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Table 6. Atomic Coordinates for Non-hydrogen Atoms with e.s.d.s for Compounds 2a, 2b and 3a.

		x	y	z	Beq
2a	N(1)	0.0396(9)	0.4908(5)	0.7466(3)	37(2)
	C(2)	-0.0576(12)	0.4918(5)	0.7993(3)	33(2)
	C(3)	-0.2724(12)	0.4889(6)	0.8049(3)	41(2)
	C(4)	-0.3955(13)	0.4848(7)	0.7553(4)	52(2)
	C(5)	-0.2936(14)	0.4844(7)	0.7021(4)	52(2)
	C(6)	-0.0791(14)	0.4858(5)	0.6981(3)	40(2)
	C(7)	0.0375(18)	0.4863(7)	0.6428(3)	59(3)
	O(8)	0.1813(9)	0.4048(4)	0.6371(2)	50(1)
	Si(9)	0.1199(4)	0.2909(2)	0.6292(1)	45(1)
	C(10)	-0.0638(24)	0.2689(10)	0.5693(4)	90(4)
	C(11)	0.3745(21)	0.2329(10)	0.6184(5)	91(4)
	O(12)	0.0016(9)	0.2477(5)	0.6873(2)	49(2)
	C(13)	0.1043(14)	0.2452(6)	0.7418(3)	46(2)
	C(14)	-0.0489(13)	0.2416(6)	0.7909(3)	40(2)
	N(15)	0.0387(11)	0.2508(5)	0.8427(3)	43(2)
	C(16)	-0.0812(15)	0.2513(7)	0.8879(3)	50(2)
	C(17)	-0.3016(14)	0.2452(7)	0.8854(3)	50(2)
	C(18)	-0.3863(15)	0.2321(8)	0.8324(4)	63(3)
	C(19)	-0.2609(13)	0.2317(7)	0.7830(3)	47(2)
	C(20)	0.0284(18)	0.2596(7)	0.9465(4)	59(3)
	O(21)	0.1228(34)	0.3346(7)	0.9587(4)	225(10)
	Si(22)	0.1020(5)	0.4514(2)	0.9605(1)	58(1)
	C(23)	0.3733(16)	0.4931(12)	0.9667(5)	102(5)
	C(24)	-0.0515(20)	0.4894(13)	1.0214(4)	116(7)
	O(25)	-0.0126(9)	0.4947(4)	0.9024(2)	46(1)
	C(26)	0.0927(14)	0.4962(6)	0.8484(3)	41(2)
2b	SI(1)	-0.0604(1)	-0.2488(1)	-0.2476(0)	2.8(0)
	O(2)	-0.1506(2)	-0.2351(2)	-0.1357(1)	3.4(1)
	C(3)	-0.2003(3)	-0.1001(3)	-0.1043(2)	3.3(1)
	C(4)	-0.3229(3)	-0.1381(3)	-0.0121(2)	2.8(1)
	C(5)	-0.4707(4)	-0.2799(3)	-0.0064(2)	3.8(1)
	C(6)	-0.5760(4)	-0.3077(3)	0.0806(2)	4.5(1)
	C(7)	-0.5304(3)	-0.1927(3)	0.1599(2)	3.8(1)
	C(8)	-0.3816(3)	-0.0533(3)	0.1487(2)	2.9(1)
	N(9)	-0.2791(3)	-0.0251(2)	0.0636(1)	2.8(1)
	C(10)	-0.3219(3)	0.0769(3)	0.2314(2)	3.4(1)
	O(11)	-0.1321(2)	0.1016(2)	0.2696(1)	3.1(1)
	C(12)	-0.2326(3)	-0.2419(3)	-0.3507(2)	3.0(1)
	C(13)	-0.1881(4)	-0.1277(3)	-0.4232(2)	4.7(1)
	C(14)	-0.3212(5)	-0.1232(4)	-0.4984(2)	6.3(2)
	C(15)	-0.4988(4)	-0.2308(4)	-0.5012(2)	5.6(1)
	C(16)	-0.5489(4)	-0.3439(4)	-0.4291(2)	5.7(1)
	C(17)	-0.4173(4)	-0.3493(3)	-0.3543(2)	4.6(1)
	C(18)	-0.0142(3)	-0.4396(3)	-0.2479(2)	3.2(1)
	C(19)	-0.0409(4)	-0.5347(3)	-0.3378(2)	4.3(1)
	C(20)	0.0010(5)	-0.6746(3)	-0.3406(3)	6.0(2)
	C(21)	0.0675(5)	-0.7215(4)	-0.2530(3)	6.8(2)
	C(22)	0.0936(5)	-0.6309(4)	-0.1622(3)	6.5(2)
	C(23)	0.0534(4)	-0.4902(3)	-0.1599(2)	4.6(1)
3a	C(1)	0.4947(2)	0.1191(2)	0.8514(4)	2.4(1)
	C(2)	0.5713(3)	0.2066(3)	0.9128(4)	3.0(1)
	C(3)	0.6921(3)	0.2117(3)	0.8699(4)	3.5(1)
	C(4)	0.7354(2)	0.1289(3)	0.7672(4)	3.0(1)

C(5)	0.6594(2)	0.0399(2)	0.7062(4)	2.3(1)
C(6)	0.5380(2)	0.0365(2)	0.7481(4)	2.5(1)
C(7)	0.3621(2)	0.1129(3)	0.8964(4)	3.1(1)
O(8)	0.2802(2)	0.1617(2)	0.7672(2)	2.7(1)
SI(9)	0.1680(1)	0.0924(1)	0.6614(1)	2.3(0)
C(10)	0.0865(3)	-0.0063(3)	0.7935(5)	4.1(2)
C(11)	0.0681(3)	0.2084(3)	0.5654(4)	3.6(1)
O(12)	0.2210(2)	0.0099(2)	0.5197(2)	2.9(1)
C(13)	0.2930(3)	0.0559(2)	0.3958(4)	3.1(1)

Table 7. Bond Distances (Å) for Compounds 2a, 2b and 3a

2a	N(1)-C(6)	1.354(9)
	N(1)-C(2)	1.369(9)
	C(2)-C(3)	1.375(11)
	C(2)-C(26)	1.486(10)
	C(3)-C(4)	1.389(11)
	C(4)-C(5)	1.392(12)
	C(5)-C(6)	1.370(13)
	C(6)-C(7)	1.478(11)
	C(7)-O(8)	1.453(11)
	O(8)-Si(9)	1.624(6)
	Si(9)-O(12)	1.651(5)
	Si(9)-C(11)	1.825(12)
	Si(9)-C(10)	1.839(12)
	O(12)-C(13)	1.421(9)
	C(13)-C(14)	1.498(10)
	C(14)-N(15)	1.326(10)
	C(14)-C(19)	1.370(12)
	N(15)-C(16)	1.294(10)
	C(16)-C(17)	1.408(13)
	C(16)-C(20)	1.530(12)
	C(17)-C(18)	1.352(12)
	C(18)-C(19)	1.393(12)
	C(20)-O(21)	1.23(2)
	O(21)-Si(22)	1.611(10)
	Si(22)-O(25)	1.642(5)
	Si(22)-C(24)	1.794(11)
	Si(22)-C(23)	1.827(12)
	O(25)-C(26)	1.417(9)
2b	Si(1)-O(2)	1.633(2)
	Si(1)-C(12)	1.857(3)
	Si(1)-C(18)	1.853(3)
	O(2)-C(3)	1.427(3)
	C(3)-C(4)	1.501(4)
	C(4)-C(5)	1.379(4)
	C(4)-N(9)	1.337(3)
	C(5)-C(6)	1.372(4)
	C(6)-C(7)	1.381(4)
	C(7)-C(8)	1.378(4)
	C(8)-N(9)	1.341(3)
	C(8)-C(10)	1.500(4)
	C(10)-O(11)	1.436(3)
3a	C(1)-C(2)	1.380(4)
	C(1)-C(6)	1.386(4)
	C(1)-C(7)	1.527(4)
	C(2)-C(3)	1.396(5)
	C(3)-C(4)	1.385(5)
	C(4)-C(5)	1.388(4)
	C(5)-C(6)	1.399(4)
	C(7)-O(8)	1.427(4)
	O(8)-Si(9)	1.638(2)
	Si(9)-C(10)	1.853(4)
	Si(9)-C(11)	1.858(3)
	Si(9)-O(12)	1.642(2)
	O(12)-C(13)	1.435(4)

Table 8. Bond Angles (°) for Compounds 2a, 2b and 3a

2a	C(6)	N(1)	C(2)	119.1(6)
	N(1)	C(2)	C(3)	122.2(7)
	N(1)	C(2)	C(26)	112.9(7)
	C(3)	C(2)	C(26)	124.9(7)
	C(2)	C(3)	C(4)	119.1(7)
	C(3)	C(4)	C(5)	117.8(7)
	C(6)	C(5)	C(4)	121.7(8)
	N(1)	C(6)	C(5)	120.1(7)
	N(1)	C(6)	C(7)	115.8(8)
	C(5)	C(6)	C(7)	124.0(8)
	O(8)	C(7)	C(6)	113.0(6)
	C(7)	O(8)	Si(9)	126.9(6)
	O(8)	Si(9)	O(12)	111.4(3)
	O(8)	Si(9)	C(11)	102.8(5)
	O(12)	Si(9)	C(11)	111.2(5)
	O(8)	Si(9)	C(10)	113.4(5)
	O(12)	Si(9)	C(10)	105.3(5)
	C(11)	Si(9)	C(10)	113.0(7)
	C(13)	O(12)	Si(9)	121.3(5)
	O(12)	C(13)	C(14)	111.9(7)
	N(15)	C(14)	C(19)	123.0(7)
	N(15)	C(14)	C(13)	114.0(7)
	C(19)	C(14)	C(13)	123.0(8)
	C(16)	N(15)	C(14)	118.7(7)
	N(15)	C(16)	C(17)	123.8(8)
	N(15)	C(16)	C(20)	116.5(8)
	C(17)	C(16)	C(20)	119.7(8)
	C(18)	C(17)	C(16)	116.2(8)
	C(17)	C(18)	C(19)	121.0(8)
	C(14)	C(19)	C(18)	117.1(8)
	O(21)	C(20)	C(16)	119.3(8)
	C(20)	O(21)	Si(22)	143(2)
	O(21)	Si(22)	O(25)	112.1(4)
	O(21)	Si(22)	C(24)	110.8(9)
	O(25)	Si(22)	C(24)	107.1(5)
	O(21)	Si(22)	C(23)	103.7(9)
	O(25)	Si(22)	C(23)	111.8(5)
	C(24)	Si(22)	C(23)	111.3(6)
	C(26)	O(25)	Si(22)	121.0(5)
	O(25)	C(26)	C(2)	111.5(7)
2b	O(2)	Si(1)	C(12)	108.9(1)
	O(2)	Si(1)	C(18)	104.7(1)
	C(12)	Si(1)	C(18)	113.5(1)
	Si(1)	O(2)	C(3)	121.9(2)
	O(2)	C(3)	C(4)	109.5(2)
	C(3)	C(4)	C(5)	122.1(2)
	C(3)	C(4)	N(9)	115.4(2)
	C(5)	C(4)	N(9)	122.5(2)
	C(4)	C(5)	C(6)	119.1(3)
	C(5)	C(6)	C(7)	118.9(3)
	C(6)	C(7)	C(8)	118.9(3)
	C(7)	C(8)	N(9)	122.4(2)
	C(7)	C(8)	C(10)	122.3(2)
	N(9)	C(8)	C(10)	115.3(2)
	C(4)	N(9)	C(8)	118.2(2)

	C(8)	C(10)	O(11)	110.9(2)
	Si(1)	C(12)	C(13)	122.4(2)
	Si(1)	C(12)	C(17)	120.4(2)
	C(13)	C(12)	C(17)	117.1(3)
	C(12)	C(13)	C(14)	121.3(3)
	C(13)	C(14)	C(15)	120.4(4)
	C(14)	C(15)	C(16)	119.8(4)
	C(15)	C(16)	C(17)	120.1(3)
	C(12)	C(17)	C(16)	121.3(3)
	Si(1)	C(18)	C(19)	120.5(2)
	Si(1)	C(18)	C(23)	121.6(2)
	C(19)	C(18)	C(23)	117.9(3)
	C(18)	C(19)	C(20)	121.3(3)
	C(19)	C(20)	C(21)	119.6(3)
	C(20)	C(21)	C(22)	120.6(4)
	C(21)	C(22)	C(23)	119.6(4)
	C(18)	C(23)	C(22)	121.0(3)
3a	C(2)	C(1)	C(6)	120.0(3)
	C(2)	C(1)	C(7)	120.3(3)
	C(6)	C(1)	C(7)	119.7(3)
	C(1)	C(2)	C(3)	119.7(3)
	C(2)	C(3)	C(4)	120.3(3)
	C(3)	C(4)	C(5)	120.4(3)
	C(4)	C(5)	C(6)	118.8(3)
	C(1)	C(6)	C(5)	120.8(3)
	C(1)	C(7)	O(8)	110.4(2)
	C(7)	O(8)	Si(9)	124.9(2)
	O(8)	Si(9)	C(10)	112.3(1)
	O(8)	Si(9)	C(11)	103.9(1)
	O(8)	Si(9)	O(12)	111.0(1)
	C(10)	Si(9)	C(11)	113.4(2)
	C(10)	Si(9)	O(12)	105.1(1)
	C(11)	Si(9)	O(12)	111.4(1)
	Si(9)	O(12)	C(13)	121.5(2)

Table 9. : Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3)

		x	y	z	U(eq)
2a	H(3)	-3345(12)	4897(6)	8413(3)	49
	H(4)	-5411(13)	4824(7)	7577(4)	62
	H(5)	-3732(14)	4832(7)	6684(4)	62
	H(7A)	-621(18)	4845(7)	6111(3)	71
	H(7B)	1161(18)	5465(7)	6398(3)	71
	H(10A)	-941(24)	2006(10)	5668(4)	136
	H(10B)	-18(24)	2905(10)	5337(4)	136
	H(10C)	-1915(24)	3042(10)	5761(4)	136
	H(11A)	3553(21)	1642(10)	6132(5)	137
	H(11B)	4616(21)	2443(10)	6516(5)	137
	H(11C)	4406(21)	2599(10)	5847(5)	137
	H(13A)	1919(14)	3025(6)	7458(3)	55
	H(13B)	1947(14)	1884(6)	7435(3)	55
	H(17)	-3843(14)	2499(7)	9184(3)	60
	H(18)	-5304(15)	2232(8)	8288(4)	76
	H(19)	-3185(13)	2250(7)	7463(3)	57
	H(20A)	-769(18)	2493(7)	9762(4)	71
	H(20B)	1275(18)	2062(7)	9494(4)	71
	H(23A)	3760(16)	5629(12)	9681(5)	153
	H(23B)	4521(16)	4710(12)	9338(5)	153
	H(23C)	4344(16)	4673(12)	10014(5)	153
	H(24A)	-620(20)	5591(13)	10217(4)	174
	H(24B)	146(20)	4678(13)	10565(4)	174
	H(24C)	-1895(20)	4617(13)	10188(4)	174
	H(26A)	1877(14)	4411(6)	8462(3)	49
	H(26B)	1755(14)	5552(6)	8454(3)	49
2b	H(103)	-840(33)	-89(26)	-836(17)	4.4
	H(203)	-2716(32)	-707(25)	-1629(17)	4.2
	H(105)	-4999(35)	-3563(28)	-652(18)	5.1
	H(106)	-6779(34)	-4124(27)	866(18)	4.9
	H(107)	-6052(35)	-2058(27)	2258(18)	5.2
	H(110)	-3252(32)	1781(26)	2007(17)	4.5
	H(210)	-4125(32)	453(26)	2936(17)	4.1
	H(113)	-573(34)	-455(27)	-4192(18)	5.1
	H(114)	-2861(36)	-381(29)	-5501(19)	6.0
	H(115)	-5868(36)	-2280(28)	-5577(19)	6.1
	H(116)	-6861(38)	-4209(29)	-4271(19)	6.4
	H(117)	-4565(35)	-4343(28)	-3031(18)	5.6
	H(119)	-903(34)	-5032(27)	-4019(18)	5.1
	H(120)	-204(36)	-7427(28)	-4086(19)	6.0
	H(121)	967(37)	-8254(29)	-2573(20)	6.3
	H(122)	1384(35)	-6594(29)	-962(19)	5.8
	H(123)	760(33)	-4247(26)	-961(18)	4.7
3a	H(103)	7475(26)	2746(26)	9175(44)	4.7
	H(104)	8219(26)	1314(27)	7369(38)	4.0
	H(106)	4832(27)	-293(26)	7045(39)	4.3
	H(107)	3414(26)	278(27)	9139(39)	4.3
	H(207)	3551(27)	1542(27)	10030(41)	4.8
	H(110)	181(31)	-471(28)	7246(44)	6.1
	H(210)	1385(27)	-652(27)	8397(39)	4.7
	H(310)	559(27)	379(29)	8805(44)	6.1
	H(111)	-8(28)	1758(27)	5013(45)	5.6
	H(211)	352(25)	2576(29)	6527(43)	5.4

H(311)	1133(27)	2549(30)	4940(45)	5.8
H(113)	2389(27)	1088(27)	3187(43)	4.9
H(213)	3684(27)	1017(26)	4516(39)	4.6

Table 10. Anisotropic displacement parameters ($Å^2 x 10^3$). The anisotropic displacement factor exponent takes the form : $-2\pi^2 [h^2 a^{*2} U11 + ... + 2 h k a^* b^* U12]$

	atoms	U11	U22	U33	U23	U13	U12
2a	N(1)	38(3)	42(4)	30(3)	5(3)	6(3)	1(3)
	C(2)	52(4)	27(4)	21(3)	4(3)	1(3)	6(3)
	C(3)	42(4)	47(5)	33(4)	1(3)	13(3)	6(4)
	C(4)	36(4)	59(5)	61(5)	-3(4)	1(4)	-5(4)
	C(5)	54(5)	63(6)	39(4)	-4(4)	-9(4)	1(5)
	C(6)	61(5)	38(4)	21(3)	2(3)	-5(3)	1(4)
	C(7)	89(7)	56(6)	31(4)	0(3)	-5(4)	17(5)
	O(8)	52(3)	53(3)	44(3)	1(2)	5(3)	-7(3)
	Si(9)	58(1)	49(1)	29(1)	-3(1)	13(1)	-3(1)
	C(10)	124(11)	116(10)	31(4)	-3(5)	1(6)	-15(9)
	C(11)	95(9)	94(9)	86(7)	15(7)	38(7)	24(8)
	O(12)	55(3)	64(4)	28(3)	3(2)	8(3)	-18(3)
	C(13)	52(5)	51(5)	35(4)	7(3)	12(4)	-3(4)
	C(14)	44(4)	39(4)	36(4)	1(3)	7(3)	3(3)
	N(15)	49(4)	43(4)	38(3)	-1(3)	4(3)	-8(3)
	C(16)	54(5)	54(5)	42(4)	16(4)	8(4)	-7(4)
	C(17)	47(5)	63(5)	39(4)	4(4)	14(4)	-4(4)
	C(18)	44(5)	96(8)	50(5)	5(5)	-3(4)	-12(6)
	C(19)	44(4)	67(6)	31(4)	5(4)	1(4)	-8(4)
	C(20)	78(7)	55(6)	45(5)	10(4)	-9(5)	0(5)
	O(21)	475(29)	63(6)	135(8)	32(5)	-203(14)	-64(11)
	Si(22)	86(2)	57(2)	30(1)	1(1)	-16(1)	-14(2)
	C(23)	48(5)	203(17)	54(6)	4(8)	-13(5)	9(9)
	C(24)	72(7)	240(20)	36(5)	-10(8)	1(5)	18(11)
	O(25)	52(3)	58(4)	28(3)	2(2)	1(2)	5(3)
	C(26)	51(4)	44(4)	29(3)	-1(3)	-2(3)	5(4)
	atoms	B11	B22	B33	B12	B13	B23
2b	SI(1)	158(1)	99(1)	38(0)	108(2)	8(1)	9(1)
	O(2)	209(4)	134(3)	40(1)	173(6)	24(3)	13(3)
	C(3)	191(6)	118(4)	44(2)	128(8)	29(5)	3(4)
	C(4)	134(5)	108(4)	42(1)	98(7)	-5(4)	3(4)
	C(5)	165(6)	125(4)	60(2)	44(8)	1(5)	-30(4)
	C(6)	164(6)	135(5)	80(2)	-12(8)	49(6)	-8(5)
	C(7)	159(6)	145(4)	55(2)	64(8)	40(5)	16(4)
	C(8)	133(5)	122(4)	43(1)	112(7)	6(4)	9(4)
	N(9)	138(4)	99(3)	43(1)	78(6)	6(4)	6(3)
	C(10)	151(5)	144(4)	49(2)	121(8)	-1(5)	-17(4)
	O(11)	154(4)	107(2)	45(1)	81(5)	-14(3)	10(3)
	C(12)	165(5)	108(4)	42(1)	116(7)	4(4)	-5(4)
	C(13)	202(7)	191(5)	64(2)	88(10)	-25(6)	73(5)
	C(14)	284(9)	281(7)	78(2)	179(13)	-60(7)	112(7)
	C(15)	231(7)	276(7)	73(2)	237(12)	-89(6)	-9(6)
	C(16)	172(7)	241(6)	89(2)	74(11)	-53(6)	-35(6)
	C(17)	193(7)	165(5)	71(2)	55(9)	-13(6)	23(5)
	C(18)	141(5)	103(4)	59(2)	83(7)	27(5)	30(4)
	C(19)	239(7)	116(4)	75(2)	143(9)	29(6)	-3(5)
	C(20)	309(9)	132(5)	128(3)	197(11)	35(9)	-31(6)
	C(21)	268(9)	128(5)	183(4)	203(11)	5(9)	37(7)
	C(22)	275(9)	172(6)	146(4)	202(12)	-65(9)	114(7)
	C(23)	219(7)	151(5)	81(2)	144(9)	-20(6)	58(5)
3a	C(1)	43(2)	55(2)	86(5)	20(4)	13(5)	7(5)
	C(2)	57(3)	60(2)	121(6)	16(4)	13(6)	-36(6)
	C(3)	66(3)	65(3)	151(7)	-15(4)	25(7)	-48(7)
	C(4)	49(2)	61(2)	131(6)	-1(4)	23(6)	-12(6)

C(5)	52(2)	40(2)	87(5)	14(3)	31(5)	7(5)
C(6)	53(2)	47(2)	94(5)	3(4)	13(6)	-2(5)
C(7)	43(2)	84(3)	108(6)	19(4)	15(6)	13(6)
O(8)	45(2)	49(2)	122(4)	8(3)	-16(4)	2(4)
SI(9)	46(1)	44(1)	98(1)	0(1)	36(1)	-10(1)
C(10)	98(4)	74(3)	154(7)	-51(5)	102(8)	-1(7)
C(11)	65(3)	69(3)	147(6)	30(4)	-14(7)	-4(7)
O(12)	76(2)	45(2)	115(4)	1(3)	85(5)	-18(4)
C(13)	82(3)	46(2)	123(6)	10(4)	104(7)	4(6)

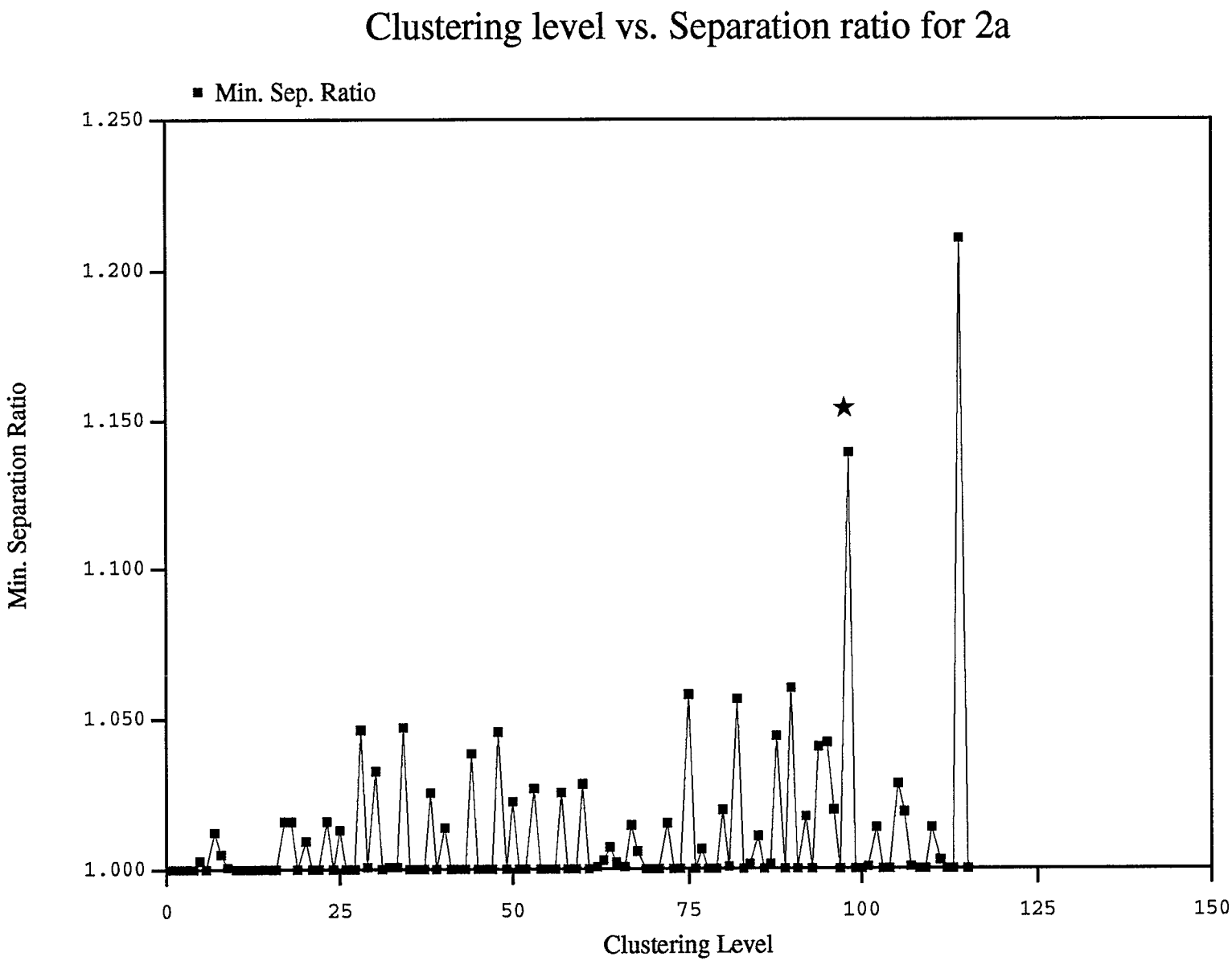
Clustering level vs. Separation ratio for 2a
Min. Sep. Ratio
1.250
1.200
1.150
1.100
1.050
1.000
Min. Separation Ratio
0
25
50
75
100
125
150
Clustering Level

Figure 6

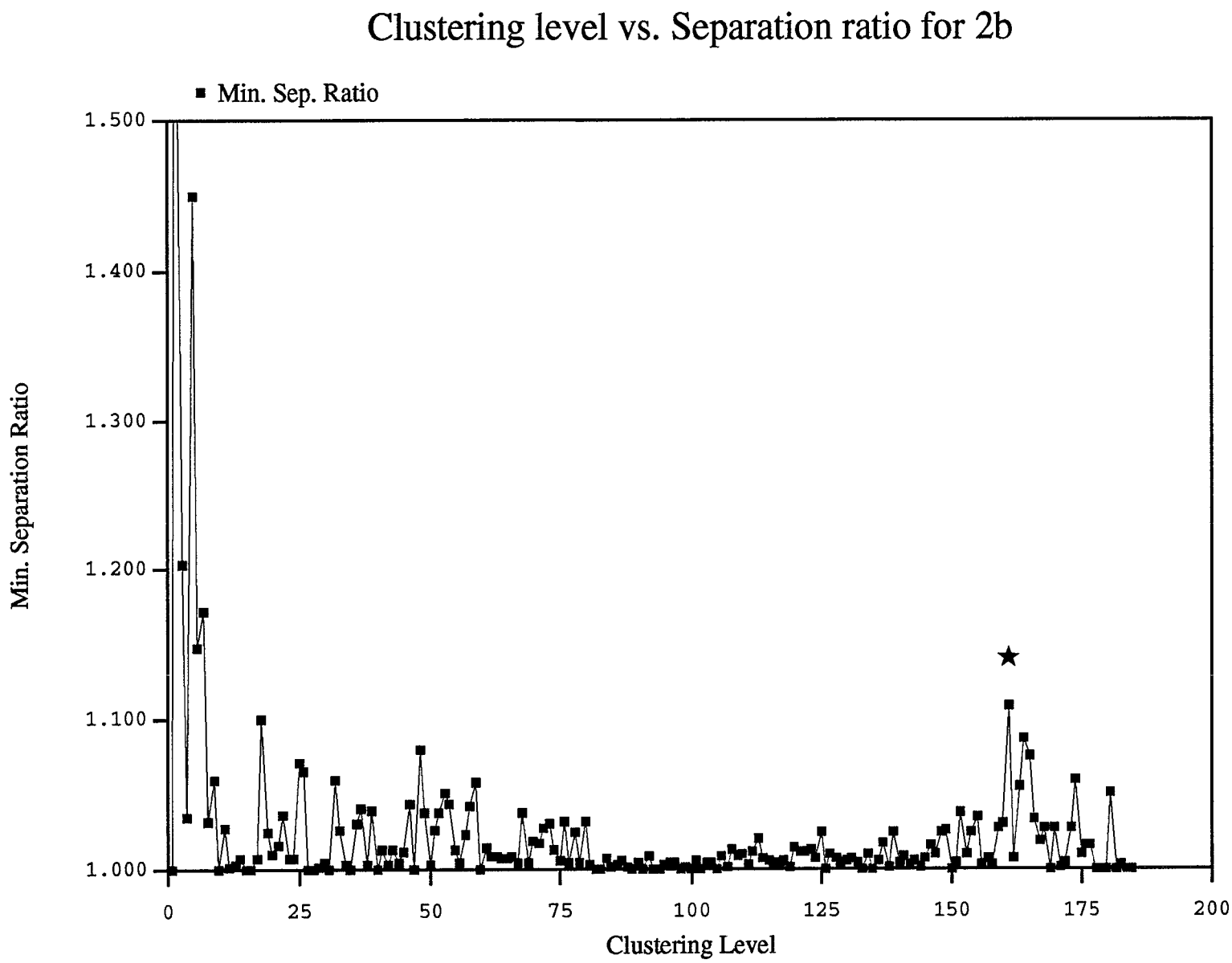
Clustering level vs. Separation ratio for 2b
Min. Sep. Ratio
1.500
1.400
1.300
1.200
1.100
1.000
Min. Separation Ratio
0
25
50
75
100
125
150
175
200
Clustering Level

Figure 7

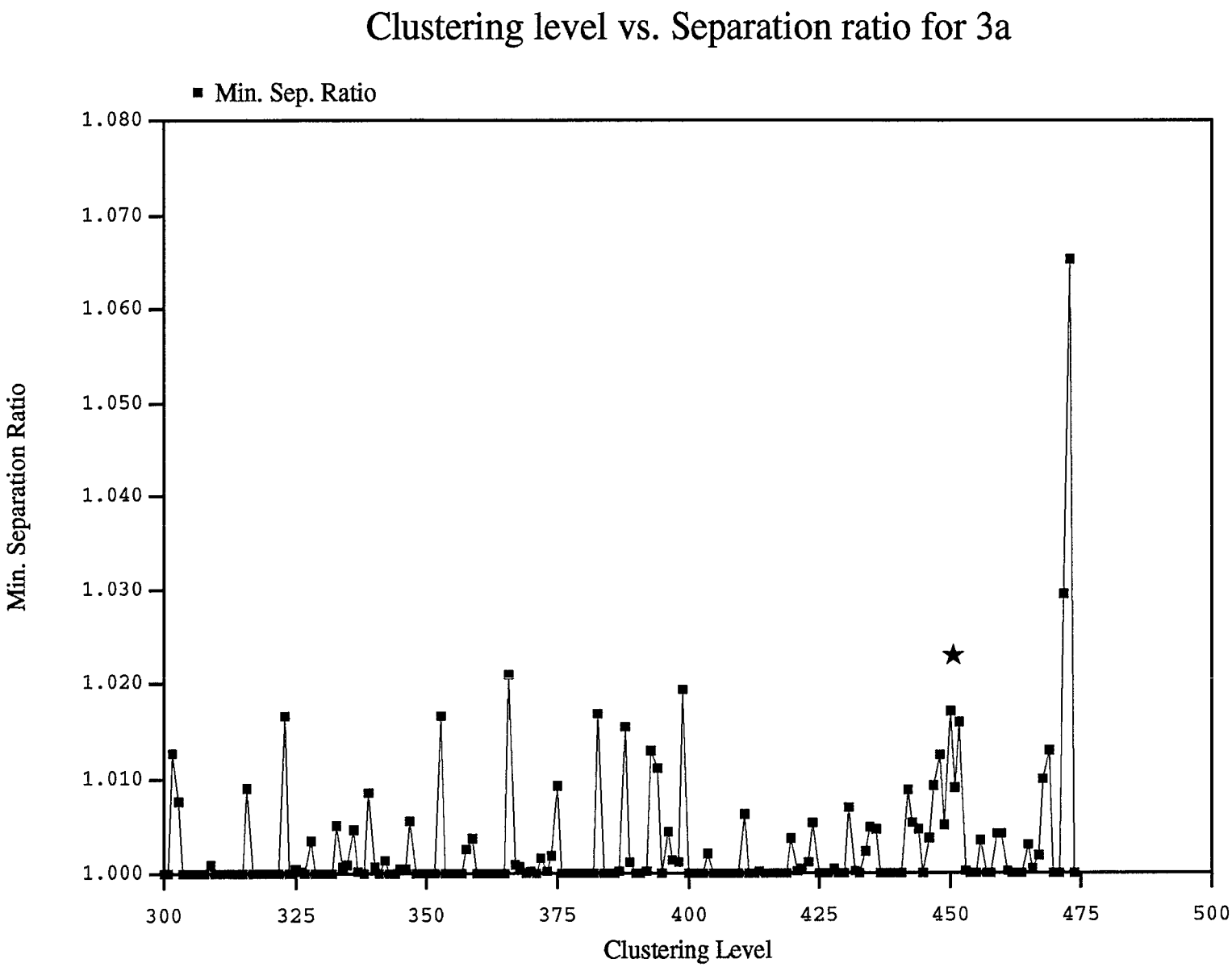
Clustering level vs. Separation ratio for 3a
Min. Sep. Ratio
1.080
1.070
1.060
1.050
1.040
1.030
1.020
1.010
1.000
Min. Separation Ratio
300
325
350
375
400
425
450
475
500
Clustering Level

Figure 8

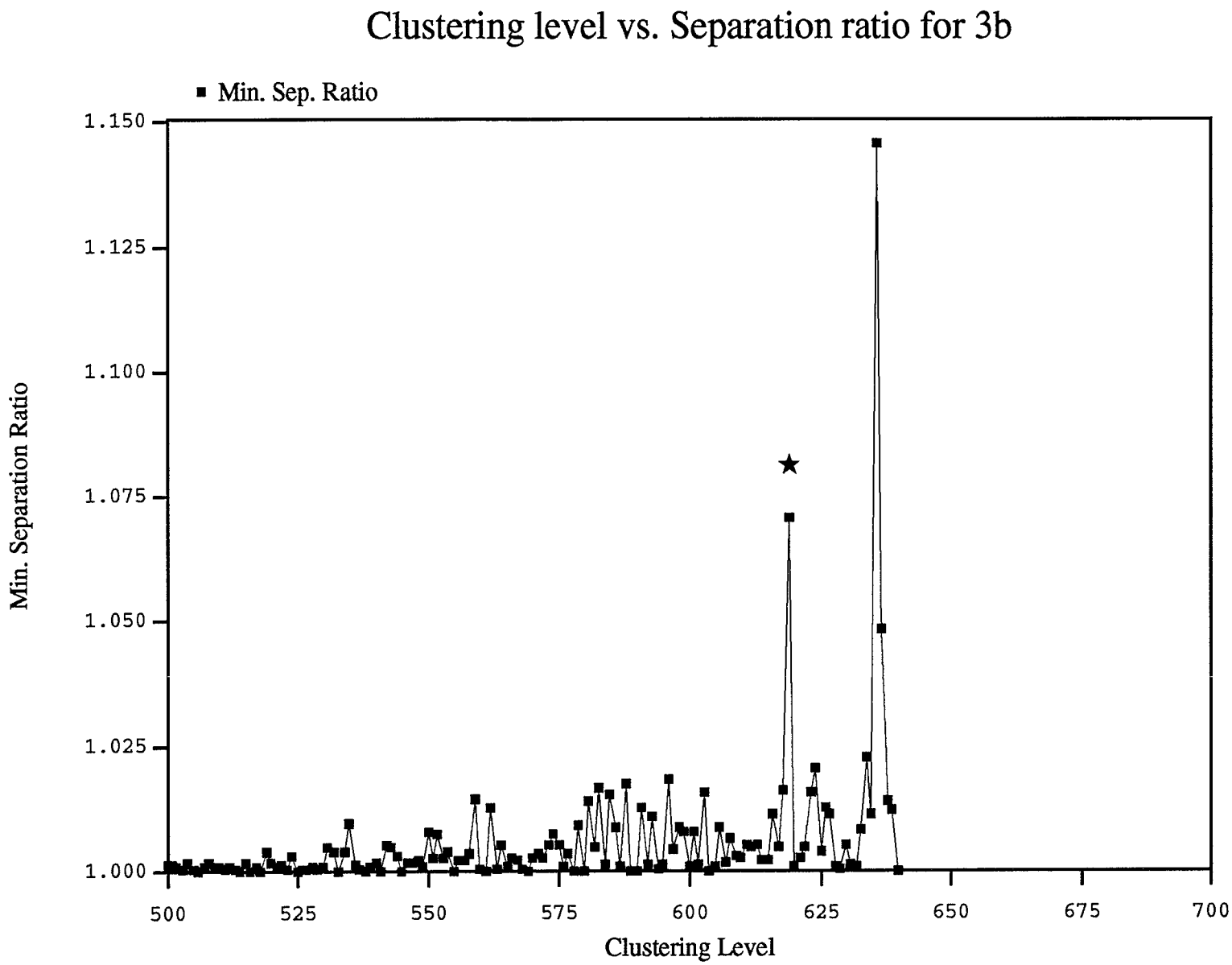
Clustering level vs. Separation ratio for 3b
Min. Sep. Ratio
1.150
1.125
1.100
1.075
1.050
1.025
1.000
Min. Separation Ratio
500
525
550
575
600
625
650
675
700
Clustering Level

Figure 9