1)	0.020(1)
O(1)	-0.0074(1)	0.0283(1)	0.5294(1)	0.018(1)
O(2)	-0.2881(2)	0.0133(1)	0.6530(1)	0.033(1)
O(3)	-0.3780(1)	-0.0950(1)	0.5659(1)	0.025(1)
O(4)	-0.6337(1)	-0.1768(1)	0.6406(1)	0.028(1)
O(5)	-0.8449(2)	-0.1949(1)	0.7648(1)	0.025(1)
O(6)	-1.0646(2)	-0.0918(1)	0.8242(1)	0.026(1)

Table 3. Bond lengths [Å] and angles [°].

C(1)-C(6)	1.401(2)	C(1)-C(2)	1.402(2)
C(1)-C(7)	1.498(2)	C(2)-C(3)	1.395(2)
C(3)-C(4)	1.391(2)	C(3)-I(1)	2.0993(17)
C(4)-C(5)	1.396(2)	C(5)-C(6)	1.395(2)
C(5)-I(2)	2.0920(16)	C(7)-O(1)	1.234(2)
C(7)-N	1.346(2)	C(8)-N	1.443(2)
C(8)-C(10)	1.529(3)	C(8)-C(9)	1.532(3)
C(10)-O(2)	1.199(2)	C(10)-O(3)	1.344(2)
C(11)-O(3)	1.447(2)	C(11)-C(12)	1.501(3)
C(12)-O(4)	1.408(3)	C(13)-O(4)	1.422(3)
C(13)-C(14)	1.502(4)	C(14)-O(5)	1.412(3)
C(15)-O(5)	1.418(2)	C(15)-C(16)	1.492(3)
C(16)-O(6)	1.422(3)	C(17)-O(6)	1.425(3)
C(6)-C(1)-C(2)	119.93(15)	C(6)-C(1)-C(7)	116.80(14)
C(2)-C(1)-C(7)	123.28(14)	C(3)-C(2)-C(1)	118.99(15)
C(4)-C(3)-C(2)	121.80(16)	C(4)-C(3)-I(1)	119.33(12)
C(2)-C(3)-I(1)	118.87(12)	C(3)-C(4)-C(5)	118.58(15)
C(6)-C(5)-C(4)	120.85(15)	C(6)-C(5)-I(2)	119.93(12)
C(4)-C(5)-I(2)	119.21(12)	C(5)-C(6)-C(1)	119.80(15)
O(1)-C(7)-N	121.45(16)	O(1)-C(7)-C(1)	121.02(15)

N-C(7)-C(1)	117.51(15)	N-C(8)-C(10)	110.59(15)
N-C(8)-C(9)	110.48(15)	C(10)-C(8)-C(9)	109.53(15)
O(2)-C(10)-O(3)	124.81(18)	O(2)-C(10)-C(8)	126.30(18)
O(3)-C(10)-C(8)	108.88(15)	O(3)-C(11)-C(12)	108.00(17)
O(4)-C(12)-C(11)	108.57(17)	O(4)-C(13)-C(14)	109.5(2)
O(5)-C(14)-C(13)	108.97(18)	O(5)-C(15)-C(16)	108.65(16)
O(6)-C(16)-C(15)	108.71(19)	C(7)-N-C(8)	119.78(15)
C(10)-O(3)-C(11)	117.61(16)	C(12)-O(4)-C(13)	112.41(18)
C(14)-O(5)-C(15)	111.64(16)	C(16)-O(6)-C(17)	112.38(17)

Table 4. Anisotropic displacement parameters (Å^2).
The anisotropic displacement factor exponent takes the form:
$-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(1)	0.016(1)	0.012(1)	0.016(1)	0.002(1)	0.002(1)	0.000
C(2)	0.019(1)	0.013(1)	0.018(1)	0.002(1)	0.001(1)	0.000
C(3)	0.019(1)	0.015(1)	0.018(1)	0.002(1)	0.001(1)	0.002
C(4)	0.017(1)	0.015(1)	0.020(1)	0.001(1)	0.002(1)	0.000
C(5)	0.018(1)	0.013(1)	0.018(1)	0.002(1)	0.004(1)	0.000
C(6)	0.018(1)	0.013(1)	0.016(1)	0.002(1)	0.003(1)	-0.001
C(7)	0.017(1)	0.014(1)	0.016(1)	0.002(1)	0.003(1)	0.000
C(8)	0.021(1)	0.018(1)	0.019(1)	0.001(1)	0.001(1)	-0.005
C(9)	0.031(1)	0.021(1)	0.035(1)	0.009(1)	-0.004(1)	-0.009
C(10)	0.023(1)	0.022(1)	0.019(1)	0.001(1)	0.004(1)	-0.005
C(11)	0.021(1)	0.030(1)	0.033(1)	0.000(1)	0.008(1)	0.004
C(12)	0.019(1)	0.036(1)	0.025(1)	-0.004(1)	-0.001(1)	0.002
C(13)	0.029(1)	0.026(1)	0.051(1)	-0.011(1)	0.011(1)	-0.004
C(14)	0.031(1)	0.018(1)	0.062(2)	0.008(1)	0.013(1)	0.005
C(15)	0.034(1)	0.030(1)	0.040(1)	0.020(1)	0.011(1)	0.005
C(16)	0.032(1)	0.035(1)	0.024(1)	0.013(1)	0.004(1)	0.003
C(17)	0.038(1)	0.023(1)	0.031(1)	0.001(1)	0.000(1)	0.002
I(1)	0.023(1)	0.019(1)	0.019(1)	0.003(1)	-0.004(1)	0.002
I(2)	0.025(1)	0.014(1)	0.021(1)	0.001(1)	0.007(1)	-0.005
N	0.025(1)	0.020(1)	0.017(1)	0.007(1)	-0.003(1)	-0.007
O(1)	0.023(1)	0.017(1)	0.015(1)	0.004(1)	0.000(1)	-0.001
O(2)	0.036(1)	0.027(1)	0.036(1)	-0.010(1)	0.003(1)	0.000(1)
O(3)	0.017(1)	0.030(1)	0.027(1)	-0.007(1)	0.004(1)	0.000
O(4)	0.019(1)	0.035(1)	0.029(1)	0.000(1)	0.001(1)	-0.004
O(5)	0.026(1)	0.018(1)	0.031(1)	0.007(1)	0.004(1)	0.001
O(6)	0.029(1)	0.024(1)	0.024(1)	0.006(1)	0.001(1)	0.002

Versicherung

Hiermit versichere ich, Christian Kaiser, geboren am 04.12.1976 in Erfurt, die vorliegende Arbeit selbstständig und nur mit Hilfe der zulässigen und angegebenen Mittel verfasst zu haben.