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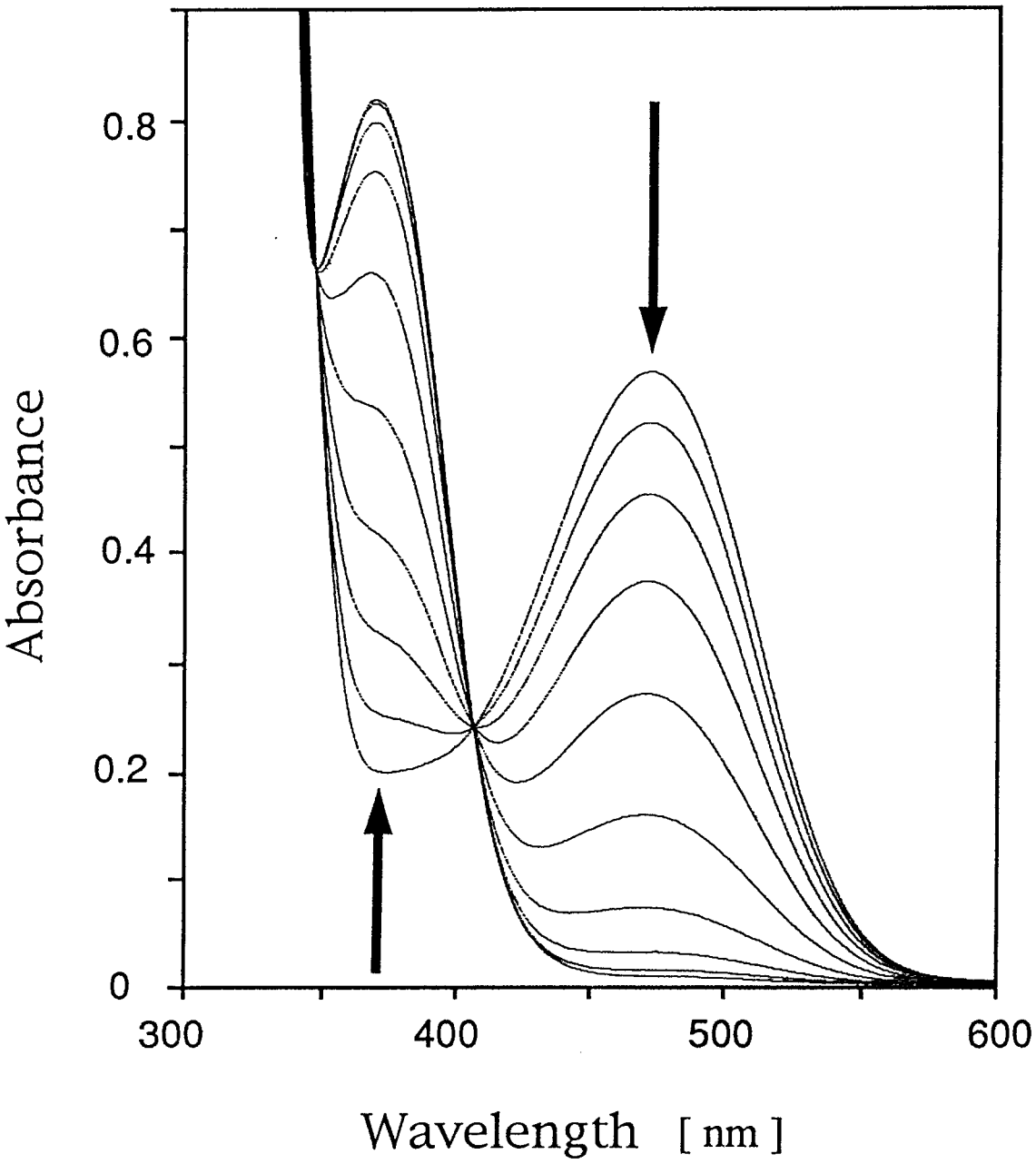
SUPPLEMENTARY MATERIAL

JA9523045

J3107-1

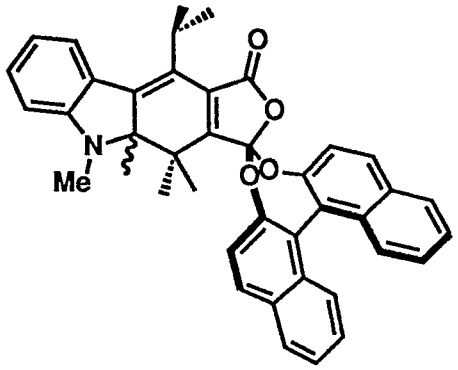


Absorption spectral change of UV-pss of 2(1.40×10^{-4} mol dm^{-3} in toluene. Cell length: 1 cm) to 2E.

Irradiation: 497-nm light from 500W Xe lamp.
Light intensity: 5.4×10^{-1} mW cm^{-2}
Irradiation time/min: 0, 0.5, 1.2, 3.7, 6, 9.3, 13.3, 20, 35, 70 (pss)

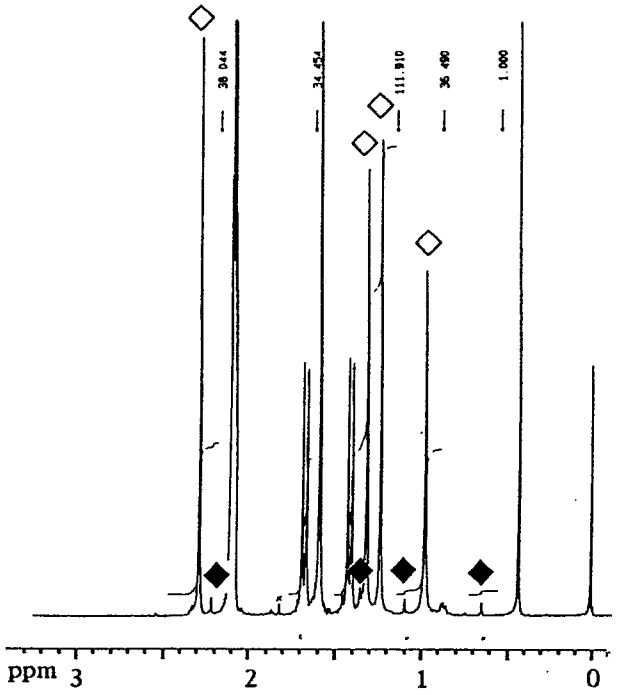
^{1}H-NMR Spectral Changes during Photoreaction of 1 in Toluene.

J3107-2



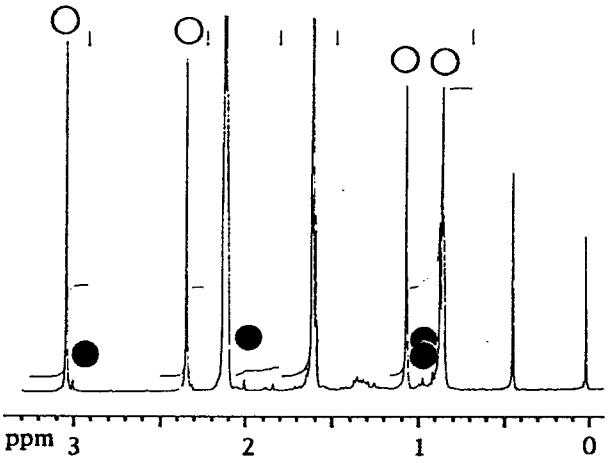
1. Before irradiation

C (◇) : C (◆) = 98 : 2



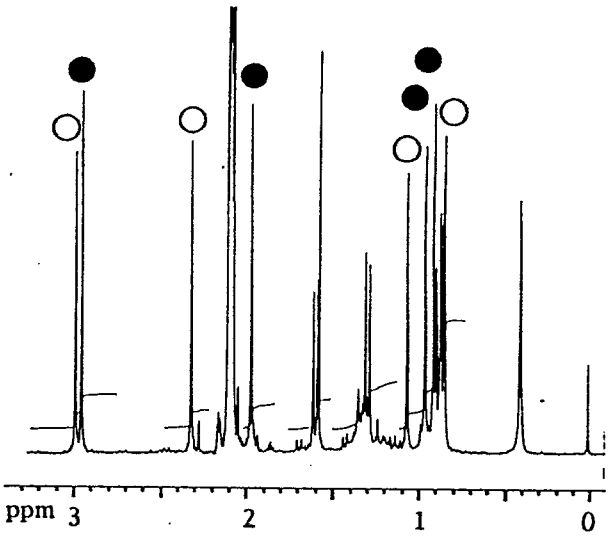
2. After Vis irradiation

E (○) : E (●) = 96 : 4

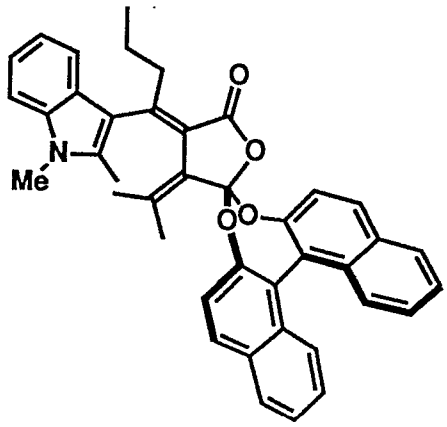


3. Thermal equilibrium

E (○) : E (●) = 48 : 52

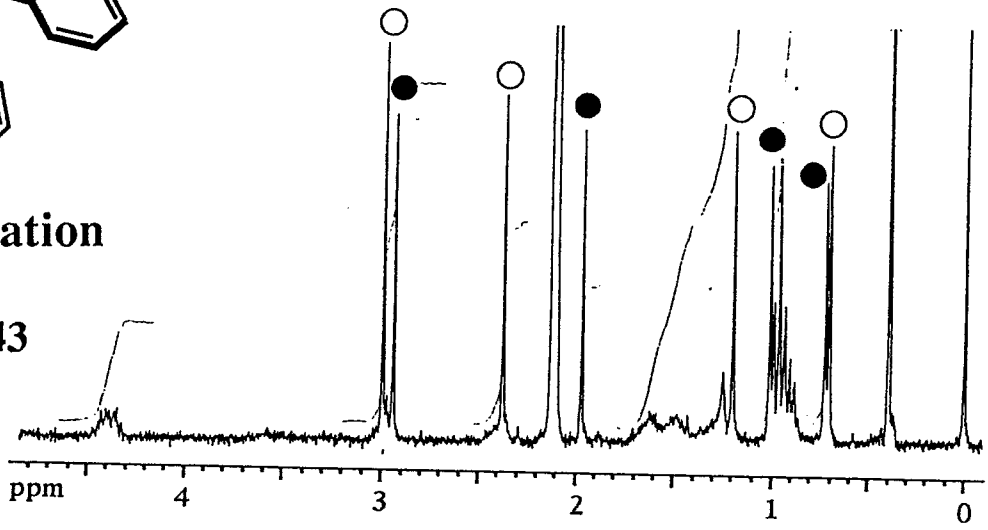


J 3107-3



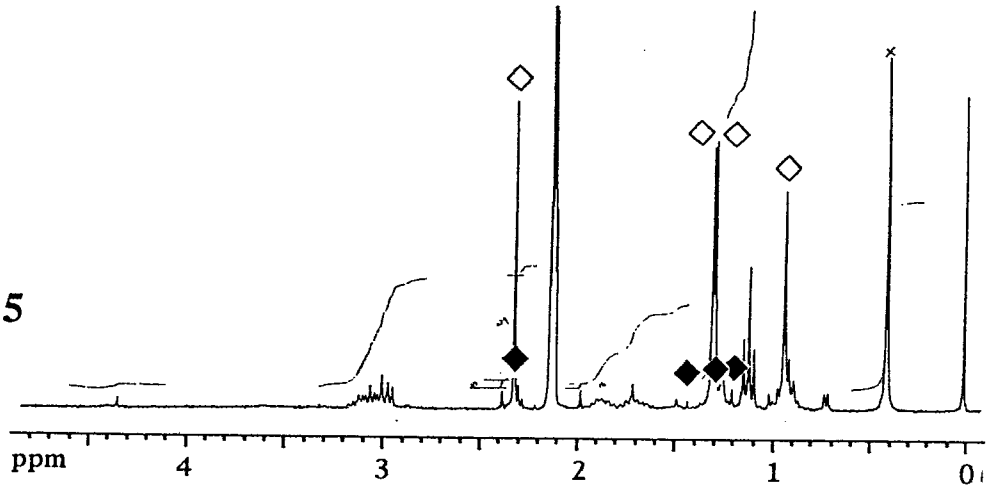
1. Before UV irradiation

E (○) : E (●) = 57 : 43



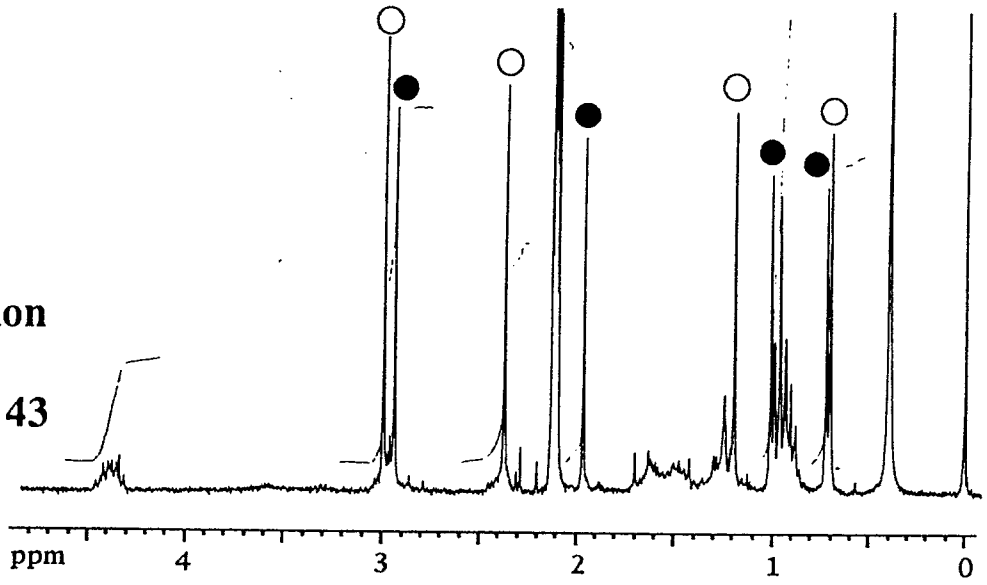
2. PSS(366)

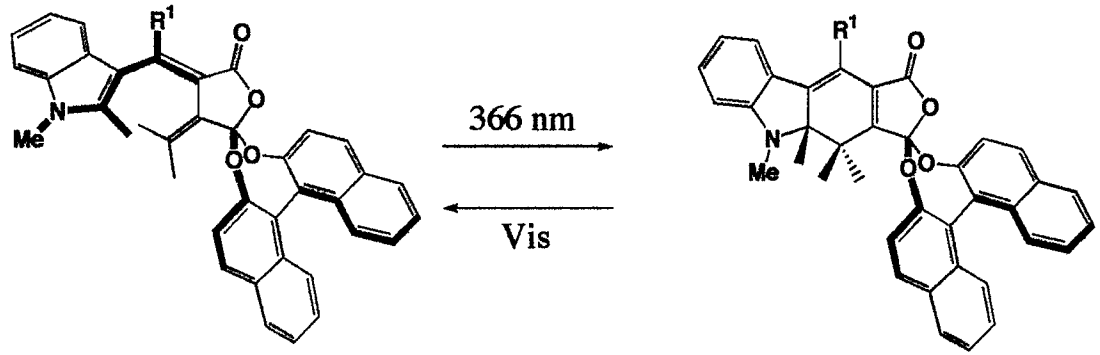
C (◇) : C (◆) = 95 : 5



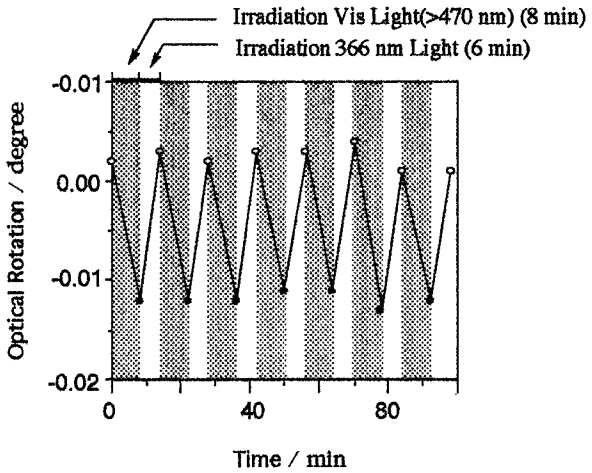
3. After Vis irradiation

E (○) : E (●) = 57 : 43

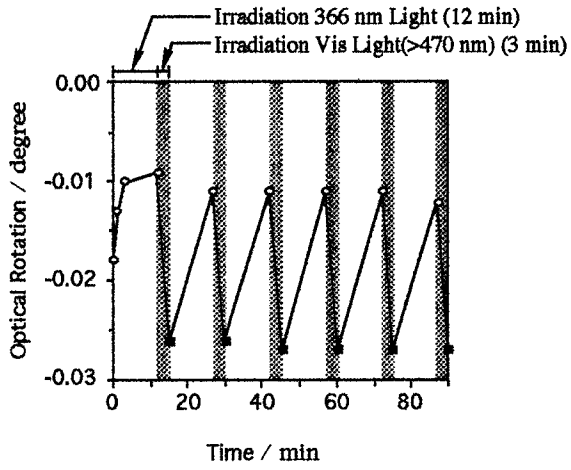




1 : $R^1 = i$-Pr



2 : $R^1 = n$-Pr



Change of optical rotation of PMMA films doped with binaphthyl-condensed indolylfulgides.

Y. Yokoyama et al., Diastereoselective Photochromism of ....

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Table 2. Anisotropic Displacement Parameters ($Å^2$) of Non-Hydrogen Atoms

atom	U11	U22	U33	U23	U13	U12
O1	0.0636(12)	0.0690(13)	0.0483(10)	-0.0012(9)	0.0050(9)	-0.0091(11)
O24	0.0604(13)	0.090(2)	0.0664(13)	-0.0014(13)	0.0019(10)	-0.0176(13)
O25	0.087(2)	0.0493(11)	0.0584(11)	-0.0007(9)	0.0288(11)	-0.0008(11)
O26	0.0691(13)	0.0519(11)	0.0501(10)	-0.0026(9)	0.0112(9)	-0.0007(10)
O85	0.174(5)	0.312(11)	0.202(6)	-0.096(7)	0.078(4)	0.059(6)
O89	0.140(4)	0.143(4)	0.211(5)	-0.005(4)	0.073(4)	-0.049(3)
N8	0.0595(15)	0.077(2)	0.069(2)	0.0063(14)	-0.0086(12)	-0.0085(14)
C2	0.0532(15)	0.065(2)	0.0504(14)	-0.0026(13)	0.0086(11)	-0.0038(14)
C3	0.0501(14)	0.061(2)	0.0501(14)	-0.0033(13)	0.0080(11)	-0.0026(13)
C4	0.0522(14)	0.057(2)	0.0496(13)	-0.0023(12)	0.0090(11)	-0.0016(12)
C5	0.060(2)	0.056(2)	0.0508(14)	-0.0040(12)	0.0141(12)	-0.0038(13)
C6	0.0524(14)	0.065(2)	0.0466(13)	0.0004(13)	0.0102(11)	-0.0033(13)
C7	0.0480(14)	0.0530(14)	0.0546(14)	-0.0038(12)	0.0074(11)	-0.0068(12)
C9	0.0509(15)	0.058(2)	0.062(2)	-0.0004(14)	0.0060(12)	-0.0037(13)
C10	0.0545(14)	0.0543(15)	0.0505(13)	-0.0011(12)	0.0092(11)	-0.0011(13)
C11	0.069(2)	0.056(2)	0.0526(15)	-0.0015(13)	0.0048(13)	0.0080(15)
C12	0.085(2)	0.068(2)	0.055(2)	0.0028(14)	0.014(2)	0.005(2)
C13	0.118(3)	0.078(2)	0.056(2)	0.009(2)	0.011(2)	0.021(3)
C14	0.117(4)	0.078(2)	0.060(2)	0.004(2)	-0.014(2)	0.018(2)
C15	0.104(3)	0.080(3)	0.072(2)	0.002(2)	-0.024(2)	0.005(2)
C16	0.073(2)	0.060(2)	0.061(2)	0.0008(14)	-0.0095(14)	0.003(2)
C17	0.059(2)	0.144(5)	0.122(4)	0.040(4)	-0.014(2)	-0.018(3)
C18	0.074(2)	0.064(2)	0.095(3)	0.002(2)	0.028(2)	0.010(2)
C19	0.063(2)	0.119(3)	0.059(2)	0.021(2)	0.0115(15)	-0.016(2)
C20	0.094(3)	0.101(4)	0.122(4)	0.033(3)	-0.005(3)	-0.039(3)
C21	0.074(2)	0.165(6)	0.085(3)	0.009(3)	0.030(2)	0.018(3)
C22	0.058(2)	0.074(2)	0.065(2)	-0.005(2)	0.0112(14)	-0.016(2)
C23	0.067(2)	0.059(2)	0.059(2)	-0.0075(14)	0.0057(14)	-0.0026(15)
C27	0.0505(13)	0.0484(13)	0.0517(13)	0.0000(12)	0.0089(10)	0.0016(12)
C28	0.064(2)	0.0495(15)	0.0531(14)	-0.0029(12)	0.0135(12)	0.0022(13)
C29	0.081(2)	0.059(2)	0.056(2)	0.0000(14)	0.0054(15)	0.016(2)
C30	0.067(2)	0.067(2)	0.076(2)	-0.006(2)	0.008(2)	0.019(2)
C31	0.054(2)	0.066(2)	0.075(2)	-0.010(2)	0.0110(14)	0.0017(15)
C32	0.054(2)	0.089(3)	0.102(3)	-0.008(2)	0.018(2)	0.003(2)
C33	0.062(2)	0.109(4)	0.125(4)	0.001(3)	0.033(2)	-0.023(2)
C34	0.073(2)	0.085(3)	0.118(3)	0.017(3)	0.030(2)	-0.015(2)
C35	0.059(2)	0.065(2)	0.095(3)	0.012(2)	0.017(2)	-0.004(2)
C36	0.0519(15)	0.056(2)	0.064(2)	-0.0026(13)	0.0121(12)	-0.0015(13)
C37	0.0481(13)	0.0457(13)	0.0539(14)	0.0020(11)	0.0109(11)	-0.0018(11)
C38	0.0536(14)	0.0499(14)	0.0536(14)	-0.0024(12)	0.0099(12)	-0.0018(12)
C39	0.055(2)	0.057(2)	0.069(2)	-0.0042(15)	0.0208(14)	0.0035(14)
C40	0.0486(15)	0.055(2)	0.080(2)	0.0023(15)	0.0135(14)	0.0066(13)
C41	0.0481(14)	0.055(2)	0.067(2)	0.0058(14)	0.0066(12)	-0.0043(13)
C42	0.060(2)	0.076(2)	0.072(2)	0.013(2)	0.0026(15)	0.000(2)
C43	0.080(2)	0.100(3)	0.063(2)	0.021(2)	0.000(2)	-0.001(2)
C44	0.081(2)	0.105(3)	0.056(2)	0.008(2)	0.020(2)	0.002(2)
C45	0.060(2)	0.074(2)	0.057(2)	0.0067(15)	0.0176(13)	-0.001(2)
C46	0.0505(14)	0.0509(15)	0.0548(14)	0.0058(12)	0.0089(11)	-0.0029(12)
C82	0.118(4)	0.147(6)	0.105(4)	-0.008(4)	-0.001(3)	0.011(4)
C83	0.112(4)	0.117(4)	0.096(3)	-0.004(3)	0.036(3)	0.025(3)
C84	0.130(5)	0.150(6)	0.125(5)	-0.028(5)	0.004(4)	-0.001(5)

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C86	0.175(7)	0.242(12)	0.117(5)	0.008(7)	-0.028(5)	-0.058(8)
C87	0.094(3)	0.091(3)	0.107(3)	-0.023(3)	0.035(3)	-0.028(3)
C88	0.140(5)	0.150(6)	0.142(6)	0.034(5)	-0.001(4)	-0.052(5)

Table 3. Positonal Parameters and Isotropic Displacement Parameters ($Å^2$) of Hydrogen Atoms

atom	x	y	z	U(iso)
H47	0.6769(4)	1.0504(3)	-0.1516(3)	0.079(12)
H48	0.5585(5)	1.0618(3)	-0.3379(3)	0.109(16)
H49	0.3763(5)	0.9766(3)	-0.3715(3)	0.139(22)
H50	0.3012(4)	0.8846(4)	-0.2607(3)	0.138(22)
H51	0.2010(4)	0.9151(5)	-0.1008(4)	0.224
H52	0.2211(4)	0.8424(5)	-0.0018(4)	0.224
H53	0.2012(4)	0.8133(5)	-0.1011(4)	0.224
H54	0.4595(4)	1.0144(3)	0.1438(4)	0.138(29)
H55	0.3378(4)	0.9843(3)	0.1217(4)	0.082(12)
H56	0.4195(4)	1.0393(3)	0.0596(4)	0.091(15)
H57	0.7995(3)	0.9816(4)	-0.0423(3)	0.072(11)
H58	0.8811(5)	1.0887(4)	0.1540(5)	0.185(33)
H59	0.7818(5)	1.1302(4)	0.0393(5)	0.178(31)
H60	0.9202(5)	1.1098(4)	0.0419(5)	0.155(26)
H61	0.9175(4)	0.8415(6)	0.0368(4)	0.139(24)
H62	0.9774(4)	0.9212(6)	0.0029(4)	0.147(22)
H63	0.9582(4)	0.9095(6)	0.1271(4)	0.107(16)
H64	0.4212(3)	0.7349(3)	0.2327(3)	0.070(10)
H65	0.3408(3)	0.8348(3)	0.2019(3)	0.062(9)
H66	0.3410(3)	0.7511(3)	0.1323(3)	0.097(15)
H67	0.6186(3)	0.7389(3)	0.0453(3)	0.063(10)
H68	0.4787(3)	0.7053(3)	0.0185(3)	0.074(11)
H69	0.5787(3)	0.6774(3)	0.1327(3)	0.085(12)
H70	0.3584(3)	0.9623(3)	0.3471(2)	0.066(10)
H71	0.1994(3)	0.9148(3)	0.4421(3)	0.069(10)
H72	0.1002(3)	0.8151(4)	0.5373(4)	0.078(11)
H73	0.1213(4)	0.6715(4)	0.6487(4)	0.142(23)
H74	0.2793(4)	0.5750(4)	0.6804(4)	0.157(25)
H75	0.4591(3)	0.6191(3)	0.6006(3)	0.090(14)
H76	0.8383(3)	0.6352(2)	0.3983(3)	0.062(9)
H77	0.8996(3)	0.5755(2)	0.5526(3)	0.101(15)
H78	0.9197(3)	0.5847(3)	0.7445(3)	0.076(12)
H79	0.8380(4)	0.6447(4)	0.8944(3)	0.081(12)
H80	0.6602(4)	0.7509(4)	0.8688(3)	0.074(11)
H81	0.5605(3)	0.7938(3)	0.7019(2)	0.069(10)