

## 7 ANHANG

Kristallstrukturdaten von 2,3-Diphenyl-1,4-dihydrocyclopenta[*b*]indol 76 (Abb. 2)

## Crystal data for 76

Crystal shape	block	Volume	1655.1(8) Å <sup>3</sup>
Crystal colour	colorless	Z	4
Crystal size	0.75 x 0.50 x 0.30 mm	Density (calculated)	1.234 g/cm <sup>3</sup>
Chemical formula	C <sub>23</sub> H <sub>17</sub> N	Radiation used	MoK <sub>α</sub>
Formula weight	307.38	Wavelength	0.71073 Å
Crystal system	Triclinic	Linear absorption coefficient	0.071 mm <sup>-1</sup>
Space group	P-1	Temperature	296(2) K
Unit cell dimensions	a = 10.400(3) Å    α = 100.263(6)° b = 11.031(3) Å    β = 94.125(5)° c = 16.304(4) Å    γ = 114.317(5)°		

## Data collection details for 76

Diffractometer	BRUKER Smart 1k CCD	Number of measured reflections	19330
Scan method	ω scans	Number of independent refl.	9287
Absorption correction	Empirical	Number of observed reflections	5271
Max. and min. transmission	0.9789 and 0.9485	Criterion of recognition (σ-limit)	>2σ(I)
R(int) =	0.0269	Index ranges	-14<=h<=14, -15<=k<=15, -22<=l<=23
Theta range for data collection	2.08 to 30.91°		
Completeness to theta = 30.91°	89.0 %		
F(000)	648		

## Refinement details for 76

Refinement method	Full-matrix least-squares on F <sup>2</sup>		
Final R indices [I>σ(I)]	R1 = 0.0464, wR2 = 0.1073		
R indices (all data)	R1 = 0.0943, wR2 = 0.1270		
R1 [=Σ( Fo - Fc )/Σ Fo ]			
wR <sup>2</sup> [=Σ(w(Fo <sup>2</sup> -Fc <sup>2</sup> ) <sup>2</sup> )/Σ(wFo <sup>4</sup> )] <sup>1/2</sup>			
H-locating and refining method	difmap/refall	Number of reflections used	9287
Number of L.S. restraints	0	Number of refined parameters	569
Goodness-of-fit on F <sup>2</sup>	1.005		
S [=Σ w(Fo <sup>2</sup> -Fc <sup>2</sup> ) <sup>2</sup> ]/(n-p) <sup>1/2</sup>	n=number of reflections, p=parameters used.		
Definition of w	calc w=1/[σ <sup>2</sup> (Fo <sup>2</sup> )+(0.0613P) <sup>2</sup> +0.0480P] where P=(Fo <sup>2</sup> +2Fc <sup>2</sup> )/3		
Maximum d/s	0.004		
Maximum e-density	0.134 e Å <sup>-3</sup>	Minimum e-density	-0.223 e Å <sup>-3</sup>

## Computer Programs used for 76

Data collection program	SMART	Structure solving program	SHELXS-97 (Sheldrick, 1990)
Cell refinement program	SAINT	Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Data reduction program	XPREP	Pictures drawn with	ZORTEP

Atomic coordinates (x 10<sup>4</sup>) and equivalent isotropic displacement parameters (Å<sup>2</sup> x 10<sup>3</sup>) for 76

U(eq) is defined as one third of the trace of the orthogonalized U<sup>ij</sup> tensor.

	x	y	z	U(eq)		x	y	z	U(eq)
N(1)	6767(1)	7412(1)	2209(1)	54(1)	N(2)	9729(1)	2032(1)	-727(1)	57(1)
C(1)	7250(1)	9260(1)	3598(1)	48(1)	C(24)	9147(1)	3177(1)	662(1)	47(1)
C(2)	7569(1)	10617(1)	3680(1)	50(1)	C(25)	7864(1)	3162(1)	809(1)	50(1)
C(3)	7660(2)	10961(1)	2810(1)	53(1)	C(26)	6733(1)	2365(2)	20(1)	56(1)
C(4)	7327(1)	9623(1)	2229(1)	50(1)	C(27)	7549(1)	1935(1)	-592(1)	49(1)
C(5)	7170(1)	8946(1)	1372(1)	49(1)	C(28)	7445(1)	1195(1)	-1424(1)	50(1)
C(6)	7310(1)	9325(2)	593(1)	58(1)	C(29)	6363(2)	473(1)	-2130(1)	62(1)
C(7)	7106(2)	8362(2)	-128(1)	64(1)	C(30)	6669(2)	-148(2)	-2847(1)	71(1)
C(8)	6733(2)	6997(2)	-103(1)	63(1)	C(31)	8037(2)	-64(2)	-2892(1)	71(1)
C(9)	6589(1)	6577(2)	648(1)	59(1)	C(32)	9139(2)	649(2)	-2216(1)	67(1)
C(10)	6818(1)	7553(1)	1379(1)	50(1)	C(33)	8838(1)	1272(1)	-1486(1)	53(1)
C(11)	7095(1)	8682(1)	2709(1)	49(1)	C(34)	8927(1)	2418(1)	-198(1)	48(1)
C(12)	7112(1)	8437(1)	4246(1)	48(1)	C(35)	10525(1)	3747(1)	1255(1)	46(1)

## Fortsetzung

C(13)	8295(2)	8289(1)	4583(1)	57(1)	C(36)	10841(1)	2916(2)	1699(1)	56(1)
C(14)	8174(2)	7485(2)	5164(1)	69(1)	C(37)	12119(2)	3433(2)	2251(1)	67(1)
C(15)	6882(2)	6813(2)	5406(1)	74(1)	C(38)	13089(2)	4773(2)	2360(1)	67(1)
C(16)	5705(2)	6944(2)	5078(1)	75(1)	C(39)	12803(2)	5597(2)	1913(1)	69(1)
C(17)	5809(2)	7746(2)	4498(1)	64(1)	C(40)	11530(1)	5085(1)	1358(1)	61(1)
C(18)	7805(1)	11669(1)	4439(1)	53(1)	C(41)	7513(1)	3740(1)	1599(1)	51(1)
C(19)	7785(2)	11444(2)	5254(1)	65(1)	C(42)	8489(2)	4942(2)	2164(1)	65(1)
C(20)	8033(2)	12481(2)	5951(1)	73(1)	C(43)	8138(2)	5443(2)	2912(1)	70(1)
C(21)	8294(2)	13767(2)	5856(1)	77(1)	C(44)	6803(2)	4774(2)	3115(1)	66(1)
C(22)	8309(2)	14012(2)	5061(1)	84(1)	C(45)	5825(2)	3602(2)	2570(1)	67(1)
C(23)	8075(2)	12991(2)	4362(1)	72(1)	C(46)	6163(2)	3086(2)	1819(1)	59(1)

## Bond lengths [Å] for 76

N(1)-C(11)	1.3797(16)	C(15)-H(15)	0.982(18)	C(29)-C(30)	1.373(2)
N(1)-C(10)	1.3909(17)	C(16)-C(17)	1.386(2)	C(29)-H(29)	1.000(15)
N(1)-H(1)	0.882(15)	C(16)-H(16)	0.911(18)	C(30)-C(31)	1.395(2)
C(1)-C(2)	1.3715(17)	C(17)-H(17)	0.939(15)	C(30)-H(30)	0.986(16)
C(1)-C(11)	1.4442(18)	C(18)-C(19)	1.395(2)	C(31)-C(32)	1.383(2)
C(1)-C(12)	1.4892(17)	C(18)-C(23)	1.398(2)	C(31)-H(31)	0.992(16)
C(2)-C(18)	1.4657(18)	C(19)-C(20)	1.385(2)	C(32)-C(33)	1.3880(19)
C(2)-C(3)	1.5314(19)	C(19)-H(19)	0.961(17)	C(32)-H(32)	0.961(16)
C(3)-C(4)	1.4929(18)	C(20)-C(21)	1.370(2)	C(35)-C(40)	1.3834(18)
C(3)-H(3A)	1.014(14)	C(20)-H(20)	0.975(16)	C(35)-C(36)	1.3878(18)
C(3)-H(3B)	0.996(15)	C(21)-C(22)	1.371(3)	C(36)-C(37)	1.3858(19)
C(4)-C(11)	1.3640(17)	C(21)-H(21)	0.938(18)	C(36)-H(36)	0.982(14)
C(4)-C(5)	1.4259(18)	C(22)-C(23)	1.379(2)	C(37)-C(38)	1.373(2)
C(5)-C(6)	1.4045(19)	C(22)-H(22)	0.975(18)	C(37)-H(37)	1.002(16)
C(5)-C(10)	1.4286(18)	C(23)-H(23)	0.983(17)	C(38)-C(39)	1.368(2)
C(6)-C(7)	1.374(2)	N(2)-C(34)	1.3732(16)	C(38)-H(38)	0.960(15)
C(6)-H(6)	0.969(15)	N(2)-C(33)	1.3858(17)	C(39)-C(40)	1.3860(19)
C(7)-C(8)	1.400(2)	N(2)-H(2)	0.900(17)	C(39)-H(39)	1.005(16)
C(7)-H(7)	0.979(15)	C(24)-C(25)	1.3671(17)	C(40)-H(40)	0.948(16)
C(8)-C(9)	1.382(2)	C(24)-C(34)	1.4477(17)	C(41)-C(46)	1.3971(19)
C(8)-H(8)	0.986(15)	C(24)-C(35)	1.4919(16)	C(41)-C(42)	1.3995(19)
C(9)-C(10)	1.3884(19)	C(25)-C(41)	1.4705(18)	C(42)-C(43)	1.384(2)
C(9)-H(9)	1.005(15)	C(25)-C(26)	1.5294(17)	C(42)-H(42)	0.995(17)
C(12)-C(17)	1.3885(19)	C(26)-C(27)	1.4918(19)	C(43)-C(44)	1.375(2)
C(12)-C(13)	1.3937(18)	C(26)-H(26A)	1.012(15)	C(43)-H(43)	0.960(16)
C(13)-C(14)	1.386(2)	C(26)-H(26B)	1.003(15)	C(44)-C(45)	1.369(2)
C(13)-H(13)	1.005(15)	C(27)-C(34)	1.3659(17)	C(44)-H(44)	0.994(16)
C(14)-C(15)	1.368(2)	C(27)-C(28)	1.4244(18)	C(45)-C(46)	1.386(2)
C(14)-H(14)	1.001(18)	C(28)-C(29)	1.4057(18)	C(45)-H(45)	0.970(17)
C(15)-C(16)	1.373(2)	C(28)-C(33)	1.4278(18)	C(46)-H(46)	0.969(14)

## Angles [°] for 76

C(11)-N(1)-C(10)	107.45(11)	C(16)-C(15)-H(15)	117.9(10)	C(29)-C(30)-H(30)	119.3(9)
C(11)-N(1)-H(1)	126.0(9)	C(15)-C(16)-C(17)	120.63(16)	C(31)-C(30)-H(30)	119.3(9)
C(10)-N(1)-H(1)	125.8(9)	C(15)-C(16)-H(16)	123.0(11)	C(32)-C(31)-C(30)	121.33(15)
C(2)-C(1)-C(11)	106.97(11)	C(17)-C(16)-H(16)	116.4(11)	C(32)-C(31)-H(31)	119.0(10)
C(2)-C(1)-C(12)	130.90(11)	C(16)-C(17)-C(12)	120.28(15)	C(30)-C(31)-H(31)	119.7(10)
C(11)-C(1)-C(12)	122.09(11)	C(16)-C(17)-H(17)	122.2(9)	C(31)-C(32)-C(33)	117.79(15)
C(1)-C(2)-C(18)	129.69(12)	C(12)-C(17)-H(17)	117.5(9)	C(31)-C(32)-H(32)	119.8(9)
C(1)-C(2)-C(3)	109.50(11)	C(19)-C(18)-C(23)	116.58(14)	C(33)-C(32)-H(32)	122.4(9)
C(18)-C(2)-C(3)	120.81(11)	C(19)-C(18)-C(2)	124.06(12)	N(2)-C(33)-C(32)	129.56(13)
C(4)-C(3)-C(2)	103.30(10)	C(23)-C(18)-C(2)	119.36(13)	N(2)-C(33)-C(28)	108.55(11)
C(4)-C(3)-H(3A)	113.1(8)	C(20)-C(19)-C(18)	121.60(15)	C(32)-C(33)-C(28)	121.90(12)
C(2)-C(3)-H(3A)	110.2(8)	C(20)-C(19)-H(19)	117.7(9)	C(27)-C(34)-N(2)	110.75(11)
C(4)-C(3)-H(3B)	114.4(8)	C(18)-C(19)-H(19)	120.7(9)	C(27)-C(34)-C(24)	112.17(11)
C(2)-C(3)-H(3B)	109.3(8)	C(21)-C(20)-C(19)	120.54(17)	N(2)-C(34)-C(24)	137.07(11)
H(3A)-C(3)-H(3B)	106.5(11)	C(21)-C(20)-H(20)	121.0(10)	C(40)-C(35)-C(36)	118.43(12)
C(11)-C(4)-C(5)	107.77(11)	C(19)-C(20)-H(20)	118.5(10)	C(40)-C(35)-C(24)	121.66(11)
C(11)-C(4)-C(3)	107.50(11)	C(20)-C(21)-C(22)	118.95(16)	C(36)-C(35)-C(24)	119.88(11)
C(5)-C(4)-C(3)	144.72(12)	C(20)-C(21)-H(21)	120.4(11)	C(37)-C(36)-C(35)	120.39(13)
C(6)-C(5)-C(4)	136.24(13)	C(22)-C(21)-H(21)	120.6(11)	C(37)-C(36)-H(36)	119.2(8)
C(6)-C(5)-C(10)	117.89(12)	C(21)-C(22)-C(23)	121.12(16)	C(35)-C(36)-H(36)	120.4(8)

## Fortsetzung

C(4)-C(5)-C(10)	105.85(11)	C(21)-C(22)-H(22)	122.6(10)	C(38)-C(37)-C(36)	120.29(14)
C(7)-C(6)-C(5)	119.70(14)	C(23)-C(22)-H(22)	116.2(10)	C(38)-C(37)-H(37)	120.7(9)
C(7)-C(6)-H(6)	119.4(9)	C(22)-C(23)-C(18)	121.20(16)	C(36)-C(37)-H(37)	119.0(9)
C(5)-C(6)-H(6)	120.8(9)	C(22)-C(23)-H(23)	119.7(10)	C(39)-C(38)-C(37)	119.95(13)
C(6)-C(7)-C(8)	121.13(14)	C(18)-C(23)-H(23)	119.1(10)	C(39)-C(38)-H(38)	121.9(9)
C(6)-C(7)-H(7)	120.8(9)	C(34)-N(2)-C(33)	107.44(11)	C(37)-C(38)-H(38)	118.1(9)
C(8)-C(7)-H(7)	118.0(9)	C(34)-N(2)-H(2)	126.7(10)	C(38)-C(39)-C(40)	120.06(14)
C(9)-C(8)-C(7)	121.26(15)	C(33)-N(2)-H(2)	125.8(10)	C(38)-C(39)-H(39)	122.3(9)
C(9)-C(8)-H(8)	119.9(9)	C(25)-C(24)-C(34)	106.97(10)	C(40)-C(39)-H(39)	117.6(9)
C(7)-C(8)-H(8)	118.8(9)	C(25)-C(24)-C(35)	129.27(11)	C(35)-C(40)-C(39)	120.84(14)
C(8)-C(9)-C(10)	117.75(14)	C(34)-C(24)-C(35)	123.61(10)	C(35)-C(40)-H(40)	119.5(9)
C(8)-C(9)-H(9)	122.4(8)	C(24)-C(25)-C(41)	128.09(11)	C(39)-C(40)-H(40)	119.6(9)
C(10)-C(9)-H(9)	119.8(8)	C(24)-C(25)-C(26)	109.98(11)	C(46)-C(41)-C(42)	116.78(13)
C(9)-C(10)-N(1)	129.43(12)	C(41)-C(25)-C(26)	121.87(11)	C(46)-C(41)-C(25)	120.39(12)
C(9)-C(10)-C(5)	122.25(12)	C(27)-C(26)-C(25)	102.89(10)	C(42)-C(41)-C(25)	122.82(12)
N(1)-C(10)-C(5)	108.32(11)	C(27)-C(26)-H(26A)	114.3(8)	C(43)-C(42)-C(41)	121.48(15)
C(4)-C(11)-N(1)	110.59(12)	C(25)-C(26)-H(26A)	111.6(8)	C(43)-C(42)-H(42)	120.0(9)
C(4)-C(11)-C(1)	112.72(11)	C(27)-C(26)-H(26B)	111.5(8)	C(41)-C(42)-H(42)	118.5(9)
N(1)-C(11)-C(1)	136.69(11)	C(25)-C(26)-H(26B)	110.4(8)	C(44)-C(43)-C(42)	120.48(16)
C(17)-C(12)-C(13)	118.35(13)	H(26A)-C(26)-H(26B)	106.3(12)	C(44)-C(43)-H(43)	119.3(9)
C(17)-C(12)-C(1)	121.65(12)	C(34)-C(27)-C(28)	107.59(11)	C(42)-C(43)-H(43)	120.2(10)
C(13)-C(12)-C(1)	119.93(11)	C(34)-C(27)-C(26)	107.99(11)	C(45)-C(44)-C(43)	119.18(15)
C(14)-C(13)-C(12)	120.66(14)	C(28)-C(27)-C(26)	144.41(11)	C(45)-C(44)-H(44)	118.8(9)
C(14)-C(13)-H(13)	122.2(8)	C(29)-C(28)-C(27)	136.02(13)	C(43)-C(44)-H(44)	122.0(9)
C(12)-C(13)-H(13)	117.2(8)	C(29)-C(28)-C(33)	118.31(12)	C(44)-C(45)-C(46)	120.95(16)
C(15)-C(14)-C(13)	120.23(15)	C(27)-C(28)-C(33)	105.67(10)	C(44)-C(45)-H(45)	121.8(10)
C(15)-C(14)-H(14)	118.0(10)	C(30)-C(29)-C(28)	119.32(14)	C(46)-C(45)-H(45)	117.3(10)
C(13)-C(14)-H(14)	121.8(10)	C(30)-C(29)-H(29)	121.2(8)	C(45)-C(46)-C(41)	121.12(14)
C(14)-C(15)-C(16)	119.85(15)	C(28)-C(29)-H(29)	119.5(8)	C(45)-C(46)-H(46)	119.8(8)
C(14)-C(15)-H(15)	122.2(10)	C(29)-C(30)-C(31)	121.35(15)	C(41)-C(46)-H(46)	119.0(8)

Symmetry transformations used to generate equivalent atoms:

**Torsion angles [°] for 76**

C(11)-C(1)-C(2)-C(18)	178.62(12)	C(34)-C(24)-C(25)-C(41)	177.16(12)
C(12)-C(1)-C(2)-C(18)	-3.5(2)	C(35)-C(24)-C(25)-C(41)	1.6(2)
C(11)-C(1)-C(2)-C(3)	-1.20(14)	C(34)-C(24)-C(25)-C(26)	-0.11(14)
C(12)-C(1)-C(2)-C(3)	176.66(12)	C(35)-C(24)-C(25)-C(26)	-175.69(12)
C(1)-C(2)-C(3)-C(4)	0.98(14)	C(24)-C(25)-C(26)-C(27)	-0.03(15)
C(18)-C(2)-C(3)-C(4)	-178.86(11)	C(41)-C(25)-C(26)-C(27)	-177.50(11)
C(2)-C(3)-C(4)-C(11)	-0.34(13)	C(25)-C(26)-C(27)-C(34)	0.17(14)
C(2)-C(3)-C(4)-C(5)	-179.38(16)	C(25)-C(26)-C(27)-C(28)	178.61(17)
C(11)-C(4)-C(5)-C(6)	-177.52(14)	C(34)-C(27)-C(28)-C(29)	-179.60(15)
C(3)-C(4)-C(5)-C(6)	1.5(3)	C(26)-C(27)-C(28)-C(29)	2.0(3)
C(11)-C(4)-C(5)-C(10)	0.60(13)	C(34)-C(27)-C(28)-C(33)	0.31(14)
C(3)-C(4)-C(5)-C(10)	179.64(17)	C(26)-C(27)-C(28)-C(33)	-178.13(18)
C(4)-C(5)-C(6)-C(7)	178.04(14)	C(27)-C(28)-C(29)-C(30)	-179.02(14)
C(10)-C(5)-C(6)-C(7)	0.09(19)	C(33)-C(28)-C(29)-C(30)	1.1(2)
C(5)-C(6)-C(7)-C(8)	1.3(2)	C(28)-C(29)-C(30)-C(31)	-0.8(2)
C(6)-C(7)-C(8)-C(9)	-1.5(2)	C(29)-C(30)-C(31)-C(32)	0.0(2)
C(7)-C(8)-C(9)-C(10)	0.4(2)	C(30)-C(31)-C(32)-C(33)	0.5(2)
C(8)-C(9)-C(10)-N(1)	-178.87(12)	C(34)-N(2)-C(33)-C(32)	-179.53(14)
C(8)-C(9)-C(10)-C(5)	0.96(19)	C(34)-N(2)-C(33)-C(28)	0.28(14)
C(11)-N(1)-C(10)-C(9)	179.08(13)	C(31)-C(32)-C(33)-N(2)	179.63(14)
C(11)-N(1)-C(10)-C(5)	-0.77(13)	C(31)-C(32)-C(33)-C(28)	-0.2(2)
C(6)-C(5)-C(10)-C(9)	-1.22(18)	C(29)-C(28)-C(33)-N(2)	179.56(12)
C(4)-C(5)-C(10)-C(9)	-179.75(11)	C(27)-C(28)-C(33)-N(2)	-0.36(14)
C(6)-C(5)-C(10)-N(1)	178.64(11)	C(29)-C(28)-C(33)-C(32)	-0.61(19)
C(4)-C(5)-C(10)-N(1)	0.11(13)	C(27)-C(28)-C(33)-C(32)	179.46(13)
C(5)-C(4)-C(11)-N(1)	-1.11(14)	C(28)-C(27)-C(34)-N(2)	-0.15(14)
C(3)-C(4)-C(11)-N(1)	179.47(10)	C(26)-C(27)-C(34)-N(2)	178.89(11)
C(5)-C(4)-C(11)-C(1)	179.04(10)	C(28)-C(27)-C(34)-C(24)	-179.30(10)
C(3)-C(4)-C(11)-C(1)	-0.38(14)	C(26)-C(27)-C(34)-C(24)	-0.25(15)
C(10)-N(1)-C(11)-C(4)	1.18(14)	C(33)-N(2)-C(34)-C(27)	-0.08(15)
C(10)-N(1)-C(11)-C(1)	-179.02(13)	C(33)-N(2)-C(34)-C(24)	178.76(14)
C(2)-C(1)-C(11)-C(4)	1.03(14)	C(25)-C(24)-C(34)-C(27)	0.23(14)

## Fortsetzung

C(12)-C(1)-C(11)-C(4)	-177.07(11)	C(35)-C(24)-C(34)-C(27)	176.13(11)
C(2)-C(1)-C(11)-N(1)	-178.77(14)	C(25)-C(24)-C(34)-N(2)	-178.60(14)
C(12)-C(1)-C(11)-N(1)	3.1(2)	C(35)-C(24)-C(34)-N(2)	-2.7(2)
C(2)-C(1)-C(12)-C(17)	91.41(17)	C(25)-C(24)-C(35)-C(40)	-89.90(17)
C(11)-C(1)-C(12)-C(17)	-91.01(16)	C(34)-C(24)-C(35)-C(40)	95.17(16)
C(2)-C(1)-C(12)-C(13)	-91.88(17)	C(25)-C(24)-C(35)-C(36)	92.12(17)
C(11)-C(1)-C(12)-C(13)	85.70(15)	C(34)-C(24)-C(35)-C(36)	-82.81(16)
C(17)-C(12)-C(13)-C(14)	-0.80(19)	C(40)-C(35)-C(36)-C(37)	1.8(2)
C(1)-C(12)-C(13)-C(14)	-177.62(11)	C(24)-C(35)-C(36)-C(37)	179.89(12)
C(12)-C(13)-C(14)-C(15)	0.8(2)	C(35)-C(36)-C(37)-C(38)	-0.4(2)
C(13)-C(14)-C(15)-C(16)	-0.5(2)	C(36)-C(37)-C(38)-C(39)	-0.9(2)
C(14)-C(15)-C(16)-C(17)	0.4(2)	C(37)-C(38)-C(39)-C(40)	0.7(2)
C(15)-C(16)-C(17)-C(12)	-0.5(2)	C(36)-C(35)-C(40)-C(39)	-2.1(2)
C(13)-C(12)-C(17)-C(16)	0.7(2)	C(24)-C(35)-C(40)-C(39)	179.92(13)
C(1)-C(12)-C(17)-C(16)	177.41(13)	C(38)-C(39)-C(40)-C(35)	0.8(2)
C(1)-C(2)-C(18)-C(19)	2.4(2)	C(24)-C(25)-C(41)-C(46)	-144.92(14)
C(3)-C(2)-C(18)-C(19)	-177.81(13)	C(26)-C(25)-C(41)-C(46)	32.05(18)
C(1)-C(2)-C(18)-C(23)	-177.91(13)	C(24)-C(25)-C(41)-C(42)	34.5(2)
C(3)-C(2)-C(18)-C(23)	1.89(18)	C(26)-C(25)-C(41)-C(42)	-148.50(14)
C(23)-C(18)-C(19)-C(20)	-0.5(2)	C(46)-C(41)-C(42)-C(43)	1.0(2)
C(2)-C(18)-C(19)-C(20)	179.18(13)	C(25)-C(41)-C(42)-C(43)	-178.44(13)
C(18)-C(19)-C(20)-C(21)	0.6(2)	C(41)-C(42)-C(43)-C(44)	-0.7(2)
C(19)-C(20)-C(21)-C(22)	-0.1(3)	C(42)-C(43)-C(44)-C(45)	0.2(2)
C(20)-C(21)-C(22)-C(23)	-0.4(3)	C(43)-C(44)-C(45)-C(46)	0.0(2)
C(21)-C(22)-C(23)-C(18)	0.4(3)	C(44)-C(45)-C(46)-C(41)	0.4(2)
C(19)-C(18)-C(23)-C(22)	0.0(2)	C(42)-C(41)-C(46)-C(45)	-0.8(2)
C(2)-C(18)-C(23)-C(22)	-179.68(15)	C(25)-C(41)-C(46)-C(45)	178.64(12)

**Kristallstrukturdaten von *anti*-10-(4,5,6,7,8,9-Hexahydrocyclooctatriazol-1-yl)-1,4,8,10-tetraphenyl-2,4,6-triazatricyclo[5.2.1.0<sup>2,6</sup>]dec-8-en-3,5-dion *anti*-79 (Abb. 3)**

**Crystal data for *anti*-79**

Crystal shape	fragment	Volume	2044.92(10) Å <sup>3</sup>
Crystal colour	colorless	Z	2
Crystal size	0.50 x 0.20 x 0.20 mm	Density (calculated)	1.397 g/cm <sup>3</sup>
Chemical formula	C <sub>39</sub> H <sub>37</sub> N <sub>6</sub> O <sub>2</sub> · 2(CHCl <sub>3</sub> )	Radiation used	MoK <sub>α</sub>
Formula weight	860.48	Wavelength	0.71073 Å
Crystal system	Triclinic	Linear absorption coefficient	0.464 mm <sup>-1</sup>
Space group	P-1	Temperature	173(2) K
Unit cell dimensions	a = 11.1015(4) Å    α = 99.140(2)° b = 12.01330(10) Å    β = 91.997(2)° c = 16.5830(5) Å    γ = 109.810(2)°		

**Data collection details for *anti*-79**

Diffractometer	BRUKER Smart CCD	Number of measured reflections	13142
Scan method	ω scans	Number of independent refl.	9093
Absorption correction	Empirical	Number of observed reflections	3366
Max. and min. transmission	0.9129 and 0.8011	Criterion of recognition (σ-limit)	>2σ(I)
R(int) =	0.0654	Index ranges	-12<=h<=14, -15<=k<=14, -21<=l<=17
θ-range for data collection	1.25 to 27.50°		
Completeness to θ = 27.50°	96.6 %		
F(000)	890		

**Refinement details for *anti*-79**

Refinement method	Full-matrix least-squares on F <sup>2</sup>		
Final R indices [I>2σ(I)]	R1 = 0.0916, wR2 = 0.1761		
R indices (all data)	R1 = 0.2556, wR2 = 0.2481		
R1 [=Σ( Fo - Fc )/Σ Fo ]			
wR2 [=Σ(w(Fo <sup>2</sup> -Fc <sup>2</sup> ) <sup>2</sup> )/Σ(wFo <sup>4</sup> )] <sup>1/2</sup>			
H-locating and refining method	geom/constr	Number of reflections used	9093

## Fortsetzung

Number of L.S. restraints	0	Number of refined parameters	506
Goodness-of-fit on $F^2$	1.009		
$S = [\sum w(F_o^2 - F_c^2)^2] / (n-p)^{1/2}$	n=number of reflections, p=parameters used.		
Definition of w			
calc $w = 1 / [\sigma^2(F_o^2) + (0.0841P)^2 + 0.4466P]$ where $P = (F_o^2 + 2F_c^2) / 3$			
Maximum d/s	0.012		
Maximum e-density	0.588 e Å <sup>-3</sup>	Minimum e-density	-0.501 e Å <sup>-3</sup>

Computer Programs used for *anti-79*

Data collection program	SMART	Structure solving program	SHELXS-97 (Sheldrick, 1990)
Cell refinement program	SAINT	Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Data reduction program	XPREP	Pictures drawn with	ZORTEP

Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters (Å<sup>2</sup> × 10<sup>3</sup>) for *anti-79*

U(eq) is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.

	x	y	z	U(eq)		x	y	z	U(eq)
Cl(1)	4317(2)	6200(2)	2504(2)	97(1)	C(16)	8345(6)	5250(6)	2030(3)	43(2)
O(1)	11980(4)	5575(3)	-89(2)	34(1)	C(17)	7111(8)	5279(10)	2315(6)	41(3)
N(1)	11817(4)	6756(4)	1123(2)	27(1)	C(17)	7410(18)	4206(19)	2281(10)	53(7)
C(1)	10563(5)	6945(5)	952(3)	26(1)	C(18)	6657(7)	4598(8)	3058(4)	67(2)
Cl(2)	5262(3)	7726(3)	4043(2)	115(1)	C(19)	7366(7)	5423(7)	3843(4)	61(2)
O(2)	14652(4)	9211(3)	1333(2)	36(1)	C(20)	8317(6)	4993(6)	4284(4)	45(2)
N(2)	12667(4)	7881(4)	1592(2)	26(1)	C(21)	9321(6)	4734(6)	3768(4)	41(2)
N(3)	13627(4)	7313(4)	523(2)	27(1)	C(22)	9971(5)	5694(5)	3308(3)	29(1)
Cl(3)	3694(3)	5257(3)	3963(2)	150(2)	C(23)	12459(5)	9724(5)	2450(3)	27(1)
C(3)	12428(6)	6456(5)	438(3)	31(1)	C(24)	12012(5)	10680(5)	2519(3)	34(1)
Cl(4)	138(2)	1795(2)	4348(1)	82(1)	C(25)	12587(6)	11698(5)	3125(4)	45(2)
N(4)	10511(4)	6919(4)	2445(2)	25(1)	C(26)	13599(6)	11763(6)	3645(4)	46(2)
C(4)	13769(6)	8274(5)	1164(3)	28(1)	C(27)	14050(6)	10825(6)	3585(4)	43(2)
Cl(5)	-2429(2)	1578(2)	3884(2)	86(1)	C(28)	13485(5)	9806(5)	2988(3)	34(1)
N(5)	11457(4)	7298(4)	3063(3)	32(1)	C(29)	8503(5)	8035(5)	1316(3)	35(1)
C(5)	10843(5)	7927(5)	435(3)	27(1)	C(30)	7476(5)	8421(5)	1479(4)	39(2)
Cl(6)	-1902(3)	416(2)	5169(1)	118(1)	C(31)	7326(6)	8861(5)	2274(4)	43(2)
N(6)	11131(5)	6563(4)	3570(3)	35(1)	C(32)	8205(6)	8926(5)	2900(4)	36(2)
C(6)	11578(5)	8945(5)	936(3)	31(1)	C(33)	9247(6)	8572(5)	2734(3)	33(1)
C(7)	11859(5)	8667(5)	1766(3)	27(1)	C(34)	9400(5)	8111(5)	1935(3)	29(1)
C(8)	10509(5)	7646(5)	1808(3)	28(1)	C(35)	10472(5)	7699(5)	-451(3)	30(1)
C(9)	14551(5)	7312(5)	-66(3)	28(1)	C(36)	9634(5)	6585(5)	-850(3)	33(1)
C(10)	14724(6)	8055(5)	-632(4)	41(2)	C(37)	9285(6)	6360(6)	-1684(3)	38(2)
C(11)	15608(6)	8035(6)	-1203(4)	48(2)	C(38)	9794(6)	7237(6)	-2134(3)	43(2)
C(12)	16285(6)	7253(6)	-1192(4)	47(2)	C(39)	10619(7)	8343(6)	-1758(4)	53(2)
C(13)	16097(6)	6524(6)	-628(4)	48(2)	C(40)	10964(7)	8583(6)	-916(4)	50(2)
C(14)	15226(6)	6542(5)	-53(4)	36(2)	C(41)	3994(7)	6512(7)	3527(5)	73(2)
C(15)	9551(5)	5924(5)	2585(3)	27(1)	C(42)	-1332(7)	1655(6)	4707(4)	64(2)

Bond lengths [Å] for *anti-79*

Cl(1)-C(41)	1.755(8)	C(5)-C(6)	1.343(7)	C(19)-C(20)	1.534(9)
O(1)-C(3)	1.204(6)	C(5)-C(35)	1.469(7)	C(20)-C(21)	1.513(8)
N(1)-C(3)	1.403(7)	Cl(6)-C(42)	1.720(7)	C(21)-C(22)	1.479(8)
N(1)-N(2)	1.439(6)	N(6)-C(22)	1.358(7)	C(23)-C(24)	1.388(7)
N(1)-C(1)	1.509(6)	C(6)-C(7)	1.514(7)	C(23)-C(28)	1.388(7)
C(1)-C(5)	1.521(7)	C(7)-C(23)	1.503(7)	C(24)-C(25)	1.396(8)
C(1)-C(8)	1.545(7)	C(7)-C(8)	1.594(7)	C(25)-C(26)	1.365(8)
Cl(2)-C(41)	1.723(8)	C(8)-C(34)	1.523(7)	C(26)-C(27)	1.371(8)
O(2)-C(4)	1.199(6)	C(9)-C(10)	1.369(8)	C(27)-C(28)	1.387(8)
N(2)-C(4)	1.414(7)	C(9)-C(14)	1.376(7)	C(29)-C(34)	1.375(7)
N(2)-C(7)	1.512(6)	C(10)-C(11)	1.390(8)	C(29)-C(30)	1.389(8)
N(3)-C(3)	1.366(7)	C(11)-C(12)	1.390(8)	C(30)-C(31)	1.376(8)
N(3)-C(4)	1.402(6)	C(12)-C(13)	1.355(9)	C(31)-C(32)	1.374(8)
N(3)-C(9)	1.440(6)	C(13)-C(14)	1.384(8)	C(32)-C(33)	1.382(7)
Cl(3)-C(41)	1.712(8)	C(15)-C(22)	1.373(7)	C(33)-C(34)	1.392(7)
Cl(4)-C(42)	1.720(7)	C(15)-C(16)	1.496(8)	C(35)-C(40)	1.385(8)

## Fortsetzung

N(4)-N(5)	1.346(6)	C(16)-C(17)	1.462(19)	C(35)-C(36)	1.388(7)
N(4)-C(15)	1.364(6)	C(16)-C(17)	1.474(11)	C(36)-C(37)	1.381(7)
N(4)-C(8)	1.474(7)	C(17)-C(18)	1.589(11)	C(37)-C(38)	1.364(8)
Cl(5)-C(42)	1.768(8)	C(17)-C(18)	1.653(19)	C(38)-C(39)	1.366(8)
N(5)-N(6)	1.288(6)	C(18)-C(19)	1.511(9)	C(39)-C(40)	1.392(8)

Angles [°] for *anti-79*

C(3)-N(1)-N(2)	107.8(4)	C(6)-C(5)-C(1)	105.8(5)	C(27)-C(28)-C(23)	120.5(6)
C(3)-N(1)-C(1)	116.7(4)	C(35)-C(5)-C(1)	123.8(5)	C(34)-C(29)-C(30)	121.1(5)
N(2)-N(1)-C(1)	105.5(4)	C(17)-C(16)-C(17)	58.3(9)	C(31)-C(30)-C(29)	119.9(6)
N(1)-C(1)-C(5)	106.6(4)	C(17)-C(16)-C(15)	117.9(9)	C(32)-C(31)-C(30)	119.6(6)
N(1)-C(1)-C(8)	98.1(4)	C(17)-C(16)-C(15)	118.6(6)	C(31)-C(32)-C(33)	120.3(5)
C(5)-C(1)-C(8)	101.7(4)	C(16)-C(17)-C(18)	115.1(7)	C(32)-C(33)-C(34)	120.6(5)
C(4)-N(2)-N(1)	107.6(4)	C(16)-C(17)-C(18)	112.0(13)	C(29)-C(34)-C(33)	118.4(5)
C(4)-N(2)-C(7)	119.6(4)	C(19)-C(18)-C(17)	108.2(7)	C(29)-C(34)-C(8)	123.8(5)
N(1)-N(2)-C(7)	106.0(4)	C(19)-C(18)-C(17)	122.6(8)	C(33)-C(34)-C(8)	117.7(5)
C(3)-N(3)-C(4)	112.2(5)	C(17)-C(18)-C(17)	52.3(8)	C(40)-C(35)-C(36)	117.9(5)
C(3)-N(3)-C(9)	123.0(4)	C(18)-C(19)-C(20)	115.0(6)	C(40)-C(35)-C(5)	121.0(5)
C(4)-N(3)-C(9)	124.1(5)	C(21)-C(20)-C(19)	115.2(5)	C(36)-C(35)-C(5)	121.1(5)
O(1)-C(3)-N(3)	128.0(5)	C(22)-C(21)-C(20)	114.0(5)	C(37)-C(36)-C(35)	121.5(6)
O(1)-C(3)-N(1)	125.5(5)	N(6)-C(22)-C(15)	107.2(5)	C(38)-C(37)-C(36)	119.7(6)
N(3)-C(3)-N(1)	106.4(5)	N(6)-C(22)-C(21)	123.6(5)	C(37)-C(38)-C(39)	120.1(6)
N(5)-N(4)-C(15)	110.0(4)	C(15)-C(22)-C(21)	129.2(5)	C(38)-C(39)-C(40)	120.5(6)
N(5)-N(4)-C(8)	121.1(4)	C(24)-C(23)-C(28)	118.8(5)	C(35)-C(40)-C(39)	120.2(6)
C(15)-N(4)-C(8)	128.2(4)	C(24)-C(23)-C(7)	118.6(5)	Cl(3)-C(41)-Cl(2)	113.0(5)
O(2)-C(4)-N(3)	127.8(5)	C(28)-C(23)-C(7)	122.4(5)	Cl(3)-C(41)-Cl(1)	110.1(4)
O(2)-C(4)-N(2)	127.2(5)	C(23)-C(24)-C(25)	120.0(6)	Cl(2)-C(41)-Cl(1)	108.8(4)
N(3)-C(4)-N(2)	104.9(5)	C(26)-C(25)-C(24)	120.2(6)	Cl(4)-C(42)-Cl(6)	111.8(5)
N(6)-N(5)-N(4)	107.3(4)	C(25)-C(26)-C(27)	120.5(6)	Cl(4)-C(42)-Cl(5)	109.0(4)
C(6)-C(5)-C(35)	130.1(5)	C(26)-C(27)-C(28)	120.0(6)	Cl(6)-C(42)-Cl(5)	110.8(4)

Symmetry transformations used to generate equivalent atoms:

Torsion angles [°] for *anti-79*

C(3)-N(1)-C(1)-C(5)	-57.0(5)	N(1)-C(1)-C(8)-N(4)	-59.4(5)	N(5)-N(6)-C(22)-C(21)	-178.4(5)
N(2)-N(1)-C(1)-C(5)	62.7(5)	C(5)-C(1)-C(8)-N(4)	-168.3(4)	N(4)-C(15)-C(22)-N(6)	1.2(6)
C(3)-N(1)-C(1)-C(8)	-161.8(4)	N(1)-C(1)-C(8)-C(34)	176.9(4)	C(16)-C(15)-C(22)-N(6)	179.3(5)
N(2)-N(1)-C(1)-C(8)	-42.1(4)	C(5)-C(1)-C(8)-C(34)	68.0(6)	N(4)-C(15)-C(22)-C(21)	179.0(5)
C(3)-N(1)-N(2)-C(4)	2.3(5)	N(1)-C(1)-C(8)-C(7)	57.8(4)	C(16)-C(15)-C(22)-C(21)	-3.0(10)
C(1)-N(1)-N(2)-C(4)	-123.1(4)	C(5)-C(1)-C(8)-C(7)	-51.2(4)	C(20)-C(21)-C(22)-N(6)	97.5(7)
C(3)-N(1)-N(2)-C(7)	131.3(4)	C(23)-C(7)-C(8)-N(4)	-65.8(6)	C(20)-C(21)-C(22)-C(15)	-79.9(8)
C(1)-N(1)-N(2)-C(7)	5.9(5)	N(2)-C(7)-C(8)-N(4)	59.6(5)	N(2)-C(7)-C(23)-C(24)	162.3(5)
C(4)-N(3)-C(3)-O(1)	174.0(5)	C(6)-C(7)-C(8)-N(4)	165.1(4)	C(6)-C(7)-C(23)-C(24)	41.5(7)
C(9)-N(3)-C(3)-O(1)	3.6(9)	C(23)-C(7)-C(8)-C(34)	57.8(7)	C(8)-C(7)-C(23)-C(24)	-79.1(7)
C(4)-N(3)-C(3)-N(1)	-9.5(6)	N(2)-C(7)-C(8)-C(34)	-176.9(4)	N(2)-C(7)-C(23)-C(28)	-14.4(7)
C(9)-N(3)-C(3)-N(1)	-179.9(4)	C(6)-C(7)-C(8)-C(34)	-71.3(5)	C(6)-C(7)-C(23)-C(28)	-135.1(5)
N(2)-N(1)-C(3)-O(1)	-179.1(5)	C(23)-C(7)-C(8)-C(1)	-179.7(5)	C(8)-C(7)-C(23)-C(28)	104.2(6)
C(1)-N(1)-C(3)-O(1)	-60.7(7)	N(2)-C(7)-C(8)-C(1)	-54.4(4)	C(28)-C(23)-C(24)-C(25)	-0.4(8)
N(2)-N(1)-C(3)-N(3)	4.2(5)	C(6)-C(7)-C(8)-C(1)	51.2(4)	C(7)-C(23)-C(24)-C(25)	-177.2(5)
C(1)-N(1)-C(3)-N(3)	122.7(5)	C(3)-N(3)-C(9)-C(10)	100.3(6)	C(23)-C(24)-C(25)-C(26)	0.7(9)
C(3)-N(3)-C(4)-O(2)	-171.5(5)	C(4)-N(3)-C(9)-C(10)	-68.9(7)	C(24)-C(25)-C(26)-C(27)	-0.7(9)
C(9)-N(3)-C(4)-O(2)	-1.3(9)	C(3)-N(3)-C(9)-C(14)	-78.6(7)	C(25)-C(26)-C(27)-C(28)	0.5(9)
C(3)-N(3)-C(4)-N(2)	10.9(6)	C(4)-N(3)-C(9)-C(14)	112.1(6)	C(26)-C(27)-C(28)-C(23)	-0.2(9)
C(9)-N(3)-C(4)-N(2)	-178.9(4)	C(14)-C(9)-C(10)-C(11)	-0.3(9)	C(24)-C(23)-C(28)-C(27)	0.2(8)
N(1)-N(2)-C(4)-O(2)	174.7(5)	N(3)-C(9)-C(10)-C(11)	-179.2(5)	C(7)-C(23)-C(28)-C(27)	176.8(5)
C(7)-N(2)-C(4)-O(2)	53.9(7)	C(9)-C(10)-C(11)-C(12)	0.6(10)	C(34)-C(29)-C(30)-C(31)	-1.7(9)
N(1)-N(2)-C(4)-N(3)	-7.6(5)	C(10)-C(11)-C(12)-C(13)	-0.5(10)	C(29)-C(30)-C(31)-C(32)	0.7(9)
C(7)-N(2)-C(4)-N(3)	-128.4(4)	C(11)-C(12)-C(13)-C(14)	0.1(10)	C(30)-C(31)-C(32)-C(33)	1.1(9)
C(15)-N(4)-N(5)-N(6)	1.2(5)	C(10)-C(9)-C(14)-C(13)	-0.1(9)	C(31)-C(32)-C(33)-C(34)	-2.0(8)
C(8)-N(4)-N(5)-N(6)	172.6(4)	N(3)-C(9)-C(14)-C(13)	178.8(5)	C(30)-C(29)-C(34)-C(33)	0.8(8)
N(1)-C(1)-C(5)-C(6)	-69.2(5)	C(12)-C(13)-C(14)-C(9)	0.2(9)	C(30)-C(29)-C(34)-C(8)	176.7(5)
C(8)-C(1)-C(5)-C(6)	33.1(5)	N(5)-N(4)-C(15)-C(22)	-1.5(5)	C(32)-C(33)-C(34)-C(29)	1.0(8)
N(1)-C(1)-C(5)-C(35)	104.5(5)	C(8)-N(4)-C(15)-C(22)	-172.1(5)	C(32)-C(33)-C(34)-C(8)	-175.1(5)
C(8)-C(1)-C(5)-C(35)	-153.3(5)	N(5)-N(4)-C(15)-C(16)	-179.7(5)	N(4)-C(8)-C(34)-C(29)	-131.3(5)
N(4)-N(5)-N(6)-C(22)	-0.4(5)	C(8)-N(4)-C(15)-C(16)	9.7(8)	C(1)-C(8)-C(34)-C(29)	-5.7(8)

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C(35)-C(5)-C(6)-C(7)	-170.3(5)	N(4)-C(15)-C(16)-C(17)	-179.4(11)	C(7)-C(8)-C(34)-C(29)	101.2(6)
C(1)-C(5)-C(6)-C(7)	2.8(6)	C(22)-C(15)-C(16)-C(17)	2.8(13)	N(4)-C(8)-C(34)-C(33)	44.6(6)
C(4)-N(2)-C(7)-C(23)	-75.6(6)	N(4)-C(15)-C(16)-C(17)	-112.3(7)	C(1)-C(8)-C(34)-C(33)	170.2(5)
N(1)-N(2)-C(7)-C(23)	162.8(4)	C(22)-C(15)-C(16)-C(17)	70.0(9)	C(7)-C(8)-C(34)-C(33)	-82.9(6)
C(4)-N(2)-C(7)-C(6)	52.1(6)	C(17)-C(16)-C(17)-C(18)	38.9(10)	C(6)-C(5)-C(35)-C(40)	4.7(9)
N(1)-N(2)-C(7)-C(6)	-69.5(5)	C(15)-C(16)-C(17)-C(18)	-68.0(10)	C(1)-C(5)-C(35)-C(40)	-167.3(5)
C(4)-N(2)-C(7)-C(8)	152.9(4)	C(17)-C(16)-C(17)-C(18)	-36.1(10)	C(6)-C(5)-C(35)-C(36)	-176.2(6)
N(1)-N(2)-C(7)-C(8)	31.3(4)	C(15)-C(16)-C(17)-C(18)	71.8(15)	C(1)-C(5)-C(35)-C(36)	11.7(8)
C(5)-C(6)-C(7)-C(23)	-168.9(5)	C(16)-C(17)-C(18)-C(19)	80.9(9)	C(40)-C(35)-C(36)-C(37)	-0.6(8)
C(5)-C(6)-C(7)-N(2)	65.4(5)	C(16)-C(17)-C(18)-C(17)	-36.6(10)	C(5)-C(35)-C(36)-C(37)	-179.7(5)
C(5)-C(6)-C(7)-C(8)	-36.0(5)	C(16)-C(17)-C(18)-C(19)	-52.5(17)	C(35)-C(36)-C(37)-C(38)	1.6(9)
N(5)-N(4)-C(8)-C(34)	-110.7(5)	C(16)-C(17)-C(18)-C(17)	36.0(10)	C(36)-C(37)-C(38)-C(39)	-1.7(9)
C(15)-N(4)-C(8)-C(34)	58.9(6)	C(17)-C(18)-C(19)-C(20)	-113.5(7)	C(37)-C(38)-C(39)-C(40)	0.9(10)
N(5)-N(4)-C(8)-C(1)	119.3(5)	C(17)-C(18)-C(19)-C(20)	-57.2(12)	C(36)-C(35)-C(40)-C(39)	-0.2(9)
C(15)-N(4)-C(8)-C(1)	-71.1(6)	C(18)-C(19)-C(20)-C(21)	55.0(8)	C(5)-C(35)-C(40)-C(39)	178.9(6)
N(5)-N(4)-C(8)-C(7)	16.7(6)	C(19)-C(20)-C(21)-C(22)	47.9(8)	C(38)-C(39)-C(40)-C(35)	0.0(10)
C(15)-N(4)-C(8)-C(7)	-173.7(4)	N(5)-N(6)-C(22)-C(15)	-0.5(6)		

**Kristallstrukturdaten von 1,1'-(2,3,4,5-Tetrachlorcyclopenta-2,4-dienyliden)-bis-(4,5,6,7,8,9-hexahydro-1H-cyclooctatriazol) 80 (Abb. 4)**
**Crystal data for 80**

Crystal shape	plate	Volume	2203.88(8) Å <sup>3</sup>
Crystal colour	colorless	Z	4
Crystal size	0.2 x 0.15 x 0.05 mm	Density (calculated)	1.514 g/cm <sup>3</sup>
Chemical formula	C <sub>21</sub> H <sub>24</sub> Cl <sub>4</sub> N <sub>6</sub>	Radiation used	MoK <sub>α</sub>
Formula weight	502.26	Wavelength	0.71073 Å
Crystal system	Monoclinic	Linear absorption coefficient	0.560 mm <sup>-1</sup>
Space group	P2(1)/n	Temperature	173(2) K
Unit cell dimensions	a = 10.1418(2) Å    α = 90° b = 13.1913(3) Å    β = 94.6290(10)° c = 16.5274(3) Å    γ = 90°		

**Data collection details for 80**

Diffractometer	BRUKER Smart CCD	Number of measured reflections	8117
Scan method	ω scans	Number of independent refl.	4210
Absorption correction	Empirical	Number of observed reflections	2930
Max. and min. transmission	0.894442 and 0.687224	Criterion of recognition (σ-limit)	>2σ(I)
R(int) =	0.0446	Index ranges	-13<=h<=8, -16<=k<=15, -7<=l<=21
Theta range for data collection	1.98 to 29.19°		
Completeness to theta = 29.19°	70.7 %		
F(000)	1040		

**Refinement details for 80**

Refinement method	Full-matrix least-squares on F <sup>2</sup>		
Final R indices [I>2σ(I)]	R1 = 0.0470, wR2 = 0.0941		
R indices (all data)	R1 = 0.0844, wR2 = 0.1060		
R1 [=Σ( Fo - Fc )/Σ Fo ]			
wR2 [=Σ(w(Fo <sup>2</sup> -Fc <sup>2</sup> ) <sup>2</sup> )/Σ(wFo <sup>4</sup> )] <sup>1/2</sup>			
H-locating and refining method	difmap/refall	Number of reflections used	4210
Number of L.S. restraints	0	Number of refined parameters	376
Goodness-of-fit on F <sup>2</sup>	1.009		
S [=Σw(Fo <sup>2</sup> -Fc <sup>2</sup> ) <sup>2</sup> ]/(n-p) <sup>1/2</sup>	n=number of reflections, p=parameters used.		
Definition of w	calc w=1/[σ <sup>2</sup> (Fo <sup>2</sup> )+(0.0456P) <sup>2</sup> +0.0000P] where P=(Fo <sup>2</sup> +2Fc <sup>2</sup> )/3		
Maximum d/s	0.004		
Maximum e-density	0.360 e Å <sup>-3</sup>	Minimum e-density	-0.365 e Å <sup>-3</sup>

**Computer Programs used for 80**

Data collection program	SMART	Structure solving program	SHELXS-97 (Sheldrick, 1990)
Cell refinement program	SAINT	Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Data reduction program	SAINT	Pictures drawn with	ZORTEP

**Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 80**U(eq) is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.

	x	y	z	U(eq)		x	y	z	U(eq)
Cl(1)	-580(1)	497(1)	2643(1)	25(1)	C(7)	-4579(3)	3032(3)	1330(2)	29(1)
Cl(2)	1553(1)	1276(1)	4160(1)	30(1)	C(8)	-5333(3)	2268(3)	1827(2)	36(1)
Cl(3)	2932(1)	3497(1)	3654(1)	30(1)	C(9)	-4701(4)	1221(3)	1941(2)	37(1)
Cl(4)	1795(1)	4186(1)	1808(1)	26(1)	C(10)	-4530(4)	618(3)	1175(2)	38(1)
N(1)	-1030(2)	2737(2)	1804(1)	17(1)	C(11)	-3613(3)	1052(3)	560(2)	30(1)
N(2)	-1287(2)	3626(2)	2189(1)	20(1)	C(12)	-2233(3)	1382(3)	909(2)	24(1)
N(3)	-2560(2)	3800(2)	2039(1)	23(1)	C(13)	-2166(3)	2337(3)	1409(2)	19(1)
N(4)	738(2)	1909(2)	1181(1)	17(1)	C(14)	1409(3)	1637(3)	-1(2)	21(1)
N(5)	1423(2)	1022(2)	1230(1)	22(1)	C(15)	1837(3)	1697(3)	-855(2)	28(1)
N(6)	1819(2)	864(2)	502(1)	26(1)	C(16)	2929(4)	2497(3)	-949(2)	34(1)
C(1)	320(3)	2339(2)	1946(2)	18(1)	C(17)	2840(3)	3479(3)	-459(2)	31(1)
C(2)	399(3)	1536(2)	2631(2)	18(1)	C(18)	1662(3)	4165(3)	-703(2)	30(1)
C(3)	1226(3)	1870(3)	3247(2)	19(1)	C(19)	276(3)	3723(3)	-670(2)	23(1)
C(4)	1796(3)	2853(3)	3039(2)	20(1)	C(20)	-50(3)	3270(3)	153(2)	23(1)
C(5)	1294(3)	3140(2)	2306(2)	18(1)	C(21)	703(3)	2340(3)	415(2)	19(1)
C(6)	-3121(3)	3041(3)	1566(2)	21(1)					

**Bond lengths [ $\text{\AA}$ ] for 80**

Cl(1)-C(2)	1.694(3)	C(6)-C(7)	1.498(4)	C(14)-C(15)	1.511(4)
Cl(2)-C(3)	1.708(3)	C(7)-C(8)	1.542(5)	C(15)-C(16)	1.547(5)
Cl(3)-C(4)	1.701(3)	C(7)-H(7A)	0.95(4)	C(15)-H(15A)	0.97(3)
Cl(4)-C(5)	1.706(3)	C(7)-H(7B)	1.03(3)	C(15)-H(15B)	1.01(4)
N(1)-N(2)	1.369(3)	C(8)-C(9)	1.528(6)	C(16)-C(17)	1.534(5)
N(1)-C(13)	1.382(4)	C(8)-H(8A)	0.97(3)	C(16)-H(16A)	0.88(3)
N(1)-C(1)	1.468(4)	C(8)-H(8B)	1.02(4)	C(16)-H(16B)	1.01(4)
N(2)-N(3)	1.316(3)	C(9)-C(10)	1.517(5)	C(17)-C(18)	1.527(5)
N(3)-C(6)	1.365(4)	C(9)-H(9A)	1.00(3)	C(17)-H(17A)	1.02(3)
N(4)-N(5)	1.359(3)	C(9)-H(9B)	0.95(4)	C(17)-H(17B)	0.96(3)
N(4)-C(21)	1.387(3)	C(10)-C(11)	1.543(5)	C(18)-C(19)	1.528(5)
N(4)-C(1)	1.478(3)	C(10)-H(10A)	1.01(4)	C(18)-H(18A)	1.02(4)
N(5)-N(6)	1.315(3)	C(10)-H(10B)	0.95(4)	C(18)-H(18B)	0.96(3)
N(6)-C(14)	1.360(4)	C(11)-C(12)	1.533(5)	C(19)-C(20)	1.545(4)
C(1)-C(5)	1.533(4)	C(11)-H(11A)	0.98(3)	C(19)-H(19A)	0.96(3)
C(1)-C(2)	1.548(4)	C(11)-H(11B)	1.03(3)	C(19)-H(19B)	0.91(3)
C(2)-C(3)	1.341(4)	C(12)-C(13)	1.505(4)	C(20)-C(21)	1.491(4)
C(3)-C(4)	1.472(4)	C(12)-H(12A)	1.04(3)	C(20)-H(20A)	0.94(3)
C(4)-C(5)	1.331(4)	C(12)-H(12B)	0.94(4)	C(20)-H(20B)	1.03(3)
C(6)-C(13)	1.381(4)	C(14)-C(21)	1.387(4)		

**Angles [ $^\circ$ ] for 80**

N(2)-N(1)-C(13)	111.4(2)	C(9)-C(8)-H(8A)	109(2)	C(14)-C(15)-H(15B)	107.4(18)
N(2)-N(1)-C(1)	116.2(2)	C(7)-C(8)-H(8A)	109(2)	C(16)-C(15)-H(15B)	110.7(18)
C(13)-N(1)-C(1)	132.1(3)	C(9)-C(8)-H(8B)	112(2)	H(15A)-C(15)-H(15B)	106(2)
N(3)-N(2)-N(1)	106.4(2)	C(7)-C(8)-H(8B)	107(2)	C(17)-C(16)-C(15)	116.7(2)
N(2)-N(3)-C(6)	109.7(2)	H(8A)-C(8)-H(8B)	104(3)	C(17)-C(16)-H(16A)	109(2)
N(5)-N(4)-C(21)	112.5(2)	C(10)-C(9)-C(8)	116.5(3)	C(15)-C(16)-H(16A)	102(2)
N(5)-N(4)-C(1)	117.4(2)	C(10)-C(9)-H(9A)	111.1(18)	C(17)-C(16)-H(16B)	107(2)
C(21)-N(4)-C(1)	129.5(3)	C(8)-C(9)-H(9A)	107(2)	C(15)-C(16)-H(16B)	106(2)
N(6)-N(5)-N(4)	106.0(2)	C(10)-C(9)-H(9B)	105(2)	H(16A)-C(16)-H(16B)	117(3)
N(5)-N(6)-C(14)	109.8(2)	C(8)-C(9)-H(9B)	108(2)	C(18)-C(17)-C(16)	116.1(3)
N(1)-C(1)-N(4)	109.2(2)	H(9A)-C(9)-H(9B)	108(3)	C(18)-C(17)-H(17A)	109.1(17)
N(1)-C(1)-C(5)	112.2(3)	C(9)-C(10)-C(11)	118.1(3)	C(16)-C(17)-H(17A)	111.8(19)
N(4)-C(1)-C(5)	112.1(2)	C(9)-C(10)-H(10A)	111.7(19)	C(18)-C(17)-H(17B)	103(2)
N(1)-C(1)-C(2)	110.8(2)	C(11)-C(10)-H(10A)	106.6(19)	C(16)-C(17)-H(17B)	114(2)
N(4)-C(1)-C(2)	111.2(2)	C(9)-C(10)-H(10B)	106(2)	H(17A)-C(17)-H(17B)	101(2)
C(5)-C(1)-C(2)	101.2(2)	C(11)-C(10)-H(10B)	106.9(19)	C(17)-C(18)-C(19)	117.8(3)
C(3)-C(2)-C(1)	108.9(3)	H(10A)-C(10)-H(10B)	106(3)	C(17)-C(18)-H(18A)	104(2)
C(3)-C(2)-Cl(1)	126.0(2)	C(12)-C(11)-C(10)	116.0(3)	C(19)-C(18)-H(18A)	111.0(18)
C(1)-C(2)-Cl(1)	124.5(2)	C(12)-C(11)-H(11A)	108.4(18)	C(17)-C(18)-H(18B)	109.8(19)
C(2)-C(3)-C(4)	110.2(2)	C(10)-C(11)-H(11A)	110.9(15)	C(19)-C(18)-H(18B)	109.2(19)
C(2)-C(3)-Cl(2)	125.8(3)	C(12)-C(11)-H(11B)	102.9(16)	H(18A)-C(18)-H(18B)	104(3)
C(4)-C(3)-Cl(2)	123.9(2)	C(10)-C(11)-H(11B)	108.3(18)	C(18)-C(19)-C(20)	116.2(3)
C(5)-C(4)-C(3)	109.6(3)	H(11A)-C(11)-H(11B)	110(2)	C(18)-C(19)-H(19A)	108.8(15)

## Fortsetzung

C(5)-C(4)-Cl(3)	126.3(3)	C(13)-C(12)-C(11)	116.3(3)	C(20)-C(19)-H(19A)	108.3(17)
C(3)-C(4)-Cl(3)	124.1(2)	C(13)-C(12)-H(12A)	107(2)	C(18)-C(19)-H(19B)	106(2)
C(4)-C(5)-C(1)	110.2(3)	C(11)-C(12)-H(12A)	103.6(19)	C(20)-C(19)-H(19B)	109.7(18)
C(4)-C(5)-Cl(4)	124.2(2)	C(13)-C(12)-H(12B)	109(2)	H(19A)-C(19)-H(19B)	108(3)
C(1)-C(5)-Cl(4)	125.3(2)	C(11)-C(12)-H(12B)	111(2)	C(21)-C(20)-C(19)	115.7(2)
N(3)-C(6)-C(13)	109.5(2)	H(12A)-C(12)-H(12B)	110(3)	C(21)-C(20)-H(20A)	110.8(18)
N(3)-C(6)-C(7)	120.7(3)	C(6)-C(13)-N(1)	103.0(3)	C(19)-C(20)-H(20A)	105.7(18)
C(13)-C(6)-C(7)	129.6(3)	C(6)-C(13)-C(12)	131.7(3)	C(21)-C(20)-H(20B)	108(2)
C(6)-C(7)-C(8)	112.9(3)	N(1)-C(13)-C(12)	125.3(3)	C(19)-C(20)-H(20B)	107.1(17)
C(6)-C(7)-H(7A)	108(2)	N(6)-C(14)-C(21)	110.0(2)	H(20A)-C(20)-H(20B)	109(2)
C(8)-C(7)-H(7A)	108(2)	N(6)-C(14)-C(15)	120.9(3)	N(4)-C(21)-C(14)	101.7(3)
C(6)-C(7)-H(7B)	111.6(16)	C(21)-C(14)-C(15)	128.8(3)	N(4)-C(21)-C(20)	125.3(2)
C(8)-C(7)-H(7B)	107.7(18)	C(14)-C(15)-C(16)	113.0(3)	C(14)-C(21)-C(20)	132.8(3)
H(7A)-C(7)-H(7B)	109(3)	C(14)-C(15)-H(15A)	110.7(16)		
C(9)-C(8)-C(7)	115.8(3)	C(16)-C(15)-H(15A)	109.1(19)		

Symmetry transformations used to generate equivalent atoms:

## Torsion angles [°] for 80

C(13)-N(1)-N(2)-N(3)	-0.6(3)	Cl(1)-C(2)-C(3)-Cl(2)	4.5(4)	C(7)-C(6)-C(13)-C(12)	5.1(6)
C(1)-N(1)-N(2)-N(3)	-174.8(2)	C(2)-C(3)-C(4)-C(5)	1.8(3)	N(2)-N(1)-C(13)-C(6)	0.8(3)
N(1)-N(2)-N(3)-C(6)	0.0(3)	Cl(2)-C(3)-C(4)-C(5)	-176.5(2)	C(1)-N(1)-C(13)-C(6)	173.8(2)
C(21)-N(4)-N(5)-N(6)	-0.8(3)	C(2)-C(3)-C(4)-Cl(3)	-177.7(2)	N(2)-N(1)-C(13)-C(12)	178.4(3)
C(1)-N(4)-N(5)-N(6)	-172.4(2)	Cl(2)-C(3)-C(4)-Cl(3)	4.1(4)	C(1)-N(1)-C(13)-C(12)	-8.7(5)
N(4)-N(5)-N(6)-C(14)	0.6(3)	C(3)-C(4)-C(5)-C(1)	-0.5(3)	C(11)-C(12)-C(13)-C(6)	-6.2(5)
N(2)-N(1)-C(1)-N(4)	-141.1(2)	Cl(3)-C(4)-C(5)-C(1)	178.9(2)	C(11)-C(12)-C(13)-N(1)	177.0(3)
C(13)-N(1)-C(1)-N(4)	46.2(4)	C(3)-C(4)-C(5)-Cl(4)	-174.6(2)	N(5)-N(6)-C(14)-C(21)	-0.2(4)
N(2)-N(1)-C(1)-C(5)	-16.1(3)	Cl(3)-C(4)-C(5)-Cl(4)	4.9(4)	N(5)-N(6)-C(14)-C(15)	174.3(3)
C(13)-N(1)-C(1)-C(5)	171.1(2)	N(1)-C(1)-C(5)-C(4)	117.4(3)	N(6)-C(14)-C(15)-C(16)	-103.6(4)
N(2)-N(1)-C(1)-C(2)	96.1(3)	N(4)-C(1)-C(5)-C(4)	-119.3(3)	C(21)-C(14)-C(15)-C(16)	69.7(5)
C(13)-N(1)-C(1)-C(2)	-76.6(3)	C(2)-C(1)-C(5)-C(4)	-0.7(3)	C(14)-C(15)-C(16)-C(17)	-36.8(5)
N(5)-N(4)-C(1)-N(1)	-138.9(3)	N(1)-C(1)-C(5)-Cl(4)	-68.6(3)	C(15)-C(16)-C(17)-C(18)	-66.7(4)
C(21)-N(4)-C(1)-N(1)	51.2(4)	N(4)-C(1)-C(5)-Cl(4)	54.7(3)	C(16)-C(17)-C(18)-C(19)	58.5(4)
N(5)-N(4)-C(1)-C(5)	96.1(3)	C(2)-C(1)-C(5)-Cl(4)	173.2(2)	C(17)-C(18)-C(19)-C(20)	55.5(4)
C(21)-N(4)-C(1)-C(5)	-73.8(4)	N(2)-N(3)-C(6)-C(13)	0.5(3)	C(18)-C(19)-C(20)-C(21)	-66.9(4)
N(5)-N(4)-C(1)-C(2)	-16.4(3)	N(2)-N(3)-C(6)-C(7)	177.7(3)	N(5)-N(4)-C(21)-C(14)	0.7(3)
C(21)-N(4)-C(1)-C(2)	173.7(3)	N(3)-C(6)-C(7)-C(8)	-103.0(4)	C(1)-N(4)-C(21)-C(14)	171.0(3)
N(1)-C(1)-C(2)-C(3)	-117.4(3)	C(13)-C(6)-C(7)-C(8)	73.6(4)	N(5)-N(4)-C(21)-C(20)	175.4(3)
N(4)-C(1)-C(2)-C(3)	121.0(3)	C(6)-C(7)-C(8)-C(9)	-44.7(4)	C(1)-N(4)-C(21)-C(20)	-14.3(5)
C(5)-C(1)-C(2)-C(3)	1.8(3)	C(7)-C(8)-C(9)-C(10)	-61.0(4)	N(6)-C(14)-C(21)-N(4)	-0.3(3)
N(1)-C(1)-C(2)-Cl(1)	54.3(3)	C(8)-C(9)-C(10)-C(11)	63.1(5)	C(15)-C(14)-C(21)-N(4)	-174.2(3)
N(4)-C(1)-C(2)-Cl(1)	-67.3(3)	C(9)-C(10)-C(11)-C(12)	50.3(5)	N(6)-C(14)-C(21)-C(20)	-174.4(3)
C(5)-C(1)-C(2)-Cl(1)	173.5(2)	C(10)-C(11)-C(12)-C(13)	-72.4(5)	C(15)-C(14)-C(21)-C(20)	11.7(6)
C(1)-C(2)-C(3)-C(4)	-2.2(3)	N(3)-C(6)-C(13)-N(1)	-0.8(3)	C(19)-C(20)-C(21)-N(4)	168.5(3)
Cl(1)-C(2)-C(3)-C(4)	-173.7(2)	C(7)-C(6)-C(13)-N(1)	-177.7(3)	C(19)-C(20)-C(21)-C(14)	-18.6(5)
C(1)-C(2)-C(3)-Cl(2)	176.0(2)	N(3)-C(6)-C(13)-C(12)	-178.1(3)		

Kristallstrukturdaten von *syn*-8-(4,5,6,7,8,9-Hexahydrocyclooctatriazol-1-yl)-1,4,7,9,10-pentaphenyl-2,4,6-triazatricyclo[5.2.1.0<sup>2,6</sup>]dec-8-en-3,5-dion *syn*-83c (Abb. 5)Crystal data for *syn*-83c

Crystal shape / colour	triclinic / colorless	Volume	1784.30(18) Å <sup>3</sup>
Crystal size	0.5 x 0.3 x 0.1 mm	Z	2
Chem. formula / weight	C <sub>45</sub> H <sub>38</sub> N <sub>6</sub> O <sub>2</sub> / 694.81	Density (calculated)	1.293 g/cm <sup>3</sup>
Crystal system	Triclinic	Radiation used	MoK <sub>α</sub>
Space group	P-1	Wavelength	0.71073 Å
Unit cell dimensions	a = 11.2139(7) Å    α = 84.7340(7)° b = 12.3398(7) Å    β = 84.3519(9)° c = 13.4954(8) Å    γ = 74.2282(12)°	Linear absorption coefficient	0.081 mm <sup>-1</sup>
		Temperature	173(2) K

**Data collection details for syn-83c**

Diffractometer	BRUKER Smart CCD	Number of measured reflections	13723
Scan method	$\omega$ scans	Number of independent refl.	9215
Absorption correction	Empirical	Number of observed reflections	3022
Max. and min. transmission	0.977859 and 0.524438	Criterion of recognition ( $\sigma$ -limit)	$>2\sigma(I)$
R(int) =	0.0912	Index ranges	$-15 \leq h \leq 15,$
Theta range for data collection	1.52 to 30.36°		$-8 \leq k \leq 17,$
Completeness to theta = 30.36°	85.7 %		$-18 \leq l \leq 17$
F(000)	732		

**Refinement details for syn-83c**

Refinement method	Full-matrix least-squares on $F^2$		
Final R indices [ $I > 2\sigma(I)$ ]	R1 = 0.0671, wR2 = 0.1413		
R indices (all data)	R1 = 0.2152, wR2 = 0.1943		
R1 [ $= \sum( F_o  -  F_c ) / \sum F_o $ ]			
wR2 [ $= [\sum(w(F_o^2 - F_c^2)^2) / \sum(wF_o^4)]^{1/2}$ ]			
H-locating and refining method	geom/mixed	Number of reflections used	9215
Number of L.S. restraints	0	Number of refined parameters	478
Goodness-of-fit on $F^2$	0.830		
S [ $= [\sum w(F_o^2 - F_c^2)^2] / (n-p)^{1/2}$ ]	n=number of reflections, p=parameters used.		
Definition of w			
calc $w = 1 / [\sigma^2(F_o^2) + (0.0518P)^2 + 0.0000P]$ where $P = (F_o^2 + 2F_c^2) / 3$			
Maximum d/s	0.002		
Maximum e-density	1.048 e Å <sup>-3</sup>	Minimum e-density	-0.454 e Å <sup>-3</sup>

**Computer Programs used for syn-83c**

Data collection program	SMART	Structure solving program	SHELXS-97 (Sheldrick, 1990)
Cell refinement program	SAINT	Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Data reduction program	SAINT	Pictures drawn with	ZORTEP

**Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters (Å<sup>2</sup> × 10<sup>3</sup>) for syn-83c**

U(eq) is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.

	x	y	z	U(eq)		x	y	z	U(eq)
O(1)	6021(2)	5056(2)	1737(2)	34(1)	C(20)	8441(3)	8311(3)	-94(2)	24(1)
O(2)	10156(2)	4105(2)	2306(2)	35(1)	C(21)	8651(3)	9136(3)	448(3)	32(1)
N(1)	7694(2)	5673(2)	994(2)	23(1)	C(22)	8531(3)	10227(3)	22(3)	35(1)
N(2)	8985(3)	5419(2)	1197(2)	24(1)	C(23)	8248(4)	10492(3)	-949(3)	38(1)
N(3)	8076(3)	4238(2)	2113(2)	26(1)	C(24)	8042(4)	9677(3)	-1500(3)	40(1)
N(4)	8829(3)	7396(2)	2938(2)	30(1)	C(25)	8145(3)	8593(3)	-1075(3)	31(1)
N(5)	9464(3)	8208(3)	2899(2)	47(1)	C(26)	10639(3)	6472(3)	1140(3)	26(1)
N(6)	9752(4)	8261(3)	3808(3)	60(1)	C(27)	11343(3)	6120(3)	1961(3)	32(1)
C(1)	7119(3)	5011(3)	1639(2)	25(1)	C(28)	12603(4)	6057(3)	1869(3)	37(1)
C(2)	9196(3)	4547(3)	1927(2)	27(1)	C(29)	13179(4)	6336(3)	961(3)	38(1)
C(3)	7229(3)	7406(3)	1814(2)	24(1)	C(30)	12479(4)	6689(3)	149(3)	33(1)
C(4)	7267(3)	6923(3)	801(2)	22(1)	C(31)	11235(3)	6754(3)	238(3)	27(1)
C(5)	8523(3)	7110(3)	286(2)	23(1)	C(32)	7926(4)	3230(3)	2683(2)	30(1)
C(6)	9271(3)	6564(3)	1198(2)	23(1)	C(33)	8758(4)	2214(3)	2475(3)	31(1)
C(7)	8397(3)	7179(3)	2043(2)	25(1)	C(34)	8608(4)	1234(3)	3008(3)	41(1)
C(8)	6126(3)	7979(3)	2444(2)	26(1)	C(35)	7639(4)	1281(4)	3735(3)	49(1)
C(9)	5049(4)	7596(3)	2575(3)	37(1)	C(36)	6844(4)	2299(4)	3929(3)	50(1)
C(10)	4051(4)	8137(3)	3181(3)	46(1)	C(37)	6973(4)	3287(3)	3403(3)	39(1)
C(11)	4096(4)	9077(4)	3663(3)	52(1)	C(38)	9309(5)	7489(3)	4429(3)	56(1)
C(12)	5132(4)	9472(3)	3529(3)	49(1)	C(39)	8709(4)	6932(3)	3886(3)	34(1)
C(13)	6157(4)	8931(3)	2924(3)	36(1)	C(40)	8082(4)	6012(3)	4146(3)	43(1)
C(14)	6217(3)	7270(3)	129(2)	25(1)	C(41)	8053(5)	5575(4)	5225(3)	74(2)
C(15)	5421(3)	8332(3)	129(3)	30(1)	C(42)	7120(6)	6391(5)	5942(4)	108(2)
C(16)	4588(3)	8710(3)	-609(3)	38(1)	C(43)	7108(6)	7626(5)	5878(4)	108(3)
C(17)	4589(4)	8021(3)	-1363(3)	40(1)	C(44)	8315(8)	7897(5)	6134(4)	131(3)
C(18)	5358(3)	6963(3)	-1359(3)	33(1)	C(45)	9470(6)	7387(4)	5519(3)	82(2)
C(19)	6196(3)	6581(3)	-638(2)	31(1)					

**Bond lengths [Å] for *syn-83c***

O(1)-C(1)	1.212(4)	C(12)-H(12)	0.9500	C(31)-H(31)	0.9500
O(2)-C(2)	1.206(4)	C(13)-H(13)	0.9500	C(32)-C(37)	1.363(5)
N(1)-C(1)	1.374(4)	C(14)-C(15)	1.370(5)	C(32)-C(33)	1.377(5)
N(1)-N(2)	1.443(3)	C(14)-C(19)	1.405(4)	C(33)-C(34)	1.391(5)
N(1)-C(4)	1.492(4)	C(15)-C(16)	1.394(4)	C(33)-H(33)	0.9500
N(2)-C(2)	1.378(4)	C(15)-H(15)	0.9500	C(34)-C(35)	1.383(6)
N(2)-C(6)	1.530(4)	C(16)-C(17)	1.384(5)	C(34)-H(34)	0.9500
N(3)-C(1)	1.392(4)	C(16)-H(16)	0.9500	C(35)-C(36)	1.359(6)
N(3)-C(2)	1.402(4)	C(17)-C(18)	1.355(5)	C(35)-H(35)	0.9500
N(3)-C(32)	1.442(4)	C(17)-H(17)	0.9500	C(36)-C(37)	1.389(5)
N(4)-C(39)	1.362(4)	C(18)-C(19)	1.381(5)	C(36)-H(36)	0.9500
N(4)-N(5)	1.373(4)	C(18)-H(18)	0.9500	C(37)-H(37)	0.9500
N(4)-C(7)	1.418(4)	C(19)-H(19)	0.9500	C(38)-C(39)	1.378(5)
N(5)-N(6)	1.310(4)	C(20)-C(25)	1.386(4)	C(38)-C(45)	1.490(5)
N(6)-C(38)	1.374(5)	C(20)-C(21)	1.389(4)	C(39)-C(40)	1.490(5)
C(3)-C(7)	1.325(4)	C(21)-C(22)	1.391(4)	C(40)-C(41)	1.506(5)
C(3)-C(8)	1.477(5)	C(21)-H(21)	0.9500	C(40)-H(40A)	0.9900
C(3)-C(4)	1.532(4)	C(22)-C(23)	1.368(5)	C(40)-H(40B)	0.9900
C(4)-C(14)	1.502(4)	C(22)-H(22)	0.9500	C(41)-C(42)	1.566(6)
C(4)-C(5)	1.573(4)	C(23)-C(24)	1.384(5)	C(41)-H(41A)	0.9900
C(5)-C(20)	1.505(4)	C(23)-H(23)	0.9500	C(41)-H(41B)	0.9900
C(5)-C(6)	1.554(4)	C(24)-C(25)	1.386(5)	C(42)-C(43)	1.514(7)
C(5)-H(5)	1.0000	C(24)-H(24)	0.9500	C(42)-H(42A)	0.9900
C(6)-C(26)	1.503(5)	C(25)-H(25)	0.9500	C(42)-H(42B)	0.9900
C(6)-C(7)	1.540(5)	C(26)-C(27)	1.391(4)	C(43)-C(44)	1.557(9)
C(8)-C(13)	1.402(4)	C(26)-C(31)	1.392(4)	C(43)-H(43A)	0.9900
C(8)-C(9)	1.402(5)	C(27)-C(28)	1.388(5)	C(43)-H(43B)	0.9900
C(9)-C(10)	1.372(5)	C(27)-H(27)	0.9500	C(44)-C(45)	1.484(8)
C(9)-H(9)	0.9500	C(28)-C(29)	1.387(5)	C(44)-H(44A)	0.9900
C(10)-C(11)	1.396(5)	C(28)-H(28)	0.9500	C(44)-H(44B)	0.9900
C(10)-H(10)	0.9500	C(29)-C(30)	1.379(5)	C(45)-H(45A)	0.9900
C(11)-C(12)	1.368(6)	C(29)-H(29)	0.9500	C(45)-H(45B)	0.9900
C(11)-H(11)	0.9500	C(30)-C(31)	1.369(5)		
C(12)-C(13)	1.390(5)	C(30)-H(30)	0.9500		

**Angles [°] for *syn-83c***

C(1)-N(1)-N(2)	109.0(2)	C(12)-C(13)-C(8)	119.9(4)	C(33)-C(32)-N(3)	118.5(3)
C(1)-N(1)-C(4)	126.6(3)	C(12)-C(13)-H(13)	120.1	C(32)-C(33)-C(34)	118.9(4)
N(2)-N(1)-C(4)	106.3(2)	C(8)-C(13)-H(13)	120.1	C(32)-C(33)-H(33)	120.5
C(2)-N(2)-N(1)	107.5(2)	C(15)-C(14)-C(19)	118.8(3)	C(34)-C(33)-H(33)	120.5
C(2)-N(2)-C(6)	127.6(3)	C(15)-C(14)-C(4)	121.0(3)	C(35)-C(34)-C(33)	120.4(4)
N(1)-N(2)-C(6)	105.6(2)	C(19)-C(14)-C(4)	119.0(3)	C(35)-C(34)-H(34)	119.8
C(1)-N(3)-C(2)	111.2(3)	C(14)-C(15)-C(16)	120.4(3)	C(33)-C(34)-H(34)	119.8
C(1)-N(3)-C(32)	123.5(3)	C(14)-C(15)-H(15)	119.8	C(36)-C(35)-C(34)	119.1(4)
C(2)-N(3)-C(32)	125.2(3)	C(16)-C(15)-H(15)	119.8	C(36)-C(35)-H(35)	120.5
C(39)-N(4)-N(5)	111.1(3)	C(17)-C(16)-C(15)	119.9(4)	C(34)-C(35)-H(35)	120.5
C(39)-N(4)-C(7)	130.5(3)	C(17)-C(16)-H(16)	120.1	C(35)-C(36)-C(37)	121.4(4)
N(5)-N(4)-C(7)	118.4(3)	C(15)-C(16)-H(16)	120.1	C(35)-C(36)-H(36)	119.3
N(6)-N(5)-N(4)	107.1(3)	C(18)-C(17)-C(16)	120.1(4)	C(37)-C(36)-H(36)	119.3
N(5)-N(6)-C(38)	108.7(3)	C(18)-C(17)-H(17)	120.0	C(32)-C(37)-C(36)	119.0(4)
O(1)-C(1)-N(1)	127.2(3)	C(16)-C(17)-H(17)	120.0	C(32)-C(37)-H(37)	120.5
O(1)-C(1)-N(3)	127.5(3)	C(17)-C(18)-C(19)	120.6(3)	C(36)-C(37)-H(37)	120.5
N(1)-C(1)-N(3)	105.2(3)	C(17)-C(18)-H(18)	119.7	N(6)-C(38)-C(39)	109.5(3)
O(2)-C(2)-N(2)	127.6(3)	C(19)-C(18)-H(18)	119.7	N(6)-C(38)-C(45)	120.5(4)
O(2)-C(2)-N(3)	126.5(3)	C(18)-C(19)-C(14)	120.1(3)	C(39)-C(38)-C(45)	130.0(4)
N(2)-C(2)-N(3)	105.9(3)	C(18)-C(19)-H(19)	120.0	N(4)-C(39)-C(38)	103.6(3)
C(7)-C(3)-C(8)	125.6(3)	C(14)-C(19)-H(19)	120.0	N(4)-C(39)-C(40)	122.8(3)
C(7)-C(3)-C(4)	106.4(3)	C(25)-C(20)-C(21)	118.5(3)	C(38)-C(39)-C(40)	133.6(4)
C(8)-C(3)-C(4)	128.0(3)	C(25)-C(20)-C(5)	116.0(3)	C(39)-C(40)-C(41)	116.1(3)
N(1)-C(4)-C(14)	112.2(2)	C(21)-C(20)-C(5)	125.5(3)	C(39)-C(40)-H(40A)	108.3
N(1)-C(4)-C(3)	105.4(2)	C(20)-C(21)-C(22)	120.5(3)	C(41)-C(40)-H(40A)	108.2
C(14)-C(4)-C(3)	123.8(3)	C(20)-C(21)-H(21)	119.8	C(39)-C(40)-H(40B)	108.3
N(1)-C(4)-C(5)	97.7(2)	C(22)-C(21)-H(21)	119.8	C(41)-C(40)-H(40B)	108.3
C(14)-C(4)-C(5)	113.2(3)	C(23)-C(22)-C(21)	120.5(3)	H(40A)-C(40)-H(40B)	107.4
C(3)-C(4)-C(5)	101.1(2)	C(23)-C(22)-H(22)	119.7	C(40)-C(41)-C(42)	114.5(4)
C(20)-C(5)-C(6)	121.1(3)	C(21)-C(22)-H(22)	119.7	C(40)-C(41)-H(41A)	108.6

## Fortsetzung

C(20)-C(5)-C(4)	113.9(3)	C(22)-C(23)-C(24)	119.6(3)	C(42)-C(41)-H(41A)	108.6
C(6)-C(5)-C(4)	93.5(2)	C(22)-C(23)-H(23)	120.2	C(40)-C(41)-H(41B)	108.6
C(20)-C(5)-H(5)	109.1	C(24)-C(23)-H(23)	120.2	C(42)-C(41)-H(41B)	108.6
C(6)-C(5)-H(5)	109.1	C(23)-C(24)-C(25)	120.1(3)	H(41A)-C(41)-H(41B)	107.6
C(4)-C(5)-H(5)	109.1	C(23)-C(24)-H(24)	119.9	C(43)-C(42)-C(41)	119.4(5)
C(26)-C(6)-N(2)	113.0(3)	C(25)-C(24)-H(24)	119.9	C(43)-C(42)-H(42A)	107.5
C(26)-C(6)-C(7)	120.3(3)	C(24)-C(25)-C(20)	120.8(3)	C(41)-C(42)-H(42A)	107.5
N(2)-C(6)-C(7)	105.6(2)	C(24)-C(25)-H(25)	119.6	C(43)-C(42)-H(42B)	107.5
C(26)-C(6)-C(5)	119.0(3)	C(20)-C(25)-H(25)	119.6	C(41)-C(42)-H(42B)	107.5
N(2)-C(6)-C(5)	95.3(2)	C(27)-C(26)-C(31)	118.2(3)	H(42A)-C(42)-H(42B)	107.0
C(7)-C(6)-C(5)	99.9(3)	C(27)-C(26)-C(6)	122.4(3)	C(42)-C(43)-C(44)	116.6(5)
C(3)-C(7)-N(4)	127.3(3)	C(31)-C(26)-C(6)	119.4(3)	C(42)-C(43)-H(43A)	108.2
C(3)-C(7)-C(6)	109.7(3)	C(28)-C(27)-C(26)	120.2(4)	C(44)-C(43)-H(43A)	108.2
N(4)-C(7)-C(6)	122.9(3)	C(28)-C(27)-H(27)	119.9	C(42)-C(43)-H(43B)	108.2
C(13)-C(8)-C(9)	119.2(3)	C(26)-C(27)-H(27)	119.9	C(44)-C(43)-H(43B)	108.2
C(13)-C(8)-C(3)	119.2(3)	C(29)-C(28)-C(27)	120.6(3)	H(43A)-C(43)-H(43B)	107.3
C(9)-C(8)-C(3)	121.7(3)	C(29)-C(28)-H(28)	119.7	C(45)-C(44)-C(43)	116.5(4)
C(10)-C(9)-C(8)	120.1(4)	C(27)-C(28)-H(28)	119.7	C(45)-C(44)-H(44A)	108.2
C(10)-C(9)-H(9)	119.9	C(30)-C(29)-C(28)	119.1(4)	C(43)-C(44)-H(44A)	108.2
C(8)-C(9)-H(9)	119.9	C(30)-C(29)-H(29)	120.4	C(45)-C(44)-H(44B)	108.2
C(9)-C(10)-C(11)	120.2(4)	C(28)-C(29)-H(29)	120.4	C(43)-C(44)-H(44B)	108.2
C(9)-C(10)-H(10)	119.9	C(31)-C(30)-C(29)	120.4(4)	H(44A)-C(44)-H(44B)	107.3
C(11)-C(10)-H(10)	119.9	C(31)-C(30)-H(30)	119.8	C(44)-C(45)-C(38)	113.6(4)
C(12)-C(11)-C(10)	120.4(4)	C(29)-C(30)-H(30)	119.8	C(44)-C(45)-H(45A)	108.8
C(12)-C(11)-H(11)	119.8	C(30)-C(31)-C(26)	121.5(3)	C(38)-C(45)-H(45A)	108.8
C(10)-C(11)-H(11)	119.8	C(30)-C(31)-H(31)	119.2	C(44)-C(45)-H(45B)	108.8
C(11)-C(12)-C(13)	120.3(4)	C(26)-C(31)-H(31)	119.2	C(38)-C(45)-H(45B)	108.8
C(11)-C(12)-H(12)	119.9	C(37)-C(32)-C(33)	121.1(3)	H(45A)-C(45)-H(45B)	107.7
C(13)-C(12)-H(12)	119.9	C(37)-C(32)-N(3)	120.4(3)		

Symmetry transformations used to generate equivalent atoms:

**Torsion angles [°] for *syn*-83c**

C(1)-N(1)-N(2)-C(2)	3.8(3)	C(4)-C(5)-C(6)-N(2)	58.8(2)	C(21)-C(22)-C(23)-C(24)	2.0(6)
C(4)-N(1)-N(2)-C(2)	143.1(3)	C(20)-C(5)-C(6)-C(7)	72.7(3)	C(22)-C(23)-C(24)-C(25)	-1.2(6)
C(1)-N(1)-N(2)-C(6)	-135.0(3)	C(4)-C(5)-C(6)-C(7)	-48.0(3)	C(23)-C(24)-C(25)-C(20)	0.7(6)
C(4)-N(1)-N(2)-C(6)	4.3(3)	C(8)-C(3)-C(7)-N(4)	2.3(5)	C(21)-C(20)-C(25)-C(24)	-1.0(5)
C(39)-N(4)-N(5)-N(6)	0.2(4)	C(4)-C(3)-C(7)-N(4)	-175.7(3)	C(5)-C(20)-C(25)-C(24)	179.8(3)
C(7)-N(4)-N(5)-N(6)	179.4(3)	C(8)-C(3)-C(7)-C(6)	179.3(3)	N(2)-C(6)-C(26)-C(27)	-77.4(4)
N(4)-N(5)-N(6)-C(38)	0.1(5)	C(4)-C(3)-C(7)-C(6)	1.3(3)	C(7)-C(6)-C(26)-C(27)	48.6(4)
N(2)-N(1)-C(1)-O(1)	173.9(3)	C(39)-N(4)-C(7)-C(3)	67.8(5)	C(5)-C(6)-C(26)-C(27)	172.1(3)
C(4)-N(1)-C(1)-O(1)	45.2(5)	N(5)-N(4)-C(7)-C(3)	-111.1(4)	N(2)-C(6)-C(26)-C(31)	103.1(3)
N(2)-N(1)-C(1)-N(3)	-9.5(3)	C(39)-N(4)-C(7)-C(6)	-108.8(4)	C(7)-C(6)-C(26)-C(31)	-131.0(3)
C(4)-N(1)-C(1)-N(3)	-138.2(3)	N(5)-N(4)-C(7)-C(6)	72.2(4)	C(5)-C(6)-C(26)-C(31)	-7.4(4)
C(2)-N(3)-C(1)-O(1)	-171.3(3)	C(26)-C(6)-C(7)-C(3)	164.3(3)	C(31)-C(26)-C(27)-C(28)	0.0(5)
C(32)-N(3)-C(1)-O(1)	11.1(5)	N(2)-C(6)-C(7)-C(3)	-66.4(3)	C(6)-C(26)-C(27)-C(28)	-179.5(3)
C(2)-N(3)-C(1)-N(1)	12.1(4)	C(5)-C(6)-C(7)-C(3)	32.0(3)	C(26)-C(27)-C(28)-C(29)	-0.4(5)
C(32)-N(3)-C(1)-N(1)	-165.5(3)	C(26)-C(6)-C(7)-N(4)	-18.5(5)	C(27)-C(28)-C(29)-C(30)	0.7(5)
N(1)-N(2)-C(2)-O(2)	-179.1(3)	N(2)-C(6)-C(7)-N(4)	110.8(3)	C(28)-C(29)-C(30)-C(31)	-0.6(5)
C(6)-N(2)-C(2)-O(2)	-52.3(5)	C(5)-C(6)-C(7)-N(4)	-150.8(3)	C(29)-C(30)-C(31)-C(26)	0.2(5)
N(1)-N(2)-C(2)-N(3)	3.5(3)	C(7)-C(3)-C(8)-C(13)	43.3(5)	C(27)-C(26)-C(31)-C(30)	0.1(5)
C(6)-N(2)-C(2)-N(3)	130.3(3)	C(4)-C(3)-C(8)-C(13)	-139.0(3)	C(6)-C(26)-C(31)-C(30)	179.7(3)
C(1)-N(3)-C(2)-O(2)	172.8(3)	C(7)-C(3)-C(8)-C(9)	-136.7(4)	C(1)-N(3)-C(32)-C(37)	-50.3(4)
C(32)-N(3)-C(2)-O(2)	-9.7(6)	C(4)-C(3)-C(8)-C(9)	41.0(5)	C(2)-N(3)-C(32)-C(37)	132.5(4)
C(1)-N(3)-C(2)-N(2)	-9.8(4)	C(13)-C(8)-C(9)-C(10)	-1.2(5)	C(1)-N(3)-C(32)-C(33)	129.0(4)
C(32)-N(3)-C(2)-N(2)	167.8(3)	C(3)-C(8)-C(9)-C(10)	178.8(3)	C(2)-N(3)-C(32)-C(33)	-48.2(5)
C(1)-N(1)-C(4)-C(14)	-77.6(4)	C(8)-C(9)-C(10)-C(11)	0.6(6)	C(37)-C(32)-C(33)-C(34)	0.5(5)
N(2)-N(1)-C(4)-C(14)	152.7(3)	C(9)-C(10)-C(11)-C(12)	0.5(6)	N(3)-C(32)-C(33)-C(34)	-178.8(3)
C(1)-N(1)-C(4)-C(3)	59.7(4)	C(10)-C(11)-C(12)-C(13)	-1.0(6)	C(32)-C(33)-C(34)-C(35)	0.0(5)
N(2)-N(1)-C(4)-C(3)	-70.1(3)	C(11)-C(12)-C(13)-C(8)	0.3(6)	C(33)-C(34)-C(35)-C(36)	-0.7(6)
C(1)-N(1)-C(4)-C(5)	163.5(3)	C(9)-C(8)-C(13)-C(12)	0.7(5)	C(34)-C(35)-C(36)-C(37)	1.0(6)
N(2)-N(1)-C(4)-C(5)	33.7(3)	C(3)-C(8)-C(13)-C(12)	-179.3(3)	C(33)-C(32)-C(37)-C(36)	-0.2(5)
C(7)-C(3)-C(4)-N(1)	67.5(3)	N(1)-C(4)-C(14)-C(15)	157.4(3)	N(3)-C(32)-C(37)-C(36)	179.1(3)
C(8)-C(3)-C(4)-N(1)	-110.5(3)	C(3)-C(4)-C(14)-C(15)	29.3(5)	C(35)-C(36)-C(37)-C(32)	-0.6(6)
C(7)-C(3)-C(4)-C(14)	-161.6(3)	C(5)-C(4)-C(14)-C(15)	-93.2(4)	N(5)-N(6)-C(38)-C(39)	-0.4(5)
C(8)-C(3)-C(4)-C(14)	20.3(5)	N(1)-C(4)-C(14)-C(19)	-34.9(4)	N(5)-N(6)-C(38)-C(45)	-178.2(4)

## Fortsetzung

C(7)-C(3)-C(4)-C(5)	-33.8(3)	C(3)-C(4)-C(14)-C(19)	-163.0(3)	N(5)-N(4)-C(39)-C(38)	-0.5(4)
C(8)-C(3)-C(4)-C(5)	148.2(3)	C(5)-C(4)-C(14)-C(19)	74.4(4)	C(7)-N(4)-C(39)-C(38)	-179.5(4)
N(1)-C(4)-C(5)-C(20)	176.1(2)	C(19)-C(14)-C(15)-C(16)	1.3(5)	N(5)-N(4)-C(39)-C(40)	-178.7(3)
C(14)-C(4)-C(5)-C(20)	57.9(4)	C(4)-C(14)-C(15)-C(16)	169.0(3)	C(7)-N(4)-C(39)-C(40)	2.2(6)
C(3)-C(4)-C(5)-C(20)	-76.5(3)	C(14)-C(15)-C(16)-C(17)	-1.9(5)	N(6)-C(38)-C(39)-N(4)	0.5(5)
N(1)-C(4)-C(5)-C(6)	-57.6(3)	C(15)-C(16)-C(17)-C(18)	3.0(6)	C(45)-C(38)-C(39)-N(4)	178.0(5)
C(14)-C(4)-C(5)-C(6)	-175.8(3)	C(16)-C(17)-C(18)-C(19)	-3.6(6)	N(6)-C(38)-C(39)-C(40)	178.5(4)
C(3)-C(4)-C(5)-C(6)	49.8(3)	C(17)-C(18)-C(19)-C(14)	3.1(5)	C(45)-C(38)-C(39)-C(40)	-4.0(8)
C(2)-N(2)-C(6)-C(26)	67.0(4)	C(15)-C(14)-C(19)-C(18)	-1.9(5)	N(4)-C(39)-C(40)-C(41)	178.7(4)
N(1)-N(2)-C(6)-C(26)	-165.5(3)	C(4)-C(14)-C(19)-C(18)	-169.9(3)	C(38)-C(39)-C(40)-C(41)	1.0(7)
C(2)-N(2)-C(6)-C(7)	-66.5(4)	C(6)-C(5)-C(20)-C(25)	158.3(3)	C(39)-C(40)-C(41)-C(42)	73.6(6)
N(1)-N(2)-C(6)-C(7)	61.0(3)	C(4)-C(5)-C(20)-C(25)	-91.5(4)	C(40)-C(41)-C(42)-C(43)	-47.7(8)
C(2)-N(2)-C(6)-C(5)	-168.4(3)	C(6)-C(5)-C(20)-C(21)	-20.7(5)	C(41)-C(42)-C(43)-C(44)	-63.4(7)
N(1)-N(2)-C(6)-C(5)	-40.8(3)	C(4)-C(5)-C(20)-C(21)	89.4(4)	C(42)-C(43)-C(44)-C(45)	58.6(7)
C(20)-C(5)-C(6)-C(26)	-60.4(4)	C(25)-C(20)-C(21)-C(22)	1.9(5)	C(43)-C(44)-C(45)-C(38)	45.3(7)
C(4)-C(5)-C(6)-C(26)	178.8(3)	C(5)-C(20)-C(21)-C(22)	-179.1(3)	N(6)-C(38)-C(45)-C(44)	104.5(6)
C(20)-C(5)-C(6)-N(2)	179.6(3)	C(20)-C(21)-C(22)-C(23)	-2.4(5)	C(39)-C(38)-C(45)-C(44)	-72.7(7)

**Kristallstrukturdaten von *anti*-/*syn*-10-Azido-1,4,7,8,9-pentaphenyl-2,4,6-triazatricyclo-[5.2.1.0<sup>2,6</sup>]dec-8-en-3,5-dion *anti*-/*syn*-82a (Abb. 6)**

## Crystal data for 82a

Crystal shape	irregular blocks	Volume	2921.1(18) Å <sup>3</sup>
Crystal colour	colorless	Z	4
Crystal size	0.4 x 0.2 x 0.2 mm	Density (calculated)	1.334 g/cm <sup>3</sup>
Chemical formula	C <sub>37</sub> H <sub>26</sub> N <sub>6</sub> O <sub>2</sub>	Radiation used	MoK <sub>α</sub>
Formula weight	586.64	Wavelength	0.71073 Å
Crystal system	Monoclinic	Linear absorption coefficient	0.085 mm <sup>-1</sup>
Space group	P2(1)/c	Temperature	173(2) K
Unit cell dimensions	a = 12.553(5) Å    α = 90° b = 19.998(6) Å    β = 104.54(3)° c = 12.022(4) Å    γ = 90°		

## Data collection details for 82a

Diffractometer	BRUKER Smart CCD	Number of measured reflections	12199
Scan method	ω scans	Number of independent refl.	6527
Absorption correction	Empirical	Number of observed reflections	2886
Max. and min. transmission	0.977848 and 0.823970	Criterion of recognition (σ-limit)	>2σ(I)
R(int) =	0.0790	Index ranges	-11 ≤ h ≤ 14, -21 ≤ k ≤ 27, -16 ≤ l ≤ 5
Theta range for data collection	1.68 to 30.18°		
Completeness to theta = 30.18°	75.3 %		
F(000)	1224		

## Refinement details for 82a

Refinement method	Full-matrix least-squares on F <sup>2</sup>		
Final R indices [I>σ(I)]	R1 = 0.0784, wR2 = 0.1256		
R indices (all data)	R1 = 0.2004, wR2 = 0.1656		
R1 [=Σ( Fo - Fc )/Σ Fo ]			
wR2 [=Σ(w(Fo <sup>2</sup> -Fc <sup>2</sup> ) <sup>2</sup> )/Σ(wFo <sup>2</sup> )] <sup>1/2</sup>			
H-locating and refining method	difmap/refall	Number of reflections used	6527
Number of L.S. restraints	0	Number of refined parameters	534
Goodness-of-fit on F <sup>2</sup>	1.042		
S [=Σ w(Fo <sup>2</sup> -Fc <sup>2</sup> ) <sup>2</sup> ]/(n-p) <sup>1/2</sup>	n=number of reflections, p=parameters used.		
Definition of w	calc w=1/[σ <sup>2</sup> (Fo <sup>2</sup> )+(0.0430P) <sup>2</sup> +0.5746P] where P=(Fo <sup>2</sup> +2Fc <sup>2</sup> )/3		
Maximum d/s	0.005		
Maximum e-density	0.263 e Å <sup>-3</sup>	Minimum e-density	-0.243 e Å <sup>-3</sup>

**Computer Programs used for 82a**

Data collection program	SMART	Structure solving program	SHELXS-97 (Sheldrick, 1990)
Cell refinement program	SAINT	Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Data reduction program	XPREP	Pictures drawn with	ZORTEP

**Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 82a**

U(eq) is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.

	x	y	z	U(eq)		x	y	z	U(eq)
O(1)	5073(2)	6351(1)	4810(2)	40(1)	C(14)	8259(3)	4280(2)	7027(2)	32(1)
O(2)	6724(2)	5317(1)	8203(2)	37(1)	C(15)	7600(4)	3824(2)	7398(3)	42(1)
N(1)	5659(2)	5917(2)	6653(2)	30(1)	C(16)	8055(4)	3248(2)	7979(3)	48(1)
N(2)	6140(2)	5382(1)	5218(2)	29(1)	C(17)	9177(4)	3135(2)	8196(3)	47(1)
N(3)	6620(2)	5038(1)	6298(2)	28(1)	C(18)	9829(4)	3587(2)	7821(3)	47(1)
N(4)	8392(4)	4431(3)	4582(3)	38(2)	C(19)	9376(4)	4154(2)	7238(3)	40(1)
N(5)	8344(6)	3799(4)	4580(4)	52(2)	C(20)	9272(3)	5776(2)	7298(3)	36(1)
N(6)	8410(8)	3227(4)	4528(6)	77(2)	C(21)	10090(3)	6176(3)	7078(3)	58(1)
N(4)	6928(6)	4209(4)	4509(5)	29(2)	C(22)	10977(4)	6396(3)	7962(4)	69(2)
N(5)	7366(9)	3663(5)	4603(6)	37(3)	C(23)	11020(4)	6209(3)	9078(4)	62(1)
N(6)	7617(12)	3112(6)	4601(9)	59(3)	C(24)	10207(4)	5827(2)	9308(3)	50(1)
C(1)	5581(3)	5943(2)	5480(2)	30(1)	C(25)	9333(3)	5596(2)	8434(3)	39(1)
C(2)	6391(3)	5426(2)	7183(3)	30(1)	C(26)	6698(3)	5508(2)	3312(2)	34(1)
C(3)	7774(3)	4868(2)	6282(2)	32(1)	C(27)	5636(3)	5669(2)	2721(3)	36(1)
C(4)	8392(3)	5526(2)	6329(2)	30(1)	C(28)	5362(4)	5721(2)	1527(3)	46(1)
C(5)	7936(3)	5861(2)	5333(2)	31(1)	C(29)	6139(4)	5615(2)	925(3)	51(1)
C(6)	7055(3)	5402(2)	4600(2)	30(1)	C(30)	7196(4)	5450(2)	1503(3)	48(1)
C(7)	7518(3)	4705(2)	4983(2)	43(1)	C(31)	7483(4)	5397(2)	2692(3)	43(1)
C(8)	5142(3)	6373(2)	7272(2)	32(1)	C(32)	8013(3)	6582(2)	5082(2)	33(1)
C(9)	5290(4)	7053(2)	7209(4)	51(1)	C(33)	8402(4)	6824(3)	4178(3)	52(1)
C(10)	4831(4)	7485(2)	7857(4)	59(1)	C(34)	8415(4)	7506(3)	3962(3)	64(1)
C(11)	4234(4)	7234(2)	8582(3)	49(1)	C(35)	8003(4)	7947(3)	4623(4)	62(1)
C(12)	4071(3)	6559(2)	8627(3)	42(1)	C(36)	7637(4)	7718(2)	5535(4)	55(1)
C(13)	4516(3)	6121(2)	7970(3)	35(1)	C(37)	7643(3)	7042(2)	5760(3)	44(1)

**Bond lengths [ $\text{\AA}$ ] for 82a**

O(1)-C(1)	1.209(4)	C(8)-C(13)	1.381(5)	C(23)-H(23)	0.99(4)
O(2)-C(2)	1.211(3)	C(9)-C(10)	1.383(6)	C(24)-C(25)	1.393(5)
N(1)-C(2)	1.386(4)	C(9)-H(9)	0.88(3)	C(24)-H(24)	0.95(3)
N(1)-C(1)	1.390(4)	C(10)-C(11)	1.379(6)	C(25)-H(25)	0.98(3)
N(1)-C(8)	1.432(4)	C(10)-H(10)	1.00(5)	C(26)-C(27)	1.381(5)
N(2)-C(1)	1.400(4)	C(11)-C(12)	1.369(6)	C(26)-C(31)	1.394(5)
N(2)-N(3)	1.459(3)	C(11)-H(11)	1.01(4)	C(27)-C(28)	1.394(5)
N(2)-C(6)	1.517(4)	C(12)-C(13)	1.388(5)	C(27)-H(27)	0.91(3)
N(3)-C(2)	1.404(4)	C(12)-H(12)	1.02(4)	C(28)-C(29)	1.368(6)
N(3)-C(3)	1.493(4)	C(13)-H(13)	0.99(4)	C(28)-H(28)	0.85(4)
N(4)-N(5)	1.265(8)	C(14)-C(15)	1.378(5)	C(29)-C(30)	1.375(6)
N(4)-C(7)	1.415(6)	C(14)-C(19)	1.383(5)	C(29)-H(29)	0.95(3)
N(5)-N(6)	1.151(9)	C(15)-C(16)	1.392(5)	C(30)-C(31)	1.387(5)
N(4)-N(5)	1.216(12)	C(15)-H(14)	0.91(3)	C(30)-H(30)	0.96(3)
N(4)-C(7)	1.283(8)	C(16)-C(17)	1.385(6)	C(31)-H(31)	0.98(3)
N(5)-N(6)	1.146(13)	C(16)-H(15)	0.97(4)	C(32)-C(37)	1.384(5)
C(3)-C(14)	1.511(5)	C(17)-C(18)	1.369(6)	C(32)-C(33)	1.385(5)
C(3)-C(4)	1.522(5)	C(17)-H(16)	1.01(4)	C(33)-C(34)	1.389(6)
C(3)-C(7)	1.547(4)	C(18)-C(19)	1.379(5)	C(33)-H(33)	0.94(4)
C(4)-C(5)	1.365(4)	C(18)-H(17)	0.86(3)	C(34)-C(35)	1.372(7)
C(4)-C(20)	1.477(5)	C(19)-H(18)	0.86(3)	C(34)-H(34)	1.03(4)
C(5)-C(32)	1.481(5)	C(20)-C(21)	1.378(5)	C(35)-C(36)	1.370(6)
C(5)-C(6)	1.534(5)	C(20)-C(25)	1.396(4)	C(35)-H(35)	1.05(4)
C(6)-C(26)	1.515(4)	C(21)-C(22)	1.403(6)	C(36)-C(37)	1.378(6)
C(6)-C(7)	1.536(5)	C(21)-H(21)	1.03(4)	C(36)-H(36)	0.94(5)
C(7)-H(7)	1.0000	C(22)-C(23)	1.381(6)	C(37)-H(37)	1.03(3)
C(7)-H(7)	1.0000	C(22)-H(22)	1.11(6)		
C(8)-C(9)	1.376(5)	C(23)-C(24)	1.357(6)		

## Angles [°] for 82a

C(2)-N(1)-C(1)	111.3(3)	N(4)-C(7)-H(7)	19.8	C(21)-C(22)-H(22)	118(3)
C(2)-N(1)-C(8)	123.1(2)	C(6)-C(7)-H(7)	107.0	C(24)-C(23)-C(22)	120.1(4)
C(1)-N(1)-C(8)	125.4(3)	C(3)-C(7)-H(7)	107.0	C(24)-C(23)-H(23)	120(2)
C(1)-N(2)-N(3)	107.2(2)	H(7)-C(7)-H(7)	127.5	C(22)-C(23)-H(23)	119(2)
C(1)-N(2)-C(6)	125.0(3)	C(9)-C(8)-C(13)	120.0(3)	C(23)-C(24)-C(25)	121.6(4)
N(3)-N(2)-C(6)	104.7(2)	C(9)-C(8)-N(1)	121.0(3)	C(23)-C(24)-H(24)	123(2)
C(2)-N(3)-N(2)	107.3(3)	C(13)-C(8)-N(1)	118.9(3)	C(25)-C(24)-H(24)	115(2)
C(2)-N(3)-C(3)	121.4(3)	C(8)-C(9)-C(10)	120.3(4)	C(24)-C(25)-C(20)	119.4(4)
N(2)-N(3)-C(3)	106.3(2)	C(8)-C(9)-H(9)	119(3)	C(24)-C(25)-H(25)	123.4(17)
N(5)-N(4)-C(7)	110.3(5)	C(10)-C(9)-H(9)	120(3)	C(20)-C(25)-H(25)	117.0(17)
N(6)-N(5)-N(4)	171.8(9)	C(11)-C(10)-C(9)	119.9(5)	C(27)-C(26)-C(31)	118.8(3)
N(5)-N(4)-C(7)	117.2(8)	C(11)-C(10)-H(10)	123(3)	C(27)-C(26)-C(6)	123.9(3)
N(6)-N(5)-N(4)	169.1(13)	C(9)-C(10)-H(10)	117(3)	C(31)-C(26)-C(6)	117.2(3)
O(1)-C(1)-N(1)	126.2(3)	C(12)-C(11)-C(10)	119.6(4)	C(26)-C(27)-C(28)	120.2(4)
O(1)-C(1)-N(2)	127.0(3)	C(12)-C(11)-H(11)	121(2)	C(26)-C(27)-H(27)	118.3(18)
N(1)-C(1)-N(2)	106.7(3)	C(10)-C(11)-H(11)	119(2)	C(28)-C(27)-H(27)	121.4(18)
O(2)-C(2)-N(1)	127.8(3)	C(11)-C(12)-C(13)	121.0(4)	C(29)-C(28)-C(27)	120.6(4)
O(2)-C(2)-N(3)	125.7(3)	C(11)-C(12)-H(12)	118(2)	C(29)-C(28)-H(28)	120(2)
N(1)-C(2)-N(3)	106.3(2)	C(13)-C(12)-H(12)	121(2)	C(27)-C(28)-H(28)	119(2)
N(3)-C(3)-C(14)	114.7(3)	C(8)-C(13)-C(12)	119.1(4)	C(28)-C(29)-C(30)	119.7(4)
N(3)-C(3)-C(4)	106.8(3)	C(8)-C(13)-H(13)	123.6(19)	C(28)-C(29)-H(29)	117(2)
C(14)-C(3)-C(4)	121.7(3)	C(12)-C(13)-H(13)	117.2(19)	C(30)-C(29)-H(29)	123(2)
N(3)-C(3)-C(7)	96.0(3)	C(15)-C(14)-C(19)	118.9(4)	C(29)-C(30)-C(31)	120.4(4)
C(14)-C(3)-C(7)	112.6(3)	C(15)-C(14)-C(3)	121.5(3)	C(29)-C(30)-H(30)	119.4(18)
C(4)-C(3)-C(7)	101.2(3)	C(19)-C(14)-C(3)	119.3(3)	C(31)-C(30)-H(30)	120.2(19)
C(5)-C(4)-C(20)	126.3(3)	C(14)-C(15)-C(16)	120.4(4)	C(30)-C(31)-C(26)	120.3(4)
C(5)-C(4)-C(3)	107.1(3)	C(14)-C(15)-H(14)	119(2)	C(30)-C(31)-H(31)	122.0(18)
C(20)-C(4)-C(3)	126.5(3)	C(16)-C(15)-H(14)	120(2)	C(26)-C(31)-H(31)	117.7(18)
C(4)-C(5)-C(32)	128.4(3)	C(17)-C(16)-C(15)	119.9(5)	C(37)-C(32)-C(33)	117.8(4)
C(4)-C(5)-C(6)	107.1(3)	C(17)-C(16)-H(15)	121(2)	C(37)-C(32)-C(5)	118.6(3)
C(32)-C(5)-C(6)	122.7(3)	C(15)-C(16)-H(15)	119(2)	C(33)-C(32)-C(5)	123.6(3)
C(26)-C(6)-N(2)	116.0(3)	C(18)-C(17)-C(16)	119.6(4)	C(32)-C(33)-C(34)	120.9(4)
C(26)-C(6)-C(5)	119.3(3)	C(18)-C(17)-H(16)	122(2)	C(32)-C(33)-H(33)	117(2)
N(2)-C(6)-C(5)	105.0(2)	C(16)-C(17)-H(16)	118(2)	C(34)-C(33)-H(33)	122(2)
C(26)-C(6)-C(7)	115.2(3)	C(17)-C(18)-C(19)	120.4(5)	C(35)-C(34)-C(33)	119.9(4)
N(2)-C(6)-C(7)	96.0(3)	C(17)-C(18)-H(17)	119(3)	C(35)-C(34)-H(34)	123(2)
C(5)-C(6)-C(7)	101.9(3)	C(19)-C(18)-H(17)	121(3)	C(33)-C(34)-H(34)	117(2)
N(4)-C(7)-N(4)	87.7(5)	C(18)-C(19)-C(14)	120.8(4)	C(36)-C(35)-C(34)	120.0(5)
N(4)-C(7)-C(6)	115.8(5)	C(18)-C(19)-H(18)	119(2)	C(36)-C(35)-H(35)	116(2)
N(4)-C(7)-C(6)	121.1(4)	C(14)-C(19)-H(18)	120(2)	C(34)-C(35)-H(35)	124(2)
N(4)-C(7)-C(3)	124.2(5)	C(21)-C(20)-C(25)	118.5(3)	C(35)-C(36)-C(37)	119.9(5)
N(4)-C(7)-C(3)	116.3(3)	C(21)-C(20)-C(4)	119.4(3)	C(35)-C(36)-H(36)	124(3)
C(6)-C(7)-C(3)	94.5(3)	C(25)-C(20)-C(4)	122.1(4)	C(37)-C(36)-H(36)	116(3)
N(4)-C(7)-H(7)	21.1	C(20)-C(21)-C(22)	121.6(4)	C(36)-C(37)-C(32)	121.5(4)
N(4)-C(7)-H(7)	107.9	C(20)-C(21)-H(21)	120(2)	C(36)-C(37)-H(37)	125(2)
C(6)-C(7)-H(7)	107.9	C(22)-C(21)-H(21)	118(2)	C(32)-C(37)-H(37)	113(2)
C(3)-C(7)-H(7)	107.9	C(23)-C(22)-C(21)	118.8(5)		
N(4)-C(7)-H(7)	107.0	C(23)-C(22)-H(22)	122(3)		

Symmetry transformations used to generate equivalent atoms:

## Torsion angles [°] for 82a

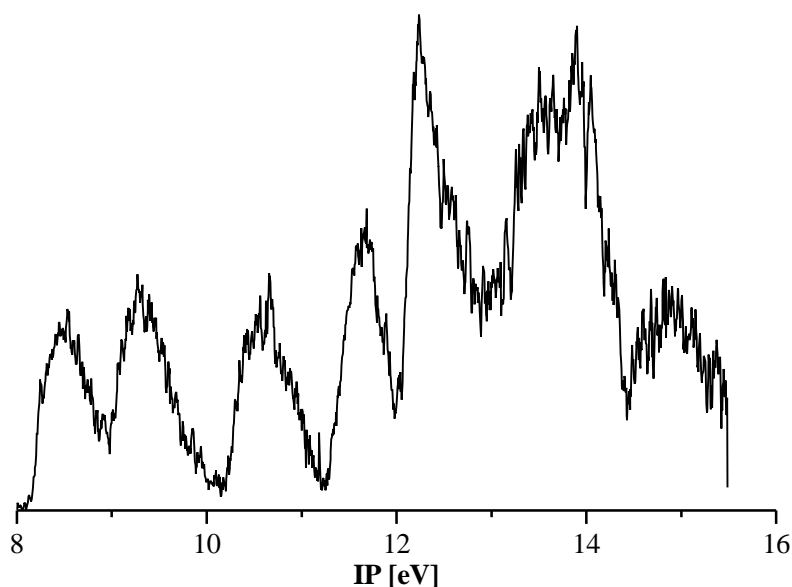
C(1)-N(2)-N(3)-C(2)	-3.5(3)	C(4)-C(5)-C(6)-N(2)	70.0(3)	C(19)-C(14)-C(15)-C(16)	0.3(5)
C(6)-N(2)-N(3)-C(2)	131.0(3)	C(32)-C(5)-C(6)-N(2)	-95.7(3)	C(3)-C(14)-C(15)-C(16)	173.1(3)
C(1)-N(2)-N(3)-C(3)	-134.7(3)	C(4)-C(5)-C(6)-C(7)	-29.7(3)	C(14)-C(15)-C(16)-C(17)	0.6(6)
C(6)-N(2)-N(3)-C(3)	-0.2(3)	C(32)-C(5)-C(6)-C(7)	164.6(3)	C(15)-C(16)-C(17)-C(18)	-0.9(6)
C(7)-N(4)-N(5)-N(6)	180(100)	N(5)-N(4)-C(7)-N(4)	41.1(8)	C(16)-C(17)-C(18)-C(19)	0.4(6)
C(7)-N(4)-N(5)-N(6)	177(6)	N(5)-N(4)-C(7)-C(6)	164.8(6)	C(17)-C(18)-C(19)-C(14)	0.5(6)
C(2)-N(1)-C(1)-O(1)	-174.2(3)	N(5)-N(4)-C(7)-C(3)	-79.4(9)	C(15)-C(14)-C(19)-C(18)	-0.8(5)
C(8)-N(1)-C(1)-O(1)	0.3(6)	N(5)-N(4)-C(7)-N(4)	-33.5(5)	C(3)-C(14)-C(19)-C(18)	-173.8(3)
C(2)-N(1)-C(1)-N(2)	9.7(4)	N(5)-N(4)-C(7)-C(6)	-152.5(4)	C(5)-C(4)-C(20)-C(21)	-35.2(6)
C(8)-N(1)-C(1)-N(2)	-175.9(3)	N(5)-N(4)-C(7)-C(3)	93.9(5)	C(3)-C(4)-C(20)-C(21)	149.0(4)
N(3)-N(2)-C(1)-O(1)	-179.7(3)	C(26)-C(6)-C(7)-N(4)	-50.2(6)	C(5)-C(4)-C(20)-C(25)	147.7(4)
C(6)-N(2)-C(1)-O(1)	57.6(5)	N(2)-C(6)-C(7)-N(4)	72.3(5)	C(3)-C(4)-C(20)-C(25)	-28.1(5)
N(3)-N(2)-C(1)-N(1)	-3.5(3)	C(5)-C(6)-C(7)-N(4)	179.1(5)	C(25)-C(20)-C(21)-C(22)	0.7(7)
C(6)-N(2)-C(1)-N(1)	-126.2(3)	C(26)-C(6)-C(7)-N(4)	53.7(5)	C(4)-C(20)-C(21)-C(22)	-176.5(4)
C(1)-N(1)-C(2)-O(2)	172.4(3)	N(2)-C(6)-C(7)-N(4)	176.2(3)	C(20)-C(21)-C(22)-C(23)	-0.5(8)

## Fortsetzung

C(8)-N(1)-C(2)-O(2)	-2.2(6)	C(5)-C(6)-C(7)-N(4)	-77.0(4)	C(21)-C(22)-C(23)-C(24)	-0.9(8)
C(1)-N(1)-C(2)-N(3)	-11.9(4)	C(26)-C(6)-C(7)-C(3)	178.2(3)	C(22)-C(23)-C(24)-C(25)	2.0(7)
C(8)-N(1)-C(2)-N(3)	173.6(3)	N(2)-C(6)-C(7)-C(3)	-59.3(3)	C(23)-C(24)-C(25)-C(20)	-1.7(6)
N(2)-N(3)-C(2)-O(2)	-175.0(3)	C(5)-C(6)-C(7)-C(3)	47.5(3)	C(21)-C(20)-C(25)-C(24)	0.4(6)
C(3)-N(3)-C(2)-O(2)	-52.7(5)	N(3)-C(3)-C(7)-N(4)	-66.3(6)	C(4)-C(20)-C(25)-C(24)	177.5(4)
N(2)-N(3)-C(2)-N(1)	9.1(3)	C(14)-C(3)-C(7)-N(4)	53.6(7)	N(2)-C(6)-C(26)-C(27)	8.5(5)
C(3)-N(3)-C(2)-N(1)	131.4(3)	C(4)-C(3)-C(7)-N(4)	-174.8(6)	C(5)-C(6)-C(26)-C(27)	-118.6(4)
C(2)-N(3)-C(3)-C(14)	82.0(4)	N(3)-C(3)-C(7)-N(4)	-172.6(4)	C(7)-C(6)-C(26)-C(27)	119.6(4)
N(2)-N(3)-C(3)-C(14)	-155.3(3)	C(14)-C(3)-C(7)-N(4)	-52.7(5)	N(2)-C(6)-C(26)-C(31)	-167.6(3)
C(2)-N(3)-C(3)-C(4)	-56.0(3)	C(4)-C(3)-C(7)-N(4)	78.8(4)	C(5)-C(6)-C(26)-C(31)	65.2(4)
N(2)-N(3)-C(3)-C(4)	66.7(3)	N(3)-C(3)-C(7)-C(6)	59.3(3)	C(7)-C(6)-C(26)-C(31)	-56.6(4)
C(2)-N(3)-C(3)-C(7)	-159.7(3)	C(14)-C(3)-C(7)-C(6)	179.2(3)	C(31)-C(26)-C(27)-C(28)	-0.3(6)
N(2)-N(3)-C(3)-C(7)	-37.0(3)	C(4)-C(3)-C(7)-C(6)	-49.2(3)	C(6)-C(26)-C(27)-C(28)	-176.4(3)
N(3)-C(3)-C(4)-C(5)	-65.4(3)	C(2)-N(1)-C(8)-C(9)	120.2(4)	C(26)-C(27)-C(28)-C(29)	0.0(6)
C(14)-C(3)-C(4)-C(5)	160.2(3)	C(1)-N(1)-C(8)-C(9)	-53.6(5)	C(27)-C(28)-C(29)-C(30)	0.5(6)
C(7)-C(3)-C(4)-C(5)	34.4(3)	C(2)-N(1)-C(8)-C(13)	-57.8(4)	C(28)-C(29)-C(30)-C(31)	-0.7(7)
N(3)-C(3)-C(4)-C(20)	111.1(3)	C(1)-N(1)-C(8)-C(13)	128.4(3)	C(29)-C(30)-C(31)-C(26)	0.4(6)
C(14)-C(3)-C(4)-C(20)	-23.3(5)	C(13)-C(8)-C(9)-C(10)	1.2(6)	C(27)-C(26)-C(31)-C(30)	0.1(6)
C(7)-C(3)-C(4)-C(20)	-149.1(3)	N(1)-C(8)-C(9)-C(10)	-176.8(4)	C(6)-C(26)-C(31)-C(30)	176.5(4)
C(20)-C(4)-C(5)-C(32)	-14.9(6)	C(8)-C(9)-C(10)-C(11)	0.9(7)	C(4)-C(5)-C(32)-C(37)	-58.6(5)
C(3)-C(4)-C(5)-C(32)	161.6(3)	C(9)-C(10)-C(11)-C(12)	-2.1(7)	C(6)-C(5)-C(32)-C(37)	103.9(4)
C(20)-C(4)-C(5)-C(6)	-179.6(3)	C(10)-C(11)-C(12)-C(13)	1.3(6)	C(4)-C(5)-C(32)-C(33)	123.7(4)
C(3)-C(4)-C(5)-C(6)	-3.1(3)	C(9)-C(8)-C(13)-C(12)	-2.0(5)	C(6)-C(5)-C(32)-C(33)	-73.8(5)
C(1)-N(2)-C(6)-C(26)	-76.7(4)	N(1)-C(8)-C(13)-C(12)	176.0(3)	C(37)-C(32)-C(33)-C(34)	-0.2(6)
N(3)-N(2)-C(6)-C(26)	159.5(3)	C(11)-C(12)-C(13)-C(8)	0.8(6)	C(5)-C(32)-C(33)-C(34)	177.6(4)
C(1)-N(2)-C(6)-C(5)	57.3(4)	N(3)-C(3)-C(14)-C(15)	18.7(4)	C(32)-C(33)-C(34)-C(35)	-2.3(7)
N(3)-N(2)-C(6)-C(5)	-66.5(3)	C(4)-C(3)-C(14)-C(15)	149.9(3)	C(33)-C(34)-C(35)-C(36)	3.7(7)
C(1)-N(2)-C(6)-C(7)	161.4(3)	C(7)-C(3)-C(14)-C(15)	-89.7(4)	C(34)-C(35)-C(36)-C(37)	-2.5(7)
N(3)-N(2)-C(6)-C(7)	37.6(3)	N(3)-C(3)-C(14)-C(19)	-168.5(3)	C(35)-C(36)-C(37)-C(32)	-0.1(7)
C(4)-C(5)-C(6)-C(26)	-157.9(3)	C(4)-C(3)-C(14)-C(19)	-37.4(4)	C(33)-C(32)-C(37)-C(36)	1.4(6)
C(32)-C(5)-C(6)-C(26)	36.4(5)	C(7)-C(3)-C(14)-C(19)	83.0(4)	C(5)-C(32)-C(37)-C(36)	-176.5(4)

## Photoelektronen-Spektrum von 2-Methyl-1-azaspiro[2.4]hepta-1,4,6-trien (57)

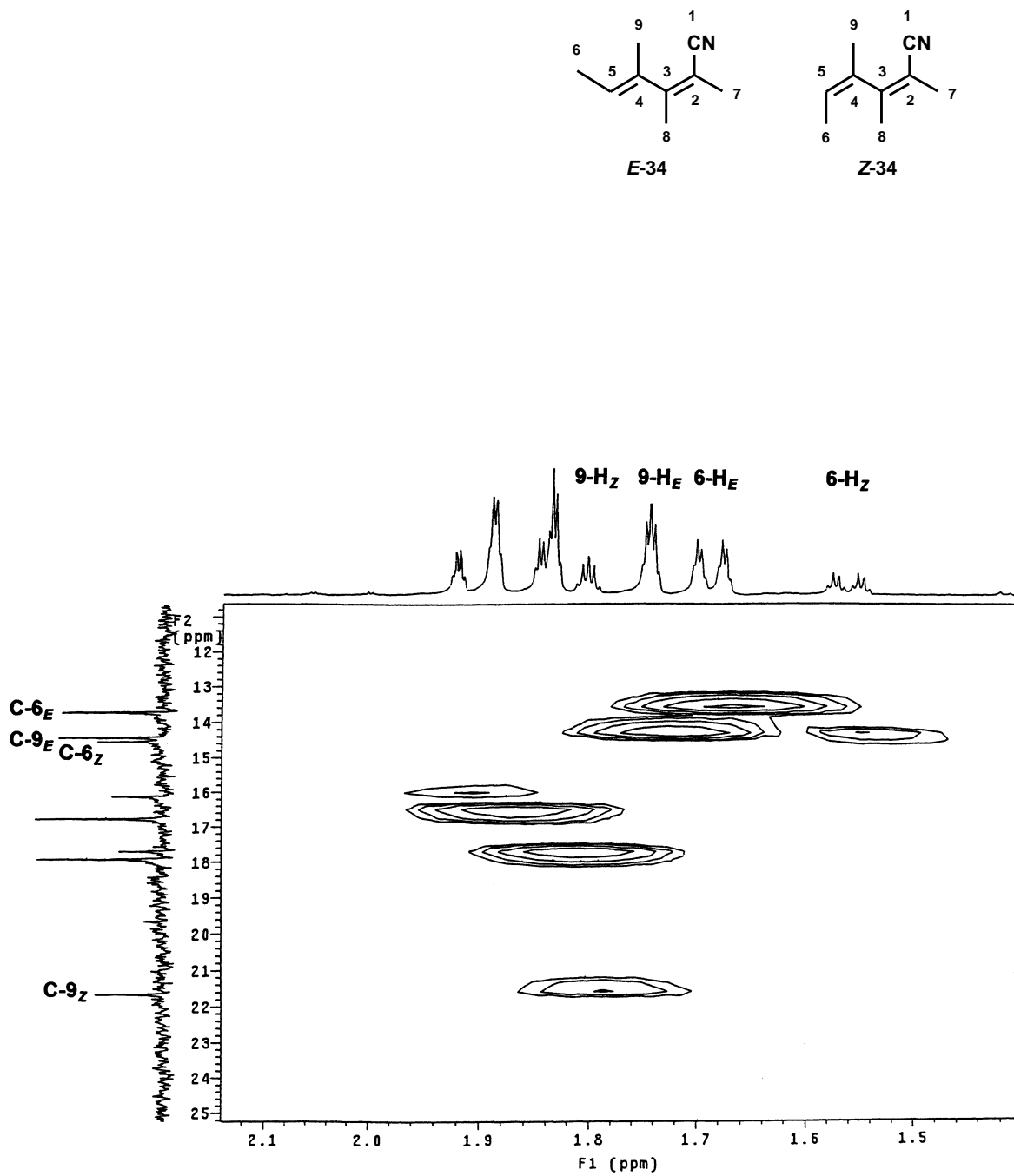
Abb. 7



$^1\text{H}$ ,  $^{13}\text{C}$ -Shift-korreliertes Spektrum der 2,3,4-Trimethylhexa-2,4-dienitrile *E*-/*Z*-34

Abb. 8

Es ist nur der aliphatische Bereich angegeben.



## **Selbständigkeitserklärung**

Hiermit erkläre ich, daß ich die vorliegende Arbeit  
selbständig und nur unter Verwendung der angegebenen  
Literatur und Hilfsmittel angefertigt habe.

Chemnitz, den 22.05.2002

Dipl.-Chem. Beate Müller

# Lebenslauf

## Privat

Name Beate Müller  
geboren am 25. 10. 1970 in Rodewisch  
Familienstand ledig, keine Kinder

## Schulbildung

09/77 – 08/87 Polytechnische Oberschule in Treuen

## Berufsausbildung

09/87 – 08/90 Facharbeiter für Textiltechnik mit Abitur in Plauen

## Studium / Beruf

09/90 – 03/92 Maschinenbau an der TU Chemnitz  
04/92 – 09/92 Urlaubssemester  
10/92 – 08/97 Diplomstudiengang Chemie an der TU Chemnitz  
09/94 Vordiplom  
10/96 – 08/97 Diplomarbeit in Organischer Chemie, Thema "Sigmatrope Umlagerungen mit Beteiligung von Stickstoff und Schwefel"  
08/97 Diplom, Gesamtprädikat: "Sehr gut"  
seit 09/97 Promotion am Lehrstuhl für Organische Chemie, TU Chemnitz  
09/97–12/97 Wissenschaftliche Hilfskraft an der TU Chemnitz  
12/97–11/00 Stipendium des Freistaates Sachsen (Graduiertenstudent)  
seit 10/00 Wissenschaftliche Mitarbeiterin an der TU Chemnitz

## weitere Tätigkeiten

- Mitarbeit in Studienkommission des Fachbereiches Chemie der TU Chemnitz als Studentenvertreter
- Erwerb des Universitätszertifikates Technikfolgen-Umwelt

## Posterpräsentationen / Publikationen

- 18th International Symposium on the Organic Chemistry of Sulfur, Florenz 1998 (Posterpräsentation)
- IUPAC / GDCh Congress, Berlin 1999 (Posterpräsentation)
- K. Banert, W. Fendel, A. Müller, B. Müller, J. Schlott, *Phosphorus, Sulfur and Silicon* **1999**, 153-154, 325–326.

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