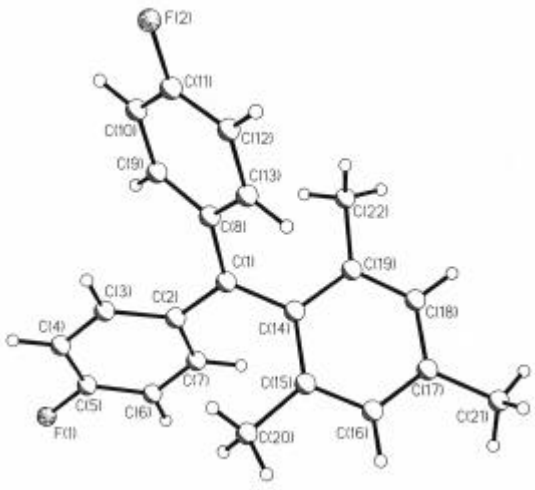
III Anhang

1. Kristallstrukturanalytische Daten

1.1 Bis(4-fluorphenyl)-(2,4,6-trimethylphenyl)-methyl-tetrafluoroborat (35)



Summenformel		$C_{22}H_{19}BF_6$
Formelgewicht		408.18 g/mol
Kristallgröße		0.35 x 0.31 x 0.28
Kristallsystem		monoklin
Raumgruppe		$P2_1/c$ (no. 14)
Gitterkonstanten	a	8.045(5) Å
	b	19.80(1) Å
	c	12.510(8) Å
	b	106.74°
Zellvolumen		1907(1) $Å^3$
Z		4
Dichte (calculated)		1.421 g/cm^3
Wellenlänge		0.71073 Å
Temperatur		150 K
Meßbereich		3.5° bis 54°
Indexbereich		-9<=h<=10; 0<=k<=25; -15<=l<=0
Absorptionskoeffizient *m*		1.22 cm^{-1}
Gesamtanzahl der Reflexe		4489
Symmetrieunabhängige Reflexe		4164 (R_{int} = 0.011)

Beobachtete Reflexe	3139 (I > 2.0)
Anzahl Variablen	264
Verfeinerungsmethode	Volle Matrix Least-Squares Verfeinerung, basierend auf F^2
*R*1	0.0473
*R*2	0.1212
Goodness-of-fit on F^2	1.031
Größter/kleinster Elektronendichte-Peak	0.41, -0.39

Bindungswinkel (Standardfehler in Klammern)

Atoms	Angle [°]	Atoms	Angle [°]
C2 - C1 - C8	120.9(2)	C14 - C1 - C2	119.2(2)
C14 - C1 - C8	119.8(2)	C3 - C2 - C7	118.3(2)
C1 - C2 - C3	122.0(2)	C1 - C2 - C7	119.6(2)
C2 - C3 - C4	120.7(2)	C3 - C4 - C5	118.3(2)
F1 - C5 - C4	117.9(2)	F1 - C5 - C6	118.3(2)
C4 - C5 - C6	123.8(2)	C5 - C6 - C7	117.6(2)
C2 - C7 - C6	121.3(2)	C13 - C8 - C9	118.8(2)
C1 - C8 - C9	122.2(2)	C1 - C8 - C13	119.0(2)
C10 - C9 - C8	120.1(2)	C11 - C10 - C9	118.7(2)
F2 - C11 - C10	118.2(2)	F2 - C11 - C12	118.1(2)
C12 - C11 - C10	123.7(2)	C13 - C12 - C11	117.7(2)
C12 - C13 - C8	121.0(2)	C19 - C14 - C15	119.3(2)
C1 - C14 - C19	120.2(2)	C1 - C14 - C15	120.5(2)
C16 - C15 - C14	118.9(2)	C16 - C15 - C20	117.8(2)
C14 - C15 - C20	123.1(2)	C17 - C16 - C15	122.1(2)
C18 - C17 - C16	118.8(2)	C18 - C17 - C21	120.5(2)
C16 - C17 - C21	120.7(2)	C19 - C18 - C17	122.2(2)
C18 - C19 - C14	118.6(2)	C18 - C19 - C22	117.3(2)
C14 - C19 - C22	123.8(2)	F5 - B - F6	111.4(2)
F4 - B - F6	108.8(2)	F4 - B - F5	107.2(2)
F3 - B - F6	109.9(2)	F3 - B - F5	110.6(2)

Bindungslängen (Standardfehler in Klammern)

Atoms			Distance [Å]	Atoms			Distance [Å]
F1	-	C5	1.347(2)	F2	-	C11	1.350(2)
C1	-	C2	1.441(3)	C1	-	C8	1.444(3)
C1	-	C14	1.453(3)	C2	-	C3	1.413(3)
C2	-	C7	1.415(3)	C3	-	C4	1.379(3)
C4	-	C5	1.380(3)	C5	-	C6	1.384(3)
C6	-	C7	1.378(3)	C8	-	C9	1.412(3)
C10	-	C9	1.381(3)	C11	-	C10	1.377(3)
C12	-	C11	1.378(3)	C13	-	C8	1.414(3)
C13	-	C12	1.382(3)	C15	-	C14	1.431(3)
C15	-	C20	1.516(3)	C17	-	C16	1.392(3)
C17	-	C21	1.504(3)	C18	-	C17	1.391(3)
C19	-	C18	1.386(3)	C19	-	C22	1.513(3)
F3	-	B	1.396(3)	F4	-	B	1.375(3)
F5	-	B	1.363(3)				

Parameter der H-Atome

Atom	X	Y	Z	U_{eq}
H3A	-0.20361	0.12599	0.48535	0.045(1)
H4A	-0.02747	0.1839	0.39435	0.045(1)
H6A	0.24638	0.26876	0.68975	0.045(1)
H7A	0.06548	0.21373	0.78062	0.045(1)
H9A	-0.42838	0.17919	0.51939	0.045(1)
H10A	-0.69614	0.13107	0.41874	0.045(1)
H12A	-0.63368	-0.01919	0.64908	0.045(1)
H13A	-0.36285	0.02684	0.7491	0.045(1)
H16A	0.22067	0.05439	1.00435	0.045(1)
H18A	-0.20388	0.14013	1.06012	0.045(1)
H20C	0.22436	0.02403	0.82748	0.045(1)
H20A	0.21624	0.09403	0.76817	0.045(1)
H20B	0.07201	0.04034	0.72072	0.045(1)
H21C	0.03946	0.11483	1.21441	0.045(1)
H21A	0.21947	0.09763	1.19401	0.045(1)
H21B	0.08816	0.04001	1.19182	0.045(1)
H22C	-0.40725	0.19683	0.9221	0.045(1)
H22A	-0.48351	0.13907	0.83621	0.045(1)
H22B	-0.39579	0.20146	0.7993	0.045(1)

Atomkoordinaten und Koeffizienten der equivalenten isotropen Temperaturfaktoren (Å), U_{eq} (ohne H-Atome, Standardfehler in Klammern)

U_{eq} ist definiert als ein Drittel der Spur des orthogonalisierten U_{ij} Tensors

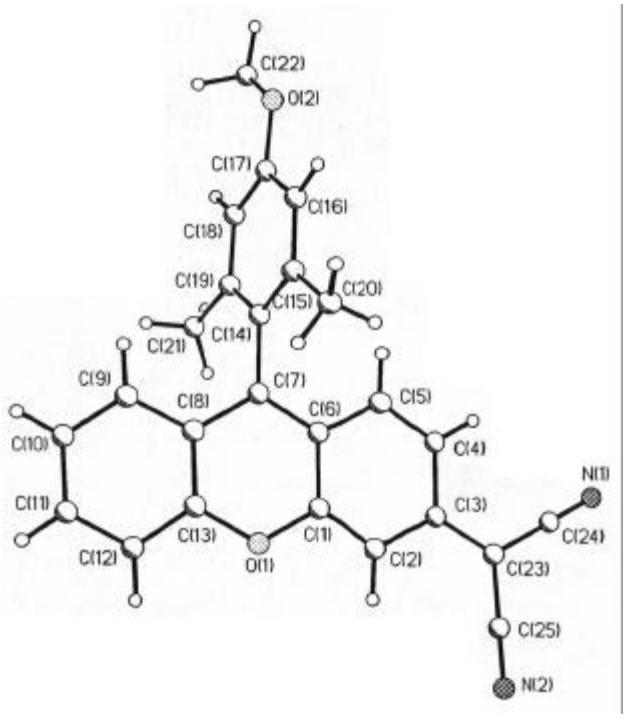
Atom	X	Y	Z	U_{eq}
F1	0.2232(2)	0.26148(6)	0.4832(1)	0.0393(3)
F2	-0.8342(2)	0.02540(7)	0.4678(1)	0.0452(3)
C1	-0.1936(2)	0.12990(9)	0.7010(2)	0.0252(4)
C2	-0.0883(2)	0.16438(9)	0.6424(2)	0.0257(4)
C3	-0.1132(2)	0.1555(1)	0.5268(2)	0.0278(4)
C4	-0.0095(2)	0.1888(1)	0.4732(2)	0.0299(4)
C5	0.1207(2)	0.23000(9)	0.5358(2)	0.0294(4)
C6	0.1534(2)	0.23996(9)	0.6495(2)	0.0299(4)
C7	0.0474(2)	0.2074(1)	0.7020(2)	0.0287(4)
C8	-0.3656(2)	0.10642(9)	0.6425(2)	0.0257(4)
C9	-0.4685(2)	0.1382(1)	0.5447(2)	0.0279(4)
C10	-0.6259(2)	0.1105(1)	0.4862(2)	0.0306(4)
C11	-0.6808(2)	0.0524(1)	0.5263(2)	0.0315(4)
C12	-0.5887(2)	0.0205(1)	0.6232(2)	0.0307(4)
C13	-0.4306(2)	0.0479(1)	0.6814(2)	0.0279(4)
C14	-0.1226(2)	0.11682(9)	0.8197(2)	0.0254(4)
C15	0.0448(2)	0.08635(9)	0.8623(2)	0.0264(4)
C16	0.1102(2)	0.07630(9)	0.9760(2)	0.0286(4)
C17	0.0207(2)	0.09665(9)	1.0506(2)	0.0282(4)
C18	-0.1419(3)	0.1262(1)	1.0088(2)	0.0290(4)
C19	-0.2179(2)	0.13577(9)	0.8954(2)	0.0272(4)
C20	0.1483(3)	0.0589(1)	0.7879(2)	0.0325(4)
C21	0.0981(3)	0.0868(1)	1.1742(2)	0.0345(5)
C22	-0.3915(3)	0.1715(1)	0.8603(2)	0.0371(5)
F3	0.5005(2)	0.16479(7)	0.2883(1)	0.0472(4)
F4	0.7430(2)	0.11395(8)	0.2722(1)	0.0553(4)
F5	0.5041(2)	0.1078(1)	0.1317(1)	0.1007(8)
F6	0.6462(3)	0.20671(9)	0.1734(2)	0.1033(8)
B	0.5968(3)	0.1489(1)	0.2150(2)	0.0368(5)

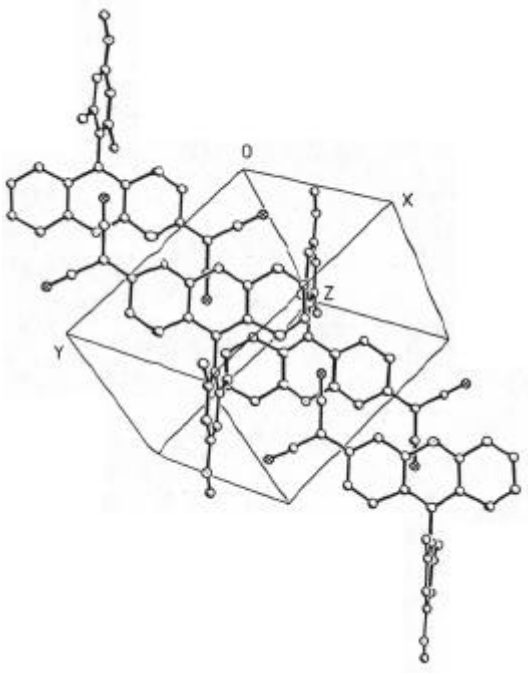
Koeffizienten der anisotropen Temperaturfaktoren (Å^2), Standardfehler in Klammern

Der anisotrope Temperaturfaktor ist definiert als $\exp(-2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}l^2c^{*2} + 2U_{12}hka^*b^* + 2U_{13}hla^*c^* + 2U_{23}klb^*c^*))$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F1	0.0375(7)	0.0389(7)	0.0447(7)	0.0088(5)	0.0170(5)	-0.0068(5)
F2	0.0275(6)	0.0542(8)	0.0499(8)	-0.0113(6)	0.0047(5)	-0.0121(6)
C1	0.0257(9)	0.0237(9)	0.0274(9)	-0.0036(7)	0.0094(7)	0.0019(7)
C2	0.0244(9)	0.0251(9)	0.0280(9)	-0.0014(7)	0.0082(7)	-0.0003(7)
C3	0.0235(9)	0.0307(10)	0.0289(10)	-0.0018(8)	0.0070(7)	-0.0003(8)
C4	0.0290(10)	0.035(1)	0.0259(9)	0.0016(8)	0.0083(8)	0.0027(8)
C5	0.0283(10)	0.0263(9)	0.036(1)	0.0065(8)	0.0135(8)	0.0016(8)
C6	0.0273(10)	0.0245(9)	0.036(1)	-0.0006(8)	0.0058(8)	-0.0022(8)
C7	0.0303(10)	0.0274(9)	0.0274(9)	-0.0035(8)	0.0067(8)	-0.0003(8)
C8	0.0247(9)	0.0281(9)	0.0252(9)	-0.0037(7)	0.0088(7)	0.0008(7)
C9	0.0265(9)	0.0320(10)	0.0268(9)	-0.0018(8)	0.0101(8)	0.0012(8)
C10	0.0242(9)	0.040(1)	0.0269(10)	-0.0025(8)	0.0065(8)	0.0034(8)
C11	0.0213(9)	0.040(1)	0.034(1)	-0.0118(9)	0.0090(8)	-0.0032(8)
C12	0.0291(10)	0.0291(10)	0.038(1)	-0.0063(8)	0.0165(9)	-0.0037(8)
C13	0.0276(9)	0.0303(10)	0.0280(9)	0.0000(8)	0.0115(8)	0.0015(8)
C14	0.0237(9)	0.0265(9)	0.0258(9)	-0.0031(7)	0.0069(7)	-0.0018(7)
C15	0.0229(9)	0.0246(9)	0.0326(10)	-0.0024(7)	0.0093(8)	-0.0035(7)
C16	0.0238(9)	0.0272(9)	0.033(1)	0.0009(8)	0.0052(8)	-0.0011(8)
C17	0.0301(10)	0.0242(9)	0.0285(10)	0.0004(7)	0.0054(8)	-0.0066(8)
C18	0.0310(10)	0.0306(10)	0.0269(9)	-0.0024(8)	0.0107(8)	-0.0031(8)
C19	0.0260(9)	0.0271(9)	0.0294(10)	-0.0017(8)	0.0092(8)	0.0000(7)
C20	0.0267(9)	0.034(1)	0.039(1)	-0.0010(9)	0.0126(8)	0.0032(8)
C21	0.036(1)	0.036(1)	0.030(1)	0.0031(8)	0.0059(8)	-0.0034(9)
C22	0.030(1)	0.049(1)	0.032(1)	-0.0042(9)	0.0100(8)	0.0082(9)
F3	0.0428(7)	0.0635(9)	0.0420(7)	0.0030(6)	0.0231(6)	0.0018(6)
F4	0.0443(8)	0.0708(10)	0.0469(8)	0.0002(7)	0.0069(6)	0.0151(7)
F5	0.0462(9)	0.190(2)	0.060(1)	-0.060(1)	0.0063(8)	-0.022(1)
F6	0.176(2)	0.0542(10)	0.132(2)	0.036(1)	0.128(2)	0.034(1)
B	0.034(1)	0.049(1)	0.029(1)	0.004(1)	0.0115(10)	0.003(1)

1.2 3-Dicyanomethylen 9-(4-methoxy-2,6-dimethylphenyl)-xanthen (134)





Summenformel		$C_{25}H_{18}N_2O_2$
Formelgewicht		378.41 g/mol
Kristallgröße		0.42 x 0.38 x 0.25
Kristallsystem		triclinic
Raumgruppe		P1 (no. 2)
Gitterkonstanten	a	8.665(3) Å
	b	10.454(3) Å
	c	11.011(3) Å
	a	94.24°
	b	105.69°
	g	98.95
Zellvolumen		1907(1) $Å^3$
Z		2
Dichte (calculated)		1.335 g/cm^3
Wellenlänge		0.71073 Å
Temperatur		150 K
Meßbereich		3.5° bis 54°
Indexbereich		-11<=h<=0; -13<=k<=13; -13<=l<=14)

Absorptionskoeffizient *m*	0.86 cm^{-1}
Gesamtanzahl der Reflexe	4377
Symmetrieunabhängige Reflexe	4099 (R_{int} = 0.012)
Beobachtete Reflexe	3201 (I > 2.0)
Anzahl Variablen	263
Verfeinerungsmethode	Volle Matrix Least-Squares Verfeinerung, basierend auf F^2
*R*1	0.0431
*R*2	0.1229
Goodness-of-fit on F^2	1.017
Größter/kleinster Elektronendichte-Peak	0.31, -0.21

Bindungswinkel (Standardfehler in Klammern)

Atoms	Angle [°]	Atoms	Angle [°]
C1 - O1 - C13	120.3(1)	C17 - O2 - C22	116.5(1)
O1 - C1 - C2	116.9(1)	C2 - C1 - C6	123.2(1)
O1 - C1 - C6	119.9(1)	C1 - C2 - C3	119.8(1)
C2 - C3 - C23	122.4(1)	C23 - C3 - C4	119.6(1)
C2 - C3 - C4	118.0(1)	C3 - C4 - C5	121.3(1)
C4 - C5 - C6	121.7(1)	C1 - C6 - C7	120.6(1)
C5 - C6 - C7	123.5(1)	C1 - C6 - C5	115.8(1)
C6 - C7 - C8	118.3(1)	C14 - C7 - C6	120.8(1)
C14 - C7 - C8	120.9(1)	C13 - C8 - C9	117.4(1)
C13 - C8 - C7	119.0(1)	C7 - C8 - C9	123.6(1)
C10 - C9 - C8	120.7(2)	C11 - C10 - C9	120.1(2)
C12 - C11 - C10	121.0(2)	C13 - C12 - C11	118.4(2)
O1 - C13 - C12	116.1(1)	O1 - C13 - C8	121.7(1)
C12 - C13 - C8	122.3(1)	C19 - C14 - C15	120.1(1)
C19 - C14 - C7	120.6(1)	C15 - C14 - C7	119.3(1)
C16 - C15 - C14	119.3(1)	C16 - C15 - C20	119.5(1)
C14 - C15 - C20	121.2(1)	C17 - C16 - C15	120.7(1)
O2 - C17 - C18	124.3(1)	O2 - C17 - C16	115.5(1)
C18 - C17 - C16	120.1(1)	C19 - C18 - C17	120.3(1)
C18 - C19 - C14	119.4(1)	C18 - C19 - C21	118.5(1)
C14 - C19 - C21	122.1(1)	C24 - C23 - C3	122.1(1)
C25 - C23 - C3	121.6(1)	C25 - C23 - C24	116.3(1)
N1 - C24 - C23	179.3(2)		

Bindungslängen (Standardfehler in Klammern)

Atoms			Distance [Å]	Atoms			Distance [Å]
O1	-	C1	1.362(2)	O1	-	C13	1.370(2)
O2	-	C17	1.367(2)	O2	-	C22	1.428(2)
N1	-	C24	1.142(2)	N2	-	C25	1.146(2)
C1	-	C2	1.361(2)	C1	-	C6	1.435(2)
C2	-	C3	1.417(2)	C3	-	C4	1.444(2)
C4	-	C5	1.345(2)	C5	-	C6	1.437(2)
C6	-	C7	1.378(2)	C7	-	C8	1.438(2)
C8	-	C9	1.411(2)	C10	-	C9	1.373(2)
C11	-	C10	1.391(2)	C12	-	C11	1.381(2)
C13	-	C8	1.399(2)	C13	-	C12	1.389(2)
C14	-	C7	1.488(2)	C15	-	C14	1.407(2)
C15	-	C20	1.509(2)	C16	-	C15	1.382(2)
C17	-	C16	1.393(2)	C19	-	C14	1.400(2)
C19	-	C18	1.395(2)	C19	-	C21	1.508(2)
C23	-	C3	1.401(2)	C24	-	C23	1.422(2)

Parameter der H-Atome

Atom	X	Y	Z	U_{eq}
H2A	0.11734	0.49625	-0.08832	0.041(1)
H4A	0.14264	0.88611	0.02418	0.041(1)
H5A	0.38368	0.89014	0.17584	0.041(1)
H9A	0.80226	0.62807	0.40152	0.041(1)
H10A	0.86927	0.42214	0.42558	0.041(1)
H11A	0.70596	0.23878	0.29107	0.041(1)
H12A	0.47356	0.25948	0.12941	0.041(1)
H16A	0.89073	1.07873	0.30379	0.041(1)
H18A	0.71622	0.97812	0.59737	0.041(1)
H20C	0.84162	0.92908	0.12055	0.041(1)
H20A	0.6506	0.89716	0.07078	0.041(1)
H20B	0.74724	0.78618	0.11103	0.041(1)
H21C	0.45687	0.68558	0.43795	0.041(1)
H21A	0.49113	0.79307	0.55513	0.041(1)
H21B	0.61322	0.69932	0.55528	0.041(1)
H22C	0.95654	1.28145	0.6838	0.041(1)
H22A	0.93174	1.13257	0.70162	0.041(1)
H22B	0.78074	1.19618	0.64779	0.041(1)

Atomkoordinaten und Koeffizienten der equivalenten isotropen Temperaturfaktoren (Å), U_{eq} (ohne H-Atome, Standardfehler in Klammern)

U_{eq} ist definiert als ein Drittel der Spur des orthogonalisierten U_{ij} Tensors

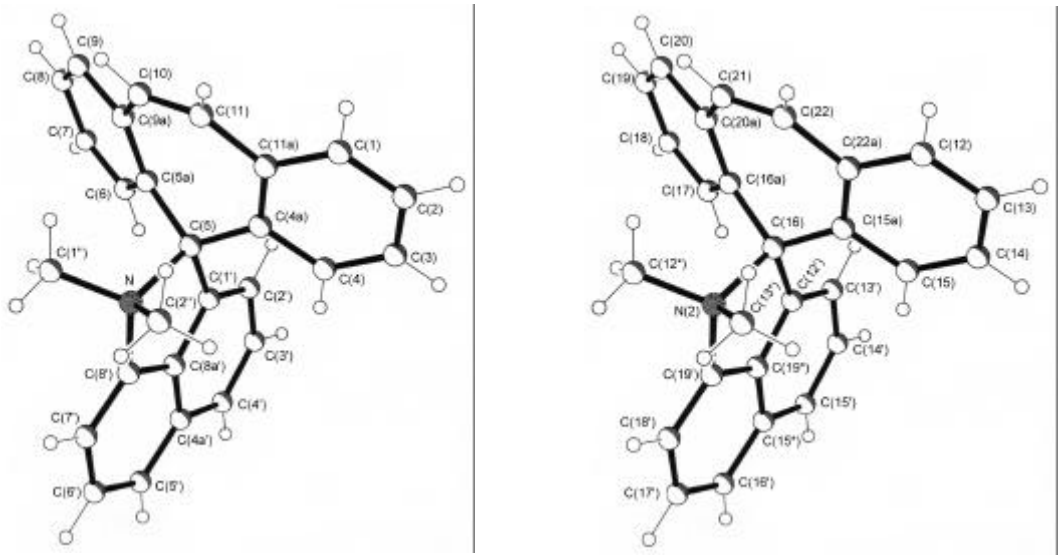
Atom	X	Y	Z	U_{eq}
O1	0.3653(1)	0.4639(1)	0.07503(9)	0.0240(2)
O2	0.9021(1)	1.1643(1)	0.5238(1)	0.0301(3)
N1	-0.1897(2)	0.4960(2)	-0.3114(1)	0.0377(4)
N2	-0.1700(2)	0.8991(1)	-0.1670(1)	0.0343(3)
C1	0.3103(2)	0.5786(1)	0.0605(1)	0.0214(3)
C2	0.1706(2)	0.5759(1)	-0.0340(1)	0.0224(3)
C3	0.1042(2)	0.6909(1)	-0.0521(1)	0.0219(3)
C4	0.1882(2)	0.8081(1)	0.0327(1)	0.0241(3)
C5	0.3289(2)	0.8100(1)	0.1230(1)	0.0242(3)
C6	0.3996(2)	0.6949(1)	0.1426(1)	0.0220(3)
C7	0.5424(2)	0.6923(1)	0.2349(1)	0.0226(3)
C8	0.5944(2)	0.5691(1)	0.2515(1)	0.0239(3)
C9	0.7344(2)	0.5532(2)	0.3463(2)	0.0283(3)
C10	0.7744(2)	0.4319(2)	0.3602(2)	0.0311(4)
C11	0.6773(2)	0.3231(2)	0.2800(2)	0.0302(4)
C12	0.5402(2)	0.3345(2)	0.1851(2)	0.0269(3)
C13	0.5009(2)	0.4576(1)	0.1718(1)	0.0231(3)
C14	0.6400(2)	0.8140(1)	0.3154(1)	0.0227(3)
C15	0.7355(2)	0.9038(1)	0.2638(1)	0.0239(3)
C16	0.8229(2)	1.0183(1)	0.3377(1)	0.0250(3)
C17	0.8144(2)	1.0466(1)	0.4611(1)	0.0241(3)
C18	0.7215(2)	0.9583(2)	0.5122(1)	0.0262(3)
C19	0.6349(2)	0.8407(2)	0.4407(1)	0.0251(3)
C20	0.7449(2)	0.8769(2)	0.1297(2)	0.0312(4)
C21	0.5394(2)	0.7454(2)	0.5019(2)	0.0338(4)
C22	0.8921(2)	1.1968(2)	0.6493(2)	0.0338(4)
C23	-0.0386(2)	0.6944(1)	-0.1482(1)	0.0234(3)
C24	-0.1216(2)	0.5842(2)	-0.2387(1)	0.0254(3)
C25	-0.1108(2)	0.8082(2)	-0.1588(1)	0.0247(3)

Koeffizienten der anisotropen Temperaturfaktoren (Å^2), Standardfehler in Klammern

Der anisotrope Temperaturfaktor ist definiert als $\exp(-2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}l^2c^{*2} + 2U_{12}hka^*b^* + 2U_{13}hla^*c^* + 2U_{23}klb^*c^*))$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	0.0266(6)	0.0213(5)	0.0231(5)	0.0023(4)	0.0050(4)	0.0053(4)
O2	0.0359(6)	0.0225(5)	0.0289(6)	-0.0013(4)	0.0068(5)	0.0028(5)
N1	0.0393(8)	0.0355(8)	0.0324(8)	-0.0015(6)	0.0037(6)	0.0040(7)
N2	0.0386(8)	0.0302(7)	0.0313(7)	0.0025(6)	0.0039(6)	0.0091(6)
C1	0.0251(7)	0.0198(7)	0.0214(7)	0.0039(5)	0.0100(6)	0.0041(6)
C2	0.0249(7)	0.0217(7)	0.0197(7)	0.0009(5)	0.0071(6)	0.0012(6)
C3	0.0232(7)	0.0231(7)	0.0190(7)	0.0028(5)	0.0068(6)	0.0015(6)
C4	0.0276(8)	0.0206(7)	0.0235(7)	0.0022(6)	0.0063(6)	0.0046(6)
C5	0.0285(8)	0.0197(7)	0.0227(7)	0.0015(5)	0.0058(6)	0.0026(6)
C6	0.0238(7)	0.0226(7)	0.0193(7)	0.0038(5)	0.0061(6)	0.0028(6)
C7	0.0237(7)	0.0244(7)	0.0202(7)	0.0043(5)	0.0082(6)	0.0019(6)
C8	0.0247(7)	0.0265(8)	0.0222(7)	0.0067(6)	0.0083(6)	0.0047(6)
C9	0.0267(8)	0.0318(8)	0.0255(8)	0.0066(6)	0.0057(6)	0.0041(6)
C10	0.0284(8)	0.0377(9)	0.0291(8)	0.0129(7)	0.0064(6)	0.0106(7)
C11	0.0353(9)	0.0303(8)	0.0327(8)	0.0138(7)	0.0159(7)	0.0132(7)
C12	0.0323(8)	0.0250(8)	0.0270(8)	0.0058(6)	0.0128(6)	0.0066(6)
C13	0.0240(7)	0.0265(7)	0.0211(7)	0.0065(6)	0.0090(6)	0.0056(6)
C14	0.0215(7)	0.0236(7)	0.0212(7)	0.0039(6)	0.0026(6)	0.0039(6)
C15	0.0258(7)	0.0248(7)	0.0202(7)	0.0046(6)	0.0035(6)	0.0060(6)
C16	0.0260(8)	0.0228(7)	0.0262(8)	0.0074(6)	0.0064(6)	0.0046(6)
C17	0.0239(7)	0.0206(7)	0.0252(7)	0.0020(6)	0.0013(6)	0.0066(6)
C18	0.0270(8)	0.0303(8)	0.0204(7)	0.0021(6)	0.0048(6)	0.0066(6)
C19	0.0232(7)	0.0294(8)	0.0206(7)	0.0038(6)	0.0033(6)	0.0039(6)
C20	0.0360(9)	0.0319(8)	0.0231(8)	0.0030(6)	0.0085(7)	-0.0017(7)
C21	0.0362(9)	0.0376(9)	0.0249(8)	0.0034(7)	0.0098(7)	-0.0026(7)
C22	0.0389(9)	0.0284(8)	0.0312(9)	-0.0066(7)	0.0081(7)	0.0053(7)
C23	0.0237(7)	0.0237(7)	0.0212(7)	0.0030(6)	0.0046(6)	0.0030(6)
C24	0.0258(8)	0.0264(8)	0.0237(7)	0.0049(6)	0.0056(6)	0.0059(6)
C25	0.0248(7)	0.0264(8)	0.0194(7)	0.0019(6)	0.0030(6)	0.0009(6)

1.3 Spiro[5*H*-dibenzo[a,d]cyclohepten-5,2'-[2*H*]-naphtho[1,8-bc]-*N*,*N*-dimethyl-pyrrolidin]-tetrafluoroborat (14)



Summenformel		$C_{27}H_{22}BF_4N$
Formelgewicht		447.27 g/mol
Kristallgröße		0.54 x 0.50 x 0.45
Kristallsystem		monoklin
Raumgruppe		$P2_1/c$ (no. 14)
Gitterkonstanten	a	22.908(3) Å
	b	12.560(2) Å
	c	15.463(2) Å
	b	94.50(2)°
Zellvolumen		4434(1) $Å^3$
Z		8
Dichte (calculated)		1.34 g/cm^3
Wellenlänge		0.71073 Å
Temperatur		293 K
Meßbereich		3° bis 50°
Indexbereich		-27<=h<=27; -1<=k<=14; -18<=l<=1)
Absorptionskoeffizient *m*		1.0 cm^{-1}
Gesamtanzahl der Reflexe		10046
Symmetrieunabhängige Reflexe		7804 (R_{int} = 0.024)

Beobachtete Reflexe	3377 (I > 2.0)
Anzahl Variablen	586
Verfeinerungsmethode	Volle Matrix Least-Squares Verfeinerung, basierend auf F^2
*R*1	0.0738
*R*2	0.2833
Goodness-of-fit on F^2	1.026
Größter/kleinster Elektronendichte-Peak	0.52, -0.3

Bindungswinkel (Standardfehler in Klammern)

Atoms	Angle [°]	Atoms	Angle [°]
C16A - C20A - C20	118.5(5)	C21 - C20A - C20	114.8(5)
C16A - C20A - C21	126.6(5)	C22 - C21 - C20A	129.5(5)
C22A - C22 - C21	129.7(5)	C15A - C22A - C12	118.8(5)
C12 - C22A - C22	115.4(5)	C15A - C22A - C22	125.8(5)
C19* - C12' - C13'	117.9(4)	C16 - C12' - C13'	130.4(4)
C19* - C12' - C16	111.6(4)	C14' - C13' - C12'	120.1(5)
C15' - C14' - C13'	122.0(5)	C15* - C15' - C14'	120.1(5)
C19* - C15* - C16'	116.2(5)	C19* - C15* - C15'	116.0(4)
C16' - C15* - C15'	127.7(5)	C17' - C16' - C15*	120.7(5)
C18' - C17' - C16'	122.8(5)	C19' - C18' - C17'	117.0(5)
C19* - C19' - C18'	121.6(4)	C18' - C19' - N2	127.9(4)
C19* - C19' - N2	110.5(4)	C19' - C19* - C12'	114.4(4)
C19' - C19* - C15*	121.7(4)	C15* - C19* - C12'	123.9(4)
F3 - B1 - F4	108.8(7)	F2 - B1 - F3	109.2(7)
F2 - B1 - F4	108.5(6)	F1 - B1 - F3	110.9(6)
F1 - B1 - F4	109.5(6)	F1 - B1 - F2	109.9(5)
F7 - B2 - F8	110.5(6)	F5 - B2 - F8	110.0(5)
F5 - B2 - F7	110.3(5)	F6 - B2 - F8	112.1(6)
F6 - B2 - F7	106.0(5)		

Atoms					Angle [°]	Atoms					Angle [°]
C1"	-	N1	-	C8'	109.1(3)	C2"	-	N1	-	C8'	108.4(3)
C1"	-	N1	-	C2"	108.9(3)	C5	-	N1	-	C8'	104.3(3)
C1"	-	N1	-	C5	112.9(3)	C2"	-	N1	-	C5	113.1(3)
C11A	-	C1	-	C2	121.0(6)	C1	-	C2	-	C3	120.3(6)
C2	-	C3	-	C4	120.2(6)	C3	-	C4	-	C4A	121.8(5)
C11A	-	C4A	-	C4	117.4(4)	C4	-	C4A	-	C5	117.4(4)
C11A	-	C4A	-	C5	125.2(4)	C1'	-	C5	-	C4A	110.8(3)
C1'	-	C5	-	C5A	110.2(3)	C4A	-	C5	-	C5A	117.1(3)
N1	-	C5	-	C1'	99.5(3)	N1	-	C5	-	C4A	108.9(3)
N1	-	C5	-	C5A	108.8(3)	C6	-	C5A	-	C9A	117.6(4)
C5	-	C5A	-	C6	117.9(4)	C5	-	C5A	-	C9A	124.4(4)
C5A	-	C6	-	C7	122.6(5)	C6	-	C7	-	C8	120.4(6)
C7	-	C8	-	C9	119.8(5)	C8	-	C9	-	C9A	121.5(5)
C5A	-	C9A	-	C9	118.1(5)	C10	-	C9A	-	C5A	126.1(4)
C10	-	C9A	-	C9	115.9(5)	C11	-	C10	-	C9A	129.4(5)
C11A	-	C11	-	C10	128.5(5)	C1	-	C11A	-	C4A	119.2(5)
C1	-	C11A	-	C11	115.1(5)	C11	-	C11A	-	C4A	125.7(5)
C2'	-	C1'	-	C8A'	119.0(4)	C2'	-	C1'	-	C5	129.7(4)
C5	-	C1'	-	C8A'	111.2(3)	C1'	-	C2'	-	C3'	118.8(4)
C2'	-	C3'	-	C4'	122.6(5)	C3'	-	C4'	-	C4A'	120.1(4)
C5'	-	C4A'	-	C8A'	116.6(4)	C4'	-	C4A'	-	C5'	127.2(4)
C4'	-	C4A'	-	C8A'	116.2(4)	C4A'	-	C5'	-	C6'	120.2(4)
C5'	-	C6'	-	C7'	122.2(4)	C6'	-	C7'	-	C8'	117.1(4)
C7'	-	C8'	-	C8A'	122.1(4)	N1	-	C8'	-	C7'	127.6(4)
N1	-	C8'	-	C8A'	110.3(3)	C1'	-	C8A'	-	C8'	114.7(4)
C4A'	-	C8A'	-	C8'	121.9(4)	C1'	-	C8A'	-	C4A'	123.3(4)
C19'	-	N2	-	C13*	108.7(3)	C19'	-	N2	-	C12*	109.0(3)
C13*	-	N2	-	C12*	109.0(4)	C19'	-	N2	-	C16	103.7(3)
C16	-	N2	-	C13*	112.8(3)	C16	-	N2	-	C12*	113.4(3)
C13	-	C12	-	C22A	122.3(7)	C14	-	C13	-	C12	119.6(7)
C15	-	C14	-	C13	120.6(7)	C15A	-	C15	-	C14	121.8(6)
C15	-	C15A	-	C22A	116.9(5)	C16	-	C15A	-	C15	118.2(4)
C16	-	C15A	-	C22A	124.6(4)	C16A	-	C16	-	C12'	110.6(4)
C16A	-	C16	-	C15A	118.3(4)	C15A	-	C16	-	C12'	109.5(4)
C16A	-	C16	-	N2	109.4(3)	C12'	-	C16	-	N2	99.6(3)
C15A	-	C16	-	N2	107.8(3)	C17	-	C16A	-	C20A	116.6(4)
C17	-	C16A	-	C16	118.4(4)	C16	-	C16A	-	C20A	124.8(4)
C18	-	C17	-	C16A	122.6(5)	C19	-	C18	-	C17	120.2(6)
C18	-	C19	-	C20	118.8(6)	C19	-	C20	-	C20A	123.2(6)

Atomkoordinaten und Koeffizienten der equivalenten isotropen Temperaturfaktoren (Å), U_{eq} (ohne H-Atome, Standardfehler in Klammern)

U_{eq} ist definiert als ein Drittel der Spur des orthogonalisierten U_{ij} Tensors

Atom	X	Y	Z	U_{eq}
N1	0.3421(1)	0.8346(3)	0.1599(2)	0.0605(9)
C1	0.2910(3)	0.5325(5)	0.3077(4)	0.096(2)
C2	0.3215(4)	0.4512(5)	0.2729(5)	0.112(2)
C3	0.3685(3)	0.4726(4)	0.2275(4)	0.101(2)
C4	0.3869(2)	0.5766(4)	0.2179(3)	0.077(1)
C4A	0.3592(2)	0.6620(3)	0.2558(3)	0.062(1)
C5	0.3838(2)	0.7728(3)	0.2425(3)	0.057(1)
C5A	0.3892(2)	0.8473(3)	0.3217(3)	0.061(1)
C6	0.4403(2)	0.9077(4)	0.3359(3)	0.077(1)
C7	0.4482(3)	0.9803(4)	0.4015(4)	0.095(2)
C8	0.4052(4)	0.9979(5)	0.4556(4)	0.107(2)
C9	0.3542(3)	0.9429(5)	0.4444(3)	0.095(2)
C9A	0.3444(2)	0.8648(4)	0.3771(3)	0.072(1)
C10	0.2880(3)	0.8117(5)	0.3726(3)	0.089(2)
C11	0.2731(2)	0.7165(5)	0.3408(3)	0.088(2)
C11A	0.3094(2)	0.6389(4)	0.3012(3)	0.071(1)
C1”	0.2926(2)	0.7671(4)	0.1228(3)	0.082(1)
C2”	0.3182(2)	0.9407(4)	0.1861(3)	0.082(1)
C1’	0.4419(2)	0.7667(3)	0.2014(3)	0.058(1)
C2’	0.4944(2)	0.7275(4)	0.2342(3)	0.076(1)
C3’	0.5430(2)	0.7344(4)	0.1833(4)	0.084(1)
C4’	0.5396(2)	0.7799(4)	0.1032(3)	0.082(1)
C4A’	0.4854(2)	0.8211(4)	0.0669(3)	0.068(1)
C5’	0.4748(2)	0.8730(4)	-0.0129(3)	0.079(1)
C6’	0.4196(2)	0.9134(4)	-0.0375(3)	0.079(1)
C7’	0.3728(2)	0.9045(4)	0.0156(3)	0.069(1)
C8’	0.3835(2)	0.8533(3)	0.0924(3)	0.056(1)
C8A’	0.4378(2)	0.8131(3)	0.1187(3)	0.057(1)
N2	0.1803(1)	0.1486(3)	0.5356(2)	0.0616(9)
C12	0.0177(3)	0.3188(5)	0.6215(5)	0.109(2)
C13	-0.0099(3)	0.3551(6)	0.5466(8)	0.130(3)
C14	0.0012(3)	0.3085(6)	0.4697(6)	0.122(2)
C15	0.0394(2)	0.2235(5)	0.4679(4)	0.088(2)
C15A	0.0679(2)	0.1808(4)	0.5445(3)	0.067(1)
C16	0.1121(2)	0.0917(3)	0.5360(3)	0.059(1)
C16A	0.1141(2)	0.0018(4)	0.6019(3)	0.064(1)
C17	0.1230(2)	-0.1028(4)	0.5726(4)	0.085(1)
C18	0.1277(3)	-0.1887(5)	0.6279(5)	0.108(2)
C19	0.1242(3)	-0.1746(6)	0.7153(6)	0.115(2)

Atom	X	Y	Z	U_{eq}
C20	0.1180(3)	-0.0747(6)	0.7460(4)	0.100(2)
C20A	0.1120(2)	0.0155(4)	0.6923(3)	0.076(1)
C21	0.1066(3)	0.1145(5)	0.7373(3)	0.092(2)
C22	0.0840(3)	0.2043(5)	0.7092(4)	0.093(2)
C22A	0.0569(2)	0.2317(4)	0.6238(4)	0.079(1)
C12*	0.1809(2)	0.2657(4)	0.5570(4)	0.090(2)
C13*	0.2255(2)	0.0932(5)	0.5949(3)	0.091(2)
C12'	0.1059(2)	0.0476(4)	0.4442(3)	0.070(1)
C13'	0.0618(2)	-0.0104(5)	0.4023(3)	0.095(2)
C14'	0.0647(3)	-0.0384(5)	0.3152(4)	0.103(2)
C15'	0.1106(3)	-0.0095(4)	0.2695(3)	0.088(2)
C15*	0.1577(2)	0.0494(4)	0.3103(3)	0.069(1)
C16'	0.2080(2)	0.0877(4)	0.2727(3)	0.080(1)
C17'	0.2491(3)	0.1455(4)	0.3204(4)	0.088(2)
C18'	0.2444(2)	0.1707(4)	0.4079(3)	0.079(1)
C19'	0.1956(2)	0.1346(3)	0.4448(3)	0.062(1)
C19*	0.1530(2)	0.0759(4)	0.3979(3)	0.063(1)
B1	0.1676(3)	0.5457(6)	0.4996(4)	0.081(2)
F1	0.1633(2)	0.6445(3)	0.4650(2)	0.132(1)
F2	0.1381(3)	0.4782(3)	0.4490(3)	0.194(2)
F3	0.1481(3)	0.5438(4)	0.5739(3)	0.246(3)
F4	0.2222(2)	0.5165(4)	0.5069(5)	0.226(3)
B2	0.3605(3)	0.2019(5)	0.0965(4)	0.081(2)
F5	0.3232(2)	0.2109(3)	0.1606(2)	0.122(1)
F6	0.4041(1)	0.1322(3)	0.1246(2)	0.122(1)
F7	0.3326(2)	0.1568(3)	0.0246(2)	0.136(1)
F8	0.3808(3)	0.2946(3)	0.0782(3)	0.211(3)

Parameter der H-Atome

Atom	X	Y	Z	U_{eq}
H14'	0.03298	-0.07815	0.28658	0.15498
H15'	0.11137	-0.02969	0.20968	0.13203
H16'	0.21358	0.07291	0.21303	0.12034
H17'	0.28315	0.16878	0.29329	0.1321
H18'	0.2738	0.2122	0.4402	0.11809

Atom	X	Y	Z	U_{eq}
H1	0.25743	0.5159	0.33859	0.14439
H2	0.30935	0.37886	0.28039	0.16858
H3	0.38843	0.41491	0.20174	0.15088
H4	0.41984	0.591	0.18495	0.11519
H6	0.47037	0.89784	0.29677	0.11562
H7	0.48461	1.01811	0.41001	0.1425
H8	0.41123	1.04907	0.50154	0.16095
H9	0.32369	0.9584	0.48172	0.14223
H10	0.25707	0.85179	0.39552	0.13294
H11	0.23317	0.69545	0.34533	0.13204
H1'A	0.27062	0.80496	0.07718	0.12359
H1'B	0.30803	0.7028	0.09996	0.12359
H1'C	0.26738	0.74961	0.16754	0.12359
H2'A	0.29537	0.97198	0.13791	0.12358
H2'B	0.29416	0.9313	0.23359	0.12358
H2'C	0.35047	0.98672	0.20358	0.12358
H2'	0.4984	0.69684	0.29126	0.11444
H3'	0.57975	0.70443	0.20555	0.12588
H4'	0.57372	0.78638	0.07144	0.12345
H5'	0.50644	0.88217	-0.04948	0.11894
H6'	0.41346	0.94822	-0.0927	0.11897
H7'	0.33475	0.93303	-0.00156	0.10407
H12	0.00932	0.35246	0.67492	0.16392
H13	-0.03624	0.41441	0.54764	0.19556
H14	-0.01821	0.33565	0.41702	0.18244
H15	0.04726	0.19197	0.41345	0.13255
H17	0.12565	-0.11365	0.51162	0.12704
H18	0.1341	-0.2588	0.60577	0.16227
H19	0.12491	-0.23446	0.75391	0.17183
H20	0.11798	-0.06459	0.80757	0.15033
H21	0.12116	0.11355	0.79725	0.13782
H22	0.0865	0.26175	0.75025	0.13962
H12A	0.21989	0.29313	0.55555	0.13529
H12B	0.15512	0.30313	0.51544	0.13529
H12C	0.16782	0.27537	0.61396	0.13529
H13A	0.2629	0.12706	0.59239	0.13702
H13B	0.21363	0.09733	0.65301	0.13702
H13C	0.22844	0.01982	0.57833	0.13702
H13'	0.02918	-0.03227	0.4335	0.14283

Bindungslängen (Standardfehler in Klammern)

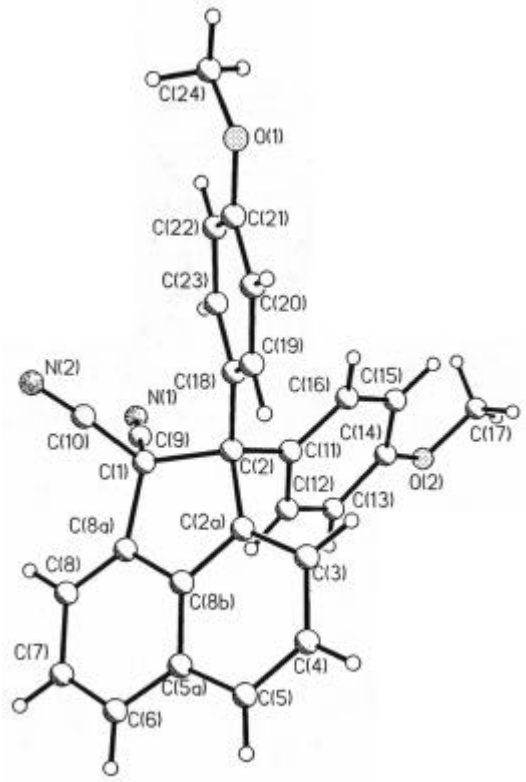
Atoms			Distance [Å]	Atoms			Distance [Å]
N1	-	C8'	1.482(5)	N1	-	C1"	1.496(5)
N1	-	C2"	1.508(5)	N1	-	C5	1.719(5)
C1	-	C2	1.371(9)	C1	-	C11A	1.407(7)
C2	-	C3	1.357(9)	C3	-	C4	1.384(7)
C4	-	C4A	1.398(6)	C4A	-	C5	1.522(6)
C5	-	C5A	1.540(5)	C5A	-	C6	1.397(6)
C5A	-	C9A	1.403(6)	C6	-	C7	1.365(6)
C7	-	C8	1.359(8)	C8	-	C9	1.358(8)
C9	-	C9A	1.435(7)	C10	-	C9A	1.451(7)
C11	-	C10	1.327(7)	C11A	-	C4A	1.416(6)
C11A	-	C11	1.449(7)	C1'	-	C5	1.520(6)
C1'	-	C2'	1.361(6)	C1'	-	C8A'	1.401(5)
C2'	-	C3'	1.416(7)	C3'	-	C4'	1.360(7)
C4'	-	C4A'	1.419(6)	C4A'	-	C5'	1.400(6)
C4A'	-	C8A'	1.407(6)	C5'	-	C6'	1.387(7)
C6'	-	C7'	1.405(6)	C7'	-	C8'	1.356(6)
C8A'	-	C8'	1.374(5)	C12	-	C22A	1.414(8)
C13	-	C12	1.35(1)	C14	-	C13	1.37(1)
C15	-	C14	1.382(9)	C15A	-	C15	1.412(6)
C15A	-	C22A	1.421(6)	C16	-	N2	1.719(5)
C16	-	C15A	1.523(6)	C16	-	C12'	1.520(6)
C16A	-	C16	1.518(6)	C17	-	C16A	1.409(6)
C18	-	C17	1.375(7)	C19	-	C18	1.372(8)
C19	-	C20	1.353(9)	C20A	-	C20	1.405(7)
C21	-	C20A	1.435(7)	C22	-	C21	1.301(7)
C22A	-	C22	1.456(7)	C12*	-	N2	1.507(6)
C13*	-	N2	1.501(5)	C14'	-	C13'	1.398(7)
C15'	-	C14'	1.363(7)	C15'	-	C15*	1.415(7)
C16'	-	C15*	1.413(7)	C17'	-	C16'	1.359(7)
C18'	-	C17'	1.402(7)	C19'	-	N2	1.483(5)
C19*	-	C12'	1.387(6)	B1	-	F3	1.265(7)
B1	-	F4	1.299(7)	B1	-	F2	1.306(7)
B1	-	F1	1.351(7)	B2	-	F8	1.293(7)
B2	-	F7	1.361(7)	B2	-	F5	1.363(7)

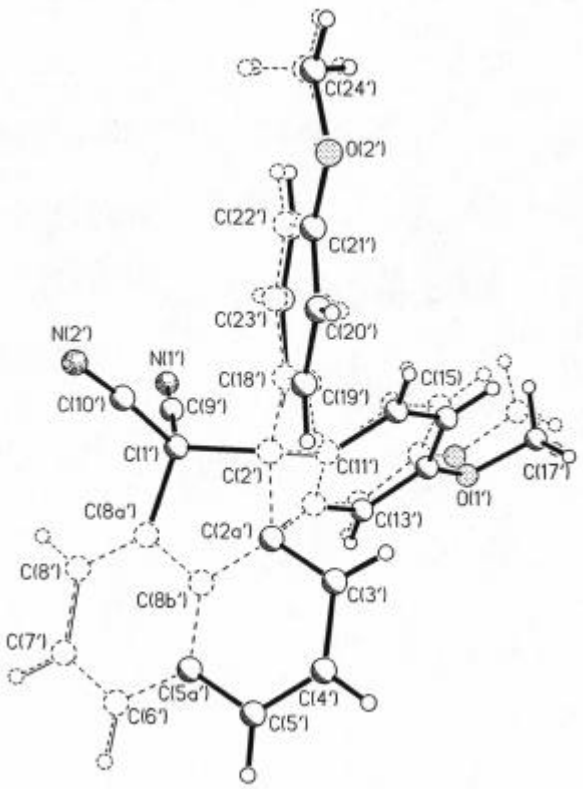
Koeffizienten der anisotropen Temperaturfaktoren (Å^2), Standardfehler in Klammern

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N1	0.063(2)	0.057(2)	0.062(2)	0.002(2)	0.005(2)	0.008(2)
C1	0.106(4)	0.090(4)	0.090(4)	0.012(3)	-0.012(3)	-0.042(4)
C2	0.156(7)	0.068(4)	0.108(5)	0.007(4)	-0.022(4)	-0.036(4)
C3	0.134(5)	0.057(3)	0.106(5)	-0.012(3)	-0.019(4)	-0.005(3)
C4	0.100(4)	0.056(3)	0.074(3)	-0.006(2)	-0.002(3)	0.002(3)
C4A	0.073(3)	0.055(3)	0.056(2)	0.003(2)	-0.002(2)	-0.006(2)
C5	0.057(2)	0.055(3)	0.058(2)	0.001(2)	0.004(2)	0.005(2)
C5A	0.070(3)	0.054(3)	0.059(3)	-0.005(2)	0.007(2)	0.005(2)
C6	0.090(4)	0.065(3)	0.076(3)	-0.008(3)	0.003(3)	-0.003(3)
C7	0.113(4)	0.080(4)	0.091(4)	-0.024(3)	0.000(3)	-0.013(3)
C8	0.157(6)	0.082(4)	0.082(4)	-0.026(3)	0.002(4)	0.000(4)
C9	0.132(5)	0.081(4)	0.073(3)	-0.006(3)	0.025(3)	0.029(4)
C9A	0.086(3)	0.067(3)	0.063(3)	-0.002(2)	0.013(2)	0.012(3)
C10	0.084(4)	0.103(4)	0.082(4)	0.002(3)	0.028(3)	0.020(4)
C11	0.071(3)	0.112(5)	0.082(4)	0.011(3)	0.014(3)	-0.007(3)
C11A	0.069(3)	0.076(3)	0.068(3)	0.007(3)	0.001(2)	-0.006(3)
C1"	0.059(3)	0.103(4)	0.082(3)	0.015(3)	-0.011(2)	-0.007(3)
C2"	0.100(4)	0.075(3)	0.074(3)	0.009(3)	0.017(3)	0.038(3)
C1'	0.055(3)	0.058(3)	0.062(3)	-0.001(2)	0.005(2)	0.003(2)
C2'	0.071(3)	0.086(3)	0.072(3)	0.002(3)	0.001(2)	0.016(3)
C3'	0.060(3)	0.102(4)	0.091(4)	-0.007(3)	0.012(3)	0.015(3)
C4'	0.062(3)	0.100(4)	0.087(4)	-0.005(3)	0.019(3)	0.003(3)
C4A'	0.070(3)	0.072(3)	0.064(3)	-0.009(2)	0.018(2)	-0.003(2)
C5'	0.089(4)	0.087(4)	0.065(3)	-0.009(3)	0.021(3)	-0.012(3)
C6'	0.089(4)	0.086(4)	0.063(3)	0.004(3)	0.007(3)	-0.012(3)
C7'	0.082(3)	0.071(3)	0.054(3)	0.002(2)	0.000(2)	0.002(2)
C8'	0.061(3)	0.054(2)	0.054(2)	-0.002(2)	0.006(2)	0.000(2)
C8A'	0.063(3)	0.052(2)	0.056(2)	-0.006(2)	0.004(2)	-0.001(2)
N2	0.050(2)	0.069(2)	0.067(2)	-0.003(2)	0.012(2)	-0.008(2)
C12	0.082(4)	0.090(4)	0.159(6)	-0.015(4)	0.031(4)	0.008(3)
C13	0.070(4)	0.093(5)	0.228(10)	-0.004(6)	0.010(5)	0.013(4)
C14	0.076(4)	0.094(5)	0.190(8)	0.023(5)	-0.020(5)	-0.003(4)
C15	0.068(3)	0.094(4)	0.102(4)	0.019(3)	-0.004(3)	-0.003(3)
C15A	0.048(2)	0.065(3)	0.086(3)	-0.002(3)	0.007(2)	-0.005(2)
C16	0.053(2)	0.068(3)	0.056(2)	-0.006(2)	0.008(2)	-0.006(2)
C16A	0.060(3)	0.066(3)	0.067(3)	-0.004(2)	0.006(2)	-0.008(2)
C17	0.082(4)	0.069(3)	0.102(4)	-0.008(3)	0.001(3)	-0.005(3)
C18	0.106(5)	0.063(4)	0.153(6)	0.012(4)	-0.009(4)	-0.005(3)
C19	0.111(5)	0.093(5)	0.135(6)	0.033(5)	-0.018(4)	-0.024(4)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C20	0.106(4)	0.104(5)	0.089(4)	0.025(4)	0.000(3)	-0.018(4)
C20A	0.087(3)	0.076(3)	0.065(3)	0.005(3)	0.008(3)	-0.021(3)
C21	0.112(5)	0.098(4)	0.067(3)	-0.009(3)	0.017(3)	-0.021(4)
C22	0.106(4)	0.095(4)	0.082(4)	-0.025(3)	0.032(3)	-0.012(4)
C22A	0.071(3)	0.069(3)	0.102(4)	-0.011(3)	0.032(3)	-0.001(3)
C12*	0.080(3)	0.082(4)	0.112(4)	-0.032(3)	0.024(3)	-0.023(3)
C13*	0.064(3)	0.128(5)	0.080(3)	0.025(3)	-0.005(3)	-0.002(3)
C12'	0.070(3)	0.079(3)	0.062(3)	-0.008(2)	0.009(2)	-0.010(3)
C13'	0.082(3)	0.134(5)	0.071(3)	-0.023(3)	0.012(3)	-0.031(3)
C14'	0.105(4)	0.132(5)	0.072(4)	-0.025(3)	0.004(3)	-0.020(4)
C15'	0.108(4)	0.095(4)	0.062(3)	-0.011(3)	0.006(3)	0.010(3)
C15*	0.071(3)	0.076(3)	0.061(3)	0.007(2)	0.012(2)	0.016(3)
C16'	0.095(4)	0.081(3)	0.067(3)	0.013(3)	0.020(3)	0.024(3)
C17'	0.090(4)	0.096(4)	0.084(4)	0.018(3)	0.043(3)	0.009(3)
C18'	0.070(3)	0.079(3)	0.089(4)	0.015(3)	0.021(3)	-0.005(3)
C19'	0.059(3)	0.064(3)	0.064(3)	0.005(2)	0.018(2)	0.007(2)
C19*	0.064(3)	0.066(3)	0.061(3)	0.001(2)	0.013(2)	0.004(2)
F1	0.159(3)	0.110(3)	0.131(3)	0.025(2)	0.042(2)	-0.006(2)
F2	0.276(6)	0.122(3)	0.166(4)	0.016(3)	-0.098(4)	-0.047(4)
F3	0.448(10)	0.186(5)	0.122(4)	0.056(3)	0.148(5)	0.055(5)
F4	0.103(3)	0.198(5)	0.369(9)	0.010(5)	-0.044(4)	0.025(3)
F5	0.122(3)	0.132(3)	0.122(2)	0.026(2)	0.067(2)	0.031(2)
F6	0.076(2)	0.155(3)	0.135(3)	-0.024(2)	-0.002(2)	0.017(2)
F7	0.135(3)	0.141(3)	0.127(3)	-0.015(2)	-0.024(2)	0.023(2)
F8	0.394(8)	0.094(3)	0.170(4)	-0.027(3)	0.171(5)	-0.085(4)

1.4 1-Dicyano-2-bis(4-methoxyphenyl)-acenaphthen (197)





Summenformel		$C_{28}H_{20}N_2B_2$
Formelgewicht		416.46 g/mol
Kristallgröße		0.42 x 0.38 x 0.25
Kristallsystem		triclinic
Raumgruppe		P1 (no. 2)
Gitterkonstanten	a	10.091(1) Å
	b	11.121(1) Å
	c	19.396(2) Å
	a	88.49°
	b	85.21°
	g	80.54
Zellvolumen		1907(1) $Å^3$
Z		4
Dichte (calculated)		1.293 g/cm^3
Wellenlänge		0.71073 Å
Temperatur		150 K
Meßbereich		3.5° bis 54°

Indexbereich	-11<=h<=12; -14<=k<=14; -24<=l<=0)
Absorptionskoeffizient *m*	0.82 cm^{-1}
Gesamtanzahl der Reflexe	9495
Symmetrieunabhängige Reflexe	9224 (R_{int} = 0.012)
Beobachtete Reflexe	7583 (I > 2.0)
Anzahl Variablen	580
Verfeinerungsmethode	Volle Matrix Least-Squares Verfeinerung, basierend auf F^2
*R*1	0.0391
*R*2	0.1007
Goodness-of-fit on F^2	1.025
Größter/kleinster Elektronendichte-Peak	0.29, -0.23

Bindungswinkel (Standardfehler in Klammern)

Atoms	Angle [°]	Atoms	Angle [°]
C6' - C7' - C8'	122.3(1)	C7' - C8' - C8A'	117.5(1)
C8' - C8A' - C8B'	121.0(1)	C1' - C8A' - C8'	131.4(1)
C1' - C8A' - C8B'	107.5(1)	C5A' - C8B' - C8A'	122.4(1)
C2A' - C8B' - C8A'	113.9(1)	C2A' - C8B' - C5A'	123.7(1)
N1' - C9' - C1'	178.7(2)	N2' - C10' - C1'	175.8(1)
C16' - C11' - C12'	117.8(1)	C16' - C11' - C2'	121.7(1)
C12' - C11' - C2'	120.3(1)	C13' - C12' - C11'	121.1(1)
C14' - C13' - C12'	120.2(1)	O1' - C14' - C15'	124.7(1)
O1' - C14' - C13'	115.6(1)	C15' - C14' - C13'	119.7(1)
C16' - C15' - C14'	119.4(1)	C15' - C16' - C11'	121.7(1)
C19' - C18' - C23'	118.0(1)	C2' - C18' - C23'	118.8(1)
C19' - C18' - C2'	123.2(1)	C18' - C19' - C20'	120.8(1)
C19' - C20' - C21'	120.2(1)	O2' - C21' - C20'	116.4(1)
O2' - C21' - C22'	123.7(1)	C22' - C21' - C20'	119.9(1)
C23' - C22' - C21'	119.3(1)		

Atoms					Angle [°]	Atoms					Angle [°]
C24	-	O1	-	C21	116.3(1)	C17	-	O2	-	C14	117.4(1)
C10	-	C1	-	C9	106.4(1)	C8A	-	C1	-	C9	114.3(1)
C10	-	C1	-	C8A	107.3(1)	C2	-	C1	-	C9	112.6(1)
C10	-	C1	-	C2	111.5(1)	C2	-	C1	-	C8A	104.7(1)
C18	-	C2	-	C2A	117.3(1)	C18	-	C2	-	C11	112.2(1)
C11	-	C2	-	C2A	107.1(1)	C1	-	C2	-	C18	108.5(1)
C1	-	C2	-	C2A	101.07(9)	C1	-	C2	-	C11	110.1(1)
C3	-	C2A	-	C8B	118.7(1)	C2	-	C2A	-	C3	130.3(1)
C2	-	C2A	-	C8B	110.3(1)	C2A	-	C3	-	C4	118.7(1)
C3	-	C4	-	C5	122.7(1)	C4	-	C5	-	C5A	119.9(1)
C5	-	C5A	-	C8B	116.3(1)	C6	-	C5A	-	C8B	116.2(1)
C5	-	C5A	-	C6	127.5(1)	C5A	-	C6	-	C7	120.9(1)
C6	-	C7	-	C8	122.1(1)	C7	-	C8	-	C8A	117.5(1)
C8	-	C8A	-	C8B	121.2(1)	C1	-	C8A	-	C8	131.0(1)
C1	-	C8A	-	C8B	107.7(1)	C2A	-	C8B	-	C8A	114.2(1)
C5A	-	C8B	-	C8A	122.1(1)	C2A	-	C8B	-	C5A	123.7(1)
N1	-	C9	-	C1	178.6(1)	N2	-	C10	-	C1	176.4(1)
C16	-	C11	-	C12	117.6(1)	C16	-	C11	-	C2	122.3(1)
C12	-	C11	-	C2	120.0(1)	C13	-	C12	-	C11	121.5(1)
C14	-	C13	-	C12	119.9(1)	O2	-	C14	-	C15	124.8(1)
O2	-	C14	-	C13	115.3(1)	C15	-	C14	-	C13	119.8(1)
C16	-	C15	-	C14	119.4(1)	C15	-	C16	-	C11	121.6(1)
C19	-	C18	-	C23	117.6(1)	C19	-	C18	-	C2	123.8(1)
C2	-	C18	-	C23	118.5(1)	C18	-	C19	-	C20	121.1(1)
C19	-	C20	-	C21	120.2(1)	O1	-	C21	-	C20	116.4(1)
O1	-	C21	-	C22	123.8(1)	C22	-	C21	-	C20	119.8(1)
C23	-	C22	-	C21	119.0(1)	C18	-	C23	-	C22	122.3(1)
C17'	-	O1'	-	C14'	117.6(1)	C24'	-	O2'	-	C21'	116.8(1)
C10'	-	C1'	-	C9'	106.8(1)	C8A'	-	C1'	-	C9'	113.7(1)
C10'	-	C1'	-	C8A'	107.4(1)	C2'	-	C1'	-	C9'	113.0(1)
C10'	-	C1'	-	C2'	111.2(1)	C2'	-	C1'	-	C8A'	104.8(1)
C18'	-	C2'	-	C2A'	116.8(1)	C18'	-	C2'	-	C11'	112.6(1)
C11'	-	C2'	-	C2A'	106.0(1)	C1'	-	C2'	-	C18'	108.9(1)
C1'	-	C2'	-	C2A'	100.8(1)	C1'	-	C2'	-	C11'	111.1(1)
C3'	-	C2A'	-	C8B'	118.9(1)	C2'	-	C2A'	-	C3'	130.1(1)
C2'	-	C2A'	-	C8B'	110.4(1)	C2A'	-	C3'	-	C4'	118.6(1)
C3'	-	C4'	-	C5'	122.6(1)	C4'	-	C5'	-	C5A'	120.1(1)
C5'	-	C5A'	-	C8B'	116.1(1)	C6'	-	C5A'	-	C8B'	116.2(1)
C5'	-	C5A'	-	C6'	127.7(1)	C5A'	-	C6'	-	C7'	120.7(1)

Bindungslängen (Standardfehler in Klammern)

Atoms			Distance [Å]	Atoms			Distance [Å]
N1	-	C9	1.140(2)	N2	-	C10	1.143(2)
O1	-	C21	1.368(2)	O1	-	C24	1.427(2)
O2	-	C14	1.366(2)	O2	-	C17	1.422(2)
C1	-	C9	1.478(2)	C1	-	C10	1.484(2)
C1	-	C8A	1.535(2)	C1	-	C2	1.643(2)
C2	-	C2A	1.530(2)	C2A	-	C3	1.370(2)
C2A	-	C8B	1.405(2)	C3	-	C4	1.417(2)
C4	-	C5	1.372(2)	C5	-	C5A	1.416(2)
C5A	-	C8B	1.407(2)	C5A	-	C6	1.419(2)
C6	-	C7	1.369(2)	C7	-	C8	1.422(2)
C8	-	C8A	1.364(2)	C8B	-	C8A	1.400(2)
C11	-	C2	1.542(2)	C12	-	C11	1.401(2)
C13	-	C12	1.378(2)	C14	-	C13	1.394(2)
C15	-	C14	1.384(2)	C16	-	C11	1.387(2)
C16	-	C15	1.398(2)	C18	-	C2	1.521(2)
C18	-	C23	1.395(2)	C19	-	C18	1.390(2)
C19	-	C20	1.388(2)	C21	-	C20	1.390(2)
C22	-	C21	1.392(2)	C23	-	C22	1.385(2)
N1'	-	C9'	1.138(2)	N2'	-	C10'	1.142(2)
O1'	-	C14'	1.369(2)	O1'	-	C17'	1.426(2)
O2'	-	C21'	1.372(2)	O2'	-	C24'	1.426(2)
C1'	-	C9'	1.474(2)	C1'	-	C10'	1.486(2)
C1'	-	C8A'	1.534(2)	C1'	-	C2'	1.636(2)
C2'	-	C2A'	1.530(2)	C2A'	-	C3'	1.370(2)
C2A'	-	C8B'	1.405(2)	C3'	-	C4'	1.416(2)
C4'	-	C5'	1.370(2)	C5'	-	C5A'	1.420(2)
C5A'	-	C8B'	1.405(2)	C5A'	-	C6'	1.421(2)
C6'	-	C7'	1.373(2)	C7'	-	C8'	1.419(2)
C8'	-	C8A'	1.366(2)	C8B'	-	C8A'	1.400(2)
C11'	-	C2'	1.542(2)	C12'	-	C11'	1.404(2)
C13'	-	C12'	1.379(2)	C14'	-	C13'	1.393(2)
C15'	-	C14'	1.388(2)	C16'	-	C11'	1.387(2)
C16'	-	C15'	1.395(2)	C18'	-	C2'	1.524(2)
C18'	-	C23'	1.392(2)	C19'	-	C18'	1.396(2)
C19'	-	C20'	1.387(2)	C21'	-	C20'	1.387(2)
C22'	-	C21'	1.390(2)				

Parameter der H-Atome

Atom	X	Y	Z	U_{eq}
H3A	-0.09337	0.16435	0.21796	0.0314(10)
H4A	-0.27299	0.07502	0.18112	0.0314(10)
H5A	-0.23728	-0.07661	0.09868	0.0314(10)
H6A	-0.05814	-0.21791	0.01581	0.0314(10)
H7A	0.16482	-0.26991	-0.02604	0.0314(10)
H8A	0.33649	-0.17029	0.01304	0.0314(10)
H12A	0.2118	-0.13431	0.21177	0.0314(10)
H13A	0.2662	-0.22997	0.31668	0.0314(10)
H15A	0.2585	0.10126	0.4025	0.0314(10)
H16A	0.21135	0.19559	0.29512	0.0314(10)
H17A	0.34451	-0.1265	0.52426	0.0314(10)
H17B	0.38691	-0.02014	0.47725	0.0314(10)
H17C	0.23437	-0.0211	0.50015	0.0314(10)
H19A	0.00918	0.31024	0.14808	0.0314(10)
H20A	0.04441	0.51349	0.14467	0.0314(10)
H22A	0.43806	0.40244	0.17937	0.0314(10)
H23A	0.39987	0.20032	0.18546	0.0314(10)
H24A	0.38355	0.71283	0.16058	0.0314(10)
H24B	0.42303	0.59482	0.20524	0.0314(10)
H24C	0.44444	0.5894	0.12433	0.0314(10)
H3'A	1.06648	-0.34526	0.27698	0.0329(10)
H4'A	1.25803	-0.4805	0.31044	0.0329(10)
H5'A	1.2407	-0.6302	0.39407	0.0329(10)
H6'A	1.07659	-0.73697	0.48198	0.0329(10)
H7'A	0.85889	-0.73602	0.53027	0.0329(10)
H8'A	0.6756	-0.58971	0.49595	0.0329(10)
H12B	0.76867	-0.57267	0.29801	0.0329(10)
H13B	0.72791	-0.6537	0.1935	0.0329(10)
H15B	0.72173	-0.32078	0.1006	0.0329(10)
H16B	0.75589	-0.23888	0.20709	0.0329(10)
H17D	0.67477	-0.53121	-0.021	0.0329(10)
H17E	0.62367	-0.41161	0.02092	0.0329(10)
H17F	0.77869	-0.45637	0.00556	0.0329(10)
H19B	0.96144	-0.18088	0.3531	0.0329(10)
H20B	0.91673	0.03271	0.35502	0.0329(10)
H22B	0.52736	0.02597	0.31767	0.0329(10)
H23B	0.5746	-0.18685	0.31303	0.0329(10)
H24D	0.56797	0.32389	0.33564	0.0329(10)
H24E	0.53218	0.21851	0.29214	0.0329(10)

Atomkoordinaten und Koeffizienten der equivalenten isotropen Temperaturfaktoren (Å), U_{eq} (ohne H-Atome, Standardfehler in Klammern)

Atom	X	Y	Z	U_{eq}
N1	0.5170(1)	-0.0787(1)	0.15395(7)	0.0299(3)
N2	0.3543(1)	0.1745(1)	0.00805(6)	0.0335(3)
O1	0.2548(1)	0.59796(8)	0.16001(5)	0.0279(2)
O2	0.3080(1)	-0.13806(9)	0.42700(5)	0.0299(2)
C1	0.2888(1)	0.0286(1)	0.10922(6)	0.0191(3)
C2	0.1854(1)	0.1000(1)	0.17046(6)	0.0185(3)
C2A	0.0506(1)	0.0684(1)	0.15236(6)	0.0194(3)
C3	-0.0770(1)	0.1036(1)	0.18268(7)	0.0224(3)
C4	-0.1831(1)	0.0484(1)	0.16092(7)	0.0248(3)
C5	-0.1628(1)	-0.0413(1)	0.11213(7)	0.0249(3)
C5A	-0.0313(1)	-0.0821(1)	0.08141(7)	0.0225(3)
C6	0.0087(2)	-0.1758(1)	0.03208(7)	0.0267(3)
C7	0.1408(2)	-0.2067(1)	0.00766(7)	0.0273(3)
C8	0.2440(1)	-0.1479(1)	0.03033(7)	0.0244(3)
C8A	0.2068(1)	-0.0578(1)	0.07781(6)	0.0198(3)
C8B	0.0718(1)	-0.0239(1)	0.10270(6)	0.0198(3)
C9	0.4168(1)	-0.0326(1)	0.13503(7)	0.0214(3)
C10	0.3253(1)	0.1138(1)	0.05342(7)	0.0228(3)
C11	0.2147(1)	0.0404(1)	0.24145(6)	0.0191(3)
C12	0.2257(1)	-0.0863(1)	0.25012(7)	0.0213(3)
C13	0.2563(1)	-0.1428(1)	0.31223(7)	0.0227(3)
C14	0.2722(1)	-0.0732(1)	0.36879(7)	0.0222(3)
C15	0.2527(1)	0.0527(1)	0.36300(7)	0.0241(3)
C16	0.2247(1)	0.1083(1)	0.29920(7)	0.0228(3)
C17	0.3193(2)	-0.0710(2)	0.48706(8)	0.0413(4)
C18	0.2006(1)	0.2340(1)	0.16787(6)	0.0193(3)
C19	0.0967(1)	0.3285(1)	0.15528(7)	0.0220(3)
C20	0.1172(1)	0.4490(1)	0.15309(7)	0.0242(3)
C21	0.2436(1)	0.4770(1)	0.16248(7)	0.0218(3)
C22	0.3501(1)	0.3838(1)	0.17378(7)	0.0229(3)
C23	0.3267(1)	0.2644(1)	0.17685(7)	0.0226(3)
C24	0.3873(2)	0.6260(1)	0.16279(8)	0.0307(3)
N1'	0.4717(1)	-0.4422(1)	0.36417(7)	0.0358(3)
N2'	0.6466(1)	-0.2342(1)	0.49844(6)	0.0302(3)
O1'	0.6951(1)	-0.55105(9)	0.07897(5)	0.0313(2)
O2'	0.7018(1)	0.17404(9)	0.33680(6)	0.0312(2)
C1'	0.7021(1)	-0.3926(1)	0.39784(7)	0.0193(3)
C2'	0.7940(1)	-0.3446(1)	0.33258(6)	0.0191(3)

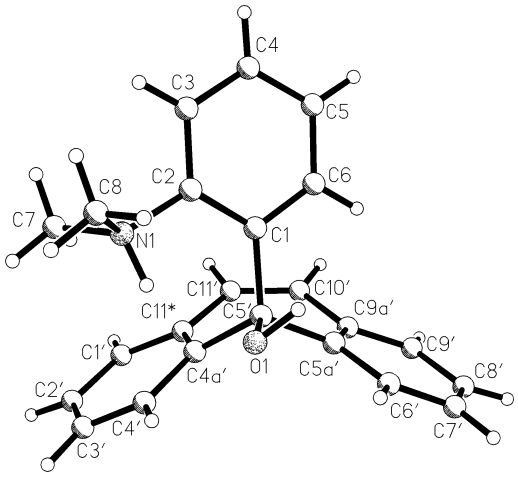
Atom	X	Y	Z	U_{eq}
C2A'	0.9342(1)	-0.4107(1)	0.34740(6)	0.0192(3)
C3'	1.0575(1)	-0.4044(1)	0.31333(7)	0.0217(3)
C4'	1.1709(1)	-0.4869(1)	0.33281(7)	0.0243(3)
C5'	1.1614(1)	-0.5757(1)	0.38246(7)	0.0247(3)
C5A'	1.0344(1)	-0.5872(1)	0.41710(7)	0.0223(3)
C6'	1.0051(2)	-0.6758(1)	0.46773(7)	0.0270(3)
C7'	0.8756(2)	-0.6757(1)	0.49572(7)	0.0287(3)
C8'	0.7657(1)	-0.5886(1)	0.47600(7)	0.0256(3)
C8A'	0.7928(1)	-0.5030(1)	0.42737(7)	0.0203(3)
C8B'	0.9243(1)	-0.5016(1)	0.39842(6)	0.0198(3)
C9'	0.5723(1)	-0.4200(1)	0.37816(7)	0.0229(3)
C10'	0.6700(1)	-0.2998(1)	0.45306(7)	0.0221(3)
C11'	0.7626(1)	-0.3959(1)	0.26372(6)	0.0189(3)
C12'	0.7566(1)	-0.5204(1)	0.25807(7)	0.0210(3)
C13'	0.7339(1)	-0.5687(1)	0.19623(7)	0.0227(3)
C14'	0.7200(1)	-0.4947(1)	0.13736(7)	0.0228(3)
C15'	0.7294(1)	-0.3720(1)	0.14117(7)	0.0246(3)
C16'	0.7502(1)	-0.3239(1)	0.20438(7)	0.0223(3)
C17'	0.6928(2)	-0.4820(2)	0.01594(8)	0.0421(4)
C18'	0.7722(1)	-0.2058(1)	0.33264(6)	0.0198(3)
C19'	0.8729(1)	-0.1388(1)	0.34527(7)	0.0226(3)
C20'	0.8466(1)	-0.0124(1)	0.34639(7)	0.0256(3)
C21'	0.7187(2)	0.0491(1)	0.33565(7)	0.0238(3)
C22'	0.6166(1)	-0.0161(1)	0.32392(7)	0.0244(3)
C23'	0.6446(1)	-0.1420(1)	0.32218(7)	0.0234(3)
C24'	0.5676(2)	0.2377(1)	0.33420(9)	0.0361(4)

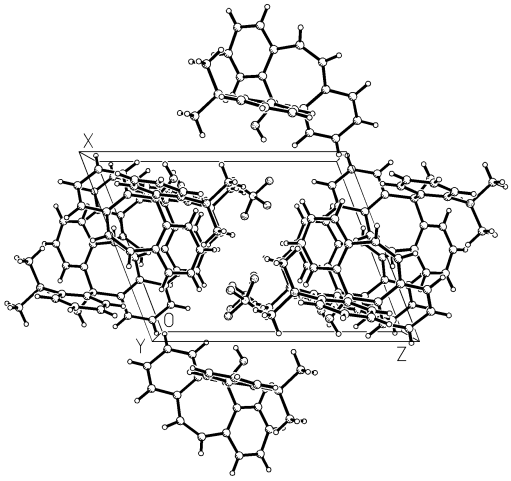
Koeffizienten der anisotropen Temperaturfaktoren (Å^2), Standardfehler in Klammern

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N1	0.0223(6)	0.0335(7)	0.0331(7)	0.0007(5)	-0.0018(5)	-0.0021(5)
N2	0.0444(8)	0.0317(7)	0.0253(6)	0.0014(5)	0.0016(6)	-0.0112(6)
O1	0.0275(5)	0.0185(5)	0.0374(6)	0.0000(4)	0.0016(4)	-0.0047(4)
O2	0.0432(6)	0.0298(5)	0.0186(5)	0.0037(4)	-0.0056(4)	-0.0109(5)
C1	0.0187(6)	0.0201(6)	0.0184(6)	0.0000(5)	-0.0004(5)	-0.0031(5)
C2	0.0174(6)	0.0201(6)	0.0176(6)	-0.0019(5)	0.0001(5)	-0.0021(5)
C2A	0.0208(6)	0.0204(6)	0.0175(6)	0.0020(5)	-0.0022(5)	-0.0044(5)
C3	0.0220(7)	0.0248(7)	0.0202(6)	-0.0001(5)	-0.0001(5)	-0.0037(5)
C4	0.0184(6)	0.0322(7)	0.0235(7)	0.0043(6)	0.0007(5)	-0.0053(5)
C5	0.0223(7)	0.0304(7)	0.0244(7)	0.0045(6)	-0.0050(5)	-0.0105(6)
C5A	0.0246(7)	0.0242(7)	0.0202(6)	0.0029(5)	-0.0047(5)	-0.0075(5)
C6	0.0323(8)	0.0254(7)	0.0247(7)	-0.0003(5)	-0.0078(6)	-0.0090(6)
C7	0.0362(8)	0.0223(7)	0.0236(7)	-0.0046(5)	-0.0046(6)	-0.0035(6)
C8	0.0264(7)	0.0238(7)	0.0220(7)	-0.0013(5)	0.0001(5)	-0.0016(5)
C8A	0.0215(6)	0.0205(6)	0.0180(6)	0.0014(5)	-0.0024(5)	-0.0048(5)
C8B	0.0217(6)	0.0198(6)	0.0181(6)	0.0022(5)	-0.0023(5)	-0.0037(5)
C9	0.0217(7)	0.0214(6)	0.0210(6)	-0.0013(5)	0.0023(5)	-0.0049(5)
C10	0.0231(7)	0.0236(7)	0.0220(7)	-0.0025(5)	-0.0010(5)	-0.0047(5)
C11	0.0161(6)	0.0222(6)	0.0190(6)	-0.0003(5)	-0.0003(5)	-0.0034(5)
C12	0.0224(7)	0.0228(6)	0.0197(6)	-0.0029(5)	-0.0007(5)	-0.0067(5)
C13	0.0251(7)	0.0206(6)	0.0228(6)	0.0013(5)	0.0005(5)	-0.0066(5)
C14	0.0204(6)	0.0287(7)	0.0182(6)	0.0034(5)	-0.0004(5)	-0.0073(5)
C15	0.0271(7)	0.0280(7)	0.0183(6)	-0.0039(5)	0.0002(5)	-0.0082(6)
C16	0.0250(7)	0.0216(6)	0.0217(6)	-0.0021(5)	0.0008(5)	-0.0042(5)
C17	0.065(1)	0.0391(9)	0.0212(7)	0.0009(6)	-0.0129(7)	-0.0083(8)
C18	0.0211(6)	0.0201(6)	0.0165(6)	-0.0017(5)	-0.0001(5)	-0.0035(5)
C19	0.0188(6)	0.0244(7)	0.0226(6)	-0.0010(5)	-0.0002(5)	-0.0032(5)
C20	0.0220(7)	0.0226(7)	0.0261(7)	0.0002(5)	-0.0005(5)	0.0011(5)
C21	0.0268(7)	0.0195(6)	0.0186(6)	-0.0010(5)	0.0028(5)	-0.0044(5)
C22	0.0222(7)	0.0233(7)	0.0241(7)	-0.0009(5)	-0.0018(5)	-0.0059(5)
C23	0.0211(7)	0.0216(6)	0.0247(7)	-0.0006(5)	-0.0036(5)	-0.0010(5)
C24	0.0320(8)	0.0225(7)	0.0388(8)	-0.0009(6)	0.0006(6)	-0.0097(6)
N1'	0.0224(7)	0.0414(8)	0.0451(8)	-0.0082(6)	-0.0018(6)	-0.0087(6)
N2'	0.0326(7)	0.0306(7)	0.0262(6)	-0.0046(5)	-0.0012(5)	-0.0016(5)
O1'	0.0481(7)	0.0265(5)	0.0192(5)	-0.0045(4)	-0.0054(4)	-0.0039(5)
O2'	0.0361(6)	0.0204(5)	0.0375(6)	-0.0011(4)	0.0009(5)	-0.0072(4)
C1'	0.0164(6)	0.0219(6)	0.0198(6)	-0.0013(5)	0.0000(5)	-0.0044(5)
C2'	0.0173(6)	0.0220(6)	0.0185(6)	-0.0006(5)	0.0001(5)	-0.0054(5)
C2A'	0.0189(6)	0.0213(6)	0.0183(6)	-0.0027(5)	-0.0025(5)	-0.0045(5)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C3'	0.0202(6)	0.0272(7)	0.0186(6)	-0.0013(5)	-0.0006(5)	-0.0069(5)
C4'	0.0167(6)	0.0342(7)	0.0226(7)	-0.0062(6)	0.0002(5)	-0.0059(5)
C5'	0.0191(7)	0.0297(7)	0.0245(7)	-0.0047(5)	-0.0049(5)	0.0004(5)
C5A'	0.0224(7)	0.0237(7)	0.0210(6)	-0.0034(5)	-0.0044(5)	-0.0030(5)
C6'	0.0299(7)	0.0244(7)	0.0266(7)	0.0012(5)	-0.0067(6)	-0.0019(6)
C7'	0.0347(8)	0.0264(7)	0.0260(7)	0.0051(6)	-0.0032(6)	-0.0087(6)
C8'	0.0245(7)	0.0286(7)	0.0245(7)	0.0006(5)	0.0019(5)	-0.0086(6)
C8A'	0.0193(6)	0.0219(6)	0.0198(6)	-0.0019(5)	-0.0012(5)	-0.0039(5)
C8B'	0.0195(6)	0.0226(6)	0.0182(6)	-0.0031(5)	-0.0021(5)	-0.0054(5)
C9'	0.0193(7)	0.0241(7)	0.0249(7)	-0.0023(5)	0.0018(5)	-0.0041(5)
C10'	0.0188(6)	0.0249(7)	0.0229(7)	0.0008(5)	-0.0013(5)	-0.0045(5)
C11'	0.0138(6)	0.0221(6)	0.0207(6)	-0.0015(5)	-0.0007(5)	-0.0025(5)
C12'	0.0186(6)	0.0223(6)	0.0214(6)	0.0010(5)	-0.0012(5)	-0.0018(5)
C13'	0.0223(7)	0.0191(6)	0.0259(7)	-0.0020(5)	-0.0013(5)	-0.0010(5)
C14'	0.0220(7)	0.0258(7)	0.0196(6)	-0.0044(5)	-0.0007(5)	-0.0011(5)
C15'	0.0289(7)	0.0247(7)	0.0198(6)	0.0022(5)	-0.0016(5)	-0.0036(5)
C16'	0.0224(7)	0.0211(6)	0.0238(7)	0.0001(5)	-0.0017(5)	-0.0050(5)
C17'	0.072(1)	0.0358(9)	0.0196(7)	-0.0024(6)	-0.0080(7)	-0.0090(8)
C18'	0.0214(6)	0.0206(6)	0.0175(6)	-0.0004(5)	0.0006(5)	-0.0049(5)
C19'	0.0214(7)	0.0261(7)	0.0213(6)	-0.0006(5)	-0.0015(5)	-0.0067(5)
C20'	0.0271(7)	0.0270(7)	0.0249(7)	-0.0006(5)	-0.0022(5)	-0.0114(6)
C21'	0.0332(7)	0.0202(6)	0.0182(6)	-0.0007(5)	0.0027(5)	-0.0073(5)
C22'	0.0227(7)	0.0251(7)	0.0245(7)	-0.0002(5)	0.0002(5)	-0.0023(5)
C23'	0.0207(7)	0.0248(7)	0.0257(7)	-0.0025(5)	-0.0016(5)	-0.0069(5)
C24'	0.0401(9)	0.0212(7)	0.0454(9)	0.0007(6)	0.0004(7)	-0.0028(6)

1.5 5-Hydroxy-5-(2-*N*,*N*-dimethylammonium-1-phenyl)-5H-dibenzo-[a,d]cyclo-hepten-tetrafluoroborat (177)





Summenformel		$C_{23}H_{22}BF_4NO$
Formelgewicht		415.23 g/mol
Kristallgröße		0.30 x 0.29 x 0.10
Kristallsystem		monoklin
Raumgruppe		$P2_1$ (no. 4)
Gitterkonstanten	a	9.896(3) Å
	b	8.453(2) Å
	c	12.998(3) Å
	b	111.05°
Zellvolumen		1014.3(6) $Å^3$
Z		2
Dichte (calculated)		1.36 g/cm^3
Wellenlänge		0.71073 Å
Temperatur		293 K
Meßbereich		3.5° bis 54°
Indexbereich		-12<=h<=1; -1<=k<=10; -15<=l<=16)
Absorptionskoeffizient *m*		1.07 cm^{-1}
Gesamtanzahl der Reflexe		3128
Symmetrieunabhängige Reflexe		2672 (R_{int} = 0.031)
Beobachtete Reflexe		1700 (I > 2.0)

Anzahl Variablen	267
Verfeinerungsmethode	Volle Matrix Least-Squares Verfeinerung, basierend auf F^2
*R*1	0.0574
*R*2	0.1716
Goodness-of-fit on F^2	1.01
Größter/kleinster Elektronendichte-Peak	0.29, -0.28

Bindungswinkel (Standardfehler in Klammern)

Atoms					Angle [°]	Atoms					Angle [°]
C2	-	C1	-	C6	116.6(4)	C5'	-	C1	-	C6	121.7(4)
C2	-	C1	-	C5'	121.3(4)	C1	-	C2	-	C3	121.4(4)
C3	-	C2	-	N1	117.4(4)	C1	-	C2	-	N1	121.1(4)
C2	-	C3	-	C4	119.9(4)	C3	-	C4	-	C5	120.6(4)
C4	-	C5	-	C6	118.5(5)	C1	-	C6	-	C5	122.8(4)
O1	-	C5'	-	C5A'	110.7(3)	O1	-	C5'	-	C4A'	106.1(3)
C4A'	-	C5'	-	C5A'	109.6(3)	O1	-	C5'	-	C1	104.8(3)
C1	-	C5'	-	C5A'	113.0(3)	C1	-	C5'	-	C4A'	112.4(3)
C6'	-	C5A'	-	C9A'	118.0(4)	C5'	-	C5A'	-	C6'	120.3(4)
C5'	-	C5A'	-	C9A'	121.7(4)	C5A'	-	C6'	-	C7'	122.4(4)
C8'	-	C9'	-	C9A'	121.6(5)	C5A'	-	C9A'	-	C9'	118.9(4)
C10'	-	C9A'	-	C9'	117.1(4)	C10'	-	C9A'	-	C5A'	124.0(4)
C11'	-	C10'	-	C9A'	127.9(4)	C11*	-	C11'	-	C10'	127.0(4)
C1'	-	C11*	-	C4A'	118.2(4)	C11'	-	C11*	-	C4A'	124.4(4)
C1'	-	C11*	-	C11'	117.4(4)	C11*	-	C1'	-	C2'	122.5(4)
C1'	-	C2'	-	C3'	118.3(4)	C2'	-	C3'	-	C4'	120.4(5)
C3'	-	C4'	-	C4A'	121.9(4)	C11*	-	C4A'	-	C4'	118.5(4)
C4'	-	C4A'	-	C5'	120.8(4)	C11*	-	C4A'	-	C5'	120.6(4)
C2	-	N1	-	C7	113.2(4)	C2	-	N1	-	C8	113.6(4)
C7	-	N1	-	C8	110.3(4)	C6'	-	C7'	-	C8'	119.4(5)
C7'	-	C8'	-	C9'	119.6(4)	F3	-	B1	-	F4	112.0(6)
F1	-	B1	-	F4	110.6(5)	F1	-	B1	-	F3	108.9(5)
F2	-	B1	-	F4	108.4(5)	F2	-	B1	-	F3	107.8(5)

Atomkoordinaten und Koeffizienten der equivalenten isotropen Temperaturfaktoren (Å), U_{eq} (ohne H-Atome, Standardfehler in Klammern)

Atom	X	Y	Z	U_{eq}
O1	0.1274(3)	0.1480(4)	0.6933(2)	0.0423(7)
C1	0.2218(4)	0.3939(5)	0.7753(3)	0.0371(9)
C2	0.2358(5)	0.4681(5)	0.6835(4)	0.042(1)
C3	0.2150(5)	0.6305(6)	0.6667(4)	0.052(1)
C4	0.1735(5)	0.7189(6)	0.7375(4)	0.055(1)
C5	0.1543(5)	0.6499(6)	0.8276(4)	0.051(1)
C6	0.1802(5)	0.4877(6)	0.8449(4)	0.046(1)
C5'	0.2369(4)	0.2128(5)	0.7905(3)	0.0340(9)
C5A'	0.2144(4)	0.1554(5)	0.8949(3)	0.0380(9)
C6'	0.0966(5)	0.0604(6)	0.8871(4)	0.046(1)
C7'	0.0696(6)	0.0098(6)	0.9785(4)	0.056(1)
C8'	0.1609(6)	0.0562(7)	1.0822(4)	0.064(1)
C9'	0.2775(6)	0.1507(7)	1.0926(4)	0.056(1)
C9A'	0.3092(5)	0.1990(6)	1.0006(3)	0.045(1)
C10'	0.4390(5)	0.2959(6)	1.0214(4)	0.051(1)
C11'	0.5253(5)	0.3020(6)	0.9625(4)	0.051(1)
C11*	0.5140(4)	0.2072(5)	0.8665(3)	0.0423(10)
C1'	0.6435(5)	0.1649(7)	0.8523(4)	0.053(1)
C2'	0.6468(5)	0.0640(7)	0.7700(4)	0.059(1)
C3'	0.5174(5)	0.0017(7)	0.6996(4)	0.054(1)
C4'	0.3888(5)	0.0455(6)	0.7090(3)	0.044(1)
C4A'	0.3833(4)	0.1512(5)	0.7897(3)	0.0377(9)
N1	0.2693(4)	0.3765(5)	0.5992(3)	0.0498(10)
C7	0.4174(6)	0.4097(9)	0.5977(5)	0.076(2)
C8	0.1570(6)	0.3934(9)	0.4849(4)	0.070(2)
B1	0.2140(6)	-0.1118(8)	0.4065(5)	0.053(1)
F1	0.3264(3)	-0.2064(6)	0.4719(3)	0.085(1)
F2	0.1261(4)	-0.1996(7)	0.3174(3)	0.110(1)
F3	0.2700(4)	0.0094(6)	0.3666(4)	0.117(2)
F4	0.1338(4)	-0.0609(9)	0.4633(3)	0.129(2)

Koeffizienten der anisotropen Temperaturfaktoren (Å^2), Standardfehler in Klammern

Der anisotrope Temperaturfaktor ist definiert als $\exp(-2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}l^2c^{*2} + 2U_{12}hka^*b^* + 2U_{13}hla^*c^* + 2U_{23}klb^*c^*))$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	0.045(2)	0.040(2)	0.040(1)	-0.002(1)	0.013(1)	-0.003(1)
C1	0.041(2)	0.032(2)	0.039(2)	0.006(2)	0.014(2)	0.000(2)
C2	0.043(2)	0.035(2)	0.049(2)	0.007(2)	0.019(2)	0.001(2)
C3	0.062(3)	0.034(2)	0.065(3)	0.020(2)	0.028(2)	0.005(2)
C4	0.064(3)	0.031(2)	0.069(3)	0.005(2)	0.024(2)	-0.003(2)
C5	0.062(3)	0.033(2)	0.057(3)	0.000(2)	0.022(2)	0.005(2)
C6	0.058(3)	0.033(2)	0.046(2)	0.005(2)	0.018(2)	0.003(2)
C5'	0.037(2)	0.030(2)	0.033(2)	0.004(2)	0.010(2)	0.001(2)
C5A'	0.052(2)	0.027(2)	0.040(2)	0.003(2)	0.022(2)	0.006(2)
C6'	0.053(2)	0.037(2)	0.053(2)	0.003(2)	0.027(2)	-0.002(2)
C7'	0.073(3)	0.041(3)	0.072(3)	0.009(3)	0.046(3)	0.001(2)
C8'	0.095(4)	0.056(3)	0.062(3)	0.014(3)	0.053(3)	0.013(3)
C9'	0.080(3)	0.053(3)	0.040(2)	0.004(2)	0.026(2)	0.010(3)
C9A'	0.061(3)	0.035(2)	0.041(2)	0.004(2)	0.019(2)	0.010(2)
C10'	0.062(3)	0.042(3)	0.042(2)	-0.005(2)	0.009(2)	0.003(3)
C11'	0.047(2)	0.041(2)	0.058(3)	-0.004(2)	0.010(2)	-0.007(2)
C11*	0.046(2)	0.036(2)	0.044(2)	0.003(2)	0.014(2)	-0.002(2)
C1'	0.044(2)	0.049(3)	0.064(3)	0.008(3)	0.016(2)	0.002(2)
C2'	0.050(3)	0.064(3)	0.070(3)	0.012(3)	0.030(2)	0.009(3)
C3'	0.068(3)	0.050(3)	0.054(3)	0.004(2)	0.032(2)	0.012(3)
C4'	0.053(2)	0.039(2)	0.046(2)	0.000(2)	0.023(2)	0.004(2)
C4A'	0.044(2)	0.032(2)	0.037(2)	0.004(2)	0.015(2)	0.003(2)
N1	0.061(2)	0.048(2)	0.050(2)	0.014(2)	0.032(2)	0.011(2)
C7	0.067(3)	0.094(5)	0.081(3)	0.028(4)	0.045(3)	0.022(4)
C8	0.083(4)	0.080(4)	0.042(2)	0.001(3)	0.017(3)	0.014(3)
F1	0.068(2)	0.104(3)	0.080(2)	0.035(2)	0.023(2)	0.004(2)
F2	0.076(2)	0.130(4)	0.107(3)	-0.039(3)	0.012(2)	-0.016(3)
F3	0.097(3)	0.096(3)	0.147(3)	0.048(3)	0.032(3)	-0.013(3)
F4	0.090(2)	0.215(7)	0.089(2)	-0.002(4)	0.043(2)	0.039(3)

Parameter der H-Atome

Atom	X	Y	Z	U_{eq}
H1A	0.05099	0.20531	0.70301	0.06339
H3A	0.22819	0.67753	0.60374	0.06251
H4A	0.16	0.83054	0.72437	0.06571
H5A	0.12486	0.71224	0.87761	0.0608
H6A	0.16608	0.43784	0.90665	0.05512
H6'	0.0322	0.03001	0.81499	0.05475
H7'	-0.01091	-0.05868	0.97076	0.06755
H8'	0.13871	0.02589	1.14557	0.07712
H9'	0.34126	0.17997	1.16521	0.06774
H10'	0.46609	0.36222	1.08558	0.06122
H11'	0.60495	0.37497	0.98563	0.06157
H1'	0.73339	0.20573	0.90283	0.06381
H2'	0.73706	0.03839	0.76202	0.07073
H3'	0.51828	-0.07316	0.6443	0.06517
H4'	0.30001	0.00515	0.65667	0.05324
H1	0.24806	0.27172	0.61874	0.07472
H7A	0.48982	0.39691	0.66979	0.09079
H7B	0.43714	0.33865	0.54717	0.09079
H7C	0.41886	0.5167	0.57334	0.09079
H8A	0.06241	0.37072	0.48579	0.08344
H8B	0.15985	0.50048	0.46113	0.08344
H8C	0.17812	0.32244	0.43496	0.08344

Bindungslängen (Standardfehler in Klammern)

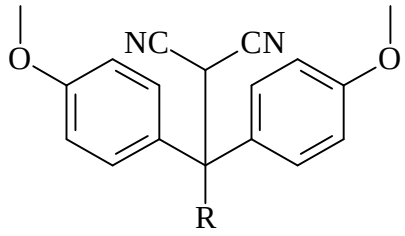
Atoms			Distance [Å]	Atoms			Distance [Å]
O1	-	C5'	1.444(5)	C1	-	C6	1.372(6)
C1	-	C2	1.398(6)	C1	-	C5'	1.544(6)
C2	-	C3	1.393(6)	C2	-	N1	1.474(6)
C3	-	C4	1.358(7)	C4	-	C5	1.381(6)
C5	-	C6	1.398(7)	C5A'	-	C5'	1.530(5)
C5A'	-	C6'	1.389(6)	C5A'	-	C9A'	1.407(6)
C6'	-	C7'	1.377(6)	C9'	-	C9A'	1.401(6)
C10'	-	C9A'	1.465(7)	C11'	-	C10'	1.337(6)
C11*	-	C11'	1.453(6)	C11*	-	C4A'	1.403(6)
C1'	-	C11*	1.405(6)	C1'	-	C2'	1.378(7)
C2'	-	C3'	1.383(7)	C3'	-	C4'	1.373(6)
C4A'	-	C5'	1.544(5)	C4A'	-	C4'	1.393(6)
N1	-	C7	1.499(6)	N1	-	C8	1.509(6)
C7'	-	C8'	1.383(7)	C8'	-	C9'	1.370(8)
B1	-	F4	1.335(6)	B1	-	F3	1.353(7)
B1	-	F1	1.386(7)				

2. NMR-Spektroskopie

2.1 Zusammenfassende Charakterisierung der Additionsprodukte

Verbindung	Typ	2'-H/2''-H/ 6'-H/6''-H	3'-H/3''-H/ 5'-H/5''-H	Alkyl-H	OCH_3	C-5'	-CN
74	IV	7.32	6.87	5.35	3.80	59.18	112.91
77	IV	7.23	6.99	5.08	3.82	58.94	112.80
123	IV	7.13	6.89	5.05	3.81	58.17	112.63
139	IV	7.26	7.11	5.85	3.50	56.95	111.47

Tabelle 11: Signifikante ^{1}H-NMR- und ^{13}C-NMR-Daten von Dicyanomethylmethanen δ [ppm]

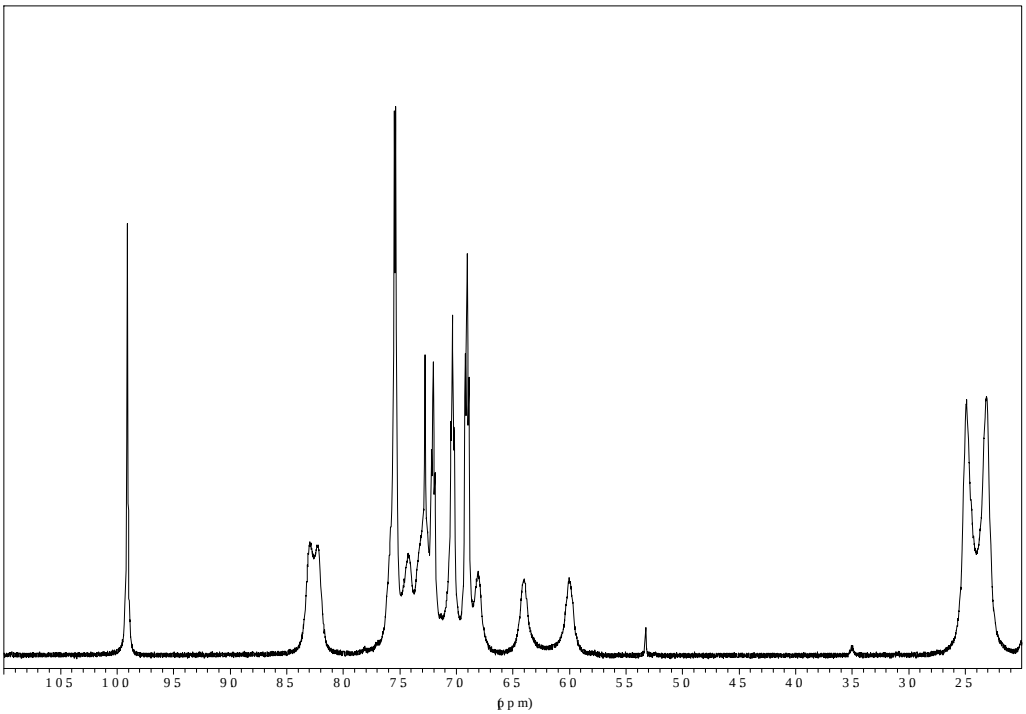


IV

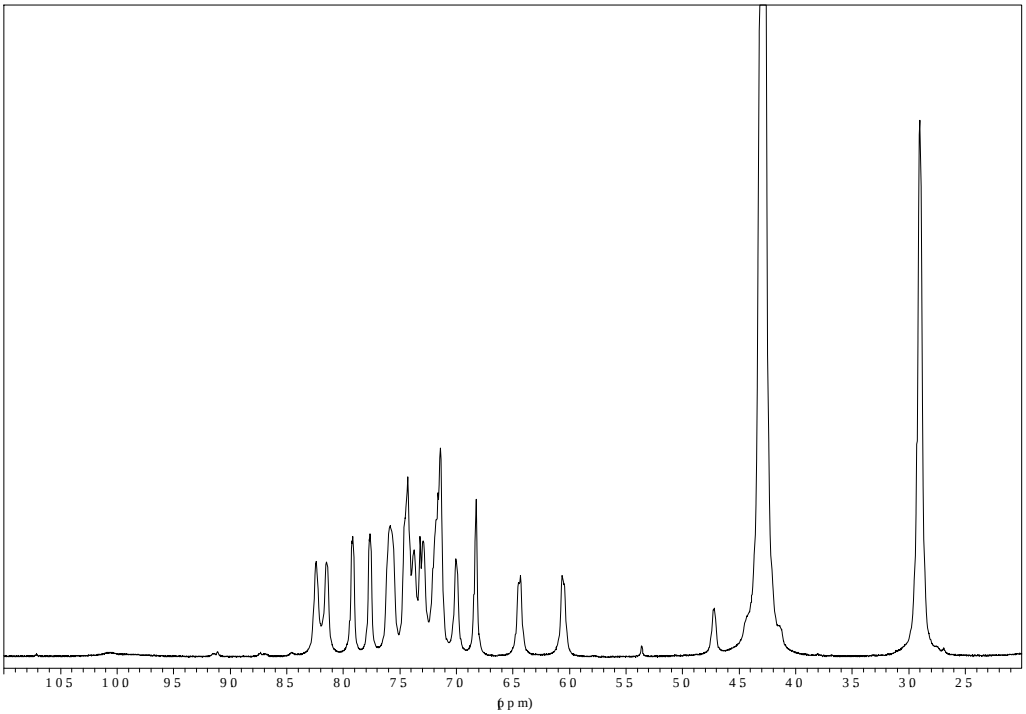
74: R = 1-naphthyl
77: R = 2-tolyl

123: R = 4-fluorphenyl
139: R = 2,4,6-trimeth-oxyphenyl

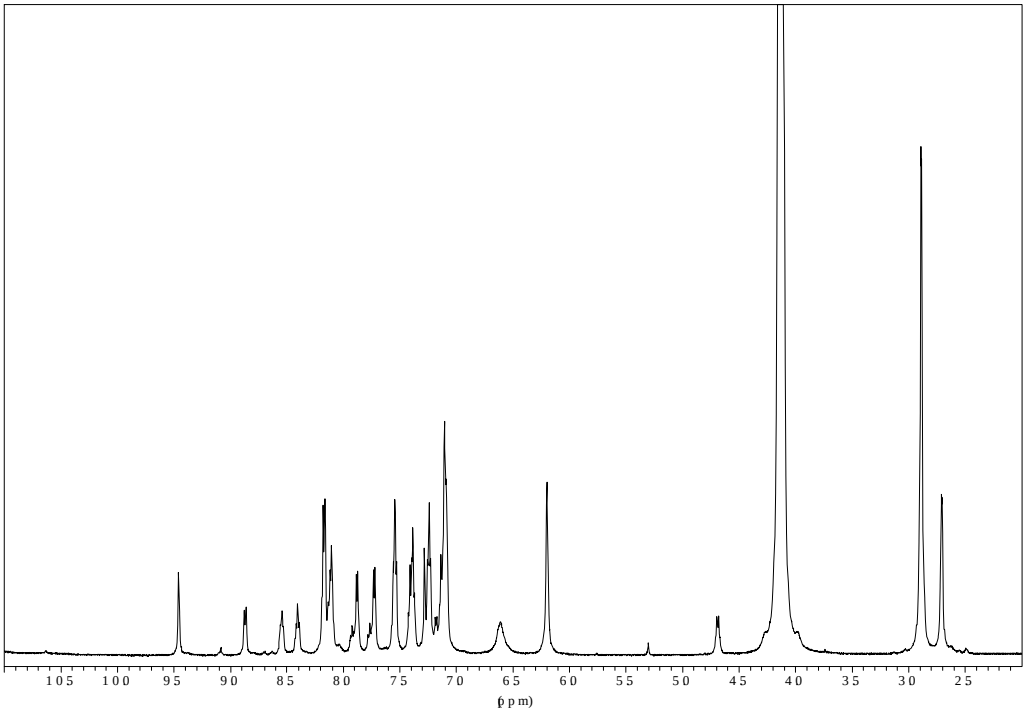
2.2 Protonenspektren: Mechanistische Untersuchung zur Bildung von Spiro[5*H*-dibenzo[a,d]cyclohepten-5,2'-[2*H*]-naphtho[1,8-bc]*N*,*N*-dimethyl-pyrrolidin]-tetrafluoroborat (14)



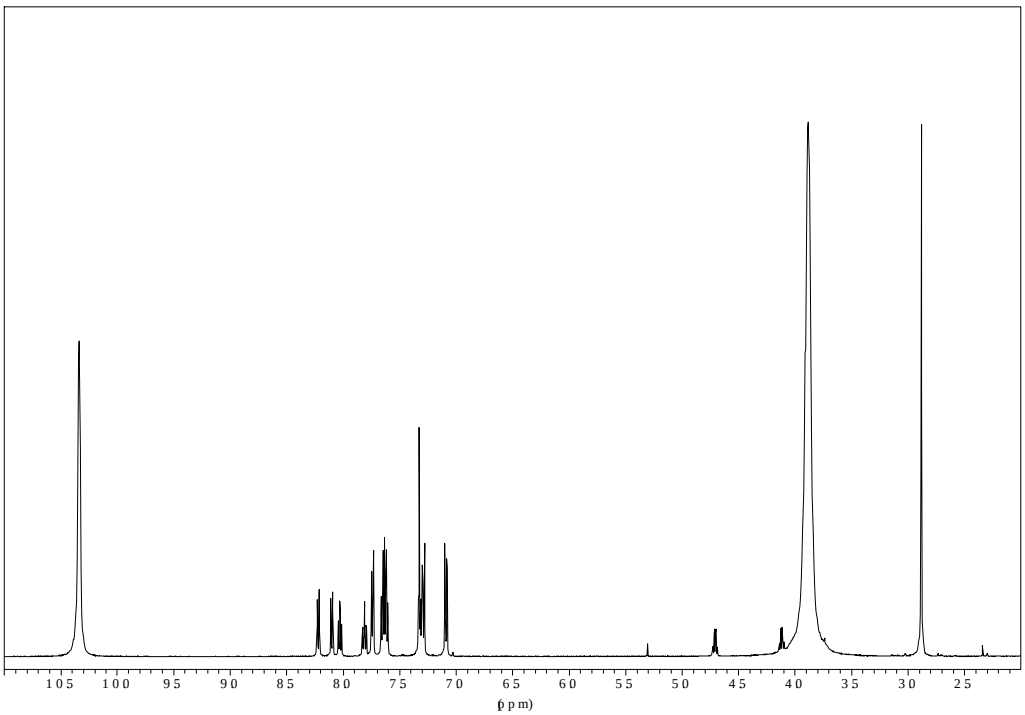
Spektrum 1: ^{1}H-NMR-Spektrum von Tritylalkohol **170** bei 228 K (t = 0)



Spektrum 2: ^{1}H-NMR-Spektrum nach Protonierung von **170** bei 228 K (t = 75 min)



Spektrum 3: ^{1}H-NMR-Spektrum nach Erwärmen auf 297 K (t = 120 min)



Spektrum 4: ^{1}H-NMR-Spektrum von **14** bei 297 K (t = 21 h)

3. ^{1}H-^{1}H-COSY-Spektren

3.1 9-Anthryl-bis(4-methoxyphenyl)-methyl-tetrafluoroborat (26)

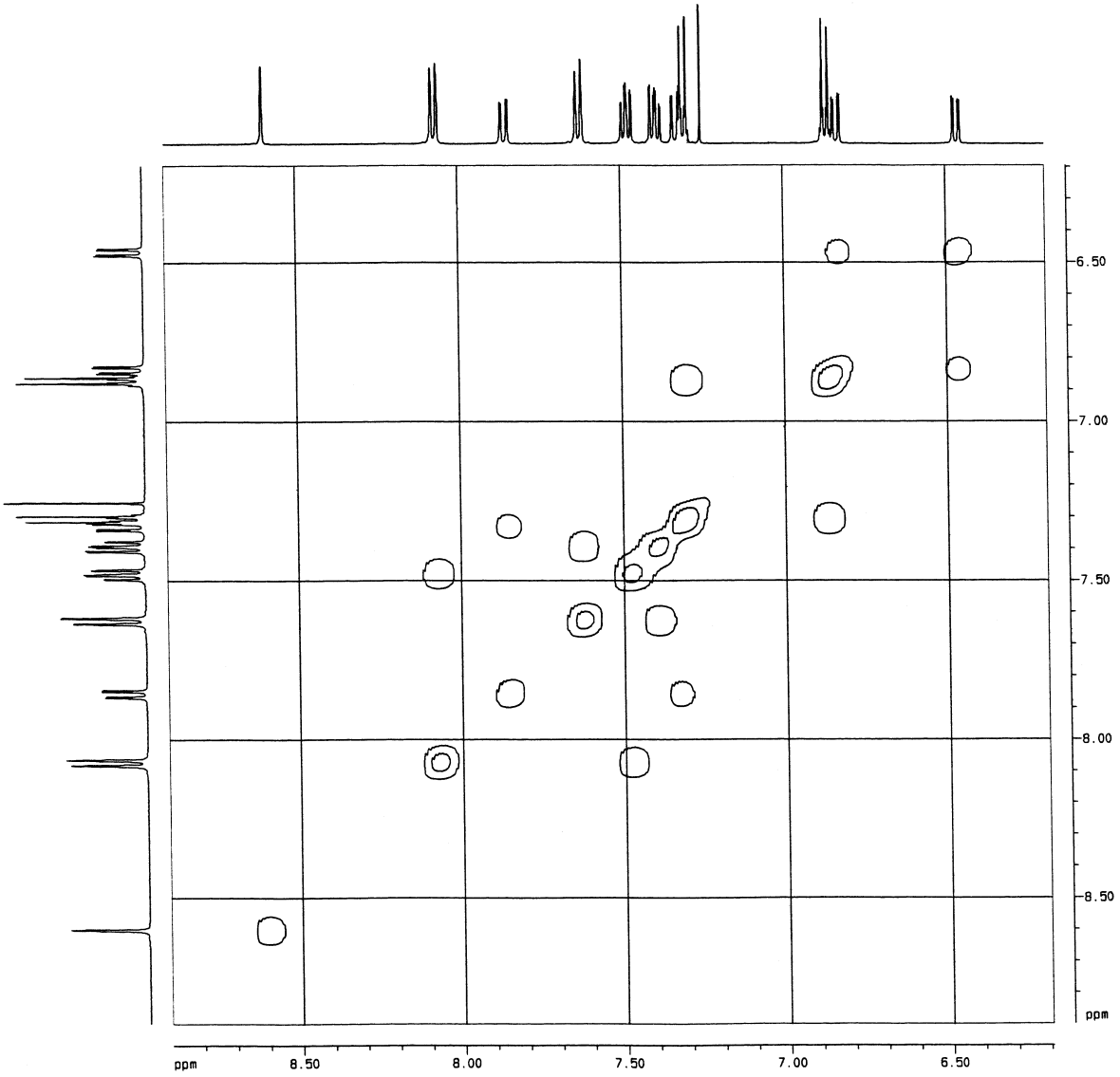


Abbildung 41: Korrelationsspektrum von **26** im Bereich δ = 6.20-8.90 ppm

3.2 1-[4-(8-Aminochinolin)-phenyl-(2,4,6-trimethylphenyl)]-methylen-4-(8-imino-chinolin)-cyclohexa-2,5-dien (110)

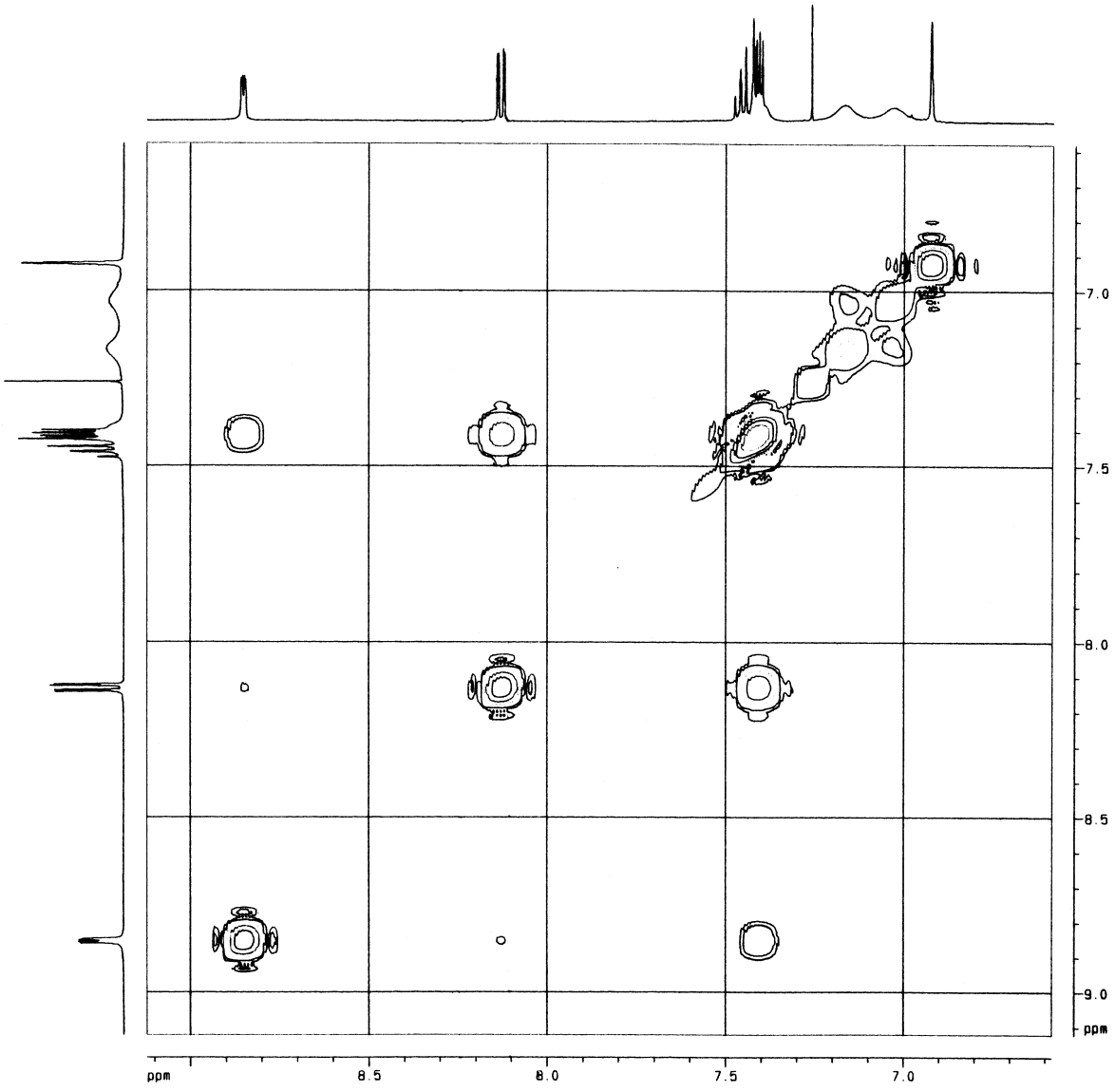


Abbildung 42: Korrelationsspektrum von **110** im Bereich δ = 6.60-9.10 ppm

3.3 5-Hydroxy-5-(1-methoxy-2-naphthyl)-5*H*-dibenzo[a,d]cyclohepten (162)

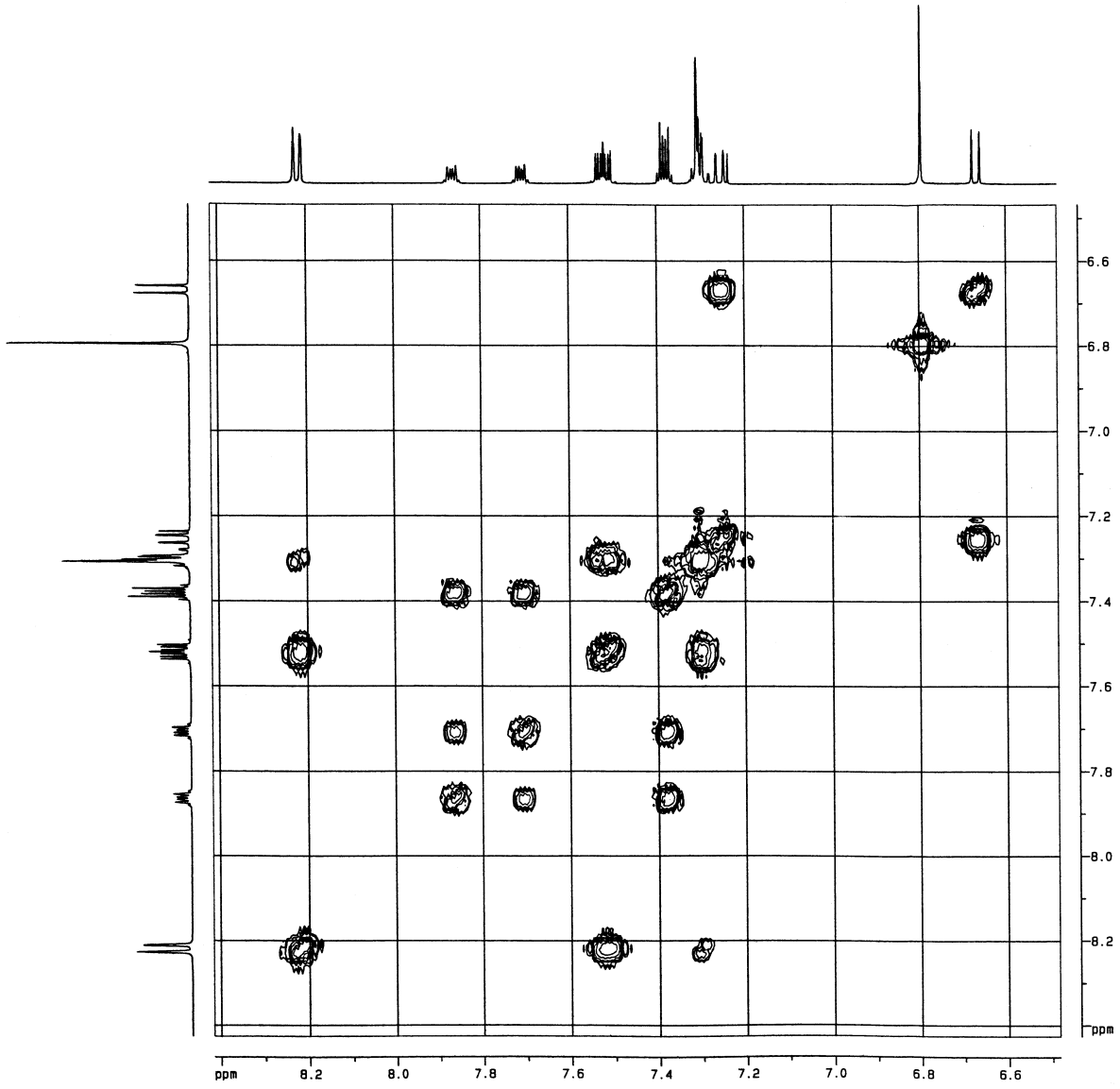


Abbildung 43: Korrelationsspektrum von **162** im Bereich δ = 6.50-8.40 ppm

3.4 5-(8-Methoxy-1-naphthyl)-5*H*-dibenzo[a,d]cycloheptenylium-tetrafluoroborat (11)

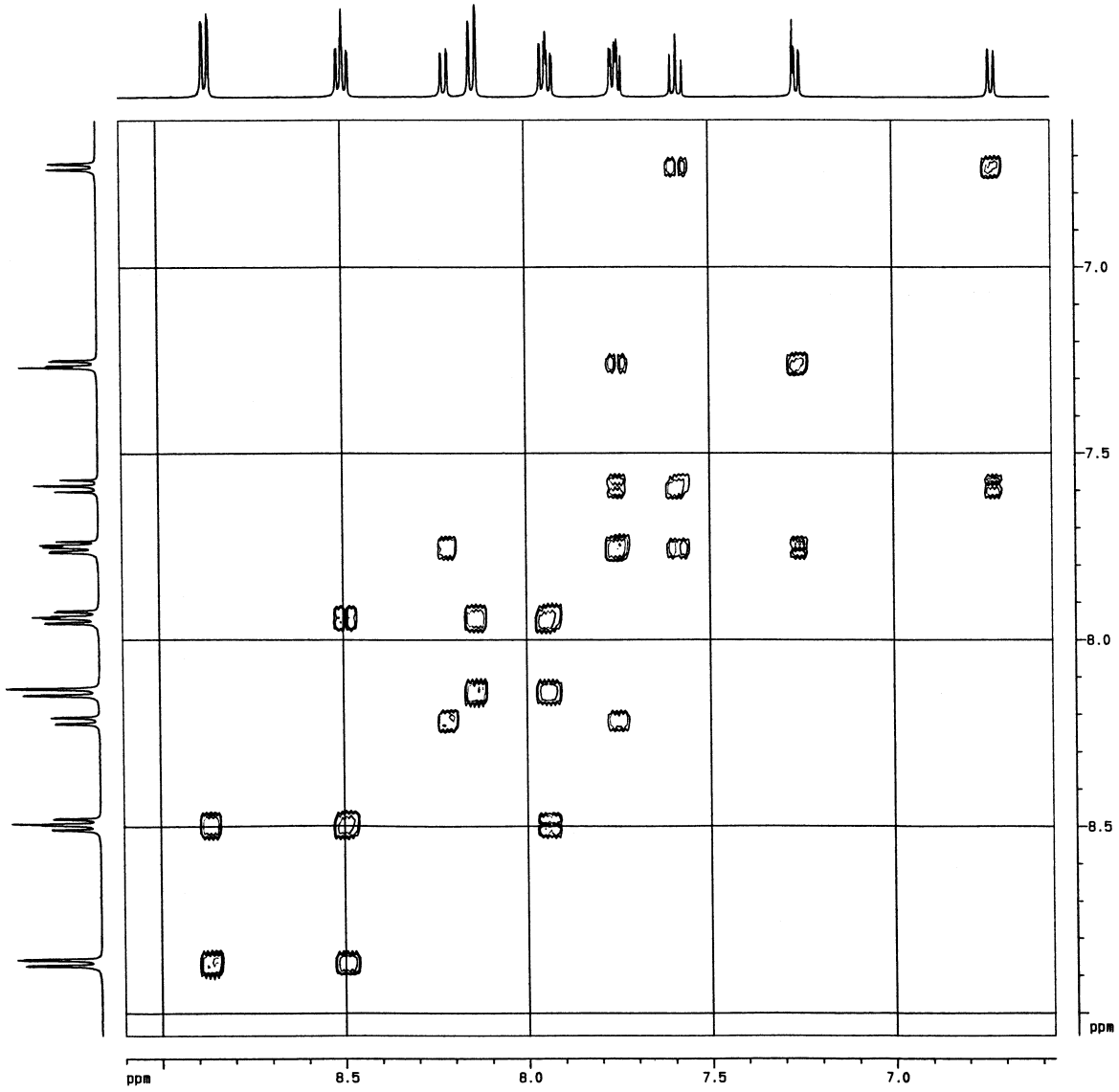


Abbildung 44: Korrelationsspektrum von **11** im Bereich δ = 6.60-9.10 ppm

3.5 Spiro[5*H*-dibenzo[a,d]cyclohepten-5,2'-[2*H*]-naphtho[1,8-bc]*N*,*N*-dimethyl-pyrrolidin]-tetrafluoroborat (14)

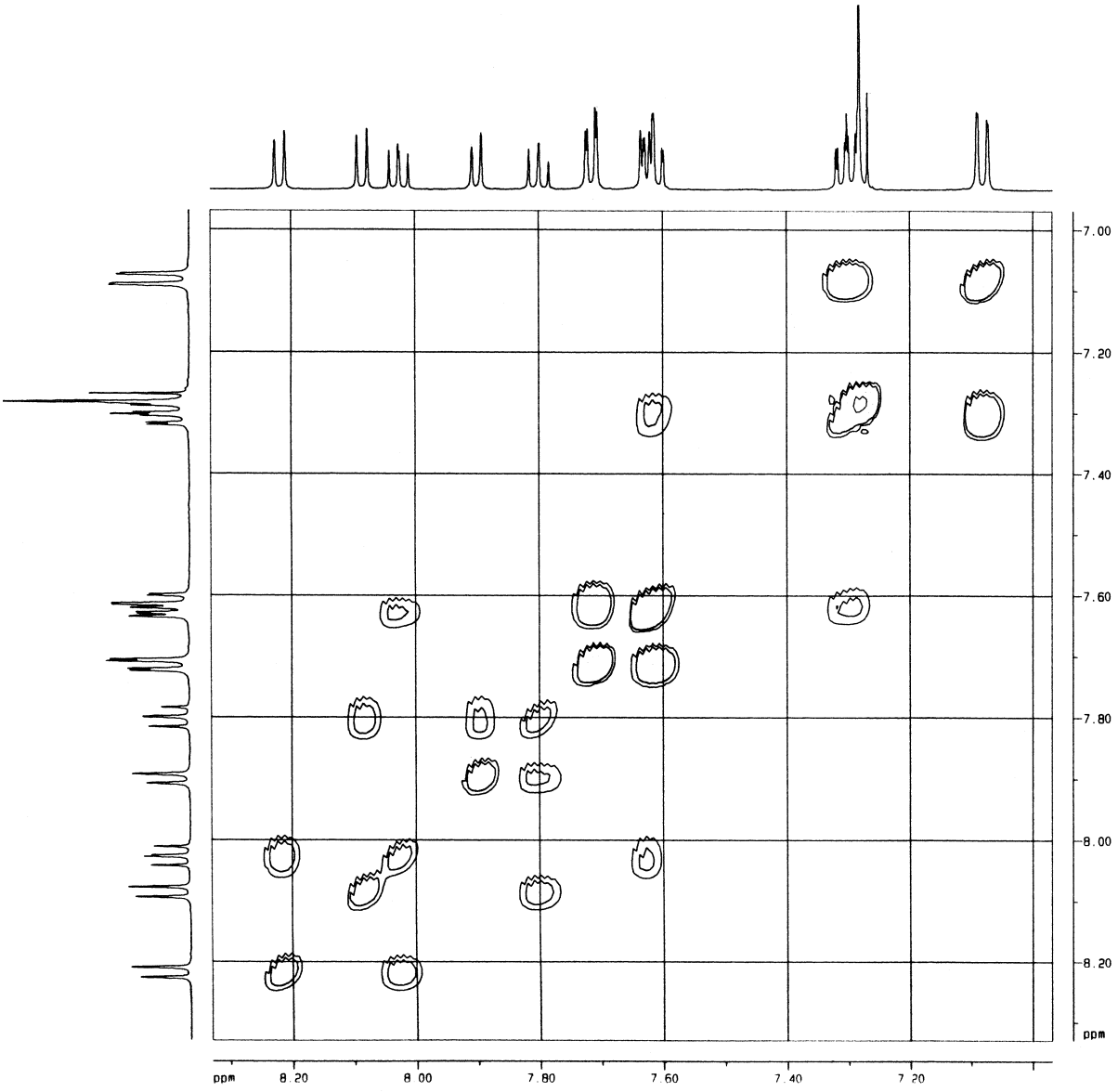


Abbildung 45: Korrelationsspektrum von **14** im Bereich δ = 7.00-8.30 ppm

3.6 Cyclische Ammoniumverbindung 182

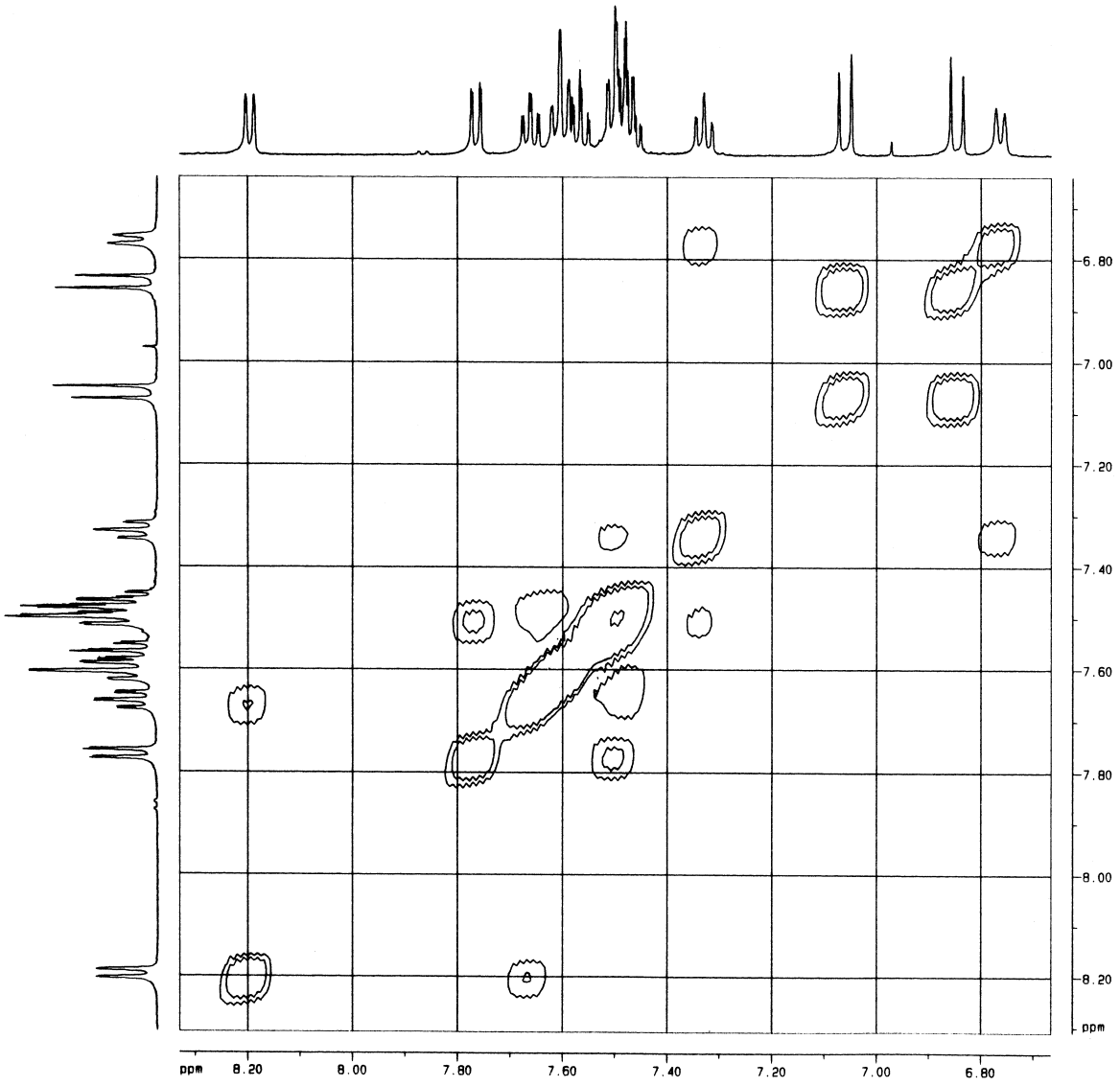


Abbildung 46: Korrelationsspektrum von **182** im Bereich δ = 6.70-8.30 ppm

3.7 [9-(10-(8-Iodnaphth-1-yl))-anthrylmethylen]-propandinitril (193)

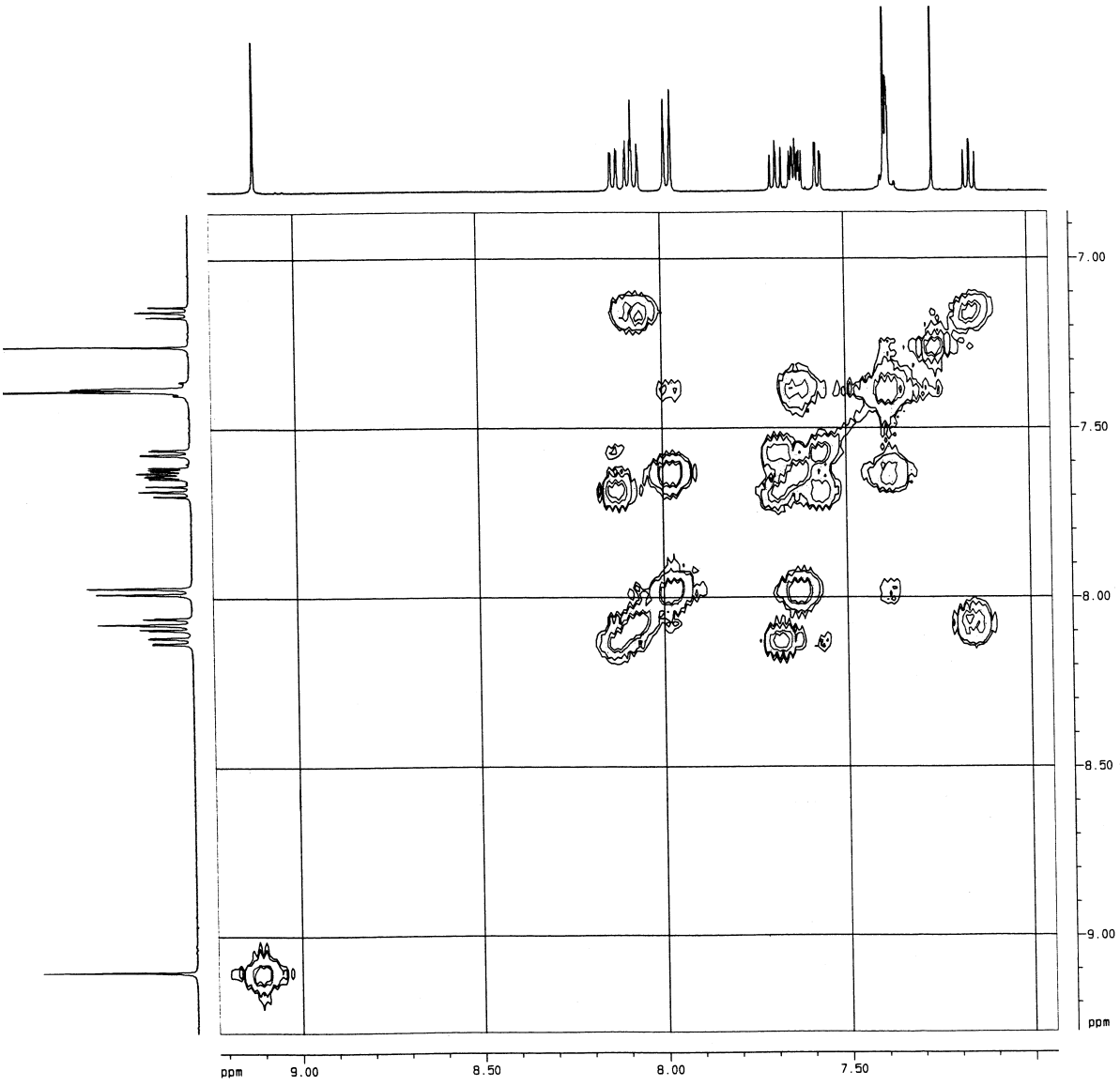


Abbildung 47: Korrelationsspektrum von **190** im Bereich δ = 7.00-9.20 ppm