

13.9 Daten der Strukturanalysen

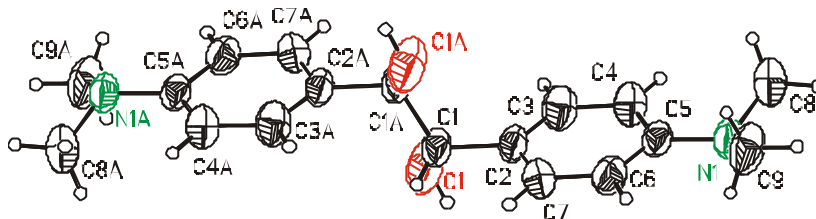
13.9.1 *meso*-1,2-Bis-(4-dimethylaminophenyl)-1,2-ethandiol

Abb. 13.9.1.1: Struktur des *meso*-1,2-Bis-(4-dimethylaminophenyl)-1,2-ethandiols. Die Ellipsoide beschreiben 50%-Aufenthaltswahrscheinlichkeit.

[C₁₈H₂₄N₂O₂], $M = 300.39 \text{ g}\cdot\text{mol}^{-1}$, triklin, Raumgruppe $P\bar{1}$, $a = 6.1806(8) \text{ \AA}$, $b = 8.2109(11) \text{ \AA}$, $c = 8.6343(9) \text{ \AA}$, $\alpha = 96.996(13)^\circ$, $\beta = 99.944(11)^\circ$, $\gamma = 107.915(12)^\circ$, $V = 403.45(9) \text{ \AA}^3$, $Z = 1$, $\rho_{\text{ber.}} = 1.236 \text{ g}\cdot\text{cm}^{-3}$, $\lambda = 0.71073 \text{ \AA}$, $T = 298(2) \text{ K}$, $m = 0.081 \text{ mm}^{-1}$, 1167 unabhängige Reflexe ($R_{\text{int}} = 0.0193$), $R = 0.0942$, $wR_2 = 0.2531$.

Tabelle 13.9.1.1: Atomkoordinaten [10^4] und äquivalente isotrope Versetzungsparameter

[$\text{\AA}^2 \cdot 10^3$] des *meso*-1,2-Bis-(4-dimethylaminophenyl)-1,2-ethandiols.

	x	y	z	U(eq)
N(1)	6888(6)	7107(4)	3550(4)	54(1)
O(1)	-77(7)	727(4)	-1871(3)	96(2)
C(1)	892(8)	545(5)	-378(4)	58(1)
C(2)	2460(7)	2260(4)	685(4)	49(1)
C(3)	1694(7)	3660(5)	907(5)	59(1)
C(4)	3122(7)	5254(5)	1860(5)	54(1)
C(5)	5384(7)	5487(4)	2614(4)	46(1)
C(6)	6153(7)	4068(5)	2394(5)	58(1)

C(7)	4715(8)	2492(5)	1439(5)	60(1)
C(8)	5744(9)	8324(6)	4104(7)	83(2)
C(9)	8757(9)	7044(6)	4806(5)	75(1)

Tabelle 13.9.1.2: Wasserstoffatomkoordinaten [10^4] und isotrope Versetzungsparameter

[$\text{\AA}^2 \cdot 10^3$] des *meso*-1,2-Bis-(4-dimethylaminophenyl)-1,2-ethandiols.

	x	y	z	U(eq)
H(10)	1089	1637	-2248	143
H(1)	1869	-125	-597	69
H(3)	132	3542	389	71
H(4)	2513	6194	1997	65
H(6)	7711	4180	2917	70
H(7)	5309	1545	1303	72
H(8A)	5218	8835	3234	124
H(8B)	6836	9225	4944	124
H(8C)	4431	7706	4504	124
H(9A)	8138	6152	5389	113
H(9B)	9423	8148	5523	113
H(9C)	9942	6791	4333	113

Tabelle 13.9.1.3: Bindungslängen [\AA] und Winkel [$^\circ$] des *meso*-1,2-Bis-(4-dimethylaminophenyl)-1,2-ethandiols.

Bindungslängen [\AA]		Winkel [$^\circ$]	
N(1)-C(5)	1.416(5)	C(5)-N(1)-C(9)	116.4(3)
N(1)-C(9)	1.460(6)	C(5)-N(1)-C(8)	115.8(3)
N(1)-C(8)	1.471(6)	C(9)-N(1)-C(8)	112.1(4)
N(1)-H(10)A	1.9653	C(5)-N(1)-H(10)A	109.0
O(1)-C(1)	1.371(5)	C(9)-N(1)-H(10)A	96.6

O(1)-H(10)	0.9962	C(8)-N(1)-H(10)A	104.3
C(1)-C(1)A	1.492(8)	C(1)-O(1)-H(10)	109.4
C(1)-C(2)	1.517(5)	O(1)-C(1)-C(1)A	111.8(5)
C(1)-H(1)	0.9600	O(1)-C(1)-C(2)	113.3(3)
C(2)-C(7)	1.377(6)	C(1)A-C(1)-C(2)	114.3(4)
C(2)-C(3)	1.377(6)	O(1)-C(1)-H(1)	103.1
C(3)-C(4)	1.395(5)	C(1)A-C(1)-H(1)	106.1
C(3)-H(3)	0.9616	C(2)-C(1)-H(1)	107.2
C(4)-C(5)	1.381(6)	C(7)-C(2)-C(3)	117.3(3)
C(4)-H(4)	0.9602	C(7)-C(2)-C(1)	121.6(4)
C(5)-C(6)	1.392(6)	C(3)-C(2)-C(1)	121.1(4)
C(6)-C(7)	1.387(6)	C(2)-C(3)-C(4)	122.0(4)
C(6)-H(6)	0.9616	C(2)-C(3)-H(3)	119.2
C(7)-H(7)	0.9602	C(4)-C(3)-H(3)	118.8
C(8)-H(8A)	0.9601	C(5)-C(4)-C(3)	120.7(4)
C(8)-H(8B)	0.9599	C(5)-C(4)-H(4)	119.9
C(8)-H(8C)	0.9602	C(3)-C(4)-H(4)	119.4
C(9)-H(9A)	0.9594	C(4)-C(5)-C(6)	117.3(3)
C(9)-H(9B)	0.9593	C(4)-C(5)-N(1)	121.8(4)
C(9)-H(9C)	0.9607	C(6)-C(5)-N(1)	120.9(4)
		C(7)-C(6)-C(5)	121.3(4)
		C(7)-C(6)-H(6)	119.3
		C(5)-C(6)-H(6)	119.4
Bindungslängen [Å]		Winkel [°]	
		C(2)-C(7)-C(6)	121.4(4)
		C(2)-C(7)-H(7)	119.5
		C(6)-C(7)-H(7)	119.1
		N(1)-C(8)-H(8A)	110.0
		N(1)-C(8)-H(8B)	109.1
		H(8A)-C(8)-H(8B)	109.5
		N(1)-C(8)-H(8C)	109.3
		H(8A)-C(8)-H(8C)	109.4
		H(8B)-C(8)-H(8C)	109.5
		N(1)-C(9)-H(9A)	109.5
		N(1)-C(9)-H(9B)	109.5
		H(9A)-C(9)-H(9B)	109.4
		N(1)-C(9)-H(9C)	109.5
		H(9A)-C(9)-H(9C)	109.5
		H(9B)-C(9)-H(9C)	109.4

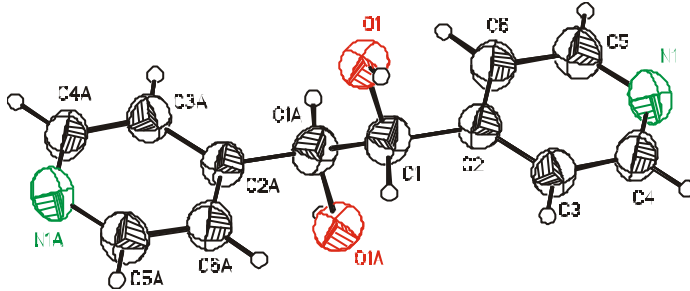
13.9.2 *meso*-1,2-Di(4-pyridyl)-1,2-ethandiol

Abb. 13.9.2.1: Struktur des *meso*-1,2-Di(4-pyridyl)-1,2-ethandiol. Die Ellipsoide beschreiben 50%-Aufenthaltswahrscheinlichkeit.

$[\text{C}_{12}\text{H}_{12}\text{N}_2\text{O}_2]$, $M = 216.24 \text{ g}\cdot\text{mol}^{-1}$, orthorhombisch, Raumgruppe $Pbca$,
 $a = 8.0537(8) \text{ \AA}$, $b = 11.2779(12) \text{ \AA}$, $c = 11.5396(12) \text{ \AA}$, $V = 1048.1(2) \text{ \AA}^3$, $Z = 4$,
 $\rho_{\text{ber.}} = 1.370 \text{ g}\cdot\text{cm}^{-3}$, $\lambda = 0.71073 \text{ \AA}$, $T = 298(2) \text{ K}$, $\mu = 0.095 \text{ mm}^{-1}$, 791
 unabhängige Reflexe ($R_{\text{int}} = 0.0323$), $R = 0.0623$, $wR_2 = 0.1454$.

Tabelle 13.9.2.1: Atomkoordinaten $[10^4]$ und äquivalente isotrope
 Versetzungsparameter

$[\text{\AA}^2 \cdot 10^3]$ des *meso*-1,2-Di(4-pyridyl)-1,2-ethandiol.

	x	y	z	U(eq)
O(1)	3154(3)	207(2)	5872(2)	50(1)
N(1)	3491(4)	3309(2)	2800(2)	55(1)
C(1)	4652(5)	551(3)	5266(3)	49(1)
C(2)	4286(4)	1512(3)	4377(2)	44(1)
C(3)	4740(4)	2672(3)	4569(3)	49(1)
C(4)	4327(4)	3529(3)	3773(3)	54(1)
C(5)	3065(5)	2183(3)	2612(3)	55(1)
C(6)	3421(5)	1276(3)	3366(3)	54(1)

Tabelle 13.9.2.2: Wasserstoffatomkoordinaten [10⁴] und isotrope Versetzungsparameter

[Å² · 10³] des *meso*-1,2-Di(4-pyridyl)-1,2-ethandiols.

	x	y	z	U(eq)
H(10)	3076	653	6596	75
H(1)	5441	846	5819	59
H(3)	5344	2878	5257	58
H(4)	4668	4330	3921	65
H(5)	2475	2000	1911	66
H(6)	3071	481	3196	64

Tabelle 13.9.2.3: Bindungslängen [Å] und Winkel [°] des *meso*-1,2-Di(4-pyridyl)-1,2-ethandiols.

Bindungslängen [Å]		Winkel [°]	
O(1)-C(1)	1.447(4)	C(4)-N(1)-C(5)	116.4(3)
N(1)-C(4)	1.333(4)	C(4)-N(1)-H(10)A	127.4
N(1)-C(5)	1.334(4)	C(5)-N(1)-H(10)A	115.8
N(1)-H(10)A	1.8467	N(1)-H(10)A-O(1)A	163.2
C(1)-C(1)A	1.495(6)	O(1)-C(1)-C(1)A	106.7(3)
C(1)-C(2)	1.521(4)	O(1)-C(1)-C(2)	110.8(3)
C(2)-C(3)	1.377(4)	C(1)A-C(1)-C(2)	112.8(3)
C(2)-C(6)	1.384(4)	C(3)-C(2)-C(6)	116.9(3)
C(3)-C(4)	1.374(4)	C(3)-C(2)-C(1)	121.2(3)

C(5)-C(6)	1.374(4)	C(6)-C(2)-C(1)	121.9(3)
		C(4)-C(3)-C(2)	119.8(3)
		N(1)-C(4)-C(3)	123.7(3)
		N(1)-C(5)-C(6)	123.5(3)
		C(5)-C(6)-C(2)	119.7(3)

13.9.3 *meso*-1,2-Dicyclohexyl-1,2-ethandiol

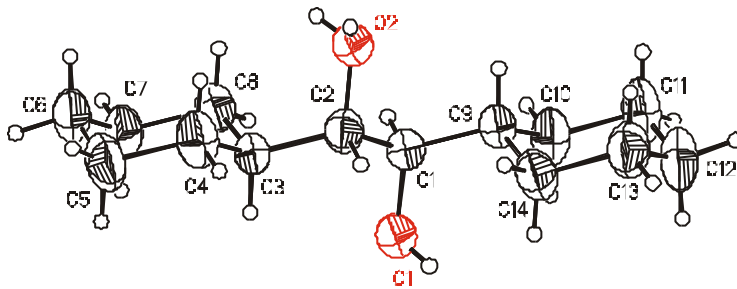


Abb. 13.9.3.1: Struktur des *meso*-1,2-Dicyclohexyl-1,2-ethandiol. Die Ellipsoide beschreiben 50%-Aufenthaltswahrscheinlichkeit.

[C₁₄H₂₆O₂], $M = 226.35 \text{ g}\cdot\text{mol}^{-1}$, orthorhombisch, Raumgruppe *Pbcn*, $a = 10.439(4) \text{ \AA}$, $b = 10.859(5) \text{ \AA}$, $c = 23.359(8) \text{ \AA}$, $V = 2648(2) \text{ \AA}^3$, $Z = 8$, $\rho_{\text{ber.}} = 1.136 \text{ g}\cdot\text{cm}^{-3}$, $\lambda = 0.71073 \text{ \AA}$, $T = 293(2) \text{ K}$, $m = 0.073 \text{ mm}^{-1}$, 1685 unabhängige Reflexe ($R_{\text{int}} = 0.0000$), $R = 0.0786$, $wR_2 = 0.2109$.

Tabelle 13.9.3.1: Atomkoordinaten [10^4] und äquivalente isotrope Versetzungsparameter

[$\text{\AA}^2 \cdot 10^3$] des *meso*-1,2-Dicyclohexyl-1,2-ethandiol.

	x	y	z	U(eq)
O(1)	1340(3)	2368(2)	2537(1)	57(1)
O(2)	3646(3)	-119(3)	2411(1)	56(1)
C(1)	2352(4)	1666(4)	2283(1)	49(1)

C(2)	2623(4)	577(4)	2662(1)	48(1)
C(3)	2901(3)	888(4)	3291(1)	48(1)
C(4)	3040(4)	-285(4)	3643(2)	66(1)
C(5)	3299(5)	-34(5)	4276(2)	76(1)
C(6)	4446(5)	782(4)	4345(2)	69(1)
C(7)	4295(4)	1954(4)	4017(2)	63(1)
C(8)	4051(4)	1695(4)	3383(1)	57(1)
C(9)	2087(4)	1374(4)	1651(1)	50(1)
C(10)	2015(4)	2550(4)	1302(2)	66(1)
C(11)	1813(5)	2292(5)	668(2)	79(2)
C(12)	636(5)	1550(5)	576(2)	79(2)
C(13)	679(5)	353(4)	911(2)	71(1)
C(14)	900(4)	602(4)	1550(2)	61(1)

Tabelle 13.9.3.2: Wasserstoffatomkoordinaten [10⁴] und isotrope Versetzungsparameter

[Å² · 10³] des *meso*-1,2-Dicyclohexyl-1,2-ethandiols.

	x	y	z	U(eq)
H(10)	1366	3172	2509	58(13)
H(10')	626	2106	2411	58(13)
H(20)	4351	106	2560	58(13)
H(20')	3704	-778	2405	58(13)
H(1)	3103	2175	2300	58
H(2)	1866	75	2655	57
H(3)	2172	1319	3442	58
H(4A)	3752	-737	3490	79
H(4B)	2286	-783	3601	79
H(5A)	3442	-798	4474	91
H(5B)	2558	353	4440	91
H(6A)	5202	360	4217	83
H(6B)	4557	983	4742	83
H(7A)	5043	2461	4061	76
H(7B)	3577	2401	4168	76

H(8A)	3931	2461	3185	68
H(8B)	4787	1293	3223	68
H(9)	2808	919	1509	60
H(10A)	2773	3036	1357	79
)				
H(10B)	1297	3016	1440	79
)				
H(11A)	2549	1864	523	95
)				
H(11B)	1737	3057	465	95
)				
H(12A)	556	1367	175	95
)				
H(12B)	-106	2008	691	95
)				
H(13A)	1375	-139	770	86
)				
H(13B)	-100	-102	856	86
)				
H(14A)	169	1033	1699	73
)				
H(14B)	975	-165	1751	73
)				

Tabelle 13.9.3.3: Bindungslängen [Å] und Winkel [°] des *meso*-1,2-Dicyclohexyl-1,2-ethandiols.

Bindungslängen [Å]		Winkel [°]	
O(1)-C(1)	1.431(4)	C(1)-O(1)-H(10)	118.5
O(1)-H(20')A	2.0372	C(1)-O(1)-H(10')	109.0
O(1)-H(10')A	2.0757	H(10)-O(1)-H(10')	109.6
O(1)-H(10)	0.8760	C(2)-O(2)-H(20)	109.1
O(1)-H(10')	0.8500	H(10)A-O(2)- H(20)	103.9
O(2)-C(2)	1.434(4)	C(2)-O(2)-H(20')	126.6
O(2)-H(10)A	1.8698	H(20)-O(2)-H(20')	102.8
O(2)-H(20)A	2.1056	O(1)-C(1)-C(2)	108.3(3)
O(2)-H(20)	0.8500	O(1)-C(1)-C(9)	112.0(3)

O(2)-H(20')	0.7183	C(2)-C(1)-C(9)	115.9(3)
C(1)-C(2)	1.503(5)	O(2)-C(2)-C(1)	108.3(3)
C(1)-C(9)	1.536(5)	O(2)-C(2)-C(3)	111.5(3)
Bindungslängen [Å]		Winkel [°]	
C(2)-C(3)	1.537(4)	C(1)-C(2)-C(3)	115.2(3)
C(3)-C(8)	1.501(5)	C(8)-C(3)-C(4)	109.6(3)
C(3)-C(4)	1.524(5)	C(8)-C(3)-C(2)	114.5(3)
C(4)-C(5)	1.527(5)	C(4)-C(3)-C(2)	110.5(3)
C(5)-C(6)	1.499(6)	C(3)-C(4)-C(5)	113.0(4)
C(6)-C(7)	1.493(6)	C(6)-C(5)-C(4)	110.5(3)
C(7)-C(8)	1.531(5)	C(7)-C(6)-C(5)	111.4(4)
C(9)-C(14)	1.515(5)	C(6)-C(7)-C(8)	111.0(4)
C(9)-C(10)	1.518(5)	C(3)-C(8)-C(7)	112.2(3)
C(10)-C(11)	1.522(5)	C(14)-C(9)-C(10)	109.9(3)
C(11)-C(12)	1.484(7)	C(14)-C(9)-C(1)	114.3(3)
C(12)-C(13)	1.518(6)	C(10)-C(9)-C(1)	110.6(3)
C(13)-C(14)	1.535(5)	C(9)-C(10)-C(11)	112.0(4)
		C(12)-C(11)-C(10)	110.8(4)
		C(11)-C(12)-C(13)	111.5(4)
		C(12)-C(13)-C(14)	110.8(4)
		C(9)-C(14)-C(13)	111.8(4)

13.9.4 5,10-Dihydrophenazin

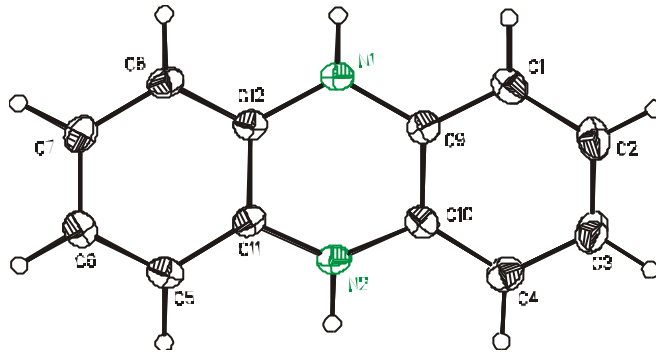


Abb. 13.9.4.1: Struktur des 5,10-Dihydrophenazins. Die Ellipsoide beschreiben 50%-Aufenthaltswahrscheinlichkeit.

$[\text{C}_{12}\text{H}_{10}\text{N}_2]$, $M = 182.22 \text{ g}\cdot\text{mol}^{-1}$, orthorhombisch, Raumgruppe $Pbca$,
 $a = 10.7727(14) \text{ \AA}$, $b = 7.5924(9) \text{ \AA}$, $c = 21.775(3) \text{ \AA}$, $V = 1781.0(4) \text{ \AA}^3$, $Z = 8$,
 $\rho_{\text{ber.}} = 1.359 \text{ g}\cdot\text{cm}^{-3}$, $\lambda = 0.71073 \text{ \AA}$, $T = 123(2) \text{ K}$, $m = 0.082 \text{ mm}^{-1}$, 1458
unabhängige Reflexe ($R_{\text{int}} = 0.0203$), $R = 0.0349$, $wR_2 = 0.0953$.

Tabelle 13.9.4.1: Atomkoordinaten [10^4] und äquivalente isotrope

Versetzungsparameter

$[\text{\AA}^2 \cdot 10^3]$ des 5,10-Dihydrophenazins.

	x	y	z	U(eq)
C(1)	3244(1)	2359(2)	8541(1)	24(1)
C(2)	2655(1)	2817(2)	7991(1)	22(1)
C(3)	3154(1)	2307(2)	7431(1)	19(1)
N(4)	2594(1)	2696(2)	6866(1)	22(1)
C(5)	3301(1)	2667(2)	6323(1)	20(1)
C(6)	2949(1)	3567(2)	5798(1)	25(1)
C(7)	3661(1)	3444(2)	5265(1)	30(1)
C(11)	4350(1)	1437(2)	8531(1)	23(1)
C(12)	4862(1)	937(2)	7968(1)	21(1)
C(13)	4265(1)	1330(2)	7422(1)	19(1)
N(14)	4676(1)	678(2)	6852(1)	22(1)
C(15)	4388(1)	1649(2)	6316(1)	20(1)
C(16)	5090(1)	1541(2)	5787(1)	26(1)
C(17)	4724(1)	2433(2)	5258(1)	31(1)

Tabelle 13.9.4.2: Wasserstoffatomkoordinaten $[10^4]$ und isotrope Versetzungsparameter $[\text{\AA}^2 \cdot 10^3]$ des 5,10-Dihydrophenazins.

	x	y	z	U(eq)
H(1)	2879	2686	8926	29
H(2)	1900	3488	8001	26
H(4)	1939	3577	6883	26
H(6)	2211	4276	5800	30
H(7)	3411	4068	4902	36
H(11)	4763	1142	8908	28
H(12)	5637	315	7960	26
H(14)	5442	94	6858	26
H(16)	5835	846	5783	31
H(17)	5210	2345	4889	37

Tabelle 13.9.4.3: Bindungslängen $[\text{\AA}]$ und Winkel $[^\circ]$ des 5,10-Dihydrophenazins.

Bindungslängen $[\text{\AA}]$		Winkel $[^\circ]$	
C(1)-C(11)	1.382(2)	C(11)-C(1)-C(2)	120.20(1)

C(1)-C(2)	1.399(2)	C(3)-C(2)-C(1)	120.51(13)
C(2)-C(3)	1.388(2)	C(2)-C(3)-N(4)	123.13(12)
C(3)-N(4)	1.401(2)	C(2)-C(3)-C(13)	119.14(12)
C(3)-C(13)	1.408(2)	N(4)-C(3)-C(13)	117.72(12)
N(4)-C(5)	1.405(2)	C(3)-N(4)-C(5)	120.09(11)
C(5)-C(6)	1.386(2)	C(6)-C(5)-C(15)	119.39(12)
C(5)-C(15)	1.403(2)	C(6)-C(5)-N(4)	122.55(12)
C(6)-C(7)	1.393(2)	C(15)-C(5)-N(4)	118.04(12)
Bindungslängen [Å]		Winkel [°]	
C(7)-C(17)	1.379(2)	C(5)-C(6)-C(7)	120.25(13)
C(11)-C(12)	1.395(2)	C(17)-C(7)-C(6)	120.28(14)
C(12)-C(13)	1.385(2)	C(1)-C(11)-C(12)	119.51(13)
C(13)-N(14)	1.410(2)	C(13)-C(12)-C(11)	120.73(13)
N(14)-C(15)	1.414(2)	C(12)-C(13)-C(3)	119.85(12)
C(15)-C(16)	1.381(2)	C(12)-C(13)-N(14)	122.35(12)
C(16)-C(17)	1.393(2)	C(3)-C(13)-N(14)	117.64(11)
		C(13)-N(14)-C(15)	118.34(11)
		C(16)-C(15)-C(5)	119.93(13)
		C(16)-C(15)-N(14)	122.48(12)
		C(5)-C(15)-N(14)	117.48(12)
		C(15)-C(16)-	120.41(1

C(17)	3)
C(7)-C(17)-C(16)	119.74(1)
	3)

13.9.5 1,4-Bis-(4-methoxyphenyl)-1,4-diaza-1,3-butadien

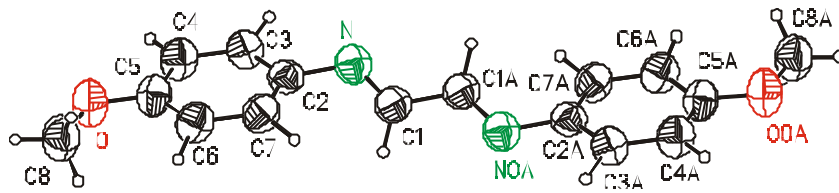


Abb. 13.9.5.1: Struktur des 1,4-Bis-(4-methoxyphenyl)-1,4-diaza-1,3-butadien. Die Ellipsoide beschreiben 50%-Aufenthaltswahrscheinlichkeit.

$[\text{C}_{16}\text{H}_{16}\text{N}_2\text{O}_2]$, $M = 268.31 \text{ g}\cdot\text{mol}^{-1}$, monoclin, Raumgruppe $P2_1/c$, $a = 10.847(7) \text{ \AA}$, $b = 4.159(3) \text{ \AA}$, $c = 15.419(11) \text{ \AA}$, $\beta = 99.55(6)^\circ$, $V = 686.0(8) \text{ \AA}^3$, $Z = 2$, $\rho_{\text{ber.}} = 1.299 \text{ g}\cdot\text{cm}^{-3}$, $\lambda = 0.71073 \text{ \AA}$, $T = 301(2) \text{ K}$, $m = 0.087 \text{ mm}^{-1}$, 1167 unabhängige Reflexe ($R_{\text{int}} = 0.0574$), $R = 0.0688$, $wR_2 = 0.1872$.

Tabelle 13.9.5.1: Atomkoordinaten $[10^4]$ und äquivalente isotrope Versetzungsparameter

$[\text{Å}^2 \cdot 10^3]$ des 1,4-Bis-(4-methoxyphenyl)-1,4-diaza-1,3-butadien.

	x	y	z	U(eq)
N(1)	6191(2)	-1432(5)	809(2)	91(1)
O(1)	8928(2)	1009(5)	4120(1)	102(1)
C(1)	5330(3)	402(6)	431(2)	88(1)
C(2)	6829(3)	-689(6)	1662(2)	82(1)
C(3)	8040(3)	-1833(7)	1904(2)	90(1)
C(4)	8711(3)	-1210(6)	2723(2)	89(1)
C(5)	8176(3)	519(6)	3327(2)	85(1)
C(6)	6960(3)	1582(6)	3114(2)	90(1)
C(7)	6302(3)	998(6)	2287(2)	88(1)
C(8)	8420(3)	2658(8)	4791(2)	109(1)

Tabelle 13.9.5.2: Wasserstoffatomkoordinaten $[10^4]$ und isotrope Versetzungsparameter

$[\text{Å}^2 \cdot 10^3]$ des 1,4-Bis-(4-methoxyphenyl)-1,4-diaza-1,3-butadien.

	x	y	z	U(eq)
H(1)	5105	2327	714	106
H(3)	8420	-3061	1491	107
H(4)	9554	-2011	2883	107
H(6)	6567	2681	3544	108
H(7)	5463	1828	2129	105
H(8A)	8152	4776	4588	163
H(8B)	9053	2833	5312	163
H(8C)	7714	1475	4929	163

Tabelle 13.9.5.3: Bindungslängen $[\text{Å}]$ und Winkel $[^\circ]$ des 1,4-Bis-(4-methoxyphenyl)-1,4-diaza-1,3-butadien.

Bindungslängen [Å]		Winkel [°]	
N(1)-C(1)	1.271(3)	C(1)-N(1)-C(2)	120.3(2)
N(1)-C(2)	1.415(4)	C(5)-O(1)-C(8)	118.4(2)
O(1)-C(5)	1.367(3)	N(1)-C(1)-C(1)A	119.9(3)
O(1)-C(8)	1.427(3)	C(3)-C(2)-C(7)	117.8(3)
C(1)-C(1)A	1.440(5)	C(3)-C(2)-N(1)	118.0(2)
C(2)-C(3)	1.388(4)	C(7)-C(2)-N(1)	124.1(3)
C(2)-C(7)	1.390(4)	C(4)-C(3)-C(2)	121.0(3)
C(3)-C(4)	1.374(4)	C(3)-C(4)-C(5)	120.1(3)
C(4)-C(5)	1.378(4)	O(1)-C(5)-C(4)	115.2(3)
C(5)-C(6)	1.378(4)	O(1)-C(5)-C(6)	124.8(3)
C(6)-C(7)	1.376(4)	C(4)-C(5)-C(6)	120.0(3)
		C(7)-C(6)-C(5)	119.6(3)
		C(6)-C(7)-C(2)	121.5(3)

13.9.6 1,4-Bis-(4-methylphenyl)-1,4-diaza-1,3-butadien

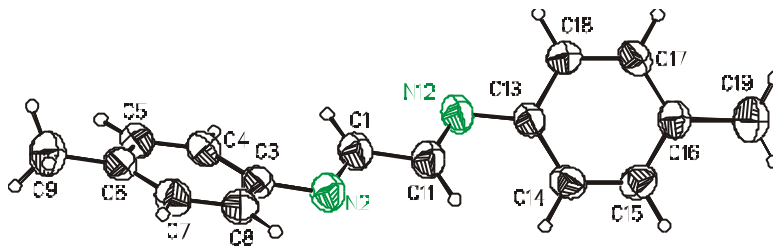


Abb. 13.9.6.1: Struktur des 1,4-Bis-(4-methylphenyl)-1,4-diaza-1,3-butadiens. Die Ellipsoide beschreiben 50%-Aufenthaltswahrscheinlichkeit.

[C₁₆H₁₆N₂], $M = 236.31 \text{ g}\cdot\text{mol}^{-1}$, triklin, Raumgruppe $P\bar{1}$, $a = 8.251(8) \text{ \AA}$, $b = 9.263(10) \text{ \AA}$, $c = 9.673(12) \text{ \AA}$, $\alpha = 93.30(5)^\circ$, $\beta = 97.45(4)^\circ$, $\gamma = 114.92(2)^\circ$, $V = 659.5(13) \text{ \AA}^3$, $Z = 2$, $\rho_{\text{ber.}} = 1.190 \text{ g}\cdot\text{cm}^{-3}$, $\lambda = 0.71073 \text{ \AA}$, $T = 293(2) \text{ K}$, $m = 0.071 \text{ mm}^{-1}$, 2075 unabhängige Reflexe ($R_{\text{int}} = 0.0205$), $R = 0.0655$, $wR_2 = 0.1560$.

Tabelle 13.9.6.1: Atomkoordinaten [10^4] und äquivalente isotrope Versetzungsparameter

[$\text{\AA}^2 \cdot 10^3$] des 1,4-Bis-(4-methylphenyl)-1,4-diaza-1,3-butadiens.

	x	y	z	U(eq)
C(1)	8429(3)	7521(3)	10156(2)	51(1)
N(2)	9563(2)	8412(2)	11211(2)	51(1)
C(3)	11002(3)	8066(2)	11803(2)	42(1)
C(4)	11773(3)	7234(2)	11072(2)	44(1)
C(5)	13154(3)	6945(2)	11756(2)	47(1)
C(6)	13820(3)	7439(2)	13188(2)	46(1)
C(7)	13071(3)	8282(3)	13901(2)	48(1)
C(8)	11707(3)	8605(2)	13224(2)	48(1)
C(9)	15314(3)	7099(3)	13935(2)	68(1)
C(11)	6913(3)	7823(3)	9577(2)	50(1)
N(12)	5686(2)	6831(2)	8604(2)	53(1)
C(13)	4156(3)	7083(2)	8070(2)	42(1)
C(14)	4098(3)	8564(2)	8108(2)	46(1)
C(15)	2520(3)	8668(3)	7574(2)	49(1)
C(16)	937(3)	7302(3)	6987(2)	45(1)
C(17)	1023(3)	5840(3)	6944(2)	47(1)
C(18)	2594(3)	5722(3)	7470(2)	48(1)
C(19)	-766(3)	7427(3)	6391(2)	65(1)

Tabelle 13.9.6.2: Wasserstoffatomkoordinaten $[10^4]$ und isotrope Versetzungsparameter

$[\text{\AA}^2 \cdot 10^3]$ des 1,4-Bis-(4-methylphenyl)-1,4-diaza-1,3-butadiens.

	x	y	z	U(eq)
H(1)	8583	6634	9734	61
H(4)	11334	6861	10089	53
H(5)	13681	6395	11230	56
H(7)	13516	8655	14883	58
H(8)	11230	9215	13733	57
H(9A)	16443	7777	13663	101
H(9B)	15052	5995	13687	101
H(9C)	15400	7308	14932	101
H(11)	6832	8777	9926	60
H(14)	5162	9522	8502	55

H(15)	2507	9700	7602	59
H(17)	-36	4885	6534	56
H(18)	2618	4693	7418	57
H(19A)	-843	7434	5392	97
)				
H(19B)	-744	8402	6810	97
)				
H(19C)	-1800	6526	6588	97
)				

Tabelle 13.9.6.3: Bindungslängen [Å] und Winkel [°] des 1,4-Bis-(4-methylphenyl)-1,4-diaza-1,3-butadiens.

Bindungslängen [Å]		Winkel [°]	
C(1)-N(2)	1.265(3)	N(2)-C(1)-C(11)	121.1(2)
C(1)-C(11)	1.445(3)	C(1)-N(2)-C(3)	120.5(2)
N(2)-C(3)	1.416(3)	C(8)-C(3)-C(4)	117.7(2)
C(3)-C(8)	1.395(3)	C(8)-C(3)-N(2)	117.1(2)
C(3)-C(4)	1.402(3)	C(4)-C(3)-N(2)	125.2(2)
C(4)-C(5)	1.375(3)	C(5)-C(4)-C(3)	120.3(2)
C(5)-C(6)	1.396(3)	C(4)-C(5)-C(6)	121.9(2)
C(6)-C(7)	1.387(3)	C(7)-C(6)-C(5)	117.5(2)
C(6)-C(9)	1.504(3)	C(7)-C(6)-C(9)	120.8(2)
C(7)-C(8)	1.378(3)	C(5)-C(6)-C(9)	121.7(2)
C(11)-N(12)	1.274(3)	C(8)-C(7)-C(6)	121.2(2)
N(12)-C(13)	1.417(3)	C(7)-C(8)-C(3)	121.2(2)
C(13)-C(14)	1.390(3)	N(12)-C(11)-C(1)	120.4(2)
C(13)-C(18)	1.393(3)	C(11)-N(12)- C(13)	120.8(2)
C(14)-C(15)	1.381(3)	C(14)-C(13)- C(18)	118.3(2)
C(15)-C(16)	1.401(3)	C(14)-C(13)- N(12)	125.3(2)
C(16)-C(17)	1.384(3)	C(18)-C(13)- N(12)	116.4(2)
C(16)-C(19)	1.502(3)	C(15)-C(14)- C(13)	120.4(2)
C(17)-C(18)	1.380(3)	C(14)-C(15)- C(16)	121.6(2)

C(17)-C(16)- C(15)	117.3(2)
C(17)-C(16)- C(19)	121.5(2)
C(15)-C(16)- C(19)	121.2(2)
C(18)-C(17)- C(16)	121.7(2)
C(17)-C(18)- C(13)	120.7(2)

13.9.7 1,4-Bis-(4-bromphenyl)-1,4-diaza-1,3-butadien

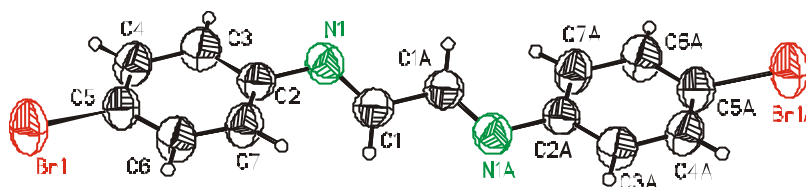


Abb. 13.9.7.1: Struktur des 1,4-Bis-(4-bromphenyl)-1,4-diaza-1,3-butadien. Die Ellipsoide beschreiben 50%-Aufenthaltswahrscheinlichkeit.

[C₁₄H₁₀N₂Br₂N₂], $M = 183.03 \text{ g mol}^{-1}$, triklin, Raumgruppe $P\bar{1}$, $a = 4.1383(6) \text{ \AA}$, $b = 6.2081(5) \text{ \AA}$, $c = 13.2786(12) \text{ \AA}$, $\alpha = 91.369(7)^\circ$, $\beta = 97.856(9)^\circ$, $\gamma = 95.634(9)^\circ$, $V = 336.06(6) \text{ \AA}^3$, $Z = 1$, $\rho_{\text{ber.}} = 1.809 \text{ g cm}^{-3}$, $\lambda = 0.71073 \text{ \AA}$, $T = 300(2) \text{ K}$, $m = 6.013 \text{ mm}^{-1}$, 1822 unabhängige Reflexe ($R_{\text{int}} = 0.0414$), $R = 0.0613$, $wR_2 = 0.1414$.

Tabelle 13.9.7.1: Atomkoordinaten [10^4] und äquivalente isotrope Versetzungsparameter

[$\text{\AA}^2 \cdot 10^3$] des 1,4-Bis-(4-bromphenyl)-1,4-diaza-1,3-butadien.

	x	y	z	U(eq)
Br(1)	1350(2)	7173(1)	9259(1)	84(1)
N(1)	-1664(9)	12887(6)	5677(3)	62(1)
C(1)	427(13)	14326(8)	5430(4)	60(1)

C(2)	-825(11)	11596(7)	6522(4)	53(1)
C(3)	-	9492(7)	6492(4)	61(1)
	2321(12)			
C(4)	-	8177(7)	7302(4)	64(1)
	1623(13)			
C(5)	446(12)	8979(7)	8148(4)	60(1)
C(6)	1923(14)	11081(8)	8205(4)	67(1)
C(7)	1260(12)	12384(7)	7379(4)	63(1)

Tabelle 13.9.7.2: Wasserstoffatomkoordinaten [10⁴] und isotrope Versetzungsparameter

[Å² · 10³] des 1,4-Bis-(4-bromphenyl)-1,4-diaza-1,3-butadien.

	x	y	z	U(eq)
H(1)	2570(111)	14629(66)	5742(36)	46(11)
))))
H(3)	-	8965(7)	5927(4)	73
	3793(12)			
H(4)	-	6749(7)	7272(4)	77
	2560(13)			
H(6)	3330(14)	11614(8)	8782(4)	80
H(7)	2234(12)	13803(7)	7406(4)	75

Tabelle 13.9.7.3: Bindungslängen [Å] und Winkel [°] des 1,4-Bis-(4-bromphenyl)-1,4-diaza-1,3-butadien.

Bindungslängen [Å]		Winkel [°]	
Br(1)-C(5)	1.894(5)	C(1)-N(1)-C(2)	119.9(4)
N(1)-C(1)	1.263(6)	N(1)-C(1)-C(1)A	120.2(6)
N(1)-C(2)	1.419(6)	C(7)-C(2)-C(3)	119.5(5)
C(1)-C(1)A	1.456(11)	C(7)-C(2)-N(1)	122.7(4)
C(2)-C(7)	1.379(6)	C(3)-C(2)-N(1)	117.7(4)
C(2)-C(3)	1.387(6)	C(4)-C(3)-C(2)	119.9(5)
C(3)-C(4)	1.382(7)	C(5)-C(4)-C(3)	119.9(4)
C(4)-C(5)	1.367(7)	C(4)-C(5)-C(6)	121.2(5)

C(5)-C(6)	1.382(7)	C(4)-C(5)-Br(1)	119.6(4)
C(6)-C(7)	1.391(7)	C(6)-C(5)-Br(1)	119.2(4)
		C(5)-C(6)-C(7)	118.6(5)
		C(2)-C(7)-C(6)	120.8(4)

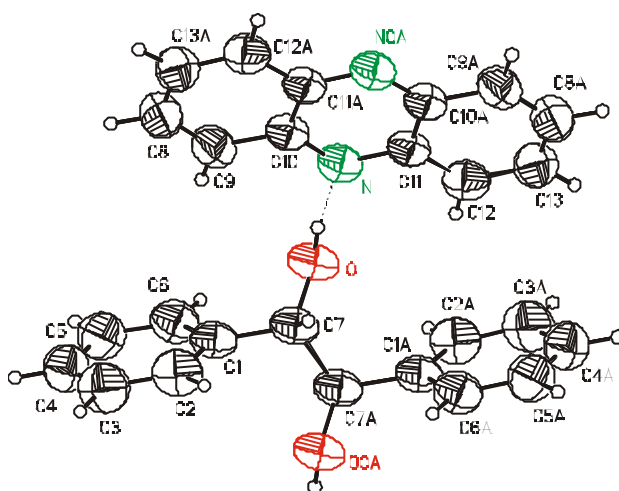
13.9.8 Phenazin und *meso*-1,2-Diphenyl-1,2-ethandiol

Abb. 13.9.8.1: Struktur des Kokristalls aus Phenazin und *meso*-1,2-Diphenyl-1,2-ethandiol. Die Ellipsoide beschreiben 50%-Aufenthaltswahrscheinlichkeit.

$[\text{C}_{12}\text{H}_8\text{N}_2] \cdot [\text{C}_{14}\text{H}_{14}\text{O}_2]$, $M = 394.46 \text{ g}\cdot\text{mol}^{-1}$, triklin, Raumgruppe $P\bar{1}$,
 $a = 5.6610(10) \text{ \AA}$, $b = 8.6428(13) \text{ \AA}$, $c = 10.524(2) \text{ \AA}$, $\alpha = 85.978(9)^\circ$,
 $\beta = 82.388(10)^\circ$, $\gamma = 86.478(12)^\circ$, $V = 508.41(14) \text{ \AA}^3$, $Z = 1$, $\rho_{\text{ber.}} = 1.288 \text{ g}\cdot\text{cm}^{-3}$,
 $\lambda = 0.71073 \text{ \AA}$, $T = 293 \text{ K}$, $m = 0.082 \text{ mm}^{-1}$, 2056 unabhängige Reflexe
 $(R_{\text{int}} = 0.0203)$, $R = 0.0532$, $wR_2 = 0.1332$.

Tabelle 13.9.8.1: Atomkoordinaten $[10^4]$ und äquivalente isotrope Versetzungsparameter

$[\text{Å}^2 \cdot 10^3]$ des Kokristalls aus Phenazin und *meso*-1,2-Diphenyl-1,2-ethandiol.

	x	y	z	U(eq)
O(1)	-717(2)	1946(1)	508(1)	72(1)
C(1)	416(3)	-345(2)	1791(2)	62(1)
C(2)	2272(3)	-1338(2)	2147(2)	75(1)
C(3)	2099(4)	-2114(2)	3344(2)	87(1)
C(4)	94(4)	-1906(2)	4209(2)	84(1)
C(5)	-1752(4)	-939(2)	3875(2)	83(1)
C(6)	-1604(3)	-159(2)	2677(2)	72(1)
C(7)	544(3)	476(2)	468(2)	63(1)
N	3087(2)	4005(1)	217(1)	60(1)
C(8)	5164(4)	3717(2)	3335(2)	78(1)
C(9)	3846(3)	3481(2)	2393(2)	70(1)
C(10)	4392(3)	4245(2)	1154(2)	58(1)
C(11)	3674(3)	4746(2)	-936(2)	57(1)
C(12)	2349(3)	4524(2)	-1960(2)	67(1)
C(13)	2932(4)	5275(2)	-3120(2)	76(1)

Tabelle 13.9.8.2: Wasserstoffatomkoordinaten $[10^4]$ und isotrope Versetzungsparameter

$[\text{Å}^2 \cdot 10^3]$ des Kokristalls aus Phenazin und *meso*-1,2-Diphenyl-1,2-ethandiol.

	x	y	z	U(eq)
H(1)	397	2753	505	107
H(2)	3673	-1471	1534	90
H(3)	3397	-2805	3564	105
H(4)	-36	-2424	5050	101
H(5)	-3155	-777	4481	100
H(6)	-2928	493	2436	87
H(7)	2187	613	139	75
H(8)	4740	3235	4178	93
H(9)	2583	2772	2545	84
H(12)	1088	3814	-1832	80

H(13) | 1978 5160 -3793 91

Tabelle 13.9.8.3: Bindungslängen [Å] und Winkel [°] des Kokristalls aus Phenazin und *meso*-1,2-Diphenyl-1,2-ethandiol.

Bindungslängen [Å]		Winkel [°]	
O(1)-C(7)	1.419(2)	C(6)-C(1)-C(2)	117.9(2)
C(1)-C(6)	1.385(2)	C(6)-C(1)-C(7)	120.5(2)
C(1)-C(2)	1.388(2)	C(2)-C(1)-C(7)	121.6(2)
C(1)-C(7)	1.513(2)	C(3)-C(2)-C(1)	120.9(2)
C(2)-C(3)	1.380(3)	C(4)-C(3)-C(2)	120.3(2)
C(3)-C(4)	1.369(3)	C(5)-C(4)-C(3)	119.6(2)
C(4)-C(5)	1.365(3)	C(4)-C(5)-C(6)	120.6(2)
C(5)-C(6)	1.383(3)	C(5)-C(6)-C(1)	120.7(2)
C(7)-C(7)A	1.537(3)	O(1)-C(7)-C(1)	111.21(13)
N-C(10)	1.342(2)	O(1)-C(7)-C(7)A	107.6(2)
N-C(11)	1.343(2)	C(1)-C(7)-C(7)A	111.4(2)
C(8)-C(9)	1.351(3)	C(10)-N-C(11)	117.53(13)
C(8)-C(13)A	1.412(3)	C(9)-C(8)-C(13)A	121.1(2)
C(9)-C(10)	1.424(2)	C(8)-C(9)-C(10)	119.7(2)
C(10)-C(11)A	1.426(2)	N-C(10)-C(9)	119.66(14)
C(11)-C(12)	1.422(2)	N-C(10)-C(11)A	121.29(14)
C(11)-C(10)A	1.426(2)	C(9)-C(10)-C(11)A	119.1(2)
C(12)-C(13)	1.352(3)	N-C(11)-C(12)	119.60(14)
C(13)-C(8)A	1.412(3)	N-C(11)-C(10)A	121.18(14)
		C(12)-C(11)- C(10)A	119.2(2)
		C(13)-C(12)-C(11)	119.6(2)
		C(12)-C(13)-C(8)A	121.2(2)

13.9.9 Phenazin und 2,2'-Dihydroxybiphenyl

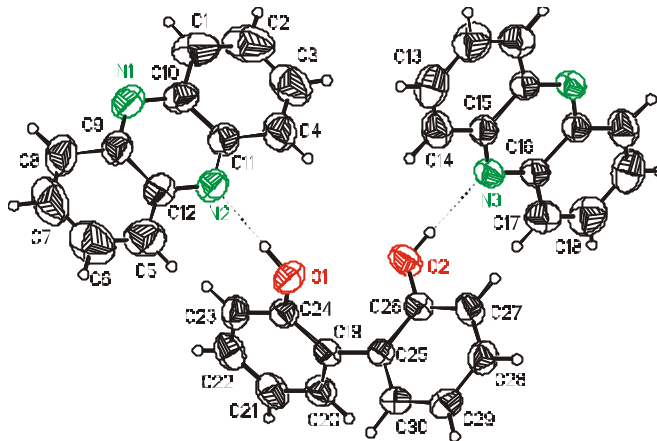


Abb. 13.9.9.1: Struktur des Kokristalls aus Phenazin und 2,2'-Dihydroxybiphenyl. Die Ellipsoide beschreiben 50%-Aufenthaltswahrscheinlichkeit.

$2[\text{C}_{12}\text{H}_{10}\text{O}_2] \cdot 3[\text{C}_{12}\text{H}_8\text{N}_2]$, $M = 456.51 \text{ g}\cdot\text{mol}^{-1}$, monoklin, Raumgruppe $P2_1/c$, $a = 19.468(2) \text{ \AA}$, $b = 7.1789(7) \text{ \AA}$, $c = 18.4599(13) \text{ \AA}$, $\beta = 115.517(5)^\circ$, $V = 2328.3(3) \text{ \AA}^3$, $Z = 4$, $\rho_{\text{ber.}} = 1.302 \text{ g}\cdot\text{cm}^{-3}$, $\lambda = 0.71073 \text{ \AA}$, $T = 298(2) \text{ K}$, $m = 0.083 \text{ mm}^{-1}$, 5354 unabhängige Reflexe ($R_{\text{int}} = 0.0137$), $R = 0.0560$, $wR_2 = 0.1171$.

Tabelle 13.9.9.1: Atomkoordinaten [10^4] und äquivalente isotrope Versetzungsparameter

$[\text{\AA}^2 \cdot 10^3]$ des Kokristalls aus Phenazin und 2,2'-Dihydroxybiphenyl.

	x	y	z	U(eq)
N(1)	-198(1)	8038(3)	2827(1)	67(1)

N(2)	967(1)	8000(3)	2309(1)	60(1)
N(3)	4582(1)	6177(3)	4347(1)	51(1)
O(1)	2119(1)	8621(2)	1807(1)	60(1)
O(2)	3730(1)	8617(2)	3067(1)	64(1)
C(1)	739(2)	8000(5)	4189(2)	92(1)
C(2)	1471(2)	7964(5)	4723(2)	112(1)
C(3)	2051(2)	7950(5)	4471(2)	105(1)
C(4)	1898(2)	7965(4)	3681(2)	81(1)
C(5)	32(2)	8021(5)	948(2)	89(1)
C(6)	-697(2)	8014(6)	420(2)	111(1)
C(7)	-1282(2)	8029(5)	675(2)	108(1)
C(8)	-1123(2)	8041(4)	1459(2)	86(1)
C(9)	-352(1)	8028(3)	2047(2)	61(1)
C(10)	533(1)	8012(4)	3348(2)	63(1)
C(11)	1128(1)	7991(3)	3094(2)	58(1)
C(12)	234(1)	8009(3)	1784(2)	59(1)
C(13)	3291(2)	2296(4)	3950(2)	80(1)
C(14)	3572(1)	3954(4)	3863(1)	66(1)
C(15)	4299(1)	4544(3)	4437(1)	49(1)
C(16)	5281(1)	6655(3)	4899(1)	49(1)
C(17)	5609(2)	8360(4)	4832(2)	69(1)
C(18)	6296(2)	8872(4)	5389(2)	82(1)
C(19)	2946(1)	10945(3)	1737(1)	44(1)
C(20)	3086(1)	12819(3)	1668(1)	56(1)
C(21)	2589(1)	14195(3)	1666(1)	63(1)
C(22)	1939(1)	13701(3)	1741(1)	63(1)
C(23)	1777(1)	11845(3)	1794(1)	56(1)
C(24)	2274(1)	10467(3)	1787(1)	46(1)
C(25)	3504(1)	9505(3)	1753(1)	41(1)
C(26)	3888(1)	8375(3)	2422(1)	45(1)
C(27)	4431(1)	7108(3)	2435(1)	55(1)
C(28)	4595(1)	6945(3)	1785(1)	59(1)
C(29)	4218(1)	8034(3)	1113(1)	58(1)
C(30)	3683(1)	9299(3)	1105(1)	50(1)

Tabelle 13.9.9.2: Wasserstoffatomkoordinaten $[10^4]$ und isotrope Versetzungsparameter[$\text{\AA}^2 \cdot 10^3$] des Kokristalls aus Phenazin und 2,2'-Dihydroxybiphenyl.

	x	y	z	U(eq)
H(10)	1747(16)	8426(39)	1987(16)	90
H(20)	3974(17)	7817(42)	3461(17)	96
H(1)	360(2)	8018(5)	4369(2)	111
H(2)	1594(2)	7948(5)	5269(2)	134
H(3)	2555(2)	7930(5)	4854(2)	126
H(4)	2293(2)	7957(4)	3526(2)	98
H(5)	411(2)	8034(5)	767(2)	106
H(6)	-822(2)	7999(6)	-126(2)	134
H(7)	-1787(2)	8031(5)	295(2)	130
H(8)	-1516(2)	8059(4)	1618(2)	104
H(13)	2816(2)	1915(4)	3568(2)	96
H(14)	3290(1)	4711(4)	3427(1)	80
H(17)	5345(2)	9137(4)	4397(2)	82
H(18)	6502(2)	10007(4)	5340(2)	99
H(20)	3526(1)	13157(3)	1621(1)	67
H(21)	2692(1)	15440(3)	1615(1)	76
H(22)	1608(1)	14619(3)	1756(1)	76
H(23)	1333(1)	11518(3)	1835(1)	67
H(27)	4684(1)	6367(3)	2885(1)	66
H(28)	4961(1)	6097(3)	1797(1)	71
H(29)	4324(1)	7915(3)	670(1)	70
H(30)	3434(1)	10038(3)	653(1)	60

Tabelle 13.9.9.3: Bindungslängen [\AA] und Winkel [$^\circ$] des Kokristalls aus Phenazin und 2,2'-Dihydroxybiphenyl.

Bindungslängen [\AA]		Winkel [$^\circ$]	
N(1)-C(10)	1.330(3)	C(10)-N(1)-C(9)	116.9(2)
N(1)-C(9)	1.339(3)	C(12)-N(2)-C(11)	117.5(2)
N(2)-C(12)	1.336(3)	C(15)-N(3)-C(16)	117.8(2)
N(2)-C(11)	1.344(3)	C(24)-O(1)-H(10)	112(2)
N(3)-C(15)	1.336(3)	C(26)-O(2)-H(20)	113(2)

N(3)-C(16)	1.346(3)	C(2)-C(1)-C(10)	120.8(3)
O(1)-C(24)	1.363(3)	C(1)-C(2)-C(3)	120.8(3)
O(1)-H(10)	0.93(3)	C(4)-C(3)-C(2)	121.6(3)
O(2)-C(26)	1.362(2)	C(3)-C(4)-C(11)	119.4(3)
O(2)-H(20)	0.89(3)	C(6)-C(5)-C(12)	120.2(3)
C(1)-C(2)	1.340(5)	C(5)-C(6)-C(7)	121.1(3)
C(1)-C(10)	1.426(4)	C(8)-C(7)-C(6)	121.1(3)
C(2)-C(3)	1.395(5)	C(7)-C(8)-C(9)	119.9(3)
C(3)-C(4)	1.356(4)	N(1)-C(9)-C(12)	121.8(2)
C(4)-C(11)	1.422(3)	N(1)-C(9)-C(8)	119.6(2)
C(5)-C(6)	1.331(4)	C(12)-C(9)-C(8)	118.6(3)
C(5)-C(12)	1.420(3)	N(1)-C(10)-C(1)	119.9(3)
C(6)-C(7)	1.407(5)	N(1)-C(10)-C(11)	122.0(2)
Bindungslängen [Å]		Winkel [°]	
C(7)-C(8)	1.343(5)	C(1)-C(10)-C(11)	118.1(3)
C(8)-C(9)	1.424(4)	N(2)-C(11)-C(4)	120.1(2)
C(9)-C(12)	1.420(3)	N(2)-C(11)-C(10)	120.7(2)
C(10)-C(11)	1.427(3)	C(4)-C(11)-C(10)	119.2(2)
C(13)-C(14)	1.348(4)	N(2)-C(12)-C(5)	119.8(2)
C(13)-	1.411(4)	N(2)-C(12)-C(9)	121.2(2)
C(18)A			
C(14)-C(15)	1.419(3)	C(5)-C(12)-C(9)	119.0(2)
C(15)-	1.430(3)	C(14)-C(13)-	121.2(3)
C(16)A		C(18)A	
C(16)-C(17)	1.410(3)	C(13)-C(14)-	120.0(2)
		C(15)	
C(16)-	1.430(3)	N(3)-C(15)-C(14)	120.1(2)
C(15)A			
C(17)-C(18)	1.341(4)	N(3)-C(15)-	121.4(2)
		C(16)A	
C(18)-	1.411(4)	C(14)-C(15)-	118.6(2)
C(13)A		C(16)A	
C(19)-C(20)	1.390(3)	N(3)-C(16)-C(17)	120.2(2)
C(19)-C(24)	1.394(3)	N(3)-C(16)-	120.9(2)
		C(15)A	
C(19)-C(25)	1.490(3)	C(17)-C(16)-	118.9(2)
		C(15)A	
C(20)-C(21)	1.381(3)	C(18)-C(17)-	120.7(3)
		C(16)	
C(21)-C(22)	1.377(3)	C(17)-C(18)-	120.6(3)
		C(13)A	

C(22)-C(23)	1.383(3)	C(20)-C(19)- C(24)	118.1(2)
C(23)-C(24)	1.387(3)	C(20)-C(19)- C(25)	120.2(2)
C(25)-C(30)	1.390(3)	C(24)-C(19)- C(25)	121.7(2)
C(25)-C(26)	1.395(3)	C(21)-C(20)- C(19)	121.9(2)
C(26)-C(27)	1.387(3)	C(22)-C(21)- C(20)	119.2(2)
C(27)-C(28)	1.373(3)	C(21)-C(22)- C(23)	120.2(2)
C(28)-C(29)	1.380(3)	C(22)-C(23)- C(24)	120.4(2)
C(29)-C(30)	1.376(3)	O(1)-C(24)-C(23)	122.0(2)
		O(1)-C(24)-C(19)	117.7(2)
		C(23)-C(24)- C(19)	120.2(2)
		C(30)-C(25)- C(26)	117.6(2)
		C(30)-C(25)- C(19)	120.5(2)
		C(26)-C(25)- C(19)	121.9(2)
		O(2)-C(26)-C(27)	121.7(2)
		O(2)-C(26)-C(25)	117.6(2)
		C(27)-C(26)- C(25)	120.6(2)
		C(28)-C(27)- C(26)	120.3(2)
		C(27)-C(28)- C(29)	120.2(2)
		C(30)-C(29)- C(28)	119.4(2)
		C(29)-C(30)- C(25)	122.0(2)

13.9.10 Phenazin mit Acridin und 2,2'-Dihydroxybiphenyl

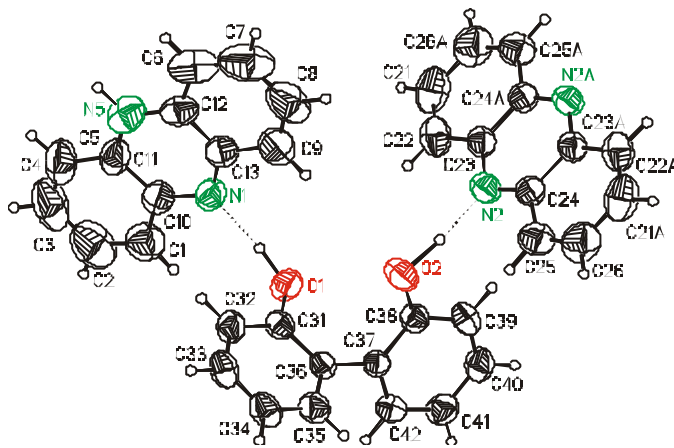


Abb. 13.9.10.1: Struktur des Kokristalls aus Phenazin, Acridin und 2,2'-Dihydroxybiphenyl. Die Ellipsoide beschreiben 50%-Aufenthaltswahrscheinlichkeit.

$[\text{C}_{13}\text{H}_9\text{N}] \cdot 2[\text{C}_{12}\text{H}_8\text{N}_2] \cdot [\text{C}_{12}\text{H}_{10}\text{O}_2]$, $M = 912.02 \text{ g}\cdot\text{mol}^{-1}$, monoklin, Raumgruppe $P2_1/c$, $a = 19.5835(2) \text{ \AA}$, $b = 7.19170(10) \text{ \AA}$, $c = 18.6027(2) \text{ \AA}$, $\beta = 115.4550(10)^\circ$, $V = 2365.64(5) \text{ \AA}^3$, $Z = 2$, $\rho_{\text{ber.}} = 1.280 \text{ g}\cdot\text{cm}^{-3}$, $\lambda = 0.71073 \text{ \AA}$, $T = 293(2) \text{ K}$, $\mu = 0.081 \text{ mm}^{-1}$, 4746 unabhängige Reflexe ($R_{\text{int}} = 0.0374$), $R = 0.0650$, $wR_2 = 0.1544$.

Tabelle 13.9.10.1: Atomkoordinaten [10^4] und äquivalente isotrope Versetzungsparameter [$\text{\AA}^2 \cdot 10^3$] des Kokristalls aus Phenazin, Acridin und 2,2'-Dihydroxybiphenyl.

	x	y	z	U(eq)
N(1)	979(1)	6937(2)	2300(1)	59(1)
N(2)	4584(1)	8812(2)	4350(1)	55(1)
O(1)	2127(1)	6375(2)	1811(1)	60(1)
O(2)	3738(1)	6397(2)	3063(1)	67(1)
C(1)	62(2)	6905(4)	945(2)	86(1)
C(2)	-668(3)	6890(6)	405(2)	117(1)
)
C(3)	-1261(2)	6847(5)	646(3)	120(2)
C(4)	-1112(2)	6804(4)	1425(3)	94(1)
C(5)	-186(2)	6794(3)	2806(2)	70(6)
N(5)	-186(2)	6794(3)	2806(2)	76(5)
C(6)	750(3)	6860(5)	4178(2)	100(1)
)
C(7)	1480(3)	6946(6)	4707(2)	124(2)
)
C(8)	2058(2)	7024(5)	4459(2)	112(1)

)
C(9)	1902(2)	6997(4)	3662(2)	88(1)
C(10)	245(1)	6895(3)	1768(2)	60(1)
C(11)	-351(1)	6824(3)	2019(2)	65(1)
C(12)	550(2)	6855(3)	3346(2)	66(1)
C(13)	1135(1)	6930(3)	3081(2)	61(1)
C(21)	3291(2)	12707(4)	3960(2)	86(1)
C(22)	3570(1)	11043(4)	3868(2)	71(1)
C(23)	4296(1)	10456(3)	4439(1)	50(1)
C(24)	5281(1)	8346(3)	4899(1)	51(1)
C(25)	5609(2)	6627(3)	4830(2)	71(1)
C(26)	6299(2)	6128(4)	5383(2)	88(1)
C(31)	2288(1)	4529(2)	1787(1)	46(1)
C(32)	1793(1)	3141(3)	1791(1)	56(1)
C(33)	1958(1)	1290(3)	1734(1)	63(1)
C(34)	2605(1)	805(3)	1665(1)	62(1)
C(35)	3101(1)	2187(3)	1665(1)	56(1)
C(36)	2956(1)	4064(2)	1735(1)	43(1)
C(37)	3511(1)	5508(2)	1749(1)	41(1)
C(38)	3892(1)	6635(2)	2420(1)	47(1)
C(39)	4436(1)	7913(3)	2432(1)	55(1)
C(40)	4600(1)	8068(3)	1786(1)	58(1)
C(41)	4230(1)	6987(3)	1120(2)	59(1)
C(42)	3691(1)	5705(3)	1111(1)	51(1)

Tabelle 13.9.10.2: Wasserstoffatomkoordinaten [10⁴] und isotrope

Versetzungparameter

[Å² · 10³] des Kokristalls aus Phenazin, Acridin und 2,2'-Dihydroxybiphenyl.

	x	y	z	U(eq)
H(10)	1709	6675	2021	105(10)
H(20)	4106	7636	3522	150(13)
H(1)	455	6912	765	103
H(2)	-802	6921	-158	140
H(3)	-1780	6840	256	144
H(4)	-1514	6746	1590	113
H(5)	-580	6728	2984	84
H(6)	361	6834	4363	120
H(7)	1608	6930	5268	149
H(8)	2577	7097	4848	135
H(9)	2301	7011	3490	105
H(21)	2801	13085	3565	103
H(22)	3281	10262	3420	85
H(25)	5338	5831	4381	85
H(26)	6511	4955	5337	105
H(32)	1340	3466	1843	67
H(33)	1617	335	1741	75
H(34)	2710	-473	1602	75
H(35)	3559	1847	1626	67
H(39)	4695	8673	2897	66
H(40)	4973	8949	1797	70
H(41)	4341	7101	667	71
H(42)	3437	4941	646	62

Tabelle 13.9.10.3: Bindungslängen [Å] und Winkel [°] des Kokristalls aus Phenazin, Acridin und 2,2'-Dihydroxybiphenyl.

Bindungslängen [Å]		Winkel [°]	
N(1)-C(13)	1.350(3)	C(13)-N(1)-C(10)	117.8(2)
N(1)-C(10)	1.350(3)	C(13)-N(1)-H(10)	119.2
N(1)-H(10)	1.7286	C(10)-N(1)-H(10)	122.3
N(2)-C(24)	1.348(3)	C(24)-N(2)-C(23)	117.7(2)
N(2)-C(23)	1.351(3)	C(24)-N(2)-H(20)	124.3
N(2)-H(20)	1.6501	C(23)-N(2)-H(20)	117.6
O(1)-C(31)	1.370(2)	C(31)-O(1)-H(10)	115.5
O(1)-H(10)	1.0708	C(38)-O(2)-H(20)	103.5
O(2)-C(38)	1.365(3)	C(2)-C(1)-C(10)	120.0(3)
O(2)-H(20)	1.2302	C(2)-C(1)-H(1)	119.4

C(1)-C(2)	1.349(5)	C(10)-C(1)-H(1)	120.6
C(1)-C(10)	1.414(4)	C(1)-C(2)-C(3)	121.0(4)
C(1)-H(1)	0.9614	C(1)-C(2)-H(2)	121.1
C(2)-C(3)	1.414(6)	C(3)-C(2)-H(2)	117.9
C(2)-H(2)	0.9632	C(4)-C(3)-C(2)	120.9(3)
C(3)-C(4)	1.349(6)	C(4)-C(3)-H(3)	118.7
C(3)-H(3)	0.9637	C(2)-C(3)-H(3)	120.4
Bindungslängen [Å]		Winkel [°]	
C(4)-C(11)	1.423(4)	C(3)-C(4)-C(11)	120.3(3)
C(4)-H(4)	0.9616	C(3)-C(4)-H(4)	121.0
C(5)-C(11)	1.357(4)	C(11)-C(4)-H(4)	118.7
C(5)-C(12)	1.359(4)	C(11)-C(5)-C(12)	118.8(2)
C(5)-H(5)	0.9613	C(11)-C(5)-H(5)	121.2
N(5)-C(11)	1.357(4)	C(12)-C(5)-H(5)	120.0
N(5)-C(12)	1.359(4)	C(11)-N(5)-C(12)	118.8(2)
N(5)-H(5)	0.9613	C(11)-N(5)-H(5)	121.2
C(6)-C(7)	1.344(6)	C(12)-N(5)-H(5)	120.0
C(6)-C(12)	1.423(4)	C(7)-C(6)-C(12)	120.4(4)
C(6)-H(6)	0.9614	C(7)-C(6)-H(6)	119.6
C(7)-C(8)	1.396(6)	C(12)-C(6)-H(6)	120.0
C(7)-H(7)	0.9630	C(6)-C(7)-C(8)	121.1(4)
C(8)-C(9)	1.380(5)	C(6)-C(7)-H(7)	119.5
C(8)-H(8)	0.9635	C(8)-C(7)-H(7)	119.3
C(9)-C(13)	1.425(4)	C(9)-C(8)-C(7)	121.3(3)
C(9)-H(9)	0.9614	C(9)-C(8)-H(8)	118.9
C(10)-C(11)	1.432(4)	C(7)-C(8)-H(8)	119.8
C(12)-C(13)	1.429(4)	C(8)-C(9)-C(13)	119.3(3)
C(21)-C(22)	1.357(4)	C(8)-C(9)-H(9)	121.4
C(21)-	1.413(4)	C(13)-C(9)-H(9)	119.4
C(26)A			
C(21)-H(21)	0.9633	N(1)-C(10)-C(1)	119.2(2)
C(22)-C(23)	1.424(3)	N(1)-C(10)-C(11)	121.4(2)
C(22)-H(22)	0.9627	C(1)-C(10)-C(11)	119.4(3)
C(23)-	1.438(3)	N(5)-C(11)-C(5)	0.0(3)
C(24)A			
C(24)-C(25)	1.424(3)	N(5)-C(11)-C(4)	121.5(3)
C(24)-	1.438(3)	C(5)-C(11)-C(4)	121.5(3)
C(23)A			
C(25)-C(26)	1.348(4)	N(5)-C(11)-C(10)	120.2(2)
C(25)-H(25)	0.9625	C(5)-C(11)-C(10)	120.2(2)
C(26)-	1.413(4)	C(4)-C(11)-C(10)	118.3(3)

C(21)A			
C(26)-H(26)	0.9604	N(5)-C(12)-C(5)	0.0(4)
C(31)-C(36)	1.392(3)	N(5)-C(12)-C(6)	120.8(3)
C(31)-C(32)	1.394(3)	C(5)-C(12)-C(6)	120.8(3)
C(32)-C(33)	1.385(3)	N(5)-C(12)-C(13)	120.0(2)
C(32)-H(32)	0.9615	C(5)-C(12)-C(13)	120.0(2)
C(33)-C(34)	1.373(3)	C(6)-C(12)-C(13)	119.2(3)
C(33)-H(33)	0.9610	N(1)-C(13)-C(9)	119.6(2)
C(34)-C(35)	1.390(3)	N(1)-C(13)-C(12)	121.8(2)
C(34)-H(34)	0.9604	C(9)-C(13)-C(12)	118.7(3)
C(35)-C(36)	1.398(3)	C(22)-C(21)-	121.4(3)
		C(26)A	
C(35)-H(35)	0.9618	C(22)-C(21)-	118.5
		H(21)	
C(36)-C(37)	1.495(2)	C(26)A-C(21)-	120.1
		H(21)	
C(37)-C(42)	1.384(3)	C(21)-C(22)-	119.7(3)
		C(23)	
C(37)-C(38)	1.405(3)	C(21)-C(22)-	120.3
		H(22)	
C(38)-C(39)	1.400(3)	C(23)-C(22)-	120.1
		H(22)	
C(39)-C(40)	1.375(3)	N(2)-C(23)-C(22)	120.2(2)
C(39)-H(39)	0.9626	N(2)-C(23)-	120.8(2)
		C(24)A	
C(40)-C(41)	1.375(3)	C(22)-C(23)-	118.9(2)
		C(24)A	
C(40)-H(40)	0.9612	N(2)-C(24)-C(25)	119.7(2)
C(41)-C(42)	1.395(3)	N(2)-C(24)-	121.5(2)
		C(23)A	
C(41)-H(41)	0.9619	C(25)-C(24)-	118.8(2)
		C(23)A	
C(42)-H(42)	0.9626	C(26)-C(25)-	120.4(3)
		C(24)	
Bindungslängen [Å]		Winkel [°]	
		C(26)-C(25)-	120.2
		H(25)	
		C(24)-C(25)-	119.5
		H(25)	
		C(25)-C(26)-	120.8(3)
		C(21)A	

C(25)-C(26)- H(26)	119.7
C(21)A-C(26)- H(26)	119.4
O(1)-C(31)-C(36)	118.1(2)
O(1)-C(31)-C(32)	121.5(2)
C(36)-C(31)- C(32)	120.3(2)
C(33)-C(32)- C(31)	120.2(2)
C(33)-C(32)- H(32)	119.8
C(31)-C(32)- H(32)	120.0
C(34)-C(33)- C(32)	120.4(2)
C(34)-C(33)- H(33)	119.6
C(32)-C(33)- H(33)	120.0
C(33)-C(34)- C(35)	119.5(2)
C(33)-C(34)- H(34)	120.7
C(35)-C(34)- H(34)	119.8
C(34)-C(35)- C(36)	121.4(2)
C(34)-C(35)- H(35)	119.5
C(36)-C(35)- H(35)	119.1
C(31)-C(36)- C(35)	118.2(2)
C(31)-C(36)- C(37)	121.9(2)
C(35)-C(36)- C(37)	119.8(2)
C(42)-C(37)- C(38)	118.0(2)
C(42)-C(37)-	120.5(2)

C(36)	
C(38)-C(37)-	121.4(2)
C(36)	
O(2)-C(38)-C(39)	121.5(2)
O(2)-C(38)-C(37)	118.3(2)
C(39)-C(38)-	120.2(2)
C(37)	
C(40)-C(39)-	120.1(2)
C(38)	
C(40)-C(39)-	120.5
H(39)	
C(38)-C(39)-	119.4
H(39)	
C(39)-C(40)-	120.7(2)
C(41)	
C(39)-C(40)-	119.7
H(40)	
C(41)-C(40)-	119.6
H(40)	
C(40)-C(41)-	119.2(2)
C(42)	
C(40)-C(41)-	120.7
H(41)	
C(42)-C(41)-	120.0
H(41)	
C(37)-C(42)-	121.8(2)
C(41)	
C(37)-C(42)-	119.1
H(42)	
C(41)-C(42)-	119.1
H(42)	

13.9.11 Phenazin und Hydrochinon

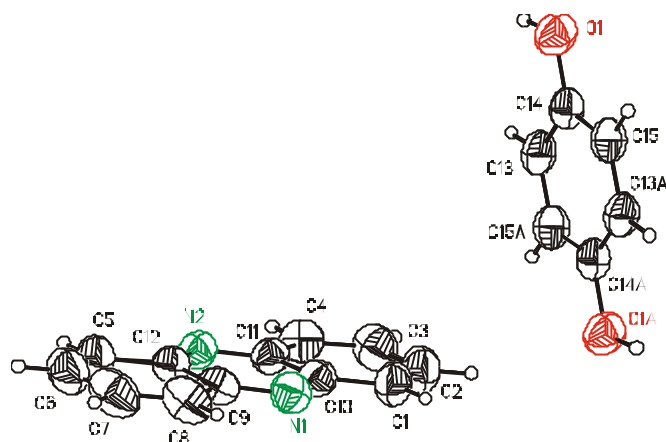


Abb. 13.9.11.1: Struktur des Kokristalls aus Phenazin und Hydrochinon. Die Ellipsoide beschreiben 50%-Aufenthaltswahrscheinlichkeit.

$[\text{C}_{12}\text{H}_8\text{N}_2] \cdot 1/2[\text{C}_6\text{H}_6\text{O}_2]$, $M = 235.26 \text{ g}\cdot\text{mol}^{-1}$, triklin, Raumgruppe $P\bar{1}$, $a = 7.286(2) \text{ \AA}$, $b = 9.004(2) \text{ \AA}$, $c = 9.23982(2) \text{ \AA}$, $\alpha = 77.418(13)^\circ$, $\beta = 74.83(3)^\circ$, $\gamma = 86.326(9)^\circ$, $V = 571.0(3) \text{ \AA}^3$, $Z = 2$, $\rho_{\text{ber.}} = 1.368 \text{ g}\cdot\text{cm}^{-3}$, $\lambda = 0.71073 \text{ \AA}$, $T = 298(2) \text{ K}$, $m = 0.088 \text{ mm}^{-1}$, 1997 unabhängige Reflexe ($R_{\text{int}} = 0.0144$), $R = 0.0393$, $wR_2 = 0.0947$.

Tabelle 13.9.11.1: Atomkoordinaten [10^4] und äquivalente isotrope Versetzungsparameter [$\text{\AA}^2 \cdot 10^3$] des Kokristalls aus Phenazin und Hydrochinon.

	x	y	z	U(eq)
N(1)	2909(2)	3664(1)	5863(1)	51(1)
N(2)	2388(2)	5996(2)	3403(2)	57(1)
O(1)	3409(2)	1410(1)	8373(1)	63(1)
C(1)	2036(3)	5402(2)	7549(2)	65(1)
C(2)	1486(3)	6820(3)	7762(2)	79(1)
C(3)	1247(3)	7981(2)	6533(3)	81(1)
C(4)	1541(3)	7722(2)	5107(2)	71(1)

C(5)	3217(3)	4235(2)	1731(2)	65(1)
C(6)	3738(3)	2817(2)	1519(2)	73(1)
C(7)	3979(3)	1656(2)	2738(2)	71(1)
C(8)	3705(2)	1927(2)	4166(2)	61(1)
C(9)	3166(2)	3398(2)	4448(2)	48(1)
C(10)	2370(2)	5073(2)	6066(2)	50(1)
C(11)	2113(2)	6248(2)	4822(2)	54(1)
C(12)	2911(2)	4580(2)	3207(2)	51(1)
C(13)	-5(2)	1216(2)	8805(2)	52(1)
C(14)	1696(2)	730(2)	9160(2)	50(1)
C(15)	1687(2)	-493(2)	10370(2)	53(1)

Tabelle 13.9.11.2: Wasserstoffatomkoordinaten $[10^4]$ und isotrope Versetzungsparameter $[\text{\AA}^2 \cdot 10^3]$ des Kokristalls aus Phenazin und Hydrochinon.

	x	y	z	U(eq)
H(10)	3344	2247	7474	94
H(1)	2189	4612	8395	78
H(2)	1265	7037	8766	94
H(3)	861	8978	6714	98
H(4)	1380	8531	4280	85
H(5)	3063	5022	884	78
H(6)	3925	2597	519	87
H(7)	4362	659	2557	85
H(8)	3866	1120	4995	73
H(13)	-1	2065	7970	63
H(15)	2858	-839	10628	64

Tabelle 13.9.11.3: Bindungslängen $[\text{\AA}]$ und Winkel $[\text{\circ}]$ des Kokristalls aus Phenazin und Hydrochinon.

Bindungslängen $[\text{\AA}]$		Winkel $[\text{\circ}]$	
N(1)-C(10)	1.342(2)	C(10)-N(1)-C(9)	117.37(13)
N(1)-C(9)	1.343(2)	C(10)-N(1)-H(10)	119.0

N(1)-H(10)	1.8193	C(9)-N(1)-H(10)	123.6
N(2)-C(11)	1.341(2)	O(1)-H(10)-N(1)	172.2
N(2)-C(12)	1.343(2)	C(11)-N(2)-C(12)	116.88(14)
)	
O(1)-H(10)	1.0019	H(10)-O(1)-C(14)	114.5
O(1)-C(14)	1.375(2)	C(2)-C(1)-C(10)	119.8(2)
C(1)-C(2)	1.353(3)	C(1)-C(2)-C(3)	121.0(2)
C(1)-C(10)	1.420(2)	C(4)-C(3)-C(2)	121.3(2)
C(2)-C(3)	1.406(3)	C(3)-C(4)-C(11)	119.9(2)
C(3)-C(4)	1.347(3)	C(6)-C(5)-C(12)	120.3(2)
C(4)-C(11)	1.424(2)	C(5)-C(6)-C(7)	121.1(2)
C(5)-C(6)	1.349(3)	C(8)-C(7)-C(6)	120.9(2)
C(5)-C(12)	1.422(2)	C(7)-C(8)-C(9)	120.2(2)
C(6)-C(7)	1.399(3)	N(1)-C(9)-C(8)	120.06(14)
)	
C(7)-C(8)	1.355(2)	N(1)-C(9)-C(12)	121.08(14)
)	
C(8)-C(9)	1.417(2)	C(8)-C(9)-C(12)	118.9(2)
C(9)-C(12)	1.427(2)	N(1)-C(10)-C(1)	119.5(2)
C(10)-C(11)	1.426(2)	N(1)-C(10)-C(11)	121.28(14)
)	
C(13)-C(15)A	1.380(2)	C(1)-C(10)-C(11)	119.2(2)
C(13)-C(14)	1.384(2)	N(2)-C(11)-C(4)	119.6(2)
C(14)-C(15)	1.387(2)	N(2)-C(11)-C(10)	121.68(14)
)	
C(15)-C(13)A	1.380(2)	C(4)-C(11)-C(10)	118.7(2)
		N(2)-C(12)-C(5)	119.7(2)
		N(2)-C(12)-C(9)	121.70(14)
)	
		C(5)-C(12)-C(9)	118.6(2)
		C(15)A-C(13)-	120.80(14)
		C(14))
		O(1)-C(14)-C(13)	123.06(14)
)	
		O(1)-C(14)-C(15)	117.92(14)
)	
Bindungslängen [Å]		Winkel [°]	
		C(13)-C(14)-C(15)	119.0(2)
		C(13)A-C(15)-	120.2(2)
		C(14)	

13.9.12 Phenazin und 1,5-Dihydroxynaphthanlin

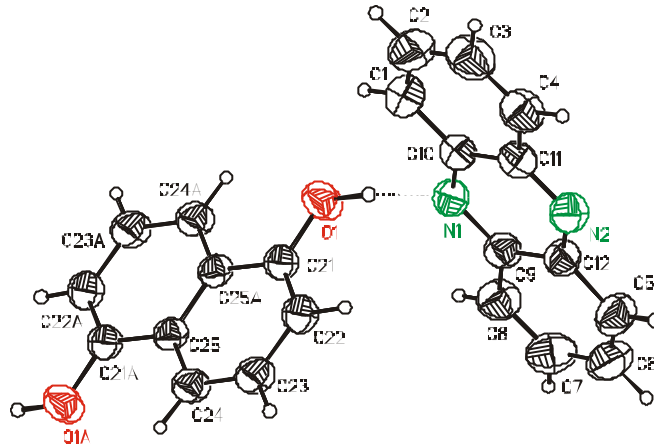


Abb. 13.9.12.1: Struktur des Kokristalls aus Phenazin und 1,5-Dihydroxynaphthanlin. Die Ellipsoide beschreiben 50%-Aufenthaltswahrscheinlichkeit.

$2[\text{C}_{12}\text{H}_8\text{N}_2] \cdot [\text{C}_{10}\text{H}_8\text{O}_2]$, $M = 520.57 \text{ g}\cdot\text{mol}^{-1}$, triklin, Raumgruppe $P\bar{1}$, $a = 7.3415(6) \text{ \AA}$, $b = 9.5933(8) \text{ \AA}$, $c = 10.1204(8) \text{ \AA}$, $\alpha = 87.680(2)^\circ$, $\beta = 70.207(2)^\circ$, $\gamma = 79.333(2)^\circ$, $V = 658.88(9) \text{ \AA}^3$, $Z = 2$, $\rho_{\text{ber.}} = 1.312 \text{ g}\cdot\text{cm}^{-3}$, $\lambda = 0.71073 \text{ \AA}$, $T = 298 \text{ K}$, $m = 0.083 \text{ mm}^{-1}$, 2208 unabhängige Reflexe ($R_{\text{int}} = 0.0575$), $R = 0.0611$, $wR_2 = 0.1326$.

Tabelle 13.9.12.1: Atomkoordinaten [10^4] und äquivalente isotrope Versetzungsparameter [$\text{Å}^2 \cdot 10^3$] des Kokristalls aus Phenazin und 1,5-Dihydroxynaphthalin.

	x	y	z	U(eq)
N(1)	3651(3)	3560(2)	8413(2)	48(1)
N(2)	2094(3)	5720(2)	10539(2)	52(1)
O(1)	5761(2)	1371(2)	6397(2)	59(1)
C(1)	2201(4)	1897(3)	10093(4)	64(1)
C(2)	1111(5)	1627(4)	11429(4)	77(1)
C(3)	330(4)	2711(4)	12487(4)	75(1)
C(4)	656(4)	4049(4)	12182(3)	63(1)
C(5)	3541(4)	7390(3)	8873(4)	61(1)
C(6)	4611(5)	7677(4)	7546(4)	71(1)
C(7)	5386(5)	6605(4)	6483(4)	71(1)
C(8)	5083(4)	5254(4)	6764(3)	60(1)
C(9)	3959(4)	4903(3)	8139(3)	46(1)
C(10)	2566(4)	3291(3)	9732(3)	47(1)
C(11)	1776(4)	4391(3)	10807(3)	47(1)
C(12)	3168(4)	5993(3)	9221(3)	46(1)
C(21)	7740(3)	1181(3)	6166(3)	43(1)
C(22)	8546(4)	1947(3)	6860(3)	49(1)
C(23)	10579(4)	1692(3)	6600(3)	51(1)
C(24)	11819(4)	672(3)	5619(3)	46(1)
C(25)	11037(3)	-116(3)	4871(3)	39(1)

Tabelle 13.9.12.2: Wasserstoffatomkoordinaten [10⁴] und isotrope Versetzungsparameter[Å² · 10³] des Kokristalls aus Phenazin und 1,5-Dihydroxynaphthalin.

	x	y	z	U(eq)
H(1)	4889(2)	2112(2)	7208(2)	126(13)
H(1A)	2718(4)	1152(3)	9388(4)	77
H(2)	874(5)	682(4)	11667(4)	92
H(3)	-436(4)	2501(4)	13424(4)	89
H(4)	128(4)	4782(4)	12899(3)	75
H(5)	3028(4)	8126(3)	9588(4)	73
H(6)	4837(5)	8627(4)	7332(4)	86
H(7)	6140(5)	6843(4)	5552(4)	85
H(8)	5620(4)	4530(4)	6038(3)	72
H(22)	7697(4)	2663(3)	7538(3)	58
H(23)	11112(4)	2247(3)	7095(3)	61
H(24)	13209(4)	491(3)	5455(3)	56

Tabelle 13.9.12.3: Bindungslängen [Å] und Winkel [°] des Kokristalls aus Phenazin und 1,5-Dihydroxynaphthalin.

Bindungslängen [Å]		Winkel [°]	
N(1)-C(10)	1.346(3)	C(10)-N(1)-C(9)	117.4(2)
N(1)-C(9)	1.351(3)	C(10)-N(1)-H(1)	118.8(2)
N(1)-H(1)	1.778(3)	C(9)-N(1)-H(1)	123.2(2)
N(1)-O(1)	2.824(3)	C(10)-N(1)-O(1)	122.1(2)
N(2)-C(11)	1.339(3)	C(9)-N(1)-O(1)	119.7(2)
N(2)-C(12)	1.344(3)	N(1)-H(1)-O(1)	170.72(10)
O(1)-H(1)	1.05	C(11)-N(2)-C(12)	117.4(3)
O(1)-C(21)	1.369(3)	H(1)-O(1)-C(21)	114.43(13)
C(1)-C(2)	1.361(4)	C(21)-O(1)-N(1)	111.3(2)

C(1)-C(10)	1.421(4)	C(21)-O(1)-H(1)	114.43(13)
C(2)-C(3)	1.418(5)	C(2)-C(1)-C(10)	120.0(3)
C(3)-C(4)	1.353(4)	C(1)-C(2)-C(3)	121.3(3)
C(4)-C(11)	1.417(4)	C(4)-C(3)-C(2)	120.3(3)
C(5)-C(6)	1.354(4)	C(3)-C(4)-C(11)	120.8(3)
C(5)-C(12)	1.423(4)	C(6)-C(5)-C(12)	120.3(3)
C(6)-C(7)	1.413(4)	C(5)-C(6)-C(7)	121.1(3)
C(7)-C(8)	1.358(4)	C(8)-C(7)-C(6)	120.9(3)
C(8)-C(9)	1.421(4)	C(7)-C(8)-C(9)	120.1(3)
C(9)-C(12)	1.438(4)	N(1)-C(9)-C(8)	119.9(3)
C(10)-C(11)	1.440(4)	N(1)-C(9)-C(12)	121.0(3)
C(21)-C(22)	1.366(3)	C(8)-C(9)-C(12)	119.1(3)
C(21)- C(25)A	1.436(3)	N(1)-C(10)-C(1)	120.2(3)
C(22)-C(23)	1.400(3)	N(1)-C(10)-C(11)	121.2(3)
C(23)-C(24)	1.381(3)	C(1)-C(10)-C(11)	118.6(3)
C(24)-C(25)	1.405(3)	N(2)-C(11)-C(4)	119.5(3)
C(25)- C(25)A	1.431(4)	N(2)-C(11)-C(10)	121.5(3)
C(25)- C(21)A	1.436(3)	C(4)-C(11)-C(10)	118.9(3)
		N(2)-C(12)-C(5)	119.9(3)
		N(2)-C(12)-C(9)	121.5(3)
		C(5)-C(12)-C(9)	118.6(3)
		C(22)-C(21)-O(1)	123.2(2)
		C(22)-C(21)-C(25)A	120.8(2)
		O(1)-C(21)-C(25)A	115.9(2)
		C(21)-C(22)-C(23)	120.9(2)
		C(24)-C(23)-C(22)	120.7(3)
		C(23)-C(24)-C(25)	119.8(2)
		C(24)-C(25)-C(25)A	120.6(3)
		C(24)-C(25)-C(21)A	122.1(2)
		C(25)A-C(25)- C(21)A	117.3(3)

13.9.13 Phenazin und 4,4'-Dihydroxybiphenyl

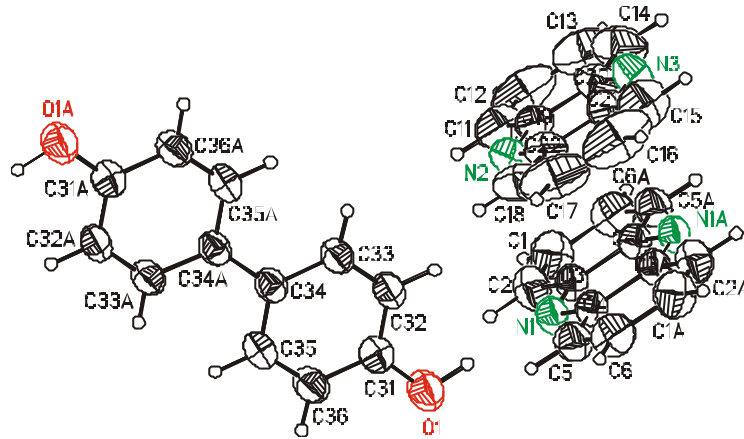


Abb. 13.9.13.1: Struktur des Kokristalls aus Phenazin und 4,4'-Dihydroxybiphenyl. Die Ellipsoide beschreiben 50%-Aufenthaltswahrscheinlichkeit.

$3[\text{C}_{12}\text{H}_8\text{N}_2] \cdot [\text{C}_{12}\text{H}_{10}\text{O}_2]$, $M = 726.81 \text{ g}\cdot\text{mol}^{-1}$, triklin, Raumgruppe $P\bar{1}$,
 $a = 9.2844(4) \text{ \AA}$, $b = 9.4909(5) \text{ \AA}$, $c = 10.7853(5) \text{ \AA}$, $\alpha = 76.669(1)^\circ$, $\beta = 87.181(1)^\circ$,
 $\gamma = 82.234(1)^\circ$, $V = 916.12(8) \text{ \AA}^3$, $Z = 1$, $\rho_{\text{ber.}} = 1.317 \text{ g}\cdot\text{cm}^{-3}$, $\lambda = 0.71073 \text{ \AA}$,
 $T = 298 \text{ K}$, $m = 0.083 \text{ mm}^{-1}$, 3091 unabhängige Reflexe ($R_{\text{int}} = 0.0205$),
 $R = 0.0777$, $wR_2 = 0.1706$.

Tabelle 13.9.13.1: Atomkoordinaten [10^4] und äquivalente isotrope Versetzungsparameter [$\text{\AA}^2 \cdot 10^3$] des Kokristalls aus Phenazin und 4,4'-Dihydroxybiphenyl.

	x	y	z	U(eq)
O(1)	3482(2)	6564(2)	5511(1)	66(1)
N(1)	1158(2)	8859(2)	5118(1)	52(1)
N(2)	485(2)	9492(2)	8373(1)	57(1)
N(3)	-1718(2)	11895(2)	8173(2)	69(1)
C(1)	-1871(3)	6991(3)	4680(2)	73(1)
C(2)	-500(2)	7225(2)	4855(2)	65(1)
C(3)	-204(2)	8625(2)	4934(2)	50(1)
C(4)	1385(2)	10205(2)	5189(2)	49(1)
C(5)	2805(2)	10505(2)	5385(2)	60(1)
C(6)	3037(2)	11863(3)	5446(2)	69(1)
C(11)	-1299(3)	8024(3)	8032(2)	77(1)
C(12)	-2721(4)	7909(4)	7839(2)	104(1)
C(13)	-3791(3)	9123(5)	7743(3)	106(1)
C(14)	-3455(3)	10397(4)	7853(2)	88(1)
C(15)	80(4)	13359(3)	8520(3)	96(1)
C(16)	1489(5)	13454(4)	8746(3)	123(1)
C(17)	2551(4)	12249(5)	8861(3)	113(1)
C(18)	2215(3)	10981(3)	8733(2)	83(1)
C(19)	-899(2)	9376(2)	8162(2)	53(1)
C(20)	-2011(2)	10589(2)	8065(2)	59(1)

C(21)	-337(2)	12010(2)	8385(2)	62(1)
C(22)	772(2)	10799(2)	8488(2)	57(1)
C(31)	3870(2)	6164(2)	6764(2)	49(1)
C(32)	3202(2)	6834(2)	7689(2)	50(1)
C(33)	3636(2)	6385(2)	8945(2)	49(1)
C(34)	4764(2)	5248(2)	9323(2)	42(1)
C(35)	5423(2)	4601(2)	8363(2)	50(1)
C(36)	5003(2)	5040(2)	7111(2)	53(1)

Tabelle 13.9.13.2: Wasserstoffatomkoordinaten $[10^4]$ und isotrope Versetzungsparameter

$[\text{\AA}^2 \cdot 10^3]$ des Kokristalls aus Phenazin und 4,4'-Dihydroxybiphenyl.

	x	y	z	U(eq)
H(10)	2700(2)	7333(2)	5409(1)	97(8)
H(1)	-2053(3)	6032(3)	4633(2)	87
H(2)	281(2)	6439(2)	4931(2)	78
H(5)	3602(2)	9734(2)	5482(2)	71
H(6)	4004(2)	12051(3)	5567(2)	83
H(11)	-569(3)	7197(3)	8073(2)	92
H(12)	-2988(4)	6984(4)	7780(2)	125
H(13)	-4775(3)	9017(5)	7585(3)	127
H(14)	-4209(3)	11207(4)	7791(2)	105
H(15)	-629(4)	14207(3)	8459(3)	116
H(16)	1769(5)	14368(4)	8821(3)	147

H(17)	3534(4)	12328(5)	9047(3)	135
H(18)	2959(3)	10161(3)	8796(2)	99
H(32)	2435(2)	7626(2)	7453(2)	61
H(33)	3149(2)	6861(2)	9572(2)	58
H(35)	6198(2)	3814(2)	8589(2)	60
H(36)	5493(2)	4570(2)	6481(2)	63

Tabelle 13.9.13.3: Bindungslängen [Å] und Winkel [°] des Kokristalls aus Phenazin und 4,4'-Dihydroxybiphenyl.

Bindungslängen [Å]		Winkel [°]	
O(1)-C(31)	1.370(2)	C(31)-O(1)-H(10)	109.24(9)
O(1)-H(10)	0.95	O(1)-H(10)-N(1)	177.13(6)
N(1)-H(10)	1.876(2)	C(4)-N(1)-C(3)	118.5(2)
N(1)-O(1)	2.824(2)	C(22)-N(2)-C(19)	116.7(2)
N(1)-C(4)	1.342(3)	C(20)-N(3)-C(21)	116.9(2)
N(1)-C(3)	1.345(2)	C(2)-C(1)-C(6)A	121.0(2)
N(2)-C(22)	1.338(3)	C(1)-C(2)-C(3)	120.5(2)
N(2)-C(19)	1.339(2)	N(1)-C(3)-C(2)	120.6(2)
N(3)-C(20)	1.336(3)	N(1)-C(3)-C(4)A	120.5(2)
N(3)-C(21)	1.337(3)	C(2)-C(3)-C(4)A	118.9(2)
C(1)-C(2)	1.351(3)	N(1)-C(4)-C(5)	120.5(2)
C(1)-C(6)A	1.415(3)	N(1)-C(4)-C(3)A	121.0(2)
C(2)-C(3)	1.414(3)	C(5)-C(4)-C(3)A	118.5(2)
C(3)-C(4)A	1.439(2)	C(6)-C(5)-C(4)	120.6(2)
C(4)-C(5)	1.421(3)	C(5)-C(6)-C(1)A	120.6(2)
C(4)-C(3)A	1.439(2)	C(12)-C(11)- C(19)	120.0(3)
C(5)-C(6)	1.351(3)	C(11)-C(12)- C(13)	120.6(3)
C(6)-C(1)A	1.415(3)	C(14)-C(13)- C(12)	120.9(3)
C(11)-C(12)	1.369(4)	C(13)-C(14)- C(20)	121.4(3)
C(11)-C(19)	1.421(3)	C(16)-C(15)- C(21)	120.2(3)
C(12)-C(13)	1.404(5)	C(15)-C(16)-	121.3(3)

C(13)-C(14)	1.321(4)	C(17)	
		C(18)-C(17)-	120.5(3)
		C(16)	
C(14)-C(20)	1.414(3)	C(17)-C(18)-	121.5(3)
		C(22)	
Bindungslängen [Å]		Winkel [°]	
C(15)-C(16)	1.362(5)	N(2)-C(19)-C(11)	120.4(2)
C(15)-C(21)	1.426(3)	N(2)-C(19)-C(20)	121.5(2)
C(16)-C(17)	1.392(5)	C(11)-C(19)-	118.1(2)
		C(20)	
C(17)-C(18)	1.321(4)	N(3)-C(20)-C(14)	119.5(2)
C(18)-C(22)	1.419(3)	N(3)-C(20)-C(19)	121.5(2)
C(19)-C(20)	1.427(3)	C(14)-C(20)-	119.0(2)
		C(19)	
C(21)-C(22)	1.423(3)	N(3)-C(21)-C(22)	121.6(2)
C(31)-C(32)	1.381(3)	N(3)-C(21)-C(15)	120.9(2)
C(31)-C(36)	1.392(2)	C(22)-C(21)-	117.4(2)
		C(15)	
C(32)-C(33)	1.386(2)	N(2)-C(22)-C(18)	119.2(2)
C(33)-C(34)	1.401(2)	N(2)-C(22)-C(21)	121.7(2)
C(34)-C(35)	1.397(2)	C(18)-C(22)-	119.1(2)
		C(21)	
C(34)-	1.496(3)	O(1)-C(31)-C(32)	123.1(2)
C(34)A			
C(35)-C(36)	1.379(2)	O(1)-C(31)-C(36)	118.0(2)
		C(32)-C(31)-	118.9(2)
		C(36)	
		C(31)-C(32)-	120.8(2)
		C(33)	
		C(32)-C(33)-	121.5(2)
		C(34)	
		C(35)-C(34)-	116.3(2)
		C(33)	
		C(35)-C(34)-	121.8(2)
		C(34)A	
		C(33)-C(34)-	121.9(2)
		C(34)A	
		C(36)-C(35)-	122.7(2)
		C(34)	
		C(35)-C(36)-	119.8(2)
		C(31)	

13.9.14 Phenazin und Fumarsäure

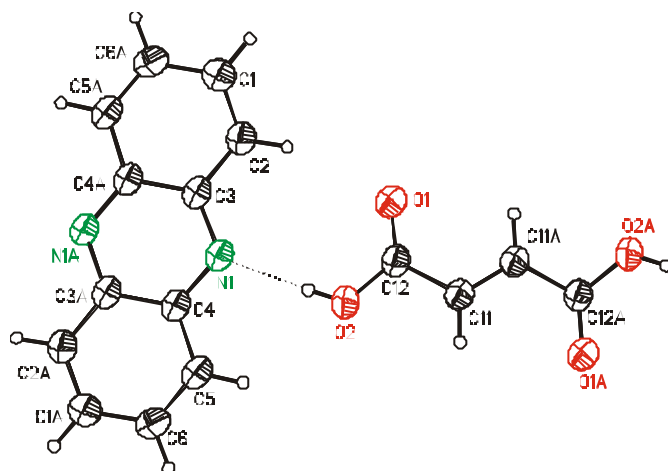


Abb. 13.9.14.1: Struktur des Kokristalls aus Phenazin und Fumarsäure. Die Ellipsoide beschreiben 50%-Aufenthaltswahrscheinlichkeit.

$[\text{C}_{12}\text{H}_8\text{N}_2] \cdot [\text{C}_4\text{H}_4\text{O}_4]$, $M = 296.28 \text{ g}\cdot\text{mol}^{-1}$, monoklin, Raumgruppe $P2_1/c$,
 $a = 5.3428(3) \text{ \AA}$, $b = 8.7784(9) \text{ \AA}$, $c = 14.9928(9) \text{ \AA}$, $\beta = 98.9500(10)^\circ$,
 $V = 694.62(7) \text{ \AA}^3$, $Z = 2$, $\rho_{\text{ber.}} = 1.417 \text{ g}\cdot\text{cm}^{-3}$, $\lambda = 0.71073 \text{ \AA}$, $T = 303 \text{ K}$, $m = 0.104$
 mm^{-1} , 968.unabhängige Reflexe ($R_{\text{int}} = 0.0115$), $R = 0.0472$, $wR_2 = 0.1257$.

Tabelle 13.9.14.1: Atomkoordinaten [10^4] und äquivalente isotrope Versetzungsparameter [$\text{\AA}^2 \cdot 10^3$] des Kokristalls aus Phenazin und Fumarsäure.

	x	y	z	U(eq)
N(1)	2894(2)	9015(2)	4928(1)	39(1)
O(1)	-901(2)	6093(2)	5829(1)	55(1)
O(2)	-1530(2)	7337(1)	4514(1)	48(1)
C(1)	5721(4)	8401(2)	7258(1)	51(1)

C(2)	4085(3)	8284(2)	6472(1)	45(1)
C(3)	4483(3)	9153(2)	5711(1)	38(1)
C(4)	3371(3)	9837(2)	4214(1)	38(1)
C(5)	1741(3)	9735(2)	3373(1)	47(1)
C(6)	2186(4)	10591(3)	2659(1)	52(1)
C(11)	-4500(3)	5494(2)	4751(1)	42(1)
C(12)	-2135(3)	6318(2)	5095(1)	39(1)

Tabelle 13.9.14.2: Wasserstoffatomkoordinaten $[10^4]$ und isotrope Versetzungsparameter

$[\text{\AA}^2 \cdot 10^3]$ des Kokristalls aus Phenazin und Fumarsäure.

	x	y	z	U(eq)
H(20)	-172(2)	7790(1)	4602(1)	71(7)
H(1)	5482(4)	7770(2)	7762(1)	61
H(2)	2638(3)	7624(2)	6426(1)	54
H(5)	295(3)	9073(2)	3311(1)	56
H(6)	1093(4)	10484(3)	2091(1)	63
H(11)	-5332(3)	5686(2)	4147(1)	50

Tabelle 13.9.14.3: Bindungslängen $[\text{\AA}]$ und Winkel $[\text{\circ}]$ des Kokristalls aus Phenazin und Fumarsäure.

Bindungslängen $[\text{\AA}]$		Winkel $[\text{\circ}]$	
N(1)-C(3)	1.343(2)	C(3)-N(1)-C(4)	118.30(14)
N(1)-C(4)	1.348(2)	C(3)-N(1)-H(20)	131.20(12)
N(1)-H(20)	1.957(2)	C(4)-N(1)-H(20)	110.50(12)
N(1)-O(2)	2.772(2)	C(3)-N(1)-O(2)	130.13(11)
O(1)-C(12)	1.208(2)	C(4)-N(1)-O(2)	111.52(11)
O(2)-C(12)	1.323(2)	C(12)-O(1)-H(6)A	154.97(14)
O(2)-H(20)	0.82	C(12)-O(2)-N(1)	119.92(10)
C(1)-C(2)	1.358(3)	C(12)-O(2)-H(20)	121.53(8)
C(1)-C(6)A	1.416(3)	N(1)-H(20)-O(2)	172.82(5)
C(2)-C(3)	1.417(2)	C(2)-C(1)-C(6)A	121.1(2)
Bindungslängen $[\text{\AA}]$		Winkel $[\text{\circ}]$	
C(3)-C(4)A	1.440(2)	C(1)-C(2)-C(3)	120.1(2)

C(4)-C(5)	1.419(2)	N(1)-C(3)-C(2)	120.1(2)
C(4)-C(3)A	1.440(2)	N(1)-C(3)-C(4)A	120.8(2)
C(5)-C(6)	1.359(3)	C(2)-C(3)-C(4)A	119.1(2)
C(6)-C(1)A	1.416(3)	N(1)-C(4)-C(5)	120.4(2)
C(11)-C(11)A	1.311(3)	N(1)-C(4)-C(3)A	120.9(2)
C(11)-C(12)	1.478(2)	C(5)-C(4)-C(3)A	118.7(2)
		C(6)-C(5)-C(4)	120.4(2)
		C(5)-C(6)-C(1)A	120.6(2)
		C(11)A-C(11)-C(12)	121.8(2)
		O(1)-C(12)-O(2)	123.8(2)

13.9.15 Phenazin und 2,3-Dihydroxyfumarsäure

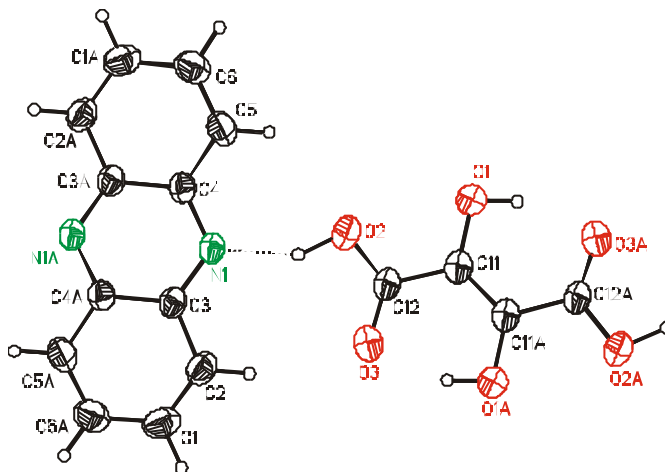


Abb. 13.9.15.1: Struktur des Kokristalls aus Phenazin und 2,3-Dihydroxyfumarsäure. Die Ellipsoide beschreiben 50%-Aufenthaltswahrscheinlichkeit.

$[\text{C}_{12}\text{H}_8\text{N}_2] \cdot [\text{C}_4\text{H}_4\text{O}_6]$, $M = 328.28 \text{ g}\cdot\text{mol}^{-1}$, monoklin, Raumgruppe $P2_1/c$, $a = 8.8138(3) \text{ \AA}$, $b = 5.3064(2) \text{ \AA}$, $c = 15.7759(5) \text{ \AA}$, $\beta = 103.2940(10)^\circ$, $V = 718.06(4) \text{ \AA}^3$, $Z = 2$, $\rho_{\text{ber.}} = 1.518 \text{ g}\cdot\text{cm}^{-3}$, $\lambda = 0.71073 \text{ \AA}$, $T = 298 \text{ K}$, $m = 0.119 \text{ mm}^{-1}$, 1224 unabhängige Reflexe ($R_{\text{int}} = 0.0255$), $R = 0.0592$, $wR_2 = 0.1487$.

Tabelle 13.9.15.1: Atomkoordinaten [10^4] und äquivalente isotrope Versetzungsparameter [$\text{\AA}^2 \cdot 10^3$] des Kokristalls aus Phenazin und 2,3-Dihydroxafumarsäure.

	x	y	z	U(eq)
N(1)	4022(2)	-2924(3)	38(1)	35(1)
O(1)	1333(2)	5105(4)	1072(1)	57(1)
O(2)	2517(2)	1202(3)	454(1)	49(1)
O(3)	706(2)	1253(3)	-804(1)	50(1)
C(1)	2479(3)	-5116(5)	-2172(2)	51(1)
C(2)	2658(3)	-3688(5)	-1443(2)	43(1)
C(3)	3856(3)	-4292(4)	-695(2)	34(1)
C(4)	5139(3)	-3592(4)	732(2)	34(1)
C(5)	5367(3)	-2189(4)	1523(2)	45(1)
C(6)	6524(3)	-2814(5)	2213(2)	50(1)
C(11)	613(3)	4393(4)	248(2)	39(1)
C(12)	1285(3)	2145(4)	-79(2)	36(1)

Tabelle 13.9.15.2: Wasserstoffatomkoordinaten [10^4] und isotrope Versetzungsparameter

[$\text{\AA}^2 \cdot 10^3$] des Kokristalls aus Phenazin und 2,3-Dihydroxyfumarsäure.

	x	y	z	U(eq)
H(10)	783(2)	6535(4)	1107(1)	11(4)
H(20)	2864(2)	-317(3)	106(1)	196(26)
H(1)	1658(3)	-4722(5)	-2670(2)	61

H(2)	1984(3)	-2274(5)	-1430(2)	52
H(5)	4698(3)	-788(4)	1565(2)	53
H(6)	6669(3)	-1847(5)	2740(2)	60

Tabelle 13.9.15.3: Bindungslängen [Å] und Winkel [°] des Kokristalls aus Phenazin und 2,3-Dihydroxyfumarsäure.

Bindungslängen [Å]		Winkel [°]	
N(1)-C(4)	1.340(3)	C(4)-N(1)-C(3)	118.3(2)
N(1)-C(3)	1.345(3)	C(4)-N(1)-H(20)	119.5(2)
N(1)-H(20)	1.737(2)	C(3)-N(1)-H(20)	122.2(2)
N(1)-O(2)	2.717(2)	C(4)-N(1)-O(2)	108.88(14)
O(1)-C(11)	1.362(3)	C(3)-N(1)-O(2)	132.8(2)
O(1)-H(10)	0.91	O(2)-H(20)-N(1)	151.83(9)
O(2)-C(12)	1.310(3)	C(11)-O(1)-H(6)1	134.3(2)
O(2)-H(20)	1.06	C(11)-O(1)-H(10)	98.73(12)
O(3)-C(12)	1.234(3)	H(6)1-O(1)-H(10)	126.71(7)
C(1)-C(2)	1.357(4)	C(12)-O(2)-N(1)	122.1(2)
C(1)-C(6)A	1.418(4)	C(12)-O(2)-H(20)	104.70(13)
C(1)-H(1)	0.96	C(2)-C(1)-C(6)A	121.2(2)
C(2)-C(3)	1.426(3)	C(1)-C(2)-C(3)	119.7(2)
C(2)-H(2)	0.96	N(1)-C(3)-C(2)	120.2(2)
Bindungslängen [Å]		Winkel [°]	
C(3)-C(4)A	1.439(3)	N(1)-C(3)-C(4)A	120.6(2)
C(4)-C(5)	1.427(3)	C(2)-C(3)-C(4)A	119.2(2)
C(4)-C(3)A	1.440(3)	N(1)-C(4)-C(5)	120.4(2)
C(5)-C(6)	1.350(4)	N(1)-C(4)-C(3)A	121.1(2)
C(5)-H(5)	0.96	C(5)-C(4)-C(3)A	118.5(2)
C(6)-C(1)A	1.418(4)	C(6)-C(5)-C(4)	120.3(2)
C(6)-H(6)	0.96	C(5)-C(6)-C(1)A	121.0(2)
C(11)-C(11)A	1.344(5)	C(11)3-C(11)-O(1)	124.0(3)
C(11)-C(12)	1.477(3)	C(11)3-C(11)-C(12)	121.1(3)
		O(1)-C(11)-C(12)	114.9(2)

O(3)-C(12)-O(2)	123.6(2)
O(3)-C(12)-C(11)	121.3(2)
O(2)-C(12)-C(11)	115.1(2)

13.9.16 Phenazin und Oxalsäure

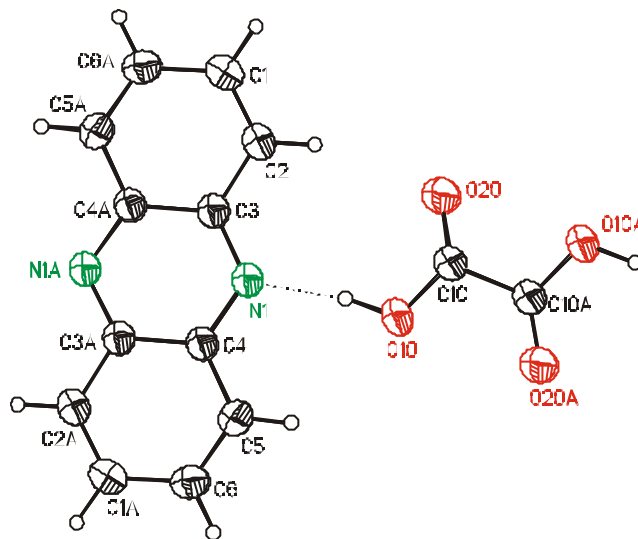


Abb. 13.9.16.1: Struktur des Kokristalls aus Phenazin und Oxalsäure. Die Ellipsoide beschreiben 50%-Aufenthaltswahrscheinlichkeit.

$[\text{C}_{12}\text{H}_8\text{N}_2] \cdot [\text{C}_2\text{H}_2\text{O}_4]$, $M = 270.24 \text{ g}\cdot\text{mol}^{-1}$, monoklin, Raumgruppe $P2_1/n$,
 $a = 3.85510(10) \text{ \AA}$, $b = 10.6381(2) \text{ \AA}$, $c = 14.7032(2) \text{ \AA}$, $\beta = 95.5910(10)^\circ$,
 $V = 600.09(2) \text{ \AA}^3$, $Z = 2$, $\rho_{\text{ber.}} = 1.496 \text{ g}\cdot\text{cm}^{-3}$, $\lambda = 0.71073 \text{ \AA}$, $T = 298 \text{ K}$, $m = 0.112$
 mm^{-1} , 1045 unabhängige Reflexe ($R_{\text{int}} = 0.0183$), $R = 0.0494$, $wR_2 = 0.1368$.

Tabelle 13.9.16.1: Atomkoordinaten [10^4] und äquivalente isotrope Versetzungsparameter [$\text{\AA}^2 \cdot 10^3$] des Kokristalls aus Phenazin und Oxalsäure.

	x	y	z	U(eq)
N(1)	926(3)	6278(1)	5000(1)	37(1)
C(1)	4910(4)	5314(2)	7222(1)	45(1)
C(2)	3922(4)	6053(2)	6496(1)	42(1)
C(3)	1922(3)	5546(1)	5719(1)	35(1)
C(4)	-976(3)	5762(1)	4278(1)	35(1)
C(5)	-2101(4)	6503(2)	3506(1)	44(1)
C(6)	-3991(4)	5982(2)	2778(1)	46(1)
C(10)	4654(4)	9346(1)	5189(1)	43(1)
O(10)	2608(3)	8690(1)	4615(1)	60(1)
O(20)	5868(4)	9003(1)	5921(1)	77(1)

Tabelle 13.9.16.2: Wasserstoffatomkoordinaten [10^4] und isotrope Versetzungsparameter [$\text{\AA}^2 \cdot 10^3$] des Kokristalls aus Phenazin und Oxalsäure.

	x	y	z	U(eq)
H(1)	6253(4)	5670(2)	7744(1)	55
H(2)	4570(4)	6924(2)	6506(1)	50
H(5)	-	7380(2)	3502(1)	52
	1524(4)			
H(6)	-	6489(2)	2253(1)	55
	4711(4)			
H(10)	2152(3)	7840(1)	4808(1)	93(7)

Tabelle 13.9.16.3: Bindungslängen [\AA] und Winkel [$^\circ$] des Kokristalls aus Phenazin und Oxalsäure.

Bindungslängen [\AA]		Winkel [$^\circ$]	
N(1)-C(3)	1.338(2)	C(3)-N(1)-C(4)	118.51(12)
N(1)-C(4)	1.346(2)	C(3)-N(1)-H(10)	128.00(10)
N(1)-H(10)	1.758(2)	C(4)-N(1)-H(10)	113.16(10)

N(1)-O(10)	2.719(2)	C(3)-N(1)-O(10)	131.08(9)
C(1)-C(2)	1.350(2)	C(4)-N(1)-O(10)	110.09(9)
C(1)-C(6)A	1.424(2)	C(2)-C(1)-C(6)A	120.84(14)
C(2)-C(3)	1.421(2)	C(1)-C(2)-C(3)	120.29(14)
C(3)-C(4)A	1.438(2)	N(1)-C(3)-C(2)	120.40(13)
C(4)-C(5)	1.416(2)	N(1)-C(3)-C(4)A	120.77(13)
C(4)-C(3)A	1.438(2)	C(2)-C(3)-C(4)A	118.83(13)
C(5)-C(6)	1.353(2)	N(1)-C(4)-C(5)	120.39(13)
C(6)-C(1)A	1.424(2)	N(1)-C(4)-C(3)A	120.72(13)
C(10)-O(20)	1.189(2)	C(5)-C(4)-C(3)A	118.89(13)
C(10)-O(10)	1.300(2)	C(6)-C(5)-C(4)	120.39(14)
C(10)-C(10)A	1.530(3)	C(5)-C(6)-C(1)A	120.75(14)
O(10)-H(10)	0.97	O(20)-C(10)-O(10)	125.63(14)
		O(20)-C(10)-C(10)A	122.7(2)
Bindungslängen [Å]		Winkel [°]	
		O(10)-C(10)-C(10)A	111.7(2)
		C(10)-O(10)-N(1)	120.92(10)
		C(10)-O(10)-H(10)	115.33(8)
		N(1)-H(10)-O(10)	171.33(5)

13.9.17 Phenazin und 5,10-Dihydrophenazin (3 : 1)

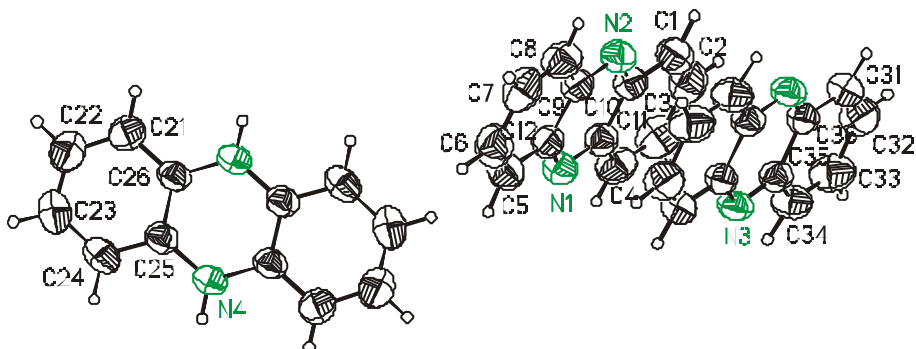


Abb. 13.9.17.1: Struktur des Kokristalls aus Phenazin und 5,10-Dihydrophenazin (3 : 1). Die Ellipsoide beschreiben 50%-Aufenthaltswahrscheinlichkeit.

$3[\text{C}_{12}\text{H}_8\text{N}_2] \cdot [\text{C}_{12}\text{H}_{10}\text{N}_2]$, $M = 722.73 \text{ g}\cdot\text{mol}^{-1}$, triklin, Raumgruppe $P\bar{1}$, $a = 9.026(2) \text{ \AA}$, $b = 9.676(2) \text{ \AA}$, $c = 11.242(2) \text{ \AA}$, $\alpha = 72.522(2)^\circ$, $\beta = 80.196(3)^\circ$, $\gamma = 77.597(3)^\circ$, $V = 908.7(3) \text{ \AA}^3$, $Z = 1$, $\rho_{\text{ber.}} = 1.321 \text{ g}\cdot\text{cm}^{-3}$, $\lambda = 0.71073 \text{ \AA}$, $T = 293(2) \text{ K}$, $\mu = 0.080 \text{ mm}^{-1}$, 2294 unabhängige Reflexe ($R_{\text{int}} = 0.0529$), $R = 0.0629$, $wR_2 = 0.1579$.

Tabelle 13.9.17.1: Atomkoordinaten [10^4] und äquivalente isotrope Versetzungsparameter [$\text{\AA}^2 \cdot 10^3$] des Kokristalls aus Phenazin und 5,10-Dihydrophenazin (3 : 1).

	x	y	z	U(eq)
C(1)	2518(5)	2671(5)	3093(4)	79(1)
C(2)	2748(4)	4032(5)	2995(3)	69(1)
C(3)	4150(4)	4261(4)	3250(3)	54(1)
N(4)	4345(3)	5624(3)	3148(2)	59(1)

C(5)	5705(4)	5776(4)	3373(3)	54(1)
C(6)	6009(5)	7181(4)	3271(3)	70(1)
C(7)	7392(6)	7347(5)	3462(4)	78(1)
C(11)	3682(6)	1445(5)	3440(4)	82(1)
C(12)	5042(5)	1607(4)	3681(3)	68(1)
C(13)	5330(4)	3017(4)	3584(3)	54(1)
N(14)	6692(3)	3157(3)	3816(3)	59(1)
C(15)	6897(4)	4532(4)	3697(3)	53(1)
C(16)	8329(4)	4756(5)	3893(3)	70(1)
C(17)	8560(5)	6119(6)	3771(4)	81(1)
C(21)	8026(5)	6703(5)	358(4)	74(1)
C(22)	7807(4)	5347(4)	430(3)	65(1)
C(23)	6394(4)	5131(4)	206(3)	51(1)
N(24)	6183(3)	3773(3)	276(2)	55(1)
C(25)	4812(4)	3629(4)	66(3)	52(1)
C(26)	4518(4)	2225(4)	143(3)	67(1)
C(27)	3155(5)	2065(5)	-69(4)	79(1)
C(31)	9857(5)	163(4)	3240(4)	72(1)
C(32)	9122(4)	886(4)	2187(4)	63(1)
C(33)	9551(4)	450(4)	1102(3)	52(1)
N(34)	8825(4)	1161(3)	27(3)	77(1)
C(35)	9255(4)	744(4)	-1073(3)	53(1)
C(36)	8520(4)	1445(4)	-2130(4)	61(1)
C(37)	8966(5)	990(4)	-3219(4)	70(1)

Tabelle 13.9.17.2: Wasserstoffatomkoordinaten $[10^4]$ und isotrope Versetzungsparameter $[\text{\AA}^2 \cdot 10^3]$ des Kokristalls aus Phenazin und 5,10-Dihydrophenazin (3 : 1).

	x	y	z	U(eq)
H(1)	1559	2532	2928	94
H(2)	1953	4861	2748	82
H(6)	5226	8032	3063	84
H(7)	7575	8313	3390	94
H(11)	3506	477	3508	98
H(12)	5819	757	3916	82
H(16)	9132	3928	4118	84
H(17)	9540	6262	3888	97
H(21)	8993	6838	509	89
H(22)	8618	4521	632	78
H(26)	5304	1375	342	81
H(27)	2976	1104	-17	94
H(31)	9546	475	3991	87
H(32)	8303	1699	2211	75
H(34)	7888	2105	66	92
H(36)	7692	2252	-2113	73
H(37)	8454	1486	-3953	84

Tabelle 13.9.17.3: Bindungslängen $[\text{\AA}]$ und Winkel $[\text{\circ}]$ des Kokristalls aus Phenazin und 5,10-Dihydrophenazin (3 : 1).

Bindungslängen $[\text{\AA}]$		Winkel $[\text{\circ}]$	
C(1)-C(2)	1.346(5)	C(2)-C(1)-C(11)	120.2(4)
C(1)-C(11)	1.411(5)	C(1)-C(2)-C(3)	121.0(4)
C(2)-C(3)	1.420(5)	N(4)-C(3)-C(2)	119.7(4)
C(3)-N(4)	1.336(4)	N(4)-C(3)-C(13)	121.8(3)
C(3)-C(13)	1.427(5)	C(2)-C(3)-C(13)	118.5(3)
N(4)-C(5)	1.341(4)	C(3)-N(4)-C(5)	117.0(3)
C(5)-C(6)	1.412(5)	N(4)-C(5)-C(6)	120.5(4)
C(5)-C(15)	1.433(5)	N(4)-C(5)-C(15)	121.3(3)

C(6)-C(7)	1.352(5)	C(6)-C(5)-C(15)	118.1(4)
C(7)-C(17)	1.408(5)	C(7)-C(6)-C(5)	120.8(4)
C(11)-C(12)	1.351(5)	C(6)-C(7)-C(17)	120.7(4)
C(12)-C(13)	1.413(5)	C(12)-C(11)-C(1)	121.1(4)
C(13)-N(14)	1.342(4)	C(11)-C(12)- C(13)	120.4(4)
N(14)-C(15)	1.346(4)	N(14)-C(13)- C(12)	119.6(3)
C(15)-C(16)	1.419(5)	N(14)-C(13)-C(3)	121.6(3)
C(16)-C(17)	1.342(5)	C(12)-C(13)-C(3)	118.8(3)
C(21)-C(22)	1.345(5)	C(13)-N(14)- C(15)	116.6(3)
C(21)- C(27)A	1.415(5)	N(14)-C(15)- C(16)	119.3(3)
C(22)-C(23)	1.410(5)	N(14)-C(15)-C(5)	121.6(3)
C(23)-N(24)	1.345(4)	C(16)-C(15)-C(5)	119.2(3)
C(23)- C(25)A	1.432(5)	C(17)-C(16)- C(15)	120.2(4)
N(24)-C(25)	1.342(4)	C(16)-C(17)-C(7)	121.1(4)
C(25)-C(26)	1.414(5)	C(22)-C(21)- C(27)A	120.9(4)
Bindungslängen [Å]		Winkel [°]	
C(25)- C(23)A	1.432(5)	C(21)-C(22)- C(23)	120.4(4)
C(26)-C(27)	1.341(5)	N(24)-C(23)- C(22)	120.1(3)
C(27)- C(21)A	1.415(5)	N(24)-C(23)- C(25)A	121.0(3)
C(31)- C(37)A	1.368(5)	C(22)-C(23)- C(25)A	118.9(3)
C(31)-C(32)	1.378(5)	C(25)-N(24)- C(23)	117.6(3)
C(32)-C(33)	1.376(5)	N(24)-C(25)- C(26)	120.1(3)
C(33)-N(34)	1.393(4)	N(24)-C(25)- C(23)A	121.4(3)
C(33)- C(35)A	1.404(4)	C(26)-C(25)- C(23)A	118.5(3)
N(34)-C(35)	1.383(4)	C(27)-C(26)- C(25)	120.7(4)
C(35)-C(36)	1.379(4)	C(26)-C(27)-	120.6(4)

C(35)- C(33)A	1.405(4)	C(21)A	
C(36)-C(37)	1.391(5)	C(37)A-C(31)- C(32)	120.6(4)
C(37)- C(31)A	1.368(5)	C(33)-C(32)- C(31)	120.5(4)
		C(32)-C(33)- N(34)	121.6(3)
		C(32)-C(33)- C(35)A	119.5(3)
		N(34)-C(33)- C(35)A	118.9(3)
		C(35)-N(34)- C(33)	122.2(3)
		C(36)-C(35)- N(34)	121.8(3)
		C(36)-C(35)- C(33)A	119.3(3)
		N(34)-C(35)- C(33)A	118.9(3)
		C(35)-C(36)- C(37)	120.5(4)
		C(31)A-C(37)- C(36)	119.6(4)

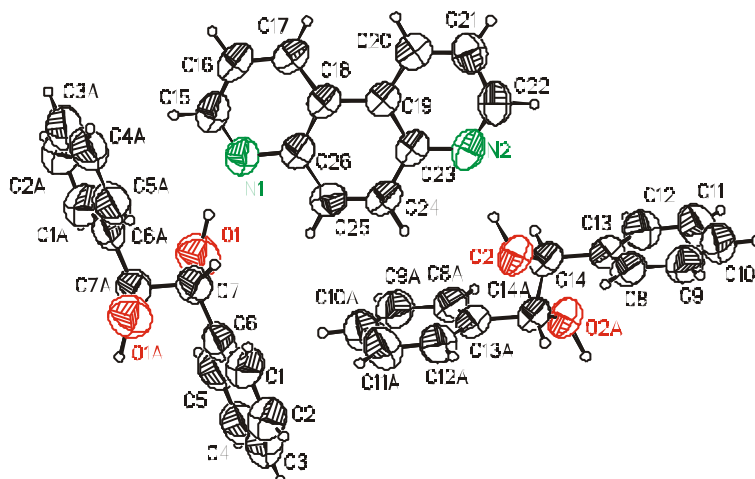
13.9.18 4,7-Phenanthrolin und *meso*-1,2-Diphenyl-1,2-ethandiol

Abb. 13.9.18.1: Struktur des Kokristalls aus 4,7-Phenanthrolin und *meso*-1,2-Diphenyl-1,2-ethandiol. Die Ellipsoide beschreiben 50%-Aufenthaltswahrscheinlichkeit.

$[\text{C}_{12}\text{H}_8\text{N}_2] \cdot [\text{C}_{14}\text{H}_{14}\text{O}_2]$, $M = 394.46 \text{ g}\cdot\text{mol}^{-1}$, triklin, Raumgruppe $P\bar{1}$, $a = 6.7805(6) \text{ \AA}$, $b = 12.1710(7) \text{ \AA}$, $c = 13.1542(9) \text{ \AA}$, $\alpha = 83.238(5)^\circ$, $\beta = 81.976(5)^\circ$, $\gamma = 80.648(4)^\circ$, $V = 1055.61(13) \text{ \AA}^3$, $Z = 2$, $\rho_{\text{ber.}} = 1.241 \text{ g}\cdot\text{cm}^{-3}$, $\lambda = 0.71073 \text{ \AA}$, $T = 293(2) \text{ K}$, $m = 0.079 \text{ mm}^{-1}$, 4187 unabhängige Reflexe ($R_{\text{int}} = 0.0225$), $R = 0.0686$, $wR_2 = 0.1834$.

Tabelle 13.9.18.1: Atomkoordinaten [10^4] und äquivalente isotrope Versetzungsparameter [$\text{\AA}^2 \cdot 10^3$] des Kokristalls aus 4,7-Phenanthrolin und *meso*-1,2-Diphenyl-1,2-ethandiol.

	x	y	z	U(eq)
C(1)	10941(9)	2206(4)	5079(3)	138(2)
O(1)	7570(5)	124(2)	5791(2)	119(1)
N(1)	8159(4)	-989(2)	7718(2)	79(1)
O(2)	7258(3)	4008(2)	10140(2)	84(1)
C(2)	10890(1)	3317(4)	4697(4)	154(2)
	2)			
N(2)	6838(3)	1768(2)	10873(2)	77(1)
C(3)	9278(15)	3831(5)	4269(4)	162(3)
C(4)	7672(11)	3319(4)	4168(3)	139(2)
C(5)	7760(8)	2154(3)	4559(3)	126(2)
C(6)	9394(7)	1615(3)	5011(2)	106(1)
C(7)	9495(6)	388(3)	5418(3)	94(1)
C(8)	7137(5)	5618(2)	11518(3)	84(1)
C(9)	7175(7)	6220(3)	12352(3)	108(1)
C(10)	5463(10)	6430(3)	13039(3)	126(2)
C(11)	3744(9)	6025(4)	12922(3)	124(1)
C(12)	3720(6)	5427(3)	12105(3)	98(1)

C(13)	5411(5)	5223(2)	11384(2)	76(1)
C(14)	5342(4)	4604(2)	10459(2)	70(1)
C(15)	8552(4)	-2085(3)	7908(3)	83(1)
C(16)	8662(4)	-2632(2)	8878(3)	80(1)
C(17)	8289(4)	-2018(2)	9707(2)	71(1)
C(18)	7862(3)	-852(2)	9556(2)	62(1)
C(19)	7468(3)	-130(2)	10381(2)	62(1)
C(20)	7342(4)	-519(2)	11430(2)	75(1)
C(21)	6972(5)	218(3)	12159(3)	86(1)
C(22)	6745(4)	1352(3)	11847(3)	86(1)
C(23)	7161(4)	1037(2)	10136(2)	66(1)
C(24)	7177(4)	1493(2)	9090(2)	73(1)
C(25)	7493(4)	821(2)	8321(2)	75(1)
C(26)	7844(4)	-363(2)	8535(2)	67(1)

Tabelle 13.9.18.2: Wasserstoffatomkoordinaten [10⁴] und isotrope Versetzungsparameter [Å² · 10³] des Kokristalls aus 4,7-Phenanthrolin und *meso*-1,2-Diphenyl-1,2-ethandiol.

	x	y	z	U(eq)
H(1)	12088	1832	5401	166
H(01)	7877	-425	6483	178
H(02)	7236	3137	10344	125
H(2)	11992	3709	4737	185
H(3)	9233	4607	4018	194

H(4)	6537	3716	3851	166
H(5)	6672	1759	4500	152
H(7)	10292	251	5981	113
H(8)	8326	5477	11034	101
H(9)	8387	6486	12447	130
H(10)	5472	6862	13603	151
H(11)	2560	6160	13410	149
H(12)	2514	5143	12028	118
H(14)	4410	4078	10651	83
H(15)	8779	-2528	7333	100
H(16)	8990	-3432	8971	96
H(17)	8323	-2387	10393	85
H(20)	7519	-1308	11635	90
H(21)	6870	-45	12879	103
H(22)	6508	1864	12369	103
H(24)	6962	2290	8928	87
H(25)	7482	1145	7619	90

Tabelle 13.9.18.3: Bindungslängen [Å] und Winkel [°] des Kokristalls aus 4,7-Phenanthrolin und *meso*-1,2-Diphenyl-1,2-ethandiol.

Bindungslängen [Å]		Winkel [°]	
C(1)-C(2)	1.383(6)	C(2)-C(1)-C(6)	122.1(5)
C(1)-C(6)	1.384(6)	C(7)-O(1)-H(01)	101.2
O(1)-C(7)	1.403(4)	C(15)-N(1)-C(26)	117.9(3)
O(1)-H(01)	10.871	C(15)-N(1)-H(01)	119.0
N(1)-C(15)	1.317(4)	C(26)-N(1)-H(01)	122.9
N(1)-C(26)	1.363(4)	C(14)-O(2)-H(02)	109.1
O(2)-C(14)	1.416(3)	C(3)-C(2)-C(1)	118.4(6)
O(2)-H(02)	10.649	C(22)-N(2)-C(23)	118.0(3)
C(2)-C(3)	1.331(8)	C(22)-N(2)-H(02)	128.1
N(2)-C(22)	1.318(4)	C(23)-N(2)-H(02)	111.9
N(2)-C(23)	1.364(3)	C(2)-C(3)-C(4)	123.8(6)
C(3)-C(4)	1.368(8)	C(3)-C(4)-C(5)	117.1(5)
C(4)-C(5)	1.445(6)	C(6)-C(5)-C(4)	119.9(5)
C(4)-H(4)	0.9599	C(5)-C(6)-C(1)	118.6(4)
C(5)-C(6)	1.367(5)	C(5)-C(6)-C(7)	120.1(4)
C(6)-C(7)	1.520(5)	C(1)-C(6)-C(7)	121.3(4)

Bindungslängen [Å]		Winkel [°]	
C(7)-C(7A)	1.547(6)	O(1)-C(7)-C(6)	111.1(3)
C(8)-C(13)	1.375(4)	O(1)-C(7)-C(7A)	109.7(4)
C(8)-C(9)	1.395(5)	C(6)-C(7)-C(7A)	111.6(4)
C(9)-C(10)	1.376(6)	C(13)-C(8)-C(9)	120.5(4)
C(10)-C(11)	1.371(6)	C(10)-C(9)-C(8)	119.6(4)
C(11)-C(12)	1.371(5)	C(11)-C(10)-C(9)	120.4(4)
C(12)-C(13)	1.391(4)	C(12)-C(11)- C(10)	119.8(4)
C(13)-C(14)	1.514(4)	C(11)-C(12)- C(13)	121.2(4)
C(14)-C(14A)	1.530(5)	C(8)-C(13)-C(12)	118.5(3)
C(15)-C(16)	1.374(5)	C(8)-C(13)-C(14)	120.7(3)
C(16)-C(17)	1.366(4)	C(12)-C(13)- C(14)	120.8(3)
C(17)-C(18)	1.398(3)	O(2)-C(14)-C(13)	111.0(2)
C(18)-C(26)	1.404(4)	O(2)-C(14)- C(14A)	108.1(3)
C(18)-C(19)	1.445(4)	C(13)-C(14)- C(14A)	112.1(2)
C(19)-C(20)	1.401(4)	N(1)-C(15)-C(16)	124.0(3)
C(19)-C(23)	1.407(4)	C(17)-C(16)- C(15)	118.8(3)
C(20)-C(21)	1.360(4)	C(16)-C(17)- C(18)	119.9(3)
C(21)-C(22)	1.383(5)	C(17)-C(18)- C(26)	117.3(3)
C(23)-C(24)	1.421(4)	C(17)-C(18)- C(19)	124.0(3)
C(24)-C(25)	1.348(4)	C(26)-C(18)- C(19)	118.7(2)
C(25)-C(26)	1.422(4)	C(20)-C(19)- C(23)	116.9(2)
		C(20)-C(19)- C(18)	124.0(2)
		C(23)-C(19)- C(18)	119.2(3)
		C(21)-C(20)- C(19)	120.3(3)
		C(20)-C(21)- C(22)	118.9(3)

Bindungslängen [Å]	Winkel [°]	
	N(2)-C(22)-C(21)	123.6(3)
	N(2)-C(23)-C(19)	122.3(3)
	N(2)-C(23)-C(24)	117.6(2)
	C(19)-C(23)- C(24)	120.1(2)
	C(25)-C(24)- C(23)	120.9(2)
	C(24)-C(25)- C(26)	120.8(3)
	N(1)-C(26)-C(18)	122.1(2)
	N(1)-C(26)-C(25)	117.5(3)
	C(18)-C(26)- C(25)	120.4(3)

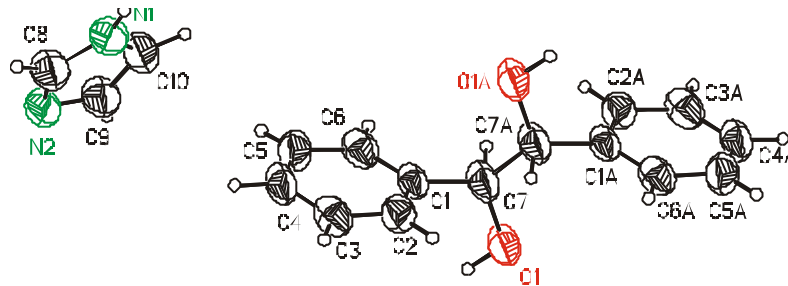
13.9.19 Imidazol und *meso*-1,2-Diphenyl-1,2-ethandiol

Abb. 13.9.19.1: Struktur des Kokristalls aus Imidazol und *meso*-1,2-Diphenyl-1,2-ethandiol. Die Ellipsoide beschreiben 50%-Aufenthaltswahrscheinlichkeit.

$[\text{C}_{14}\text{H}_{14}\text{O}_2] \cdot 2[\text{C}_3\text{H}_4\text{N}_2]$, $M = 350.42 \text{ g}\cdot\text{mol}^{-1}$, monoklin, Raumgruppe $P2_1/c$,
 $a = 5.6362(2) \text{ \AA}$, $b = 11.50390(10) \text{ \AA}$, $c = 14.4279(4) \text{ \AA}$, $\beta = 96.640(2)^\circ$,
 $V = 929.21(4) \text{ \AA}^3$, $Z = 2$, $\rho_{\text{ber.}} = 1.252 \text{ g}\cdot\text{cm}^{-3}$, $\lambda = 0.71073 \text{ \AA}$, $T = 293(2) \text{ K}$,
 $m = 0.083 \text{ mm}^{-1}$, 1597 unabhängige Reflexe ($R_{\text{int}} = 0.0402$), $R = 0.0643$,
 $wR_2 = 0.1478$.

Tabelle 13.9.19.1: Atomkoordinaten [10^4] und äquivalente isotrope Versetzungsparameter [$\text{\AA}^2 \cdot 10^3$] des Kokristalls aus Imidazol und *meso*-1,2-Diphenyl-1,2-ethandiol.

	x	y	z	U(eq)
N(1)	6816(4)	2611(2)	2943(2)	65(1)
N(2)	4759(4)	1263(2)	2135(1)	66(1)
O(1)	8436(4)	4636(1)	3884(1)	72(1)
C(1)	9321(5)	4509(2)	4800(2)	68(1)
C(2)	10449(4)	3329(2)	5019(2)	50(1)
C(3)	9374(4)	2561(2)	5578(2)	57(1)
C(4)	10281(5)	1463(2)	5746(2)	64(1)
C(5)	12290(5)	1119(2)	5372(2)	65(1)
C(6)	13406(5)	1872(2)	4822(2)	62(1)
C(7)	12490(5)	2980(2)	4652(2)	56(1)
C(8)	4818(6)	2359(2)	2425(2)	70(1)
C(9)	6856(6)	779(2)	2479(2)	74(1)
C(10)	8086(5)	1607(2)	2977(2)	66(1)

Tabelle 13.9.19.2: Wasserstoffatomkoordinaten [10^4] und isotrope Versetzungsparameter [$\text{\AA}^2 \cdot 10^3$] des Kokristalls aus Imidazol und *meso*-1,2-Diphenyl-1,2-ethandiol.

	x	y	z	U(eq)
H(2)	3551	913	1778	80
H(10)	7799	3849	3655	108
H(1)	7925	4513	5123	82
H(3)	7983	2802	5854	68
H(4)	9493	932	6122	77
H(5)	12935	355	5499	77
H(6)	14803	1627	4552	74
H(7)	13283	3514	4280	68
H(8)	3546	2906	2277	84
H(9)	7367	-4	2384	88
H(10A)	9648	1512	3312	79

Tabelle 13.9.19.3: Bindungslängen [Å] und Winkel [°] des Kokristalls aus Imidazol und *meso*-1,2-Diphenyl-1,2-ethandiol.

Bindungslängen [Å]		Winkel [°]	
N(1)-C(8)	1.310(4)	C(8)-N(1)-C(10)	104.3(2)
N(1)-C(10)	1.357(3)	C(8)-N(1)-H(10)	133.4
N(1)-H(10)	1.8055	C(10)-N(1)- H(10)	121.6
N(2)-C(8)	1.327(3)	C(10)-N(1)- H(10)	121.6
N(2)-C(9)	1.348(4)	O(1)-H(10)- N(1)	164.3
O(1)-C(1)	1.365(3)	O(1)-C(1)-C(1)A	114.8(3)
C(1)-C(1)A	1.447(5)	O(1)-C(1)-C(2)	113.3(2)
C(1)-C(2)	1.516(3)	C(1)A-C(1)-C(2)	115.2(3)
C(2)-C(7)	1.380(4)	C(7)-C(2)-C(3)	118.6(2)
C(2)-C(3)	1.383(4)	C(7)-C(2)-C(1)	121.9(2)
C(3)-C(4)	1.373(3)	C(3)-C(2)-C(1)	119.5(2)
C(4)-C(5)	1.369(4)	C(4)-C(3)-C(2)	120.8(3)
C(5)-C(6)	1.376(4)	C(5)-C(4)-C(3)	120.3(3)
C(6)-C(7)	1.386(3)	C(4)-C(5)-C(6)	119.9(2)
C(9)-C(10)	1.338(4)	C(5)-C(6)-C(7)	119.7(3)
		C(2)-C(7)-C(6)	120.7(2)
		N(1)-C(8)-N(2)	112.3(3)
		C(10)-C(9)-N(2)	106.3(2)
		C(9)-C(10)-N(1)	110.4(2)

13.9.20 1,4-Bis-(4-methoxyphenyl)-1,4-diaza-1,3-butadien und *meso*-1,2-Diphenyl-1,2-ethandiol

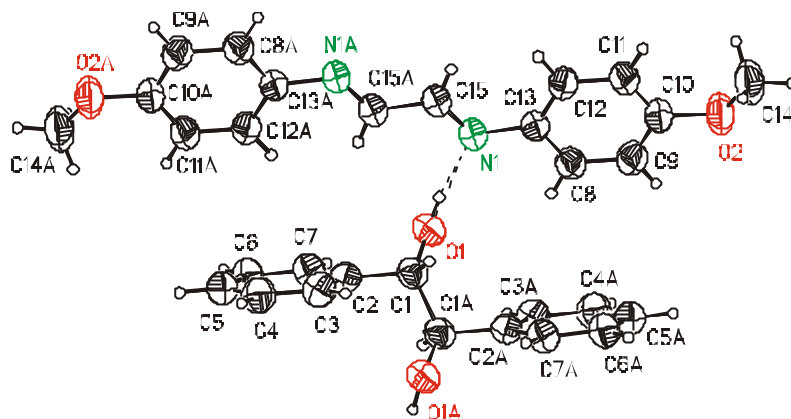


Abb. 13.9.20.1: Struktur des Kokristalls aus 1,4-Bis-(4-methoxyphenyl)-1,4-diaza-1,3-butadien und *meso*-1,2-Diphenyl-1,2-ethandiol. Die Ellipsoide beschreiben 50%-Aufenthaltswahrscheinlichkeit.

$[\text{C}_{16}\text{H}_{16}\text{N}_2\text{O}_2] \cdot [\text{C}_{14}\text{H}_{14}\text{O}_2]$, $M = 482.56 \text{ g}\cdot\text{mol}^{-1}$, triklin, Raumgruppe $P\bar{1}$,
 $a = 5.6939(13) \text{ \AA}$, $b = 7.4233(14) \text{ \AA}$, $c = 15.030(3) \text{ \AA}$, $\alpha = 98.09(2)^\circ$, $\beta = 90.08(2)^\circ$,
 $\gamma = 90.619(14)^\circ$, $V = 628.8(2) \text{ \AA}^3$, $Z = 1$, $\rho_{\text{ber.}} = 1.274 \text{ g}\cdot\text{cm}^{-3}$, $\lambda = 0.71073 \text{ \AA}$,
 $T = 293(2) \text{ K}$, $m = 0.085 \text{ mm}^{-1}$, 3647 unabhängige Reflexe ($R_{\text{int}} = 0.0576$),
 $R = 0.0709$, $wR_2 = 0.1785$.

Tabelle 13.9.20.1: Atomkoordinaten [10^4] und äquivalente isotrope Versetzungsparameter [$\text{\AA}^2 \cdot 10^3$] des Kokristalls aus 1,4-Bis-(4-methoxyphenyl)-1,4-diaza-1,3-butadien und *meso*-1,2-Diphenyl-1,2-ethandiol.

	x	y	z	U(eq)
O(1)	-264(2)	2341(2)	4798(1)	60(1)
C(1)	755(3)	849(2)	5151(1)	50(1)
N(1)	3714(3)	3886(2)	4015(1)	51(1)
C(2)	927(3)	1222(2)	6163(1)	49(1)
O(2)	4166(3)	2352(2)	292(1)	76(1)
C(3)	2777(3)	556(3)	6618(1)	58(1)
C(4)	2885(4)	853(3)	7544(1)	64(1)
C(5)	1160(4)	1839(3)	8038(1)	61(1)

C(6)	-688(4)	2512(3)	7587(1)	61(1)
C(7)	-796(3)	2210(3)	6661(1)	55(1)
C(8)	2194(3)	2585(2)	2587(1)	53(1)
C(9)	2305(3)	2205(3)	1661(1)	58(1)
C(10)	4208(4)	2800(3)	1211(1)	56(1)
C(11)	6007(4)	3766(3)	1681(1)	59(1)
C(12)	5883(4)	4151(3)	2606(1)	57(1)
C(13)	3983(3)	3560(2)	3072(1)	47(1)
C(14)	6292(5)	2536(4)	-177(2)	86(1)
C(15)	5182(3)	4833(2)	4519(1)	53(1)

Tabelle 13.9.20.2: Wasserstoffatomkoordinaten [10⁴] und isotrope Versetzungsparameter [Å² · 10³] des Kokristalls aus 1,4-Bis-(4-methoxyphenyl)-1,4-diaza-1,3-butadien und *meso*-1,2-Diphenyl-1,2-ethandiol.

	x	y	z	U(eq)
H(10)	942	2962	4595	90

H(1)	2308	646	4912	60
H(3)	3986	-93	6266	69
H(4)	4190	389	7844	77
H(5)	1180	2051	8683	74
H(6)	-1885	3232	7910	74
H(7)	-2126	2635	6360	66
H(8)	923	2134	2915	64
H(9)	1036	1549	1337	70
H(11)	7325	4190	1367	71
H(12)	7082	4867	2944	68
H(14A)	6810	3781	-48	129
)				
H(14B)	5957	2244	-807	129
H(14C)	7504	1754	-13	129
)				
H(15)	6532	5340	4258	63

Tabelle 13.9.20.3: Bindungslängen [Å] und Winkel [°] des Kokristalls aus 1,4-Bis-(4-methoxyphenyl)-1,4-diaza-1,3-butadien und *meso*-1,2-Diphenyl-1,2-ethandiol.

Bindungslängen [Å]		Winkel [°]	
O(1)-C(1)	1.422(2)	O(1)-C(1)-C(2)	110.99(14)
C(1)-C(2)	1.511(2)	O(1)-C(1)-C(1)A	108.2(2)
C(1)-C(1)A	1.532(3)	C(2)-C(1)-C(1)A	111.0(2)
N(1)-C(15)	1.266(2)	C(15)-N(1)-C(13)	121.9(2)
N(1)-C(13)	1.412(2)	C(15)-N(1)-H(10)	117.1
N(1)-H(10)	1.9675	C(13)-N(1)-H(10)	120.9
C(2)-C(7)	1.387(3)	C(7)-C(2)-C(3)	118.5(2)
C(2)-C(3)	1.388(3)	C(7)-C(2)-C(1)	120.5(2)
O(2)-C(10)	1.374(2)	C(3)-C(2)-C(1)	121.0(2)
O(2)-C(14)	1.416(3)	C(10)-O(2)-C(14)	117.5(2)
C(3)-C(4)	1.380(3)	C(4)-C(3)-C(2)	120.7(2)
C(4)-C(5)	1.384(3)	C(3)-C(4)-C(5)	120.6(2)
C(5)-C(6)	1.386(3)	C(4)-C(5)-C(6)	118.9(2)

C(6)-C(7)	1.379(3)	C(7)-C(6)-C(5)	120.4(2)
C(8)-C(9)	1.381(2)	C(6)-C(7)-C(2)	120.9(2)
C(8)-C(13)	1.389(2)	C(9)-C(8)-C(13)	120.7(2)
C(9)-C(10)	1.379(3)	C(10)-C(9)-C(8)	119.9(2)
C(10)-C(11)	1.379(3)	O(2)-C(10)-C(9)	115.7(2)
C(11)-C(12)	1.382(3)	O(2)-C(10)-	124.0(2)
		C(11)	
C(12)-C(13)	1.390(2)	C(9)-C(10)-	120.3(2)
		C(11)	
C(15)-	1.449(3)	C(12)-C(11)-	119.6(2)
C(15)A		C(10)	
		C(11)-C(12)-	121.0(2)
		C(13)	
		C(8)-C(13)-	118.5(2)
		C(12)	
Bindungslängen [Å]		Winkel [°]	
		C(8)-C(13)-N(1)	116.7(2)
		C(12)-C(13)-	124.8(2)
		N(1)	
		N(1)-C(15)-	120.3(2)
		C(15)A	

13.9.21 1,4-Bis-(4-methoxyphenyl)-1,4-diaza-1,3-butadien und *meso*-1,2-Bis-(4-methoxyphenyl)-1,2-ethandiol

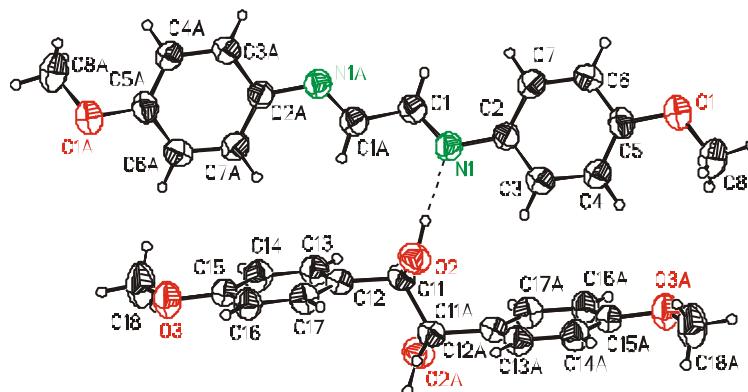


Abb. 13.9.21.1: Struktur des Kokristalls aus 1,4-Bis-(4-methoxyphenyl)-1,4-diaza-1,3-butadien und *meso*-1,2-Bis-(4-methoxyphenyl)-1,2-ethandiol. Die Ellipsoide beschreiben 50%-Aufenthaltswahrscheinlichkeit.

$[\text{C}_{16}\text{H}_{16}\text{N}_2\text{O}_2] \cdot [\text{C}_{16}\text{H}_{18}\text{O}_2]$, $M = 542.61 \text{ g}\cdot\text{mol}^{-1}$, monoklin, Raumgruppe $P2_1/n$, $a = 5.668(2) \text{ \AA}$, $b = 7.431(2) \text{ \AA}$, $c = 33.146(6) \text{ \AA}$, $\beta = 93.24(2)^\circ$, $V = 1393.8(7) \text{ \AA}^3$, $Z = 2$, $\rho_{\text{ber.}} = 1.293 \text{ g}\cdot\text{cm}^{-3}$, $\lambda = 0.71073 \text{ \AA}$, $T = 298(2) \text{ K}$, $\mu = 0.089 \text{ mm}^{-1}$, 2576.unabhängige Reflexe ($R_{\text{int}} = 0.0373$), $R = 0.0729$, $wR_2 = 0.1648$.

Tabelle 13.9.21.1: Atomkoordinaten [10^4] und äquivalente isotrope Versetzungsparameter [$\text{\AA}^2 \cdot 10^3$] des Kokristalls aus 1,4-Bis-(4-methoxyphenyl)-1,4-diaza-1,3-butadien und *meso*-1,2-Bis-(4-methoxyphenyl)-1,2-ethandiol.

	x	y	z	U(eq)
O(1)	-289(4)	2401(3)	5077(1)	57(1)
O(2)	857(4)	989(3)	3217(1)	63(1)
O(3)	4298(4)	4031(3)	7117(1)	67(1)
N(1)	3752(4)	4176(3)	5435(1)	48(1)
C(1)	5173(6)	4995(4)	5218(1)	50(1)
C(2)	3995(5)	4155(3)	5860(1)	43(1)
C(3)	2214(5)	3308(4)	6060(1)	48(1)

C(4)	2250(6)	3245(4)	6478(1)	52(1)
C(5)	4076(6)	4031(4)	6703(1)	50(1)
C(6)	5888(6)	4890(4)	6509(1)	52(1)
C(7)	5843(6)	4956(4)	6096(1)	51(1)
C(8)	2509(8)	3141(6)	7325(1)	89(1)
C(11)	740(5)	801(4)	4929(1)	44(1)
C(12)	846(5)	852(4)	4476(1)	43(1)
C(13)	2704(5)	71(4)	4282(1)	48(1)
C(14)	2779(6)	87(4)	3865(1)	51(1)
C(15)	980(5)	903(4)	3633(1)	45(1)
C(16)	-887(6)	1702(4)	3820(1)	49(1)
C(17)	-941(5)	1664(4)	4235(1)	48(1)
C(18)	2795(7)	306(6)	3013(1)	85(1)

Tabelle 13.9.21.2: Wasserstoffatomkoordinaten $[10^4]$ und isotrope Versetzungsparameter

$[\text{\AA}^2 \cdot 10^3]$ des Kokristalls aus 1,4-Bis-(4-methoxyphenyl)-1,4-diaza-1,3-butadien und *meso*-1,2-Bis-(4-methoxyphenyl)-1,2-ethandiol.

	x	y	z	U(eq)
H(10)	1031	3212	5192	85
H(1)	6493	5632	5343	60
H(3)	938	2745	5905	58
H(4)	1009	2647	6611	62
H(6)	7181	5420	6667	63
H(7)	7078	5565	5964	61
H(8A)	1116	3879	7320	133
H(8B)	3067	2939	7600	133
H(8C)	2138	2008	7198	133
H(11)	2318	679	5046	53
H(13)	3974	-478	4442	58
H(14)	4068	-473	3737	61
H(16)	-2131	2286	3661	59
H(17)	-2240	2211	4363	58
H(18A)	4226	874	3116	127
H(18B)	2551	561	2730	127
H(18C)	2916	-971	3052	127

Tabelle 13.9.21.3: Bindungslängen [Å] und Winkel [°] des Kokristalls aus 1,4-Bis-(4-methoxyphenyl)-1,4-diaza-1,3-butadien und *meso*-1,2-Bis-(4-methoxyphenyl)-1,2-ethandiol.

Bindungslängen [Å]		Winkel [°]	
O(1)-H(10)	1.0176	H(10)-O(1)-C(11)	108.5
O(1)-C(11)	1.424(3)	C(15)-O(2)-C(18)	117.7(3)
O(2)-C(15)	1.379(3)	C(5)-O(3)-C(8)	117.3(3)
O(2)-C(18)	1.415(4)	C(1)-N(1)-C(2)	123.1(3)
O(3)-C(5)	1.372(4)	C(1)-N(1)-H(10)	118.8
O(3)-C(8)	1.421(4)	C(2)-N(1)-H(10)	117.7
N(1)-C(1)	1.266(4)	O(1)-H(10)-N(1)	166.5
N(1)-C(2)	1.409(4)	N(1)-C(1)-C(1)A	121.0(4)
N(1)-H(10)	1.8437	C(3)-C(2)-C(7)	117.8(3)
C(1)-C(1)A	1.444(6)	C(3)-C(2)-N(1)	116.7(3)
C(2)-C(3)	1.389(4)	C(7)-C(2)-N(1)	125.4(3)
C(2)-C(7)	1.403(4)	C(4)-C(3)-C(2)	121.5(3)
C(3)-C(4)	1.385(4)	C(5)-C(4)-C(3)	119.8(3)
C(4)-C(5)	1.372(5)	C(4)-C(5)-O(3)	124.6(3)
C(5)-C(6)	1.396(4)	C(4)-C(5)-C(6)	119.8(3)
C(6)-C(7)	1.370(4)	O(3)-C(5)-C(6)	115.6(3)
C(11)-C(12)	1.505(4)	C(7)-C(6)-C(5)	120.2(3)
C(11)- C(11)A	1.546(5)	C(6)-C(7)-C(2)	120.8(3)
C(12)-C(13)	1.391(4)	O(1)-C(11)-C(12)	111.4(2)
C(12)-C(17)	1.392(4)	O(1)-C(11)- C(11)A	107.3(3)
C(13)-C(14)	1.386(4)	C(12)-C(11)- C(11)A	112.2(3)
C(14)-C(15)	1.382(4)	C(13)-C(12)- C(17)	117.5(3)
C(15)-C(16)	1.389(4)	C(13)-C(12)- C(11)	121.6(3)
C(16)-C(17)	1.380(4)	C(17)-C(12)- C(11)	120.9(3)
		C(14)-C(13)- C(12)	121.6(3)
		C(15)-C(14)- C(13)	119.7(3)

O(2)-C(15)-C(14)	124.8(3)
O(2)-C(15)-C(16)	115.4(3)
C(14)-C(15)-	119.8(3)
C(16)	
C(17)-C(16)-	119.8(3)
C(15)	
C(16)-C(17)-	121.7(3)
C(12)	

13.9.22 1,4-Bis-(4-methylphenyl)-1,4-diaza-1,3-butadien und *meso*-1,2-Diphenyl-1,2-ethandiol

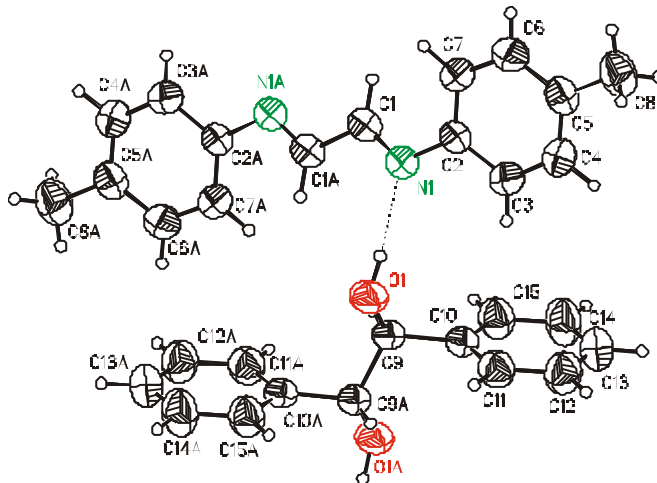


Abb. 13.9.22.1: Struktur des Kokristalls aus 1,4-Bis-(4-methylphenyl)-1,4-diaza-1,3-butadien und *meso*-1,2-Diphenyl-1,2-ethandiol. Die Ellipsoide beschreiben 50%-Aufenthaltswahrscheinlichkeit.

$[\text{C}_{16}\text{H}_{16}\text{N}_2] \cdot [\text{C}_{14}\text{H}_{14}\text{O}_2]$, $M = 225.28 \text{ g}\cdot\text{mol}^{-1}$, triklin, Raumgruppe $P\bar{1}$,
 $a = 5.5402(10) \text{ \AA}$, $b = 9.6281(14) \text{ \AA}$, $c = 12.164(2) \text{ \AA}$, $\alpha = 100.563(9)^\circ$,
 $\beta = 100.873(10)^\circ$, $\gamma = 96.428(10)^\circ$, $V = 619.2(2) \text{ \AA}^3$, $Z = 2$, $\rho_{\text{ber.}} = 1.208 \text{ g}\cdot\text{cm}^{-3}$,
 $\lambda = 0.71073 \text{ \AA}$, $T = 300(2) \text{ K}$, $m = 0.076 \text{ mm}^{-1}$, 3612 unabhängige Reflexe
($R_{\text{int}} = 0.0394$), $R = 0.0716$, $wR_2 = 0.1886$.

Tabelle 13.9.22.1: Atomkoordinaten [10^4] und äquivalente isotrope Versetzungsparameter [$\text{\AA}^2 \cdot 10^3$] des Kokristalls aus 1,4-Bis-(4-methylphenyl)-1,4-diaza-1,3-butadien und *meso*-1,2-Diphenyl-1,2-ethandiol.

	x	y	z	U(eq)
N(1)	1740(3)	9081(2)	9128(1)	54(1)
O(1)	2220(3)	6550(2)	10099(1)	68(1)
C(1)	695(4)	10089(2)	9557(2)	55(1)
C(2)	3202(4)	9273(2)	8308(2)	49(1)
C(3)	3507(5)	8049(2)	7571(2)	65(1)
C(4)	4974(5)	8163(2)	6783(2)	68(1)
C(5)	6205(4)	9462(2)	6707(2)	57(1)
C(6)	5886(4)	10673(2)	7444(2)	60(1)
C(7)	4372(3)	10582(2)	8234(1)	55(1)
C(8)	7907(3)	9560(2)	5867(1)	79(1)
C(9)	25(4)	5550(2)	9625(2)	51(1)
C(10)	-90(4)	4882(2)	8382(2)	49(1)
C(11)	1734(4)	4128(2)	8063(2)	62(1)
C(12)	1627(5)	3564(3)	6923(2)	72(1)
C(13)	-263(5)	3759(3)	6091(2)	75(1)
C(14)	-2072(5)	4504(3)	6400(2)	81(1)
C(15)	-1980(4)	5063(3)	7538(2)	66(1)

Tabelle 13.9.22.2: Wasserstoffatomkoordinaten [10⁴] und isotrope Versetzungsparameter

[Å² · 10³] des Kokristalls aus 1,4-Bis-(4-methylphenyl)-1,4-diaza-1,3-butadien und *meso*-1,2-Diphenyl-1,2-ethandiol.

	x	y	z	U(eq)
H(01)	2064(47)	7309(29)	9782(23)	81(8)
H(1)	684(39)	10980(2)	9307(20)	63(6)
		4)		
H(3)	2726(5)	7157(2)	7610(2)	78
H(4)	5140(5)	7338(2)	6287(2)	82
H(6)	6692(4)	11562(2)	7413(2)	72
H(7)	4154(3)	11409(2)	8712(1)	66
H(8A)	8591(3)	10542(2)	5939(1)	118
H(8B)	6971(3)	9185(2)	5100(1)	118
H(8C)	9231(3)	9017(2)	6033(1)	118
H(9)	-	6121(23)	9696(18)	58(6)
	1352(38)			
H(11)	3043(4)	4000(2)	8620(2)	75

H(12)	2852(5)	3046(3)	6720(2)	86
H(13)	-316(5)	3389(3)	5324(2)	90
H(14)	-3372(5)	4635(3)	5840(2)	97
H(15)	-3221(4)	5572(3)	7737(2)	79

Tabelle 13.9.22.3: Bindungslängen [Å] und Winkel [°] des Kokristalls aus 1,4-Bis-(4-methylphenyl)-1,4-diaza-1,3-butadien und *meso*-1,2-Diphenyl-1,2-ethandiol.

Bindungslängen [Å]		Winkel [°]	
N(1)-C(1)	1.266(3)	C(1)-N(1)-C(2)	120.6(2)
N(1)-C(2)	1.423(2)	N(1)-C(1)-C(1A)	120.3(2)
O(1)-C(9)	1.417(2)	C(7)-C(2)-C(3)	119.2(2)
C(1)-C(1A)	1.461(4)	C(7)-C(2)-N(1)	123.7(2)
C(2)-C(7)	1.377(2)	C(3)-C(2)-N(1)	117.1(2)
C(2)-C(3)	1.391(3)	C(4)-C(3)-C(2)	119.7(2)
C(3)-C(4)	1.380(3)	C(3)-C(4)-C(5)	122.2(2)
C(4)-C(5)	1.383(3)	C(4)-C(5)-C(6)	117.5(2)
C(5)-C(6)	1.385(3)	C(4)-C(5)-C(8)	121.5(2)
C(5)-C(8)	1.523(2)	C(6)-C(5)-C(8)	120.9(2)
C(6)-C(7)	1.397(2)	C(5)-C(6)-C(7)	121.0(2)
C(9)-C(10)	1.517(3)	C(2)-C(7)-C(6)	120.3(2)
C(9)-C(9A)	1.520(3)	O(1)-C(9)-C(10)	111.4(2)
C(10)-C(15)	1.372(3)	O(1)-C(9)-C(9A)	107.2(2)
C(10)-C(11)	1.381(3)	C(10)-C(9)-C(9A)	112.7(2)
C(11)-C(12)	1.381(3)	C(15)-C(10)- C(11)	118.2(2)
C(12)-C(13)	1.368(3)	C(15)-C(10)-C(9)	120.3(2)
C(13)-C(14)	1.365(4)	C(11)-C(10)-C(9)	121.5(2)
C(14)-C(15)	1.380(3)	C(12)-C(11)- C(10)	120.5(2)
		C(13)-C(12)- C(11)	120.6(2)
		C(14)-C(13)- C(12)	119.3(2)
		C(13)-C(14)- C(15)	120.3(2)
		C(10)-C(15)- C(14)	121.1(2)

13.9.23 1,4-Bis-(4-dimethylaminophenyl)-1,4-diaza-1,3-butadien und *meso*-1,2-Diphenyl-1,2-ethandiol

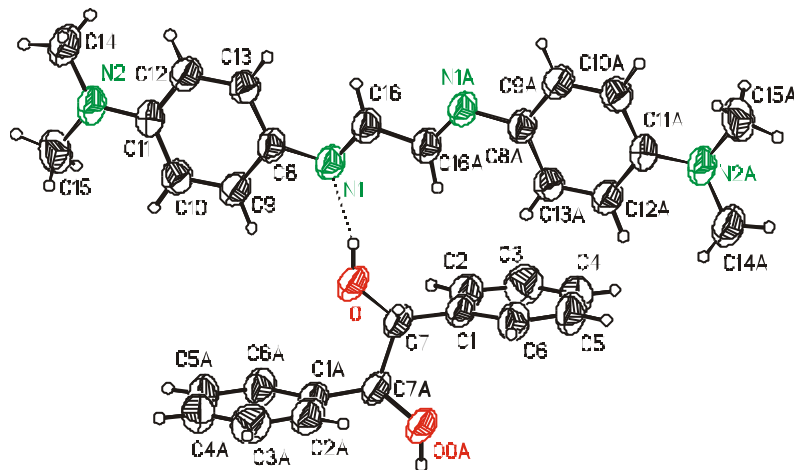


Abb. 13.9.23.1: Struktur des Kokristalls aus 1,4-Bis-(4-dimethylaminophenyl)-1,4-diaza-1,3-butadien und *meso*-1,2-Diphenyl-1,2-ethandiol. Die Ellipsoide beschreiben 50%-Aufenthaltswahrscheinlichkeit.

$[\text{C}_{16}\text{H}_{22}\text{N}_4] \cdot [\text{C}_{14}\text{H}_{12}\text{O}_2]$, $M = 508.65 \text{ g}\cdot\text{mol}^{-1}$, triklin, Raumgruppe $P\bar{1}$,
 $a = 6.35330(10) \text{ \AA}$, $b = 9.8233(2) \text{ \AA}$, $c = 11.2533(3) \text{ \AA}$, $\alpha = 88.84^\circ$, $\beta = 77.348(2)^\circ$,
 $\gamma = 85.090(2)^\circ$, $V = 682.75(3) \text{ \AA}^3$, $Z = 1$, $\rho_{\text{ber.}} = 1.237 \text{ g}\cdot\text{cm}^{-3}$, $\lambda = 0.71073 \text{ \AA}$,
 $T = 298(2) \text{ K}$, $\mu = 0.078 \text{ mm}^{-1}$, 1968 unabhängige Reflexe ($R_{\text{int}} = 0.0832$),
 $R = 0.0787$, $wR_2 = 0.2249$.

Tabelle 13.9.23.1: Atomkoordinaten [10^4] und äquivalente isotrope Versetzungsparameter [$\text{\AA}^2 \cdot 10^3$] des Kokristalls aus 1,4-Bis-(4-dimethylaminophenyl)-1,4-diaza-1,3-butadien und *meso*-1,2-Diphenyl-1,2-ethandiol.

	x	y	z	U(eq)
N(1)	2386(3)	9035(2)	4302(2)	53(1)
N(2)	10859(4)	9161(2)	1527(2)	66(1)
O(1)	1944(3)	6238(2)	4887(2)	72(1)
C(1)	-132(4)	5749(2)	5205(2)	55(1)
C(2)	-1084(4)	5884(2)	6555(2)	53(1)

C(3)	239(5)	5841(3)	7377(3)	65(1)
C(4)	-623(5)	5922(3)	8620(3)	74(1)
C(5)	-2833(6)	6054(3)	9048(3)	74(1)
C(6)	-4148(5)	6099(3)	8239(3)	74(1)
C(7)	-3309(4)	6009(3)	7000(3)	63(1)
C(8)	5788(4)	7934(3)	3271(2)	59(1)
C(9)	7858(4)	7931(3)	2587(2)	60(1)
C(10)	8779(4)	9154(3)	2194(2)	51(1)
C(11)	7480(4)	10369(3)	2539(2)	57(1)
C(12)	5410(4)	10354(3)	3219(2)	56(1)
C(13)	4492(4)	9144(2)	3611(2)	50(1)
C(14)	11787(5)	10424(3)	1132(3)	75(1)
C(15)	12164(5)	7906(4)	1183(3)	80(1)
C(16)	1070(4)	10076(3)	4650(2)	54(1)

Tabelle 13.9.23.2: Wasserstoffatomkoordinaten $[10^4]$ und isotrope Versetzungsparameter

$[\text{\AA}^2 \cdot 10^3]$ des Kokristalls aus 1,4-Bis-(4-dimethylaminophenyl)-1,4-diaza-1,3-butadien und *meso*-1,2-Diphenyl-1,2-ethandiol.

	x	y	z	U(eq)
H(10)	2127	7222	4980	108
H(1)	-1078	6254	4765	66
H(3)	1781	5765	7081	78
H(4)	319	5875	9183	89
H(5)	-3440	6123	9906	88
H(6)	-5687	6195	8545	89
H(7)	-4274	6034	6451	76
H(8)	5219	7077	3531	71
H(9)	8693	7075	2373	72
H(11)	8047	11230	2292	68
H(12)	4571	11208	3435	67
H(14A)	10912	10940	658	112
)				
H(14B)	13223	10231	647	112
)				
H(14C)	11852	10945	1834	112
)				

H(15A)	12254	7371	1896	121
)				
H(15B)	13589	8117	772	121
)				
H(15C)	11538	7398	648	121
)				
H(16)	1509	10978	4445	64

Tabelle 13.9.23.3: Bindungslängen [Å] und Winkel [°] des Kokristalls aus 1,4-Bis-(4-dimethylaminophenyl)-1,4-diaza-1,3-butadien und *meso*-1,2-Diphenyl-1,2-ethandiol.

Bindungslängen [Å]		Winkel [°]	
(1)-C(16)	1.275(3)	C(16)-N(1)-C(13)	122.5(2)
N(1)-C(13)	1.405(3)	C(16)-N(1)-H(10)	125.4
N(1)-H(10)	19.293	C(13)-N(1)-H(10)	110.0
N(2)-C(10)	1.370(3)	C(10)-N(2)-C(15)	120.9(2)
N(2)-C(15)	1.435(4)	C(10)-N(2)-C(14)	121.1(2)
N(2)-C(14)	1.441(4)	C(15)-N(2)-C(14)	118.0(2)
O(1)-H(10)	0.9932	H(10)-O(1)-C(1)	120.4
O(1)-C(1)	1.412(3)	O(1)-H(10)-N(1)	150.3
C(1)-C(2)	1.511(3)	O(1)-C(1)-C(2)	111.7(2)
C(1)-C(1A)	1.535(5)	O(1)-C(1)-C(1A)	106.6(2)
C(2)-C(3)	1.377(4)	C(2)-C(1)-C(1A)	111.5(2)
C(2)-C(7)	1.388(4)	C(3)-C(2)-C(7)	118.4(2)
C(3)-C(4)	1.387(4)	C(3)-C(2)-C(1)	120.6(2)
C(4)-C(5)	1.377(4)	C(7)-C(2)-C(1)	120.9(3)
C(5)-C(6)	1.361(5)	C(2)-C(3)-C(4)	121.0(3)
C(6)-C(7)	1.381(4)	C(5)-C(4)-C(3)	120.0(3)
C(8)-C(9)	1.370(3)	C(6)-C(5)-C(4)	119.2(3)
C(8)-C(13)	1.396(4)	C(5)-C(6)-C(7)	121.3(3)
C(9)-C(10)	1.403(4)	C(6)-C(7)-C(2)	120.1(3)
C(10)-C(11)	1.402(4)	C(9)-C(8)-C(13)	122.1(2)
C(11)-C(12)	1.370(3)	C(8)-C(9)-C(10)	121.2(2)
C(12)-C(13)	1.390(3)	N(2)-C(10)-C(11)	121.7(2)
C(16)-C(16A)	1.432(5)	N(2)-C(10)-C(9)	121.6(2)
		C(11)-C(10)-C(9)	116.7(2)
		C(12)-C(11)-	121.4(2)
		C(10)	

C(11)-C(12)- C(13)	122.1(2)
C(12)-C(13)-C(8)	116.5(2)
C(12)-C(13)-N(1)	125.9(2)
C(8)-C(13)-N(1)	117.6(2)
N(1)-C(16)- C(16A)	120.9(3)