

9 Anhang

Kristallstrukturdaten von 3-Azido-1,2-diphenyl-1*H*-inden **55a** (Darstellung siehe S. 24)

Kristall-, Aufnahme- und Verfeinerungsdaten der Verbindung 55a			
Summenformel	C ₂₁ H ₁₅ N ₃ (309.36)	Diffraktometer	Bruker SMART CCD
Kristallform, -farbe	Block, gelb	Strahlung (λ [Å])	Mo K _α (0.71073)
Kristallgröße	0.4×0.3×0.3 mm	Temperatur [K]	173(2)
Kristallsystem	monoklin	Scan-Modus	ω scans
Raumgruppe	P2(1)/c	Scan-Bereich θ [°]	1.84–30.22
Gitterkonstanten		Absorptionskorrektur	empirisch
a [Å]	11.3640(6)	max./min. Transmission	0.977861/0.642621
b [Å]	9.4497(4)	Reflexe {N (hkl)}	
c [Å]	15.50900(10)	gemessen	6383
α [°]	90	unabhängig	3584
β [°]	103.363(2)	beobachtet >2σ(I)	1737
γ [°]	90	Verfeinerungsmethode	kleinste Fehlerquadrate (F ²)
Volumen [Å³]	1620.36(11)	Verfeinerte Parameter	277
Z (Zellbesetzung)	4	R(int)	0.0468
Dichte, ber. [g·cm⁻³]	1.268	S	1.012
Indexbereich	-3≤h≤15	R1, wR2 {I>2σ(I)}	R1=0.0656, wR2=0.1231
	-9≤k≤13	R1, wR2 (alle Daten)	R1=0.1587, wR2=0.1630
	-21≤l≤14	Maximum δ/σ	0.001
linearer Absorptionskoeffizient [mm⁻¹]	0.076	max./min. Restelektro- nendichte [e·Å⁻³]	0.191/-0.203

Lageparameter (Atomkoordinaten) (×10⁴)

Atom	X	Y	Z	Atom	X	Y	Z
N(1)	7878(2)	10744(3)	2807(2)	C(10)	5718(2)	9113(3)	1769(2)
N(2)	8780(2)	11364(3)	3253(2)	C(11)	5610(2)	10452(4)	1380(2)
N(3)	9494(2)	12121(4)	3631(2)	C(12)	4506(2)	10932(4)	882(2)
C(1)	7884(2)	9259(3)	2728(2)	C(13)	3486(2)	10080(4)	762(2)
C(2)	6893(2)	8537(3)	2275(2)	C(14)	3574(2)	8767(4)	1141(2)
C(3)	7140(2)	6964(3)	2337(2)	C(15)	4675(2)	8259(4)	1639(2)
C(4)	8428(2)	6898(3)	2908(2)	C(16)	7031(2)	6228(3)	1448(2)
C(5)	9126(3)	5724(4)	3193(2)	C(17)	7570(2)	6844(3)	815(2)
C(6)	10293(3)	5923(4)	3717(2)	C(18)	7505(2)	6183(4)	5(2)
C(7)	10737(3)	7269(4)	3925(2)	C(19)	6900(2)	4915(4)	-186(2)
C(8)	10040(2)	8476(4)	3635(2)	C(20)	6375(3)	4298(4)	436(2)
C(9)	8862(2)	8267(3)	3121(2)	C(21)	6439(2)	4950(4)	1250(2)

interatomare Abstände (Bindungslängen) [Å]

N(1)-N(2)	1.242(3)	C(6)-C(7)	1.378(5)	C(14)-C(15)	1.395(4)
N(1)-C(1)	1.409(4)	C(6)-H(6)	1.01(4)	C(14)-H(14)	0.97(3)
N(2)-N(3)	1.138(4)	C(7)-C(8)	1.402(5)	C(15)-H(15)	1.01(3)
C(1)-C(2)	1.364(4)	C(7)-H(7)	1.01(3)	C(16)-C(21)	1.382(4)
C(1)-C(9)	1.474(4)	C(8)-C(9)	1.405(4)	C(16)-C(17)	1.399(4)
C(2)-C(10)	1.487(4)	C(8)-H(8)	0.94(3)	C(17)-C(18)	1.389(4)
C(2)-C(3)	1.513(4)	C(10)-C(11)	1.394(4)	C(17)-H(17)	0.97(3)
C(3)-C(16)	1.523(4)	C(10)-C(15)	1.410(4)	C(18)-C(19)	1.379(5)
C(3)-C(4)	1.527(3)	C(11)-C(12)	1.389(4)	C(18)-H(18)	0.99(3)
C(3)-H(3)	0.99(3)	C(11)-H(11)	1.01(3)	C(19)-C(20)	1.376(5)
C(4)-C(5)	1.376(4)	C(12)-C(13)	1.388(4)	C(19)-H(19)	0.92(3)
C(4)-C(9)	1.396(4)	C(12)-H(12)	0.97(3)	C(20)-C(21)	1.391(4)
C(5)-C(6)	1.399(4)	C(13)-C(14)	1.367(5)	C(20)-H(20)	0.98(4)
C(5)-H(5)	0.90(3)	C(13)-H(13)	1.01(3)	C(21)-H(21)	0.97(3)

intermolekulare Winkel [°]

N(2)-N(1)-C(1)	119.9(3)	C(6)-C(7)-C(8)	121.8(3)	C(15)-C(14)-H(14)	119.6(19)
N(3)-N(2)-N(1)	169.0(3)	C(6)-C(7)-H(7)	119(2)	C(14)-C(15)-C(10)	119.9(3)
C(2)-C(1)-N(1)	121.5(3)	C(8)-C(7)-H(7)	120(2)	C(14)-C(15)-H(15)	119.9(16)
C(2)-C(1)-C(9)	110.4(3)	C(7)-C(8)-C(9)	117.5(3)	C(10)-C(15)-H(15)	120.1(16)
N(1)-C(1)-C(9)	128.0(2)	C(7)-C(8)-H(8)	121.0(19)	C(21)-C(16)-C(17)	118.5(3)
C(1)-C(2)-C(10)	128.5(3)	C(9)-C(8)-H(8)	121.5(19)	C(21)-C(16)-C(3)	122.3(2)
C(1)-C(2)-C(3)	109.9(2)	C(4)-C(9)-C(8)	120.2(3)	C(17)-C(16)-C(3)	119.3(3)
C(10)-C(2)-C(3)	121.6(2)	C(4)-C(9)-C(1)	107.5(2)	C(18)-C(17)-C(16)	120.5(3)
C(2)-C(3)-C(16)	114.6(2)	C(8)-C(9)-C(1)	132.3(3)	C(18)-C(17)-H(17)	121.9(15)
C(2)-C(3)-C(4)	102.5(2)	C(11)-C(10)-C(15)	118.1(3)	C(16)-C(17)-H(17)	117.6(15)
C(16)-C(3)-C(4)	111.9(2)	C(11)-C(10)-C(2)	122.6(2)	C(19)-C(18)-C(17)	120.3(3)
C(2)-C(3)-H(3)	108.8(17)	C(15)-C(10)-C(2)	119.2(3)	C(19)-C(18)-H(18)	121.4(19)
C(16)-C(3)-H(3)	108.4(16)	C(12)-C(11)-C(10)	121.0(3)	C(17)-C(18)-H(18)	118.3(19)
C(4)-C(3)-H(3)	110.6(14)	C(12)-C(11)-H(11)	118.5(19)	C(20)-C(19)-C(18)	119.5(3)
C(5)-C(4)-C(9)	121.7(3)	C(10)-C(11)-H(11)	120.5(19)	C(20)-C(19)-H(19)	124.0(19)
C(5)-C(4)-C(3)	128.5(3)	C(13)-C(12)-C(11)	120.3(3)	C(18)-C(19)-H(19)	116.4(19)
C(9)-C(4)-C(3)	109.8(2)	C(13)-C(12)-H(12)	121.2(16)	C(19)-C(20)-C(21)	120.5(3)
C(4)-C(5)-C(6)	118.4(3)	C(11)-C(12)-H(12)	118.4(17)	C(19)-C(20)-H(20)	116.7(17)
C(4)-C(5)-H(5)	120.8(19)	C(14)-C(13)-C(12)	119.6(3)	C(21)-C(20)-H(20)	122.8(17)
C(6)-C(5)-H(5)	120.7(19)	C(14)-C(13)-H(13)	121.2(18)	C(16)-C(21)-C(20)	120.7(3)
C(7)-C(6)-C(5)	120.4(3)	C(12)-C(13)-H(13)	119.2(18)	C(16)-C(21)-H(21)	114.4(18)
C(7)-C(6)-H(6)	119.2(19)	C(13)-C(14)-C(15)	121.2(3)	C(20)-C(21)-H(21)	124.8(18)
C(5)-C(6)-H(6)	120.3(19)	C(13)-C(14)-H(14)	119.1(19)		

Torsionswinkel

C(1)-N(1)-N(2)-N(3)	-175.9(16)	C(5)-C(6)-C(7)-C(8)	1.0(5)	C(10)-C(11)-C(12)-C(13)	0.0(5)
N(2)-N(1)-C(1)-C(2)	177.2(2)	C(6)-C(7)-C(8)-C(9)	0.0(5)	C(11)-C(12)-C(13)-C(14)	0.2(5)
N(2)-N(1)-C(1)-C(9)	0.2(4)	C(5)-C(4)-C(9)-C(8)	0.3(4)	C(12)-C(13)-C(14)-C(15)	-0.6(4)
N(1)-C(1)-C(2)-C(10)	3.5(4)	C(3)-C(4)-C(9)-C(8)	-179.2(2)	C(13)-C(14)-C(15)-C(10)	0.8(4)
C(9)-C(1)-C(2)-C(10)	-178.9(2)	C(5)-C(4)-C(9)-C(1)	-179.0(2)	C(11)-C(10)-C(15)-C(14)	-0.5(4)
N(1)-C(1)-C(2)-C(3)	-177.3(2)	C(3)-C(4)-C(9)-C(1)	1.5(3)	C(2)-C(10)-C(15)-C(14)	-177.9(2)
C(9)-C(1)-C(2)-C(3)	0.2(3)	C(7)-C(8)-C(9)-C(4)	-0.6(4)	C(2)-C(3)-C(16)-C(21)	-135.6(3)
C(1)-C(2)-C(3)-C(16)	-120.7(2)	C(7)-C(8)-C(9)-C(1)	178.4(3)	C(4)-C(3)-C(16)-C(21)	108.3(3)
C(10)-C(2)-C(3)-C(16)	58.5(3)	C(2)-C(1)-C(9)-C(4)	-1.1(3)	C(2)-C(3)-C(16)-C(17)	45.9(3)
C(1)-C(2)-C(3)-C(4)	0.7(3)	N(1)-C(1)-C(9)-C(4)	176.2(2)	C(4)-C(3)-C(16)-C(17)	-70.2(3)
C(10)-C(2)-C(3)-C(4)	179.88(19)	C(2)-C(1)-C(9)-C(8)	179.7(3)	C(21)-C(16)-C(17)-C(18)	0.2(4)
C(2)-C(3)-C(4)-C(5)	179.2(3)	N(1)-C(1)-C(9)-C(8)	-2.9(5)	C(3)-C(16)-C(17)-C(18)	178.7(2)
C(16)-C(3)-C(4)-C(5)	-57.6(3)	C(1)-C(2)-C(10)-C(11)	27.0(4)	C(16)-C(17)-C(18)-C(19)	0.5(4)
C(2)-C(3)-C(4)-C(9)	-1.4(3)	C(3)-C(2)-C(10)-C(11)	-152.0(3)	C(17)-C(18)-C(19)-C(20)	-1.0(5)
C(16)-C(3)-C(4)-C(9)	121.9(2)	C(1)-C(2)-C(10)-C(15)	-155.7(3)	C(18)-C(19)-C(20)-C(21)	0.7(5)
C(9)-C(4)-C(5)-C(6)	0.7(4)	C(3)-C(2)-C(10)-C(15)	25.2(3)	C(17)-C(16)-C(21)-C(20)	-0.4(4)
C(3)-C(4)-C(5)-C(6)	-179.9(2)	C(15)-C(10)-C(11)-C(12)	0.1(4)	C(3)-C(16)-C(21)-C(20)	-178.9(3)
C(4)-C(5)-C(6)-C(7)	-1.3(4)	C(2)-C(10)-C(11)-C(12)	177.4(2)	C(19)-C(20)-C(21)-C(16)	0.0(5)

Kristallstrukturdaten von *E,E*-[1,2-Bis-(1-azidoethyliden)-ethan-1,2-diy]-bis(diphenylphosphinoxid) *E,E*-**83** (Darstellung siehe S. 34)

Kristall-, Aufnahme- und Verfeinerungsdaten der Verbindung *E,E*-**83**

Summenformel	C ₃₂ H ₃₂ Cl ₄ N ₆ O ₃ P ₂ (752.38)	Diffraktometer	Bruker SMART CCD
Kristallform, -farbe	Plättchen, farblos	Strahlung (λ [Å])	Mo K _α (0.71073)
Kristallgröße	1.30×0.30×0.08mm	Temperatur [K]	173(2)
Kristallsystem	monoklin	Scan-Modus	ω scans
Raumgruppe	P2(1)/n	Scan-Bereich θ [°]	1.83–31.00
Gitterkonstanten		Absorptionskorrektur	empirisch
a [Å]	14.475(3)	max./min. Transmission	0.9639/0.5842
b [Å]	17.223(3)	Reflexe {N (hkl)}	
c [Å]	14.548(2)	gemessen	27477
α [°]	90	unabhängig	10217
β [°]	100.084(4)	beobachtet >2σ(I)	5414
γ [°]	90	Verfeinerungsmethode	kleinste Fehlerquadrate (F ²)
Volumen [Å³]	3570.7(11)	Verfeinerte Parameter	552
Z (Zellbesetzung)	4	R(int)	0.0590
Dichte, ber. [g·cm⁻³]	1.400	S	0.983
Indexbereich	-19<=h<=17	R1, wR2 {I>2σ(I)}	R1=0.0496, wR2=0.1049
	-15<=k<=24	R1, wR2 (alle Daten)	R1=0.1233, wR2=0.1307
	-18<=l<=20	Maximum δ/σ	0.005
linearer Absorptionskoeffizient [mm⁻¹]	0.463	max./min. Restelektro- nendichte [e·Å⁻³]	0.743/-0.629

Lageparameter (Atomkoordinaten) (×10⁴)

Atom	X	Y	Z	Atom	X	Y	Z
P(1)	8721(1)	1324(1)	8228(1)	C(6)	10517(2)	2949(2)	10490(2)
P(2)	8720(1)	2015(1)	10881(1)	C(7)	9977(2)	1272(1)	8582(2)
O(1)	8276(1)	561(1)	8365(1)	C(8)	10604(2)	1570(2)	8043(2)
O(2)	9370(1)	1385(1)	11278(1)	C(9)	11562(2)	1482(2)	8328(2)
N(1)	7218(1)	3017(1)	9215(1)	C(10)	11903(2)	1100(2)	9153(2)
N(2)	6372(2)	3190(1)	9155(1)	C(11)	11295(2)	816(2)	9702(2)
N(3)	5645(2)	3400(2)	9195(2)	C(12)	10336(2)	897(2)	9420(2)
N(4)	9792(1)	3050(1)	8810(1)	C(13)	8519(2)	1610(1)	7014(2)
N(5)	10544(2)	3359(1)	8712(2)	C(14)	8496(2)	2382(2)	6734(2)
N(6)	11178(2)	3642(2)	8511(2)	C(15)	8341(2)	2559(2)	5789(2)
C(1)	6665(2)	2095(2)	7919(2)	C(16)	8213(2)	1975(2)	5129(2)
C(2)	7432(2)	2385(1)	8664(2)	C(17)	8241(2)	1213(2)	5402(2)
C(3)	8309(2)	2103(1)	8894(2)	C(18)	8398(2)	1028(2)	6341(2)
C(4)	8944(2)	2362(1)	9763(2)	C(19)	8787(2)	2844(1)	11648(2)
C(5)	9719(2)	2776(1)	9714(2)	C(20)	9072(2)	2715(2)	12598(2)

Fortsetzung

Atom	X	Y	Z	Atom	X	Y	Z
C(21)	9151(2)	3329(2)	13221(2)	C(30)	6815(2)	2104(2)	11047(2)
C(22)	8949(2)	4064(2)	12904(2)	O(3)	11154(2)	935(2)	12234(2)
C(23)	8657(2)	4203(2)	11967(3)	Cl(1)	8036(1)	752(1)	2895(1)
C(24)	8577(2)	3596(2)	11336(2)	Cl(2)	9206(1)	-440(1)	3906(1)
C(25)	7510(2)	1695(1)	10703(2)	C(31)	9073(2)	233(2)	2968(3)
C(26)	7283(2)	991(2)	10253(2)	Cl(3)	4149(1)	526(1)	2160(1)
C(27)	6375(2)	706(2)	10138(2)	Cl(4)	3924(1)	128(1)	4060(1)
C(28)	5690(2)	1116(2)	10483(2)	C(32)	3360(2)	444(2)	2962(3)
C(29)	5910(2)	1806(2)	10932(2)				

interatomare Abstände (Bindungslängen) [Å]

P(1)-O(1)	1.4928(17)	C(8)-C(9)	1.383(4)	C(22)-H(22)	0.95(3)
P(1)-C(7)	1.804(2)	C(8)-H(8)	0.95(3)	C(23)-C(24)	1.383(4)
P(1)-C(13)	1.807(2)	C(9)-C(10)	1.383(4)	C(23)-H(23)	0.89(3)
P(1)-C(3)	1.815(2)	C(9)-H(9)	0.98(3)	C(24)-H(24)	0.95(3)
P(2)-O(2)	1.4863(17)	C(10)-C(11)	1.378(4)	C(25)-C(26)	1.390(3)
P(2)-C(19)	1.803(2)	C(10)-H(10)	0.97(3)	C(25)-C(30)	1.392(3)
P(2)-C(25)	1.810(2)	C(11)-C(12)	1.384(4)	C(26)-C(27)	1.385(4)
P(2)-C(4)	1.816(2)	C(11)-H(11)	0.95(2)	C(26)-H(26)	0.97(3)
N(1)-N(2)	1.248(3)	C(12)-H(12)	0.87(3)	C(27)-C(28)	1.381(4)
N(1)-C(2)	1.419(3)	C(13)-C(14)	1.389(4)	C(27)-H(27)	0.92(3)
N(2)-N(3)	1.125(3)	C(13)-C(18)	1.391(4)	C(28)-C(29)	1.367(4)
N(4)-N(5)	1.243(3)	C(14)-C(15)	1.387(4)	C(28)-H(28)	0.94(3)
N(4)-C(5)	1.418(3)	C(14)-H(14)	0.95(3)	C(29)-C(30)	1.389(4)
N(5)-N(6)	1.121(3)	C(15)-C(16)	1.380(4)	C(29)-H(29)	0.86(3)
C(1)-C(2)	1.494(3)	C(15)-H(15)	0.91(3)	C(30)-H(30)	0.97(3)
C(1)-H(1A)	0.99(3)	C(16)-C(17)	1.371(5)	O(3)-H(103)	0.86(4)
C(1)-H(1B)	0.92(3)	C(16)-H(16)	0.93(3)	O(3)-H(203)	0.76(3)
C(1)-H(1C)	0.92(3)	C(17)-C(18)	1.383(4)	Cl(1)-C(31)	1.734(3)
C(2)-C(3)	1.346(3)	C(17)-H(17)	0.97(3)	Cl(2)-C(31)	1.775(4)
C(3)-C(4)	1.494(3)	C(18)-H(18)	0.90(3)	C(31)-H(31A)	0.88(4)
C(4)-C(5)	1.341(3)	C(19)-C(24)	1.389(4)	C(31)-H(31B)	1.01(3)
C(5)-C(6)	1.497(3)	C(19)-C(20)	1.389(3)	Cl(3)-C(32)	1.776(4)
C(6)-H(6A)	0.98(3)	C(20)-C(21)	1.384(4)	Cl(4)-C(32)	1.748(4)
C(6)-H(6B)	0.98(3)	C(20)-H(20)	0.96(3)	C(32)-H(32A)	0.94(3)
C(6)-H(6C)	1.00(3)	C(21)-C(22)	1.361(5)	C(32)-H(32B)	0.85(3)
C(7)-C(12)	1.397(3)	C(21)-H(21)	0.90(3)		
C(7)-C(8)	1.397(3)	C(22)-C(23)	1.376(5)		

intermolekulare Winkel [°]

O(1)-P(1)-C(7)	110.79(10)	N(1)-C(2)-C(1)	117.3(2)	C(8)-C(9)-H(9)	117.2(16)
O(1)-P(1)-C(13)	111.76(10)	C(2)-C(3)-C(4)	121.1(2)	C(11)-C(10)-C(9)	120.4(2)
C(7)-P(1)-C(13)	105.97(11)	C(2)-C(3)-P(1)	121.15(17)	C(11)-C(10)-H(10)	117.0(16)
O(1)-P(1)-C(3)	112.96(10)	C(4)-C(3)-P(1)	117.48(16)	C(9)-C(10)-H(10)	122.5(16)
C(7)-P(1)-C(3)	107.04(10)	C(5)-C(4)-C(3)	120.7(2)	C(10)-C(11)-C(12)	120.1(3)
C(13)-P(1)-C(3)	107.96(11)	C(5)-C(4)-P(2)	120.32(17)	C(10)-C(11)-H(11)	119.4(15)
O(2)-P(2)-C(19)	112.11(11)	C(3)-C(4)-P(2)	118.64(16)	C(12)-C(11)-H(11)	120.4(15)
O(2)-P(2)-C(25)	111.37(11)	C(4)-C(5)-N(4)	115.1(2)	C(11)-C(12)-C(7)	120.4(2)
C(19)-P(2)-C(25)	106.01(11)	C(4)-C(5)-C(6)	127.5(2)	C(11)-C(12)-H(12)	118.5(18)
O(2)-P(2)-C(4)	112.84(10)	N(4)-C(5)-C(6)	117.4(2)	C(7)-C(12)-H(12)	121.0(18)
C(19)-P(2)-C(4)	107.15(11)	C(5)-C(6)-H(6A)	110.0(16)	C(14)-C(13)-C(18)	119.3(2)
C(25)-P(2)-C(4)	106.96(10)	C(5)-C(6)-H(6B)	112.9(18)	C(14)-C(13)-P(1)	122.63(19)
N(2)-N(1)-C(2)	116.8(2)	H(6A)-C(6)-H(6B)	108(2)	C(18)-C(13)-P(1)	118.1(2)
N(3)-N(2)-N(1)	171.4(3)	C(5)-C(6)-H(6C)	108.2(15)	C(15)-C(14)-C(13)	119.5(3)
N(5)-N(4)-C(5)	117.2(2)	H(6A)-C(6)-H(6C)	111(2)	C(15)-C(14)-H(14)	118.6(16)
N(6)-N(5)-N(4)	171.5(3)	H(6B)-C(6)-H(6C)	107(2)	C(13)-C(14)-H(14)	121.8(16)
C(2)-C(1)-H(1A)	112.6(18)	C(12)-C(7)-C(8)	118.8(2)	C(16)-C(15)-C(14)	120.5(3)
C(2)-C(1)-H(1B)	108.7(18)	C(12)-C(7)-P(1)	118.31(18)	C(16)-C(15)-H(15)	123.9(19)

H(1A)-C(1)-H(1B)	105(3)	C(8)-C(7)-P(1)	122.91(18)	C(14)-C(15)-H(15)	116(2)
C(2)-C(1)-H(1C)	110.4(19)	C(9)-C(8)-C(7)	120.5(2)	C(17)-C(16)-C(15)	120.2(3)
H(1A)-C(1)-H(1C)	112(3)	C(9)-C(8)-H(8)	118.8(16)	C(17)-C(16)-H(16)	118(2)
H(1B)-C(1)-H(1C)	108(3)	C(7)-C(8)-H(8)	120.7(16)	C(15)-C(16)-H(16)	122(2)
C(3)-C(2)-N(1)	115.2(2)	C(10)-C(9)-C(8)	119.9(3)	C(16)-C(17)-C(18)	119.9(3)
C(3)-C(2)-C(1)	127.5(2)	C(10)-C(9)-H(9)	122.8(16)	C(16)-C(17)-H(17)	119.0(19)
C(18)-C(17)-H(17)	121.0(19)	C(24)-C(23)-H(23)	117(2)	C(30)-C(29)-H(29)	117(2)
C(17)-C(18)-C(13)	120.5(3)	C(23)-C(24)-C(19)	120.0(3)	C(29)-C(30)-C(25)	119.7(3)
C(17)-C(18)-H(18)	118.4(17)	C(23)-C(24)-H(24)	118.5(18)	C(29)-C(30)-H(30)	121.2(15)
C(13)-C(18)-H(18)	121.0(17)	C(19)-C(24)-H(24)	121.5(18)	C(25)-C(30)-H(30)	119.0(15)
C(24)-C(19)-C(20)	118.9(2)	C(26)-C(25)-C(30)	119.0(2)	H(103)-O(3)-H(203)	104(3)
C(24)-C(19)-P(2)	123.5(2)	C(26)-C(25)-P(2)	118.44(19)	Cl(1)-C(31)-Cl(2)	111.17(18)
C(20)-C(19)-P(2)	117.6(2)	C(30)-C(25)-P(2)	122.45(19)	Cl(1)-C(31)-H(31A)	108(3)
C(21)-C(20)-C(19)	120.4(3)	C(27)-C(26)-C(25)	120.4(3)	Cl(2)-C(31)-H(31A)	107(3)
C(21)-C(20)-H(20)	119.9(17)	C(27)-C(26)-H(26)	117.1(15)	Cl(1)-C(31)-H(31B)	108(2)
C(19)-C(20)-H(20)	119.7(17)	C(25)-C(26)-H(26)	122.5(15)	Cl(2)-C(31)-H(31B)	108.0(19)
C(22)-C(21)-C(20)	120.1(3)	C(28)-C(27)-C(26)	120.1(3)	H(31A)-C(31)-H(31B)	115(3)
C(22)-C(21)-H(21)	124(2)	C(28)-C(27)-H(27)	121.0(19)	Cl(4)-C(32)-Cl(3)	111.95(19)
C(20)-C(21)-H(21)	116(2)	C(26)-C(27)-H(27)	118.8(19)	Cl(4)-C(32)-H(32A)	109(2)
C(21)-C(22)-C(23)	120.5(3)	C(29)-C(28)-C(27)	119.8(3)	Cl(3)-C(32)-H(32A)	107(2)
C(21)-C(22)-H(22)	120.5(18)	C(29)-C(28)-H(28)	122(2)	Cl(4)-C(32)-H(32B)	109(2)
C(23)-C(22)-H(22)	119.0(18)	C(27)-C(28)-H(28)	119(2)	Cl(3)-C(32)-H(32B)	106(2)
C(22)-C(23)-C(24)	120.2(3)	C(28)-C(29)-C(30)	120.9(3)	H(32A)-C(32)-H(32B)	114(3)
C(22)-C(23)-H(23)	123(2)	C(28)-C(29)-H(29)	122(2)		

Torsionswinkel

C(2)-N(1)-N(2)-N(3)	167.7(18)	N(5)-N(4)-C(5)-C(6)	5.6(3)	O(2)-P(2)-C(19)-C(24)	153.0(2)
C(5)-N(4)-N(5)-N(6)	175(2)	O(1)-P(1)-C(7)-C(12)	-44.3(2)	C(25)-P(2)-C(19)-C(24)	-85.3(2)
N(2)-N(1)-C(2)-C(3)	-165.8(2)	C(13)-P(1)-C(7)-C(12)	-165.66(19)	C(4)-P(2)-C(19)-C(24)	28.7(2)
N(2)-N(1)-C(2)-C(1)	12.9(3)	C(3)-P(1)-C(7)-C(12)	79.3(2)	O(2)-P(2)-C(19)-C(20)	-26.5(2)
N(1)-C(2)-C(3)-C(4)	9.4(3)	O(1)-P(1)-C(7)-C(8)	133.8(2)	C(25)-P(2)-C(19)-C(20)	95.2(2)
C(1)-C(2)-C(3)-C(4)	-169.1(2)	C(13)-P(1)-C(7)-C(8)	12.4(2)	C(4)-P(2)-C(19)-C(20)	-150.79(19)
N(1)-C(2)-C(3)-P(1)	-177.03(16)	C(3)-P(1)-C(7)-C(8)	-102.7(2)	C(24)-C(19)-C(20)-C(21)	-0.5(4)
C(1)-C(2)-C(3)-P(1)	4.5(4)	C(12)-C(7)-C(8)-C(9)	1.0(4)	P(2)-C(19)-C(20)-C(21)	179.0(2)
O(1)-P(1)-C(3)-C(2)	-70.6(2)	P(1)-C(7)-C(8)-C(9)	-177.0(2)	C(19)-C(20)-C(21)-C(22)	0.0(4)
C(7)-P(1)-C(3)-C(2)	167.17(19)	C(7)-C(8)-C(9)-C(10)	-0.2(4)	C(20)-C(21)-C(22)-C(23)	0.6(4)
C(13)-P(1)-C(3)-C(2)	53.5(2)	C(8)-C(9)-C(10)-C(11)	-1.0(4)	C(21)-C(22)-C(23)-C(24)	-0.7(5)
O(1)-P(1)-C(3)-C(4)	103.16(18)	C(9)-C(10)-C(11)-C(12)	1.3(4)	C(22)-C(23)-C(24)-C(19)	0.2(4)
C(7)-P(1)-C(3)-C(4)	-19.0(2)	C(10)-C(11)-C(12)-C(7)	-0.5(4)	C(20)-C(19)-C(24)-C(23)	0.3(4)
C(13)-P(1)-C(3)-C(4)	-132.74(17)	C(8)-C(7)-C(12)-C(11)	-0.7(4)	P(2)-C(19)-C(24)-C(23)	-179.1(2)
C(2)-C(3)-C(4)-C(5)	-113.5(3)	P(1)-C(7)-C(12)-C(11)	177.4(2)	O(2)-P(2)-C(25)-C(26)	-48.1(2)
P(1)-C(3)-C(4)-C(5)	72.7(3)	O(1)-P(1)-C(13)-C(14)	152.5(2)	C(19)-P(2)-C(25)-C(26)	-170.25(19)
C(2)-C(3)-C(4)-P(2)	73.4(3)	C(7)-P(1)-C(13)-C(14)	-86.7(2)	C(4)-P(2)-C(25)-C(26)	75.7(2)
P(1)-C(3)-C(4)-P(2)	-100.42(17)	C(3)-P(1)-C(13)-C(14)	27.7(2)	O(2)-P(2)-C(25)-C(30)	128.0(2)
O(2)-P(2)-C(4)-C(5)	-70.4(2)	O(1)-P(1)-C(13)-C(18)	-28.6(2)	C(19)-P(2)-C(25)-C(30)	5.8(2)
C(19)-P(2)-C(4)-C(5)	53.4(2)	C(7)-P(1)-C(13)-C(18)	92.2(2)	C(4)-P(2)-C(25)-C(30)	-108.3(2)
C(25)-P(2)-C(4)-C(5)	166.75(19)	C(3)-P(1)-C(13)-C(18)	-153.4(2)	C(30)-C(25)-C(26)-C(27)	0.9(4)
O(2)-P(2)-C(4)-C(3)	102.70(18)	C(18)-C(13)-C(14)-C(15)	0.9(4)	P(2)-C(25)-C(26)-C(27)	177.1(2)
C(19)-P(2)-C(4)-C(3)	-133.43(17)	P(1)-C(13)-C(14)-C(15)	179.8(2)	C(25)-C(26)-C(27)-C(28)	-1.0(4)
C(25)-P(2)-C(4)-C(3)	-20.1(2)	C(13)-C(14)-C(15)-C(16)	-0.2(4)	C(26)-C(27)-C(28)-C(29)	0.5(4)
C(3)-C(4)-C(5)-N(4)	10.2(3)	C(14)-C(15)-C(16)-C(17)	-0.2(5)	C(27)-C(28)-C(29)-C(30)	0.0(5)
P(2)-C(4)-C(5)-N(4)	-176.79(15)	C(15)-C(16)-C(17)-C(18)	0.1(5)	C(28)-C(29)-C(30)-C(25)	-0.1(4)
C(3)-C(4)-C(5)-C(6)	-167.2(2)	C(16)-C(17)-C(18)-C(13)	0.5(5)	C(26)-C(25)-C(30)-C(29)	-0.4(4)
P(2)-C(4)-C(5)-C(6)	5.8(4)	C(14)-C(13)-C(18)-C(17)	-1.0(4)	P(2)-C(25)-C(30)-C(29)	-176.4(2)
N(5)-N(4)-C(5)-C(4)	-172.1(2)	P(1)-C(13)-C(18)-C(17)	-180.0(2)		

Kristallstrukturdaten von *rac*-Bi-2*H*-azirin-2-yl *rac*-**85** (Darstellung siehe S. 37)

Kristall-, Aufnahme- und Verfeinerungsdaten der Verbindung <i>rac</i> - 85			
Summenformel	C ₃₀ H ₂₈ N ₂ O ₃ P ₂ (526.48)	Diffraktometer	Bruker SMART CCD
Kristallform, -farbe	Plättchen, farblos	Strahlung (λ [Å])	Mo K _α (0.71073)
Kristallgröße	0.58×0.26×0.10mm	Temperatur [K]	173(2)
Kristallsystem	monoklin	Scan-Modus	ω scans
Raumgruppe	P2(1)/c	Scan-Bereich θ [°]	1.75–31.01
Gitterkonstanten		Absorptionskorrektur	empirisch
a [Å]	9.02180(10)	max./min. Transmission	0.9802/0.8926
b [Å]	20.6574(5)	Reflexe {N (hkl)}	
c [Å]	14.1817(3)	gemessen	12782
α [°]	90	unabhängig	7319
β [°]	94.8780(10)	beobachtet >2σ(I)	4281
γ [°]	90	Verfeinerungsmethode	kleinste Fehlerquadrate (F ²)
Volumen [Å³]	2633.43(9)	Verfeinerte Parameter	446
Z (Zellbesetzung)	4	R(int)	0.0401
Dichte, ber. [g·cm⁻³]	1.328	S	0.976
Indexbereich	-13<=h<=12	R1, wR2 {I>2σ(I)}	R1=0.0510, wR2=0.1047
	-29<=k<=12	R1, wR2 (alle Daten)	R1=0.1086, wR2=0.1276
	-19<=l<=8	Maximum δ/σ	0.006
linearer Absorptionskoeffizient [mm⁻¹]	0.200	max./min. Restelektro- nendichte [e·Å⁻³]	0.421/−0.352

Lageparameter (Atomkoordinaten) (×10⁴)

Atom	X	Y	Z	Atom	X	Y	Z
P(1)	3235(1)	6310(1)	7825(1)	C(14)	5777(3)	7025(1)	7995(2)
P(2)	-750(1)	6354(1)	5681(1)	C(15)	6629(3)	7581(1)	8098(2)
O(1)	3999(2)	5800(1)	7307(1)	C(16)	5953(3)	8178(1)	8105(2)
O(2)	-1540(2)	5843(1)	6181(1)	C(17)	4413(3)	8226(1)	8011(2)
N(1)	341(2)	6911(1)	7825(1)	C(18)	3546(3)	7669(1)	7919(2)
N(2)	2160(2)	6952(1)	5717(1)	C(19)	-1728(2)	7118(1)	5659(2)
C(1)	-775(3)	5836(1)	8336(2)	C(20)	-1049(3)	7716(1)	5550(2)
C(2)	121(2)	6313(1)	7870(1)	C(21)	-1914(3)	8276(1)	5502(2)
C(3)	1356(2)	6444(1)	7285(1)	C(22)	-3431(3)	8241(1)	5559(2)
C(4)	1140(2)	6464(1)	6218(1)	C(23)	-4098(3)	7648(1)	5668(2)
C(5)	2387(2)	6357(1)	5627(1)	C(24)	-3255(3)	7089(1)	5724(2)
C(6)	3308(3)	5901(1)	5138(2)	C(25)	-581(2)	6148(1)	4458(2)
C(7)	3001(2)	6069(1)	9028(1)	C(26)	-1070(3)	5535(1)	4168(2)
C(8)	2643(2)	6504(1)	9721(2)	C(27)	-1052(3)	5354(1)	3231(2)
C(9)	2511(3)	6294(1)	10639(2)	C(28)	-539(3)	5780(1)	2579(2)
C(10)	2739(3)	5646(1)	10874(2)	C(29)	-51(3)	6388(1)	2863(2)
C(11)	3086(3)	5213(1)	10187(2)	C(30)	-71(2)	6574(1)	3801(2)
C(12)	3213(3)	5416(1)	9263(2)	O(3)	6388(2)	4976(1)	6894(1)
C(13)	4232(2)	7064(1)	7912(2)				

interatomare Abstände (Bindungslängen) [Å]

P(1)-O(1)	1.4866(15)	C(7)-C(8)	1.390(3)	C(20)-C(21)	1.395(3)
P(1)-C(13)	1.799(2)	C(7)-C(12)	1.398(3)	C(20)-H(20)	0.96(2)
P(1)-C(7)	1.807(2)	C(8)-C(9)	1.386(3)	C(21)-C(22)	1.380(3)
P(1)-C(3)	1.8212(19)	C(8)-H(8)	1.00(2)	C(21)-H(21)	0.94(2)
P(2)-O(2)	1.4874(15)	C(9)-C(10)	1.391(3)	C(22)-C(23)	1.379(4)
P(2)-C(25)	1.805(2)	C(9)-H(9)	0.96(3)	C(22)-H(22)	0.94(2)
P(2)-C(19)	1.806(2)	C(10)-C(11)	1.380(4)	C(23)-C(24)	1.381(3)
P(2)-C(4)	1.8218(19)	C(10)-H(10)	0.99(3)	C(23)-H(23)	0.95(3)
O(1)-H(1O3)	1.95(4)	C(11)-C(12)	1.389(3)	C(24)-H(24)	0.98(2)
N(1)-C(2)	1.254(3)	C(11)-H(11)	1.01(2)	C(25)-C(30)	1.388(3)
N(1)-C(3)	1.573(3)	C(12)-H(12)	0.97(3)	C(25)-C(26)	1.392(3)
N(2)-C(5)	1.254(3)	C(13)-C(14)	1.391(3)	C(26)-C(27)	1.382(3)
N(2)-C(4)	1.575(3)	C(13)-C(18)	1.396(3)	C(26)-H(26)	0.99(3)
C(1)-C(2)	1.467(3)	C(14)-C(15)	1.383(3)	C(27)-C(28)	1.384(4)
C(1)-H(1A)	0.89(3)	C(14)-H(14)	0.98(2)	C(27)-H(27)	0.92(2)
C(1)-H(1B)	1.01(3)	C(15)-C(16)	1.376(4)	C(28)-C(29)	1.381(3)
C(1)-H(1C)	1.00(3)	C(15)-H(15)	1.00(3)	C(28)-H(28)	0.93(3)
C(2)-C(3)	1.470(3)	C(16)-C(17)	1.388(3)	C(29)-C(30)	1.387(3)
C(3)-C(4)	1.509(3)	C(16)-H(16)	0.88(2)	C(29)-H(29)	0.94(2)
C(4)-C(5)	1.476(3)	C(17)-C(18)	1.390(3)	C(30)-H(30)	1.03(2)
C(5)-C(6)	1.468(3)	C(17)-H(17)	0.93(2)	O(3)-H(2O3)	0.83(3)
C(6)-H(6A)	0.97(3)	C(18)-H(18)	0.94(3)	O(3)-H(1O3)	0.90(4)
C(6)-H(6B)	0.96(3)	C(19)-C(24)	1.390(3)		
C(6)-H(6C)	0.94(3)	C(19)-C(20)	1.393(3)		

intermolekulare Winkel [°]

O(1)-P(1)-C(13)	113.43(10)	N(2)-C(4)-P(2)	116.94(12)	C(16)-C(15)-H(15)	119.8(14)
O(1)-P(1)-C(7)	111.54(9)	N(2)-C(5)-C(6)	141.3(2)	C(14)-C(15)-H(15)	119.7(14)
C(13)-P(1)-C(7)	105.78(9)	N(2)-C(5)-C(4)	69.92(16)	C(15)-C(16)-C(17)	120.3(2)
O(1)-P(1)-C(3)	110.77(9)	C(6)-C(5)-C(4)	148.6(2)	C(15)-C(16)-H(16)	122.8(17)
C(13)-P(1)-C(3)	109.82(9)	C(5)-C(6)-H(6A)	111.0(16)	C(17)-C(16)-H(16)	116.9(17)
C(7)-P(1)-C(3)	105.07(9)	C(5)-C(6)-H(6B)	108.7(18)	C(16)-C(17)-C(18)	120.1(2)
O(2)-P(2)-C(25)	111.92(9)	H(6A)-C(6)-H(6B)	110(2)	C(16)-C(17)-H(17)	119.8(14)
O(2)-P(2)-C(19)	112.08(10)	C(5)-C(6)-H(6C)	109.6(17)	C(18)-C(17)-H(17)	120.1(14)
C(25)-P(2)-C(19)	105.69(9)	H(6A)-C(6)-H(6C)	107(2)	C(17)-C(18)-C(13)	119.6(2)
O(2)-P(2)-C(4)	110.98(9)	H(6B)-C(6)-H(6C)	111(3)	C(17)-C(18)-H(18)	118.7(14)
C(25)-P(2)-C(4)	106.17(10)	C(8)-C(7)-C(12)	119.3(2)	C(13)-C(18)-H(18)	121.7(14)
C(19)-P(2)-C(4)	109.71(9)	C(8)-C(7)-P(1)	122.86(15)	C(24)-C(19)-C(20)	119.5(2)
P(1)-O(1)-H(1O3)	155.9(10)	C(12)-C(7)-P(1)	117.80(17)	C(24)-C(19)-P(2)	116.56(16)
C(2)-N(1)-C(3)	61.46(14)	C(9)-C(8)-C(7)	120.4(2)	C(20)-C(19)-P(2)	123.87(17)
C(5)-N(2)-C(4)	61.67(14)	C(9)-C(8)-H(8)	119.8(14)	C(19)-C(20)-C(21)	119.5(2)
C(2)-C(1)-H(1A)	109(2)	C(7)-C(8)-H(8)	119.7(14)	C(19)-C(20)-H(20)	123.2(13)
C(2)-C(1)-H(1B)	109.3(16)	C(8)-C(9)-C(10)	120.2(2)	C(21)-C(20)-H(20)	117.3(13)
H(1A)-C(1)-H(1B)	110(2)	C(8)-C(9)-H(9)	118.7(15)	C(22)-C(21)-C(20)	120.4(2)
C(2)-C(1)-H(1C)	107.5(16)	C(10)-C(9)-H(9)	121.0(15)	C(22)-C(21)-H(21)	116.4(15)
H(1A)-C(1)-H(1C)	112(2)	C(11)-C(10)-C(9)	119.5(2)	C(20)-C(21)-H(21)	123.1(16)
H(1B)-C(1)-H(1C)	108(2)	C(11)-C(10)-H(10)	121.9(13)	C(23)-C(22)-C(21)	119.9(2)
N(1)-C(2)-C(1)	141.3(2)	C(9)-C(10)-H(10)	118.5(13)	C(23)-C(22)-H(22)	124.3(15)
N(1)-C(2)-C(3)	70.02(15)	C(10)-C(11)-C(12)	120.8(2)	C(21)-C(22)-H(22)	115.7(15)
C(1)-C(2)-C(3)	148.4(2)	C(10)-C(11)-H(11)	118.4(14)	C(22)-C(23)-C(24)	120.3(2)
C(2)-C(3)-C(4)	122.11(16)	C(12)-C(11)-H(11)	120.7(14)	C(22)-C(23)-H(23)	120.8(18)
C(2)-C(3)-N(1)	48.52(12)	C(11)-C(12)-C(7)	119.7(2)	C(24)-C(23)-H(23)	118.9(18)
C(4)-C(3)-N(1)	116.16(15)	C(11)-C(12)-H(12)	122.1(16)	C(23)-C(24)-C(19)	120.3(2)
C(2)-C(3)-P(1)	117.20(14)	C(7)-C(12)-H(12)	118.1(16)	C(23)-C(24)-H(24)	121.4(14)
C(4)-C(3)-P(1)	117.51(14)	C(14)-C(13)-C(18)	119.6(2)	C(19)-C(24)-H(24)	118.3(14)
N(1)-C(3)-P(1)	116.63(12)	C(14)-C(13)-P(1)	116.55(16)	C(30)-C(25)-C(26)	119.5(2)
C(5)-C(4)-C(3)	121.73(16)	C(18)-C(13)-P(1)	123.82(17)	C(30)-C(25)-P(2)	123.75(15)
C(5)-C(4)-N(2)	48.40(12)	C(15)-C(14)-C(13)	120.3(2)	C(26)-C(25)-P(2)	116.62(17)
C(3)-C(4)-N(2)	116.03(15)	C(15)-C(14)-H(14)	120.9(13)	C(27)-C(26)-C(25)	120.1(2)
C(5)-C(4)-P(2)	118.39(14)	C(13)-C(14)-H(14)	118.7(13)	C(27)-C(26)-H(26)	119.7(15)
C(3)-C(4)-P(2)	116.90(14)	C(16)-C(15)-C(14)	120.1(2)	C(25)-C(26)-H(26)	119.9(15)
C(26)-C(27)-C(28)	120.1(2)	C(27)-C(28)-H(28)	119.4(16)	C(29)-C(30)-H(30)	119.2(14)

C(26)-C(27)-H(27)	119.7(17)	C(28)-C(29)-C(30)	120.1(2)	C(25)-C(30)-H(30)	120.7(14)
C(28)-C(27)-H(27)	120.2(16)	C(28)-C(29)-H(29)	118.9(14)	H(2O3)-O(3)-H(1O3)	100(3)
C(29)-C(28)-C(27)	120.1(2)	C(30)-C(29)-H(29)	120.8(14)		
C(29)-C(28)-H(28)	120.5(16)	C(29)-C(30)-C(25)	120.0(2)		

Torsionswinkel

C(13)-P(1)-O(1)-H(1O3)	60(2)	O(2)-P(2)-C(4)-C(3)	-40.61(17)	C(13)-C(14)-C(15)-C(16)	-0.9(4)
C(7)-P(1)-O(1)-H(1O3)	-60(2)	C(25)-P(2)-C(4)-C(3)	-162.44(14)	C(14)-C(15)-C(16)-C(17)	0.1(4)
C(3)-P(1)-O(1)-H(1O3)	-176(2)	C(19)-P(2)-C(4)-C(3)	83.80(16)	C(15)-C(16)-C(17)-C(18)	0.7(4)
C(3)-N(1)-C(2)-C(1)	174.6(3)	O(2)-P(2)-C(4)-N(2)	175.32(14)	C(16)-C(17)-C(18)-C(13)	-0.7(4)
N(1)-C(2)-C(3)-C(4)	-98.0(2)	C(25)-P(2)-C(4)-N(2)	53.49(16)	C(14)-C(13)-C(18)-C(17)	-0.1(3)
C(1)-C(2)-C(3)-C(4)	88.3(4)	C(19)-P(2)-C(4)-N(2)	-60.27(17)	P(1)-C(13)-C(18)-C(17)	178.50(18)
C(1)-C(2)-C(3)-N(1)	-173.6(4)	C(4)-N(2)-C(5)-C(6)	175.7(3)	O(2)-P(2)-C(19)-C(24)	-25.7(2)
N(1)-C(2)-C(3)-P(1)	102.61(15)	C(3)-C(4)-C(5)-N(2)	-98.1(2)	C(25)-P(2)-C(19)-C(24)	96.50(19)
C(1)-C(2)-C(3)-P(1)	-71.0(4)	P(2)-C(4)-C(5)-N(2)	102.05(16)	C(4)-P(2)-C(19)-C(24)	-149.43(17)
C(2)-N(1)-C(3)-C(4)	110.87(19)	C(3)-C(4)-C(5)-C(6)	87.0(4)	O(2)-P(2)-C(19)-C(20)	156.68(18)
C(2)-N(1)-C(3)-P(1)	-103.84(16)	N(2)-C(4)-C(5)-C(6)	-174.9(4)	C(25)-P(2)-C(19)-C(20)	-81.2(2)
O(1)-P(1)-C(3)-C(2)	118.06(15)	P(2)-C(4)-C(5)-C(6)	-72.8(4)	C(4)-P(2)-C(19)-C(20)	32.9(2)
C(13)-P(1)-C(3)-C(2)	-115.87(16)	O(1)-P(1)-C(7)-C(8)	164.65(16)	C(24)-C(19)-C(20)-C(21)	-0.3(3)
C(7)-P(1)-C(3)-C(2)	-2.52(17)	C(13)-P(1)-C(7)-C(8)	40.89(19)	P(2)-C(19)-C(20)-C(21)	177.29(17)
O(1)-P(1)-C(3)-C(4)	-42.25(17)	C(3)-P(1)-C(7)-C(8)	-75.28(18)	C(19)-C(20)-C(21)-C(22)	-0.2(4)
C(13)-P(1)-C(3)-C(4)	83.81(16)	O(1)-P(1)-C(7)-C(12)	-14.44(19)	C(20)-C(21)-C(22)-C(23)	0.3(4)
C(7)-P(1)-C(3)-C(4)	-162.83(14)	C(13)-P(1)-C(7)-C(12)	-138.21(17)	C(21)-C(22)-C(23)-C(24)	0.2(4)
O(1)-P(1)-C(3)-N(1)	172.94(13)	C(3)-P(1)-C(7)-C(12)	105.62(17)	C(22)-C(23)-C(24)-C(19)	-0.7(4)
C(13)-P(1)-C(3)-N(1)	-61.00(17)	C(12)-C(7)-C(8)-C(9)	0.6(3)	C(20)-C(19)-C(24)-C(23)	0.8(4)
C(7)-P(1)-C(3)-N(1)	52.36(16)	P(1)-C(7)-C(8)-C(9)	-178.49(16)	P(2)-C(19)-C(24)-C(23)	-177.0(2)
C(2)-C(3)-C(4)-C(5)	-157.30(18)	C(7)-C(8)-C(9)-C(10)	0.1(3)	O(2)-P(2)-C(25)-C(30)	171.20(16)
N(1)-C(3)-C(4)-C(5)	146.96(18)	C(8)-C(9)-C(10)-C(11)	-0.5(3)	C(19)-P(2)-C(25)-C(30)	48.93(19)
P(1)-C(3)-C(4)-C(5)	2.0(2)	C(9)-C(10)-C(11)-C(12)	0.1(4)	C(4)-P(2)-C(25)-C(30)	-67.58(19)
C(2)-C(3)-C(4)-N(2)	147.22(17)	C(10)-C(11)-C(12)-C(7)	0.6(4)	O(2)-P(2)-C(25)-C(26)	-5.41(19)
N(1)-C(3)-C(4)-N(2)	91.5(2)	C(8)-C(7)-C(12)-C(11)	-0.9(3)	C(19)-P(2)-C(25)-C(26)	-127.68(17)
P(1)-C(3)-C(4)-N(2)	-53.5(2)	P(1)-C(7)-C(12)-C(11)	178.21(18)	C(4)-P(2)-C(25)-C(26)	115.82(17)
C(2)-C(3)-C(4)-P(2)	2.8(2)	O(1)-P(1)-C(13)-C(14)	-34.0(2)	C(30)-C(25)-C(26)-C(27)	-0.2(3)
N(1)-C(3)-C(4)-P(2)	-52.9(2)	C(7)-P(1)-C(13)-C(14)	88.57(19)	P(2)-C(25)-C(26)-C(27)	176.55(19)
P(1)-C(3)-C(4)-P(2)	162.10(10)	C(3)-P(1)-C(13)-C(14)	-158.53(17)	C(25)-C(26)-C(27)-C(28)	0.4(4)
C(5)-N(2)-C(4)-C(3)	110.43(19)	O(1)-P(1)-C(13)-C(18)	147.37(19)	C(26)-C(27)-C(28)-C(29)	-0.3(4)
C(5)-N(2)-C(4)-P(2)	-105.19(17)	C(7)-P(1)-C(13)-C(18)	-90.1(2)	C(27)-C(28)-C(29)-C(30)	0.1(4)
O(2)-P(2)-C(4)-C(5)	120.20(16)	C(3)-P(1)-C(13)-C(18)	22.8(2)	C(28)-C(29)-C(30)-C(25)	0.0(3)
C(25)-P(2)-C(4)-C(5)	-1.63(18)	C(18)-C(13)-C(14)-C(15)	0.9(4)	C(26)-C(25)-C(30)-C(29)	0.0(3)
C(19)-P(2)-C(4)-C(5)	-115.39(17)	P(1)-C(13)-C(14)-C(15)	-177.8(2)	P(2)-C(25)-C(30)-C(29)	-176.50(16)

Kristallstrukturdaten von *meso*-Bi-[3-methyl-2-(diphenylphosphinoyl)-2*H*-azirin-2-yl]
meso-**85** (Darstellung siehe S. 37)

Kristall-, Aufnahme- und Verfeinerungsdaten der Verbindung *meso*-**85**

Summenformel	C ₃₆ H ₃₂ N ₂ O ₂ P ₂ (586.58)	Diffraktometer	Bruker SMART CCD
Kristallform, -farbe	Block, farblos	Strahlung (λ [Å])	Mo K α (0.71073)
Kristallgröße	0.40×0.36×0.18 mm	Temperatur [K]	173(2)
Kristallsystem	monoklin	Scan-Modus	ω scans
Raumgruppe	P2(1)/n	Scan-Bereich θ [°]	2.06–30.81
Gitterkonstanten		Absorptionskorrektur	empirisch
a [Å]	8.9905(12)	max./min. Transmission	0.9686/0.9321
b [Å]	8.5595(12)	Reflexe {N (hkl)}	
c [Å]	20.115(3)	gemessen	7358
α [°]	90	unabhängig	3575
β [°]	100.060(3)	beobachtet $>2\sigma(I)$	2695
γ [°]	90	Verfeinerungsmethode	kleinste Fehlerquadrate (F ²)
Volumen [Å³]	1524.1(4)	Verfeinerte Parameter	254
Z (Zellbesetzung)	2	R(int)	0.0280
Dichte, ber. [g·cm⁻³]	1.278	S	1.019
Indexbereich	-12 \leq h \leq 5	R1, wR2 {I$>2\sigma(I)$}	R1=0.0396, wR2=0.1009
	-12 \leq k \leq 11	R1, wR2 (alle Daten)	R1=0.0598, wR2=0.1102
	-28 \leq l \leq 11	Maximum δ/σ	0.008
linearer Absorptionskoeffizient [mm⁻¹]	0.178	max./min. Restelektro- nendichte [e\cdotÅ⁻³]	0.363/-0.291

Lageparameter (Atomkoordinaten) ($\times 10^4$)

Atom	X	Y	Z	Atom	X	Y	Z
P(1)	-15(1)	408(1)	8883(1)	C(9)	1919(3)	-1196(2)	8211(1)
O(1)	-1210(1)	-706(1)	8577(1)	C(10)	-613(2)	2415(2)	8764(1)
N(1)	1940(2)	-1132(2)	9944(1)	C(11)	82(2)	3661(2)	9150(1)
C(1)	597(2)	73(2)	9786(1)	C(12)	-404(2)	5180(2)	9001(1)
C(2)	2202(2)	277(2)	10091(1)	C(13)	-1593(2)	5474(2)	8474(1)
C(3)	3419(2)	1357(3)	10383(1)	C(14)	-2298(2)	4247(2)	8094(1)
C(4)	1689(2)	212(2)	8531(1)	C(15)	-1819(2)	2724(2)	8239(1)
C(5)	2804(2)	1367(2)	8581(1)	C(16)	4833(2)	4986(2)	9301(1)
C(6)	4109(3)	1124(3)	8322(1)	C(17)	3802(2)	5778(2)	9614(1)
C(7)	4331(3)	-276(3)	8010(1)	C(18)	3960(2)	5792(2)	10310(1)
C(8)	3236(3)	-1434(3)	7955(1)				

interatomare Abstände (Bindungslängen) [Å]

P(1)-O(1)	1.4879(11)	C(5)-C(6)	1.380(3)	C(12)-H(12)	0.947(19)
P(1)-C(10)	1.8040(15)	C(5)-H(5)	1.01(2)	C(13)-C(14)	1.385(2)
P(1)-C(4)	1.804(2)	C(6)-C(7)	1.383(4)	C(13)-H(13)	1.000(19)
P(1)-C(1)	1.8258(15)	C(6)-H(6)	0.93(3)	C(14)-C(15)	1.388(2)
N(1)-C(2)	1.254(2)	C(7)-C(8)	1.388(4)	C(14)-H(14)	0.95(2)
N(1)-C(1)	1.5771(19)	C(7)-H(7)	0.87(3)	C(15)-H(15)	0.938(16)
C(1)-C(2)	1.477(2)	C(8)-C(9)	1.386(3)	C(16)-C(17)	1.385(3)
C(1)-C(1)#1	1.495(3)	C(8)-H(8)	0.95(2)	C(16)-C(18)#2	1.392(3)
C(2)-C(3)	1.473(3)	C(9)-H(9)	0.95(2)	C(16)-H(16)	1.02(2)
C(3)-H(3A)	0.95(3)	C(10)-C(11)	1.400(2)	C(17)-C(18)	1.382(3)
C(3)-H(3B)	0.94(3)	C(10)-C(15)	1.401(2)	C(17)-H(17)	0.98(2)
C(3)-H(3C)	1.02(3)	C(11)-C(12)	1.388(2)	C(18)-C(16)#2	1.392(3)
C(4)-C(5)	1.398(3)	C(11)-H(11)	0.948(19)	C(18)-H(18)	0.93(2)
C(4)-C(9)	1.399(3)	C(12)-C(13)	1.391(2)		

intermolekulare Winkel [°]

O(1)-P(1)-C(10)	112.22(7)	C(5)-C(4)-P(1)	123.62(14)	C(11)-C(12)-C(13)	120.35(15)
O(1)-P(1)-C(4)	112.30(8)	C(9)-C(4)-P(1)	117.65(15)	C(11)-C(12)-H(12)	118.1(11)
C(10)-P(1)-C(4)	106.88(8)	C(6)-C(5)-C(4)	120.9(2)	C(13)-C(12)-H(12)	121.5(11)
O(1)-P(1)-C(1)	112.48(7)	C(6)-C(5)-H(5)	121.7(13)	C(14)-C(13)-C(12)	119.97(15)
C(10)-P(1)-C(1)	108.20(7)	C(4)-C(5)-H(5)	117.4(13)	C(14)-C(13)-H(13)	117.7(10)
C(4)-P(1)-C(1)	104.29(7)	C(5)-C(6)-C(7)	120.1(2)	C(12)-C(13)-H(13)	122.4(11)
C(2)-N(1)-C(1)	61.63(10)	C(5)-C(6)-H(6)	121.7(17)	C(13)-C(14)-C(15)	120.11(14)
C(2)-C(1)-C(1)#1	121.25(16)	C(7)-C(6)-H(6)	118.2(17)	C(13)-C(14)-H(14)	121.7(12)
C(2)-C(1)-N(1)	48.36(10)	C(6)-C(7)-C(8)	119.9(3)	C(15)-C(14)-H(14)	118.2(12)
C(1)#1-C(1)-N(1)	115.50(14)	C(6)-C(7)-H(7)	117.6(15)	C(14)-C(15)-C(10)	120.41(14)
C(2)-C(1)-P(1)	119.87(13)	C(8)-C(7)-H(7)	122.5(15)	C(14)-C(15)-H(15)	119.7(9)
C(1)#1-C(1)-P(1)	117.64(13)	C(9)-C(8)-C(7)	120.4(2)	C(10)-C(15)-H(15)	119.8(9)
N(1)-C(1)-P(1)	112.98(10)	C(9)-C(8)-H(8)	119.2(15)	C(17)-C(16)-C(18)#2	119.8(2)
N(1)-C(2)-C(3)	142.47(17)	C(7)-C(8)-H(8)	120.4(14)	C(17)-C(16)-H(16)	120.9(13)
N(1)-C(2)-C(1)	70.01(12)	C(8)-C(9)-C(4)	120.1(2)	C(18)#2-C(16)-H(16)	119.2(13)
C(3)-C(2)-C(1)	147.51(16)	C(8)-C(9)-H(9)	120.6(13)	C(18)-C(17)-C(16)	120.42(17)
C(2)-C(3)-H(3A)	102.8(16)	C(4)-C(9)-H(9)	119.3(13)	C(18)-C(17)-H(17)	120.6(13)
C(2)-C(3)-H(3B)	110.5(18)	C(11)-C(10)-C(15)	119.09(14)	C(16)-C(17)-H(17)	119.0(13)
H(3A)-C(3)-H(3B)	112(2)	C(11)-C(10)-P(1)	123.92(11)	C(17)-C(18)-C(16)#2	119.7(2)
C(2)-C(3)-H(3C)	112.9(16)	C(15)-C(10)-P(1)	116.96(11)	C(17)-C(18)-H(18)	120.3(12)
H(3A)-C(3)-H(3C)	109(2)	C(12)-C(11)-C(10)	120.05(14)	C(16)#2-C(18)-H(18)	119.9(13)
H(3B)-C(3)-H(3C)	110(2)	C(12)-C(11)-H(11)	120.3(12)		
C(5)-C(4)-C(9)	118.70(19)	C(10)-C(11)-H(11)	119.6(12)		

#1 -x, -y, -z+2 #2 -x+1, -y+1, -z+2

Torsionswinkel

C(2)-N(1)-C(1)-C(1)#1	-110.18(18)	P(1)-C(1)-C(2)-C(3)	84.0(3)	C(4)-P(1)-C(10)-C(11)	-75.31(16)
C(2)-N(1)-C(1)-P(1)	110.29(14)	O(1)-P(1)-C(4)-C(5)	161.14(13)	C(1)-P(1)-C(10)-C(11)	36.48(17)
O(1)-P(1)-C(1)-C(2)	143.08(12)	C(10)-P(1)-C(4)-C(5)	37.66(15)	O(1)-P(1)-C(10)-C(15)	-20.83(16)
C(10)-P(1)-C(1)-C(2)	-92.38(13)	C(1)-P(1)-C(4)-C(5)	-76.80(15)	C(4)-P(1)-C(10)-C(15)	102.70(14)
C(4)-P(1)-C(1)-C(2)	21.14(14)	O(1)-P(1)-C(4)-C(9)	-20.98(15)	C(1)-P(1)-C(10)-C(15)	-145.51(14)
O(1)-P(1)-C(1)-C(1)#1	-49.45(17)	C(10)-P(1)-C(4)-C(9)	-144.46(13)	C(15)-C(10)-C(11)-C(12)	-1.3(3)
C(10)-P(1)-C(1)-C(1)#1	75.09(16)	C(1)-P(1)-C(4)-C(9)	101.08(13)	P(1)-C(10)-C(11)-C(12)	176.68(14)
C(4)-P(1)-C(1)-C(1)#1	-171.39(14)	C(9)-C(4)-C(5)-C(6)	-0.3(3)	C(10)-C(11)-C(12)-C(13)	0.7(3)
O(1)-P(1)-C(1)-N(1)	89.15(12)	P(1)-C(4)-C(5)-C(6)	177.60(15)	C(11)-C(12)-C(13)-C(14)	0.1(3)
C(10)-P(1)-C(1)-N(1)	-146.32(11)	C(4)-C(5)-C(6)-C(7)	-0.1(3)	C(12)-C(13)-C(14)-C(15)	-0.2(3)
C(4)-P(1)-C(1)-N(1)	-32.80(12)	C(5)-C(6)-C(7)-C(8)	0.2(3)	C(13)-C(14)-C(15)-C(10)	-0.5(3)
C(1)-N(1)-C(2)-C(3)	-179.4(3)	C(6)-C(7)-C(8)-C(9)	0.0(3)	C(11)-C(10)-C(15)-C(14)	1.2(3)
C(1)#1-C(1)-C(2)-N(1)	97.72(19)	C(7)-C(8)-C(9)-C(4)	-0.4(3)	P(1)-C(10)-C(15)-C(14)	-176.92(14)
P(1)-C(1)-C(2)-N(1)	-95.27(13)	C(5)-C(4)-C(9)-C(8)	0.5(3)	C(18)#2-C(16)-C(17)-C(18)	-0.4(3)
C(1)#1-C(1)-C(2)-C(3)	-83.0(4)	P(1)-C(4)-C(9)-C(8)	-177.45(15)	C(16)-C(17)-C(18)-C(16)#2	0.4(3)
N(1)-C(1)-C(2)-C(3)	179.3(4)	O(1)-P(1)-C(10)-C(11)	161.17(14)		

#1 -x, -y, -z+2 #2 -x+1, -y+1, -z+2

Kristallstrukturdaten von *trans*-6-*t*-Butyl-2-phenyl-1-azaspiro[2.5]oct-1-en *trans*-97
(Darstellung siehe S. 45)

Kristall-, Aufnahme- und Verfeinerungsdaten der Verbindung *trans*-97

Summenformel	C ₁₇ H ₂₃ N (241.36)	Diffraktometer	Bruker SMART CCD
Kristallform, -farbe	Stäbchen, gelblich	Strahlung (λ [Å])	Mo K _α (0.71073)
Kristallgröße	0.50×0.12×0.10mm	Temperatur [K]	173(2)
Kristallsystem	triklin	Scan-Modus	ω scans
Raumgruppe	P-1	Scan-Bereich θ [°]	1.61–30.70
Gitterkonstanten		Absorptionskorrektur	empirisch
a [Å]	10.057(2)	max./min. Transmission	0.9938/0.9693
b [Å]	12.290(3)	Reflexe {N (hkl)}	
c [Å]	13.299(3)	gemessen	11002
α [°]	73.578(5)	unabhängig	7969
β [°]	89.969(5)	beobachtet >2σ(I)	2619
γ [°]	69.060(5)	Verfeinerungsmethode	kleinste Fehlerquadrate (F ²)
Volumen [Å³]	1463.2(6)	Verfeinerte Parameter	443
Z (Zellbesetzung)	4	R(int)	0.0696
Dichte, ber. [g·cm⁻³]	1.096	S	0.905
Indexbereich	-9<=h<=14	R1, wR2 {I>2σ(I)}	R1=0.0884, wR2=0.1909
	-17<=k<=17	R1, wR2 (alle Daten)	R1=0.2602, wR2=0.2630
	-17<=l<=18	Maximum δ/σ	0.006
linearer Absorptionskoeffizient [mm⁻¹]	0.063	max./min. Restelektronendichte [e·Å⁻³]	0.414/-0.299

Lageparameter (Atomkoordinaten) (×10⁴)

Atom	X	Y	Z	Atom	X	Y	Z
N(1)	4806(3)	153(3)	3011(2)	N(2)	9806(3)	219(3)	1745(3)
C(1)	3856(4)	1211(3)	2857(3)	C(18)	8828(4)	1284(3)	1398(3)
C(2)	4118(4)	919(3)	1863(3)	C(19)	9119(4)	930(3)	2538(3)
C(3)	5025(4)	1441(4)	1120(3)	C(20)	8189(4)	446(4)	3273(3)
C(4)	4093(4)	2443(4)	148(3)	C(21)	7260(4)	1421(4)	3737(3)
C(5)	3136(4)	2012(4)	-410(3)	C(22)	8138(4)	1911(3)	4298(3)
C(6)	2220(4)	1518(4)	379(3)	C(23)	9080(4)	2396(4)	3528(3)
C(7)	3131(4)	506(4)	1348(3)	C(24)	10025(4)	1436(4)	3038(3)
C(8)	2268(4)	2975(4)	-1460(3)	C(25)	7211(4)	2829(4)	4864(3)
C(9)	1212(6)	4119(4)	-1255(4)	C(26)	5994(5)	3873(4)	4099(4)
C(10)	3291(6)	3339(6)	-2202(4)	C(27)	6587(5)	2172(4)	5777(3)
C(11)	1458(5)	2421(4)	-2008(3)	C(28)	8147(5)	3350(4)	5344(4)
C(12)	3163(4)	2041(3)	3456(3)	C(29)	8101(4)	2164(4)	392(3)
C(13)	2397(4)	3271(4)	2955(3)	C(30)	7297(4)	3350(4)	325(3)
C(14)	1794(5)	4058(4)	3528(3)	C(31)	6640(5)	4200(4)	-644(4)
C(15)	1929(5)	3618(4)	4619(4)	C(32)	6793(5)	3843(5)	-1548(4)
C(16)	2684(5)	2380(4)	5130(3)	C(33)	7576(5)	2638(5)	-1478(3)
C(17)	3283(4)	1614(4)	4554(3)	C(34)	8232(4)	1808(4)	-521(3)

interatomare Abstände (Bindungslängen) [Å]

N(1)-C(1)	1.267(4)	C(11)-H(11A)	0.9800	C(23)-C(24)	1.533(5)
N(1)-C(2)	1.555(5)	C(11)-H(11B)	0.9800	C(23)-H(23A)	1.04(4)
C(1)-C(12)	1.453(5)	C(11)-H(11C)	0.9800	C(23)-H(23B)	1.00(4)
C(1)-C(2)	1.464(5)	C(12)-C(13)	1.386(5)	C(24)-H(24A)	1.04(4)
C(2)-C(7)	1.507(5)	C(12)-C(17)	1.395(5)	C(24)-H(24B)	1.02(3)
C(2)-C(3)	1.509(5)	C(13)-C(14)	1.371(6)	C(25)-C(26)	1.523(6)
C(3)-C(4)	1.531(5)	C(13)-H(13)	0.91(4)	C(25)-C(27)	1.525(5)
C(3)-H(3A)	0.95(4)	C(14)-C(15)	1.385(6)	C(25)-C(28)	1.539(6)
C(3)-H(3B)	1.11(4)	C(14)-H(14)	0.98(4)	C(26)-H(26A)	0.9800
C(4)-C(5)	1.531(5)	C(15)-C(16)	1.394(6)	C(26)-H(26B)	0.9800
C(4)-H(4A)	1.03(4)	C(15)-H(15)	0.92(4)	C(26)-H(26C)	0.9800
C(4)-H(4B)	1.00(4)	C(16)-C(17)	1.355(6)	C(27)-H(27A)	0.9800
C(5)-C(6)	1.535(5)	C(16)-H(16)	1.03(4)	C(27)-H(27B)	0.9800
C(5)-C(8)	1.562(5)	C(17)-H(17)	0.98(3)	C(27)-H(27C)	0.9800
C(5)-H(5)	0.87(4)	N(2)-C(18)	1.277(4)	C(28)-H(28A)	0.9800
C(6)-C(7)	1.526(5)	N(2)-C(19)	1.563(4)	C(28)-H(28B)	0.9800
C(6)-H(6A)	1.04(4)	C(18)-C(19)	1.453(5)	C(28)-H(28C)	0.9800
C(6)-H(6B)	1.09(4)	C(18)-C(29)	1.453(5)	C(29)-C(30)	1.368(5)
C(7)-H(7A)	1.02(4)	C(19)-C(20)	1.500(5)	C(29)-C(34)	1.394(5)
C(7)-H(7B)	0.98(3)	C(19)-C(24)	1.515(5)	C(30)-C(31)	1.391(6)
C(8)-C(10)	1.520(6)	C(20)-C(21)	1.519(5)	C(30)-H(30)	0.87(4)
C(8)-C(9)	1.526(6)	C(20)-H(20A)	1.05(4)	C(31)-C(32)	1.383(6)
C(8)-C(11)	1.529(5)	C(20)-H(20B)	0.97(4)	C(31)-H(31)	0.81(3)
C(9)-H(9A)	0.9800	C(21)-C(22)	1.528(5)	C(32)-C(33)	1.382(6)
C(9)-H(9B)	0.9800	C(21)-H(21A)	1.01(3)	C(32)-H(32)	1.06(5)
C(9)-H(9C)	0.9800	C(21)-H(21B)	0.99(4)	C(33)-C(34)	1.372(6)
C(10)-H(10A)	0.9800	C(22)-C(23)	1.535(5)	C(33)-H(33)	0.98(4)
C(10)-H(10B)	0.9800	C(22)-C(25)	1.561(5)	C(34)-H(34)	0.93(4)
C(10)-H(10C)	0.9800	C(22)-H(22)	1.01(4)		

intermolekulare Winkel [°]

C(1)-N(1)-C(2)	61.5(2)	C(5)-C(6)-H(6A)	104(2)	H(11A)-C(11)-H(11B)	109.5
N(1)-C(1)-C(12)	139.0(3)	C(7)-C(6)-H(6B)	106.1(18)	C(8)-C(11)-H(11C)	109.5
N(1)-C(1)-C(2)	68.9(3)	C(5)-C(6)-H(6B)	108.5(18)	H(11A)-C(11)-H(11C)	109.5
C(12)-C(1)-C(2)	152.0(3)	H(6A)-C(6)-H(6B)	117(3)	H(11B)-C(11)-H(11C)	109.5
C(1)-C(2)-C(7)	121.9(3)	C(2)-C(7)-C(6)	111.2(3)	C(13)-C(12)-C(17)	118.6(4)
C(1)-C(2)-C(3)	120.4(3)	C(2)-C(7)-H(7A)	112(2)	C(13)-C(12)-C(1)	121.1(3)
C(7)-C(2)-C(3)	114.1(3)	C(6)-C(7)-H(7A)	113(2)	C(17)-C(12)-C(1)	120.3(3)
C(1)-C(2)-N(1)	49.5(2)	C(2)-C(7)-H(7B)	113(2)	C(14)-C(13)-C(12)	120.8(4)
C(7)-C(2)-N(1)	117.6(3)	C(6)-C(7)-H(7B)	108(2)	C(14)-C(13)-H(13)	117(3)
C(3)-C(2)-N(1)	117.6(3)	H(7A)-C(7)-H(7B)	99(3)	C(12)-C(13)-H(13)	122(3)
C(2)-C(3)-C(4)	110.8(3)	C(10)-C(8)-C(9)	108.6(4)	C(13)-C(14)-C(15)	119.7(4)
C(2)-C(3)-H(3A)	112(2)	C(10)-C(8)-C(11)	107.7(4)	C(13)-C(14)-H(14)	127(2)
C(4)-C(3)-H(3A)	105(2)	C(9)-C(8)-C(11)	109.7(4)	C(15)-C(14)-H(14)	114(2)
C(2)-C(3)-H(3B)	109.7(18)	C(10)-C(8)-C(5)	109.6(3)	C(14)-C(15)-C(16)	120.0(4)
C(4)-C(3)-H(3B)	112.8(18)	C(9)-C(8)-C(5)	111.1(3)	C(14)-C(15)-H(15)	126(2)
H(3A)-C(3)-H(3B)	106(3)	C(11)-C(8)-C(5)	110.1(3)	C(16)-C(15)-H(15)	114(2)
C(5)-C(4)-C(3)	112.5(3)	C(8)-C(9)-H(9A)	109.5	C(17)-C(16)-C(15)	119.7(4)
C(5)-C(4)-H(4A)	109(2)	C(8)-C(9)-H(9B)	109.5	C(17)-C(16)-H(16)	123(2)
C(3)-C(4)-H(4A)	108(2)	H(9A)-C(9)-H(9B)	109.5	C(15)-C(16)-H(16)	117(2)
C(5)-C(4)-H(4B)	112(2)	C(8)-C(9)-H(9C)	109.5	C(16)-C(17)-C(12)	121.2(4)
C(3)-C(4)-H(4B)	108(2)	H(9A)-C(9)-H(9C)	109.5	C(16)-C(17)-H(17)	117.2(19)
H(4A)-C(4)-H(4B)	107(3)	H(9B)-C(9)-H(9C)	109.5	C(12)-C(17)-H(17)	121.5(19)
C(4)-C(5)-C(6)	109.5(3)	C(8)-C(10)-H(10A)	109.5	C(18)-N(2)-C(19)	60.6(2)
C(4)-C(5)-C(8)	113.9(3)	C(8)-C(10)-H(10B)	109.5	N(2)-C(18)-C(19)	69.5(3)
C(6)-C(5)-C(8)	114.3(3)	H(10A)-C(10)-H(10B)	109.5	N(2)-C(18)-C(29)	138.7(4)
C(4)-C(5)-H(5)	109(3)	C(8)-C(10)-H(10C)	109.5	C(19)-C(18)-C(29)	151.7(4)
C(6)-C(5)-H(5)	108(2)	H(10A)-C(10)-H(10C)	109.5	C(18)-C(19)-C(20)	122.6(3)
C(8)-C(5)-H(5)	102(2)	H(10B)-C(10)-H(10C)	109.5	C(18)-C(19)-C(24)	120.4(3)
C(7)-C(6)-C(5)	112.2(3)	C(8)-C(11)-H(11A)	109.5	C(20)-C(19)-C(24)	113.7(3)
C(7)-C(6)-H(6A)	109(2)	C(8)-C(11)-H(11B)	109.5	C(18)-C(19)-N(2)	49.9(2)
C(20)-C(19)-N(2)	117.3(3)	H(23A)-C(23)-H(23B)	101(3)	C(25)-C(28)-H(28A)	109.5

C(24)-C(19)-N(2)	117.6(3)	C(19)-C(24)-C(23)	110.4(3)	C(25)-C(28)-H(28B)	109.5
C(19)-C(20)-C(21)	110.3(3)	C(19)-C(24)-H(24A)	109(2)	H(28A)-C(28)-H(28B)	109.5
C(19)-C(20)-H(20A)	110(2)	C(23)-C(24)-H(24A)	109(2)	C(25)-C(28)-H(28C)	109.5
C(21)-C(20)-H(20A)	107(2)	C(19)-C(24)-H(24B)	110.7(19)	H(28A)-C(28)-H(28C)	109.5
C(19)-C(20)-H(20B)	118(2)	C(23)-C(24)-H(24B)	109.8(18)	H(28B)-C(28)-H(28C)	109.5
C(21)-C(20)-H(20B)	107(3)	H(24A)-C(24)-H(24B)	108(3)	C(30)-C(29)-C(34)	119.2(4)
H(20A)-C(20)-H(20B)	104(3)	C(26)-C(25)-C(27)	109.2(3)	C(30)-C(29)-C(18)	120.8(3)
C(20)-C(21)-C(22)	112.6(3)	C(26)-C(25)-C(28)	109.5(4)	C(34)-C(29)-C(18)	120.0(4)
C(20)-C(21)-H(21A)	112.1(18)	C(27)-C(25)-C(28)	106.7(3)	C(29)-C(30)-C(31)	120.6(4)
C(22)-C(21)-H(21A)	103.3(19)	C(26)-C(25)-C(22)	110.9(3)	C(29)-C(30)-H(30)	117(3)
C(20)-C(21)-H(21B)	113(2)	C(27)-C(25)-C(22)	110.2(3)	C(31)-C(30)-H(30)	122(3)
C(22)-C(21)-H(21B)	106(2)	C(28)-C(25)-C(22)	110.2(3)	C(32)-C(31)-C(30)	119.8(5)
H(21A)-C(21)-H(21B)	109(3)	C(25)-C(26)-H(26A)	109.5	C(32)-C(31)-H(31)	121(3)
C(21)-C(22)-C(23)	109.3(3)	C(25)-C(26)-H(26B)	109.5	C(30)-C(31)-H(31)	119(3)
C(21)-C(22)-C(25)	113.2(3)	H(26A)-C(26)-H(26B)	109.5	C(33)-C(32)-C(31)	119.6(4)
C(23)-C(22)-C(25)	114.7(3)	C(25)-C(26)-H(26C)	109.5	C(33)-C(32)-H(32)	121(2)
C(21)-C(22)-H(22)	113(2)	H(26A)-C(26)-H(26C)	109.5	C(31)-C(32)-H(32)	119(2)
C(23)-C(22)-H(22)	103(2)	H(26B)-C(26)-H(26C)	109.5	C(34)-C(33)-C(32)	120.2(4)
C(25)-C(22)-H(22)	103(2)	C(25)-C(27)-H(27A)	109.5	C(34)-C(33)-H(33)	120(2)
C(24)-C(23)-C(22)	112.5(3)	C(25)-C(27)-H(27B)	109.5	C(32)-C(33)-H(33)	120(2)
C(24)-C(23)-H(23A)	109(2)	H(27A)-C(27)-H(27B)	109.5	C(33)-C(34)-C(29)	120.5(4)
C(22)-C(23)-H(23A)	112(2)	C(25)-C(27)-H(27C)	109.5	C(33)-C(34)-H(34)	118(3)
C(24)-C(23)-H(23B)	113(2)	H(27A)-C(27)-H(27C)	109.5	C(29)-C(34)-H(34)	121(3)
C(22)-C(23)-H(23B)	110(2)	H(27B)-C(27)-H(27C)	109.5		

Torsionswinkel

C(2)-N(1)-C(1)-C(12)	-177.0(6)	N(1)-C(1)-C(12)-C(13)	163.6(4)	C(21)-C(22)-C(23)-C(24)	-54.8(4)
N(1)-C(1)-C(2)-C(7)	100.8(4)	C(2)-C(1)-C(12)-C(13)	-10.5(9)	C(25)-C(22)-C(23)-C(24)	177.0(3)
C(12)-C(1)-C(2)-C(7)	-83.4(8)	N(1)-C(1)-C(12)-C(17)	-15.1(7)	C(18)-C(19)-C(24)-C(23)	106.1(4)
N(1)-C(1)-C(2)-C(3)	-101.9(4)	C(2)-C(1)-C(12)-C(17)	170.8(6)	C(20)-C(19)-C(24)-C(23)	-53.7(4)
C(12)-C(1)-C(2)-C(3)	74.0(8)	C(17)-C(12)-C(13)-C(14)	1.3(6)	N(2)-C(19)-C(24)-C(23)	163.7(3)
C(12)-C(1)-C(2)-N(1)	175.8(8)	C(1)-C(12)-C(13)-C(14)	-177.4(4)	C(22)-C(23)-C(24)-C(19)	53.6(5)
C(1)-N(1)-C(2)-C(7)	-109.7(4)	C(12)-C(13)-C(14)-C(15)	-1.1(6)	C(21)-C(22)-C(25)-C(26)	-54.7(4)
C(1)-N(1)-C(2)-C(3)	107.7(4)	C(13)-C(14)-C(15)-C(16)	0.4(6)	C(23)-C(22)-C(25)-C(26)	71.6(4)
C(1)-C(2)-C(3)-C(4)	-106.8(4)	C(14)-C(15)-C(16)-C(17)	0.1(6)	C(21)-C(22)-C(25)-C(27)	66.4(4)
C(7)-C(2)-C(3)-C(4)	52.2(5)	C(15)-C(16)-C(17)-C(12)	0.1(6)	C(23)-C(22)-C(25)-C(27)	-167.3(3)
N(1)-C(2)-C(3)-C(4)	-164.0(3)	C(13)-C(12)-C(17)-C(16)	-0.8(5)	C(21)-C(22)-C(25)-C(28)	-176.1(3)
C(2)-C(3)-C(4)-C(5)	-53.8(5)	C(1)-C(12)-C(17)-C(16)	177.9(4)	C(23)-C(22)-C(25)-C(28)	-49.8(5)
C(3)-C(4)-C(5)-C(6)	55.6(4)	C(19)-N(2)-C(18)-C(29)	176.8(5)	N(2)-C(18)-C(29)-C(30)	-165.4(4)
C(3)-C(4)-C(5)-C(8)	-175.0(3)	N(2)-C(18)-C(19)-C(20)	-100.0(4)	C(19)-C(18)-C(29)-C(30)	8.2(9)
C(4)-C(5)-C(6)-C(7)	-55.6(4)	C(29)-C(18)-C(19)-C(20)	84.5(8)	N(2)-C(18)-C(29)-C(34)	13.8(7)
C(8)-C(5)-C(6)-C(7)	175.1(3)	N(2)-C(18)-C(19)-C(24)	102.0(4)	C(19)-C(18)-C(29)-C(34)	-172.6(6)
C(1)-C(2)-C(7)-C(6)	106.1(4)	C(29)-C(18)-C(19)-C(24)	-73.5(8)	C(34)-C(29)-C(30)-C(31)	-1.3(6)
C(3)-C(2)-C(7)-C(6)	-52.6(4)	C(29)-C(18)-C(19)-N(2)	-175.5(8)	C(18)-C(29)-C(30)-C(31)	178.0(4)
N(1)-C(2)-C(7)-C(6)	163.6(3)	C(18)-N(2)-C(19)-C(20)	110.9(4)	C(29)-C(30)-C(31)-C(32)	0.3(6)
C(5)-C(6)-C(7)-C(2)	54.1(4)	C(18)-N(2)-C(19)-C(24)	-107.9(4)	C(30)-C(31)-C(32)-C(33)	1.3(7)
C(4)-C(5)-C(8)-C(10)	56.5(5)	C(18)-C(19)-C(20)-C(21)	-104.5(4)	C(31)-C(32)-C(33)-C(34)	-1.9(7)
C(6)-C(5)-C(8)-C(10)	-176.6(4)	C(24)-C(19)-C(20)-C(21)	54.8(4)	C(32)-C(33)-C(34)-C(29)	0.9(6)
C(4)-C(5)-C(8)-C(9)	-63.6(5)	N(2)-C(19)-C(20)-C(21)	-162.6(3)	C(30)-C(29)-C(34)-C(33)	0.7(6)
C(6)-C(5)-C(8)-C(9)	63.3(5)	C(19)-C(20)-C(21)-C(22)	-56.1(4)	C(18)-C(29)-C(34)-C(33)	-178.6(4)
C(4)-C(5)-C(8)-C(11)	174.7(3)	C(20)-C(21)-C(22)-C(23)	56.0(4)		
C(6)-C(5)-C(8)-C(11)	-58.3(5)	C(20)-C(21)-C(22)-C(25)	-174.9(3)		

Selbständigkeitserklärung

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

Chemnitz, den 31.07. 2001

Antje Melzer