IV. ANHANG 179

IV. Anhang

1. Röntgenstrukturanalysen (Tabellen)

1.1. Diastereomer A (Diplomarbeit)

Table 1: Crystal data and structure refinement.

Empirical formula:	C_{23} H_{33} N O_4	
Formula weight:	387.50	
Temperature:	20(2) °C	
Wavelength:	1.54180 Å	
Crystal system:	orthorhombic	
Space group:	P212121	
Unit cell dimensions:	a = 6.126(2) Å	α = 90 deg.
	b = 16.336(4) Å	β = 90 deg.
	c = 21.842(4) Å	γ = 90 deg.
Volume:	2185.8(10) $Å^3$	
Z:	4	
Density (calculated):	1.178 Mg/m^3	
Absorption coefficient:	6.37 cm^{-1}	
F(000):	840	
Crystal size:	0.38 x 0.25 x 0.16 mm	
2 Θ range for data collection:	6.76 to 120.06 deg.	
Index ranges:	08h86, 08k818, 08l824	
Reflections collected:	1898	
Independent reflections:	1898 [R_{int} = 0.0000]	
Refinement method:	Full-matrix least-squares on F^2	
Data / restraints / parameters:	1898 / 0 / 386	

Goodness-of-fit on F^2, S:	1.043
Final R indices [I>2σ (I)]:	R1 = 0.0322, wR2 = 0.0893
R indices (all data):	R1 = 0.0397, wR2 = 0.0927
Absolute structure parameter:	0.6 (4)
Extinction coefficient:	0.0051 (5)
Largest diff. peak and hole:	0.107 and -0.125 e/Å^3

Table 2: Atomic coordinates ($\cdot 10^4$) and equivalent isotropic displacement parameters (Å$^2 \cdot 10^3$)

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor

	X		Y		Z		U (eq)	
C(1)	-944	(5)	8323	(2)	6036	(1)	57	(1)
C(2)	-135	(5)	7466	(2)	6252	(1)	49	(1)
C(3)	-887	(5)	6766	(2)	5829	(1)	50	(1)
C(4)	-118	(5)	5925	(2)	6044	(1)	49	(1)
C(5)	-797	(4)	5753	(2)	6705	(1)	45	(1)
C(6)	72	(6)	6431	(2)	7117	(1)	54	(1)
C(7)	-756	(6)	7268	(2)	6915	(1)	52	(1)
O(8)	276	(3)	5001	(1)	6919	(1)	48	(1)
C(9)	-448	(4)	4261	(2)	6760	(1)	42	(1)
O(90)	643	(3)	3665	(1)	6878	(1)	52	(1)
N(10)	-2434	(3)	4203	(1)	6459	(1)	42	(1)
C(11)	-3834	(4)	4871	(2)	6401	(1)	46	(1)
O(110)	-5451	(3)	4829	(1)	6081	(1)	65	(1)
C(12)	-3247	(5)	5606	(2)	6770	(1)	48	(1)
C(120)	-4055	(7)	5494	(3)	7429	(2)	65	(1)
C(13)	-3252	(5)	3386	(2)	6272	(1)	47	(1)
C(14)	-1761	(6)	2935	(2)	5830	(1)	53	(1)
C(15)	-1206	(5)	3419	(2)	5262	(1)	48	(1)
C(16)	-2679	(7)	3467	(2)	4783	(2)	67	(1)
C(17)	-2183	(9)	3904	(3)	4263	(2)	84	(1)
C(18)	-244	(8)	4309	(2)	4212	(2)	82	(1)
C(19)	1217	(7)	4274	(2)	4685	(2)	72	(1)
C(20)	748	(6)	3831	(2)	5207	(2)	59	(1)
C(21)	-3853	(6)	2865	(2)	6825	(2)	62	(1)
O(22)	-5000	(4)	3300	(2)	7280	(1)	78	(1)
C(23)	-137	(11)	8494	(3)	5385	(2)	86	(1)
C(24)	-11	(9)	8986	(2)	6460	(2)	79	(1)
C(25)	-3415	(6)	8384	(3)	6041	(2)	71	(1)

Table 3a: Bond lengths [Å].

C(1)-C(25)	1.518	(5)	N(10)-C(11)	1.395	(3)
C(1)-C(24)	1.535	(5)	N(10)-C(13)	1.483	(4)
C(1)-C(23)	1.530	(5)	C(11)-O(110)	1.214	(3)
C(1)-C(2)	1.559	(4)	C(11)-C(12)	1.490	(4)
C(2)-C(7)	1.532	(4)	C(12)-C(120)	1.533	(4)
C(2)-C(3)	1.539	(4)	C(13)-C(14)	1.520	(4)
C(3)-C(4)	1.527	(4)	C(13)-C(21)	1.522	(4)
C(4)-C(5)	1.529	(4)	C(14)-C(15)	1.510	(4)
C(5)-O(8)	1.469	(3)	C(15)-C(20)	1.378	(5)
C(5)-C(6)	1.522	(4)	C(15)-C(16)	1.384	(4)
C(5)-C(12)	1.526	(4)	C(16)-C(17)	1.377	(5)
C(6)-C(7)	1.524	(4)	C(17)-C(18)	1.363	(6)
O(8)-C(9)	1.333	(3)	C(18)-C(19)	1.368	(6)
C(9)-O(90)	1.209	(3)	C(19)-C(20)	1.381	(5)
C(9)-N(10)	1.386	(3)	C(21)-O(22)	1.409	(5)

Table 3b: Bond angles [deg].

C(25)-C(1)-C(24)	108.7	(3)	C(9)-N(10)-C(11)	121.9	(2)
C(25)-C(1)-C(23)	108.5	(4)	C(9)-N(10)-C(13)	119.3	(2)
C(24)-C(1)-C(23)	108.2	(4)	C(11)-N(10)-C(13)	118.2	(2)
C(25)-C(1)-C(2)	112.0	(3)	O(110)-C(11)-N(10)	120.7	(3)
C(24)-C(1)-C(2)	109.4	(3)	O(110)-C(11)-C(12)	123.6	(3)
C(23)-C(1)-C(2)	110.1	(3)	N(10)-C(11)-C(12)	115.7	(2)
C(7)-C(2)-C(3)	109.7	(3)	C(11)-C(12)-C(5)	108.2	(2)
C(7)-C(2)-C(1)	113.4	(2)	C(11)-C(12)-C(120)	109.5	(3)
C(3)-C(2)-C(1)	113.0	(2)	C(5)-C(12)-C(120)	115.0	(3)
C(4)-C(3)-C(2)	113.0	(2)	N(10)-C(13)-C(14)	114.1	(2)
C(3)-C(4)-C(5)	111.9	(2)	N(10)-C(13)-C(21)	111.5	(2)
O(8)-C(5)-C(6)	105.4	(2)	C(14)-C(13)-C(21)	112.2	(2)
O(8)-C(5)-C(12)	106.3	(2)	C(15)-C(14)-C(13)	113.8	(2)
C(6)-C(5)-C(12)	113.8	(2)	C(20)-C(15)-C(16)	118.2	(3)
O(8)-C(5)-C(4)	109.4	(2)	C(20)-C(15)-C(14)	121.6	(3)
C(6)-C(5)-C(4)	109.1	(3)	C(16)-C(15)-C(14)	120.3	(3)
C(12)-C(5)-C(4)	112.6	(2)	C(17)-C(16)-C(15)	120.7	(4)
C(5)-C(6)-C(7)	111.5	(2)	C(18)-C(17)-C(16)	120.7	(4)
C(6)-C(7)-C(2)	112.3	(3)	C(17)-C(18)-C(19)	119.3	(4)
C(9)-O(8)-C(5)	121.8	(2)	C(18)-C(19)-C(20)	120.6	(4)
O(90)-C(9)-O(8)	119.4	(2)	C(15)-C(20)-C(19)	120.6	(3)
O(90)-C(9)-N(10)	122.0	(2)	O(22)-C(21)-C(13)	113.5	(3)
O(8)-C(9)-N(10)	118.5	(2)			

Table 4: Anisotropic displacement parameters ($Å^2 \cdot 10^3$).

The anisotropic displacement factor exponent takes the form:

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

	U11	U22	U33	U23	U13	U12
C(1)	63 (2)	48 (2)	58 (2)	0 (1)	6 (2)	9 (2)
C(2)	45 (2)	49 (2)	52 (2)	-5 (1)	-2 (1)	5 (1)
C(3)	56 (2)	50 (2)	44 (2)	-5 (1)	2 (1)	6 (2)
C(4)	50 (2)	46 (2)	51 (2)	-9 (1)	3 (1)	6 (1)
C(5)	49 (2)	42 (1)	46 (1)	-2 (1)	-6 (1)	12 (1)
C(6)	60 (2)	52 (2)	49 (2)	-5 (1)	-13 (2)	6 (2)
C(7)	62 (2)	47 (2)	48 (2)	-9 (1)	-9 (2)	5 (1)
O(8)	43 (1)	45 (1)	57 (1)	-2 (1)	-13 (1)	7 (1)
C(9)	39 (1)	46 (1)	42 (1)	1 (1)	-2 (1)	6 (1)
O(90)	45 (1)	48 (1)	63 (1)	9 (1)	-7 (1)	9 (1)
N(10)	37 (1)	45 (1)	44 (1)	1 (1)	-2 (1)	7 (1)
C(11)	38 (1)	54 (2)	46 (1)	0 (1)	2 (1)	8 (1)
O(110)	47 (1)	67 (1)	83 (1)	-9 (1)	-23 (1)	13 (1)
C(12)	42 (2)	53 (2)	49 (1)	-1 (1)	-1 (1)	15 (1)
C(120)	63 (2)	76 (2)	55 (2)	-2 (2)	10 (2)	16 (2)
C(13)	46 (2)	44 (1)	51 (2)	3 (1)	-8 (1)	1 (1)
C(14)	62 (2)	40 (2)	58 (2)	-1 (1)	-6 (2)	3 (2)
C(15)	56 (2)	38 (1)	51 (2)	-10 (1)	-2 (1)	-1 (1)
C(16)	75 (2)	61 (2)	64 (2)	-2 (2)	-14 (2)	-11 (2)
C(17)	112 (3)	77 (2)	63 (2)	9 (2)	-23 (2)	-10 (3)
C(18)	120 (3)	58 (2)	67 (2)	7 (2)	8 (2)	-8 (3)
C(19)	78 (2)	58 (2)	79 (2)	-4 (2)	12 (2)	-16 (2)
C(20)	54 (2)	57 (2)	66 (2)	-12 (2)	-3 (2)	-6 (2)
C(21)	49 (2)	69 (2)	69 (2)	15 (2)	-2 (2)	-7 (2)
O(22)	52 (1)	125 (2)	58 (1)	14 (1)	4 (1)	0 (2)
C(23)	115 (4)	68 (2)	74 (2)	17 (2)	30 (3)	18 (3)
C(24)	101 (3)	46 (2)	91 (3)	-6 (2)	-1 (3)	-6 (2)
C(25)	68 (2)	63 (2)	81 (3)	6 (2)	-1 (2)	24 (2)

Table 5: Hydrogen coordinates ($\cdot 10^4$) and isotropic displacement parameters ($Å^2 \cdot 10^3$).

	X		Y		Z		U	
H(2)	1603	(59)	7458	(19)	6205	(14)	64	(9)
H(31)	-2538	(55)	6761	(18)	5839	(12)	49	(8)
H(32)	-342	(48)	6856	(16)	5398	(13)	48	(7)
H(41)	1624	(70)	5915	(24)	6057	(17)	89	(12)
H(42)	-658	(48)	5496	(16)	5775	(11)	42	(7)
H(61)	1599	(65)	6404	(21)	7030	(15)	63	(10)
H(62)	-194	(52)	6285	(17)	7561	(14)	51	(8)
H(71)	-2439	(70)	7329	(20)	6913	(14)	68	(10)
H(72)	-163	(51)	7679	(17)	7221	(12)	48	(7)
H(12)	-3854	(56)	6043	(18)	6589	(13)	55	(8)
H(121)	-5508	(85)	5273	(28)	7430	(19)	96	(13)
H(122)	-3357	(59)	5082	(22)	7641	(15)	68	(10)
H(123)	-4018	(63)	5983	(23)	7656	(16)	72	(10)
H(13)	-4486	(54)	3515	(18)	6053	(13)	52	(8)
H(141)	-507	(67)	2772	(21)	6039	(15)	70	(10)
H(142)	-2516	(60)	2419	(20)	5717	(13)	64	(9)
H(16)	-4203	(68)	3182	(21)	4849	(15)	75	(10)
H(17)	-3149	(84)	3978	(28)	3916	(21)	115	(15)
H(18)	107	(68)	4641	(23)	3858	(16)	81	(11)
H(19)	2693	(93)	4597	(30)	4634	(21)	133	(17)
H(20)	1739	(64)	3810	(20)	5569	(16)	79	(10)
H(211)	-4731	(77)	2405	(24)	6662	(17)	83	(12)
H(212)	-2520	(70)	2672	(21)	6991	(13)	68	(10)
H(22)	-6044	(85)	3423	(28)	7133	(20)	93	(16)
H(231)	-287	(71)	9100	(24)	5238	(16)	85	(11)
H(232)	-445	(74)	8078	(25)	5085	(19)	93	(13)
H(233)	1135	(99)	8384	(34)	5362	(24)	117	(21)
H(241)	-818	(69)	8936	(22)	6900	(17)	86	(12)
H(242)	1919	(102)	8905	(33)	6434	(22)	139	(18)
H(243)	-435	(70)	9521	(25)	6264	(17)	92	(12)
H(251)	-3837	(93)	8303	(31)	6419	(24)	123	(18)
H(252)	-3829	(71)	8894	(25)	5823	(18)	89	(12)
H(253)	-4111	(68)	7928	(25)	5774	(18)	86	(12)

Table 6: Torsion angles [deg].

C(25)-C(1)-C(2)-C(7)	-62.8	(4)
C(24)-C(1)-C(2)-C(7)	57.8	(4)
C(23)-C(1)-C(2)-C(7)	176.5	(4)
C(25)-C(1)-C(2)-C(3)	62.8	(4)
C(24)-C(1)-C(2)-C(3)	-176.7	(3)
C(23)-C(1)-C(2)-C(3)	-58.0	(4)
C(7)-C(2)-C(3)-C(4)	-51.8	(3)
C(1)-C(2)-C(3)-C(4)	-179.3	(2)
C(2)-C(3)-C(4)-C(5)	54.6	(3)
C(3)-C(4)-C(5)-O(8)	-171.0	(2)
C(3)-C(4)-C(5)-C(6)	-56.2	(3)
C(3)-C(4)-C(5)-C(12)	71.2	(3)
O(8)-C(5)-C(6)-C(7)	175.2	(3)
C(12)-C(5)-C(6)-C(7)	-68.8	(4)
C(4)-C(5)-C(6)-C(7)	57.8	(3)
C(5)-C(6)-C(7)-C(2)	-58.0	(4)
C(3)-C(2)-C(7)-C(6)	53.3	(4)
C(1)-C(2)-C(7)-C(6)	-179.4	(3)
C(6)-C(5)-O(8)-C(9)	164.5	(2)
C(12)-C(5)-O(8)-C(9)	43.4	(3)
C(4)-C(5)-O(8)-C(9)	-78.3	(3)
C(5)-O(8)-C(9)-O(90)	170.3	(2)
C(5)-O(8)-C(9)-N(10)	-9.1	(3)
O(90)-C(9)-N(10)-C(11)	170.7	(2)
O(8)-C(9)-N(10)-C(11)	-9.9	(3)
O(90)-C(9)-N(10)-C(13)	-0.2	(4)
O(8)-C(9)-N(10)-C(13)	179.2	(2)
C(9)-N(10)-C(11)-O(110)	172.2	(2)
C(13)-N(10)-C(11)-O(110)	-16.8	(4)
C(9)-N(10)-C(11)-C(12)	-10.1	(3)
C(13)-N(10)-C(11)-C(12)	160.9	(2)
O(110)-C(11)-C(12)-C(5)	-137.7	(3)
N(10)-C(11)-C(12)-C(5)	44.6	(3)
O(110)-C(11)-C(12)-C(120)	96.2	(3)
N(10)-C(11)-C(12)-C(120)	-81.5	(3)
O(8)-C(5)-C(12)-C(11)	-58.1	(3)
C(6)-C(5)-C(12)-C(11)	-173.6	(2)
C(4)-C(5)-C(12)-C(11)	61.6	(3)
O(8)-C(5)-C(12)-C(120)	64.7	(3)
C(6)-C(5)-C(12)-C(120)	-50.8	(4)
C(4)-C(5)-C(12)-C(120)	-175.6	(3)
C(9)-N(10)-C(13)-C(14)	-60.5	(3)
C(11)-N(10)-C(13)-C(14)	128.3	(3)
C(9)-N(10)-C(13)-C(21)	67.9	(3)
C(11)-N(10)-C(13)-C(21)	-103.3	(3)

N(10)-C(13)-C(14)-C(15)	-54.4	(3)
C(21)-C(13)-C(14)-C(15)	177.6	(3)
C(13)-C(14)-C(15)-C(20)	99.6	(3)
C(13)-C(14)-C(15)-C(16)	-79.7	(4)
C(20)-C(15)-C(16)-C(17)	1.0	(5)
C(14)-C(15)-C(16)-C(17)	-179.7	(3)
C(15)-C(16)-C(17)-C(18)	-1.0	(6)
C(16)-C(17)-C(18)-C(19)	0.2	(6)
C(17)-C(18)-C(19)-C(20)	0.5	(6)
C(16)-C(15)-C(20)-C(19)	-0.3	(4)
C(14)-C(15)-C(20)-C(19)	-179.6	(3)
C(18)-C(19)-C(20)-C(15)	-0.4	(5)
N(10)-C(13)-C(21)-O(22)	42.9	(4)
C(14)-C(13)-C(21)-O(22)	172.3	(3)

1.2. Diastereomer B (Diplomarbeit)

Table 1: Crystal data and structure refinement.

Empirical formula:	$C_{23}\ H_{33}\ N\ O_4$	
Formula weight:	387.50	
Temperature:	20(2) °C	
Wavelength:	1.54180 Å	
Crystal system:	orthorhombic	
Space group:	P212121	
Unit cell dimensions:	a = 5.986(2) Å	α = 90 deg.
	b = 13.139(3) Å	β = 90 deg.
	c = 28.171(7) Å	γ = 90 deg.
Volume:	2215.7(11) $Å^3$	
Z:	4	
Density (calculated):	1.162 Mg/m^3	
Absorption coefficient:	6.28 cm^{-1}	
F(000):	840	
Crystal size:	0.70 x 0.10 x 0.05 mm	
2 Θ range for data collection:	9.20 to 109.86 deg.	
Index ranges:	08h85, 08k813, 08l829	
Reflections collected:	1351	
Independent reflections:	1351 [R_{int} = 0.0000]	
Refinement method:	Full-matrix least-squares on F^2	
Data / restraints / parameters:	1351 / 0 / 256	
Goodness-of-fit on F^2, S:	0.785	
Final R indices [I>2σ (I)]:	R1 = 0.0594, wR2 = 0,1270	
R indices (all data):	R1 = 0.1917, wR2 = 0.1506	
Absolute structure parameter:	-0.9 (12)	
Extinction coefficient:	0.0020 (5)	
Largest diff. peak and hole:	0.216 and -0.175 e/$Å^3$	

Table 2: Atomic coordinates ($\cdot 10^4$) and equivalent isotropic displacement parameters ($Å^2 \cdot 10^3$)

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor

	X		Y		Z		U (eq)	
C(1)	5595	(23)	2896	(14)	1108	(5)	78	(5)
C(2)	6116	(22)	3396	(11)	1584	(5)	57	(4)
C(3)	7671	(21)	2734	(10)	1894	(4)	65	(4)
C(4)	8446	(20)	3309	(10)	2332	(4)	73	(5)
C(5)	6605	(22)	3753	(10)	2625	(4)	50	(4)
C(6)	4928	(21)	4333	(8)	2322	(4)	60	(4)
C(7)	4181	(21)	3676	(11)	1895	(5)	73	(4)
O(8)	5232	(14)	2899	(7)	2825	(3)	66	(3)
C(9)	5992	(29)	2457	(12)	3217	(6)	67	(5)
O(90)	4899	(16)	1666	(7)	3356	(3)	74	(3)
N(10)	7822	(21)	2777	(11)	3464	(4)	59	(4)
C(11)	8653	(28)	3725	(16)	3376	(5)	74	(5)
O(110)	10399	(21)	4014	(7)	3572	(3)	102	(4)
C(12)	7281	(26)	4403	(10)	3039	(5)	72	(5)
C(120)	8587	(24)	5363	(9)	2908	(4)	94	(6)
C(13)	8835	(27)	2120	(11)	3829	(5)	73	(5)
C(14)	7398	(23)	2032	(10)	4291	(4)	72	(5)
C(15)	6642	(35)	3103	(12)	4469	(5)	66	(5)
C(16)	4677	(34)	3484	(17)	4335	(6)	89	(6)
C(17)	4129	(34)	4454	(18)	4529	(7)	104	(7)
C(18)	5424	(46)	4928	(18)	4832	(7)	124	(9)
C(19)	7402	(49)	4579	(16)	4968	(6)	116	(8)
C(20)	8053	(28)	3590	(16)	4782	(5)	104	(7)
C(21)	9395	(25)	1095	(11)	3651	(4)	78	(5)
O(22)	10362	(18)	1082	(10)	3192	(3)	100	(4)
C(23)	7705	(23)	2628	(12)	822	(4)	111	(6)
C(24)	4016	(23)	3607	(11)	817	(4)	96	(6)
C(25)	4296	(28)	1851	(12)	1175	(4)	103	(6)

Table 3a: Bond lengths [Å].

C(1)-C(2)	1.526	(14)	N(10)-C(11)	1.36	(2)
C(1)-C(24)	1.56	(2)	N(10)-C(13)	1.47	(2)
C(1)-C(23)	1.54	(2)	C(11)-O(110)	1.24	(2)
C(1)-C(25)	1.59	(2)	C(11)-C(12)	1.54	(2)
C(2)-C(7)	1.50	(2)	C(12)-C(120)	1.529	(14)
C(2)-C(3)	1.545	(14)	C(13)-C(21)	1.48	(2)
C(3)-C(4)	1.518	(13)	C(13)-C(14)	1.56	(2)
C(4)-C(5)	1.495	(14)	C(14)-C(15)	1.56	(2)
C(5)-O(8)	1.500	(12)	C(15)-C(16)	1.33	(2)
C(5)-C(12)	1.50	(2)	C(15)-C(20)	1.38	(2)
C(5)-C(6)	1.522	(13)	C(16)-C(17)	1.42	(2)
C(6)-C(7)	1.547	(14)	C(17)-C(18)	1.31	(2)
O(8)-C(9)	1.327	(14)	C(18)-C(19)	1.33	(3)
C(9)-O(90)	1.290	(14)	C(19)-C(20)	1.45	(2)
C(9)-N(10)	1.36	(2)	C(21)-O(22)	1.415	(12)

Table 3b: Bond angles [deg].

C(2)-C(1)-C(24)	109.1	(12)	C(11)-N(10)-C(9)	118.8	(14)
C(2)-C(1)-C(23)	113.0	(12)	C(11)-N(10)-C(13)	120.7	(13)
C(24)-C(1)-C(23)	111.0	(13)	C(9)-N(10)-C(13)	120.4	(14)
C(2)-C(1)-C(25)	111.6	(12)	O(110)-C(11)-N(10)	121	(2)
C(24)-C(1)-C(25)	106.4	(11)	O(110)-C(11)-C(12)	123	(2)
C(23)-C(1)-C(25)	105.4	(13)	N(10)-C(11)-C(12)	117	(2)
C(7)-C(2)-C(1)	117.4	(11)	C(5)-C(12)-C(120)	114.8	(12)
C(7)-C(2)-C(3)	105.9	(11)	C(5)-C(12)-C(11)	107.1	(12)
C(1)-C(2)-C(3)	112.2	(12)	C(120)-C(12)-C(11)	110.7	(14)
C(4)-C(3)-C(2)	111.3	(11)	N(10)-C(13)-C(21)	112.9	(12)
C(5)-C(4)-C(3)	114.6	(10)	N(10)-C(13)-C(14)	113.5	(12)
C(4)-C(5)-O(8)	108.6	(10)	C(21)-C(13)-C(14)	109.9	(12)
C(4)-C(5)-C(12)	116.9	(12)	C(13)-C(14)-C(15)	111.1	(11)
O(8)-C(5)-C(12)	106.4	(10)	C(16)-C(15)-C(20)	123	(2)
C(4)-C(5)-C(6)	111.8	(10)	C(16)-C(15)-C(14)	120	(2)
O(8)-C(5)-C(6)	102.9	(10)	C(20)-C(15)-C(14)	117	(2)
C(12)-C(5)-C(6)	109.1	(12)	C(15)-C(16)-C(17)	116	(2)
C(5)-C(6)-C(7)	110.3	(10)	C(18)-C(17)-C(16)	123	(2)
C(2)-C(7)-C(6)	111.6	(10)	C(17)-C(18)-C(19)	123	(2)
C(9)-O(8)-C(5)	116.8	(11)	C(18)-C(19)-C(20)	116	(2)
O(90)-C(9)-O(8)	116	(2)	C(15)-C(20)-C(19)	119	(2)
O(90)-C(9)-N(10)	120	(2)	O(22)-C(21)-C(13)	114.5	(12)
O(8)-C(9)-N(10)	124.4	(14)			

Table 4: Anisotropic displacement parameters ($Å^2 \cdot 10^3$).

The anisotropic displacement factor exponent takes the form:

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

	U11	U22	U33	U23	U13	U12
C(1)	40 (10)	113 (16)	80 (12)	-16 (11)	0 (10)	1 (12)
C(2)	65 (11)	59 (10)	48 (9)	4 (9)	-21 (9)	-11 (9)
C(3)	67 (9)	87 (12)	41 (8)	2 (9)	33 (9)	5 (11)
C(4)	61 (11)	84 (11)	75 (11)	-14 (10)	17 (9)	14 (9)
C(5)	54 (10)	56 (10)	38 (9)	17 (9)	1 (8)	-17 (10)
C(6)	71 (10)	39 (9)	69 (10)	5 (8)	-5 (11)	-23 (10)
C(7)	56 (10)	87 (12)	76 (10)	18 (10)	6 (10)	14 (10)
O(8)	80 (7)	67 (7)	51 (6)	7 (5)	3 (6)	-7 (7)
C(9)	73 (13)	77 (14)	50 (11)	25 (10)	51 (10)	-1 (12)
O(90)	85 (8)	78 (7)	58 (6)	-4 (6)	-6 (5)	-3 (7)
N(10)	44 (8)	65 (11)	66 (9)	-4 (8)	-21 (7)	-17 (8)
C(11)	73 (14)	103 (17)	47 (10)	-37 (11)	23 (9)	-35 (14)
O(110)	134 (9)	67 (8)	105 (8)	5 (6)	-41 (9)	-41 (8)
C(12)	97 (12)	54 (12)	65 (11)	-12 (9)	-5 (11)	33 (11)
C(120)	148 (16)	35 (10)	100 (11)	-5 (8)	13 (11)	-38 (11)
C(13)	102 (12)	39 (11)	78 (11)	-5 (10)	2 (11)	19 (10)
C(14)	80 (11)	88 (14)	50 (9)	14 (9)	8 (9)	-7 (11)
C(15)	87 (14)	74 (14)	37 (9)	3 (9)	17 (10)	8 (13)
C(16)	70 (14)	106 (18)	91 (14)	5 (13)	-11 (12)	-1 (14)
C(17)	100 (18)	138 (21)	73 (14)	37 (15)	-6 (14)	4 (17)
C(18)	145 (23)	150 (22)	76 (16)	28 (15)	-39 (15)	9 (19)
C(19)	190 (27)	86 (17)	72 (13)	-25 (12)	-44 (15)	-49 (19)
C(20)	115 (14)	158 (20)	39 (10)	2 (11)	-22 (11)	-99 (16)
C(21)	83 (11)	79 (13)	71 (11)	10 (10)	20 (10)	-2 (12)
O(22)	61 (8)	144 (10)	95 (8)	-9 (7)	-7 (7)	2 (9)
C(23)	79 (11)	177 (17)	77 (11)	-40 (11)	13 (11)	-4 (15)
C(24)	89 (13)	137 (14)	62 (10)	11 (11)	-19 (10)	-21 (13)
C(25)	113 (14)	120 (14)	75 (11)	-28 (10)	6 (11)	-29 (15)

Table 5: Hydrogen coordinates ($\cdot 10^4$) and isotropic displacement parameters ($Å^2 \cdot 10^3$).

	X		Y		Z		U	
H(2)	6925	(22)	4027	(11)	1515	(5)	69	
H(3A)	6883	(21)	2124	(10)	1991	(4)	78	
H(3B)	8961	(21)	2530	(10)	1709	(4)	78	
H(4A)	9309	(20)	2849	(10)	2530	(4)	88	
H(4B)	9432	(20)	3855	(10)	2233	(4)	88	
H(6A)	5603	(21)	4958	(8)	2208	(4)	72	
H(6B)	3638	(21)	4511	(8)	2513	(4)	72	
H(7A)	3471	(21)	3060	(11)	2011	(5)	88	
H(7B)	3090	(21)	4050	(11)	1710	(5)	88	
H(12)	5920	(26)	4613	(10)	3206	(5)	86	
H(12A)	9790	(24)	5457	(9)	3129	(4)	141	
H(12B)	7609	(24)	5941	(9)	2919	(4)	141	
H(12C)	9182	(24)	5292	(9)	2593	(4)	141	
H(13)	10248	(27)	2442	(11)	3921	(5)	87	
H(14A)	8267	(23)	1699	(10)	4537	(4)	87	
H(14B)	6092	(23)	1616	(10)	4228	(4)	87	
H(16)	3728	(34)	3140	(17)	4129	(6)	107	
H(17)	2800	(34)	4762	(18)	4437	(7)	125	
H(18)	4929	(46)	5541	(18)	4959	(7)	148	
H(19)	8324	(49)	4947	(16)	5170	(6)	139	
H(20)	9395	(28)	3292	(16)	4873	(5)	125	
H(21A)	10424	(25)	776	(11)	3871	(4)	93	
H(21B)	8044	(25)	688	(11)	3645	(4)	93	
H(22)	11723	(26)	1132	(95)	3215	(4)	56	(47)
H(23A)	8000	(23)	3157	(12)	596	(4)	167	
H(23B)	7478	(23)	1996	(12)	658	(4)	167	
H(23C)	8953	(23)	2564	(12)	1034	(4)	167	
H(24A)	2669	(23)	3247	(11)	740	(4)	144	
H(24B)	4753	(23)	3814	(11)	531	(4)	144	
H(24C)	3656	(23)	4197	(11)	1003	(4)	144	
H(25A)	4658	(28)	1400	(12)	918	(4)	154	
H(25B)	2716	(28)	1978	(12)	1177	(4)	154	
H(25C)	4728	(28)	1545	(12)	1471	(4)	154	

Table 6: Torsion angles [deg].

C(24)-C(1)-C(2)-C(7)	57	(2)
C(23)-C(1)-C(2)-C(7)	-179.2	(14)
C(25)-C(1)-C(2)-C(7)	-61	(2)
C(24)-C(1)-C(2)-C(3)	179.8	(10)
C(23)-C(1)-C(2)-C(3)	-56	(2)
C(25)-C(1)-C(2)-C(3)	62.5	(14)
C(7)-C(2)-C(3)-C(4)	-59.1	(13)
C(1)-C(2)-C(3)-C(4)	171.5	(11)
C(2)-C(3)-C(4)-C(5)	54	(2)
C(3)-C(4)-C(5)-O(8)	64.8	(14)
C(3)-C(4)-C(5)-C(12)	-174.9	(11)
C(3)-C(4)-C(5)-C(6)	-48	(2)
C(4)-C(5)-C(6)-C(7)	49.7	(14)
O(8)-C(5)-C(6)-C(7)	-66.7	(12)
C(12)-C(5)-C(6)-C(7)	-179.4	(11)
C(1)-C(2)-C(7)-C(6)	-170.4	(11)
C(3)-C(2)-C(7)-C(6)	63.4	(14)
C(5)-C(6)-C(7)-C(2)	-60.2	(13)
C(4)-C(5)-O(8)-C(9)	82.7	(12)
C(12)-C(5)-O(8)-C(9)	-43.9	(13)
C(6)-C(5)-O(8)-C(9)	-158.6	(10)
C(5)-O(8)-C(9)-O(90)	-173.7	(10)
C(5)-O(8)-C(9)-N(10)	5	(2)
O(90)-C(9)-N(10)-C(11)	-165.7	(12)
O(8)-C(9)-N(10)-C(11)	16	(2)
O(90)-C(9)-N(10)-C(13)	12	(2)
O(8)-C(9)-N(10)-C(13)	-166.4	(12)
C(9)-N(10)-C(11)-O(110)	-175.2	(12)
C(13)-N(10)-C(11)-O(110)	7	(2)
C(9)-N(10)-C(11)-C(12)	6	(2)
C(13)-N(10)-C(11)-C(12)	-171.8	(11)
C(4)-C(5)-C(12)-C(120)	62	(2)
O(8)-C(5)-C(12)-C(120)	-176.4	(10)
C(6)-C(5)-C(12)-C(120)	-66.0	(14)
C(4)-C(5)-C(12)-C(11)	-61	(2)
O(8)-C(5)-C(12)-C(11)	60.2	(13)
C(6)-C(5)-C(12)-C(11)	170.7	(11)
O(110)-C(11)-C(12)-C(5)	137.0	(14)
N(10)-C(11)-C(12)-C(5)	-45	(2)
O(110)-C(11)-C(12)-C(120)	11	(2)
N(10)-C(11)-C(12)-C(120)	-170.5	(11)
C(11)-N(10)-C(13)-C(21)	-128.2	(14)
C(9)-N(10)-C(13)-C(21)	54	(2)
C(11)-N(10)-C(13)-C(14)	105.8	(14)
C(9)-N(10)-C(13)-C(14)	-72.2	(14)

N(10)-C(13)-C(14)-C(15)	-49	(2)
C(21)-C(13)-C(14)-C(15)	-176.1	(14)
C(13)-C(14)-C(15)-C(16)	93	(2)
C(13)-C(14)-C(15)-C(20)	-90	(2)
C(20)-C(15)-C(16)-C(17)	1	(2)
C(14)-C(15)-C(16)-C(17)	178.3	(12)
C(15)-C(16)-C(17)-C(18)	-2	(3)
C(16)-C(17)-C(18)-C(19)	4	(3)
C(17)-C(18)-C(19)-C(20)	-3	(3)
C(16)-C(15)-C(20)-C(19)	-2	(2)
C(14)-C(15)-C(20)-C(19)	-178.5	(14)
C(18)-C(19)-C(20)-C(15)	2	(3)
N(10)-C(13)-C(21)-O(22)	42	(2)
C(14)-C(13)-C(21)-O(22)	169.8	(11)

1.3. Aldoladdukt 5A

Table 1: Crystal data and structure refinement.

Empirical formula:	$C_{24}\ H_{36}\ N_2\ O_3$	
Formula weight:	400.57	
Temperature:	-140 °C	
Radiation:	Mo-K_α	
Crystal system:	orthorhombic	
Space group:	P212121	
Unit cell dimensions:	a = 6.296(1) Å	α = 90 deg.
	b = 10.551(2) Å	β = 90 deg.
	c = 35.58(1) Å	γ = 90 deg.
Volume:	2363.2(9) $Å^3$	
Z:	4	
Density (calculated):	1.126 g/cm^3	
Absorption coefficient:	0.7 cm^{-1}	
Crystal color:	colorless, transparent	
Crystal size:	0.04 x 0.15 x 1.20 mm	
Scan range:	sphere	
(2 Θ)max:	52 deg.	
Resolution:	0.80 Å	
Reflections collected:	30998	
Independent reflections:	2596	
Reflections used with I > 0:	2510	
Number of variables:	407	
R (F):	0.097	
wR (F):	0.048	
S:	0.76	

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

Starred atoms were refined isotropically. Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as:

$(4/3) \cdot [a^2 \cdot B(1,1) + b^2 \cdot B(2,2) + c^2 \cdot B(3,3) + a \cdot b \cdot (\cos \gamma) \cdot B(1,2) + a \cdot c \cdot (\cos \beta) \cdot B(1,3) + b \cdot c \cdot (\cos \alpha) \cdot B(2,3)]$

	X		Y		Z		U (eq)	
O1	0.5416	(4)	0.3165	(2)	0.03654	(5)	1.97	(5)
O2	0.0275	(4)	0.5535	(2)	0.06147	(6)	2.69	(5)
O3	0.2488	(4)	0.7740	(2)	0.07916	(6)	2.55	(5)
N1	0.2033	(4)	0.3685	(2)	0.05965	(7)	1.71	(5)
N2	0.2895	(4)	0.1653	(2)	0.05113	(7)	1.75	(6)
C1	0.3662	(5)	0.2840	(3)	0.04767	(8)	1.93	(7)
C2	0.0580	(5)	0.1634	(3)	0.05680	(8)	1.79	(7)
C3	0.0134	(6)	0.2978	(3)	0.07220	(8)	1.97	(7)
C4	0.2007	(6)	0.5000	(3)	0.05935	(8)	1.95	(7)
C5	0.4069	(6)	0.5729	(3)	0.05814	(9)	1.98	(7)
C6	0.4019	(6)	0.6779	(3)	0.08870	(9)	2.00	(7)
C7	0.6169	(6)	0.7440	(3)	0.09145	(9)	2.18	(8)
C8	0.6268	(6)	0.8408	(3)	0.12359	(9)	2.40	(8)
C9	0.5716	(6)	0.7846	(3)	0.16170	(9)	2.46	(8)
C10	0.3548	(6)	0.7201	(3)	0.15880	(9)	2.50	(8)
C11	0.3471	(6)	0.6221	(3)	0.1272	(1)	2.41	(8)
C12	0.3980	(6)	0.0598	(3)	0.03250	(9)	2.38	(8)
C13	-0.0158	(6)	0.0553	(3)	0.08148	(9)	2.65	(8)
C14	-0.0155	(6)	0.3075	(3)	0.11376	(8)	1.80	(7)
C15	-0.2101	(6)	0.3417	(4)	0.12917	(9)	2.84	(8)
C16	-0.2367	(7)	0.3520	(4)	0.1674	(1)	4.4	(1)
C17	-0.0706	(7)	0.3279	(4)	0.19146	(9)	3.9	(1)
C18	0.1231	(6)	0.2936	(4)	0.17689	(9)	3.32	(9)
C19	0.1488	(6)	0.2849	(4)	0.13875	(9)	2.76	(8)
C20	0.4365	(7)	0.6255	(3)	0.01794	(9)	3.05	(9)
C21	0.5928	(6)	0.8797	(3)	0.19477	(9)	2.81	(9)
C22	0.4551	(8)	0.9971	(4)	0.1890	(1)	4.2	(1)
C23	0.8260	(7)	0.9239	(4)	0.1983	(1)	3.9	(1)
C24	0.5341	(8)	0.8162	(4)	0.23179	(9)	4.7	(1)

Table 3a: Bond lengths [Å].

Numbers in parentheses are estimated standard deviations in the least significant digits.

O1-C1	1.222	(4)	C6-C11	1.532	(5)
O2-C4	1.230	(4)	C7-C8	1.535	(5)
O3-C6	1.439	(4)	C8-C9	1.520	(5)
N1-C1	1.424	(4)	C9-C10	1.529	(5)
N1-C3	1.478	(4)	C9-C21	1.552	(5)
N1-C4	1.387	(4)	C10-C11	1.528	(5)
N2-C1	1.348	(4)	C14-C15	1.390	(5)
N2-C2	1.471	(4)	C14-C19	1.384	(5)
N2-C12	1.465	(4)	C15-C16	1.373	(5)
C2-C3	1.546	(4)	C16-C17	1.376	(6)
C2-C13	1.513	(5)	C17-C18	1.374	(6)
C3-C14	1.493	(4)	C18-C19	1.370	(5)
C4-C5	1.510	(5)	C21-C22	1.527	(6)
C5-C6	1.552	(4)	C21-C23	1.545	(6)
C5-C20	1.545	(5)	C21-C24	1.523	(5)
C6-C7	1.526	(5)			

Table 3b: Bond angles [deg].

C1-N1-C3	110.9	(2)	C5-C6-C7	110.7	(3)
C1-N1-C4	129.2	(3)	C5-C6-C11	110.9	(3)
C3-N1-C4	119.8	(3)	C7-C6-C11	108.5	(3)
C1-N2-C2	112.3	(3)	C6-C7-C8	112.9	(3)
C1-N2-C12	119.9	(3)	C7-C8-C9	113.3	(3)
C2-N2-C12	120.9	(3)	C8-C9-C10	108.5	(3)
O1-C1-N1	124.9	(3)	C8-C9-C21	113.9	(3)
O1-C1-N2	127.9	(3)	C10-C9-C21	114.6	(3)
N1-C1-N2	107.2	(3)	C9-C10-C11	112.3	(3)
N2-C2-C3	102.5	(3)	C6-C11-C10	113.0	(3)
N2-C2-C13	113.2	(3)	C3-C14-C15	121.0	(3)
C3-C2-C13	115.5	(3)	C3-C14-C19	122.2	(3)
N1-C3-C2	102.1	(3)	C15-C14-C19	116.7	(3)
N1-C3-C14	111.3	(3)	C14-C15-C16	121.2	(3)
C2-C3-C14	115.8	(3)	C15-C16-C17	120.6	(4)
O2-C4-N1	118.0	(3)	C16-C17-C18	119.2	(3)
O2-C4-C5	122.0	(3)	C17-C18-C19	119.8	(3)
N1-C4-C5	120.0	(3)	C14-C19-C18	122.4	(3)
C4-C5-C6	109.1	(3)	C9-C21-C22	111.9	(3)
C4-C5-C20	108.3	(3)	C9-C21-C23	109.8	(3)
C6-C5-C20	113.2	(3)	C9-C21-C24	110.5	(3)
O3-C6-C5	110.5	(3)	C22-C21-C23	107.8	(3)
O3-C6-C7	106.7	(3)	C22-C21-C24	109.7	(3)
O3-C6-C11	109.3	(3)	C23-C21-C24	107.0	(3)

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

The form of the anisotropic displacement parameter is:

$\exp [-2\pi^2 \cdot (h^2 \cdot a^2 \cdot U_{11} + k^2 \cdot b^2 \cdot U_{22} + l^2 \cdot c^2 \cdot U_{33} + 2 \cdot h \cdot k \cdot a \cdot b \cdot U_{12} + 2 \cdot h \cdot l \cdot a \cdot c \cdot U_{13} + 2 \cdot k \cdot l \cdot b \cdot c \cdot U_{23})]$ where a, b, and c are reciprocal lattice constants.

	U11	U22	U33	U23	U13	U12
O1	0.017 (1)	0.026 (1)	0.031 (1)	0.001 (1)	0.004 (1)	0.001 (1)
O2	0.021 (1)	0.027 (1)	0.054 (1)	0.007 (1)	-0.001 (1)	-0.001 (1)
O3	0.031 (1)	0.022 (1)	0.043 (1)	0.005 (1)	0.000 (1)	-0.001 (1)
N1	0.015 (2)	0.023 (1)	0.027 (1)	-0.004 (2)	0.004 (1)	0.007 (1)
N2	0.021 (2)	0.018 (1)	0.028 (1)	-0.000 (2)	-0.000 (1)	-0.002 (1)
C1	0.024 (2)	0.026 (2)	0.023 (2)	0.006 (2)	-0.006 (2)	-0.004 (2)
C2	0.015 (2)	0.025 (2)	0.028 (2)	-0.002 (2)	-0.000 (2)	0.002 (2)
C3	0.015 (2)	0.026 (2)	0.033 (2)	0.003 (2)	-0.005 (2)	0.004 (2)
C4	0.032 (2)	0.022 (2)	0.020 (2)	0.001 (2)	-0.002 (2)	-0.002 (2)
C5	0.023 (2)	0.020 (2)	0.033 (2)	0.000 (2)	0.003 (2)	-0.002 (2)
C6	0.026 (2)	0.015 (2)	0.035 (2)	0.001 (2)	0.009 (2)	0.004 (2)
C7	0.026 (2)	0.027 (2)	0.030 (2)	-0.002 (2)	0.009 (2)	0.003 (2)
C8	0.032 (2)	0.028 (2)	0.031 (2)	0.001 (2)	0.003 (2)	0.005 (2)
C9	0.018 (2)	0.035 (2)	0.041 (2)	0.006 (2)	0.001 (2)	0.007 (2)
C10	0.033 (2)	0.035 (2)	0.027 (2)	0.003 (2)	0.001 (2)	0.010 (2)
C11	0.024 (2)	0.025 (2)	0.043 (2)	0.004 (2)	0.007 (2)	-0.002 (2)
C12	0.036 (2)	0.021 (2)	0.034 (2)	-0.001 (2)	0.001 (2)	-0.003 (2)
C13	0.032 (2)	0.031 (2)	0.038 (2)	-0.006 (2)	0.005 (2)	0.003 (2)
C14	0.026 (2)	0.017 (2)	0.025 (2)	-0.000 (2)	-0.002 (2)	0.004 (2)
C15	0.023 (2)	0.052 (2)	0.033 (2)	0.009 (2)	0.006 (2)	0.003 (2)
C16	0.033 (3)	0.086 (3)	0.047 (2)	0.015 (3)	0.015 (2)	-0.000 (2)
C17	0.050 (3)	0.076 (3)	0.022 (2)	0.001 (3)	0.005 (2)	0.004 (2)
C18	0.037 (2)	0.063 (3)	0.027 (2)	0.004 (3)	-0.006 (2)	-0.001 (2)
C19	0.022 (2)	0.047 (2)	0.036 (2)	0.004 (2)	0.007 (2)	0.001 (2)
C20	0.048 (3)	0.031 (2)	0.036 (2)	-0.010 (2)	0.005 (2)	-0.003 (2)
C21	0.026 (2)	0.046 (2)	0.035 (2)	-0.001 (2)	0.001 (2)	-0.013 (2)
C22	0.050 (3)	0.057 (3)	0.052 (2)	0.007 (3)	-0.005 (3)	-0.028 (2)
C23	0.043 (3)	0.065 (3)	0.040 (2)	-0.011 (3)	-0.002 (2)	-0.010 (2)
C24	0.070 (3)	0.079 (3)	0.032 (2)	-0.015 (3)	0.007 (2)	-0.010 (2)

Table 5: Hydrogen coordinates ($\cdot 10^4$) and isotropic displacement parameters ($Å^2 \cdot 10^3$).
Starred atoms were refined isotropically. Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as:

$(4/3) \cdot [a^2 \cdot B(1,1) + b^2 \cdot B(2,2) + c^2 \cdot B(3,3) + a \cdot b \cdot (\cos \gamma) \cdot B(1,2) + a \cdot c \cdot (\cos \beta) \cdot B(1,3) + b \cdot c \cdot (\cos \alpha) \cdot B(2,3)]$

	X		Y		Z		U	
H2	-0.009	(5)	0.158	(2)	0.0313	(6)	2.3	(7)*
H3	-0.088	(4)	0.324	(2)	0.0616	(5)	-0.8	(5)*
H5	0.524	(5)	0.517	(2)	0.0626	(7)	2.5	(7)*
H7a	0.640	(4)	0.780	(3)	0.0678	(7)	2.2	(7)*
H7b	0.731	(5)	0.682	(3)	0.0955	(7)	3.0	(7)*
H8a	0.534	(5)	0.912	(3)	0.1163	(7)	2.6	(7)*
H8b	0.765	(5)	0.884	(3)	0.1235	(8)	4.3	(8)*
H9	0.667	(4)	0.726	(2)	0.1671	(6)	1.0	(6)*
H10a	0.256	(4)	0.783	(2)	0.1515	(5)	-0.2	(5)*
H10b	0.321	(4)	0.678	(2)	0.1819	(6)	0.9	(6)*
H11a	0.444	(4)	0.555	(2)	0.1316	(6)	0.9	(6)*
H11b	0.205	(5)	0.582	(3)	0.1268	(8)	3.8	(8)*
H15	-0.322	(5)	0.358	(3)	0.1126	(7)	2.7	(7)*
H16	-0.349	(5)	0.371	(3)	0.1767	(7)	2.5	(7)*
H17	-0.090	(5)	0.334	(3)	0.2172	(7)	2.4	(7)*
H18	0.225	(5)	0.268	(3)	0.1947	(8)	4.1	(8)*
H19	0.266	(4)	0.263	(2)	0.1301	(5)	-0.6	(5)*
H20a	0.431	(4)	0.554	(2)	-0.0001	(6)	2.2	(7)*
H20b	0.342	(6)	0.700	(3)	0.0125	(9)	7	(1)*
H20c	0.566	(5)	0.667	(2)	0.0177	(7)	1.9	(7)*
H22a	0.470	(5)	1.054	(3)	0.2097	(7)	3.2	(8)*
H22b	0.500	(5)	1.041	(3)	0.1643	(7)	3.1	(8)*
H22c	0.320	(7)	0.978	(4)	0.186	(1)	8	(1)*
H23a	0.842	(6)	0.980	(3)	0.2211	(9)	6	(1)*
H23b	0.900	(7)	0.847	(4)	0.200	(1)	8	(1)*
H23c	0.856	(5)	0.970	(3)	0.1765	(7)	2.5	(7)*
H24a	0.550	(6)	0.874	(3)	0.2529	(8)	4.5	(8)*
H24b	0.392	(6)	0.788	(3)	0.2331	(9)	6	(1)*
H24c	0.622	(6)	0.727	(4)	0.2319	(9)	7	(1)*
H0	0.153	(6)	0.732	(3)	0.0742	(9)	6	(1)*
H12a	0.371	(5)	-0.017	(3)	0.0466	(8)	3.4	(8)*
H12b	0.345	(4)	0.044	(2)	0.0062	(6)	1.3	(6)*
H13a	0.056	(6)	0.051	(3)	0.1071	(8)	4.6	(9)*
H13b	0.014	(5)	-0.020	(2)	0.0681	(7)	2.6	(7)*
H12c	0.565	(5)	0.082	(3)	0.0309	(7)	3.8	(8)*
H13c	-0.160	(5)	0.061	(3)	0.0849	(8)	4.9	(9)*

Table 6: Torsion angles [deg].

C3-N1-C1-O1	-178.61	(0.28)
C3-N1-C1-N2	1.26	(0.32)
C4-N1-C1-O1	4.18	(0.49)
C4-N1-C1-N2	-175.96	(0.27)
C1-N1-C3-C2	-14.18	(0.30)
C1-N1-C3-C14	109.96	(0.29)
C4-N1-C3-C2	163.33	(0.25)
C4-N1-C3-C14	-72.53	(0.35)
C1-N1-C4-O2	161.10	(0.28)
C1-N1-C4-C5	-21.47	(0.44)
C3-N1-C4-O2	-15.90	(0.40)
C3-N1-C4-C5	161.54	(0.26)
C2-N2-C1-O1	-166.46	(0.29)
C2-N2-C1-N1	13.68	(0.32)
C12-N2-C1-O1	-15.28	(0.47)
C12-N2-C1-N1	164.86	(0.25)
C1-N2-C2-C3	-22.07	(0.30)
C1-N2-C2-C13	-147.14	(0.26)
C12-N2-C2-C3	-172.91	(0.25)
C12-N2-C2-C13	62.02	(0.35)
N2-C2-C3-N1	20.47	(0.28)
N2-C2-C3-C14	-100.58	(0.31)
C13-C2-C3-N1	144.01	(0.28)
C13-C2-C3-C14	22.97	(0.43)
N1-C3-C14-C15	130.05	(0.33)
N1-C3-C14-C19	-49.02	(0.42)
C2-C3-C14-C15	-114.01	(0.36)
C2-C3-C14-C19	66.92	(0.43)
O2-C4-C5-C6	45.58	(0.39)
O2-C4-C5-C20	-78.01	(0.36)
N1-C4-C5-C6	-131.75	(0.28)
N1-C4-C5-C20	104.66	(0.32)
C4-C5-C6-O3	-68.51	(0.32)
C4-C5-C6-C7	173.51	(0.26)
C4-C5-C6-C11	52.95	(0.36)
C20-C5-C6-O3	52.08	(0.38)
C20-C5-C6-C7	-65.91	(0.37)
C20-C5-C6-C11	173.53	(0.30)
O3-C6-C7-C8	64.68	(0.32)
C5-C6-C7-C8	-175.00	(0.26)
C11-C6-C7-C8	-53.03	(0.35)
O3-C6-C11-C10	-61.70	(0.36)
C5-C6-C11-C10	176.13	(0.29)
C7-C6-C11-C10	54.31	(0.37)

C6-C7-C8-C9	55.67	(0.39)
C7-C8-C9-C10	-54.27	(0.39)
C7-C8-C9-C21	176.88	(0.30)
C8-C9-C10-C11	54.90	(0.37)
C21-C9-C10-C11	-176.64	(0.28)
C8-C9-C21-C22	57.27	(0.41)
C8-C9-C21-C23	-62.37	(0.39)
C8-C9-C21-C24	179.81	(0.32)
C10-C9-C21-C22	-68.44	(0.39)
C10-C9-C21-C23	171.92	(0.29)
C10-C9-C21-C24	54.09	(0.42)
C9-C10-C11-C6	-57.32	(0.39)
C3-C14-C15-C16	-179.31	(0.35)
C19-C14-C15-C16	-0.19	(0.54)
C3-C14-C19-C18	180.00	(0.66)
C15-C14-C19-C18	0.88	(0.55)
C14-C15-C16-C17	-0.31	(0.64)
C15-C16-C17-C18	0.16	(0.67)
C16-C17-C18-C19	0.50	(0.64)
C17-C18-C19-C14	-1.05	(0.62)

1.4. Aldoladdukt 13A

Table 1: Crystal data and structure refinement.

Empirical formula:	$C_{35}\ H_{60}\ N_2\ O_5\ Si_2$	
Formula weight:	645.05	
Temperature:	-139 °C	
Radiation:	Mo-K_α	
Crystal system:	orthorhombic	
Space group:	P212121	
Unit cell dimensions:	a = 6.4521(9) Å	α = 90 deg.
	b = 10.085(2) Å	β = 90 deg.
	c = 56.915(9) Å	γ = 90 deg.
Volume:	3703(1) $Å^3$	
Z:	4	
Density (calculated):	1.157 g/cm^3	
Absorption coefficient:	1.31 cm^{-1}	
Crystal color:	colorless, transparent	
Crystal size:	0.04 x 0.12 x 0.84 mm	
Scan range:	sphere	
(2 Θ)max:	49 deg.	
Resolution:	0.86 Å	
Reflections collected:	39092	
Independent reflections:	5540	
Reflections used with I > 0:	5516	
Number of variables:	637	
R (F):	0.090	
wR (F):	0.065	
S:	1.10	

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

Starred atoms were refined isotropically. Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as:

$(4/3) \cdot [a^2 \cdot B(1,1) + b^2 \cdot B(2,2) + c^2 \cdot B(3,3) + a \cdot b \cdot (\cos \gamma) \cdot B(1,2) + a \cdot c \cdot (\cos \beta) \cdot B(1,3) + b \cdot c \cdot (\cos \alpha) \cdot B(2,3)]$

	X		Y		Z		U (eq)	
SI1	0.0129	(2)	-0.0898	(2)	0.20622	(2)	2.30	(3)
SI2	0.4458	(2)	0.3187	(1)	0.14653	(2)	1.61	(3)
O1	0.1830	(5)	-0.1698	(3)	0.02012	(5)	1.82	(7)
O2	0.6818	(5)	-0.1907	(4)	0.06782	(5)	2.20	(7)
O3	0.4535	(5)	-0.2794	(3)	0.10738	(5)	1.82	(7)
O4	0.1626	(5)	-0.1150	(3)	0.18304	(5)	1.87	(7)
O5	0.3555	(5)	0.1745	(3)	0.15526	(5)	2.33	(7)
N1	0.4260	(6)	-0.0437	(4)	0.00077	(6)	1.81	(9)
N2	0.5136	(6)	-0.1227	(4)	0.03573	(6)	1.19	(8)
C1	0.3534	(7)	-0.1179	(5)	0.01868	(7)	1.6	(1)
C2	0.6503	(7)	-0.0225	(5)	0.00179	(8)	1.7	(1)
C3	0.6965	(7)	-0.0456	(5)	0.02821	(8)	1.7	(1)
C4	0.5158	(7)	-0.1858	(5)	0.05753	(7)	1.6	(1)
C5	0.3192	(7)	-0.2420	(5)	0.06780	(8)	1.4	(1)
C6	0.3007	(7)	-0.2073	(5)	0.09388	(7)	1.4	(1)
C7	0.0889	(7)	-0.2447	(5)	0.10402	(7)	1.4	(1)
C8	0.0154	(7)	-0.1312	(5)	0.12010	(7)	1.6	(1)
C9	-0.0286	(7)	-0.1659	(5)	0.14627	(8)	2.0	(1)
C10	0.1085	(7)	-0.0718	(5)	0.16010	(7)	1.4	(1)
C11	0.2991	(7)	-0.0534	(5)	0.14444	(7)	1.3	(1)
C12	0.1961	(8)	-0.0311	(5)	0.12042	(8)	1.6	(1)
C13	0.3188	(7)	-0.0585	(5)	0.09841	(7)	1.4	(1)
C14	0.3220	(8)	-0.0465	(6)	-0.02174	(8)	3.1	(1)
C15	0.7190	(8)	0.1110	(6)	-0.00773	(8)	2.5	(1)
C16	0.7262	(7)	0.0753	(5)	0.04322	(7)	1.5	(1)
C17	0.9207	(7)	0.1039	(5)	0.05245	(8)	2.2	(1)
C18	0.9508	(8)	0.2129	(6)	0.06620	(9)	3.3	(1)
C19	0.7852	(9)	0.2961	(5)	0.07123	(8)	2.8	(1)
C20	0.5946	(8)	0.2701	(5)	0.06248	(9)	2.7	(1)
C21	0.5635	(8)	0.1602	(5)	0.04827	(8)	1.8	(1)
C22	0.3192	(8)	-0.3931	(5)	0.06356	(8)	2.4	(1)
C23	-0.1011	(8)	0.0789	(5)	0.20508	(8)	2.6	(1)
C24	-0.1941	(9)	-0.2190	(6)	0.2071	(1)	3.9	(1)
C25	0.1830	(8)	-0.1109	(5)	0.23269	(8)	2.5	(1)
C26	0.0551	(9)	-0.0984	(6)	0.25507	(8)	3.5	(1)
C27	0.3526	(9)	-0.0036	(6)	0.23226	(9)	3.6	(1)
C28	0.2809	(8)	-0.2489	(6)	0.23243	(8)	3.0	(1)

C29	0.4500	(8)	0.0480	(5)	0.15295	(8)	1.9 (1)
C30	0.7271	(8)	0.3046	(6)	0.13900	(8)	2.6 (1)
C31	0.3043	(8)	0.3682	(6)	0.11956	(8)	2.7 (1)
C32	0.4036	(7)	0.4386	(5)	0.17141	(8)	1.6 (1)
C33	0.514	(1)	0.3922	(5)	0.19360	(8)	3.3 (1)
C34	0.4843	(9)	0.5761	(5)	0.16439	(8)	3.4 (1)
C35	0.1722	(9)	0.4495	(6)	0.17731	(8)	3.0 (1)

Table 3a: Bond lengths [Å].

Numbers in parentheses are estimated standard deviations in the least significant digits.

SI1-O4	1.655	(3)	C5-C22	1.543	(7)
SI1-C23	1.855	(6)	C6-C7	1.530	(6)
SI1-C24	1.867	(6)	C6-C13	1.527	(7)
SI1-C25	1.876	(5)	C7-C8	1.540	(6)
SI2-O5	1.643	(4)	C8-C9	1.556	(6)
SI2-C30	1.871	(5)	C8-C12	1.542	(7)
SI2-C31	1.854	(5)	C9-C10	1.518	(6)
SI2-C32	1.882	(5)	C10-C11	1.530	(6)
O1-C1	1.220	(6)	C11-C12	1.537	(6)
O2-C4	1.222	(5)	C11-C29	1.493	(7)
O3-C6	1.446	(5)	C12-C13	1.507	(6)
O4-C10	1.420	(5)	C16-C17	1.391	(7)
O5-C29	1.421	(6)	C16-C21	1.384	(7)
N1-C1	1.349	(6)	C17-C18	1.363	(7)
N1-C2	1.464	(6)	C18-C19	1.389	(8)
N1-C14	1.447	(6)	C19-C20	1.352	(8)
N2-C1	1.418	(6)	C20-C21	1.387	(7)
N2-C3	1.477	(6)	C25-C26	1.523	(7)
N2-C4	1.395	(5)	C25-C27	1.539	(8)
C2-C3	1.550	(6)	C25-C28	1.529	(8)
C2-C15	1.517	(7)	C32-C33	1.525	(7)
C3-C16	1.501	(7)	C32-C34	1.534	(7)
C4-C5	1.507	(6)	C32-C35	1.534	(8)
C5-C6	1.530	(6)			

Table 3b: Bond angles [deg].

O4-SI1-C23	110.1	(2)
O4-SI1-C24	109.4	(2)
O4-SI1-C25	106.3	(2)
C23-SI1-C24	111.0	(2)
C23-SI1-C25	111.4	(2)
C24-SI1-C25	108.5	(2)
O5-SI2-C30	110.2	(2)
O5-SI2-C31	108.3	(2)
O5-SI2-C32	106.8	(2)
C30-SI2-C31	108.0	(2)
C30-SI2-C32	111.2	(2)
C31-SI2-C32	112.3	(2)
SI1-O4-C10	122.9	(3)
SI2-O5-C29	127.9	(3)
C1-N1-C2	113.2	(4)
C1-N1-C14	119.8	(4)
C2-N1-C14	119.8	(4)
C1-N2-C3	111.5	(3)
C1-N2-C4	129.2	(4)
C3-N2-C4	119.4	(3)
O1-C1-N1	127.0	(4)
O1-C1-N2	126.6	(4)
N1-C1-N2	106.4	(4)
N1-C2-C3	101.9	(3)
N1-C2-C15	113.8	(4)
C3-C2-C15	115.1	(4)
N2-C3-C2	101.9	(3)
N2-C3-C16	111.4	(4)
C2-C3-C16	117.0	(4)
O2-C4-N2	117.0	(4)
O2-C4-C5	122.5	(4)
N2-C4-C5	120.5	(4)
C4-C5-C6	110.8	(4)
C4-C5-C22	108.1	(4)
C6-C5-C22	112.2	(4)
O3-C6-C5	110.3	(4)
O3-C6-C7	106.5	(3)
O3-C6-C13	110.6	(3)
C5-C6-C7	112.3	(4)
C5-C6-C13	112.5	(4)
C7-C6-C13	104.3	(4)
C6-C7-C8	108.4	(4)
C7-C8-C9	117.2	(4)
C7-C8-C12	105.1	(4)
C9-C8-C12	105.9	(3)
C8-C9-C10	104.4	(4)
O4-C10-C9	115.3	(4)
O4-C10-C11	112.0	(4)
C9-C10-C11	104.0	(3)
C10-C11-C12	100.8	(4)
C10-C11-C29	114.7	(4)
C12-C11-C29	118.1	(4)
C8-C12-C11	104.0	(4)
C8-C12-C13	105.5	(4)
C11-C12-C13	119.0	(4)
C6-C13-C12	106.3	(4)
C3-C16-C17	119.9	(4)
C3-C16-C21	121.6	(4)
C17-C16-C21	118.5	(4)
C16-C17-C18	120.8	(5)
C17-C18-C19	119.7	(5)
C18-C19-C20	120.4	(5)
C19-C20-C21	120.1	(5)
C16-C21-C20	120.4	(4)
SI1-C25-C26	110.2	(4)
SI1-C25-C27	108.9	(3)
SI1-C25-C28	109.7	(3)
C26-C25-C27	109.9	(4)
C26-C25-C28	107.9	(4)
C27-C25-C28	110.3	(4)
O5-C29-C11	111.4	(4)
SI2-C32-C33	111.0	(3)
SI2-C32-C34	109.6	(3)
SI2-C32-C35	110.6	(3)
C33-C32-C34	109.5	(4)
C33-C32-C35	107.3	(4)
C34-C32-C35	108.8	(4)

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

The form of the anisotropic displacement parameter is:

$\exp [-2\pi^2 \cdot (h^2 \cdot a^2 \cdot U_{11} + k^2 \cdot b^2 \cdot U_{22} + l^2 \cdot c^2 \cdot U_{33} + 2 \cdot h \cdot k \cdot a \cdot b \cdot U_{12} + 2 \cdot h \cdot l \cdot a \cdot c \cdot U_{13} + 2 \cdot k \cdot l \cdot b \cdot c \cdot U_{23})]$ where a, b, and c are reciprocal lattice constants.

	U11	U22	U33	U23	U13	U12
SI1	0.0338 (8)	0.0323 (8)	0.0211 (6)	0.0057 (8)	0.0016 (7)	-0.0002 (7)
SI2	0.0238 (7)	0.0189 (7)	0.0184 (6)	-0.0042 (7)	0.0001 (6)	-0.0016 (7)
O1	0.015 (2)	0.033 (2)	0.021 (2)	-0.003 (2)	0.002 (2)	0.001 (2)
O2	0.024 (2)	0.039 (2)	0.021 (2)	0.005 (2)	-0.001 (2)	0.004 (2)
O3	0.026 (2)	0.022 (2)	0.021 (2)	0.002 (2)	0.003 (2)	0.008 (2)
O4	0.028 (2)	0.026 (2)	0.018 (2)	0.001 (2)	0.002 (2)	0.002 (2)
O5	0.031 (2)	0.020 (2)	0.037 (2)	0.001 (2)	0.012 (2)	-0.005 (2)
N1	0.027 (2)	0.032 (2)	0.009 (2)	-0.005 (2)	-0.005 (2)	0.004 (2)
N2	0.019 (2)	0.013 (2)	0.013 (2)	0.004 (2)	0.003 (2)	-0.000 (2)
C1	0.029 (3)	0.015 (3)	0.016 (2)	0.014 (2)	0.001 (2)	-0.002 (2)
C2	0.025 (3)	0.022 (3)	0.019 (2)	0.002 (3)	0.011 (2)	-0.006 (2)
C3	0.012 (2)	0.028 (3)	0.023 (2)	0.001 (2)	0.009 (2)	-0.003 (2)
C4	0.021 (3)	0.022 (3)	0.020 (2)	0.010 (3)	0.002 (2)	-0.009 (2)
C5	0.022 (3)	0.015 (2)	0.018 (2)	0.001 (2)	-0.012 (2)	0.002 (2)
C6	0.025 (3)	0.017 (3)	0.012 (2)	0.007 (3)	-0.007 (2)	0.007 (2)
C7	0.019 (3)	0.017 (3)	0.017 (2)	-0.004 (2)	0.004 (2)	0.002 (2)
C8	0.022 (3)	0.026 (3)	0.015 (2)	0.001 (2)	-0.003 (2)	0.003 (2)
C9	0.031 (3)	0.015 (3)	0.031 (2)	-0.005 (3)	0.012 (3)	-0.002 (2)
C10	0.025 (3)	0.010 (2)	0.018 (2)	-0.003 (2)	0.001 (2)	0.008 (2)
C11	0.022 (3)	0.013 (3)	0.017 (2)	0.007 (2)	0.000 (2)	0.002 (2)
C12	0.028 (3)	0.009 (3)	0.023 (2)	0.003 (2)	-0.003 (2)	-0.001 (2)
C13	0.013 (2)	0.029 (3)	0.012 (2)	-0.003 (3)	-0.007 (2)	0.004 (2)
C14	0.023 (3)	0.063 (4)	0.032 (3)	-0.004 (3)	-0.003 (3)	0.021 (3)
C15	0.040 (3)	0.034 (3)	0.022 (3)	-0.001 (3)	0.003 (3)	0.007 (3)
C16	0.030 (3)	0.016 (3)	0.012 (2)	-0.003 (2)	0.003 (2)	0.007 (2)
C17	0.023 (3)	0.032 (3)	0.029 (3)	-0.004 (3)	-0.001 (2)	-0.012 (3)
C18	0.043 (3)	0.044 (4)	0.038 (3)	-0.008 (3)	-0.027 (3)	-0.001 (3)
C19	0.068 (4)	0.019 (3)	0.018 (2)	-0.012 (3)	-0.001 (3)	-0.005 (2)
C20	0.048 (3)	0.022 (3)	0.033 (3)	0.011 (3)	0.017 (3)	0.005 (3)
C21	0.026 (3)	0.019 (3)	0.026 (2)	0.003 (3)	0.005 (2)	0.004 (2)
C22	0.038 (3)	0.029 (3)	0.024 (3)	0.004 (3)	-0.006 (3)	-0.004 (3)
C23	0.034 (3)	0.040 (3)	0.027 (3)	0.017 (3)	0.000 (3)	-0.005 (3)
C24	0.036 (3)	0.053 (4)	0.057 (4)	-0.023 (3)	0.008 (3)	0.003 (4)
C25	0.037 (3)	0.031 (3)	0.027 (3)	0.012 (3)	0.004 (3)	0.003 (3)
C26	0.048 (4)	0.064 (4)	0.020 (3)	0.013 (4)	-0.003 (3)	-0.000 (3)
C27	0.045 (4)	0.048 (4)	0.045 (3)	-0.014 (3)	-0.018 (3)	0.003 (3)
C28	0.037 (3)	0.053 (4)	0.022 (3)	-0.000 (3)	0.001 (3)	0.005 (3)
C29	0.026 (3)	0.020 (3)	0.026 (2)	0.004 (3)	0.001 (2)	-0.004 (2)

C30	0.030	(3)	0.037	(3)	0.033	(3)	-0.006	(3)	-0.001	(2)	-0.003	(3)
C31	0.033	(3)	0.039	(4)	0.030	(3)	0.000	(3)	0.003	(3)	0.004	(3)
C32	0.027	(3)	0.010	(3)	0.025	(2)	-0.003	(2)	-0.003	(2)	-0.002	(2)
C33	0.074	(4)	0.029	(3)	0.024	(2)	0.017	(4)	-0.016	(3)	-0.012	(3)
C34	0.071	(4)	0.028	(3)	0.030	(3)	0.001	(4)	-0.012	(3)	-0.013	(3)
C35	0.057	(4)	0.028	(3)	0.027	(3)	0.000	(3)	-0.002	(3)	-0.011	(3)

Table 5: Hydrogen coordinates ($\cdot 10^4$) and isotropic displacement parameters ($Å^2 \cdot 10^3$).
Starred atoms were refined isotropically. Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as:

$(4/3) \cdot [a^2 \cdot B(1,1) + b^2 \cdot B(2,2) + c^2 \cdot B(3,3) + a \cdot b \cdot (\cos \gamma) \cdot B(1,2) + a \cdot c \cdot (\cos \beta) \cdot B(1,3) + b \cdot c \cdot (\cos \alpha) \cdot B(2,3)]$

	X		Y		Z		U	
H2	0.711	(5)	-0.089	(3)	-0.0070	(5)	-0.6	(7)*
H3	0.819	(5)	-0.102	(3)	0.0292	(5)	0.3	(8)*
H03	0.557	(5)	-0.251	(3)	0.1029	(6)	0.5	(8)*
H5	0.220	(5)	-0.213	(3)	0.0584	(5)	-0.3	(7)*
H7A	0.102	(5)	-0.319	(3)	0.1123	(5)	0.1	(8)*
H7B	-0.027	(6)	-0.261	(4)	0.0911	(7)	3	(1)*
H8	-0.095	(5)	-0.103	(3)	0.1133	(5)	-0.5	(7)*
H9B	-0.195	(7)	-0.162	(5)	0.1516	(7)	4	(1)*
H9A	0.008	(5)	-0.248	(3)	0.1487	(5)	0.0	(7)*
H10	0.044	(5)	0.016	(3)	0.1615	(6)	0.7	(8)*
H11	0.355	(5)	-0.129	(3)	0.1459	(5)	0.1	(8)*
H12	0.154	(5)	0.047	(3)	0.1199	(5)	-0.2	(7)*
H13A	0.254	(5)	-0.010	(4)	0.0841	(5)	0.3	(8)*
H13B	0.453	(5)	-0.031	(3)	0.1002	(5)	-0.6	(7)*
H14A	0.307	(6)	0.038	(4)	-0.0294	(6)	2	(1)*
H14B	0.411	(7)	-0.102	(5)	-0.0320	(8)	5	(1)*
H14C	0.189	(5)	-0.067	(4)	-0.0195	(6)	0.8	(8)*
H15C	0.677	(5)	0.123	(3)	-0.0237	(5)	-0.0	(7)*
H15A	0.872	(5)	0.127	(4)	-0.0063	(6)	1.4	(9)*
H15B	0.647	(7)	0.179	(4)	-0.0006	(8)	4	(1)*
H17	1.030	(5)	0.051	(3)	0.0480	(5)	0.3	(8)*
H18	1.083	(6)	0.234	(4)	0.0731	(6)	2	(1)*
H19	0.804	(5)	0.357	(3)	0.0795	(5)	-0.4	(7)*
H20	0.485	(5)	0.329	(4)	0.0650	(6)	0.9	(8)*
H21	0.438	(6)	0.145	(4)	0.0411	(6)	2	(1)*
H22A	0.327	(6)	-0.407	(4)	0.0452	(6)	1.3	(9)*
H22C	0.186	(8)	-0.432	(5)	0.0679	(8)	6	(1)*
H22B	0.408	(4)	-0.434	(3)	0.0711	(5)	-1.0	(7)*
H23C	-0.198	(7)	0.088	(4)	0.1944	(7)	3	(1)*
H23A	-0.165	(8)	0.102	(6)	0.2218	(9)	7	(2)*
H23B	-0.00	(1)	0.136	(7)	0.204	(1)	13	(2)*
H24B	-0.275	(8)	-0.212	(6)	0.1950	(9)	8	(2)*
H24C	-0.289	(6)	-0.229	(4)	0.2230	(7)	3	(1)*
H24A	-0.129	(6)	-0.307	(4)	0.2121	(7)	3	(1)*
H26B	-0.065	(5)	-0.158	(3)	0.2537	(5)	0.2	(8)*
H26A	-0.005	(9)	0.000	(5)	0.2560	(8)	7	(2)*
H26C	0.118	(7)	-0.098	(5)	0.2678	(7)	4	(1)*

H27C	0.423	(6)	0.003	(4)	0.2173	(6)	2 (1)*
H27B	0.458	(9)	-0.023	(5)	0.2472	(8)	6 (1)*
H27A	0.301	(6)	0.083	(4)	0.2282	(6)	2 (1)*
H28B	0.167	(5)	-0.316	(4)	0.2338	(6)	0.6 (8)*
H28A	0.357	(5)	-0.271	(3)	0.2176	(5)	-0.4 (7)*
H28C	0.367	(8)	-0.258	(6)	0.2485	(9)	7 (2)*
H29A	0.572	(5)	0.058	(4)	0.1432	(6)	0.8 (8)*
H29B	0.509	(6)	0.024	(4)	0.1709	(5)	0.7 (8)*
H30B	0.815	(7)	0.280	(5)	0.1521	(7)	4 (1)*
H30C	0.785	(7)	0.394	(5)	0.1373	(7)	4 (1)*
H30A	0.736	(7)	0.258	(6)	0.1256	(9)	6 (2)*
H31A	0.354	(5)	0.441	(3)	0.1138	(5)	-0.1 (8)*
H31C	0.156	(6)	0.374	(4)	0.1239	(7)	3 (1)*
H31B	0.353	(7)	0.312	(5)	0.1076	(7)	4 (1)*
H33A	0.489	(6)	0.456	(4)	0.2065	(7)	3 (1)*
H33C	0.498	(5)	0.301	(4)	0.1983	(6)	0.9 (9)*
H33B	0.673	(8)	0.384	(5)	0.1936	(8)	6 (1)*
H34C	0.437	(5)	0.602	(4)	0.1521	(6)	1.1 (9)*
H34B	0.456	(7)	0.650	(4)	0.1766	(7)	4 (1)*
H34A	0.653	(7)	0.586	(5)	0.1664	(8)	6 (1)*
H35A	0.100	(5)	0.472	(3)	0.1652	(5)	-0.2 (8)*
H35C	0.110	(6)	0.355	(4)	0.1810	(6)	1 (1)*
H35B	0.155	(8)	0.511	(5)	0.1950	(8)	5 (1)*

Table 6: Torsion angles [deg].

C23-SI1-O4-C10	-40.68	(0.39)
C24-SI1-O4-C10	81.52	(0.38)
C25-SI1-O4-C10	-161.48	(0.34)
O4-SI1-C25-C26	-176.29	(0.37)
O4-SI1-C25-C27	63.11	(0.39)
O4-SI1-C25-C28	-57.64	(0.38)
C23-SI1-C25-C26	63.70	(0.44)
C23-SI1-C25-C27	-56.90	(0.41)
C23-SI1-C25-C28	-177.65	(0.33)
C24-SI1-C25-C26	-58.71	(0.45)
C24-SI1-C25-C27	-179.31	(0.36)
C24-SI1-C25-C28	59.94	(0.40)
C30-SI2-O5-C29	-13.73	(0.40)
C31-SI2-O5-C29	104.19	(0.37)
C32-SI2-O5-C29	-134.68	(0.35)
O5-SI2-C32-C33	59.07	(0.38)
O5-SI2-C32-C34	-179.87	(0.33)
O5-SI2-C32-C35	-59.90	(0.36)
C30-SI2-C32-C33	-61.25	(0.41)
C30-SI2-C32-C34	59.81	(0.40)
C30-SI2-C32-C35	179.78	(0.33)
C31-SI2-C32-C33	177.65	(0.35)
C31-SI2-C32-C34	-61.28	(0.40)
C31-SI2-C32-C35	58.68	(0.39)
SI1-O4-C10-C9	-85.28	(0.44)
SI1-O4-C10-C11	156.00	(0.30)
SI2-O5-C29-C11	-134.48	(0.33)
C2-N1-C1-O1	-166.33	(0.45)
C2-N1-C1-N2	14.35	(0.50)
C14-N1-C1-O1	-16.00	(0.73)
C14-N1-C1-N2	164.68	(0.40)
C1-N1-C2-C3	-22.45	(0.49)
C1-N1-C2-C15	-146.95	(0.40)
C14-N1-C2-C3	-172.79	(0.42)
C14-N1-C2-C15	62.72	(0.56)
C3-N2-C1-O1	-178.58	(0.45)
C3-N2-C1-N1	0.75	(0.49)
C4-N2-C1-O1	0.14	(0.76)
C4-N2-C1-N1	179.46	(0.41)
C1-N2-C3-C2	-13.82	(0.47)
C1-N2-C3-C16	111.76	(0.40)
C4-N2-C3-C2	167.32	(0.37)
C4-N2-C3-C16	-67.09	(0.51)
C1-N2-C4-O2	170.56	(0.42)

C1-N2-C4-C5	-10.81	(0.68)
C3-N2-C4-O2	-10.82	(0.61)
C3-N2-C4-C5	167.81	(0.40)
N1-C2-C3-N2	20.30	(0.43)
N1-C2-C3-C16	-101.48	(0.44)
C15-C2-C3-N2	143.96	(0.40)
C15-C2-C3-C16	22.19	(0.59)
N2-C3-C16-C17	131.88	(0.43)
N2-C3-C16-C21	-47.96	(0.56)
C2-C3-C16-C17	-111.41	(0.49)
C2-C3-C16-C21	68.74	(0.57)
O2-C4-C5-C6	42.72	(0.61)
O2-C4-C5-C22	-80.60	(0.53)
N2-C4-C5-C6	-135.82	(0.42)
N2-C4-C5-C22	100.85	(0.47)
C4-C5-C6-O3	-69.79	(0.47)
C4-C5-C6-C7	171.55	(0.38)
C4-C5-C6-C13	54.28	(0.50)
C22-C5-C6-O3	51.13	(0.50)
C22-C5-C6-C7	-67.53	(0.50)
C22-C5-C6-C13	175.20	(0.39)
O3-C6-C7-C8	101.28	(0.39)
C5-C6-C7-C8	-137.84	(0.38)
C13-C6-C7-C8	-15.77	(0.44)
O3-C6-C13-C12	-84.25	(0.42)
C5-C6-C13-C12	151.84	(0.38)
C7-C6-C13-C12	29.92	(0.43)
C6-C7-C8-C9	-120.99	(0.42)
C6-C7-C8-C12	-3.73	(0.45)
C7-C8-C9-C10	123.86	(0.41)
C12-C8-C9-C10	7.02	(0.47)
C7-C8-C12-C11	-103.83	(0.38)
C7-C8-C12-C13	22.18	(0.45)
C9-C8-C12-C11	20.92	(0.46)
C9-C8-C12-C13	146.92	(0.37)
C8-C9-C10-O4	-155.69	(0.36)
C8-C9-C10-C11	-32.60	(0.44)
O4-C10-C11-C12	170.77	(0.35)
O4-C10-C11-C29	-61.20	(0.50)
C9-C10-C11-C12	45.55	(0.42)
C9-C10-C11-C29	173.58	(0.38)
C10-C11-C12-C8	-40.43	(0.42)
C10-C11-C12-C13	-157.37	(0.40)
C29-C11-C12-C8	-166.23	(0.39)
C29-C11-C12-C13	76.83	(0.54)
C10-C11-C29-O5	-58.42	(0.48)
C12-C11-C29-O5	60.30	(0.51)

C8-C12-C13-C6	-32.74	(0.45)
C11-C12-C13-C6	83.41	(0.47)
C3-C16-C17-C18	-179.72	(0.44)
C21-C16-C17-C18	0.13	(0.71)
C3-C16-C21-C20	179.03	(0.43)
C17-C16-C21-C20	-0.82	(0.67)
C16-C17-C18-C19	0.44	(0.75)
C17-C18-C19-C20	-0.32	(0.76)
C18-C19-C20-C21	-0.37	(0.75)
C19-C20-C21-C16	0.95	(0.73)

1.5. Aldoladdukt 13B

Table 1: Crystal data and structure refinement.

Empirical formula:	$C_{35}\ H_{60}\ N_2\ O_5\ Si_2$	
Formula weight:	645.05	
Temperature:	-139 °C	
Radiation:	Mo-K_α	
Crystal system:	monoclinic	
Space group:	P21	
Unit cell dimensions:	a = 6.4304(7) Å	α = 90 deg.
	b = 12.510(2) Å	β = 95.73(1) deg.
	c = 23.203(3) Å	γ = 90 deg.
Volume:	1857.3(5) $Å^3$	
Z:	2	
Density (calculated):	1.153 g/cm^3	
Absorption coefficient:	1.3 cm^{-1}	
Crystal color:	colorless, transparent	
Crystal size:	0.05 x 0.40 x 0.80 mm	
Scan range:	sphere	
(2 Θ)max:	61 deg.	
Resolution:	0.70 Å	
Reflections collected:	28509	
Independent reflections:	9274	
Reflections used with I > 0:	9058	
Number of variables:	637	
R (F):	0.054	
wR (F):	0.046	
S:	1.17	

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

Starred atoms were refined isotropically. Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as:

$(4/3) \cdot [a^2 \cdot B(1,1) + b^2 \cdot B(2,2) + c^2 \cdot B(3,3) + a \cdot b \cdot (\cos \gamma) \cdot B(1,2) + a \cdot c \cdot (\cos \beta) \cdot B(1,3) + b \cdot c \cdot (\cos \alpha) \cdot B(2,3)]$

	X		Y		Z		U (eq)	
Si1	0.18399	(8)	0.61857	(0)	0.09859	(2)	1.604	(9)
Si2	0.56322	(8)	1.01012	(5)	0.21917	(2)	1.601	(9)
O1	0.4812	(2)	0.2696	(1)	0.42297	(6)	1.77	(2)
O2	-0.1106	(2)	0.4127	(1)	0.38285	(6)	1.90	(3)
O3	0.4117	(2)	0.4841	(1)	0.38207	(5)	1.66	(2)
O4	0.2989	(2)	0.5950	(1)	0.16423	(5)	1.86	(3)
O5	0.4193	(2)	0.9003	(1)	0.21774	(6)	2.13	(3)
N1	0.3225	(2)	0.2238	(1)	0.50376	(6)	1.48	(3)
N2	0.1366	(2)	0.3193	(1)	0.43666	(6)	1.26	(3)
C1	0.3309	(3)	0.2692	(1)	0.45128	(8)	1.37	(3)
C2	0.1090	(3)	0.2157	(2)	0.51960	(8)	1.60	(3)
C3	0.0030	(3)	0.3107	(2)	0.48504	(7)	1.41	(3)
C4	0.0570	(3)	0.3675	(1)	0.38478	(8)	1.32	(3)
C5	0.1783	(3)	0.3569	(1)	0.33193	(7)	1.28	(3)
C6	0.3087	(3)	0.4594	(1)	0.32588	(7)	1.19	(3)
C7	0.4723	(3)	0.4524	(2)	0.28249	(8)	1.42	(3)
C8	0.5578	(3)	0.5675	(2)	0.28238	(8)	1.42	(3)
C9	0.6258	(3)	0.6100	(2)	0.22481	(8)	1.91	(4)
C10	0.4369	(3)	0.6701	(2)	0.19565	(8)	1.68	(4)
C11	0.3321	(3)	0.7199	(2)	0.24580	(8)	1.50	(3)
C12	0.3698	(3)	0.6393	(1)	0.29644	(7)	1.38	(3)
C13	0.1919	(3)	0.5607	(2)	0.30581	(8)	1.38	(3)
C14	0.4853	(3)	0.1509	(2)	0.52787	(8)	1.92	(4)
C15	0.0986	(3)	0.2159	(2)	0.58475	(8)	2.24	(4)
C16	-0.0024	(3)	0.4090	(2)	0.52243	(8)	1.50	(3)
C17	-0.1807	(3)	0.4291	(2)	0.54959	(9)	2.13	(4)
C18	-0.1816	(4)	0.5068	(2)	0.59213	(9)	2.90	(4)
C19	-0.0036	(4)	0.5660	(2)	0.60782	(9)	2.89	(5)
C20	0.1743	(4)	0.5489	(2)	0.57992	(9)	2.37	(4)
C21	0.1751	(3)	0.4707	(2)	0.53725	(8)	1.79	(4)
C22	0.0278	(3)	0.3309	(2)	0.27828	(8)	1.69	(4)
C23	-0.0236	(4)	0.7211	(2)	0.1019	(1)	2.86	(5)
C24	0.3755	(3)	0.6702	(2)	0.05003	(9)	2.50	(4)
C25	0.0780	(3)	0.4843	(2)	0.07228	(8)	2.11	(4)
C26	-0.0771	(4)	0.4430	(2)	0.1128	(1)	3.70	(5)
C27	0.2586	(4)	0.4054	(2)	0.0703	(1)	3.58	(5)
C28	-0.0366	(4)	0.4962	(2)	0.01145	(9)	3.00	(5)

C29	0.4301	(3)	0.8264	(2)	0.26464	(8)	2.12 (4)
C30	0.4836	(4)	1.1030	(2)	0.27555	(9)	2.59 (4)
C31	0.8444	(4)	0.9759	(2)	0.2356	(1)	2.95 (5)
C32	0.5063	(3)	1.0696	(2)	0.14482	(8)	1.90 (4)
C33	0.6395	(4)	1.1702	(2)	0.1392	(1)	3.06 (5)
C34	0.2748	(4)	1.0998	(2)	0.1344	(1)	2.83 (5)
C35	0.5568	(4)	0.9879	(2)	0.0990	(1)	3.35 (5)

Table 3a: Bond lengths [Å].

Numbers in parentheses are estimated standard deviations in the least significant digits.

Si1-O4	1.652	(1)	C5-C22	1.534	(2)
Si1-C23	1.858	(2)	C6-C7	1.529	(3)
Si1-C24	1.866	(2)	C6-C13	1.523	(3)
Si1-C25	1.891	(2)	C7-C8	1.541	(3)
Si2-O5	1.655	(2)	C8-C9	1.541	(3)
Si2-C30	1.859	(2)	C8-C12	1.567	(3)
Si2-C31	1.860	(2)	C9-C10	1.528	(3)
Si2-C32	1.881	(2)	C10-C11	1.534	(3)
O1-C1	1.222	(2)	C11-C12	1.549	(3)
O2-C4	1.214	(2)	C11-C29	1.520	(3)
O3-C6	1.436	(2)	C12-C13	1.540	(3)
O4-C10	1.439	(2)	C16-C17	1.385	(3)
O5-C29	1.424	(2)	C16-C21	1.393	(3)
N1-C1	1.349	(2)	C17-C18	1.385	(3)
N1-C2	1.460	(3)	C18-C19	1.381	(3)
N1-C14	1.458	(2)	C19-C20	1.386	(3)
N2-C1	1.409	(2)	C20-C21	1.392	(3)
N2-C3	1.484	(2)	C25-C26	1.527	(3)
N2-C4	1.397	(2)	C25-C27	1.528	(3)
C2-C3	1.552	(3)	C25-C28	1.533	(3)
C2-C15	1.520	(3)	C32-C33	1.535	(3)
C3-C16	1.508	(3)	C32-C34	1.532	(3)
C4-C5	1.523	(3)	C32-C35	1.532	(3)
C5-C6	1.546	(3)			

Table 3b: Bond angles [deg].

O4-Si1-C23	109.98	(9)
O4-Si1-C24	110.93	(8)
O4-Si1-C25	104.65	(8)
C23-Si1-C24	107.8	(1)
C23-Si1-C25	112.9	(1)
C24-Si1-C25	110.6	(1)
O5-Si2-C30	109.88	(9)
O5-Si2-C31	110.1	(1)
O5-Si2-C32	104.63	(8)
C30-Si2-C31	109.3	(1)
C30-Si2-C32	110.9	(1)
C31-Si2-C32	112.0	(1)
Si1-O4-C10	123.2	(1)
Si2-O5-C29	122.6	(1)
C1-N1-C2	112.3	(1)
C1-N1-C14	121.2	(2)
C2-N1-C14	121.2	(2)
C1-N2-C3	110.6	(1)
C1-N2-C4	129.8	(2)
C3-N2-C4	119.5	(1)
O1-C1-N1	126.3	(2)
O1-C1-N2	126.8	(2)
N1-C1-N2	106.9	(2)
N1-C2-C3	101.1	(1)
N1-C2-C15	112.7	(2)
C3-C2-C15	116.9	(2)
N2-C3-C2	100.9	(1)
N2-C3-C16	115.1	(2)
C2-C3-C16	111.2	(1)
O2-C4-N2	118.7	(2)
O2-C4-C5	122.4	(2)
N2-C4-C5	118.9	(2)
C4-C5-C6	109.1	(1)
C4-C5-C22	109.8	(1)
C6-C5-C22	114.0	(1)
O3-C6-C5	107.5	(1)
O3-C6-C7	109.0	(1)
O3-C6-C13	105.5	(1)
C5-C6-C7	115.3	(1)
C5-C6-C13	117.6	(1)
C7-C6-C13	101.3	(1)
C6-C7-C8	102.5	(1)
C7-C8-C9	117.1	(2)
C7-C8-C12	104.6	(1)
C9-C8-C12	105.9	(1)
C8-C9-C10	105.7	(2)
O4-C10-C9	109.1	(2)
O4-C10-C11	110.7	(2)
C9-C10-C11	104.7	(1)
C10-C11-C12	105.3	(2)
C10-C11-C29	111.9	(2)
C12-C11-C29	108.9	(1)
C8-C12-C11	106.3	(1)
C8-C12-C13	105.2	(1)
C11-C12-C13	117.4	(1)
C6-C13-C12	103.0	(1)
C3-C16-C17	118.5	(2)
C3-C16-C21	122.0	(2)
C17-C16-C21	118.8	(2)
C16-C17-C18	120.9	(2)
C17-C18-C19	120.1	(2)
C18-C19-C20	119.7	(2)
C19-C20-C21	120.2	(2)
C16-C21-C20	120.3	(2)
Si1-C25-C26	109.8	(1)
Si1-C25-C27	109.5	(1)
Si1-C25-C28	109.6	(2)
C26-C25-C27	110.2	(2)
C26-C25-C28	108.4	(2)
C27-C25-C28	109.4	(2)
O5-C29-C11	111.2	(1)
Si2-C32-C33	110.1	(1)
Si2-C32-C34	109.9	(1)
Si2-C32-C35	109.7	(1)
C33-C32-C34	109.0	(2)
C33-C32-C35	109.2	(2)
C34-C32-C35	109.0	(2)

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

The form of the anisotropic displacement parameter is:

$\exp [-2\pi^2 \cdot (h^2 \cdot a^2 \cdot U_{11} + k^2 \cdot b^2 \cdot U_{22} + l^2 \cdot c^2 \cdot U_{33} + 2 \cdot h \cdot k \cdot a \cdot b \cdot U_{12} + 2 \cdot h \cdot l \cdot a \cdot c \cdot U_{13} + 2 \cdot k \cdot l \cdot b \cdot c \cdot U_{23})]$ where a, b, and c are reciprocal lattice constants.

	U11	U22	U33	U23	U13	U12
Si1	0.0250 (2)	0.0223 (2)	0.0134 (2)	0.0017 (2)	0.0009 (2)	0.0012 (2)
Si2	0.0252 (2)	0.0173 (2)	0.0185 (2)	-0.0030 (2)	0.0024 (2)	0.0019 (2)
O1	0.0195 (6)	0.0272 (7)	0.0206 (6)	0.0039 (6)	0.0034 (5)	0.0058 (6)
O2	0.0211 (6)	0.0303 (7)	0.0208 (6)	0.0058 (6)	0.0022 (5)	0.0077 (6)
O3	0.0301 (7)	0.0187 (6)	0.0128 (5)	-0.0040 (6)	-0.0040 (5)	0.0009 (5)
O4	0.0339 (7)	0.0202 (7)	0.0151 (6)	-0.0047 (6)	-0.0037 (5)	0.0007 (5)
O5	0.0373 (8)	0.0199 (7)	0.0227 (6)	-0.0076 (6)	-0.0020 (6)	0.0074 (6)
N1	0.0210 (7)	0.0171 (7)	0.0181 (7)	0.0040 (6)	0.0011 (6)	0.0048 (6)
N2	0.0167 (7)	0.0173 (7)	0.0141 (6)	0.0015 (6)	0.0027 (6)	0.0021 (6)
C1	0.0202 (8)	0.0118 (8)	0.0188 (8)	-0.0019 (7)	-0.0042 (7)	0.0010 (7)
C2	0.0234 (9)	0.0185 (9)	0.0186 (8)	-0.0040 (8)	0.0011 (7)	0.0040 (8)
C3	0.0175 (8)	0.0228 (9)	0.0134 (7)	-0.0018 (7)	0.0024 (7)	0.0052 (8)
C4	0.0195 (8)	0.0136 (8)	0.0166 (8)	-0.0026 (7)	-0.0005 (7)	0.0017 (7)
C5	0.0174 (8)	0.0154 (8)	0.0152 (8)	0.0021 (7)	-0.0012 (7)	0.0015 (7)
C6	0.0202 (8)	0.0135 (8)	0.0112 (7)	-0.0000 (7)	-0.0001 (7)	0.0005 (7)
C7	0.0156 (8)	0.0203 (9)	0.0173 (8)	0.0026 (7)	-0.0011 (7)	-0.0004 (7)
C8	0.0153 (8)	0.0220 (9)	0.0161 (8)	-0.0030 (8)	-0.0012 (7)	0.0013 (8)
C9	0.0219 (8)	0.029 (1)	0.0224 (8)	-0.0027 (9)	0.0052 (7)	0.0038 (9)
C10	0.0253 (9)	0.0194 (9)	0.0187 (9)	-0.0061 (8)	0.0002 (7)	0.0032 (8)
C11	0.0237 (9)	0.0186 (8)	0.0143 (8)	-0.0027 (8)	0.0004 (7)	0.0020 (7)
C12	0.0243 (9)	0.0153 (9)	0.0124 (7)	-0.0018 (7)	0.0005 (7)	0.0002 (7)
C13	0.0204 (8)	0.0144 (8)	0.0183 (8)	0.0028 (7)	0.0052 (7)	0.0005 (7)
C14	0.029 (1)	0.022 (1)	0.0208 (9)	0.0054 (8)	-0.0031 (8)	0.0071 (8)
C15	0.036 (1)	0.030 (1)	0.0194 (9)	0.0039 (9)	0.0059 (8)	0.0095 (9)
C16	0.0225 (9)	0.0180 (8)	0.0158 (8)	0.0032 (8)	-0.0008 (7)	0.0065 (7)
C17	0.026 (1)	0.031 (1)	0.0245 (9)	0.0045 (9)	0.0065 (8)	0.0071 (9)
C18	0.046 (1)	0.038 (1)	0.0280 (9)	0.018 (1)	0.0161 (9)	0.007 (1)
C19	0.067 (1)	0.024 (1)	0.0190 (9)	0.013 (1)	0.004 (1)	0.0005 (9)
C20	0.041 (1)	0.023 (1)	0.0236 (9)	0.0006 (9)	-0.0067 (9)	0.0003 (8)
C21	0.0241 (9)	0.0203 (9)	0.0232 (9)	0.0029 (8)	0.0004 (8)	0.0026 (8)
C22	0.0250 (9)	0.0231 (9)	0.0154 (8)	-0.0047 (8)	-0.0008 (7)	0.0007 (8)
C23	0.040 (1)	0.033 (1)	0.035 (1)	0.008 (1)	0.003 (1)	0.001 (1)
C24	0.035 (1)	0.040 (1)	0.0199 (9)	-0.005 (1)	0.0039 (9)	-0.0001 (9)
C25	0.032 (1)	0.027 (1)	0.0202 (9)	-0.0020 (9)	-0.0022 (8)	-0.0027 (8)
C26	0.064 (2)	0.046 (1)	0.032 (1)	-0.026 (1)	0.008 (1)	-0.004 (1)
C27	0.053 (1)	0.030 (1)	0.050 (1)	0.006 (1)	-0.006 (1)	-0.009 (1)
C28	0.038 (1)	0.052 (1)	0.0222 (9)	-0.003 (1)	-0.0065 (9)	-0.010 (1)
C29	0.042 (1)	0.0196 (9)	0.0182 (9)	-0.0078 (9)	0.0005 (9)	0.0029 (8)

C30	0.043 (1)	0.032 (1)	0.0244 (9)	-0.004 (1)	0.0075 (9)	-0.0056 (9)
C31	0.030 (1)	0.046 (1)	0.036 (1)	0.004 (1)	0.002 (1)	0.006 (1)
C32	0.033 (1)	0.0211 (9)	0.0186 (8)	-0.0027 (9)	0.0048 (8)	0.0035 (8)
C33	0.046 (1)	0.035 (1)	0.035 (1)	-0.012 (1)	0.002 (1)	0.017 (1)
C34	0.036 (1)	0.040 (1)	0.031 (1)	-0.000 (1)	-0.0036 (9)	0.007 (1)
C35	0.063 (1)	0.040 (1)	0.026 (1)	0.006 (1)	0.010 (1)	0.003 (1)

Table 5: Hydrogen coordinates ($\cdot 10^4$) and isotropic displacement parameters ($Å^2 \cdot 10^3$).
Starred atoms were refined isotropically. Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as:

$(4/3) \cdot [a^2 \cdot B(1,1) + b^2 \cdot B(2,2) + c^2 \cdot B(3,3) + a \cdot b \cdot (\cos \gamma) \cdot B(1,2) + a \cdot c \cdot (\cos \beta) \cdot B(1,3) + b \cdot c \cdot (\cos \alpha) \cdot B(2,3)]$

	X		Y		Z		U	
H2	0.049	(3)	0.153	(1)	0.5041	(8)	1.3	(4)*
H3	-0.133	(3)	0.294	(2)	0.4685	(8)	1.1	(4)*
H03	0.500	(4)	0.444	(2)	0.390	(1)	3.6	(6)*
H5	0.274	(3)	0.301	(1)	0.3378	(7)	0.8	(4)*
H7A	0.576	(3)	0.402	(2)	0.2951	(9)	1.8	(4)*
H7B	0.403	(3)	0.436	(2)	0.2445	(8)	1.4	(4)*
H8	0.672	(3)	0.574	(1)	0.3130	(8)	0.7	(4)*
H9A	0.737	(3)	0.658	(2)	0.2336	(9)	2.0	(4)*
H9B	0.670	(3)	0.555	(2)	0.2004	(9)	1.9	(4)*
H10	0.481	(3)	0.725	(2)	0.1715	(7)	0.8	(3)*
H11	0.189	(3)	0.732	(2)	0.2364	(8)	1.1	(4)*
H12	0.397	(3)	0.677	(2)	0.3320	(8)	1.7	(4)*
H13B	0.107	(3)	0.585	(2)	0.3327	(8)	1.6	(4)*
H13A	0.112	(3)	0.545	(1)	0.2680	(8)	1.2	(4)*
H14A	0.609	(3)	0.158	(2)	0.5069	(9)	2.3	(5)*
H14C	0.513	(3)	0.163	(2)	0.5676	(9)	2.4	(5)*
H14B	0.434	(3)	0.075	(2)	0.5249	(9)	2.2	(5)*
H15A	0.157	(3)	0.152	(2)	0.602	(1)	3.2	(5)*
H15C	0.167	(3)	0.277	(2)	0.6033	(9)	2.2	(5)*
H15B	-0.053	(3)	0.218	(2)	0.5917	(9)	2.8	(5)*
H17	-0.299	(3)	0.387	(2)	0.5389	(9)	2.2	(5)*
H18	-0.292	(4)	0.520	(2)	0.610	(1)	4.0	(6)*
H19	-0.003	(3)	0.615	(2)	0.6389	(9)	3.0	(5)*
H20	0.285	(3)	0.592	(2)	0.5877	(9)	2.4	(5)*
H21	0.293	(3)	0.457	(2)	0.5186	(9)	2.1	(4)*
H22B	0.103	(3)	0.323	(2)	0.2482	(8)	2.2	(4)*
H22A	-0.046	(3)	0.262	(2)	0.2850	(9)	2.6	(5)*
H22C	-0.078	(3)	0.385	(2)	0.2705	(9)	2.3	(5)*
H23B	0.036	(4)	0.779	(2)	0.118	(1)	3.8	(6)*
H23A	-0.102	(4)	0.730	(2)	0.063	(1)	5.3	(7)*
H23C	-0.134	(4)	0.692	(2)	0.124	(1)	5.5	(7)*
H24A	0.431	(4)	0.741	(2)	0.062	(1)	5.3	(7)*
H24B	0.315	(4)	0.673	(2)	0.011	(1)	3.6	(6)*
H24C	0.494	(4)	0.620	(2)	0.047	(1)	4.5	(6)*
H26A	-0.007	(4)	0.433	(2)	0.153	(1)	4.1	(6)*
H26C	-0.209	(4)	0.499	(3)	0.112	(1)	6.4	(8)*
H26B	-0.109	(4)	0.373	(2)	0.102	(1)	5.3	(7)*

H27A	0.335	(4)	0.393	(2)	0.109	(1)	4.4 (6)*
H27C	0.205	(4)	0.331	(2)	0.057	(1)	4.7 (6)*
H27B	0.350	(5)	0.428	(3)	0.044	(1)	7.0 (9)*
H28B	-0.089	(4)	0.425	(2)	-0.005	(1)	5.3 (7)*
H28C	0.065	(4)	0.512	(2)	-0.018	(1)	5.1 (7)*
H28A	-0.160	(3)	0.547	(2)	0.010	(1)	3.8 (6)*
H29B	0.582	(3)	0.814	(2)	0.280	(1)	3.4 (5)*
H29A	0.347	(3)	0.852	(2)	0.296	(1)	3.2 (5)*
H30B	0.546	(4)	1.171	(2)	0.275	(1)	5.8 (8)*
H30A	0.510	(4)	1.068	(2)	0.313	(1)	5.7 (7)*
H30C	0.339	(3)	1.118	(2)	0.271	(1)	4.0 (6)*
H31C	0.936	(4)	1.033	(2)	0.228	(1)	5.5 (7)*
H31A	0.873	(4)	0.947	(2)	0.272	(1)	3.7 (6)*
H31B	0.890	(4)	0.928	(2)	0.207	(1)	4.1 (6)*
H33B	0.794	(3)	1.151	(2)	0.143	(1)	3.6 (6)*
H33C	0.612	(3)	1.225	(2)	0.1667	(9)	3.0 (5)*
H33A	0.608	(3)	1.203	(2)	0.1019	(9)	3.0 (5)*
H34C	0.242	(4)	1.158	(2)	0.162	(1)	4.5 (6)*
H34B	0.191	(4)	1.034	(2)	0.138	(1)	4.0 (6)*
H34A	0.240	(4)	1.131	(2)	0.096	(1)	5.5 (7)*
H35C	0.695	(4)	0.967	(2)	0.104	(1)	3.8 (6)*
H35B	0.480	(4)	0.925	(2)	0.103	(1)	4.8 (7)*
H35A	0.530	(4)	1.020	(2)	0.059	(1)	4.9 (7)*

Table 6: Torsion angles [deg].

C23-Si1-O4-C10	-71.54	(0.16)
C24-Si1-O4-C10	47.66	(0.16)
C25-Si1-O4-C10	166.91	(0.14)
O4-Si1-C25-C26	60.10	(0.16)
O4-Si1-C25-C27	-60.98	(0.16)
O4-Si1-C25-C28	179.08	(0.14)
C23-Si1-C25-C26	-59.50	(0.18)
C23-Si1-C25-C27	179.42	(0.15)
C23-Si1-C25-C28	59.48	(0.17)
C24-Si1-C25-C26	179.59	(0.15)
C24-Si1-C25-C27	58.52	(0.17)
C24-Si1-C25-C28	-61.42	(0.17)
C30-Si2-O5-C29	-66.19	(0.17)
C31-Si2-O5-C29	54.20	(0.17)
C32-Si2-O5-C29	174.73	(0.15)
O5-Si2-C32-C33	-177.20	(0.14)
O5-Si2-C32-C34	62.76	(0.16)
O5-Si2-C32-C35	-57.00	(0.17)
C30-Si2-C32-C33	64.39	(0.17)
C30-Si2-C32-C34	-55.65	(0.17)
C30-Si2-C32-C35	-175.41	(0.15)
C31-Si2-C32-C33	-57.98	(0.18)
C31-Si2-C32-C34	-178.02	(0.15)
C31-Si2-C32-C35	62.22	(0.18)
Si1-O4-C10-C9	-137.16	(0.13)
Si1-O4-C10-C11	108.13	(0.15)
Si2-O5-C29-C11	-163.72	(0.13)
C2-N1-C1-O1	-166.65	(0.18)
C2-N1-C1-N2	15.69	(0.20)
C14-N1-C1-O1	-12.21	(0.29)
C14-N1-C1-N2	170.13	(0.16)
C1-N1-C2-C3	-27.40	(0.19)
C1-N1-C2-C15	-152.95	(0.17)
C14-N1-C2-C3	178.15	(0.15)
C14-N1-C2-C15	52.60	(0.23)
C3-N2-C1-O1	-173.68	(0.18)
C3-N2-C1-N1-	3.97	(0.20)
C4-N2-C1-O1-	9.91	(0.31)
C4-N2-C1-N1	-172.44	(0.17)
C1-N2-C3-C2	-19.82	(0.18)
C1-N2-C3-C16	99.95	(0.18)
C4-N2-C3-C2	157.01	(0.15)
C4-N2-C3-C16	-83.22	(0.20)
C1-N2-C4-O2	-175.06	(0.17)

C1-N2-C4-C5-	7.85	(0.27)
C3-N2-C4-O2-	8.80	(0.25)
C3-N2-C4-C5	-168.29	(0.16)
N1-C2-C3-N2	26.57	(0.16)
N1-C2-C3-C16	-95.95	(0.17)
C15-C2-C3-N2	149.27	(0.16)
C15-C2-C3-C16	26.75	(0.23)
N2-C3-C16-C17	151.03	(0.17)
N2-C3-C16-C21	-38.64	(0.24)
C2-C3-C16-C17	-95.05	(0.20)
C2-C3-C16-C21	75.28	(0.22)
O2-C4-C5-C6	84.48	(0.21)
O2-C4-C5-C22	-41.12	(0.24)
N2-C4-C5-C6	-98.53	(0.18)
N2-C4-C5-C22	135.87	(0.17)
C4-C5-C6-O3	46.42	(0.18)
C4-C5-C6-C7	168.19	(0.15)
C4-C5-C6-C13	-72.34	(0.19)
C22-C5-C6-O3	169.58	(0.14)
C22-C5-C6-C7	-68.65	(0.20)
C22-C5-C6-C13	50.82	(0.21)
O3-C6-C7-C8	-64.15	(0.17)
C5-C6-C7-C8	174.83	(0.14)
C13-C6-C7-C8	46.76	(0.16)
O3-C6-C13-C12	68.04	(0.16)
C5-C6-C13-C12	-172.12	(0.14)
C7-C6-C13-C12	-45.49	(0.16)
C6-C7-C8-C9	-146.64	(0.15)
C6-C7-C8-C12	-29.74	(0.17)
C7-C8-C9-C10	94.58	(0.19)
C12-C8-C9-C10	-21.61	(0.19)
C7-C8-C12-C11	-123.26	(0.15)
C7-C8-C12-C13	1.96	(0.17)
C9-C8-C12-C11	1.11	(0.19)
C9-C8-C12-C13	126.32	(0.15)
C8-C9-C10-O4	-84.41	(0.18)
C8-C9-C10-C11	34.13	(0.20)
O4-C10-C11-C12	84.18	(0.17)
O4-C10-C11-C29	-157.67	(0.15)
C9-C10-C11-C12	-33.23	(0.19)
C9-C10-C11-C29	84.92	(0.19)
C10-C11-C12-C8	19.67	(0.18)
C10-C11-C12-C13	-97.69	(0.18)
C29-C11-C12-C8	-100.51	(0.17)
C29-C11-C12-C13	142.13	(0.16)
C10-C11-C29-O5	57.87	(0.21)
C12-C11-C29-O5	173.87	(0.15)

C8-C12-C13-C6	26.71	(0.17)
C11-C12-C13-C6	144.66	(0.15)
C3-C16-C17-C18	168.54	(0.19)
C21-C16-C17-C18	-2.09	(0.30)
C3-C16-C21-C20	-168.32	(0.18)
C17-C16-C21-C20	1.98	(0.29)
C16-C17-C18-C19	0.42	(0.33)
C17-C18-C19-C20	1.39	(0.34)
C18-C19-C20-C21	-1.49	(0.33)
C19-C20-C21-C16	-0.21	(0.31)

1.6. Olefin (E)-17

Table 1: Crystal data and structure refinement.

Empirical formula:	$C_{11}\ H_{18}\ O_2$	
Formula weight:	182.26	
Temperature:	-140 °C	
Radiation:	Mo-K_α	
Crystal system:	orthorhombic	
Space group:	P212121	
Unit cell dimensions:	a = 6.3068(9) Å	α = 90 deg.
	b = 8.429(2) Å	β = 90 deg.
	c = 19.409(3) Å	γ = 90 deg.
Volume:	1031.8(3) $Å^3$	
Z:	4	
Density (calculated):	1.173 g/cm^3	
Absorption coefficient:	0.74 cm^{-1}	
Crystal color:	colorless, transparent	
Crystal size:	0.18 x 0.30 x 1.00 mm	
Scan range:	sphere	
(2 Θ)max:	63 deg.	
Resolution:	0.68 Å	
Reflections collected:	16002	
Independent reflections:	1825	
Reflections used with I > 0:	1809	
Number of variables:	191	
R (F):	0.036	
wR (F):	0.041	
S:	1.50	

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

Starred atoms were refined isotropically. Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as:

$(4/3) \cdot [a^2 \cdot B(1,1) + b^2 \cdot B(2,2) + c^2 \cdot B(3,3) + a \cdot b \cdot (\cos \gamma) \cdot B(1,2) + a \cdot c \cdot (\cos \beta) \cdot B(1,3) + b \cdot c \cdot (\cos \alpha) \cdot B(2,3)]$

	X		Y		Z		U (eq)	
O1	0.8812	(1)	0.0796	(1)	0.02427	(5)	1.96	(2)
O2	0.2954	(2)	0.1406	(1)	0.03779	(5)	2.23	(2)
C1	0.4700	(2)	-0.1107	(1)	0.13309	(6)	1.39	(2)
C2	0.4031	(2)	-0.2867	(1)	0.13824	(6)	1.67	(2)
C3	0.5936	(2)	-0.3684	(1)	0.16905	(6)	1.52	(2)
C4	0.6926	(2)	-0.2527	(1)	0.21895	(6)	1.72	(2)
C5	0.6590	(2)	-0.0892	(1)	0.18488	(6)	1.47	(2)
C6	0.8458	(2)	-0.0328	(1)	0.14023	(6)	1.61	(2)
C7	0.7380	(2)	0.0507	(1)	0.08030	(6)	1.42	(2)
C8	0.5590	(2)	-0.0633	(1)	0.06212	(6)	1.38	(2)
C9	0.3983	(2)	0.0014	(2)	0.01152	(6)	1.93	(2)
C10	0.6632	(2)	-0.5125	(1)	0.15224	(6)	1.82	(2)
C11	0.8519	(2)	-0.5945	(2)	0.18292	(7)	2.40	(2)

Table 3a: Bond lengths [Å].

Numbers in parentheses are estimated standard deviations in the least significant digits.

O1-C7	1.435	(1)	C3-C10	1.332	(2)
O2-C9	1.435	(2)	C4-C5	1.543	(2)
C1-C2	1.545	(2)	C5-C6	1.537	(2)
C1-C5	1.570	(2)	C6-C7	1.520	(2)
C1-C8	1.540	(2)	C7-C8	1.524	(2)
C2-C3	1.509	(2)	C8-C9	1.513	(2)
C3-C4	1.510	(2)	C10-C11	1.500	(2)

Table 3b: Bond angles [deg].

C2-C1-C5	106.07	(9)	C4-C5-C6	114.4	(1)
C2-C1-C8	114.00	(9)	C5-C6-C7	103.41	(9)
C5-C1-C8	105.41	(9)	O1-C7-C6	112.2	(1)
C1-C2-C3	104.3	(1)	O1-C7-C8	113.47	(9)
C2-C3-C4	106.8	(1)	C6-C7-C8	102.50	(9)
C2-C3-C10	125.6	(1)	C1-C8-C7	103.11	(9)
C4-C3-C10	127.6	(1)	C1-C8-C9	115.5	(1)
C3-C4-C5	104.19	(9)	C7-C8-C9	114.8	(1)
C1-C5-C4	106.00	(9)	O2-C9-C8	111.5	(1)
C1-C5-C6	104.87	(9)	C3-C10-C11	125.8	(1)

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

The form of the anisotropic displacement parameter is:

$\exp [-2\pi^2 \cdot (h^2 \cdot a^2 \cdot U_{11} + k^2 \cdot b^2 \cdot U_{22} + l^2 \cdot c^2 \cdot U_{33} + 2 \cdot h \cdot k \cdot a \cdot b \cdot U_{12} + 2 \cdot h \cdot l \cdot a \cdot c \cdot U_{13} + 2 \cdot k \cdot l \cdot b \cdot c \cdot U_{23})]$ where a, b, and c are reciprocal lattice constants.

	U11	U22	U33	U23	U13	U12
O1	0.0154 (4)	0.0268 (4)	0.0325 (4)	0.0022 (4)	0.0044 (4)	0.0117 (4)
O2	0.0150 (4)	0.0276 (4)	0.0423 (5)	0.0011 (4)	-0.0027 (4)	0.0146 (4)
C1	0.0137 (5)	0.0179 (4)	0.0213 (5)	0.0017 (4)	0.0005 (5)	0.0024 (4)
C2	0.0179 (6)	0.0206 (5)	0.0251 (5)	-0.0032 (5)	-0.0012 (5)	0.0057 (4)
C3	0.0211 (5)	0.0199 (5)	0.0166 (5)	-0.0027 (5)	0.0005 (5)	0.0041 (4)
C4	0.0273 (6)	0.0195 (5)	0.0185 (5)	-0.0001 (5)	-0.0036 (5)	0.0026 (4)
C5	0.0208 (6)	0.0167 (4)	0.0183 (5)	0.0009 (5)	-0.0011 (5)	-0.0012 (4)
C6	0.0149 (5)	0.0210 (5)	0.0252 (5)	-0.0004 (5)	-0.0047 (5)	0.0025 (5)
C7	0.0124 (5)	0.0172 (4)	0.0242 (5)	-0.0001 (4)	0.0005 (4)	0.0033 (4)
C8	0.0148 (5)	0.0180 (5)	0.0198 (5)	-0.0003 (4)	-0.0002 (4)	0.0014 (4)
C9	0.0194 (6)	0.0311 (6)	0.0230 (5)	-0.0023 (6)	-0.0043 (5)	0.0064 (5)
C10	0.0298 (7)	0.0208 (5)	0.0187 (5)	-0.0007 (5)	-0.0029 (5)	0.0017 (4)
C11	0.0388 (8)	0.0251 (5)	0.0272 (6)	0.0088 (6)	-0.0050 (6)	0.0008 (5)

Table 5: Hydrogen coordinates ($\cdot 10^4$) and isotropic displacement parameters ($Å^2 \cdot 10^3$).
Starred atoms were refined isotropically. Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as:

$(4/3) \cdot [a^2 \cdot B(1,1) + b^2 \cdot B(2,2) + c^2 \cdot B(3,3) + a \cdot b \cdot (\cos \gamma) \cdot B(1,2) + a \cdot c \cdot (\cos \beta) \cdot B(1,3) + b \cdot c \cdot (\cos \alpha) \cdot B(2,3)]$

	X		Y		Z		U	
H1	0.352	(2)	-0.050	(2)	0.1440	(7)	1.6	(3)*
H01	0.845	(2)	0.165	(2)	0.0047	(8)	2.8	(3)*
H2B	0.361	(2)	-0.331	(2)	0.0954	(6)	1.6	(3)*
H2A	0.278	(3)	-0.300	(2)	0.1680	(7)	2.7	(3)*
H02	0.167	(3)	0.114	(2)	0.0392	(8)	4.8	(5)*
H4A	0.850	(2)	-0.274	(2)	0.2304	(6)	1.9	(3)*
H4B	0.615	(2)	-0.259	(2)	0.2622	(6)	1.9	(3)*
H5	0.634	(2)	-0.005	(2)	0.2199	(6)	1.5	(3)*
H6B	0.925	(2)	-0.124	(2)	0.1220	(7)	1.9	(3)*
H6A	0.948	(2)	0.033	(2)	0.1623	(7)	2.6	(3)*
H7	0.676	(2)	0.149	(2)	0.0958	(6)	1.6	(3)*
H8	0.619	(2)	-0.163	(2)	0.0377	(7)	2.2	(3)*
H9A	0.471	(2)	0.024	(2)	-0.0311	(7)	2.3	(3)*
H9B	0.290	(3)	-0.085	(2)	-0.0008	(8)	2.4	(3)*
H10	0.579	(2)	-0.567	(2)	0.1186	(7)	2.3	(3)*
H11A	0.800	(3)	-0.691	(2)	0.2169	(7)	3.7	(4)*
H11C	0.929	(3)	-0.522	(2)	0.2167	(8)	5.0	(5)*
H11B	0.947	(3)	-0.640	(2)	0.1450	(8)	3.7	(4)*

Table 6: Torsion angles [deg].

C5-C1-C2-C3	-20.18	(0.12)
C8-C1-C2-C3	95.35	(0.11)
C2-C1-C5-C4	-0.83	(0.12)
C2-C1-C5-C6	120.49	(0.10)
C8-C1-C5-C4	-122.06	(0.10)
C8-C1-C5-C6	-0.73	(0.11)
C2-C1-C8-C7	-141.90	(0.10)
C2-C1-C8-C9	92.09	(0.12)
C5-C1-C8-C7	-25.99	(0.11)
C5-C1-C8-C9	-152.00	(0.10)
C1-C2-C3-C4	34.71	(0.12)
C1-C2-C3-C10	-142.55	(0.12)
C2-C3-C4-C5	-35.25	(0.12)
C10-C3-C4-C5	141.94	(0.13)
C2-C3-C10-C11	-179.74	(0.13)
C4-C3-C10-C11	3.57	(0.21)
C3-C4-C5-C1	21.51	(0.12)
C3-C4-C5-C6	-93.51	(0.12)
C1-C5-C6-C7	27.29	(0.11)
C4-C5-C6-C7	142.97	(0.10)
C5-C6-C7-O1	-166.14	(0.09)
C5-C6-C7-C8	-44.09	(0.11)
O1-C7-C8-C1	164.59	(0.09)
O1-C7-C8-C9	-68.97	(0.13)
C6-C7-C8-C1	43.42	(0.11)
C6-C7-C8-C9	169.85	(0.10)
C1-C8-C9-O2	59.36	(0.13)
C7-C8-C9-O2	-60.43	(0.13)

1.7. Aldoladdukt 27

Table 1: Crystal data and structure refinement.

Empirical formula:	$C_{28}\ H_{44}\ N_2\ O_4$	
Formula weight:	472.67	
Temperature:	-140 °C	
Radiation:	Mo-K_α	
Crystal system:	orthorhombic	
Space group:	P212121	
Unit cell dimensions:	a = 6.3525(5) Å	α = 90 deg.
	b = 13.562(1) Å	β = 90 deg.
	c = 31.229(3) Å	γ = 90 deg.
Volume:	2690.5(5) $Å^3$	
Z:	4	
Density (calculated):	1.167 g/cm^3	
Absorption coefficient:	0.72 cm^{-1}	
Crystal color:	colorless, transparent	
Crystal size:	0.12 x 0.44 x 1.20 mm	
Scan range:	sphere	
(2 Θ)max:	58 deg.	
Resolution:	0.73 Å	
Reflections collected:	40562	
Independent reflections:	3773	
Reflections used with I > 0:	3773	
Number of variables:	464	
R (F):	0.090	
wR (F):	0.076	
S:	1.48	

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

Starred atoms were refined isotropically. Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as:

$(4/3) \cdot [a^2 \cdot B(1,1) + b^2 \cdot B(2,2) + c^2 \cdot B(3,3) + a \cdot b \cdot (\cos \gamma) \cdot B(1,2) + a \cdot c \cdot (\cos \beta) \cdot B(1,3) + b \cdot c \cdot (\cos \alpha) \cdot B(2,3)]$

	X		Y		Z		U (eq)	
O1	-0.4870	(4)	-0.4031	(2)	-0.18570	(8)	2.49	(5)
O2	-1.0699	(4)	-0.5437	(2)	-0.16541	(7)	2.12	(5)
O3	-0.5504	(4)	-0.6221	(2)	-0.16330	(7)	2.00	(5)
O4	-1.2556	(6)	-0.1972	(2)	-0.0820	(1)	6.79	(9)
N1	-0.8433	(5)	-0.4404	(2)	-0.19758	(8)	1.73	(6)
N2	-0.6881	(5)	-0.3251	(2)	-0.23699	(9)	1.86	(6)
C1	-0.6516	(6)	-0.3898	(3)	-0.2043	(1)	1.80	(7)
C2	-0.9112	(6)	-0.3135	(2)	-0.2460	(1)	1.78	(7)
C3	-0.9982	(5)	-0.4148	(3)	-0.2309	(1)	1.66	(6)
C4	-0.5345	(7)	-0.2487	(3)	-0.2473	(1)	2.46	(8)
C5	-0.9558	(6)	-0.2848	(3)	-0.2915	(1)	2.42	(8)
C6	-1.0208	(6)	-0.4899	(2)	-0.2664	(1)	1.87	(7)
C7	-1.2083	(6)	-0.4944	(3)	-0.2887	(1)	2.15	(7)
C8	-1.2285	(6)	-0.5536	(3)	-0.3247	(1)	2.71	(8)
C9	-1.0566	(7)	-0.6082	(3)	-0.3388	(1)	2.52	(8)
C10	-0.8722	(7)	-0.6062	(3)	-0.3164	(1)	2.46	(8)
C11	-0.8498	(6)	-0.5467	(3)	-0.2800	(1)	2.21	(7)
C12	-0.9005	(6)	-0.5013	(2)	-0.1634	(1)	1.77	(6)
C13	-0.7608	(6)	-0.5042	(3)	-0.1241	(1)	1.68	(6)
C14	-0.6422	(5)	-0.6044	(2)	-0.1218	(1)	1.51	(6)
C15	-0.4687	(6)	-0.6004	(3)	-0.0877	(1)	1.80	(7)
C16	-0.3507	(6)	-0.6994	(3)	-0.0828	(1)	1.93	(7)
C17	-0.5047	(6)	-0.7853	(2)	-0.0734	(1)	1.68	(6)
C18	-0.6663	(6)	-0.7892	(2)	-0.1091	(1)	1.87	(7)
C19	-0.7868	(6)	-0.6923	(3)	-0.1126	(1)	1.82	(7)
C20	-0.3890	(6)	-0.8853	(3)	-0.0644	(1)	1.96	(7)
C21	-0.2381	(8)	-0.8738	(3)	-0.0272	(1)	3.41	(9)
C22	-0.5562	(8)	-0.9621	(3)	-0.0512	(1)	3.47	(9)
C23	-0.2716	(7)	-0.9234	(3)	-0.1034	(1)	2.73	(8)
C24	-0.8973	(6)	-0.4798	(3)	-0.0851	(1)	1.87	(7)
C25	-0.9909	(7)	-0.3750	(3)	-0.0879	(1)	2.84	(8)
C26	-1.1211	(8)	-0.3479	(3)	-0.0488	(1)	3.29	(9)
C27	-1.177	(1)	-0.2348	(5)	-0.0489	(2)	8.2	(2)
C28	-1.4673	(9)	-0.2399	(5)	-0.0890	(2)	6.8	(2)

Table 3a: Bond lengths [Å].

Numbers in parentheses are estimated standard deviations in the least significant digits.

O1-C1	1.210	(4)	C9-C10	1.365	(6)
O2-C12	1.222	(4)	C10-C11	1.401	(5)
O3-C14	1.441	(4)	C12-C13	1.515	(5)
O4-C27	1.257	(7)	C13-C14	1.554	(5)
O4-C28	1.481	(7)	C13-C24	1.532	(5)
N1-C1	1.414	(5)	C14-C15	1.533	(5)
N1-C3	1.474	(4)	C14-C19	1.532	(5)
N1-C12	1.397	(4)	C15-C16	1.546	(5)
N2-C1	1.365	(4)	C16-C17	1.549	(5)
N2-C2	1.453	(5)	C17-C18	1.518	(5)
N2-C4	1.460	(5)	C17-C20	1.569	(5)
C2-C3	1.554	(5)	C18-C19	1.525	(5)
C2-C5	1.501	(5)	C20-C21	1.513	(6)
C3-C6	1.512	(5)	C20-C22	1.543	(6)
C6-C7	1.382	(5)	C20-C23	1.519	(5)
C6-C11	1.397	(5)	C24-C25	1.543	(5)
C7-C8	1.387	(5)	C25-C26	1.521	(6)
C8-C9	1.391	(6)	C26-C27	1.575	(7)

Table 3b: Bond angles [deg].

C27-O4-C28	108.7	(5)
C1-N1-C3	110.8	(3)
C1-N1-C12	128.6	(3)
C3-N1-C12	120.3	(3)
C1-N2-C2	112.3	(3)
C1-N2-C4	120.5	(3)
C2-N2-C4	122.1	(3)
O1-C1-N1	126.9	(3)
O1-C1-N2	127.0	(3)
N1-C1-N2	106.1	(3)
N2-C2-C3	101.1	(3)
N2-C2-C5	113.3	(3)
C3-C2-C5	116.7	(3)
N1-C3-C2	100.6	(3)
N1-C3-C6	115.0	(3)
C2-C3-C6	114.1	(3)
C3-C6-C7	118.8	(3)
C3-C6-C11	121.4	(3)
C7-C6-C11	119.5	(3)
C6-C7-C8	120.9	(3)
C7-C8-C9	119.5	(4)
C8-C9-C10	120.0	(3)
C9-C10-C11	121.0	(4)
C6-C11-C10	119.0	(3)
O2-C12-N1	117.9	(3)
O2-C12-C13	123.0	(3)
N1-C12-C13	118.8	(3)

C12-C13-C14	110.1	(3)
C12-C13-C24	107.9	(3)
C14-C13-C24	115.3	(3)
O3-C14-C13	107.5	(3)
O3-C14-C15	109.8	(3)
O3-C14-C19	106.4	(3)
C13-C14-C15	110.5	(3)
C13-C14-C19	113.4	(3)
C15-C14-C19	109.1	(3)
C14-C15-C16	112.8	(3)
C15-C16-C17	111.5	(3)
C16-C17-C18	108.4	(3)
C16-C17-C20	112.9	(3)
C18-C17-C20	114.8	(3)
C17-C18-C19	111.1	(3)
C14-C19-C18	112.6	(3)
C17-C20-C21	110.2	(3)
C17-C20-C22	108.0	(3)
C17-C20-C23	112.3	(3)
C21-C20-C22	107.5	(3)
C21-C20-C23	109.8	(3)
C22-C20-C23	108.8	(3)
C13-C24-C25	111.8	(3)
C24-C25-C26	112.7	(3)
C25-C26-C27	110.9	(4)
O4-C27-C26	119.2	(5)

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

The form of the anisotropic displacement parameter is:

$\exp [-2\pi^2 \cdot (h^2 \cdot a^2 \cdot U_{11} + k^2 \cdot b^2 \cdot U_{22} + l^2 \cdot c^2 \cdot U_{33} + 2 \cdot h \cdot k \cdot a \cdot b \cdot U_{12} + 2 \cdot h \cdot l \cdot a \cdot c \cdot U_{13} + 2 \cdot k \cdot l \cdot b \cdot c \cdot U_{23})]$ where a, b, and c are reciprocal lattice constants.

	U11	U22	U33	U23	U13	U12
O1	0.026 (1)	0.028 (1)	0.041 (1)	-0.002 (1)	-0.000 (1)	0.009 (1)
O2	0.029 (1)	0.017 (1)	0.035 (1)	-0.002 (1)	0.001 (1)	0.005 (1)
O3	0.036 (1)	0.012 (1)	0.028 (1)	0.001 (1)	0.006 (1)	-0.000 (1)
O4	0.108 (3)	0.045 (2)	0.105 (2)	0.040 (2)	0.056 (2)	0.037 (2)
N1	0.026 (2)	0.017 (1)	0.023 (1)	0.002 (1)	0.004 (1)	0.001 (1)
N2	0.028 (2)	0.013 (1)	0.029 (1)	-0.001 (1)	0.003 (1)	0.004 (1)
C1	0.023 (2)	0.017 (2)	0.029 (2)	0.000 (2)	0.006 (2)	-0.001 (2)
C2	0.029 (2)	0.011 (1)	0.027 (2)	0.002 (2)	0.003 (2)	-0.001 (1)
C3	0.022 (2)	0.017 (2)	0.024 (2)	0.002 (2)	0.003 (2)	0.001 (1)
C4	0.042 (2)	0.019 (2)	0.033 (2)	-0.007 (2)	0.010 (2)	0.004 (2)
C5	0.034 (2)	0.020 (2)	0.039 (2)	-0.001 (2)	0.000 (2)	0.003 (2)
C6	0.032 (2)	0.014 (2)	0.025 (2)	0.000 (2)	0.004 (2)	0.005 (1)
C7	0.029 (2)	0.022 (2)	0.030 (2)	-0.002 (2)	0.004 (2)	0.002 (2)
C8	0.038 (2)	0.027 (2)	0.038 (2)	-0.009 (2)	-0.005 (2)	0.005 (2)
C9	0.051 (2)	0.016 (2)	0.029 (2)	-0.008 (2)	0.003 (2)	0.000 (2)
C10	0.044 (2)	0.015 (2)	0.035 (2)	-0.002 (2)	0.009 (2)	0.000 (2)
C11	0.033 (2)	0.017 (2)	0.034 (2)	0.000 (2)	0.001 (2)	0.004 (2)
C12	0.028 (2)	0.013 (1)	0.026 (2)	0.007 (2)	0.006 (2)	-0.001 (1)
C13	0.029 (2)	0.011 (1)	0.024 (2)	-0.002 (2)	0.000 (2)	0.000 (1)
C14	0.022 (2)	0.011 (1)	0.025 (2)	-0.001 (2)	0.003 (2)	0.000 (1)
C15	0.028 (2)	0.014 (2)	0.027 (2)	-0.001 (2)	-0.001 (2)	-0.002 (1)
C16	0.023 (2)	0.019 (2)	0.031 (2)	-0.002 (2)	0.002 (2)	-0.000 (2)
C17	0.028 (2)	0.013 (2)	0.023 (2)	-0.001 (2)	0.002 (2)	0.001 (1)
C18	0.026 (2)	0.011 (2)	0.034 (2)	-0.003 (2)	0.001 (2)	0.002 (2)
C19	0.025 (2)	0.014 (2)	0.030 (2)	-0.002 (2)	-0.008 (2)	0.002 (2)
C20	0.033 (2)	0.017 (2)	0.025 (2)	0.005 (2)	0.000 (2)	0.002 (2)
C21	0.063 (3)	0.032 (2)	0.035 (2)	0.014 (2)	-0.015 (2)	0.004 (2)
C22	0.059 (3)	0.022 (2)	0.051 (2)	0.002 (2)	0.001 (3)	0.017 (2)
C23	0.038 (2)	0.030 (2)	0.036 (2)	0.008 (2)	-0.002 (2)	-0.002 (2)
C24	0.033 (2)	0.014 (2)	0.025 (2)	0.002 (2)	0.004 (2)	0.001 (1)
C25	0.048 (2)	0.021 (2)	0.038 (2)	0.015 (2)	0.009 (2)	0.003 (2)
C26	0.057 (3)	0.025 (2)	0.042 (2)	0.017 (2)	0.010 (2)	0.000 (2)
C27	0.156 (5)	0.086 (4)	0.070 (3)	0.072 (4)	0.039 (4)	0.003 (3)
C28	0.064 (4)	0.084 (4)	0.111 (4)	-0.006 (4)	0.010 (4)	-0.004 (4)

Table 5: Hydrogen coordinates ($\cdot 10^4$) and isotropic displacement parameters ($Å^2 \cdot 10^3$).
Starred atoms were refined isotropically. Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as:

$(4/3) \cdot [a^2 \cdot B(1,1) + b^2 \cdot B(2,2) + c^2 \cdot B(3,3) + a \cdot b \cdot (\cos \gamma) \cdot B(1,2) + a \cdot c \cdot (\cos \beta) \cdot B(1,3) + b \cdot c \cdot (\cos \alpha) \cdot B(2,3)]$

	X		Y		Z		U	
H2	-0.990	(5)	-0.267	(2)	-0.2271	(9)	1.9	(7)*
H3	-1.125	(4)	-0.410	(2)	-0.2170	(7)	-1.0	(5)*
H03	-0.441	(7)	-0.584	(3)	-0.172	(1)	7	(1)*
H4B	-0.377	(5)	-0.282	(2)	-0.2360	(9)	2.2	(8)*
H4A	-0.545	(4)	-0.245	(2)	-0.2759	(7)	-0.3	(5)*
H4C	-0.586	(7)	-0.201	(3)	-0.234	(1)	6	(1)*
H5C	-1.118	(5)	-0.283	(2)	-0.2919	(9)	1.0	(6)*
H5B	-0.882	(7)	-0.216	(3)	-0.296	(1)	5	(1)*
H5A	-0.870	(6)	-0.324	(3)	-0.310	(1)	3.3	(9)*
H7	-1.323	(6)	-0.463	(3)	-0.274	(1)	4.1	(9)*
H8	-1.363	(5)	-0.553	(3)	-0.342	(1)	2.8	(8)*
H9	-1.058	(5)	-0.639	(2)	-0.3656	(9)	1.5	(7)*
H10	-0.740	(5)	-0.634	(2)	-0.3277	(9)	2.1	(8)*
H11	-0.709	(7)	-0.543	(3)	-0.264	(1)	6	(1)*
H13	-0.635	(6)	-0.445	(3)	-0.131	(1)	5	(1)*
H15A	-0.536	(4)	-0.589	(2)	-0.0584	(8)	0.4	(6)*
H15B	-0.343	(7)	-0.538	(3)	-0.095	(1)	5	(1)*
H16A	-0.221	(5)	-0.694	(2)	-0.0589	(9)	1.9	(7)*
H16B	-0.278	(4)	-0.711	(2)	-0.1084	(8)	0.6	(6)*
H17	-0.599	(5)	-0.773	(2)	-0.0475	(9)	1.3	(7)*
H18B	-0.761	(5)	-0.840	(2)	-0.102	(1)	2.2	(8)*
H18A	-0.576	(5)	-0.802	(2)	-0.1381	(9)	1.3	(7)*
H19A	-0.877	(5)	-0.690	(2)	-0.1340	(8)	0.7	(6)*
H19B	-0.884	(6)	-0.674	(3)	-0.080	(1)	4	(1)*
H21C	-0.328	(6)	-0.852	(3)	-0.001	(1)	4	(1)*
H21A	-0.096	(7)	-0.850	(3)	-0.038	(1)	5	(1)*
H21B	-0.187	(6)	-0.938	(3)	-0.018	(1)	4	(1)*
H22B	-0.662	(6)	-0.964	(3)	-0.071	(1)	3.4	(9)*
H22C	-0.643	(5)	-0.934	(2)	-0.0226	(9)	2.1	(8)*
H22A	-0.475	(7)	-1.004	(3)	-0.039	(1)	7	(1)*
H23C	-0.188	(7)	-0.984	(3)	-0.100	(1)	6	(1)*
H23B	-0.168	(7)	-0.888	(3)	-0.109	(1)	6	(1)*
H23A	-0.364	(5)	-0.927	(2)	-0.130	(1)	2.5	(8)*
H24B	-0.805	(4)	-0.488	(2)	-0.0581	(8)	-0.0	(5)*
H24A	-1.015	(5)	-0.533	(2)	-0.0813	(8)	0.9	(6)*
H25A	-1.083	(6)	-0.371	(3)	-0.116	(1)	3.5	(9)*
H25B	-0.849	(7)	-0.339	(3)	-0.087	(1)	4	(1)*

H26A	-1.250 (5)	-0.375 (2)	-0.049 (1)	2.5 (8)*
H26B	-1.049 (5)	-0.362 (2)	-0.0230 (9)	1.2 (7)*
H27A	-1.2605	-0.2206	-0.0232	8 *
H27B	-1.0329	-0.1989	-0.0431	8 *
H28B	-1.5502	-0.1995	-0.1099	8 *
H28C	-1.5503	-0.2406	-0.0619	8 *
H28A	-1.4588	-0.3067	-0.0999	8 *

Table 6: Torsion angles [deg].

C28-O4-C27-C26	66.41	(0.67)
C3-N1-C1-O1	-170.89	(0.33)
C3-N1-C1-N2	7.26	(0.36)
C12-N1-C1-O1	14.10	(0.57)
C12-N1-C1-N2	-167.75	(0.31)
C1-N1-C3-C2	-22.90	(0.33)
C1-N1-C3-C6	100.14	(0.33)
C12-N1-C3-C2	152.59	(0.28)
C12-N1-C3-C6	-84.37	(0.37)
C1-N1-C12-O2	-174.83	(0.31)
C1-N1-C12-C13	10.86	(0.50)
C3-N1-C12-O2	10.57	(0.46)
C3-N1-C12-C13	-163.74	(0.29)
C2-N2-C1-O1	-168.15	(0.33)
C2-N2-C1-N1	13.70	(0.36)
C4-N2-C1-O1	-12.71	(0.53)
C4-N2-C1-N1	169.14	(0.28)
C1-N2-C2-C3	-27.31	(0.34)
C1-N2-C2-C5	-152.90	(0.29)
C4-N2-C2-C3	177.69	(0.28)
C4-N2-C2-C5	52.10	(0.41)
N2-C2-C3-N1	28.42	(0.30)
N2-C2-C3-C6	-95.24	(0.32)
C5-C2-C3-N1	151.71	(0.30)
C5-C2-C3-C6	28.05	(0.44)
N1-C3-C6-C7	154.71	(0.31)
N1-C3-C6-C11	-32.45	(0.45)
C2-C3-C6-C7	-89.78	(0.39)
C2-C3-C6-C11	83.06	(0.40)
C3-C6-C7-C8	172.25	(0.33)
C11-C6-C7-C8	-0.72	(0.54)
C3-C6-C11-C10	-172.20	(0.32)
C7-C6-C11-C10	0.58	(0.52)
C6-C7-C8-C9	-0.78	(0.56)
C7-C8-C9-C10	2.45	(0.56)
C8-C9-C10-C11	-2.62	(0.56)
C9-C10-C11-C6	1.09	(0.54)
O2-C12-C13-C14	77.60	(0.41)
O2-C12-C13-C24	-49.02	(0.42)
N1-C12-C13-C14	-108.39	(0.33)
N1-C12-C13-C24	124.99	(0.32)
C12-C13-C14-O3	48.72	(0.35)
C12-C13-C14-C15	168.54	(0.28)
C12-C13-C14-C19	-68.60	(0.35)

C24-C13-C14-O3	171.10	(0.28)
C24-C13-C14-C15	-69.08	(0.37)
C24-C13-C14-C19	53.78	(0.39)
C12-C13-C24-C25	-62.26	(0.37)
C14-C13-C24-C25	174.20	(0.30)
O3-C14-C15-C16	-63.78	(0.34)
C13-C14-C15-C16	177.80	(0.27)
C19-C14-C15-C16	52.44	(0.36)
O3-C14-C19-C18	63.74	(0.34)
C13-C14-C19-C18	-178.27	(0.27)
C15-C14-C19-C18	-54.66	(0.36)
C14-C15-C16-C17	-55.11	(0.36)
C15-C16-C17-C18	56.62	(0.35)
C15-C16-C17-C20	-175.15	(0.26)
C16-C17-C18-C19	-58.82	(0.36)
C20-C17-C18-C19	174.03	(0.28)
C16-C17-C20-C21	57.31	(0.37)
C16-C17-C20-C22	174.52	(0.28)
C16-C17-C20-C23	-65.47	(0.37)
C18-C17-C20-C21	-177.88	(0.31)
C18-C17-C20-C22	-60.67	(0.37)
C18-C17-C20-C23	59.34	(0.41)
C17-C18-C19-C14	59.83	(0.37)
C13-C24-C25-C26	-178.10	(0.33)
C24-C25-C26-C27	169.31	(0.39)
C25-C26-C27-O4	50.08	(0.72)

1.8. Aldoladdukt 32A

Table 1: Crystal data and structure refinement.

Empirical formula:	$C_{25}\ H_{38}\ N_2\ O_3$	
Formula weight:	414.59	
Temperature:	-115 °C	
Radiation:	Mo-K_α	
Crystal system:	monoclinic	
Space group:	P21	
Unit cell dimensions:	a = 6.2585(6) Å	α = 90 deg.
	b = 10.081(1) Å	β = 90.27(1) deg.
	c = 18.789(3) Å	γ = 90 deg.
Volume:	1185.4(3) $Å^3$	
Z:	2	
Density (calculated):	1.162 g/cm^3	
Absorption coefficient:	0.71 cm^{-1}	
Crystal color:	colorless, transparent	
Crystal size:	0.03 x 0.11 x 1.40 mm	
Scan range:	sphere	
(2 Θ)max:	59 deg.	
Resolution:	0.72 Å	
Reflections collected:	15108	
Independent reflections:	3120	
Reflections used with I > 0:	3048	
Number of variables:	423	
R (F):	0.072	
wR (F):	0.045	
S:	0.87	

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

Starred atoms were refined isotropically. Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as:

$(4/3) \cdot [a^2 \cdot B(1,1) + b^2 \cdot B(2,2) + c^2 \cdot B(3,3) + a \cdot b \cdot (\cos \gamma) \cdot B(1,2) + a \cdot c \cdot (\cos \beta) \cdot B(1,3) + b \cdot c \cdot (\cos \alpha) \cdot B(2,3)]$

	X		Y		Z		U (eq)	
O1	0.5005	(3)	0.8475	(0)	0.08778	(9)	1.98	(4)
O2	-0.0714	(3)	0.8800	(2)	0.20659	(9)	2.14	(4)
O3	0.4998	(3)	0.7940	(2)	0.24842	(9)	1.66	(3)
N1	0.1560	(3)	0.7909	(2)	0.1281	(1)	1.46	(4)
N2	0.3107	(3)	0.6724	(2)	0.0423	(1)	1.96	(4)
C1	0.3417	(4)	0.7777	(3)	0.0859	(1)	1.62	(5)
C2	0.0837	(4)	0.6307	(3)	0.0396	(1)	1.98	(5)
C3	-0.0057	(4)	0.6894	(3)	0.1101	(1)	1.49	(5)
C4	0.4462	(5)	0.6568	(3)	-0.0201	(2)	2.90	(6)
C5	0.0593	(5)	0.4832	(3)	0.0287	(2)	2.79	(6)
C6	-0.0417	(4)	0.5909	(3)	0.1704	(1)	1.64	(5)
C7	-0.2424	(4)	0.5346	(3)	0.1784	(2)	2.35	(6)
C8	-0.2810	(5)	0.4473	(3)	0.2345	(2)	3.09	(7)
C9	-0.1235	(5)	0.4177	(3)	0.2827	(2)	2.99	(6)
C10	0.0770	(5)	0.4735	(3)	0.2752	(1)	2.67	(6)
C11	0.1186	(4)	0.5598	(3)	0.2193	(1)	2.03	(5)
C12	0.1088	(4)	0.8819	(3)	0.1815	(1)	1.60	(5)
C13	0.2773	(4)	0.9776	(3)	0.2095	(1)	1.53	(5)
C14	0.3971	(4)	0.9127	(3)	0.2738	(1)	1.47	(5)
C15	0.5611	(4)	1.0089	(3)	0.3050	(1)	1.49	(5)
C16	0.6891	(4)	0.9478	(3)	0.3665	(1)	1.67	(5)
C17	0.5430	(4)	0.8995	(3)	0.4268	(1)	1.60	(5)
C18	0.3759	(4)	0.8049	(3)	0.3955	(1)	1.90	(5)
C19	0.2490	(4)	0.8671	(3)	0.3339	(1)	1.69	(5)
C20	0.6677	(4)	0.8404	(3)	0.4915	(1)	1.78	(5)
C21	0.8388	(5)	0.9392	(3)	0.5172	(2)	2.70	(6)
C22	0.5119	(5)	0.8172	(3)	0.5539	(1)	2.72	(6)
C23	0.7759	(5)	0.7089	(3)	0.4732	(2)	2.53	(6)
C24	0.1704	(4)	1.1117	(3)	0.2242	(1)	1.94	(5)
C25	0.0694	(5)	1.1709	(3)	0.1570	(2)	2.77	(6)

Table 3a: Bond lengths [Å].

Numbers in parentheses are estimated standard deviations in the least significant digits.

O1-C1	1.218	(3)	C9-C10	1.383	(4)
O2-C12	1.225	(3)	C10-C11	1.389	(4)
O3-C14	1.441	(3)	C12-C13	1.521	(4)
N1-C1	1.416	(3)	C13-C14	1.563	(3)
N1-C3	1.478	(3)	C13-C24	1.535	(4)
N1-C12	1.392	(3)	C14-C15	1.527	(4)
N2-C1	1.354	(3)	C14-C19	1.534	(3)
N2-C2	1.482	(3)	C15-C16	1.532	(4)
N2-C4	1.459	(4)	C16-C17	1.539	(4)
C2-C3	1.557	(4)	C17-C18	1.531	(4)
C2-C5	1.509	(4)	C17-C20	1.560	(4)
C3-C6	1.523	(4)	C18-C19	1.534	(4)
C6-C7	1.387	(4)	C20-C21	1.538	(4)
C6-C11	1.394	(4)	C20-C22	1.546	(4)
C7-C8	1.395	(4)	C20-C23	1.529	(4)
C8-C9	1.368	(4)	C24-C25	1.529	(4)

Table 3b: Bond angles [deg].

C1-N1-C3	111.7	(2)
C1-N1-C12	130.0	(2)
C3-N1-C12	118.3	(2)
C1-N2-C2	112.2	(2)
C1-N2-C4	119.3	(2)
C2-N2-C4	120.2	(2)
O1-C1-N1	127.0	(2)
O1-C1-N2	125.8	(2)
N1-C1-N2	107.3	(2)
N2-C2-C3	102.2	(2)
N2-C2-C5	112.4	(2)
C3-C2-C5	117.0	(2)
N1-C3-C2	102.1	(2)
N1-C3-C6	112.7	(2)
C2-C3-C6	116.1	(2)
C3-C6-C7	119.0	(2)
C3-C6-C11	121.9	(2)
C7-C6-C11	119.0	(2)
C6-C7-C8	120.1	(3)
C7-C8-C9	120.7	(3)
C8-C9-C10	119.7	(3)
C9-C10-C11	120.3	(3)
C6-C11-C10	120.2	(3)
O2-C12-N1	117.8	(2)
O2-C12-C13	121.0	(2)

N1-C12-C13	121.2	(2)
C12-C13-C14	109.4	(2)
C12-C13-C24	108.6	(2)
C14-C13-C24	115.9	(2)
O3-C14-C13	107.7	(2)
O3-C14-C15	110.7	(2)
O3-C14-C19	105.5	(2)
C13-C14-C15	110.5	(2)
C13-C14-C19	113.9	(2)
C15-C14-C19	108.4	(2)
C14-C15-C16	112.5	(2)
C15-C16-C17	111.9	(2)
C16-C17-C18	108.7	(2)
C16-C17-C20	113.5	(2)
C18-C17-C20	113.6	(2)
C17-C18-C19	112.7	(2)
C14-C19-C18	111.4	(2)
C17-C20-C21	110.0	(2)
C17-C20-C22	109.5	(2)
C17-C20-C23	112.1	(2)
C21-C20-C22	107.5	(2)
C21-C20-C23	108.9	(2)
C22-C20-C23	108.8	(2)
C13-C24-C25	112.0	(2)

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

The form of the anisotropic displacement parameter is:

$\exp [-2\pi^2 \cdot (h^2 \cdot a^2 \cdot U_{11} + k^2 \cdot b^2 \cdot U_{22} + l^2 \cdot c^2 \cdot U_{33} + 2 \cdot h \cdot k \cdot a \cdot b \cdot U_{12} + 2 \cdot h \cdot l \cdot a \cdot c \cdot U_{13} + 2 \cdot k \cdot l \cdot b \cdot c \cdot U_{23})]$ where a, b, and c are reciprocal lattice constants.

	U11	U22	U33	U23	U13	U12
O1	0.0195(9)	0.029 (1)	0.0266(9)	-0.0032(9)	0.0045(8)	-0.0031(9)
O2	0.0150(8)	0.038 (1)	0.0289(9)	-0.0002(9)	0.0056(8)	-0.008 (1)
O3	0.0152(8)	0.0214(8)	0.0264(8)	0.0024(8)	0.0030(7)	-0.0051(8)
N1	0.015 (1)	0.021 (1)	0.0193(9)	-0.001 (1)	0.0008(8)	-0.001 (1)
N2	0.022 (1)	0.031 (1)	0.022 (1)	0.001 (1)	0.0069(9)	-0.006 (1)
C1	0.023 (1)	0.024 (1)	0.014 (1)	0.004 (1)	0.000 (1)	0.004 (1)
C2	0.026 (1)	0.026 (1)	0.023 (1)	-0.003 (1)	-0.003 (1)	0.002 (1)
C3	0.018 (1)	0.020 (1)	0.019 (1)	0.001 (1)	-0.003 (1)	-0.001 (1)
C4	0.036 (2)	0.046 (2)	0.029 (1)	-0.006 (2)	0.012 (1)	-0.013 (1)
C5	0.046 (2)	0.030 (1)	0.030 (1)	-0.006 (2)	0.009 (1)	-0.009 (1)
C6	0.021 (1)	0.021 (1)	0.020 (1)	-0.001 (1)	0.003 (1)	-0.002 (1)
C7	0.022 (1)	0.030 (2)	0.037 (2)	0.000 (1)	0.001 (1)	-0.000 (1)
C8	0.030 (2)	0.037 (2)	0.050 (2)	-0.004 (1)	0.016 (1)	0.006 (2)
C9	0.046 (2)	0.037 (2)	0.031 (1)	-0.002 (2)	0.012 (1)	0.010 (1)
C10	0.043 (2)	0.035 (2)	0.023 (1)	0.003 (2)	-0.000 (1)	0.003 (1)
C11	0.028 (1)	0.024 (1)	0.024 (1)	-0.002 (1)	0.001 (1)	-0.002 (1)
C12	0.021 (1)	0.023 (1)	0.017 (1)	0.003 (1)	0.001 (1)	0.002 (1)
C13	0.018 (1)	0.023 (1)	0.017 (1)	0.000 (1)	0.003 (1)	-0.002 (1)
C14	0.012 (1)	0.023 (1)	0.020 (1)	-0.000 (1)	0.002 (1)	-0.000 (1)
C15	0.018 (1)	0.021 (1)	0.018 (1)	-0.003 (1)	0.007 (1)	-0.002 (1)
C16	0.019 (1)	0.022 (1)	0.023 (1)	-0.003 (1)	0.001 (1)	0.000 (1)
C17	0.018 (1)	0.019 (1)	0.024 (1)	0.005 (1)	0.004 (1)	-0.001 (1)
C18	0.022 (1)	0.027 (1)	0.024 (1)	-0.004 (1)	0.004 (1)	0.003 (1)
C19	0.015 (1)	0.025 (1)	0.024 (1)	-0.002 (1)	0.002 (1)	-0.002 (1)
C20	0.022 (1)	0.025 (1)	0.020 (1)	0.001 (1)	-0.001 (1)	0.000 (1)
C21	0.037 (2)	0.036 (2)	0.029 (1)	-0.003 (1)	-0.012 (1)	0.003 (1)
C22	0.040 (2)	0.041 (2)	0.022 (1)	0.002 (2)	0.003 (1)	0.009 (1)
C23	0.030 (2)	0.027 (1)	0.040 (2)	0.005 (1)	-0.000 (1)	0.006 (1)
C24	0.026 (1)	0.025 (1)	0.022 (1)	0.001 (1)	-0.003 (1)	-0.003 (1)
C25	0.045 (2)	0.028 (2)	0.032 (1)	0.011 (2)	-0.007 (1)	-0.002 (1)

Table 5: Hydrogen coordinates ($\cdot 10^4$) and isotropic displacement parameters ($Å^2 \cdot 10^3$).

Starred atoms were refined isotropically. Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as:

$(4/3) \cdot [a^2 \cdot B(1,1) + b^2 \cdot B(2,2) + c^2 \cdot B(3,3) + a \cdot b \cdot (\cos \gamma) \cdot B(1,2) + a \cdot c \cdot (\cos \beta) \cdot B(1,3) + b \cdot c \cdot (\cos \alpha) \cdot B(2,3)]$

	X		Y		Z		U	
H2	0.018	(4)	0.677	(2)	-0.000	(1)	1.1	(5)*
H3	-0.137	(4)	0.736	(2)	0.100	(1)	1.0	(5)*
H03	0.599	(4)	0.821	(3)	0.228	(2)	4.3	(8)*
H4A	0.586	(4)	0.704	(3)	-0.010	(1)	3.3	(7)*
H4C	0.386	(4)	0.696	(3)	-0.064	(1)	2.8	(6)*
H4B	0.454	(5)	0.567	(3)	-0.031	(1)	4.2	(8)*
H5A	-0.097	(5)	0.465	(3)	0.032	(2)	4.8	(8)*
H5B	0.133	(4)	0.433	(3)	0.067	(1)	3.5	(7)*
H5C	0.115	(4)	0.462	(3)	-0.017	(1)	2.9	(6)*
H7	-0.349	(4)	0.552	(2)	0.142	(1)	1.7	(5)*
H8	-0.402	(4)	0.414	(3)	0.238	(1)	3.4	(7)*
H9	-0.149	(4)	0.364	(3)	0.321	(1)	3.5	(7)*
H10	0.193	(4)	0.449	(2)	0.312	(1)	1.9	(6)*
H11	0.250	(4)	0.605	(3)	0.216	(1)	2.4	(6)*
H13	0.379	(4)	0.987	(3)	0.175	(1)	1.7	(5)*
H15A	0.649	(3)	1.040	(2)	0.269	(1)	0.7	(5)*
H15B	0.492	(4)	1.088	(3)	0.323	(1)	2.1	(6)*
H16A	0.775	(4)	0.868	(3)	0.347	(1)	2.0	(5)*
H16B	0.785	(4)	1.015	(3)	0.384	(1)	2.7	(6)*
H17	0.473	(3)	0.979	(2)	0.443	(1)	1.3	(5)*
H18B	0.277	(4)	0.777	(3)	0.432	(1)	3.2	(7)*
H18A	0.446	(4)	0.721	(3)	0.379	(1)	2.1	(6)*
H19B	0.164	(4)	0.947	(2)	0.349	(1)	1.7	(5)*
H19A	0.154	(4)	0.801	(3)	0.316	(1)	2.2	(6)*
H21B	0.773	(4)	1.028	(3)	0.526	(1)	3.5	(7)*
H21C	0.904	(5)	0.907	(3)	0.562	(1)	4.2	(7)*
H21A	0.950	(4)	0.944	(3)	0.480	(1)	2.4	(6)*
H22B	0.435	(4)	0.904	(3)	0.566	(2)	4.3	(8)*
H22A	0.594	(4)	0.784	(3)	0.594	(1)	1.9	(5)*
H22C	0.406	(4)	0.754	(3)	0.542	(1)	2.6	(6)*
H23B	0.672	(4)	0.636	(3)	0.462	(1)	2.9	(6)*
H23A	0.848	(4)	0.677	(3)	0.514	(1)	3.7	(7)*
H23C	0.867	(4)	0.715	(3)	0.431	(1)	2.8	(6)*
H24B	0.058	(4)	1.104	(3)	0.261	(1)	2.1	(6)*
H24A	0.284	(4)	1.173	(2)	0.241	(1)	1.6	(5)*
H25B	0.017	(4)	1.260	(3)	0.169	(1)	3.4	(7)*
H25A	0.166	(5)	1.173	(4)	0.116	(2)	6.1	(9)*
H25C	-0.040	(4)	1.110	(3)	0.141	(1)	2.6	(6)*

Table 6: Torsion angles [deg].

C3-N1-C1-O1	178.97	(0.23)
C3-N1-C1-N2	-0.71	(0.28)
C12-N1-C1-O1	-1.30	(0.43)
C12-N1-C1-N2	179.02	(0.24)
C1-N1-C3-C2	-12.13	(0.26)
C1-N1-C3-C6	113.09	(0.23)
C12-N1-C3-C2	168.11	(0.21)
C12-N1-C3-C6	-66.67	(0.29)
C1-N1-C12-O2	174.20	(0.24)
C1-N1-C12-C13	-7.73	(0.39)
C3-N1-C12-O2	-6.09	(0.34)
C3-N1-C12-C13	171.99	(0.22)
C2-N2-C1-O1	-165.02	(0.24)
C2-N2-C1-N1	14.66	(0.28)
C4-N2-C1-O1	-16.74	(0.39)
C4-N2-C1-N1	162.94	(0.22)
C1-N2-C2-C3	-21.63	(0.27)
C1-N2-C2-C5	-147.85	(0.23)
C4-N2-C2-C3	-169.59	(0.24)
C4-N2-C2-C5	64.19	(0.32)
N2-C2-C3-N1	18.97	(0.24)
N2-C2-C3-C6	-103.94	(0.24)
C5-C2-C3-N1	142.13	(0.23)
C5-C2-C3-C6	19.22	(0.34)
N1-C3-C6-C7	148.90	(0.24)
N1-C3-C6-C11	-28.46	(0.34)
C2-C3-C6-C7	-93.91	(0.30)
C2-C3-C6-C11	88.73	(0.31)
C3-C6-C7-C8	-178.04	(0.26)
C11-C6-C7-C8	-0.61	(0.42)
C3-C6-C11-C10	177.41	(0.26)
C7-C6-C11-C10	0.05	(0.45)
C6-C7-C8-C9	1.04	(0.46)
C7-C8-C9-C10	-0.89	(0.48)
C8-C9-C10-C11	0.33	(0.47)
C9-C10-C11-C6	0.10	(0.44)
O2-C12-C13-C14	87.47	(0.29)
O2-C12-C13-C24	-39.94	(0.31)
N1-C12-C13-C14	-90.55	(0.26)
N1-C12-C13-C24	142.04	(0.23)
C12-C13-C14-O3	61.23	(0.24)
C12-C13-C14-C15	-177.65	(0.20)
C12-C13-C14-C19	-55.39	(0.28)
C24-C13-C14-O3	-175.61	(0.20)

C24-C13-C14-C15	-54.49	(0.28)
C24-C13-C14-C19	67.76	(0.29)
C12-C13-C24-C25	-59.94	(0.27)
C14-C13-C24-C25	176.51	(0.22)
O3-C14-C15-C16	-58.44	(0.26)
C13-C14-C15-C16	-177.75	(0.20)
C19-C14-C15-C16	56.81	(0.27)
O3-C14-C19-C18	62.26	(0.25)
C13-C14-C19-C18	-179.81	(0.21)
C15-C14-C19-C18	-56.38	(0.28)
C14-C15-C16-C17	-57.47	(0.27)
C15-C16-C17-C18	54.31	(0.28)
C15-C16-C17-C20	-178.23	(0.21)
C16-C17-C18-C19	-54.99	(0.27)
C20-C17-C18-C19	177.64	(0.20)
C16-C17-C20-C21	52.43	(0.28)
C16-C17-C20-C22	170.37	(0.22)
C16-C17-C20-C23	-68.85	(0.28)
C18-C17-C20-C21	177.28	(0.21)
C18-C17-C20-C22	-64.79	(0.28)
C18-C17-C20-C23	55.99	(0.28)
C17-C18-C19-C14	57.79	(0.28)

1.9. Trifluoressigsäurester 35

Table 1: Crystal data and structure refinement.

Empirical formula:	$C_{25}\ H_{33}\ N_2\ O_4\ F_3$	
Formula weight:	482.55	
Temperature:	-140 °C	
Radiation:	Mo-K_α	
Crystal system:	monoclinic	
Space group:	C2	
Unit cell dimensions:	a = 22.231(4) Å	α = 90 deg.
	b = 6.3899(8) Å	β = 104.80(1) deg.
	c = 17.602(3) Å	γ = 90 deg.
Volume:	2417.5(8) $Å^3$	
Z:	4	
Density (calculated):	1.326 g/cm^3	
Absorption coefficient:	0.99 cm^{-1}	
Crystal color:	colorless, transparent	
Crystal size:	0.02 x 0.34 x 1.60 mm	
Scan range:	sphere	
(2 Θ)max:	57 deg.	
Resolution:	0.74 Å	
Reflections collected:	14792	
Independent reflections:	2965	
Reflections used with I > 0:	2887	
Number of variables:	306	
R (F):	0.161	
wR (F):	0.120	
S:	1.16	

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

Starred atoms were refined isotropically. Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as:

$(4/3) \cdot [a^2 \cdot B(1,1) + b^2 \cdot B(2,2) + c^2 \cdot B(3,3) + a \cdot b \cdot (\cos \gamma) \cdot B(1,2) + a \cdot c \cdot (\cos \beta) \cdot B(1,3) + b \cdot c \cdot (\cos \alpha) \cdot B(2,3)]$

	X		Y		Z		U (eq)	
F1	0.4609	(2)	0.3890	(0)	0.3798	(3)	3.0	(1)
F2	0.3856	(2)	0.303	(1)	0.2819	(3)	3.0	(1)
F3	0.4517	(2)	0.532	(1)	0.2665	(3)	3.2	(1)
O1	0.7231	(3)	0.0299	(9)	0.2017	(4)	2.4	(1)
O2	0.5740	(2)	0.449	(1)	0.1978	(3)	1.7	(1)
O3	0.5418	(2)	0.199	(1)	0.3216	(3)	1.4	(1)
O4	0.4633	(3)	0.062	(1)	0.2263	(3)	2.6	(1)
N1	0.6658	(3)	0.347	(1)	0.1784	(3)	1.7	(1)
N2	0.7583	(3)	0.326	(1)	0.1544	(4)	1.9	(2)
C1	0.7169	(2)	0.215	(2)	0.1806	(4)	2.7	(2)
C2	0.7442	(4)	0.558	(2)	0.1473	(5)	1.5	(2)
C3	0.6749	(4)	0.557	(1)	0.1453	(4)	1.4	(2)
C4	0.8215	(4)	0.255	(2)	0.1599	(6)	2.7	(2)
C5	0.7625	(4)	0.658	(2)	0.0783	(5)	2.4	(2)
C6	0.6305	(3)	0.591	(2)	0.0650	(5)	1.6	(2)
C7	0.6100	(4)	0.792	(1)	0.0413	(5)	1.8	(2)
C8	0.5693	(4)	0.832	(2)	-0.0309	(5)	2.1	(2)
C9	0.5461	(4)	0.670	(2)	-0.0817	(4)	1.8	(2)
C10	0.5664	(4)	0.462	(1)	-0.0589	(5)	2.0	(2)
C11	0.6072	(4)	0.428	(2)	0.0121	(5)	2.1	(2)
C12	0.6119	(3)	0.310	(2)	0.1981	(4)	1.4	(2)
C13	0.5981	(3)	0.088	(2)	0.2207	(5)	1.6	(2)
C14	0.5935	(3)	0.075	(1)	0.3068	(5)	1.3	(2)
C15	0.5861	(4)	-0.163	(1)	0.3271	(5)	1.1	(2)
C16	0.5875	(4)	-0.189	(2)	0.4131	(5)	1.9	(2)
C17	0.6465	(4)	-0.102	(2)	0.4693	(4)	1.5	(2)
C18	0.6517	(4)	0.132	(2)	0.4496	(5)	1.7	(2)
C19	0.6501	(4)	0.163	(2)	0.3629	(5)	1.7	(2)
C20	0.6525	(4)	-0.148	(2)	0.5582	(4)	1.5	(2)
C21	0.7066	(4)	-0.023	(2)	0.6101	(5)	2.4	(2)
C22	0.6689	(4)	-0.382	(2)	0.5739	(5)	2.3	(2)
C23	0.5924	(5)	-0.101	(2)	0.5814	(5)	2.6	(2)
C24	0.4851	(4)	0.179	(2)	0.2801	(5)	1.8	(2)
C25	0.4448	(3)	0.350	(1)	0.3038	(4)	1.7	(1)

Table 3a: Bond lengths [Å].

Numbers in parentheses are estimated standard deviations in the least significant digits.

F1-C25	1.317	(9)	C6-C11	1.41	(1)
F2-C25	1.309	(8)	C7-C8	1.38	(1)
F3-C25	1.36	(1)	C8-C9	1.38	(1)
O1-C1	1.23	(1)	C9-C10	1.43	(1)
O2-C12	1.23	(1)	C10-C11	1.36	(1)
O3-C14	1.47	(1)	C12-C13	1.53	(1)
O3-C24	1.291	(9)	C13-C14	1.55	(1)
O4-C24	1.21	(1)	C14-C15	1.58	(1)
N1-C1	1.41	(1)	C14-C19	1.50	(1)
N1-C3	1.49	(1)	C15-C16	1.52	(1)
N1-C12	1.35	(1)	C16-C17	1.53	(1)
N2-C1	1.33	(1)	C17-C18	1.55	(1)
N2-C2	1.51	(1)	C17-C20	1.56	(1)
N2-C4	1.46	(1)	C18-C19	1.53	(1)
C2-C3	1.53	(1)	C20-C21	1.53	(1)
C2-C5	1.52	(1)	C20-C22	1.55	(1)
C3-C6	1.52	(1)	C20-C23	1.52	(1)
C6-C7	1.39	(1)	C24-C25	1.54	(1)

Table 3b: Bond angles [deg].

C14-O3-C24	122.7	(7)	O3-C14-C13	113.2	(6)
C1-N1-C3	111.0	(7)	O3-C14-C15	110.4	(7)
C1-N1-C12	130.4	(8)	O3-C14-C19	104.1	(7)
C3-N1-C12	118.5	(8)	C13-C14-C15	108.0	(7)
C1-N2-C2	113.8	(8)	C13-C14-C19	111.8	(7)
C1-N2-C4	123.3	(8)	C15-C14-C19	109.3	(6)
C2-N2-C4	119.1	(8)	C14-C15-C16	110.8	(7)
O1-C1-N1	127.5	(8)	C15-C16-C17	113.6	(7)
O1-C1-N2	125.5	(8)	C16-C17-C18	107.9	(6)
N1-C1-N2	107.0	(9)	C16-C17-C20	114.8	(7)
N2-C2-C3	100.5	(7)	C18-C17-C20	114.3	(7)
N2-C2-C5	112.6	(8)	C17-C18-C19	111.5	(7)
C3-C2-C5	117.2	(6)	C14-C19-C18	114.2	(7)
N1-C3-C2	103.4	(7)	C17-C20-C21	110.7	(7)
N1-C3-C6	111.9	(7)	C17-C20-C22	108.3	(7)
C2-C3-C6	115.6	(7)	C17-C20-C23	112.1	(6)
C3-C6-C7	120.0	(8)	C21-C20-C22	106.3	(7)
C3-C6-C11	123.3	(8)	C21-C20-C23	110.3	(7)
C7-C6-C11	116.7	(7)	C22-C20-C23	109.0	(8)
C6-C7-C8	122.4	(8)	O3-C24-O4	130.0	(9)
C7-C8-C9	120.4	(9)	O3-C24-C25	109.3	(7)
C8-C9-C10	118.5	(7)	O4-C24-C25	120.5	(7)
C9-C10-C11	119.8	(8)	F1-C25-F2	109.5	(6)
C6-C11-C10	122.2	(9)	F1-C25-F3	107.1	(6)
O2-C12-N1	121.5	(9)	F1-C25-C24	112.7	(6)
O2-C12-C13	119.6	(7)	F2-C25-F3	106.4	(6)
N1-C12-C13	118.9	(8)	F2-C25-C24	111.7	(7)
C12-C13-C14	111.9	(7)	F3-C25-C24	109.2	(7)

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

The form of the anisotropic displacement parameter is:

$\exp [-2\pi^2 \cdot (h^2 \cdot a^2 \cdot U_{11} + k^2 \cdot b^2 \cdot U_{22} + l^2 \cdot c^2 \cdot U_{33} + 2 \cdot h \cdot k \cdot a \cdot b \cdot U_{12} + 2 \cdot h \cdot l \cdot a \cdot c \cdot U_{13} + 2 \cdot k \cdot l \cdot b \cdot c \cdot U_{23})]$ where a, b, and c are reciprocal lattice constants.

	U11	U22	U33	U23	U13	U12
F1	0.057 (3)	0.019 (3)	0.037 (2)	0.013 (3)	0.013 (2)	-0.000 (3)
F2	0.033 (2)	0.017 (3)	0.065 (3)	0.004 (3)	0.014 (2)	0.009 (3)
F3	0.039 (3)	0.023 (3)	0.058 (3)	0.004 (3)	0.012 (2)	0.012 (3)
O1	0.066 (4)	-0.025 (2)	0.045 (3)	0.002 (3)	0.001 (3)	0.003 (3)
O2	0.031 (3)	0.012 (3)	0.025 (3)	0.004 (3)	0.012 (2)	0.002 (3)
O3	0.027 (2)	0.004 (3)	0.022 (2)	0.004 (3)	0.006 (2)	0.003 (3)
O4	0.038 (3)	0.022 (4)	0.028 (3)	0.002 (3)	-0.008 (3)	-0.007 (3)
N1	0.041 (4)	0.010 (4)	0.009 (3)	-0.007 (4)	-0.002 (3)	0.001 (3)
N2	0.033 (3)	0.010 (4)	0.026 (3)	0.010 (4)	-0.000 (3)	-0.000 (4)
C1	-0.023 (2)	0.089 (8)	0.038 (4)	-0.001 (4)	0.003 (2)	-0.031 (5)
C2	0.020 (3)	0.008 (5)	0.023 (4)	0.004 (4)	-0.004 (3)	-0.003 (4)
C3	0.035 (4)	-0.003 (4)	0.017 (3)	-0.001 (4)	0.002 (3)	-0.007 (4)
C4	0.013 (3)	0.030 (6)	0.062 (5)	0.000 (4)	0.016 (3)	-0.004 (5)
C5	0.023 (4)	0.034 (7)	0.031 (4)	0.001 (5)	-0.002 (3)	0.009 (5)
C6	0.017 (3)	0.016 (5)	0.027 (4)	-0.000 (4)	0.007 (3)	-0.002 (4)
C7	0.049 (5)	-0.004 (4)	0.020 (4)	0.011 (4)	0.002 (3)	-0.000 (4)
C8	0.036 (4)	0.019 (5)	0.022 (4)	-0.001 (5)	0.001 (3)	-0.007 (5)
C9	0.025 (4)	0.022 (6)	0.013 (3)	-0.001 (5)	-0.006 (3)	0.002 (4)
C10	0.040 (5)	0.001 (5)	0.029 (4)	-0.011 (4)	-0.004 (4)	0.002 (4)
C11	0.047 (5)	0.006 (5)	0.022 (4)	0.005 (5)	0.002 (4)	0.001 (4)
C12	0.019 (3)	0.018 (5)	0.014 (3)	-0.002 (4)	-0.004 (3)	-0.002 (4)
C13	0.020 (3)	0.015 (5)	0.027 (4)	-0.000 (4)	0.008 (3)	0.002 (4)
C14	0.020 (4)	-0.006 (4)	0.030 (4)	-0.003 (4)	-0.001 (3)	0.008 (4)
C15	0.036 (4)	-0.028 (3)	0.032 (4)	0.003 (3)	0.005 (3)	0.005 (3)
C16	0.031 (4)	0.007 (5)	0.030 (4)	-0.003 (4)	-0.000 (3)	-0.005 (4)
C17	0.026 (3)	0.012 (5)	0.021 (3)	0.009 (4)	0.006 (3)	0.002 (4)
C18	0.023 (4)	0.019 (5)	0.016 (4)	-0.004 (4)	-0.002 (3)	-0.010 (4)
C19	0.021 (3)	0.014 (5)	0.028 (4)	0.004 (4)	0.002 (3)	-0.001 (4)
C20	0.026 (4)	0.010 (5)	0.017 (3)	0.004 (4)	-0.002 (3)	-0.011 (4)
C21	0.036 (5)	0.028 (7)	0.022 (4)	0.004 (5)	-0.003 (4)	0.007 (5)
C22	0.036 (4)	0.009 (5)	0.034 (5)	0.009 (5)	-0.003 (4)	0.007 (4)
C23	0.056 (5)	0.014 (6)	0.026 (4)	0.007 (5)	0.005 (4)	0.001 (5)
C24	0.033 (4)	0.017 (5)	0.015 (3)	0.002 (4)	-0.004 (3)	0.006 (4)
C25	0.017 (2)	0.014 (4)	0.046 (3)	0.015 (3)	0.033 (2)	0.035 (3)

Table 5: Hydrogen coordinates ($\cdot 10^4$) and isotropic displacement parameters ($Å^2 \cdot 10^3$).
Starred atoms were refined isotropically. Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as:

$(4/3) \cdot [a^2 \cdot B(1,1) + b^2 \cdot B(2,2) + c^2 \cdot B(3,3) + a \cdot b \cdot (\cos \gamma) \cdot B(1,2) + a \cdot c \cdot (\cos \beta) \cdot B(1,3) + b \cdot c \cdot (\cos \alpha) \cdot B(2,3)]$

	X	Y	Z	U	
H2	0.7678	0.6477	0.1900	2	*
H3	0.6643	0.6791	0.1746	1	*
H4b	0.8337	0.3041	0.1135	3	*
H4a	0.8216	0.1147	0.1642	3	*
H4c	0.8493	0.3237	0.2053	3	*
H5a	0.7517	0.8097	0.0768	2	*
H5b	0.8070	0.6440	0.0853	2	*
H5c	0.7395	0.5931	0.0298	2	*
H7	0.6265	0.9115	0.0765	2	*
H8	0.5557	0.9761	-0.0457	2	*
H9	0.5178	0.6969	-0.1329	2	*
H10	0.5505	0.3452	-0.0932	2	*
H11	0.6205	0.2857	0.0268	2	*
H13b	0.5575	0.0452	0.1866	1	*
H13a	0.6304	-0.0042	0.2136	1	*
H15b	0.5455	-0.2168	0.2948	1	*
H15a	0.6194	-0.2479	0.3155	1	*
H16b	0.5509	-0.1153	0.4226	2	*
H16a	0.5843	-0.3379	0.4246	2	*
H17	0.6814	-0.1770	0.4600	1	*
H18a	0.6922	0.1847	0.4814	1	*
H18b	0.6183	0.2117	0.4622	1	*
H19b	0.6869	0.0996	0.3529	1	*
H19a	0.6502	0.3150	0.3532	1	*
H21b	0.7457	-0.0623	0.5964	3	*
H21c	0.6995	0.1272	0.6004	3	*
H21a	0.7105	-0.0539	0.6652	3	*
H22a	0.6725	-0.4115	0.6299	2	*
H22b	0.6345	-0.4667	0.5421	2	*
H22c	0.7071	-0.4139	0.5606	2	*
H23a	0.5977	-0.1309	0.6374	3	*
H23b	0.5812	0.0472	0.5715	3	*
H23c	0.5586	-0.1882	0.5502	3	*

Table 6: Torsion angles [deg].

C24-O3-C14-C13	53.23	(1.02)
C24-O3-C14-C15	-67.98	(0.91)
C24-O3-C14-C19	174.83	(0.74)
C14-O3-C24-O4	2.13	(1.45)
C14-O3-C24-C25	-172.75	(0.64)
C3-N1-C1-O1	-177.07	(0.77)
C3-N1-C1-N2	2.29	(0.85)
C12-N1-C1-O1	0.03	(1.38)
C12-N1-C1-N2	179.39	(0.72)
C1-N1-C3-C2	-14.33	(0.79)
C1-N1-C3-C6	110.74	(0.75)
C12-N1-C3-C2	168.18	(0.64)
C12-N1-C3-C6	-66.75	(0.88)
C1-N1-C12-O2	174.65	(0.72)
C1-N1-C12-C13	-5.66	(1.15)
C3-N1-C12-O2	-8.43	(1.04)
C3-N1-C12-C13	171.26	(0.63)
C2-N2-C1-O1	-169.04	(0.77)
C2-N2-C1-N1	11.59	(0.87)
C4-N2-C1-O1	-11.08	(1.33)
C4-N2-C1-N1	169.54	(0.72)
C1-N2-C2-C3	-19.83	(0.81)
C1-N2-C2-C5	-145.37	(0.70)
C4-N2-C2-C3	-178.78	(0.67)
C4-N2-C2-C5	55.68	(0.94)
N2-C2-C3-N1	18.79	(0.69)
N2-C2-C3-C6	-103.86	(0.81)
C5-C2-C3-N1	141.11	(0.80)
C5-C2-C3-C6	18.47	(1.22)
N1-C3-C6-C7	149.26	(0.77)
N1-C3-C6-C11	-29.47	(1.09)
C2-C3-C6-C7	-92.70	(0.99)
C2-C3-C6-C11	88.57	(1.05)
C3-C6-C7-C8	-179.66	(0.80)
C11-C6-C7-C8	-0.85	(1.29)
C3-C6-C11-C10	178.54	(0.84)
C7-C6-C11-C10	-0.22	(1.31)
C6-C7-C8-C9	1.85	(1.38)
C7-C8-C9-C10	-1.71	(1.30)
C8-C9-C10-C11	0.66	(1.32)
C9-C10-C11-C6	0.31	(1.41)
O2-C12-C13-C14	-63.61	(0.91)
N1-C12-C13-C14	116.69	(0.75)
C12-C13-C14-O3	63.27	(0.84)

C12-C13-C14-C15	-174.20	(0.63)
C12-C13-C14-C19	-53.93	(0.92)
O3-C14-C15-C16	-61.15	(0.82)
C13-C14-C15-C16	174.64	(0.65)
C19-C14-C15-C16	52.81	(0.87)
O3-C14-C19-C18	64.19	(0.91)
C13-C14-C19-C18	-173.30	(0.76)
C15-C14-C19-C18	-53.77	(0.95)
C14-C15-C16-C17	-57.04	(0.96)
C15-C16-C17-C18	57.37	(0.92)
C15-C16-C17-C20	-173.89	(0.74)
C16-C17-C18-C19	-55.06	(0.85)
C20-C17-C18-C19	175.94	(0.66)
C16-C17-C20-C21	-170.18	(0.79)
C16-C17-C20-C22	73.62	(0.92)
C16-C17-C20-C23	-46.62	(1.10)
C18-C17-C20-C21	-44.74	(0.97)
C18-C17-C20-C22	-160.94	(0.69)
C18-C17-C20-C23	78.83	(0.93)
C17-C18-C19-C14	56.85	(0.96)
O3-C24-C25-F1	-37.34	(0.95)
O3-C24-C25-F2	-161.10	(0.67)
O3-C24-C25-F3	81.55	(0.77)
O4-C24-C25-F1	147.22	(0.79)
O4-C24-C25-F2	23.46	(1.13)
O4-C24-C25-F3	-93.90	(0.96)

1.10. endocyclisches Olefin 36A

Table 1: Crystal data and structure refinement.

Empirical formula:	$C_{23}\ H_{32}\ N_2\ O_2$	
Formula weight:	368.52	
Temperature:	-101 °C	
Radiation:	Mo-K_α	
Crystal system:	orthorhombic	
Space group:	P212121	
Unit cell dimensions:	a = 6.1039(6) Å	α = 90 deg.
	b = 16.321(2) Å	β = 90 deg.
	c = 21.359(3) Å	γ = 90 deg.
Volume:	2127.8(5) $Å^3$	
Z:	4	
Density (calculated):	1.150 g/cm^3	
Absorption coefficient:	0.68 cm^{-1}	
Crystal color:	colorless, transparent	
Crystal size:	0.16 x 0.17 x 1.20 mm	
Scan range:	sphere	
(2 Θ)max:	58 deg.	
Index ranges:	-88h88, -208k822, -258l828	
Resolution:	0.74 Å	
Reflections collected:	26936	
Independent reflections:	2952	
Reflections used with I > 0:	2918	
Number of variables:	336	
R (F):	0.102	
wR (F):	0.078	
S:	1.32	

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

Starred atoms were refined isotropically. Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as:

$(4/3) \cdot [a^2 \cdot B(1,1) + b^2 \cdot B(2,2) + c^2 \cdot B(3,3) + a \cdot b \cdot (\cos \gamma) \cdot B(1,2) + a \cdot c \cdot (\cos \beta) \cdot B(1,3) + b \cdot c \cdot (\cos \alpha) \cdot B(2,3)]$

	X		Y		Z		U (eq)	
O1	-0.9174	(4)	-0.4422	(2)	-0.1821	(1)	3.24	(6)
O2	-0.4899	(5)	-0.2410	(2)	-0.1696	(1)	3.06	(5)
N1	-0.5921	(5)	-0.3672	(2)	-0.1989	(1)	1.94	(5)
N2	-0.6218	(6)	-0.4937	(2)	-0.2362	(1)	2.62	(6)
C1	-0.7292	(7)	-0.4365	(2)	-0.2030	(2)	2.51	(7)
C2	-0.3878	(7)	-0.4752	(2)	-0.2430	(2)	2.34	(7)
C3	-0.3831	(7)	-0.3808	(2)	-0.2308	(2)	2.15	(7)
C4	-0.6962	(8)	-0.5779	(2)	-0.2393	(2)	3.9	(1)
C5	-0.2894	(8)	-0.5036	(3)	-0.3037	(2)	3.69	(9)
C6	-0.3557	(7)	-0.3287	(2)	-0.2897	(2)	2.53	(7)
C7	-0.1517	(7)	-0.2914	(2)	-0.2995	(2)	3.19	(8)
C8	-0.1151	(8)	-0.2457	(3)	-0.3540	(2)	4.0	(1)
C9	-0.2768	(9)	-0.2356	(3)	-0.3964	(2)	4.3	(1)
C10	-0.4814	(9)	-0.2714	(3)	-0.3880	(2)	4.3	(1)
C11	-0.5209	(7)	-0.3189	(3)	-0.3327	(2)	3.25	(8)
C12	-0.6263	(6)	-0.2951	(2)	-0.1657	(2)	2.18	(7)
C13	-0.8267	(7)	-0.2901	(2)	-0.1243	(2)	2.59	(7)
C14	-0.8457	(7)	-0.2099	(2)	-0.0888	(2)	2.21	(7)
C15	-1.0156	(7)	-0.1601	(2)	-0.0984	(2)	2.48	(7)
C16	-1.0530	(6)	-0.0812	(2)	-0.0642	(2)	2.61	(8)
C17	-0.8439	(7)	-0.0521	(2)	-0.0283	(2)	2.88	(8)
C18	-0.7487	(8)	-0.1229	(3)	0.0049	(2)	3.71	(9)
C19	-0.6757	(7)	-0.1916	(2)	-0.0399	(2)	2.94	(8)
C20	-0.8809	(8)	0.0253	(2)	0.0114	(2)	3.22	(8)
C21	-1.015	(1)	0.0095	(3)	0.0694	(2)	5.3	(1)
C22	-0.987	(1)	0.0917	(3)	-0.0284	(2)	4.7	(1)
C23	-0.657	(1)	0.0602	(3)	0.0307	(3)	5.7	(1)

Table 3a: Bond lengths [Å].

Numbers in parentheses are estimated standard deviations in the least significant digits.

O1-C1	1.236	(5)	C9-C10	1.391	(7)
O2-C12	1.217	(5)	C10-C11	1.432	(6)
N1-C1	1.409	(5)	C12-C13	1.513	(5)
N1-C3	1.464	(5)	C13-C14	1.516	(5)
N1-C12	1.389	(4)	C14-C15	1.334	(5)
N2-C1	1.343	(5)	C14-C19	1.503	(5)
N2-C2	1.467	(5)	C15-C16	1.498	(5)
N2-C4	1.448	(5)	C16-C17	1.563	(6)
C2-C3	1.563	(5)	C17-C18	1.475	(6)
C2-C5	1.503	(6)	C17-C20	1.539	(5)
C3-C6	1.527	(5)	C18-C19	1.540	(6)
C6-C7	1.402	(6)	C20-C21	1.508	(7)
C6-C11	1.374	(6)	C20-C22	1.524	(6)
C7-C8	1.401	(6)	C20-C23	1.537	(7)
C8-C9	1.349	(7)			

Table 3b: Bond angles [deg].

C1-N1-C3	111.5	(3)	C6-C11-C10	119.4	(4)
C1-N1-C12	128.5	(3)	O2-C12-N1	118.6	(3)
C3-N1-C12	119.8	(3)	O2-C12-C13	123.6	(3)
C1-N2-C2	112.6	(3)	N1-C12-C13	117.8	(3)
C1-N2-C4	122.1	(3)	C12-C13-C14	113.7	(3)
C2-N2-C4	119.7	(3)	C13-C14-C15	120.6	(3)
O1-C1-N1	126.1	(3)	C13-C14-C19	117.8	(3)
O1-C1-N2	126.3	(3)	C15-C14-C19	121.5	(3)
N1-C1-N2	107.5	(3)	C14-C15-C16	124.6	(3)
N2-C2-C3	101.8	(3)	C15-C16-C17	112.0	(3)
N2-C2-C5	114.3	(3)	C16-C17-C18	108.7	(3)
C3-C2-C5	116.1	(3)	C16-C17-C20	113.5	(3)
N1-C3-C2	102.2	(3)	C18-C17-C20	115.8	(3)
N1-C3-C6	113.3	(3)	C17-C18-C19	112.6	(3)
C2-C3-C6	114.4	(3)	C14-C19-C18	112.2	(3)
C3-C6-C7	117.5	(3)	C17-C20-C21	113.1	(3)
C3-C6-C11	122.4	(4)	C17-C20-C22	109.8	(3)
C7-C6-C11	120.1	(3)	C17-C20-C23	108.8	(4)
C6-C7-C8	119.8	(4)	C21-C20-C22	110.4	(4)
C7-C8-C9	120.4	(4)	C21-C20-C23	109.0	(4)
C8-C9-C10	121.2	(4)	C22-C20-C23	105.4	(4)
C9-C10-C11	119.0	(4)			

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

The form of the anisotropic displacement parameter is:

$\exp [-2\pi^2 \cdot (h^2 \cdot a^2 \cdot U_{11} + k^2 \cdot b^2 \cdot U_{22} + l^2 \cdot c^2 \cdot U_{33} + 2 \cdot h \cdot k \cdot a \cdot b \cdot U_{12} + 2 \cdot h \cdot l \cdot a \cdot c \cdot U_{13} + 2 \cdot k \cdot l \cdot b \cdot c \cdot U_{23})]$ where a, b, and c are reciprocal lattice constants.

	U11	U22	U33	U23	U13	U12
O1	0.031 (1)	0.034 (1)	0.059 (2)	-0.002 (1)	0.001 (2)	-0.003 (1)
O2	0.043 (2)	0.030 (1)	0.044 (1)	-0.007 (1)	0.012 (2)	-0.005 (1)
N1	0.024 (1)	0.023 (1)	0.027 (1)	-0.003 (1)	0.005 (1)	-0.003 (1)
N2	0.039 (2)	0.026 (1)	0.034 (2)	0.000 (2)	-0.004 (2)	-0.005 (1)
C1	0.042 (2)	0.024 (2)	0.030 (2)	0.005 (2)	-0.005 (2)	0.000 (2)
C2	0.036 (2)	0.026 (2)	0.028 (2)	0.011 (2)	-0.002 (2)	0.005 (2)
C3	0.033 (2)	0.025 (2)	0.024 (2)	0.003 (2)	0.006 (2)	-0.002 (1)
C4	0.050 (3)	0.032 (2)	0.064 (3)	-0.006 (2)	-0.010 (3)	-0.013 (2)
C5	0.060 (3)	0.034 (2)	0.047 (2)	0.016 (2)	0.009 (2)	-0.005 (2)
C6	0.037 (2)	0.024 (2)	0.036 (2)	0.007 (2)	0.008 (2)	-0.002 (2)
C7	0.046 (2)	0.035 (2)	0.040 (2)	0.007 (2)	0.015 (2)	0.002 (2)
C8	0.048 (3)	0.041 (2)	0.062 (3)	0.012 (3)	0.015 (3)	0.013 (2)
C9	0.069 (3)	0.046 (2)	0.050 (2)	0.021 (3)	0.026 (3)	0.016 (2)
C10	0.062 (3)	0.051 (2)	0.050 (2)	0.021 (3)	-0.003 (3)	0.008 (2)
C11	0.040 (2)	0.047 (2)	0.036 (2)	0.010 (2)	0.005 (2)	0.005 (2)
C12	0.025 (2)	0.028 (2)	0.029 (2)	0.000 (2)	0.001 (2)	0.004 (2)
C13	0.038 (2)	0.025 (2)	0.035 (2)	-0.004 (2)	0.009 (2)	-0.005 (2)
C14	0.033 (2)	0.028 (2)	0.023 (1)	-0.003 (2)	0.006 (2)	-0.000 (1)
C15	0.033 (2)	0.034 (2)	0.027 (2)	-0.004 (2)	-0.002 (2)	-0.001 (2)
C16	0.027 (2)	0.034 (2)	0.038 (2)	0.006 (2)	0.002 (2)	-0.002 (2)
C17	0.036 (2)	0.040 (2)	0.034 (2)	0.003 (2)	-0.002 (2)	-0.009 (2)
C18	0.048 (3)	0.046 (2)	0.047 (2)	0.014 (2)	-0.021 (2)	-0.019 (2)
C19	0.040 (2)	0.035 (2)	0.037 (2)	0.013 (2)	-0.008 (2)	0.000 (2)
C20	0.056 (3)	0.030 (2)	0.036 (2)	0.008 (2)	0.003 (2)	-0.011 (2)
C21	0.123 (4)	0.032 (2)	0.046 (2)	0.007 (3)	0.033 (3)	-0.009 (2)
C22	0.101 (4)	0.039 (2)	0.041 (2)	-0.007 (3)	0.019 (3)	-0.000 (2)
C23	0.068 (3)	0.066 (3)	0.081 (3)	-0.011 (3)	-0.006 (3)	-0.028 (3)

Table 5: Hydrogen coordinates ($\cdot 10^4$) and isotropic displacement parameters ($Å^2 \cdot 10^3$).
Starred atoms were refined isotropically. Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as:

$(4/3) \cdot [a^2 \cdot B(1,1) + b^2 \cdot B(2,2) + c^2 \cdot B(3,3) + a \cdot b \cdot (\cos \gamma) \cdot B(1,2) + a \cdot c \cdot (\cos \beta) \cdot B(1,3) + b \cdot c \cdot (\cos \alpha) \cdot B(2,3)]$

	X	Y	Z	U
H2	-0.318 (4)	-0.497 (1)	-0.212 (1)	-0.5 (5)*
H3	-0.259 (5)	-0.371 (2)	-0.199 (1)	1.8 (7)*
H4A	-0.607 (8)	-0.607 (3)	-0.214 (2)	6 (1)*
H4C	-0.697 (7)	-0.593 (2)	-0.281 (2)	4 (1)*
H4B	-0.821 (8)	-0.585 (3)	-0.225 (2)	6 (1)*
H5B	-0.149 (6)	-0.487 (2)	-0.304 (2)	4 (1)*
H5A	-0.321 (6)	-0.565 (2)	-0.304 (2)	3.6 (9)*
H5C	-0.407 (9)	-0.485 (3)	-0.341 (2)	10 (2)*
H7	-0.041 (9)	-0.301 (3)	-0.262 (2)	7 (1)*
H8	0.022 (6)	-0.221 (2)	-0.357 (2)	3.5 (9)*
H9	-0.26 (1)	-0.209 (3)	-0.438 (3)	11 (2)*
H10	-0.628 (8)	-0.282 (3)	-0.415 (2)	6 (1)*
H11	-0.663 (5)	-0.350 (2)	-0.325 (1)	1.4 (7)*
H13A	-0.963 (5)	-0.294 (2)	-0.153 (1)	0.8 (6)*
H13B	-0.820 (7)	-0.343 (2)	-0.096 (2)	4 (1)*
H15	-1.114 (6)	-0.175 (2)	-0.134 (1)	2.7 (8)*
H16A	-1.183 (6)	-0.090 (2)	-0.034 (1)	2.6 (8)*
H16B	-1.087 (5)	-0.037 (2)	-0.092 (1)	1.8 (7)*
H17	-0.697 (9)	-0.043 (3)	-0.056 (2)	8 (1)*
H18A	-0.643 (6)	-0.107 (2)	0.031 (1)	3.2 (8)*
H18B	-0.909 (9)	-0.135 (3)	0.032 (2)	11 (2)*
H19A	-0.668 (6)	-0.241 (2)	-0.016 (1)	3.1 (9)*
H19B	-0.537 (6)	-0.172 (2)	-0.064 (1)	2.1 (7)*
H21a	-1.0355	0.0596	0.0933	6 *
H21b	-1.1605	-0.0124	0.0572	6 *
H21c	-0.9414	-0.0318	0.0956	6 *
H22a	-1.0142	0.1414	-0.0039	6 *
H22b	-0.8966	0.1050	-0.0648	6 *
H22c	-1.1325	0.0717	-0.0443	6 *
H23a	-0.6735	0.1099	0.0566	7 *
H23b	-0.5741	0.0192	0.0560	7 *
H23c	-0.5674	0.0739	-0.0060	7 *

Table 6: Torsion angles [deg].

C3-N1-C1-O1	-177.79	(0.34)
C3-N1-C1-N2	-0.47	(0.38)
C12-N1-C1-O1	7.42	(0.59)
C12-N1-C1-N2	-175.26	(0.31)
C1-N1-C3-C2	-11.99	(0.34)
C1-N1-C3-C6	111.62	(0.32)
C12-N1-C3-C2	163.31	(0.28)
C12-N1-C3-C6	-73.07	(0.38)
C1-N1-C12-O2	-177.90	(0.33)
C1-N1-C12-C13	5.01	(0.51)
C3-N1-C12-O2	7.69	(0.47)
C3-N1-C12-C13	-169.40	(0.29)
C2-N2-C1-O1	-168.33	(0.35)
C2-N2-C1-N1	14.35	(0.39)
C4-N2-C1-O1	-14.77	(0.59)
C4-N2-C1-N1	167.92	(0.33)
C1-N2-C2-C3	-21.10	(0.36)
C1-N2-C2-C5	-147.14	(0.32)
C4-N2-C2-C3	-175.35	(0.31)
C4-N2-C2-C5	58.62	(0.44)
N2-C2-C3-N1	18.62	(0.31)
N2-C2-C3-C6	-104.22	(0.35)
C5-C2-C3-N1	143.45	(0.33)
C5-C2-C3-C6	20.60	(0.50)
N1-C3-C6-C7	136.91	(0.34)
N1-C3-C6-C11	-44.07	(0.46)
C2-C3-C6-C7	-106.49	(0.40)
C2-C3-C6-C11	72.53	(0.48)
C3-C6-C7-C8	177.44	(0.35)
C11-C6-C7-C8	-1.61	(0.58)
C3-C6-C11-C10	-177.88	(0.36)
C7-C6-C11-C10	1.12	(0.59)
C6-C7-C8-C9	1.77	(0.63)
C7-C8-C9-C10	-1.45	(0.68)
C8-C9-C10-C11	0.95	(0.67)
C9-C10-C11-C6	-0.77	(0.62)
O2-C12-C13-C14	1.46	(0.50)
N1-C12-C13-C14	178.40	(0.30)
C12-C13-C14-C15	117.87	(0.39)
C12-C13-C14-C19	-66.18	(0.41)
C13-C14-C15-C16	177.84	(0.33)
C19-C14-C15-C16	2.05	(0.57)
C13-C14-C19-C18	-163.36	(0.32)
C15-C14-C19-C18	12.55	(0.50)

C14-C15-C16-C17	14.38	(0.51)
C15-C16-C17-C18	-45.18	(0.42)
C15-C16-C17-C20	-175.61	(0.30)
C16-C17-C18-C19	61.83	(0.44)
C20-C17-C18-C19	-168.97	(0.36)
C16-C17-C20-C21	72.78	(0.47)
C16-C17-C20-C22	-51.07	(0.47)
C16-C17-C20-C23	-165.91	(0.33)
C18-C17-C20-C21	-54.02	(0.55)
C18-C17-C20-C22	-177.87	(0.40)
C18-C17-C20-C23	67.29	(0.46)
C17-C18-C19-C14	-45.73	(0.47)

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Table 1: Crystal data and structure refinement.

Empirical formula:	$C_{24}\ H_{36}\ N_2\ O_3$	
Formula weight:	400.55	
Temperature:	22(2) °C	
Wavelength:	0.71068 Å	
Crystal system:	monoclinic	
Space group:	P21	
Unit cell dimensions:	a = 11.321(2) Å	α = 90 deg.
	b = 7.1420(10) Å	β = 106.63(1) deg.
	c = 14.550(2) Å	γ = 90 deg.
Volume:	1127.2(3) $Å^3$	
Z:	2	
Density (calculated):	1.180 Mg/m^3	
Absorption coefficient:	0.77 cm^{-1}	
F(000):	436	
Crystal size:	0.92 x 0.69 x 0.65 mm	
2 Θ range for data collection:	4.04 to 60.02 deg.	
Index ranges:	-158h85, 08k810, -208l820	
Reflections collected:	4721	
Independent reflections:	3528 [R_{int} = 0.0258]	
Refinement method:	Full-matrix least-squares on F^2	
Data / restraints / parameters:	3528 / 1 / 406	
Goodness-of-fit on F^2, S:	1.060	
Final R indices [I>2σ (I)]:	R1 = 0.0391, wR2 = 0.1126	
R indices (all data):	R1 = 0.0476, wR2 = 0.1188	
Absolute structure parameter:	-0.7 (13)	
Extinction coefficient:	0.0051 (5)	
Largest diff. peak and hole:	0.280 and -0.161 e/$Å^3$	

Table 2: Atomic coordinates ($\cdot 10^4$) and equivalent isotropic displacement parameters ($Å^2 \cdot 10^3$)

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor

	X		Y		Z		U (eq)	
C(1)	1059	(2)	6031	(3)	8683	(2)	53	(1)
C(2)	1833	(2)	4715	(2)	8232	(1)	39	(1)
C(3)	2459	(2)	5681	(2)	7557	(1)	42	(1)
C(4)	3288	(1)	4354	(2)	7187	(1)	39	(1)
C(5)	2629	(1)	2578	(2)	6684	(1)	33	(1)
C(6)	1974	(2)	1675	(2)	7375	(1)	39	(1)
C(7)	1128	(2)	3007	(3)	7710	(1)	43	(1)
C(8)	3512	(1)	1032	(2)	6542	(1)	36	(1)
N(9)	4770	(1)	1398	(2)	6621	(1)	39	(1)
C(10)	5245	(2)	2781	(3)	6131	(1)	46	(1)
N(11)	6418	(1)	2329	(3)	6207	(1)	55	(1)
C(12)	6851	(2)	675	(3)	6789	(1)	50	(1)
C(13)	5613	(1)	-235	(3)	6809	(1)	41	(1)
C(14)	5708	(1)	-1255	(3)	7733	(1)	42	(1)
C(15)	6199	(2)	-3062	(3)	7847	(2)	60	(1)
C(16)	6432	(3)	-3985	(4)	8713	(2)	75	(1)
C(17)	6155	(3)	-3173	(4)	9478	(2)	70	(1)
C(18)	5634	(2)	-1407	(4)	9374	(2)	62	(1)
C(19)	5420	(2)	-447	(3)	8507	(1)	50	(1)
O(20)	3196	(1)	-593	(2)	6472	(1)	47	(1)
C(21)	560	(4)	4921	(5)	9396	(3)	81	(1)
C(22)	-19	(3)	6923	(6)	7920	(3)	83	(1)
C(23)	1880	(3)	7609	(4)	9239	(2)	71	(1)
C(24)	1694	(2)	3062	(3)	5696	(1)	47	(1)
C(25)	739	(2)	1563	(4)	5280	(2)	64	(1)
O(26)	2303	(2)	3354	(4)	4983	(1)	82	(1)
O(27)	4698	(1)	4132	(3)	5697	(1)	59	(1)
C(28)	7190	(3)	3433	(6)	5772	(2)	78	(1)
C(29)	7715	(2)	1217	(4)	7760	(2)	59	(1)

Table 3a: Bond lengths [Å].

C(1)-C(22)	1.535	(4)	C(10)-O(27)	1.221	(3)
C(1)-C(23)	1.535	(3)	C(10)-N(11)	1.339	(2)
C(1)-C(21)	1.535	(3)	N(11)-C(28)	1.450	(3)
C(1)-C(2)	1.553	(2)	N(11)-C(12)	1.454	(3)
C(2)-C(3)	1.530	(2)	C(12)-C(29)	1.521	(3)
C(2)-C(7)	1.534	(2)	C(12)-C(13)	1.553	(2)
C(3)-C(4)	1.536	(2)	C(13)-C(14)	1.505	(2)
C(4)-C(5)	1.546	(2)	C(14)-C(19)	1.384	(2)
C(5)-C(8)	1.543	(2)	C(14)-C(15)	1.396	(3)
C(5)-C(6)	1.550	(2)	C(15)-C(16)	1.378	(4)
C(5)-C(24)	1.561	(2)	C(16)-C(17)	1.369	(5)
C(6)-C(7)	1.525	(2)	C(17)-C(18)	1.382	(4)
C(8)-O(20)	1.210	(2)	C(18)-C(19)	1.395	(3)
C(8)-N(9)	1.420	(2)	C(24)-O(26)	1.415	(3)
N(9)-C(10)	1.412	(2)	C(24)-C(25)	1.519	(3)
N(9)-C(13)	1.482	(2)			

Table 3b: Bond angles [deg].

C(22)-C(1)-C(23)	108.3	(3)	C(8)-N(9)-C(13)	116.61	(14)
C(22)-C(1)-C(21)	109.4	(3)	O(27)-C(10)-N(11)	125.3	(2)
C(23)-C(1)-C(21)	107.9	(2)	O(27)-C(10)-N(9)	127.2	(2)
C(22)-C(1)-C(2)	111.9	(2)	N(11)-C(10)-N(9)	107.5	(2)
C(23)-C(1)-C(2)	109.7	(2)	C(10)-N(11)-C(28)	122.6	(2)
C(21)-C(1)-C(2)	109.5	(2)	C(10)-N(11)-C(12)	113.9	(2)
C(3)-C(2)-C(7)	108.15	(12)	C(28)-N(11)-C(12)	123.4	(2)
C(3)-C(2)-C(1)	114.8	(2)	N(11)-C(12)-C(29)	110.7	(2)
C(7)-C(2)-C(1)	114.48	(14)	N(11)-C(12)-C(13)	101.23	(14)
C(2)-C(3)-C(4)	112.87	(14)	C(29)-C(12)-C(13)	115.6	(2)
C(3)-C(4)-C(5)	114.30	(12)	N(9)-C(13)-C(14)	115.03	(13)
C(8)-C(5)-C(4)	114.02	(12)	N(9)-C(13)-C(12)	101.8	(2)
C(8)-C(5)-C(6)	103.78	(12)	C(14)-C(13)-C(12)	112.69	(13)
C(4)-C(5)-C(6)	106.85	(11)	C(19)-C(14)-C(15)	117.8	(2)
C(8)-C(5)-C(24)	109.23	(12)	C(19)-C(14)-C(13)	123.5	(2)
C(4)-C(5)-C(24)	111.26	(14)	C(15)-C(14)-C(13)	118.6	(2)
C(6)-C(5)-C(24)	111.47	(12)	C(16)-C(15)-C(14)	121.1	(2)
C(7)-C(6)-C(5)	114.12	(13)	C(17)-C(16)-C(15)	120.8	(3)
C(6)-C(7)-C(2)	111.64	(13)	C(16)-C(17)-C(18)	119.2	(2)
O(20)-C(8)-N(9)	116.7	(2)	C(17)-C(18)-C(19)	120.4	(2)
O(20)-C(8)-C(5)	120.69	(13)	C(14)-C(19)-C(18)	120.7	(2)
N(9)-C(8)-C(5)	122.05	(14)	O(26)-C(24)-C(25)	104.7	(2)
C(10)-N(9)-C(8)	127.29	(13)	O(26)-C(24)-C(5)	111.35	(14)
C(10)-N(9)-C(13)	108.99	(13)	C(25)-C(24)-C(5)	115.4	(2)

Table 4: Anisotropic displacement parameters ($Å^2 \cdot 10^3$).

The anisotropic displacement factor exponent takes the form:

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

	U11	U22	U33	U23	U13	U12
C(1)	56 (1)	48 (1)	60 (1)	-11 (1)	27 (1)	-1 (1)
C(2)	40 (1)	39 (1)	40 (1)	-1 (1)	13 (1)	-2 (1)
C(3)	44 (1)	36 (1)	47 (1)	0 (1)	15 (1)	-7 (1)
C(4)	36 (1)	40 (1)	41 (1)	-1 (1)	13 (1)	-10 (1)
C(5)	30 (1)	38 (1)	32 (1)	1 (1)	7 (1)	-4 (1)
C(6)	39 (1)	36 (1)	45 (1)	-1 (1)	18 (1)	-7 (1)
C(7)	38 (1)	41 (1)	54 (1)	-5 (1)	20 (1)	-8 (1)
C(8)	33 (1)	45 (1)	29 (1)	-1 (1)	7 (1)	-2 (1)
N(9)	35 (1)	48 (1)	36 (1)	2 (1)	12 (1)	1 (1)
C(10)	41 (1)	65 (1)	33 (1)	6 (1)	13 (1)	-5 (1)
N(11)	39 (1)	86 (1)	45 (1)	12 (1)	19 (1)	-4 (1)
C(12)	39 (1)	71 (1)	45 (1)	-7 (1)	19 (1)	3 (1)
C(13)	37 (1)	51 (1)	36 (1)	-8 (1)	10 (1)	4 (1)
C(14)	35 (1)	46 (1)	41 (1)	-4 (1)	7 (1)	2 (1)
C(15)	66 (1)	47 (1)	61 (1)	-7 (1)	9 (1)	5 (1)
C(16)	88 (2)	47 (1)	78 (2)	8 (1)	2 (1)	5 (1)
C(17)	70 (1)	70 (1)	60 (1)	20 (1)	2 (1)	-5 (1)
C(18)	58 (1)	84 (2)	46 (1)	11 (1)	15 (1)	12 (1)
C(19)	48 (1)	62 (1)	40 (1)	3 (1)	12 (1)	13 (1)
O(20)	43 (1)	43 (1)	53 (1)	-6 (1)	14 (1)	-4 (1)
C(21)	105 (2)	73 (2)	91 (2)	-18 (2)	69 (2)	-15 (2)
C(22)	69 (2)	81 (2)	98 (2)	-10 (2)	21 (2)	28 (2)
C(23)	86 (2)	58 (1)	78 (2)	-26 (1)	36 (2)	-12 (1)
C(24)	41 (1)	56 (1)	38 (1)	2 (1)	2 (1)	3 (1)
C(25)	46 (1)	80 (2)	55 (1)	-14 (1)	-3 (1)	-6 (1)
O(26)	68 (1)	133 (2)	39 (1)	22 (1)	4 (1)	-19 (1)
O(27)	54 (1)	74 (1)	53 (1)	22 (1)	22 (1)	-2 (1)
C(28)	56 (1)	122 (3)	67 (1)	22 (2)	33 (1)	-12 (2)
C(29)	37 (1)	80 (2)	56 (1)	2 (1)	4 (1)	-6 (1)

Table 5: Hydrogen coordinates ($\cdot 10^4$) and isotropic displacement parameters ($Å^2 \cdot 10^3$).

	X		Y		Z		U	
H(2)	2450	(25)	4224	(44)	8763	(20)	54	(7)
H(31)	2980	(25)	6677	(46)	7878	(19)	59	(7)
H(32)	1857	(27)	6176	(47)	6995	(20)	64	(7)
H(41)	3985	(20)	4048	(32)	7695	(14)	35	(4)
H(42)	3681	(25)	5099	(47)	6758	(19)	62	(7)
H(61)	2594	(21)	1293	(37)	7946	(17)	42	(5)
H(62)	1463	(20)	579	(36)	7098	(16)	41	(5)
H(71)	402	(26)	3449	(47)	7160	(20)	63	(8)
H(72)	694	(26)	2347	(47)	8104	(20)	64	(8)
H(12)	7327	(31)	-63	(57)	6441	(25)	76	(8)
H(13)	5325	(20)	-1043	(35)	6273	(15)	38	(5)
H(15)	6335	(38)	-3487	(77)	7359	(30)	108	(14)
H(16)	6868	(63)	-5248	(140)	8717	(51)	175	(24)
H(17)	6326	(38)	-3948	(72)	10048	(29)	101	(12)
H(18)	5419	(28)	-819	(54)	9966	(25)	78	(9)
H(19)	5174	(25)	784	(49)	8503	(18)	60	(7)
H(211)	143	(37)	5861	(66)	9759	(25)	95	(11)
H(212)	1196	(47)	4195	(81)	9812	(31)	112	(16)
H(213)	-160	(36)	4005	(66)	8995	(27)	92	(11)
H(221)	-436	(32)	7613	(61)	8261	(25)	83	(10)
H(222)	-576	(29)	6015	(55)	7563	(22)	67	(8)
H(223)	346	(34)	7615	(64)	7463	(26)	84	(10)
H(231)	1551	(33)	8480	(65)	9544	(26)	84	(10)
H(232)	2362	(49)	7110	(101)	9546	(37)	127	(21)
H(233)	2092	(34)	8493	(59)	8785	(27)	80	(10)
H(24)	1265	(24)	4086	(43)	5765	(18)	51	(6)
H(251)	155	(35)	1641	(62)	5624	(26)	90	(11)
H(252)	1103	(31)	453	(59)	5155	(23)	75	(9)
H(253)	203	(28)	2141	(50)	4652	(21)	67	(8)
H(26)	3053	(32)	3663	(51)	5279	(23)	67	(8)
H(281)	6930	(36)	4698	(67)	5639	(27)	86	(11)
H(282)	6729	(75)	3497	(159)	4995	(58)	209	(32)
H(283)	7837	(44)	3230	(90)	5812	(31)	117	(16)
H(291)	8395	(30)	1939	(54)	7717	(21)	72	(8)
H(292)	8036	(35)	228	(74)	8170	(28)	92	(11)
H(293)	7229	(40)	1922	(77)	8135	(30)	108	(13)

Table 6: Torsion angles [deg].

C(22)-C(1)-C(2)-C(3)	62.4	(3)
C(23)-C(1)-C(2)-C(3)	-57.7	(2)
C(21)-C(1)-C(2)-C(3)	-176.0	(2)
C(22)-C(1)-C(2)-C(7)	-63.5	(3)
C(23)-C(1)-C(2)-C(7)	176.3	(2)
C(21)-C(1)-C(2)-C(7)	58.0	(3)
C(7)-C(2)-C(3)-C(4)	-55.0	(2)
C(1)-C(2)-C(3)-C(4)	175.8	(2)
C(2)-C(3)-C(4)-C(5)	55.5	(2)
C(3)-C(4)-C(5)-C(8)	-165.45	(13)
C(3)-C(4)-C(5)-C(6)	-51.4	(2)
C(3)-C(4)-C(5)-C(24)	70.5	(2)
C(8)-C(5)-C(6)-C(7)	174.34	(13)
C(4)-C(5)-C(6)-C(7)	53.5	(2)
C(24)-C(5)-C(6)-C(7)	-68.2	(2)
C(5)-C(6)-C(7)-C(2)	-59.0	(2)
C(3)-C(2)-C(7)-C(6)	56.5	(2)
C(1)-C(2)-C(7)-C(6)	-174.1	(2)
C(4)-C(5)-C(8)-O(20)	154.73	(14)
C(6)-C(5)-C(8)-O(20)	38.9	(2)
C(24)-C(5)-C(8)-O(20)	-80.1	(2)
C(4)-C(5)-C(8)-N(9)	-16.3	(2)
C(6)-C(5)-C(8)-N(9)	-132.13	(13)
C(24)-C(5)-C(8)-N(9)	108.9	(2)
O(20)-C(8)-N(9)-C(10)	134.9	(2)
C(5)-C(8)-N(9)-C(10)	-53.7	(2)
O(20)-C(8)-N(9)-C(13)	-12.1	(2)
C(5)-C(8)-N(9)-C(13)	159.25	(12)
C(8)-N(9)-C(10)-O(27)	15.4	(3)
C(13)-N(9)-C(10)-O(27)	164.4	(2)
C(8)-N(9)-C(10)-N(11)	-163.4	(2)
C(13)-N(9)-C(10)-N(11)	-14.4	(2)
O(27)-C(10)-N(11)-C(28)	0.2	(4)
N(9)-C(10)-N(11)-C(28)	179.0	(2)
O(27)-C(10)-N(11)-C(12)	178.3	(2)
N(9)-C(10)-N(11)-C(12)	-2.8	(2)
C(10)-N(11)-C(12)-C(29)	-105.7	(2)
C(28)-N(11)-C(12)-C(29)	72.5	(3)
C(10)-N(11)-C(12)-C(13)	17.5	(2)
C(28)-N(11)-C(12)-C(13)	-164.4	(2)
C(10)-N(9)-C(13)-C(14)	146.24	(14)
C(8)-N(9)-C(13)-C(14)	-61.0	(2)
C(10)-N(9)-C(13)-C(12)	24.1	(2)
C(8)-N(9)-C(13)-C(12)	176.81	(12)

N(11)-C(12)-C(13)-N(9)	-23.8	(2)
C(29)-C(12)-C(13)-N(9)	95.9	(2)
N(11)-C(12)-C(13)-C(14)	-147.5	(2)
C(29)-C(12)-C(13)-C(14)	-27.8	(2)
N(9)-C(13)-C(14)-C(19)	-22.1	(2)
C(12)-C(13)-C(14)-C(19)	93.9	(2)
N(9)-C(13)-C(14)-C(15)	162.9	(2)
C(12)-C(13)-C(14)-C(15)	-81.0	(2)
C(19)-C(14)-C(15)-C(16)	-2.3	(3)
C(13)-C(14)-C(15)-C(16)	172.9	(2)
C(14)-C(15)-C(16)-C(17)	1.9	(4)
C(15)-C(16)-C(17)-C(18)	0.0	(4)
C(16)-C(17)-C(18)-C(19)	-1.4	(4)
C(15)-C(14)-C(19)-C(18)	1.0	(3)
C(13)-C(14)-C(19)-C(18)	-174.0	(2)
C(17)-C(18)-C(19)-C(14)	0.9	(3)
C(8)-C(5)-C(24)-O(26)	-48.5	(2)
C(4)-C(5)-C(24)-O(26)	78.3	(2)
C(6)-C(5)-C(24)-O(26)	-162.6	(2)
C(8)-C(5)-C(24)-C(25)	70.6	(2)
C(4)-C(5)-C(24)-C(25)	-162.7	(2)
C(6)-C(5)-C(24)-C(25)	-43.5	(2)

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Table 1: Crystal data and structure refinement.

Empirical formula:	$C_{24}\ H_{42}\ N_2\ O_3$	
Formula weight:	406.61	
Radiation:	Cu-K_α	
Crystal system:	monoclinic	
Space group:	P21/c	
Unit cell dimensions:	a = 16.479(1) Å	α = 90 deg.
	b = 8.0170(7) Å	β = 110.913(7) deg.
	c = 19.145(2) Å	γ = 90 deg.
Volume:	2382.8(7) $Å^3$	
Z:	4	
Density (calculated):	1.143 g/cm^3	
Absorption coefficient:	5.5 cm^{-1}	
Crystal color:	colorless, transparent	
Crystal size:	0.22 x 0.25 x 0.27 mm	
Scan range:	+h ±k ±l hemi-sphere	
(2 Θ)max:	120 deg.	
Reflections collected:	6738	
Independent reflections:	3488	
Reflections used with I > 0:	3403	
Number of variables:	423	
R (F):	0.052	
wR (F):	0.069	
S:	3.28	

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

Starred atoms were refined isotropically. Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as:

$(4/3) \cdot [a^2 \cdot B(1,1) + b^2 \cdot B(2,2) + c^2 \cdot B(3,3) + a \cdot b \cdot (\cos \gamma) \cdot B(1,2) + a \cdot c \cdot (\cos \beta) \cdot B(1,3) + b \cdot c \cdot (\cos \alpha) \cdot B(2,3)]$

	X		Y		Z		U (eq)	
O1	0.05948	(8)	0.6445	(2)	0.75739	(8)	6.06	(4)
O2	0.23882	(7)	1.0037	(2)	0.81883	(6)	4.03	(3)
O3	0.1660	(1)	0.5871	(3)	0.68420	(8)	7.36	(5)
N1	0.14335	(8)	0.8390	(2)	0.84549	(7)	3.23	(3)
N2	0.01010	(9)	0.7768	(2)	0.83944	(8)	4.46	(4)
C1	0.0698	(1)	0.7415	(3)	0.8095	(1)	4.02	(4)
C2	0.0438	(1)	0.8856	(3)	0.9042	(1)	3.91	(4)
C3	0.1147	(1)	0.9770	(2)	0.88431	(9)	3.28	(4)
C4	0.2132	(1)	0.8631	(2)	0.82029	(8)	3.04	(4)
C5	0.2628	(1)	0.7129	(2)	0.80389	(8)	2.89	(3)
C6	0.3603	(1)	0.7630	(2)	0.8384	(1)	3.49	(4)
C7	0.4235	(1)	0.6261	(2)	0.8368	(1)	3.69	(4)
C8	0.4106	(1)	0.4655	(2)	0.87436	(9)	3.14	(4)
C9	0.3147	(1)	0.4146	(2)	0.8404	(1)	3.53	(4)
C10	0.2528	(1)	0.5524	(2)	0.84434	(9)	3.37	(4)
C11	-0.0734	(1)	0.6932	(4)	0.8175	(2)	7.37	(7)
C12	0.0708	(1)	0.7824	(3)	0.9754	(1)	5.05	(5)
C13	0.1846	(1)	1.0740	(2)	0.94507	(9)	3.40	(4)
C14	0.1409	(1)	1.2022	(3)	0.9796	(1)	4.49	(5)
C15	0.2069	(1)	1.3170	(3)	1.0332	(1)	5.18	(5)
C16	0.2754	(1)	1.2206	(3)	1.0935	(1)	5.01	(5)
C17	0.3197	(1)	1.0936	(3)	1.0602	(1)	5.02	(5)
C18	0.2540	(1)	0.9767	(2)	1.0057	(1)	3.90	(4)
C19	0.2393	(1)	0.6876	(2)	0.71818	(9)	3.73	(4)
C20	0.2373	(2)	0.8447	(3)	0.6756	(1)	7.58	(7)
C21	0.4748	(1)	0.3223	(2)	0.87605	(9)	3.67	(4)
C22	0.4534	(1)	0.2423	(3)	0.7989	(1)	5.36	(5)
C23	0.5679	(1)	0.3882	(3)	0.9034	(1)	5.30	(5)
C24	0.4698	(1)	0.1883	(3)	0.9308	(1)	4.95	(5)

Table 3a: Bond lengths [Å].

Numbers in parentheses are estimated standard deviations in the least significant digits.

O1-C1	1.228	(3)	C6-C7	1.520	(3)
O2-C4	1.207	(2)	C7-C8	1.526	(3)
O3-C19	1.405	(2)	C8-C9	1.534	(2)
N1-C1	1.399	(2)	C8-C21	1.554	(3)
N1-C3	1.500	(2)	C9-C10	1.524	(3)
N1-C4	1.412	(2)	C13-C14	1.533	(3)
N2-C1	1.334	(3)	C13-C18	1.522	(2)
N2-C2	1.454	(2)	C14-C15	1.511	(3)
N2-C11	1.452	(3)	C15-C16	1.509	(3)
C2-C3	1.538	(3)	C16-C17	1.519	(3)
C2-C12	1.519	(3)	C17-C18	1.526	(3)
C3-C13	1.526	(2)	C19-C20	1.494	(3)
C4-C5	1.548	(3)	C21-C22	1.532	(3)
C5-C6	1.557	(2)	C21-C23	1.527	(3)
C5-C10	1.540	(2)	C21-C24	1.524	(3)
C5-C19	1.559	(2)			

Table 3b: Bond angles [deg].

C1-N1-C3	106.6	(1)	C5-C6-C7	114.5	(1)
C1-N1-C4	125.2	(2)	C6-C7-C8	112.8	(2)
C3-N1-C4	120.5	(1)	C7-C8-C9	108.6	(1)
C1-N2-C2	112.2	(1)	C7-C8-C21	115.1	(2)
C1-N2-C11	123.2	(2)	C9-C8-C21	113.8	(1)
C2-N2-C11	123.8	(2)	C8-C9-C10	113.1	(1)
O1-C1-N1	126.8	(2)	C5-C10-C9	112.7	(2)
O1-C1-N2	125.0	(2)	C3-C13-C14	109.1	(1)
N1-C1-N2	108.2	(2)	C3-C13-C18	118.6	(1)
N2-C2-C3	99.6	(2)	C14-C13-C18	110.8	(1)
N2-C2-C12	109.8	(2)	C13-C14-C15	111.5	(2)
C3-C2-C12	118.5	(1)	C14-C15-C16	111.6	(2)
N1-C3-C2	99.9	(1)	C15-C16-C17	111.3	(2)
N1-C3-C13	117.9	(1)	C16-C17-C18	111.6	(2)
C2-C3-C13	119.2	(2)	C13-C18-C17	111.3	(2)
O2-C4-N1	118.0	(2)	O3-C19-C5	114.3	(2)
O2-C4-C5	120.5	(2)	O3-C19-C20	112.5	(2)
N1-C4-C5	121.1	(1)	C5-C19-C20	114.4	(2)
C4-C5-C6	104.6	(1)	C8-C21-C22	111.6	(1)
C4-C5-C10	112.9	(2)	C8-C21-C23	110.2	(2)
C4-C5-C19	111.4	(1)	C8-C21-C24	109.3	(2)
C6-C5-C10	106.3	(1)	C22-C21-C23	109.5	(2)
C6-C5-C19	108.1	(2)	C22-C21-C24	108.5	(2)
C10-C5-C19	112.9	(1)	C23-C21-C24	107.6	(1)

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

The form of the anisotropic displacement parameter is:

$\exp [-2\pi^2 \cdot (h^2 \cdot a^2 \cdot U_{11} + k^2 \cdot b^2 \cdot U_{22} + l^2 \cdot c^2 \cdot U_{33} + 2 \cdot h \cdot k \cdot a \cdot b \cdot U_{12} + 2 \cdot h \cdot l \cdot a \cdot c \cdot U_{13} + 2 \cdot k \cdot l \cdot b \cdot c \cdot U_{23})]$ where a, b, and c are reciprocal lattice constants.

	U11	U22	U33	U23	U13	U12
O1	0.0420 (6)	0.098 (1)	0.0844 (8)	-0.0084 (7)	0.0150 (6)	-0.0536 (7)
O2	0.0651 (6)	0.0375 (6)	0.0573 (6)	0.0020 (6)	0.0302 (4)	-0.0011 (6)
O3	0.0741 (8)	0.149 (1)	0.0555 (7)	-0.037 (1)	0.0214 (6)	-0.0361 (9)
N1	0.0358 (6)	0.0463 (8)	0.0391 (6)	0.0013 (6)	0.0117 (5)	-0.0108 (6)
N2	0.0333 (7)	0.073 (1)	0.0615 (8)	-0.0068 (7)	0.0141 (6)	-0.0223 (8)
C1	0.0355 (8)	0.060 (1)	0.0520 (9)	0.0007 (9)	0.0089 (7)	-0.0162 (9)
C2	0.0364 (8)	0.062 (1)	0.0492 (9)	0.0045 (8)	0.0135 (6)	-0.0120 (9)
C3	0.0407 (8)	0.0445 (9)	0.0369 (7)	0.0095 (8)	0.0107 (6)	-0.0024 (8)
C4	0.0380 (8)	0.0448 (9)	0.0297 (7)	0.0021 (8)	0.0082 (6)	-0.0029 (7)
C5	0.0373 (7)	0.0363 (9)	0.0370 (7)	-0.0006 (7)	0.0141 (5)	-0.0016 (7)
C6	0.0404 (8)	0.0375 (9)	0.0551 (9)	-0.0029 (8)	0.0174 (6)	0.0015 (8)
C7	0.0390 (8)	0.045 (1)	0.0586 (9)	-0.0010 (8)	0.0205 (6)	0.0036 (8)
C8	0.0405 (7)	0.0426 (9)	0.0393 (7)	0.0017 (7)	0.0177 (5)	-0.0000 (7)
C9	0.0444 (8)	0.0363 (9)	0.0562 (9)	-0.0026 (8)	0.0216 (6)	0.0026 (8)
C10	0.0392 (7)	0.0421 (9)	0.0503 (8)	-0.0022 (7)	0.0202 (6)	0.0023 (8)
C11	0.040 (1)	0.122 (2)	0.117 (2)	-0.023 (1)	0.027 (1)	-0.055 (1)
C12	0.056 (1)	0.076 (1)	0.064 (1)	-0.009 (1)	0.0277 (7)	0.000 (1)
C13	0.0456 (8)	0.044 (1)	0.0399 (8)	0.0026 (8)	0.0159 (6)	-0.0046 (8)
C14	0.062 (1)	0.051 (1)	0.0533 (9)	0.0127 (9)	0.0166 (8)	-0.0091 (9)
C15	0.089 (1)	0.052 (1)	0.058 (1)	-0.002 (1)	0.0283 (9)	-0.015 (1)
C16	0.073 (1)	0.065 (1)	0.0498 (9)	-0.013 (1)	0.0190 (8)	-0.017 (1)
C17	0.050 (1)	0.080 (1)	0.055 (1)	-0.004 (1)	0.0115 (8)	-0.014 (1)
C18	0.0427 (9)	0.053 (1)	0.0465 (9)	0.0058 (9)	0.0082 (7)	-0.0081 (9)
C19	0.0494 (9)	0.051 (1)	0.0418 (8)	0.0056 (9)	0.0168 (6)	-0.0044 (8)
C20	0.181 (2)	0.069 (1)	0.048 (1)	0.012 (2)	0.054 (1)	0.006 (1)
C21	0.0460 (8)	0.048 (1)	0.0476 (8)	0.0087 (8)	0.0201 (6)	0.0031 (8)
C22	0.084 (1)	0.068 (1)	0.058 (1)	0.024 (1)	0.0326 (8)	-0.004 (1)
C23	0.0458 (9)	0.071 (1)	0.085 (1)	0.014 (1)	0.0232 (8)	0.009 (1)
C24	0.067 (1)	0.056 (1)	0.068 (1)	0.019 (1)	0.0276 (8)	0.017 (1)

Table 5: Hydrogen coordinates ($\cdot 10^4$) and isotropic displacement parameters ($Å^2 \cdot 10^3$).
Starred atoms were refined isotropically. Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as:

$(4/3) \cdot [a^2 \cdot B(1,1) + b^2 \cdot B(2,2) + c^2 \cdot B(3,3) + a \cdot b \cdot (\cos \gamma) \cdot B(1,2) + a \cdot c \cdot (\cos \beta) \cdot B(1,3) + b \cdot c \cdot (\cos \alpha) \cdot B(2,3)]$

	X		Y		Z		U	
H2	0.000	(1)	0.969	(2)	0.907	(1)	5.2	(5)*
H3	0.0869	(9)	1.060	(2)	0.8476	(8)	3.4	(4)*
H6a	0.372	(1)	0.854	(2)	0.8122	(9)	4.1	(4)*
H6b	0.372	(1)	0.789	(2)	0.890	(1)	4.7	(4)*
H7a	0.418	(1)	0.600	(2)	0.784	(1)	4.9	(4)*
H7b	0.485	(1)	0.670	(2)	0.865	(1)	4.6	(4)*
H8	0.425	(1)	0.494	(2)	0.9274	(9)	3.9	(4)*
H9a	0.298	(1)	0.381	(2)	0.7852	(9)	3.8	(4)*
H9b	0.302	(1)	0.315	(2)	0.8629	(9)	4.2	(4)*
H10a	0.264	(1)	0.584	(2)	0.8966	(9)	4.1	(4)*
H10b	0.193	(1)	0.505	(2)	0.822	(1)	4.7	(4)*
H14a	0.099	(1)	1.265	(2)	0.939	(1)	5.0	(5)*
H14b	0.108	(1)	1.139	(3)	1.007	(1)	6.4	(5)*
H15a	0.238	(1)	1.377	(2)	1.007	(1)	5.6	(5)*
H15b	0.176	(1)	1.394	(3)	1.056	(1)	7.1	(6)*
H16a	0.322	(1)	1.308	(3)	1.128	(1)	7.9	(6)*
H16b	0.246	(1)	1.158	(2)	1.123	(1)	5.0	(5)*
H17a	0.349	(1)	1.161	(3)	1.035	(1)	7.3	(6)*
H17b	0.364	(1)	1.027	(3)	1.104	(1)	6.4	(5)*
H18a	0.229	(1)	0.911	(2)	1.0358	(9)	4.4	(4)*
H18b	0.286	(1)	0.901	(2)	0.9833	(9)	4.1	(4)*
H13	0.214	(1)	1.146	(2)	0.9171	(9)	4.7	(4)*
H19	0.284	(1)	0.619	(2)	0.712	(1)	5.3	(5)*
H11a	-0.069	(2)	0.581	(4)	0.804	(2)	13	(1)*
H11b	-0.108	(2)	0.745	(3)	0.835	(1)	9.7	(8)*
H12a	0.118	(1)	0.704	(3)	0.978	(1)	6.2	(5)*
H12b	0.084	(1)	0.857	(3)	1.018	(1)	5.7	(5)*
H11c	-0.107		0.709		0.763		9.2	*
H12c	0.024	(1)	0.705	(3)	0.975	(1)	6.1	(5)*
H20a	0.237	(1)	0.821	(3)	0.628	(1)	8.7	(7)*
H20b	0.275	(2)	0.934	(4)	0.700	(2)	10	(1)*
H20c	0.177	(2)	0.888	(5)	0.674	(2)	16	(1)*
H22a	0.497	(1)	0.154	(3)	0.802	(1)	7.4	(6)*
H22b	0.458	(1)	0.325	(2)	0.767	(1)	5.3	(5)*
H22c	0.393	(1)	0.171	(3)	0.781	(1)	8.4	(7)*
H23a	0.606	(1)	0.287	(3)	0.909	(1)	7.1	(6)*
H23b	0.580	(1)	0.452	(3)	0.951	(1)	8.0	(7)*

H23c	0.579	(1)	0.460	(3)	0.862	(1)	7.2 (6)*
H24a	0.512	(1)	0.103	(3)	0.935	(1)	7.3 (6)*
H24b	0.414	(1)	0.137	(3)	0.918	(1)	6.6 (5)*
H24c	0.483	(1)	0.251	(3)	0.984	(1)	7.8 (6)*
H0	0.1258		0.6153		0.7121		9 *

Table 6: Torsion angles [deg].

C3-N1-C1-O1	160.07	(0.19)
C3-N1-C1-N2	-17.31	(0.19)
C4-N1-C1-O1	10.85	(0.30)
C4-N1-C1-N2	-166.53	(0.16)
C1-N1-C3-C2	32.68	(0.16)
C1-N1-C3-C13	163.47	(0.15)
C4-N1-C3-C2	-176.35	(0.13)
C4-N1-C3-C13	-45.57	(0.20)
C1-N1-C4-O2	132.51	(0.18)
C1-N1-C4-C5	-54.58	(0.22)
C3-N1-C4-O2	-12.78	(0.21)
C3-N1-C4-C5	160.14	(0.14)
C2-N2-C1-O1	175.35	(0.19)
C2-N2-C1-N1	-7.21	(0.22)
C11-N2-C1-O1	5.16	(0.32)
C11-N2-C1-N1	-177.40	(0.19)
C1-N2-C2-C3	27.34	(0.20)
C1-N2-C2-C12	-97.76	(0.19)
C11-N2-C2-C3	-162.55	(0.19)
C11-N2-C2-C12	72.35	(0.24)
N2-C2-C3-N1	-34.34	(0.15)
N2-C2-C3-C13	-164.28	(0.15)
C12-C2-C3-N1	84.56	(0.18)
C12-C2-C3-C13	-45.38	(0.25)
N1-C3-C13-C14	-177.27	(0.14)
N1-C3-C13-C18	-49.21	(0.21)
C2-C3-C13-C14	-55.96	(0.21)
C2-C3-C13-C18	72.09	(0.22)
O2-C4-C5-C6	35.89	(0.19)
O2-C4-C5-C10	151.08	(0.15)
O2-C4-C5-C19	-80.64	(0.19)
N1-C4-C5-C6	-136.85	(0.14)
N1-C4-C5-C10	-21.66	(0.20)
N1-C4-C5-C19	106.62	(0.16)
C4-C5-C6-C7	173.73	(0.14)
C10-C5-C6-C7	54.04	(0.18)
C19-C5-C6-C7	-67.52	(0.18)
C4-C5-C10-C9	-169.06	(0.13)
C6-C5-C10-C9	-54.91	(0.17)
C19-C5-C10-C9	63.50	(0.19)
C4-C5-C19-O3	-87.40	(0.19)
C4-C5-C19-C20	44.33	(0.24)
C6-C5-C19-O3	158.23	(0.16)
C6-C5-C19-C20	-70.05	(0.22)

C10-C5-C19-O3	40.85	(0.22)
C10-C5-C19-C20	172.58	(0.19)
C5-C6-C7-C8	-55.53	(0.19)
C6-C7-C8-C9	52.50	(0.19)
C6-C7-C8-C21	-178.60	(0.14)
C7-C8-C9-C10	-54.60	(0.18)
C21-C8-C9-C10	175.73	(0.14)
C7-C8-C21-C22	-73.77	(0.20)
C7-C8-C21-C23	48.05	(0.20)
C7-C8-C21-C24	166.11	(0.15)
C9-C8-C21-C22	52.56	(0.20)
C9-C8-C21-C23	174.38	(0.15)
C9-C8-C21-C24	-67.56	(0.18)
C8-C9-C10-C5	58.82	(0.18)
C3-C13-C14-C15	-172.71	(0.15)
C18-C13-C14-C15	55.01	(0.21)
C3-C13-C18-C17	178.34	(0.16)
C14-C13-C18-C17	-54.41	(0.21)
C13-C14-C15-C16	-55.71	(0.23)
C14-C15-C16-C17	55.55	(0.25)
C15-C16-C17-C18	-55.04	(0.24)
C16-C17-C18-C13	54.81	(0.22)

2. Abkürzungen

abs.	absolut / absolutiert
Ar	Aryl / Aromat
Ber.	Berechnet
Bn	Benzyl
BuLi	n-Buthyllithium
c.	Konzentration
d	Tag(e)
DC	Dünnschichtchromatographie
de	Diastereomerenüberschuß (diasteromeric excess)
dest.	destilliert
DMAP	4-(N,N-Dimethylamino)pyridin
DMF	N,N-Dimetylformamid
DMS	Dimethylsulfid
DMSO	Dimethylsulfoxid
E	entgegengesetzt (Doppelbindungsgeometrie)
ee	Enantiomerenüberschuß (enantiomeric excess)
EA	Elementaranalyse
EE	Essigsäureethylester
EI	Elektronenstoßionisation
eq.	(Mol-) Äquivalent
Ether	Diethylether
FAB	fast atom bombardment
Fp.	Schmelzpunkt
GC	Gaschromatographie
Gef.	Gefunden
ges.	gesättigt
h	Stunde(n)
Hex	Hexan
HPLC	Hochdruckflüssigkeitschromatographie
IR	Infrarotspektrum
J	Kopplungskonstante

kat.	katalytisch / katalytische Menge
KDA	Kaliumdiisopropylamid
KHMDS	Kaliumhexamethyldisilazid
konz.	konzentriert
LAH	Lthiumaluminiumhydrid
LDA	Lithiumdiisopropylamid
LHMDS	Lithiumhexamethyldisilazid
Me	Methyl
min	Minute(n)
MS	Massenspektrum
NMR	kernmagnetische Resonanz
Ph	Phenyl
ppm	parts per million
RT	Raumtemperatur
s	Sekunde(n)
SEM	β-(Trimethylsilyl)ethoxymethyl
TBS	*t*Butyldimethylsilyl
THF	Tetrahydrofuran
Z	Zusammen (Doppelbindungsgeometrie)