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JM9702692

	Dye 32/EtOH	Dye 33/CH_3CN
Formula	$C_{29}H_{34}ClN_3O_3S_2$	$C_{26}H_{28}F_3IN_4OS_3$
Formula weight	572.18	692.61
Crystal System	Monoclinic	Triclinic
Space Group	$P2_1/c$	P1
Z	4	2
Calculated density	1.371Mg/m^3	1.582Mg/m^3
Cell dimensions		
a	17.439(3)Å	11.243(1)Å
b	7.164(1)Å	15.375(2)Å
c	23.535(4)Å	8.744(1)Å
α	90°	91.70(1)°
β	109.44(1)°	105.27(1)°
γ	90°	93.55(1)°
V	2772(2)Å^3	1453.7(3)Å^3
Radiation	Cu$K\alpha$	Cu$K\alpha$
No. of observed reflections	1824	4033
No. of unobserved weak reflections	3509	454
Data collection method	2θ-ω scan	2θ-ω scan
Structure determination	Direct method	Direct method
Refinement procedure	Full-matrix LS	Full-matrix LS
Final R	0.183	0.051
Rw	0.272	0.070
Maximum peak height in the final D-Fourier map	1.0e$^-$/Å^3	0.68e$^-$/Å^3

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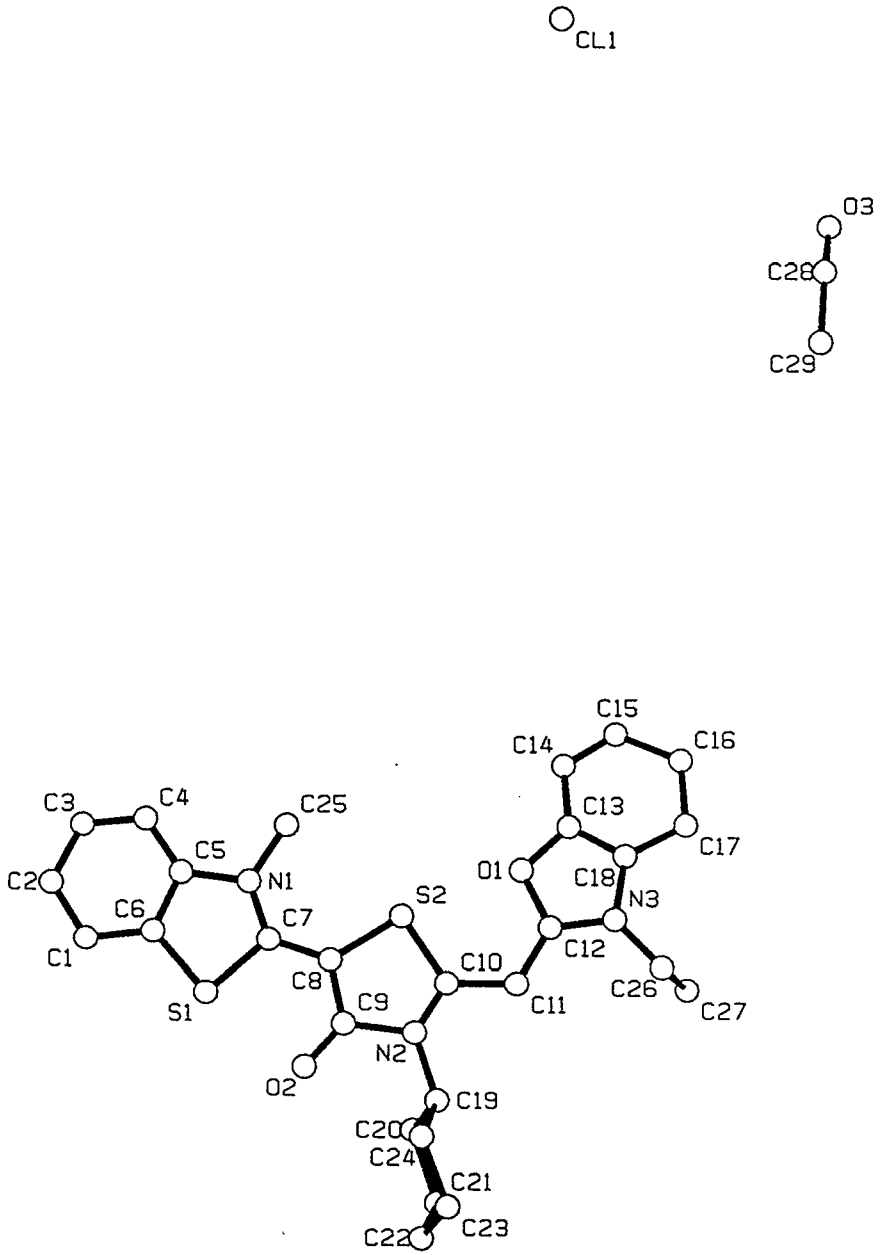
Supporting information for Rhodacyanine Dye 32

RHODACYANIN-DYE-32



Positional parameters and B(eq) for Positional Parameters for Rhodacyanine Dye 32

atom	x	y	z	B(eq)
Cl(1)	0.6421(4)	0.051(2)	0.1197(3)	8.6(5)
S(1)	1.1463(4)	0.221(1)	1.1121(3)	4.6(3)
S(2)	0.8919(3)	0.234(1)	0.9883(3)	5.3(4)
O(1)	0.736(1)	0.255(3)	0.9137(8)	4.7(8)
O(2)	1.025(1)	0.185(3)	1.1533(8)	6(1)
N(1)	1.084(1)	0.264(3)	0.998(1)	3.7(9)
N(2)	0.884(1)	0.184(4)	1.092(1)	5(1)
N(3)	0.623(1)	0.153(4)	0.932(1)	5(1)
C(1)	1.296(1)	0.263(5)	1.096(1)	6(1)
C(2)	1.337(1)	0.298(4)	1.054(2)	5(1)
C(3)	1.295(2)	0.350(6)	0.993(1)	7(2)
C(4)	1.213(2)	0.308(5)	0.970(1)	5(1)
C(5)	1.170(2)	0.292(5)	1.009(1)	6(2)
C(6)	1.210(2)	0.255(3)	1.070(1)	4(1)
C(7)	1.062(1)	0.230(3)	1.046(1)	2.7(9)
C(8)	0.985(1)	0.224(4)	1.048(1)	4(1)
C(9)	0.972(1)	0.202(4)	1.103(1)	4(1)
C(10)	0.839(1)	0.206(4)	1.038(1)	4(1)
C(11)	0.752(1)	0.163(5)	1.019(1)	6(1)
C(12)	0.705(2)	0.187(6)	0.958(1)	8(2)
C(13)	0.672(1)	0.270(5)	0.860(1)	5(1)
C(14)	0.673(2)	0.337(5)	0.805(1)	6(1)
C(15)	0.603(2)	0.343(4)	0.761(1)	6(2)
C(16)	0.524(2)	0.263(8)	0.767(1)	11(3)
C(17)	0.524(2)	0.20(1)	0.826(2)	16(4)
C(18)	0.603(1)	0.220(7)	0.872(1)	10(2)
C(19)	0.860(1)	0.151(6)	1.148(1)	6(1)
C(20)	0.889(2)	0.336(6)	1.188(2)	7(2)
C(21)	0.862(2)	0.341(6)	1.250(1)	7(2)
C(22)	0.888(1)	0.129(6)	1.279(1)	6(1)
C(23)	0.857(2)	-0.022(7)	1.237(1)	8(2)
C(24)	0.885(2)	-0.02(1)	1.180(1)	13(3)
C(25)	1.032(1)	0.284(4)	0.936(1)	3(1)
C(26)	0.568(1)	0.105(3)	0.963(1)	3(1)
C(27)	0.528(1)	0.286(2)	0.980(1)	4(1)
O(3)	0.304(3)	0.185(8)	0.229(3)	19(2)
C(28)	0.319(4)	0.09(1)	0.276(4)	17(2)
C(29)	0.331(4)	0.04(1)	0.345(3)	16(2)

U values for Positional Parameters for Rhodacyanine Dye 32

ATOM	U11	U22	U33	U12	U13	U23
Cl(1)	0.047(4)	0.23(1)	0.056(4)	-0.029(6)	0.021(3)	0.009(6)
S(1)	0.034(3)	0.089(6)	0.057(4)	-0.004(4)	0.021(3)	-0.001(4)
S(2)	0.028(3)	0.132(8)	0.046(3)	0.005(4)	0.016(3)	0.009(5)
O(1)	0.05(1)	0.08(2)	0.06(1)	-0.02(1)	0.020(8)	0.02(1)
O(2)	0.05(1)	0.13(2)	0.05(1)	-0.01(1)	0.018(9)	-0.00(1)
N(1)	0.03(1)	0.05(2)	0.06(1)	-0.02(1)	0.02(1)	-0.03(1)
N(2)	0.015(9)	0.12(2)	0.05(1)	-0.00(1)	0.016(9)	-0.00(1)
N(3)	0.020(8)	0.10(2)	0.05(1)	0.02(1)	0.011(8)	-0.02(1)
C(1)	0.03(1)	0.12(3)	0.07(2)	0.02(2)	0.02(1)	0.03(2)
C(2)	0.03(1)	0.07(2)	0.10(2)	0.03(1)	0.04(1)	0.01(2)
C(3)	0.04(2)	0.14(3)	0.08(2)	0.02(2)	0.02(2)	-0.01(2)
C(4)	0.04(1)	0.09(3)	0.07(2)	-0.02(2)	0.03(1)	-0.02(2)
C(5)	0.05(2)	0.15(3)	0.05(1)	-0.01(2)	0.04(1)	-0.05(2)
C(6)	0.05(2)	0.03(2)	0.07(2)	0.02(1)	0.04(1)	-0.01(1)
C(7)	0.04(1)	0.01(1)	0.07(2)	-0.03(1)	0.05(1)	-0.02(1)
C(8)	0.015(9)	0.10(2)	0.03(1)	0.04(1)	0.010(9)	0.06(1)
C(9)	0.03(1)	0.08(2)	0.06(2)	-0.02(1)	0.03(1)	-0.03(2)
C(10)	0.02(1)	0.05(2)	0.08(2)	0.02(1)	0.03(1)	0.01(2)
C(11)	0.01(1)	0.14(3)	0.06(2)	-0.01(2)	0.02(1)	0.01(2)
C(12)	0.03(1)	0.22(5)	0.04(1)	0.04(2)	0.02(1)	-0.00(2)
C(13)	0.03(1)	0.12(3)	0.04(1)	-0.02(2)	0.00(1)	0.00(2)
C(14)	0.06(2)	0.10(3)	0.06(2)	0.01(2)	0.04(2)	0.02(2)
C(15)	0.12(3)	0.07(2)	0.04(1)	0.06(2)	0.03(2)	0.05(2)
C(16)	0.07(2)	0.27(6)	0.05(2)	0.01(3)	0.00(2)	0.06(3)
C(17)	0.07(2)	0.5(1)	0.05(2)	-0.05(4)	0.02(2)	0.09(4)
C(18)	0.01(1)	0.28(6)	0.07(2)	0.04(2)	-0.00(1)	0.01(3)
C(19)	0.03(1)	0.16(4)	0.02(1)	-0.02(2)	0.00(1)	0.00(2)
C(20)	0.04(2)	0.13(3)	0.12(3)	0.02(2)	0.04(2)	0.05(3)
C(21)	0.05(2)	0.16(4)	0.05(2)	-0.05(2)	0.03(1)	-0.01(2)
C(22)	0.04(1)	0.15(3)	0.04(1)	0.02(2)	0.02(1)	-0.02(2)
C(23)	0.06(2)	0.22(5)	0.04(2)	0.01(2)	0.03(2)	-0.02(3)
C(24)	0.08(2)	0.38(8)	0.04(2)	-0.08(4)	0.05(2)	-0.02(3)
C(25)	0.05(1)	0.05(2)	0.04(1)	-0.02(1)	0.02(1)	0.01(1)
C(26)	0.05(1)	-0.02(1)	0.09(2)	-0.03(1)	0.01(1)	0.02(1)
C(27)	0.06(1)	-0.026(8)	0.13(2)	0.05(1)	0.07(2)	0.05(1)
O(3)	0.24(2)					
C(28)	0.21(3)					
C(29)	0.21(3)					

Intramolecular Distances Involving the Nonhydrogen Atoms Rhodacyanine Dye 32

atom	atom	distance	atom	atom	distance
S1	C6	1.73(2)	C5	C6	1.40(4)
S1	C7	1.75(3)	C7	C8	1.37(3)
S2	C8	1.77(2)	C8	C9	1.39(3)
S2	C10	1.72(2)	C10	C11	1.47(3)
O1	C12	1.41(3)	C11	C12	1.41(3)
O1	C13	1.38(3)	C13	C14	1.39(4)
O2	C9	1.24(3)	C13	C18	1.36(4)
N1	C5	1.46(3)	C14	C15	1.32(4)
N1	C7	1.31(3)	C15	C16	1.55(5)
N1	C25	1.44(3)	C16	C17	1.45(4)
N2	C9	1.49(2)	C17	C18	1.45(4)
N2	C10	1.26(3)	C19	C20	1.60(5)
N2	C19	1.51(3)	C19	C24	1.45(7)
N3	C12	1.38(3)	C20	C21	1.68(4)
N3	C18	1.43(4)	C21	C22	1.67(5)
N3	C26	1.43(3)	C22	C23	1.44(5)
C1	C2	1.41(4)	C23	C24	1.58(3)
C1	C6	1.42(3)	C26	C27	1.58(3)
C2	C3	1.43(4)	O3	C28	1.24(8)
C3	C4	1.37(4)	C28	C29	1.60(9)
C4	C5	1.37(3)			

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Nonhydrogen Atoms Rhodacyanine Dye 32

atom	atom	atom	angle	atom	atom	atom	angle
C6	S1	C7	90(1)	S2	C8	C9	111(2)
C8	S2	C10	90(1)	C7	C8	C9	121(2)
C12	O1	C13	108(2)	O2	C9	N2	124(2)
C5	N1	C7	117(2)	O2	C9	C8	127(2)
C5	N1	C25	115(2)	N2	C9	C8	109(2)
C7	N1	C25	128(2)	S2	C10	N2	115(2)
C9	N2	C10	115(2)	S2	C10	C11	123(2)
C9	N2	C19	115(2)	N2	C10	C11	121(2)
C10	N2	C19	130(2)	C10	C11	C12	119(2)
C12	N3	C18	104(2)	O1	C12	N3	110(2)
C12	N3	C26	127(2)	O1	C12	C11	124(2)
C18	N3	C26	127(2)	N3	C12	C11	126(3)
C2	C1	C6	115(3)	O1	C13	C14	128(2)
C1	C2	C3	122(2)	O1	C13	C18	107(2)
C2	C3	C4	118(3)	C14	C13	C18	124(3)
C3	C4	C5	118(3)	C13	C14	C15	117(2)
N1	C5	C4	131(3)	C14	C15	C16	122(2)
N1	C5	C6	106(2)	C15	C16	C17	119(3)
C4	C5	C6	121(3)	C16	C17	C18	113(3)
S1	C6	C1	124(2)	N3	C18	C13	110(2)
S1	C6	C5	115(2)	N3	C18	C17	124(3)
C1	C6	C5	121(2)	C13	C18	C17	124(3)
S1	C7	N1	112(1)	N2	C19	C20	105(3)
S1	C7	C8	120(2)	N2	C19	C24	118(3)
N1	C7	C8	128(2)	C20	C19	C24	115(2)
S2	C8	C7	128(2)	C19	C20	C21	114(2)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Nonhydrogen Atoms (cont)

atom	atom	atom	angle	atom	atom	atom	angle
C20	C21	C22	102(3)				
C21	C22	C23	114(2)				
C22	C23	C24	115(3)				
C19	C24	C23	108(4)				
N3	C26	C27	111(2)				
O3	C28	C29	159(8)				

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

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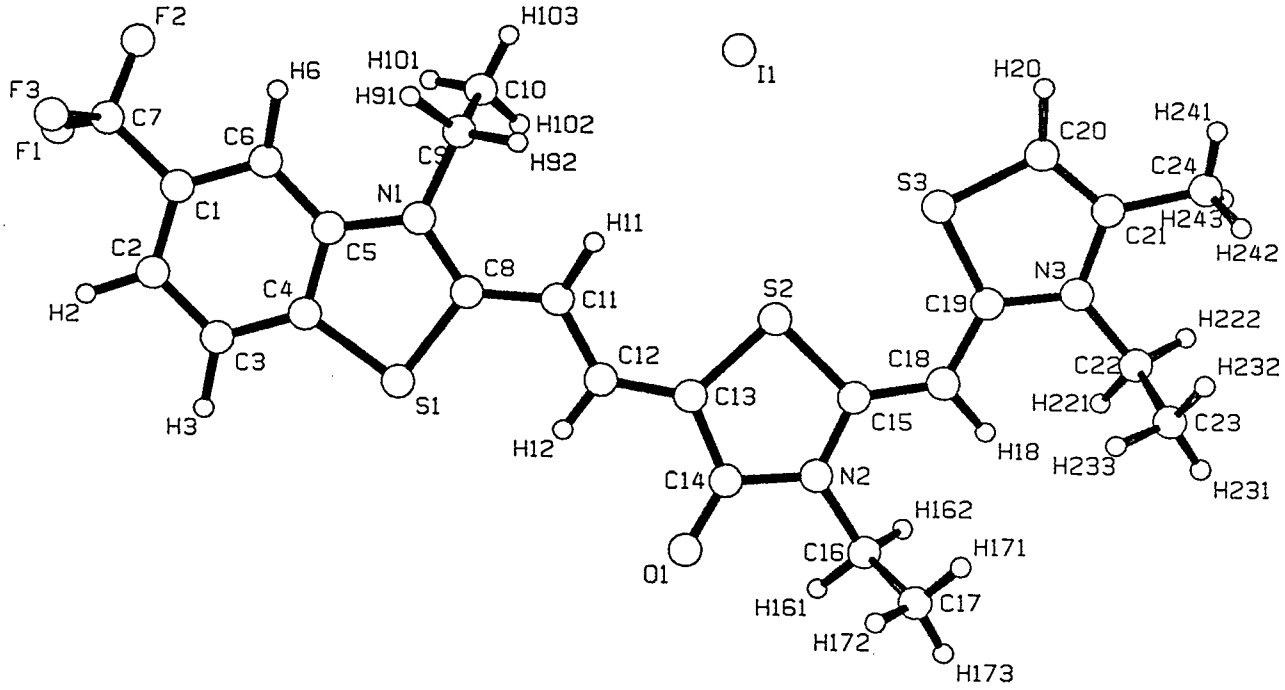
Supporting information for Rhodacyanine Dye 33

RHODACYANIN-DYE-33



Positional parameters and B(eq) forRhodacyanine Dye 33

atom	x	y	z	B(eq)
I1	0.13891(5)	0.29523(3)	0.43800(7)	5.22(2)
S1	-0.5075(1)	0.3458(1)	0.4042(2)	3.37(6)
S2	-0.0954(1)	0.13409(9)	0.6318(2)	2.85(5)
S3	0.1706(1)	0.0908(1)	0.6900(2)	3.21(6)
F1	-0.5845(7)	0.6926(4)	-0.0309(7)	10.0(3)
F2	-0.3990(6)	0.7064(4)	0.065(1)	10.6(4)
F3	-0.5144(9)	0.7533(3)	0.1927(8)	11.3(4)
O1	-0.4207(4)	0.0559(3)	0.6509(6)	4.3(2)
N1	-0.3117(4)	0.4327(3)	0.3781(6)	2.9(2)
N2	-0.2305(4)	0.0023(3)	0.6775(6)	2.8(2)
N3	0.1953(4)	-0.0658(3)	0.7687(5)	2.5(2)
C1	-0.5073(6)	0.6028(4)	0.1790(7)	3.3(2)
C2	-0.6219(6)	0.5672(4)	0.1879(8)	3.7(3)
C3	-0.6314(6)	0.4874(4)	0.2576(8)	3.6(2)
C4	-0.5236(6)	0.4459(4)	0.3147(7)	3.1(2)
C5	-0.4087(5)	0.4829(4)	0.3083(7)	2.7(2)
C6	-0.3978(6)	0.5625(4)	0.2399(7)	3.2(2)
C7	-0.5000(7)	0.6883(5)	0.1055(9)	4.3(3)
C8	-0.3469(5)	0.3557(4)	0.4307(7)	2.8(2)
C9	-0.1820(6)	0.4590(4)	0.3851(8)	3.6(2)
C10	-0.1510(7)	0.4310(5)	0.234(1)	5.2(3)
C11	-0.2702(6)	0.2925(4)	0.4964(7)	3.0(2)
C12	-0.3151(6)	0.2163(4)	0.5507(7)	3.0(2)
C13	-0.2520(5)	0.1459(4)	0.6080(7)	2.8(2)
C14	-0.3124(6)	0.0680(4)	0.6468(7)	2.9(2)
C15	-0.1111(5)	0.0258(3)	0.6810(6)	2.5(2)
C16	-0.2746(6)	-0.0869(4)	0.7023(7)	3.3(2)
C17	-0.2493(7)	-0.1066(5)	0.876(1)	4.7(3)
C18	-0.0181(5)	-0.0296(4)	0.7187(7)	2.8(2)
C19	0.1070(5)	-0.0085(4)	0.7277(6)	2.6(2)
C20	0.3163(6)	0.0523(4)	0.7320(8)	3.6(3)
C21	0.3142(6)	-0.0308(4)	0.7727(7)	3.1(2)
C22	0.1692(5)	-0.1567(4)	0.8035(7)	2.9(2)
C23	0.1659(7)	-0.1648(5)	0.9741(8)	4.5(3)
C24	0.4235(6)	-0.0840(5)	0.8236(9)	4.2(3)
H2	-0.7045	0.6000	0.1577	4.4
H3	-0.7212	0.4522	0.2616	4.4
H6	-0.3027	0.6054	0.2613	3.8
H11	-0.1675	0.3136	0.5394	3.5
H12	-0.4017	0.2128	0.5472	3.7
H18	-0.0376	-0.0969	0.7327	3.4
H20	0.3920	0.0994	0.7388	4.3
H91	-0.1712	0.5328	0.4236	4.4
H92	-0.1226	0.4345	0.5042	4.4
H101	-0.1995	0.4591	0.1465	6.1
H102	-0.1644	0.3697	0.2160	6.1
H103	-0.0650	0.4473	0.2433	6.1
H161	-0.3694	-0.0941	0.6335	4.0
H162	-0.2362	-0.1296	0.6309	4.0

Positional parameters and B(eq) for Rhodacyanine Dye 33

atom	x	y	z	B(eq)
H171	-0.1639	-0.1043	0.9231	5.7
H172	-0.2881	-0.0673	0.9286	5.7
H173	-0.2843	-0.1653	0.8835	5.7
H221	0.0835	-0.1811	0.7240	3.5
H222	0.2324	-0.1961	0.7647	3.5
H231	0.1375	-0.2258	0.9770	5.6
H232	0.2474	-0.1404	1.0535	5.6
H233	0.1048	-0.1219	1.0096	5.6
H241	0.4977	-0.0498	0.8308	5.0
H242	0.4263	-0.1064	0.9263	5.0
H243	0.4166	-0.1325	0.7504	5.0
C25	1.118(1)	0.3304(9)	0.951(2)	9.4(7)
C26	1.005(1)	0.3700(8)	0.892(1)	7.1(5)
N26	0.917(1)	0.404(1)	0.846(2)	11.5(7)

U values for Rhodacyanine Dye 33

ATOM	U11	U22	U33	U12	U13	U23
I1	0.0725(4)	0.0341(3)	0.0822(4)	-0.0037(2)	0.0065(3)	-0.0071(2)
S1	0.0465(9)	0.0365(8)	0.0467(9)	0.0031(7)	0.0142(7)	0.0105(7)
S2	0.0458(8)	0.0296(7)	0.0346(8)	0.0017(6)	0.0134(6)	0.0082(6)
S3	0.0494(9)	0.0331(8)	0.0416(8)	-0.0027(6)	0.0163(7)	0.0091(6)
F1	0.153(6)	0.096(4)	0.095(4)	-0.008(4)	-0.029(4)	0.052(4)
F2	0.120(5)	0.108(5)	0.213(8)	0.050(4)	0.094(5)	0.111(5)
F3	0.30(1)	0.039(3)	0.128(5)	0.025(4)	0.123(6)	0.014(3)
O1	0.048(3)	0.043(3)	0.079(3)	0.007(2)	0.026(2)	0.011(2)
N1	0.038(3)	0.031(3)	0.039(3)	0.005(2)	0.009(2)	0.004(2)
N2	0.040(3)	0.027(2)	0.040(3)	0.003(2)	0.012(2)	0.008(2)
N3	0.034(3)	0.033(3)	0.028(2)	-0.001(2)	0.009(2)	0.002(2)
C1	0.056(4)	0.032(3)	0.035(3)	0.009(3)	0.009(3)	0.005(3)
C2	0.054(4)	0.044(4)	0.042(4)	0.014(3)	0.008(3)	0.007(3)
C3	0.047(4)	0.045(4)	0.046(4)	0.010(3)	0.011(3)	0.004(3)
C4	0.048(4)	0.033(3)	0.035(3)	0.004(3)	0.009(3)	0.007(3)
C5	0.043(3)	0.028(3)	0.033(3)	0.006(2)	0.009(3)	0.001(2)
C6	0.048(4)	0.037(3)	0.035(3)	0.004(3)	0.010(3)	0.000(3)
C7	0.070(5)	0.042(4)	0.052(4)	0.017(3)	0.014(4)	0.012(3)
C8	0.044(3)	0.031(3)	0.030(3)	0.005(3)	0.010(3)	-0.000(2)
C9	0.040(3)	0.037(3)	0.057(4)	0.001(3)	0.007(3)	0.005(3)
C10	0.059(5)	0.067(5)	0.077(5)	0.008(4)	0.031(4)	0.010(4)
C11	0.047(4)	0.030(3)	0.035(3)	0.006(3)	0.009(3)	0.002(3)
C12	0.046(4)	0.036(3)	0.034(3)	0.009(3)	0.012(3)	0.002(3)
C13	0.042(3)	0.032(3)	0.032(3)	0.003(3)	0.011(3)	0.004(2)
C14	0.042(4)	0.035(3)	0.035(3)	0.006(3)	0.012(3)	0.005(3)
C15	0.041(3)	0.026(3)	0.029(3)	-0.002(2)	0.012(2)	0.005(2)
C16	0.048(4)	0.031(3)	0.047(4)	0.001(3)	0.016(3)	0.006(3)
C17	0.064(5)	0.063(5)	0.060(5)	0.006(4)	0.027(4)	0.025(4)
C18	0.040(3)	0.031(3)	0.037(3)	0.002(2)	0.013(3)	0.007(2)
C19	0.040(3)	0.032(3)	0.026(3)	0.001(2)	0.010(2)	0.003(2)
C20	0.046(4)	0.046(4)	0.048(4)	-0.008(3)	0.020(3)	0.003(3)
C21	0.041(3)	0.044(4)	0.033(3)	0.000(3)	0.012(3)	0.002(3)
C22	0.045(3)	0.031(3)	0.033(3)	0.002(3)	0.012(3)	0.005(2)
C23	0.082(5)	0.051(4)	0.041(4)	0.003(4)	0.022(4)	0.014(3)
C24	0.038(4)	0.059(4)	0.062(4)	0.004(3)	0.012(3)	0.001(4)

U values for Rhodacyanine Dye 33

ATOM	U11	U22	U33	U12	U13	U23
H2	0.0559					
H3	0.0560					
H6	0.0482					
H11	0.0447					
H12	0.0469					
H18	0.0432					
H20	0.0549					
H91	0.0553					
H92	0.0553					
H101	0.0768					
H102	0.0768					
H103	0.0768					
H161	0.0500					
H162	0.0500					
H171	0.0718					
H172	0.0718					
H173	0.0718					
H221	0.0442					
H222	0.0442					
H231	0.0707					
H232	0.0707					
H233	0.0707					
H241	0.0638					
H242	0.0638					
H243	0.0638					
C25	0.091(8)	0.13(1)	0.14(1)	0.023(7)	0.022(8)	0.029(8)
C26	0.081(7)	0.101(8)	0.088(7)	-0.019(6)	0.026(6)	0.003(6)
N26	0.086(7)	0.19(1)	0.15(1)	0.022(8)	0.024(7)	0.02(1)

Intramolecular Distances Involving the Nonhydrogen Atoms Rhodacyanine Dye 33

atom	atom	distance	atom	atom	distance
S1	C4	1.745(6)	N3	C22	1.467(7)
S1	C8	1.755(6)	C1	C2	1.390(9)
S2	C13	1.739(6)	C1	C6	1.398(9)
S2	C15	1.742(5)	C1	C7	1.487(9)
S3	C19	1.723(6)	C2	C3	1.397(9)
S3	C20	1.728(7)	C3	C4	1.387(9)
F1	F2	2.028(9)	C4	C5	1.395(8)
F1	F3	2.075(9)	C5	C6	1.390(8)
F1	C7	1.322(9)	C8	C11	1.376(8)
F2	F3	2.070(9)	C9	C10	1.51(1)
F2	C7	1.293(9)	C11	C12	1.392(8)
F3	C7	1.283(9)	C12	C13	1.365(8)
O1	C14	1.230(7)	C13	C14	1.435(8)
N1	C5	1.392(7)	C15	C18	1.368(8)
N1	C8	1.357(7)	C16	C17	1.516(9)
N1	C9	1.474(8)	C18	C19	1.405(8)
N2	C14	1.394(7)	C20	C21	1.338(9)
N2	C15	1.360(7)	C21	C24	1.495(9)
N2	C16	1.471(7)	C22	C23	1.511(8)
N3	C19	1.353(7)	C25	C26	1.43(2)
N3	C21	1.401(7)	C26	N26	1.13(1)

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Distances Involving the Hydrogen Atoms Rhodacyanine Dye 33

atom	atom	distance	atom	atom	distance
N1	H91	2.087	C16	H162	1.077
N2	H161	2.036	C16	H171	2.038
N2	H162	2.049	C16	H172	2.039
N3	H221	2.074	C16	H173	2.040
N3	H222	2.072	C17	H171	0.937
C2	H2	1.059	C17	H172	0.941
C3	H2	2.079	C17	H173	0.972
C3	H3	1.125	C18	H18	1.063
C6	H6	1.189	C19	H18	2.064
C9	H91	1.165	C20	H20	1.070
C9	H92	1.166	C21	H241	2.032
C9	H101	2.044	C21	H242	2.030
C9	H102	2.043	C21	H243	2.031
C9	H103	2.044	C22	H221	1.068
C10	H101	0.947	C22	H222	1.075
C10	H102	0.947	C22	H231	1.972
C10	H103	0.965	C23	H231	0.976
C11	H11	1.139	C23	H232	1.035
C11	H12	2.010	C23	H233	1.077
C12	H12	0.965	C24	H241	0.945
C13	H12	1.987	C24	H242	0.964
C16	H161	1.075	C24	H243	0.954

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Nonhydrogen Atoms Rhodacyanine Dye 33

atom	atom	atom	angle	atom	atom	atom	angle
C4	S1	C8	91.2(3)	S1	C4	C3	127.7(5)
C13	S2	C15	91.6(3)	S1	C4	C5	110.4(4)
C19	S3	C20	91.4(3)	C3	C4	C5	121.9(5)
F2	F1	F3	60.6(4)	N1	C5	C4	112.9(5)
F2	F1	C7	38.6(4)	N1	C5	C6	125.9(5)
F3	F1	C7	36.6(4)	C4	C5	C6	121.2(5)
F1	F2	F3	60.8(4)	C1	C6	C5	116.5(6)
F1	F2	C7	39.7(4)	F1	C7	F2	101.7(7)
F3	F2	C7	36.4(4)	F1	C7	F3	105.6(7)
F1	F3	F2	58.6(3)	F1	C7	C1	112.9(6)
F1	F3	C7	37.9(4)	F2	C7	F3	106.9(8)
F2	F3	C7	36.7(5)	F2	C7	C1	115.0(6)
C5	N1	C8	114.7(5)	F3	C7	C1	113.6(6)
C5	N1	C9	122.4(5)	S1	C8	N1	110.7(4)
C8	N1	C9	122.8(5)	S1	C8	C11	123.1(5)
C14	N2	C15	116.2(5)	N1	C8	C11	126.2(5)
C14	N2	C16	120.3(5)	N1	C9	C10	111.1(6)
C15	N2	C16	123.5(5)	C8	C11	C12	121.8(6)
C19	N3	C21	113.9(5)	C11	C12	C13	128.2(6)
C19	N3	C22	123.3(5)	S2	C13	C12	126.6(5)
C21	N3	C22	122.9(5)	S2	C13	C14	111.0(4)
C2	C1	C6	122.7(6)	C12	C13	C14	122.3(5)
C2	C1	C7	118.9(6)	O1	C14	N2	122.0(5)
C6	C1	C7	118.4(6)	O1	C14	C13	127.8(5)
C1	C2	C3	120.2(6)	N2	C14	C13	110.1(5)
C2	C3	C4	117.5(6)	S2	C15	N2	110.7(4)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Nonhydrogen Atoms (cont)

atom	atom	atom	angle	atom	atom	atom	angle
S2	C15	C18	125.9(4)				
N2	C15	C18	123.4(5)				
N2	C16	C17	112.8(5)				
C15	C18	C19	126.0(5)				
S3	C19	N3	110.4(4)				
S3	C19	C18	126.3(4)				
N3	C19	C18	123.3(5)				
S3	C20	C21	111.5(5)				
N3	C21	C20	112.9(5)				
N3	C21	C24	120.8(5)				
C20	C21	C24	126.3(6)				
N3	C22	C23	111.5(5)				
C25	C26	N26	178(1)				

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Hydrogen Atoms Rhodacyanine Dye 33

atom	atom	atom	angle	atom	atom	atom	angle
C5	N1	H91	97.14	N1	C9	H91	103.94
C8	N1	H91	143.23	N1	C9	H92	106.27
C9	N1	H91	32.79	N1	C9	H101	98.02
C14	N2	H161	92.95	N1	C9	H102	96.62
C14	N2	H162	137.30	N1	C9	H103	137.59
C15	N2	H161	147.37	C10	C9	H91	118.95
C15	N2	H162	100.58	C10	C9	H92	117.75
C16	N2	H161	30.63	C10	C9	H101	25.75
C16	N2	H162	30.31	C10	C9	H102	25.76
H161	N2	H162	47.07	C10	C9	H103	26.48
C19	N3	H221	99.04	H91	C9	H92	96.93
C19	N3	H222	145.19	H91	C9	H101	103.49
C21	N3	H221	142.41	H91	C9	H102	144.71
C21	N3	H222	97.07	H91	C9	H103	104.26
C22	N3	H221	29.18	H92	C9	H101	143.32
C22	N3	H222	29.52	H92	C9	H102	104.51
H221	N3	H222	46.92	H92	C9	H103	101.04
C1	C2	H2	124.43	H101	C9	H102	44.62
C3	C2	H2	114.97	H101	C9	H103	44.61
C2	C3	H2	27.50	H102	C9	H103	44.62
C2	C3	H3	124.43	C9	C10	H101	110.34
C4	C3	H2	144.78	C9	C10	H102	110.30
C4	C3	H3	117.83	C9	C10	H103	109.21
H2	C3	H3	97.39	H101	C10	H102	109.99
C1	C6	H6	118.05	H101	C10	H103	108.47
C5	C6	H6	123.29	H102	C10	H103	108.47

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Hydrogen Atoms (cont)

atom	atom	atom	angle	atom	atom	atom	angle
C8	C11	H11	116.25	H162	C16	H173	100.72
C8	C11	H12	96.30	H171	C16	H172	44.74
C12	C11	H11	119.32	H171	C16	H173	44.73
C12	C11	H12	25.60	H172	C16	H173	44.72
H11	C11	H12	141.85	C16	C17	H171	110.09
C11	C12	H12	115.83	C16	C17	H172	109.94
C13	C12	H12	116.00	C16	C17	H173	108.12
S2	C13	H12	152.44	H171	C17	H172	111.46
C12	C13	H12	25.87	H171	C17	H173	108.74
C14	C13	H12	96.51	H172	C17	H173	108.41
N2	C16	H161	105.16	C15	C18	H18	120.92
N2	C16	H162	106.09	C19	C18	H18	112.80
N2	C16	H171	100.14	S3	C19	H18	154.25
N2	C16	H172	98.31	N3	C19	H18	95.12
N2	C16	H173	139.73	C18	C19	H18	28.34
C17	C16	H161	116.68	S3	C20	H20	116.71
C17	C16	H162	115.85	C21	C20	H20	131.06
C17	C16	H171	25.58	N3	C21	H241	146.30
C17	C16	H172	25.71	N3	C21	H242	103.34
C17	C16	H173	26.93	N3	C21	H243	107.30
H161	C16	H162	98.63	C20	C21	H241	100.58
H161	C16	H171	142.06	C20	C21	H242	136.93
H161	C16	H172	103.17	C20	C21	H243	134.05
H161	C16	H173	99.79	C24	C21	H241	25.77
H162	C16	H171	100.97	C24	C21	H242	26.60
H162	C16	H172	141.54	C24	C21	H243	26.14

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Hydrogen Atoms (cont)

atom	atom	atom	angle	atom	atom	atom	angle
H241	C21	H242	44.91				
H241	C21	H243	44.89				
H242	C21	H243	44.91				
N3	C22	H221	108.74				
N3	C22	H222	108.20				
N3	C22	H231	140.06				
C23	C22	H221	110.98				
C23	C22	H222	115.91				
C23	C22	H231	28.83				
H221	C22	H222	100.79				
H221	C22	H231	91.92				
H222	C22	H231	100.58				
C22	C23	H231	102.88				
C22	C23	H232	112.43				
C22	C23	H233	113.48				
H231	C23	H232	119.39				
H231	C23	H233	111.17				
H232	C23	H233	97.98				
C21	C24	H241	110.77				
C21	C24	H242	109.43				
C21	C24	H243	110.18				
H241	C24	H242	108.75				
H241	C24	H243	109.62				
H242	C24	H243	108.02				

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.