Visualized acid-base discoloration and optoelectronic investigations for azines and azomethines having double 4-[*N*,*N*-di(4-methoxyphenyl)amino]phenyl terminals

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Electronic Supporting Information

Compound	MS-1	MS-2
Formula	$C_{42}H_{38}N_4O_4$	$C_{41}H_{37}N_3O_4$
Mr	662.76	635.74
Crystal system	Monoclinic	Monoclinic
Space group	$P2_{1}/n$	$P2_{1}/c$
<i>a</i> / Å	11.061(7)	20.928(2)
<i>b</i> / Å	9.663(6)	10.0003(11)
<i>c</i> / Å	16.800(10)	33.930(4)
lpha / °	90°	90
eta / °	91.609(10)	102.537(2)
γ / $^{\circ}$	90	90
V / Å ³	1794.9(19)	6931.6(13)
Ζ	2	8
T / \mathbf{K}	123(2)	123(2)
Refinement	full-matrix	full-matrix
Method	least-squares	least-squares
D_{calcd} , g/cm ⁻³	1.226	1.218
μ / mm ⁻¹	0.080	0.079
<i>F</i> (000)	700	2688
Crystal size / mm ³	0.12×0.10×0.10	$0.06 \times 0.04 \times 0.04$
Reflections measured	9571	37473
Unique reflections	3161	12198

Table SI1 Crystallographic data of compounds MS-1 and MS-2.

$R_{ m int}$	0.0311	0.0970
Data / parameter	3161 / 237	12198 / 873
Goof on F^2	1.026	0.996
$R_1^{a}, wR_2^{b} [I > 2\sigma(I)]$	0.0775, 0.2160	0.0679, 0.1061
R_1 , wR_2 (all data)	0.1353, 0.2435	0.2189, 0.1280
$\Delta ho_{ m max,} \Delta ho_{ m min}$ / e·Å ⁻³	0.339, -0.300	0.481, -0.337

^{*a*} $R_1 = \Sigma ||Fo| - |Fc|| / \Sigma |Fo|, \ ^{b} w R_2 = [\Sigma [w(Fo^2 - Fc^2)^2] / \Sigma w(Fo^2)^2]^{1/2}$

Table SI2 Selected bond distances (Å) and angles (°) for compounds**MS-1** and **MS-2**.

MS-1		MS-2	
Bond distances	Bond angles	Bond distances	Bond angles
C(1)-N(1) 1.254(5)	N(1)-C(1)-C(2)123.3(4)	C(1)-C(6) 1.357(6)	C(6)-C(1)-C(2)117.3(5)
C(1)-C(2) 1.464(5)	C(3)-C(2)-C(7)118.1(4)	C(1)-C(2) 1.387(6)	C(6)-C(1)-C(7)135.7(7)
C(2)-C(3) 1.360(5)	C(3)-C(2)-C(1)119.5(4)	C(1)-C(7) 1.405(6)	C(2)-C(1)-C(7)106.9(6)
C(2)-C(7) 1.383(6)	C(7)-C(2)-C(1)122.3(4)	C(2)-C(3) 1.378(5)	C(3)-C(2)-C(1)120.9(5)
C(3)-C(4) 1.376(5)	C(2)-C(3)-C(4)121.9(5)	C(3)-C(4) 1.377(5)	C(4)-C(3)-C(2)121.3(5)
C(4)-C(5) 1.384(6)	C(3)-C(4)-C(5)120.5(4)	C(4)-C(5) 1.375(5)	C(5)-C(4)-C(3)117.4(4)
C(5)-C(6) 1.375(6)	C(6)-C(5)-C(4)118.1(4)	C(4)-N(1) 1.406(5)	C(5)-C(4)-N(1)122.2(4)
C(5)-N(2) 1.392(5)	C(6)-C(5)-N(2)121.4(4)	C(5)-C(6) 1.377(5)	C(3)-C(4)-N(1)120.4(5)
C(6)-C(7) 1.388(5)	C(4)-C(5)-N(2)120.5(4)	C(8)-C(13) 1.358(5)	C(4)-C(5)-C(6)121.0(5)
C(8)-C(13) 1.373(6)	C(5)-C(6)-C(7)120.9(4)	C(8)-C(9) 1.366(5)	C(1)-C(6)-C(5)122.0(5)
C(8)-C(9) 1.374(6)	C(2)-C(7)-C(6)120.5(4)	C(8)-N(1) 1.424(5)	C(13)-C(8)-C(9)119.2(5)
C(8)-N(2) 1.431(5)	C(13)-C(8)-C(9)117.7(5)	C(9)-C(10) 1.365(5)	C(13)-C(8)-N(1)122.8(5)
C(9)-C(10) 1.365(6)	C(13)-C(8)-N(2)121.0(4)	C(10)-C(11) 1.356(6)	C(9)-C(8)-N(1)118.0(5)
C(10)-C(11) 1.353(6)	C(9)-C(8)-N(2)121.3(4)	C(11)-C(12) 1.354(6)	C(10)-C(9)-C(8)121.7(5)
C(11)-C(12) 1.366(7)	C(10)-C(9)-C(8)121.5(4)	C(11)-O(1) 1.414(5)	C(11)-C(10)-C(9)118.8(5)
C(11)-O(1) 1.373(6)	C(11)-C(10)-C(9)120.2(5)	C(12)-C(13) 1.428(5)	C(12)-C(11)-C(10)122.6(5)
C(12)-C(13) 1.375(6)	C(10)-C(11)-C(12)119.6(5)	C(14)-O(1) 1.384(5)	C(12)-C(11)-O(1)122.3(5)
C(14)-O(1) 1.428(6)	C(10)-C(11)-O(1)115.8(5)	C(15)-C(16) 1.375(5)	C(10)-C(11)-O(1)115.0(6)
C(15)-C(20) 1.357(7)	C(12)-C(11)-O(1)124.6(5)	C(15)-C(20) 1.382(5)	C(11)-C(12)-C(13)117.4(5)
C(15)-C(16) 1.379(6)	C(11)-C(12)-C(13)120.2(5)	C(15)-N(1) 1.425(4)	C(8)-C(13)-C(12)120.3(5)

C(15)-N(2) 1.411(6)	C(8)-C(13)-C(12)120.8(5)	C(16)-C(17) 1.375(4)	C(16)-C(15)-C(20)118.1(4)
C(16)-C(17) 1.389(7)	C(20)-C(15)-C(16)116.5(5)	C(17)-C(18) 1.361(5)	C(16)-C(15)-N(1)121.7(4)
C(17)-C(18) 1.355(8)	C(20)-C(15)-N(2)122.9(4)	C(18)-O(2) 1.375(4)	C(20)-C(15)-N(1)120.2(4)
C(18)-C(19) 1.363(6)	C(16)-C(15)-N(2)120.6(5)	C(18)-C(19) 1.386(5)	C(15)-C(16)-C(17)121.4(4)
C(18)-O(2') 1.374(13)	C(15)-C(16)-C(17)118.0(6)	C(19)-C(20) 1.365(5)	C(18)-C(17)-C(16)120.0(4)
C(18)-O(2) 1.438(8)	C(18)-C(17)-C(16)126.2(7)	C(21)-O(2) 1.410(4)	C(17)-C(18)-O(2)125.2(4)
C(19)-C(20) 1.331(8)	C(17)-C(18)-C(19)111.4(7)	C(22)-C(27) 1.359(7)	C(17)-C(18)-C(19)119.5(4)
C(21)-O(2) 1.113(9)	C(17)-C(18)-O(2')84.0(8)	C(22)-C(23) 1.371(7)	O(2)-C(18)-C(19)115.2(4)
C(21)-O(2') 1.365(12)	C(19)-C(18)-O(2')164.1(9)	C(22)-N(3) 1.483(6)	C(20)-C(19)-C(18)120.1(4)
N(1)-N(1)#1 1.416(6)	C(17)-C(18)-O(2)140.9(9)	C(23)-C(24) 1.391(6)	C(19)-C(20)-C(15)120.9(4)
C(1)-N(1) 1.254(5)	C(19)-C(18)-O(2)107.4(8)	C(24)-C(25) 1.391(5)	C(27)-C(22)-C(23)115.7(6)
C(1)-C(2) 1.464(5)	O(2')-C(18)-O(2)56.9(5)	C(25)-C(26) 1.389(6)	C(27)-C(22)-N(3)118.6(7)
C(2)-C(3) 1.360(5)	C(20)-C(19)-C(18)125.3(7)	C(25)-N(2) 1.401(5)	C(23)-C(22)-N(3)125.7(7)
C(2)-C(7) 1.383(6)	C(19)-C(20)-C(15)122.1(6)	C(26)-C(27) 1.396(6)	C(22)-C(23)-C(24)123.0(6)
C(3)-C(4) 1.376(5)	O(2)-C(21)-O(2')64.6(7)	C(28)-C(29) 1.358(5)	C(25)-C(24)-C(23)119.8(5)
C(4)-C(5) 1.384(6)	C(1)-N(1)-N(1)#1112.7(5)	C(28)-C(33) 1.381(5)	C(26)-C(25)-C(24)118.4(5)
C(5)-C(6) 1.375(6)	C(5)-N(2)-C(15)122.4(4)	C(28)-N(2) 1.427(5)	C(26)-C(25)-N(2)122.0(5)
C(5)-N(2) 1.392(5)	C(5)-N(2)-C(8)119.4(4)	C(29)-C(30) 1.382(5)	C(24)-C(25)-N(2)119.6(5)
C(6)-C(7) 1.388(5)	C(15)-N(2)-C(8)118.1(3)	C(30)-C(31) 1.373(6)	C(25)-C(26)-C(27)118.6(5)
C(8)-C(13) 1.373(6)	C(11)-O(1)-C(14)117.6(5)	C(31)-C(32) 1.363(6)	C(22)-C(27)-C(26)124.4(6)
C(8)-C(9) 1.374(6)	C(21)-O(2)-C(18)119.4(9)	C(31)-O(3) 1.380(6)	C(29)-C(28)-C(33)117.6(5)
C(8)-N(2) 1.431(5)	C(21)-O(2')-C(18)107.5(8)	C(32)-C(33) 1.383(6)	C(29)-C(28)-N(2)120.4(5)
C(9)-C(10) 1.365(6)	N(1)-C(1)-C(2)123.3(4)	C(34)-O(3) 1.381(6)	C(33)-C(28)-N(2)122.0(5)
C(10)-C(11) 1.353(6)	C(3)-C(2)-C(7)118.1(4)	C(35)-C(40) 1.363(5)	C(28)-C(29)-C(30)122.2(5)
C(11)-C(12) 1.366(7)	C(3)-C(2)-C(1)119.5(4)	C(35)-C(36) 1.386(5)	C(31)-C(30)-C(29)119.2(5)
C(11)-O(1) 1.373(6)	C(7)-C(2)-C(1)122.3(4)	C(35)-N(2) 1.411(5)	C(32)-C(31)-C(30)119.9(6)
C(12)-C(13) 1.375(6)	C(2)-C(3)-C(4)121.9(5)	C(36)-C(37) 1.395(6)	C(32)-C(31)-O(3)126.2(6)
C(14)-O(1) 1.428(6)	C(3)-C(4)-C(5)120.5(4)	C(37)-C(38) 1.350(5)	C(30)-C(31)-O(3)113.9(6)
C(15)-C(20) 1.357(7)	C(6)-C(5)-C(4)118.1(4)	C(38)-C(39) 1.353(5)	C(31)-C(32)-C(33)119.9(6)
C(15)-C(16) 1.379(6)	C(6)-C(5)-N(2)121.4(4)	C(38)-O(4) 1.414(5)	C(28)-C(33)-C(32)121.2(5)
	C(4)-C(5)-N(2)120.5(4)	C(39)-C(40) 1.368(5)	C(40)-C(35)-C(36)118.4(4)
	C(5)-C(6)-C(7)120.9(4)	C(41)-O(4) 1.377(4)	C(40)-C(35)-N(2)120.0(4)
	C(2)-C(7)-C(6)120.5(4)	C(42)-C(43) 1.384(5)	C(36)-C(35)-N(2)121.6(5)
	C(13)-C(8)-C(9)117.7(5)	C(42)-C(47) 1.385(5)	C(35)-C(36)-C(37)120.9(4)
	C(13)-C(8)-N(2)121.0(4)	C(42)-N(6) 1.460(5)	C(38)-C(37)-C(36)118.5(5)

C(9)-C(8)-N(2)121.3(4)
C(11)-C(10)-C(9)120.2(5)
C(10)-C(11)-C(12)119.6(5)
C(10)-C(11)-O(1)115.8(5)
C(12)-C(11)-O(1)124.6(5)
C(11)-C(12)-C(13)120.2(5)
C(8)-C(13)-C(12)120.8(5)
C(20)-C(15)-C(16)116.5(5)
C(20)-C(15)-N(2)122.9(4)

C(43)-C(44) 1.394(5)	C(37)-C(38)-C(39)121.0(5)
C(44)-C(45) 1.398(4)	C(37)-C(38)-O(4)124.1(5)
C(45)-C(46) 1.389(5)	C(39)-C(38)-O(4)114.8(5)
C(45)-N(4) 1.410(4)	C(38)-C(39)-C(40)120.9(4)
C(46)-C(47) 1.377(5)	C(35)-C(40)-C(39)120.3(4)
C(48)-C(49) 1.364(5)	C(43)-C(42)-C(47)117.8(4)
C(48)-C(53) 1.379(5)	C(43)-C(42)-N(6)118.9(4)
C(48)-N(4) 1.428(4)	C(47)-C(42)-N(6)123.1(4)
C(49)-C(50) 1.390(5)	C(42)-C(43)-C(44)122.7(4)
C(50)-C(51) 1.370(5)	C(43)-C(44)-C(45)119.0(4)
C(51)-C(52) 1.366(5)	C(46)-C(45)-C(44)117.9(4)
C(51)-O(5) 1.382(5)	C(46)-C(45)-N(4)121.9(4)
C(52)-C(53) 1.379(5)	C(44)-C(45)-N(4)120.1(4)
C(54)-O(5) 1.409(4)	C(47)-C(46)-C(45)122.4(4)
C(55)-C(60) 1.370(5)	C(46)-C(47)-C(42)120.2(4)
C(55)-C(56) 1.385(5)	C(49)-C(48)-C(53)118.2(4)
C(55)-N(4) 1.431(4)	C(49)-C(48)-N(4)121.6(4)
C(56)-C(57) 1.389(5)	C(53)-C(48)-N(4)120.2(4)
C(57)-C(58) 1.362(5)	C(48)-C(49)-C(50)121.7(4)
C(58)-C(59) 1.360(6)	C(51)-C(50)-C(49)119.1(4)
C(58)-O(6) 1.394(5)	C(52)-C(51)-C(50)119.9(5)
C(59)-C(60) 1.385(5)	C(52)-C(51)-O(5)115.7(5)
C(61)-O(6) 1.352(5)	C(50)-C(51)-O(5)124.4(5)
C(62)-N(6) 1.278(4)	C(51)-C(52)-C(53)120.4(5)
C(62)-C(63) 1.445(5)	C(52)-C(53)-C(48)120.6(4)
C(63)-C(64) 1.382(5)	C(60)-C(55)-C(56)118.9(4)
C(63)-C(68) 1.383(5)	C(60)-C(55)-N(4)120.4(4)
C(64)-C(65) 1.386(5)	C(56)-C(55)-N(4)120.7(4)
C(65)-C(66) 1.385(5)	C(55)-C(56)-C(57)120.4(4)
C(66)-C(67) 1.387(5)	C(58)-C(57)-C(56)119.1(4)
C(66)-N(5) 1.405(4)	C(59)-C(58)-C(57)121.4(5)
C(67)-C(68) 1.382(5)	C(59)-C(58)-O(6)114.6(6)
C(69)-C(74) 1.373(5)	C(57)-C(58)-O(6)124.0(5)
C(69)-C(70) 1.388(5)	C(58)-C(59)-C(60)119.5(5)
C(69)-N(5) 1.426(4)	C(55)-C(60)-C(59)120.7(4)

C(70)-C(71) 1.372(5)	N(6)-C(62)-C(63)121.6(4)
C(71)-C(72) 1.375(5)	C(64)-C(63)-C(68)117.6(4)
C(72)-O(7) 1.372(4)	C(64)-C(63)-C(62)122.7(4)
C(72)-C(73) 1.376(5)	C(68)-C(63)-C(62)119.6(4)
C(73)-C(74) 1.387(5)	C(63)-C(64)-C(65)121.3(4)
C(75)-O(7) 1.411(5)	C(66)-C(65)-C(64)120.8(4)
C(76)-C(77) 1.359(5)	C(65)-C(66)-C(67)117.9(4)
C(76)-C(81) 1.364(5)	C(65)-C(66)-N(5)119.9(4)
C(76)-N(5) 1.421(4)	C(67)-C(66)-N(5)122.2(4)
C(77)-C(78) 1.390(5)	C(68)-C(67)-C(66)120.8(4)
C(78)-C(79) 1.380(5)	C(67)-C(68)-C(63)121.4(4)
C(79)-C(80) 1.358(5)	C(74)-C(69)-C(70)117.8(4)
C(79)-O(8) 1.383(5)	C(74)-C(69)-N(5)120.7(4)
C(80)-C(81) 1.387(5)	C(70)-C(69)-N(5)121.4(4)
C(82)-O(8) 1.408(5)	C(71)-C(70)-C(69)120.9(4)
C(7)-N(3) 0.964(5)	C(70)-C(71)-C(72)120.5(4)
C(1)-C(6) 1.357(6)	O(7)-C(72)-C(71)115.8(4)
C(1)-C(2) 1.387(6)	O(7)-C(72)-C(73)124.5(4)
C(1)-C(7) 1.405(6)	C(71)-C(72)-C(73)119.8(4)
C(2)-C(3) 1.378(5)	C(72)-C(73)-C(74)119.2(4)
C(3)-C(4) 1.377(5)	C(69)-C(74)-C(73)121.8(4)
C(4)-C(5) 1.375(5)	C(77)-C(76)-C(81)118.4(4)
C(4)-N(1) 1.406(5)	C(77)-C(76)-N(5)120.2(4)
C(5)-C(6) 1.377(5)	C(81)-C(76)-N(5)121.3(4)
C(8)-C(13) 1.358(5)	C(76)-C(77)-C(78)120.8(4)
C(8)-C(9) 1.366(5)	C(79)-C(78)-C(77)119.9(5)
C(8)-N(1) 1.424(5)	C(80)-C(79)-C(78)119.5(5)
C(9)-C(10) 1.365(5)	C(80)-C(79)-O(8)124.7(5)
C(10)-C(11) 1.356(6)	C(78)-C(79)-O(8)115.8(5)
C(11)-C(12) 1.354(6)	C(79)-C(80)-C(81)119.5(4)
C(11)-O(1) 1.414(5)	C(76)-C(81)-C(80)121.8(4)
C(12)-C(13) 1.428(5)	C(4)-N(1)-C(8)118.6(4)
C(14)-O(1) 1.384(5)	C(4)-N(1)-C(15)120.3(4)
C(15)-C(16) 1.375(5)	C(8)-N(1)-C(15)118.9(3)
C(15)-C(20) 1.382(5)	C(25)-N(2)-C(35)122.6(4)

C(15)-N(1) 1.425(4)	C(25)-N(2)-C(28)118.4(4)
C(16)-C(17) 1.375(4)	C(35)-N(2)-C(28)117.9(4)
C(17)-C(18) 1.361(5)	C(45)-N(4)-C(48)121.2(3)
C(18)-O(2) 1.375(4)	C(45)-N(4)-C(55)118.7(4)
C(18)-C(19) 1.386(5)	C(48)-N(4)-C(55)117.7(3)
C(19)-C(20) 1.365(5)	C(66)-N(5)-C(76)119.9(3)
C(21)-O(2) 1.410(4)	C(66)-N(5)-C(69)120.7(4)
C(22)-C(27) 1.359(7)	C(76)-N(5)-C(69)117.8(3)
C(22)-C(23) 1.371(7)	C(62)-N(6)-C(42)119.8(4)
C(22)-N(3) 1.483(6)	C(14)-O(1)-C(11)118.5(5)
C(23)-C(24) 1.391(6)	C(18)-O(2)-C(21)116.8(3)
C(24)-C(25) 1.391(5)	C(31)-O(3)-C(34)116.7(5)
C(25)-C(26) 1.389(6)	C(41)-O(4)-C(38)117.2(4)
C(25)-N(2) 1.401(5)	C(51)-O(5)-C(54)118.5(4)
C(26)-C(27) 1.396(6)	C(61)-O(6)-C(58)117.2(5)
C(28)-C(29) 1.358(5)	C(72)-O(7)-C(75)117.9(4)
C(28)-C(33) 1.381(5)	C(79)-O(8)-C(82)118.2(4)
C(28)-N(2) 1.427(5)	N(3)-C(7)-C(1)131.6(10)
C(29)-C(30) 1.382(5)	C(7)-N(3)-C(22)142.2(10)
C(30)-C(31) 1.373(6)	C(6)-C(1)-C(2)117.3(5)
C(31)-C(32) 1.363(6)	C(6)-C(1)-C(7)135.7(7)
C(31)-O(3) 1.380(6)	C(2)-C(1)-C(7)106.9(6)
C(32)-C(33) 1.383(6)	C(3)-C(2)-C(1)120.9(5)
C(34)-O(3) 1.381(6)	C(4)-C(3)-C(2)121.3(5)
C(35)-C(40) 1.363(5)	C(5)-C(4)-C(3)117.4(4)
C(35)-C(36) 1.386(5)	C(5)-C(4)-N(1)122.2(4)
C(35)-N(2) 1.411(5)	C(3)-C(4)-N(1)120.4(5)
C(36)-C(37) 1.395(6)	C(4)-C(5)-C(6)121.0(5)
C(37)-C(38) 1.350(5)	C(1)-C(6)-C(5)122.0(5)
C(38)-C(39) 1.353(5)	C(13)-C(8)-C(9)119.2(5)
C(38)-O(4) 1.414(5)	C(13)-C(8)-N(1)122.8(5)
C(39)-C(40) 1.368(5)	C(9)-C(8)-N(1)118.0(5)
C(41)-O(4) 1.377(4)	C(10)-C(9)-C(8)121.7(5)
C(42)-C(43) 1.384(5)	C(11)-C(10)-C(9)118.8(5)
C(42)-C(47) 1.385(5)	C(12)-C(11)-C(10)122.6(5)

C(42)-N(6) 1.460(5)	C(12)-C(11)-O(1)122.3(5)
C(43)-C(44) 1.394(5)	C(10)-C(11)-O(1)115.0(6)
C(44)-C(45) 1.398(4)	C(11)-C(12)-C(13)117.4(5)
C(45)-C(46) 1.389(5)	C(8)-C(13)-C(12)120.3(5)
C(45)-N(4) 1.410(4)	C(16)-C(15)-C(20)118.1(4)
C(46)-C(47) 1.377(5)	C(16)-C(15)-N(1)121.7(4)
C(48)-C(49) 1.364(5)	C(20)-C(15)-N(1)120.2(4)
C(48)-C(53) 1.379(5)	C(15)-C(16)-C(17)121.4(4)
C(48)-N(4) 1.428(4)	C(18)-C(17)-C(16)120.0(4)
C(49)-C(50) 1.390(5)	C(17)-C(18)-O(2)125.2(4)
C(50)-C(51) 1.370(5)	C(17)-C(18)-C(19)119.5(4)
C(51)-C(52) 1.366(5)	O(2)-C(18)-C(19)115.2(4)
C(51)-O(5) 1.382(5)	C(20)-C(19)-C(18)120.1(4)
C(52)-C(53) 1.379(5)	C(19)-C(20)-C(15)120.9(4)
C(54)-O(5) 1.409(4)	C(27)-C(22)-C(23)115.7(6)
C(55)-C(60) 1.370(5)	C(27)-C(22)-N(3)118.6(7)
C(55)-C(56) 1.385(5)	C(23)-C(22)-N(3)125.7(7)
C(55)-N(4) 1.431(4)	C(22)-C(23)-C(24)123.0(6)
C(56)-C(57) 1.389(5)	C(25)-C(24)-C(23)119.8(5)
C(57)-C(58) 1.362(5)	C(26)-C(25)-C(24)118.4(5)
C(58)-C(59) 1.360(6)	C(26)-C(25)-N(2)122.0(5)
C(58)-O(6) 1.394(5)	C(24)-C(25)-N(2)119.6(5)
C(61)-O(6) 1.352(5)	C(25)-C(26)-C(27)118.6(5)
C(62)-N(6) 1.278(4)	C(22)-C(27)-C(26)124.4(6)
C(62)-C(63) 1.445(5)	C(29)-C(28)-C(33)117.6(5)
C(63)-C(64) 1.382(5)	C(29)-C(28)-N(2)120.4(5)
C(63)-C(68) 1.383(5)	C(33)-C(28)-N(2)122.0(5)
C(64)-C(65) 1.386(5)	C(28)-C(29)-C(30)122.2(5)
C(65)-C(66) 1.385(5)	C(31)-C(30)-C(29)119.2(5)
C(66)-C(67) 1.387(5)	C(32)-C(31)-C(30)119.9(6)
C(66)-N(5) 1.405(4)	C(32)-C(31)-O(3)126.2(6)
C(67)-C(68) 1.382(5)	C(30)-C(31)-O(3)113.9(6)
C(69)-C(74) 1.373(5)	C(31)-C(32)-C(33)119.9(6)
C(69)-C(70) 1.388(5)	C(28)-C(33)-C(32)121.2(5)
C(69)-N(5) 1.426(4)	C(40)-C(35)-C(36)118.4(4)

C(70)-C(71) 1.372(5)	C(40)-C(35)-N(2)120.0(4)
C(71)-C(72) 1.375(5)	C(36)-C(35)-N(2)121.6(5)
C(72)-O(7) 1.372(4)	C(35)-C(36)-C(37)120.9(4)
C(72)-C(73) 1.376(5)	C(38)-C(37)-C(36)118.5(5)
C(73)-C(74) 1.387(5)	C(37)-C(38)-C(39)121.0(5)
C(75)-O(7) 1.411(5)	C(37)-C(38)-O(4)124.1(5)
C(76)-C(77) 1.359(5)	C(39)-C(38)-O(4)114.8(5)
C(76)-C(81) 1.364(5)	C(38)-C(39)-C(40)120.9(4)
C(76)-N(5) 1.421(4)	C(35)-C(40)-C(39)120.3(4)
C(77)-C(78) 1.390(5)	C(43)-C(42)-C(47)117.8(4)
C(78)-C(79) 1.380(5)	C(43)-C(42)-N(6)118.9(4)
C(79)-C(80) 1.358(5)	C(47)-C(42)-N(6)123.1(4)
C(79)-O(8) 1.383(5)	C(42)-C(43)-C(44)122.7(4)
C(80)-C(81) 1.387(5)	C(43)-C(44)-C(45)119.0(4)
C(82)-O(8) 1.408(5)	C(46)-C(45)-C(44)117.9(4)
C(7)-N(3) 0.964(5)	C(46)-C(45)-N(4)121.9(4)
	C(44)-C(45)-N(4)120.1(4)
	C(47)-C(46)-C(45)122.4(4)
	C(46)-C(47)-C(42)120.2(4)
	C(49)-C(48)-C(53)118.2(4)
	C(49)-C(48)-N(4)121.6(4)
	C(53)-C(48)-N(4)120.2(4)



Fig. SI1 Thermograms of compounds MS-1 and MS-2.



Fig. SI2Alteration in the UV-Vis spectrum at 520 nm of MS-1 (a) andMS-2 (b) in CH_2Cl_2 solutions with the same concentration of 1.0×10^{-5} MuponadditionofTFA.









b



c



Fig. SI3 ESI-MS (a), ESI-MS+TFA (b), ¹H NMR (c) and ¹H NMR+TFA (d) spectra of compound MS-1.





a





b







Fig. SI4 ESI-MS (a), ESI-MS+TFA (b), ¹H NMR (c) and ¹H NMR+TFA (d) spectra of compound MS-2.



Fig. SI5 Fluorescence emission spectra and fluorescence intensity vs p[TFA] curve (Inset) for compound **MS-1** in CH₂Cl₂ at 1.0×10^{-4} M concentration (excited at 350 nm).



Fig. SI6 I-V curves for single-crystal sample of **MS-2** (black line) and its hydrochloric adduct (red line) at room temperature.



Fig. SI7 The calculated UV-Vis spectrum of MS-1 (a) and MS- 1^{2+} (b); the calculated UV-Vis spectrum of MS-2 (c), MS- 2^{+} (d) and MS- 2^{2+} (e).



Fig. SI8 Plots of electron-recombination lifetime as a function of bias voltage.



Fig. SI9 Space charge limitation of current J-V characteristic of **MS-2** obtained in the dark for the hole-only device.