Supporting Information for

Spectroscopic and ExcitedState Properties of Tr-9-anthrylborane III: Crystal and Spectroscopic Polymorphisms

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Table S1. Atomic Coordinates, Isotropic Thermal Parameter, and Occupancy of **TAB** (**R**–Form).

	x	y	z	U_{iso}	Occ
C1	0.91529(9)	0.01262(9)	0.86610(5)	0.0210(3)	1.00
C2	0.91144(9)	0.07719(9)	0.89957(5)	0.0212(3)	1.00
C3	0.9759(1)	0.12393(10)	0.94027(6)	0.0246(3)	1.00
C4	0.9726(1)	0.1876(1)	0.97087(6)	0.0284(4)	1.00
C5	0.9046(1)	0.2099(1)	0.96298(6)	0.0327(4)	1.00
C6	0.8396(1)	0.1646(1)	0.92641(6)	0.0321(4)	1.00
C7	0.8394(1)	0.0961(1)	0.89444(6)	0.0262(4)	1.00
C8	0.7707(1)	0.0472(1)	0.85847(6)	0.0304(4)	1.00
C9	0.77008(10)	-0.0189(1)	0.82664(6)	0.0275(4)	1.00
C10	0.6975(1)	-0.0697(1)	0.79084(7)	0.0365(4)	1.00
C11	0.6975(1)	-0.1325(1)	0.75891(7)	0.0399(5)	1.00
C12	0.7715(1)	-0.1469(1)	0.75951(7)	0.0377(5)	1.00
C13	0.8418(1)	-0.1003(1)	0.79293(6)	0.0300(4)	1.00
C14	0.84369(9)	-0.03587(9)	0.82967(5)	0.0231(3)	1.00
C15	0.8716(2)	0.2638(2)	0.7125(2)	0.096(1)	1.00
C16	0.8328(2)	0.2304(2)	0.7593(1)	0.0846(10)	1.00
C17	0.7491(3)	0.2125(2)	0.7683(2)	0.113(1)	1.00
C18	0.7016(2)	0.2258(2)	0.7317(3)	0.132(2)	1.00
C19	0.7346(4)	0.2558(3)	0.6847(2)	0.114(2)	1.00
C20	0.8213(4)	0.2760(3)	0.6718(1)	0.118(2)	1.00
B1	1.0000	0.0000	0.8671(1)	0.0210(3)	1.00

Table S2. Bond Distance (Å) of **TAB** (**R**–Form).

C1	C2	1.424(2)
C1	C14	1.426(2)
C1	B1	1.580(1)
C2	C3	1.429(2)
C2	C7	1.437(2)
C3	C4	1.366(2)
C4	C5	1.416(2)
C5	C6	1.357(2)
C6	C7	1.429(2)
C7	C8	1.392(2)
C8	C9	1.390(2)
C9	C10	1.432(2)
C9	C14	1.439(2)
C10	C11	1.349(3)
C11	C12	1.416(2)
C12	C13	1.360(2)
C13	C14	1.434(2)
C15	C16	1.336(5)
C15	C20	1.425(6)
C16	C17	1.334(5)
C17	C18	1.329(6)
C18	C19	1.303(7)
C19	C20	1.394(7)

Table S3. Bond Angles (deg) of **TAB** (**R**–Form).

C2	C1	C14	118.4(1)
C2	C1	B1	120.4(1)
C14	C1	B1	121.2(1)
C1	C2	C3	122.6(1)
C1	C2	C7	120.4(1)
C3	C2	C7	117.0(1)
C2	C3	C4	121.7(1)
C3	C4	C5	120.7(1)
C4	C5	C6	119.8(1)
C5	C6	C7	121.2(1)
C2	C7	C6	119.4(1)
C2	C7	C8	119.4(1)
C6	C7	C8	121.2(1)
C7	C8	C9	121.9(1)
C8	C9	C10	120.7(1)
C8	C9	C14	119.3(1)
C10	C9	C14	119.9(1)
C9	C10	C11	121.1(2)
C10	C11	C12	119.7(1)
C11	C12	C13	121.2(2)
C12	C13	C14	121.7(1)
C1	C14	C9	120.5(1)
C1	C14	C13	123.2(1)
C9	C14	C13	116.2(1)
C16	C15	C20	119.3(4)
C15	C16	C17	120.2(3)
C16	C17	C18	121.8(4)
C17	C18	C19	121.2(4)
C18	C19	C20	120.8(4)
C15	C20	C19	116.7(3)
C1	B1	C1*	119.975(6)
C1	B1	C1’	119.975(9)
C1*	B1	C1’	119.975(8)

Symmetry notation ; * : -y, x-y, z, ‘ : -x+y, -x, z

Figure S1. ORTEP drawing showing **TAB** (**R**–Form).

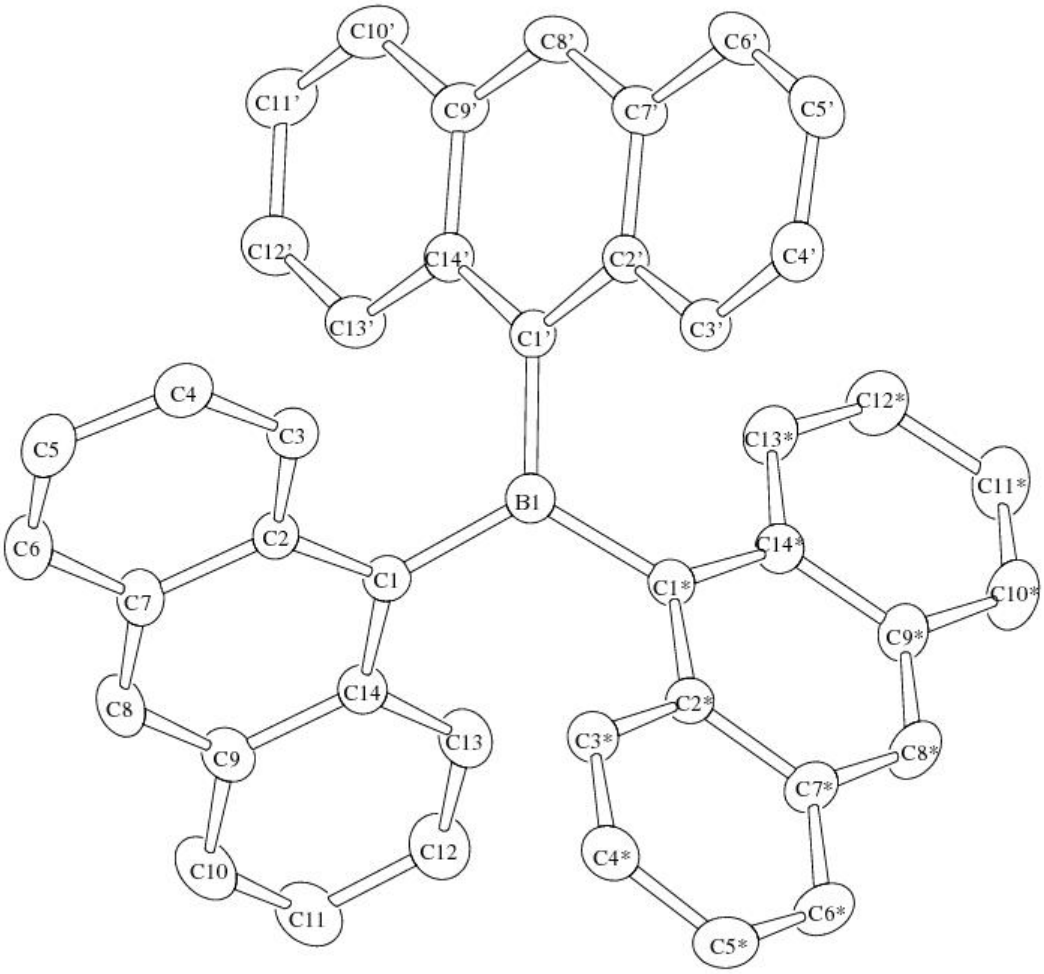

Table S4. Atomic Coordinates, Isotropic Thermal Parameter, and Occupancy of **TAB** (**O**–Form).

	x	y	z	U_{iso}	Occ
C1	0.4353(1)	0.6720(1)	0.01223(3)	0.0377(5)	1.00
C2	0.5080(1)	0.7303(1)	0.02653(2)	0.0394(5)	1.00
C3	0.4899(1)	0.7754(1)	0.04309(3)	0.0423(5)	1.00
C4	0.5597(1)	0.8291(1)	0.05686(3)	0.0501(6)	1.00
C5	0.6536(2)	0.8410(2)	0.05521(3)	0.0600(7)	1.00
C6	0.6746(1)	0.7986(2)	0.04000(3)	0.0597(7)	1.00
C7	0.6040(1)	0.7422(1)	0.02516(3)	0.0465(5)	1.00
C8	0.6249(1)	0.6973(2)	0.00963(3)	0.0518(6)	1.00
C9	0.5557(1)	0.6386(1)	-0.00429(3)	0.0453(5)	1.00
C10	0.5786(1)	0.5916(2)	-0.01987(3)	0.0540(6)	1.00
C11	0.5114(2)	0.5337(2)	-0.03338(3)	0.0589(7)	1.00
C12	0.4163(2)	0.5187(2)	-0.03217(3)	0.0582(7)	1.00
C13	0.3915(1)	0.5629(2)	-0.01772(3)	0.0498(6)	1.00
C14	0.4592(1)	0.6241(1)	-0.00288(3)	0.0402(5)	1.00
C15	0.8560(4)	0.1984(3)	0.07458(7)	0.137(2)	1.00
C16	0.9298(3)	0.1844(3)	0.08179(5)	0.111(1)	1.00
C17	0.9527(2)	0.1243(3)	0.07187(5)	0.103(1)	1.00
C18	0.9049(3)	0.0774(2)	0.05495(5)	0.103(1)	1.00
C19	0.8321(3)	0.0911(3)	0.04777(6)	0.119(1)	1.00
C20	0.8064(3)	0.1505(3)	0.05751(8)	0.146(2)	1.00
C21	0.0374(8)	-0.0606(6)	0.00000(7)	0.138(2)	1.00
C22	0.0000	0.0000	0.2299(1)	0.164(2)	1.00
C23	0.0783(7)	0.0091(7)	0.2400(1)	0.196(4)	0.67
B1	0.3333	0.6667	0.01253(5)	0.0371(5)	1.00

Table S5. Bond Distance (Å) of **TAB** (**O**–Form).

C1	C2	1.425(2)
C1	C14	1.425(2)
C1	B1	1.581(2)
C2	C3	1.423(2)
C2	C7	1.444(3)
C3	C4	1.362(3)
C4	C5	1.412(3)
C5	C6	1.348(3)
C6	C7	1.426(3)
C7	C8	1.389(3)
C8	C9	1.384(3)
C9	C10	1.429(3)
C9	C14	1.436(3)
C10	C11	1.347(3)
C11	C12	1.410(3)
C12	C13	1.362(3)
C13	C14	1.427(3)
C15	C16	1.386(5)
C15	C20	1.377(6)
C16	C17	1.353(5)
C17	C18	1.356(4)
C18	C19	1.366(5)
C19	C20	1.366(6)
C21	C21’	1.362(4)
C21	C21†	1.362(4)
C22	C23	1.359(9)
C22	C23*	1.359(9)
C22	C23‡	1.359(9)
C23	C23§	1.35(1)

Symmetry notation ; ‘ : y, -x+y, -z, † : x-y, x, -z

* : -y, x-y, z, ‡: -x+y, -x, z

§ : x-y, -y, 1/2-z,

Table S6. Bond Angles (deg) of **TAB** (**O**–Form).

C2	C1	C14	118.3(2)
C2	C1	B1	120.2(2)
C14	C1	B1	121.4(2)
C1	C2	C3	122.9(2)
C1	C2	C7	120.3(2)
C3	C2	C7	116.8(2)
C2	C3	C4	122.1(2)
C3	C4	C5	120.5(2)
C4	C5	C6	120.0(2)
C5	C6	C7	121.5(2)
C2	C7	C6	119.1(2)
C2	C7	C8	119.3(2)
C6	C7	C8	121.6(2)
C7	C8	C9	122.1(2)
C8	C9	C10	121.0(2)
C8	C9	C14	119.4(2)
C10	C9	C14	119.6(2)
C9	C10	C11	121.4(2)
C10	C11	C12	119.6(2)
C11	C12	C13	121.1(2)
C12	C13	C14	121.8(2)
C1	C14	C9	120.6(2)
C1	C14	C13	122.9(2)
C9	C14	C13	116.5(2)
C16	C15	C20	119.6(4)
C15	C16	C17	119.5(3)
C16	C17	C18	121.3(4)
C17	C18	C19	119.4(4)
C18	C19	C20	120.9(3)
C15	C20	C19	119.3(4)
C21	C21’	C21†	120.0000(5)
C23	C22	C23*	97.6(6)
C23	C22	C23‡	97.6(6)
C23*	C22	C23‡	97.6(6)
C22	C23	C23§	118.1(5)
C1	B1	C1”	119.984(6)
C1	B1	C1□	119.984(6)
C1”	B1	C1□	119.985(6)

Symmetry notation ;
‘ : y, -x+y, -z, † : x-y, x, -z, * : -y, x-y, z,
‡: -x+y, -x, z, § : x-y, -y, 1/2-z,
“ : -x+y, 1-x, z, □: 1-y,1+x-y, z,
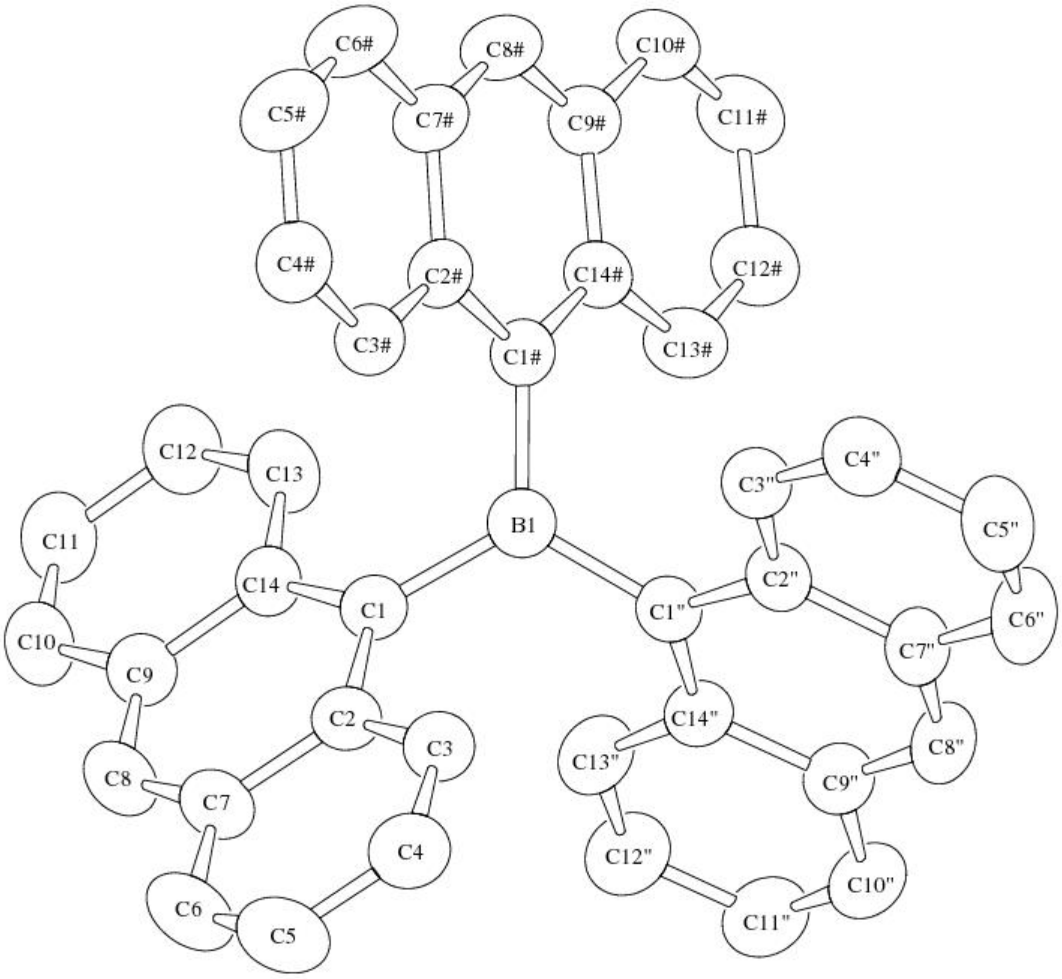
Figure S2. ORTEP drawing showing **TAB** (**O**–Form).