Supporting Information for

Synthesis and electrochemical and spectroscopic characterization of 4,7-diamino-1,10-phenanthrolines and their precursors

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$\begin{array}{cccc} 2CaH_8O(0, S(C_2H_8O_2)) & 2C(AH_8O) \\ 2(CaH_8O), S(C_2H_8O_2) & 2(CaH_8O) \\ 1 \\ Temperature [K] & 295(2) & 295(2) & 295(2) \\ 2 \\ Wavelength (Å) & 0.71073 & 0.71073 & 0.71073 \\ Crystal system & triclinic & triclinic & monoclinic \\ Space group & P-1 & P-1 & P2_{1/c} \\ Unit cell dimensions & a \\ a [Å] & 9.1767(13) & 12.1394(7) & 9.0665(4) \\ b [Å] & 10.3249(14) & 12.6397(5) & 27.0123(10) \\ c [Å] & 14.9935(12) & 12.9635(6) & 15.0843(5) \\ a [P] & 83.725(9) & 89.230(4) & 90 \\ \beta [P] & 82.567(9) & 75.454(4) & 91.867(4) \\ \gamma [P] & 87.109(12) & 79.332(4) & 90 \\ Volume [Å^3] & 1399.3(3) & 1890.91(16) & 3692.3(2) \\ Z & 2 & 4 \\ Calculated density [Mg/m^3] & 1.432 & 1.278 & 1.367 \\ Absorption coefficient [mm^-1] & 0.642 & 0.083 & 0.195 \\ F(000) & 620 & 768 & 1592 \\ Crystal dimensions [mm] & 0.36 x 0.08 x 0.06 & 0.17 x 0.08 x 0.07 & 0.37 x 0.15 x 0.14 \\ \theta range for data collection [P] & 3.33 - 25.05 & 3.57 - 27.95 & 3.46 - 29.56 \\ Index ranges & -12 \le h \le 12 & -16 \le h \le 15 & -10 \le h \le 11 \\ -12 \le k \le 14 & -15 \le k \le 14 & -36 \le k \le 27 \\ -18 \le 1 \le 21 & -17 \le 1 \le 14 & -20 \le 1 \le 15 \\ Independent reflections & 6529 (R(int) = 0.0784] & 8928 [R(int) = 0.0412] & 9010 [R(int) = 0.0310] \\ Data / restraints / parameters & 6529 (0.328 & 8928/2/516 & 90100/0500 \\ Goodness-of-fit on F^2 & 0.912 & 1.019 & 1.034 \\ R indices (all data) & R_1 = 0.0650, & R_1 = 0.0667, & R_1 = 0.0604, \\ W_8 = 0.209 & W_8 = 0.1589 & W_8 = 0.1438 \\ R indices (all data) & R_1 = 0.0650, & R_1 = 0.0667, & R_1 = 0.0604, \\ W_8 = 0.209 & W_8 = 0.1589 & W_8 = 0.1438 \\ R indices (all data) & R_1 = 0.0650, & R_1 = 0.0667, & R_1 = 0.0604, \\ W_8 = 0.209 & W_8 = 0.1599 & W_8 = 0.1438 \\ R indices (all data) & R_1 = 0.0650, & R_1 = 0.0667, & R_1 = 0.0604, \\ W_8 = 0.209 & W_8 = 0.1589 & W_8 = 0.1655 \\ Largest diff. Peak and hole & 0.530/-0.437 & 0.312/-0.266 & 0.401/-0.329 \\ CCDC number & 4479401 & 1917090 & 1919692 \\ \end{array}$	Empirical formula	$C_{22}H_{25}EN_4 2(CHCl_2)$	$C_{27}H_{21}N_{5}O$	$C_{27}H_{21}N_5OS_2$
Formula weight603.19727.84759.91Temperature [K]295(2)295(2)295(2)Wavelength (Å)0.710730.710730.71073Crystal systemtriclinictriclinicmonoclinicSpace group $P-1$ $P-1$ P_{-1} Unit cell dimensionsa[Å]9.1767(13)12.1394(7)9.0665(4)a [Å]9.1767(13)12.6397(5)27.0123(10)c [Å]10.3249(14)12.6397(5)27.0123(10)c [Å]14.9935(12)12.9635(6)15.0843(5)a [°]83.725(9)89.230(4)90b [Å]1.399.3(3)1890.91(16)3692.3(2)Z224Calculated density [Mg/m³]1.4321.2781.3370.36 x 0.08 x 0.060.17 x 0.08 x 0.070.37 x 0.15 x 0.14 θ range for data collection [°]3.33 - 25.053.57 - 27.953.46 - 29.56Index ranges $-12 \le h \le 12$ $-16 \le h \le 15$ $-10 \le h \le 11$ $-12 \le h \le 12$ $-17 \le 1 \le 14$ $-36 \le 4 \le 27$ $-18 \le 1 \ge 21$ $-17 \le 1 \le 14$ $-20 \le 1 \le 15$ Reflections collected112851691822276Independent reflections6529 [R(int) = 0.0784]8928 [R(int) = 0.0412]9010 [R(int) = 0.0310]Data / restraints / parameters6529 (0.0288228/25169010/0/500Goodness-of-fit on F ² 0.9121.0191.034Final R indices [I-2 σ (I)]*R ₁ = 0.0650, R ₁ = 0.0667, R ₁ = 0.0664, wR ₂ = 0.1458wR ₂ = 0.1589 </td <td>Empirical formala</td> <td>C2211231 114, 2(CIICI3)</td> <td>$2(C_4H_0O_1) = 5(C_2H_0O_2)$</td> <td>$2(C_4H_{\circ}O)$</td>	Empirical formala	C2211231 114, 2(CIICI3)	$2(C_4H_0O_1) = 5(C_2H_0O_2)$	$2(C_4H_{\circ}O)$
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$ \begin{array}{c ccccc} Wavelength (Å) & 0.71073 & 0.71073 & 0.71073 \\ \hline Wavelength (Å) & 0.71073 & 0.71073 & 0.71073 \\ \hline Crystal system & triclinic & triclinic & monoclinic \\ \hline Space group & P-1 & P-1 & P_{1}/c \\ \hline With cell dimensions & a [Å] & 9.1767(13) & 12.1394(7) & 9.0665(4) \\ \hline b [Å] & 10.3249(14) & 12.6397(5) & 27.0123(10) \\ \hline c [Å] & 14.9935(12) & 12.9635(6) & 15.0843(5) \\ \hline a [°] & 83.725(9) & 89.230(4) & 90 \\ \hline \beta [°] & 82.567(9) & 75.454(4) & 91.867(4) \\ \hline \gamma [°] & 87.109(12) & 79.332(4) & 90 \\ \hline Volume [Å^3] & 1399.3(3) & 1890.91(16) & 3692.3(2) \\ Z & 2 & 2 & 4 \\ \hline Calculated density [Mg/m^3] & 1.432 & 1.278 & 1.367 \\ \hline Absorption coefficient [mm-1] & 0.642 & 0.083 & 0.195 \\ \hline F(000) & 620 & 768 & 1592 \\ \hline Crystal dimensions [mm] & 0.36 x 0.08 x 0.06 & 0.17 x 0.08 x 0.07 & 0.37 x 0.15 x 0.14 \\ \hline a range for data collection [°] & 3.33 - 25.05 & 3.57 - 27.95 & 3.46 - 29.56 \\ \hline Index ranges & -12 \leq h \leq 12 & -16 \leq h \leq 15 & -10 \leq h \leq 11 \\ -12 \leq k \leq 14 & -15 \leq k \leq 14 & -36 \leq k \leq 27 \\ -18 \leq 1 \leq 21 & -17 \leq 1 \leq 14 & -20 \leq 1 \leq 15 \\ \hline Independent reflections & 6529 [R(int) = 0.0784] & 8928 [R(int) = 0.0412] & 9010 [R(int) = 0.0310] \\ \hline Data / restraints / parameters & 6529 /0/328 & 8928/2/516 & 90100/0500 \\ \hline Goodness-of-fit on F^2 & 0.912 & 1.019 & 1.034 \\ \hline Final R indices ([1>2\sigma(I)])^* & R_1 = 0.0650, & R_1 = 0.0667, & R_1 = 0.0604, \\ wR_2 = 0.1458 & wR_2 = 0.1589 & wR_2 = 0.1438 \\ R indices (all data) & R_1 = 0.1830, & R_1 = 0.1391, & R_1 = 0.0991, \\ wR_2 = 0.0291 & wR_2 = 0.1599 & wR_2 = 0.1438 \\ R indices (all data) & R_1 = 0.1830, & R_1 = 0.1391, & R_1 = 0.0991, \\ wR_2 = 0.0291 & WR_2 = 0.1589 & wR_2 = 0.1438 \\ R indices (all data) & R_1 = 0.1830, & R_1 = 0.1391, & R_1 = 0.0991, \\ wR_2 = 0.0291 & WR_2 = 0.1589 & WR_2 = 0.1458 \\ Largest diff. Peak and hole & 0.530 /-0.437 & 0.312/-0.266 & 0.401/-0.329 \\ \hline CDC number & 1479401 & 1917090 & 1919692 \\ \hline \end{array}$	Temperature [K]	295(2)	295(2)	295(2)
Crystal systemtriclinictriclinictriclinicmonoclinicSpace group $P-1$ $P-1$ $P-1$ $P_{21/c}$ Unit cell dimensions $a[\Lambda]$ 9.1767(13)12.1394(7)9.0665(4)b [Å]10.3249(14)12.6397(5)27.0123(10)c [Å]14.9935(12)12.9635(6)15.0843(5)a [V]83.725(9)89.230(4)90 β [°]82.567(9)75.454(4)91.867(4) γ [°]87.109(12)79.332(4)90Volume [ų]1399.3(3)1890.91(16)3692.3(2)Z224Calculated density [Mg/m³]1.4321.2781.367Absorption coefficient [mm ⁻¹]0.6420.0830.195F(000)6207681592Crystal dimensions [mm]0.36 x 0.08 x 0.060.17 x 0.08 x 0.070.37 x 0.15 x 0.14 θ range for data collection [°]3.33 - 25.05 $3.57 - 27.95$ $3.46 - 29.56$ Index ranges $-12 \le h \le 12$ $-16 \le h \le 15$ $-10 \le h \le 11$ $-12 \le k \le 14$ $-15 \le k \le 14$ $-36 \le k \ge 77$ $-18 \le 1 \ge 21$ $-17 \le 1 \le 14$ $-20 \le 1 \le 15$ Independent reflections6529 /0/3288928/2/51690100/0500Goodness-of-fit on F²0.9121.0191.034Final R indices (all data) $R_1 = 0.0650$, $R_1 = 0.0667$, $R_1 = 0.0604$, w $R_2 = 0.1438$ $R_1 = 0.1391$, $R_1 = 0.0991$, w $R_2 = 0.1438$ R indices (all data) $R_1 = 0.1201$ $W_2 = 0.1299$ $W_2 = 0.1438$ R indices (all	Wavelength (Å)	0.71073	0.71073	0.71073
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	Crystal system	triclinic	triclinic	monoclinic
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Space group	P-1	P-1	$P2_1/c$
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$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	a [Å]	9,1767(13)	12,1394(7)	9.0665(4)
$ \begin{bmatrix} \alpha \\ 1 \\ \alpha \end{bmatrix} = 10000000000000000000000000000000000$	b [Å]	10 3249(14)	12.6397(5)	27 0123(10)
$ \begin{array}{c} \alpha \left[\frac{n}{2} \right] & 83.725(9) & 89.230(4) & 90 \\ \beta \left[\frac{n}{2} \right] & 83.725(9) & 89.230(4) & 90 \\ \gamma \left[\frac{n}{2} \right] & 83.725(9) & 75.454(4) & 91.867(4) \\ \gamma \left[\frac{n}{2} \right] & 87.109(12) & 79.332(4) & 90 \\ Volume \left[\mathbb{Å}^3 \right] & 1399.3(3) & 1890.91(16) & 3692.3(2) \\ Z & 2 & 2 & 4 \\ Calculated density [Mg/m^3] & 1.432 & 1.278 & 1.367 \\ Absorption coefficient [mm^{-1}] & 0.642 & 0.083 & 0.195 \\ F(000) & 620 & 768 & 1592 \\ Crystal dimensions [mm] & 0.36 x 0.08 x 0.06 & 0.17 x 0.08 x 0.07 & 0.37 x 0.15 x 0.14 \\ \theta \ range \ for \ data \ collection \left[\frac{n}{2} \right] & 3.33 - 25.05 & 3.57 - 27.95 & 3.46 - 29.56 \\ Index \ ranges & -12 \le h \le 12 & -16 \le h \le 15 & -10 \le h \le 11 \\ -12 \le k \le 14 & -15 \le k \le 14 & -36 \le k \le 27 \\ -18 \le 12 1 & -17 \le 1 \le 14 & -20 \le 1 \le 15 \\ \end{array} $ Reflections collected & 11285 & 16918 & 22276 \\ Independent \ reflections & 6529 \ [R(int) = 0.0784] \ 8928 \ [R(int) = 0.0412] & 9010 \ [R(int) = 0.0310] \\ Data / \ restraints / \ parameters \\ Goodness-of-fit \ n \ F^2 & 0.912 & 1.019 & 1.034 \\ Final \ R \ indices \ [I>2\sigma(I)]^* & R_1 = 0.0650, \ R_1 = 0.0667, \ R_1 = 0.0604, \\ w_{R_2} = 0.1458 & w_{R_2} = 0.1589 & w_{R_2} = 0.1438 \\ R \ indices \ (all \ dat) & R_1 = 0.1830, \ R_1 = 0.1391, \ w_{R_2} = 0.1438 \\ R \ indices \ (all \ dat) & R_1 = 0.1830, \ R_1 = 0.1391, \ w_{R_2} = 0.1665 \\ Largest \ diff. \ Peak \ and \ hole \ 0.530 \ .0.437 & 0.312 \ .0.266 & 0.401 \ .0.329 \\ \hline \ CDC n \ number & 1479401 \ 1917090 & 1919692 \\ \hline \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \	c [Å]	14.9935(12)	12,9635(6)	15 0843(5)
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $		83 725(9)	89 230(4)	90
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	~ [] β [º]	82 567(9)	75 454(4)	91 867(4)
111399.3(3)1399.3(3)1399.3(1)Volume [Å ³]1399.3(3)1890.91(16)3692.3(2)Z24Calculated density [Mg/m ³]1.4321.2781.367Absorption coefficient [mm ⁻¹]0.6420.0830.195F(000)6207681592Crystal dimensions [mm]0.36 x 0.08 x 0.060.17 x 0.08 x 0.070.37 x 0.15 x 0.14 θ range for data collection [°] $3.33 - 25.05$ $3.57 - 27.95$ $3.46 - 29.56$ Index ranges $-12 \le h \le 12$ $-16 \le h \le 15$ $-10 \le h \le 11$ $-12 \le k \le 14$ $-15 \le k \le 14$ $-36 \le k \le 27$ $-18 \le 1 \le 21$ $-17 \le 1 \le 4$ $-20 \le 1 \le 15$ Reflections collected112851691822276Independent reflections6529 /0/3288928/2/5169010/0/500Goodness-of-fit on F ² 0.9121.0191.034Final R indices [I>2\sigma(I)]*R ₁ = 0.0650, R ₁ = 0.0667, R ₁ = 0.0667, R ₁ = 0.0604, wR ₂ = 0.1438R ₁ = 0.1391, R ₁ = 0.0991, wR ₂ = 0.1999wR ₂ = 0.2091wR ₂ = 0.1999wR ₂ = 0.1665Largest diff. Peak and hole0.530 /-0.4370.312/-0.2660.401/-0.329CCDC number1479401191709019170901919692	v [°]	87 109(12)	79 332(4)	90
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$\begin{array}{c c c c c c c c c c c c c c c c c c c $	7	2	2	4
Absorption coefficient [mm] 1.452 1.637 Absorption coefficient [mm] 0.642 0.083 0.195 F(000) 620 768 1592 Crystal dimensions [mm] $0.36 \ge 0.08 \ge 0.06$ $0.17 \ge 0.08 \ge 0.07$ $0.37 \ge 0.15 \ge 0.14$ θ range for data collection [°] $3.33 - 25.05$ $3.57 - 27.95$ $3.46 - 29.56$ Index ranges $-12 \le h \le 12$ $-16 \le h \le 15$ $-10 \le h \le 11$ $-12 \le k \le 14$ $-15 \le k \le 14$ $-36 \le k \le 27$ $-18 \le 1 \le 21$ $-17 \le 1 \le 14$ $-20 \le 1 \le 15$ Reflections collected 11285 16918 22276 Independent reflections 6529 [R(int) = 0.0784] 8928 [R(int) = 0.0412] 9010 [R(int) =Data / restraints / parameters $6529 / 0/328$ $8928/2/516$ $9010/0/500$ Goodness-of-fit on F ² 0.912 1.019 1.034 Final R indices [I> 2σ (I)]* $R_1 = 0.0650$, $R_1 = 0.0667$, $R_1 = 0.0604$, $wR_2 = 0.1438$ $R_1 = 0.1830$, $R_1 = 0.1391$, $R_1 = 0.0991$, $wR_2 = 0.2091$ $wR_2 = 0.2091$ $wR_2 = 0.1999$ $wR_2 = 0.1665$ Largest diff. Peak and hole $0.530 / 0.437$ $0.312 / 0.266$ $0.401 / -0.329$ CCDC number 1479401 197090 1919692	Calculated density $[Mg/m^3]$	1 432	1 278	1 367
F(000)6207681592Crystal dimensions [mm]0.36 x 0.08 x 0.060.17 x 0.08 x 0.070.37 x 0.15 x 0.14 θ range for data collection [°]3.33 - 25.053.57 - 27.953.46 - 29.56Index ranges $-12 \le h \le 12$ $-16 \le h \le 15$ $-10 \le h \le 11$ $-12 \le k \le 14$ $-15 \le k \le 14$ $-36 \le k \le 27$ $-18 \le 1 \le 21$ $-17 \le 1 \le 14$ $-20 \le 1 \le 15$ Reflections collected112851691822276Independent reflections6529 [R(int) = 0.0784]8928 [R(int) = 0.0412]9010 [R(int) =0.0310]0.34529 [N/3288928/2/5169010/0/500Goodness-of-fit on F²0.9121.0191.034Final R indices [I>2\sigma(I)]*R ₁ = 0.0650,R ₁ = 0.0667,R ₁ = 0.0604,wR ₂ = 0.1458wR ₂ = 0.1589wR ₂ = 0.1438R indices (all data)R ₁ = 0.1391,R ₁ = 0.0991,wR ₂ = 0.2091wR ₂ = 0.1999wR ₂ = 0.1665Largest diff. Peak and hole0.530 /-0.4370.312/-0.2660.401/-0.329147940119170901919692	Absorption coefficient [mm ⁻¹]	0.642	0.083	0.195
Crystal dimensions [mm] θ range for data collection [°]0.36 x 0.08 x 0.06 3.33 - 25.050.17 x 0.08 x 0.07 3.57 - 27.950.37 x 0.15 x 0.14 	F(000)	620	768	1592
$\begin{array}{c} 0.117 \times 0.107 \times 0.117 \times 0.107 \times 0.107 \times 0.117 \times 0.107 \times 0.117 \times 0.107 \times 0.117 \times 0.107 \times 0.117 \times 0.107 \times 0.107 \times 0.117 \times 0.107 \times 0.117 \times 0.107 \times 0.117 \times$	Crystal dimensions [mm]	0.20 0.36 x 0.08 x 0.06	$0.17 \times 0.08 \times 0.07$	$0.37 \ge 0.15 \ge 0.14$
o funge for data concertion [1] $5.53^{-} 2.5.53^{-}$	θ range for data collection [°]	333 - 2505	357 - 2795	3.46 - 29.56
Index ranges $12 \ge n \ge 12$ $10 \ge n \ge 13$ $10 \ge n \ge 11$ $-12 \le k \le 14$ $-15 \le k \le 14$ $-36 \le k \le 27$ $-18 \le 1 \le 21$ $-17 \le 1 \le 14$ $-20 \le 1 \le 15$ Reflections collected 11285 16918 22276 Independent reflections $6529 [R(int) = 0.0784]$ $8928 [R(int) = 0.0412]$ $9010 [R(int) = 0.0310]$ Data / restraints / parameters $6529 / 0/328$ $8928 / 2/516$ $9010 / 0/500$ Goodness-of-fit on F ² 0.912 1.019 1.034 Final R indices $[I > 2\sigma(I)]^*$ $R_1 = 0.0650$, $R_1 = 0.0667$, $R_1 = 0.0604$,wR ₂ = 0.1458wR ₂ = 0.1589wR ₂ = 0.1438R indices (all data) $R_1 = 0.1830$, $R_1 = 0.1391$, $R_1 = 0.0991$,wR ₂ = 0.2091wR ₂ = 0.1999wR ₂ = 0.1665Largest diff. Peak and hole $0.530 / -0.437$ $0.312 / -0.266$ $0.401 / -0.329$ CCDC number 1479401 1917090 1919692	Index ranges	-12 < h < 12	-16 < h < 15	-10 < h < 11
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Index Tunges	$-12 \le h \le 12$ -12 < k < 14	-15 < k < 14	-36 < k < 27
Reflections collected 11285 16918 22276 Independent reflections $6529 [R(int) = 0.0784]$ $8928 [R(int) = 0.0412]$ $9010 [R(int) = 0.0310]$ Data / restraints / parameters $6529 / 0/328$ $8928 / 2/516$ $9010 / 0/500$ Goodness-of-fit on F ² 0.912 1.019 1.034 Final R indices $[I > 2\sigma(I)]^*$ $R_1 = 0.0650$, $R_1 = 0.0667$, $R_1 = 0.0604$, $wR_2 = 0.1458$ $wR_2 = 0.1458$ R indices (all data) $R_1 = 0.1830$, $R_1 = 0.1391$, $R_1 = 0.0991$, $wR_2 = 0.1665$ Largest diff. Peak and hole $0.530 / -0.437$ $0.312 / -0.266$ $0.401 / -0.329$ CCDC number 1479401 1917090 1919692		-18 < 1 < 21	-17 < 1 < 14	-20 < 1 < 15
Independent reflections 11203 10510 10510 12210 Independent reflections $6529 [R(int) = 0.0784]$ $8928 [R(int) = 0.0412]$ $9010 [R(int) = 0.0310]$ Data / restraints / parameters $6529 / 0/328$ $8928 / 2/516$ $9010 / 0/500$ Goodness-of-fit on F ² 0.912 1.019 1.034 Final R indices $[I>2\sigma(I)]^*$ $R_1 = 0.0650$, $R_1 = 0.0667$, $R_1 = 0.0604$, $wR_2 = 0.1458$ $wR_2 = 0.1458$ R indices (all data) $R_1 = 0.1830$, $R_1 = 0.1391$, $R_1 = 0.0991$, $wR_2 = 0.1665$ Largest diff. Peak and hole $0.530 / -0.437$ $0.312 / -0.266$ $0.401 / -0.329$ CCDC number 1479401 1917090 1919692	Reflections collected	11285	16918	20 _ 1 _ 13
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Independent reflections	6529 [R(int) - 0.0784]	8928 [R(int) - 0.0412]	9010 [R(int) -
Data / restraints / parameters $6529 / 0/328$ $8928/2/516$ $9010/0/500$ Goodness-of-fit on F2 0.912 1.019 1.034 Final R indices $[I>2\sigma(I)]^*$ $R_1 = 0.0650$, $R_1 = 0.0667$, $R_1 = 0.0604$, $wR_2 = 0.1458$ $wR_2 = 0.1458$ R indices (all data) $R_1 = 0.1830$, $R_1 = 0.1391$, $R_1 = 0.0991$, $wR_2 = 0.1665$ Largest diff. Peak and hole $0.530 / -0.437$ $0.312/-0.266$ CCDC number 1479401 1917090 1919692	independent reflections	0.027 [R(IIII) = 0.0704]	0.0412	0.03101
Goodness-of-fit on F^2 0.912 1.019 1.034 Final R indices $[I>2\sigma(I)]^*$ R ₁ = 0.0650, R ₁ = 0.0667, R ₁ = 0.0604, WR ₂ = 0.1458 WR ₂ = 0.1589 WR ₂ = 0.1438 R indices (all data) R ₁ = 0.1830, R ₁ = 0.1391, WR ₂ = 0.1999 WR ₂ = 0.1665 0.401/-0.329 Largest diff. Peak and hole 0.530 /-0.437 0.312/-0.266 0.401/-0.329 *Structure process of fixed on E 2 and fixed on	Data / restraints / parameters	6529 /0/328	8928/2/516	9010/0/500
Final R indices $[I>2\sigma(I)]^*$ R i = 0.0650, wR2 = 0.1458R i = 0.0667, wR2 = 0.1589R i = 0.0604, wR2 = 0.1438R indices (all data)R i = 0.1830, WR2 = 0.2091R i = 0.1391, wR2 = 0.1999R i = 0.0991, wR2 = 0.1665Largest diff. Peak and hole0.530 /-0.4370.312/-0.2660.401/-0.329CCDC number147940119170901919692	Goodness-of-fit on F^2	0.912	1.019	1.034
R indices (all data) $R_1 = 0.1458$ $wR_2 = 0.1589$ $wR_2 = 0.1438$ R indices (all data) $R_1 = 0.1830$, $R_1 = 0.1391$, $R_1 = 0.0991$, $wR_2 = 0.2091$ $wR_2 = 0.1999$ $wR_2 = 0.1665$ Largest diff. Peak and hole $0.530 / -0.437$ $0.312 / -0.266$ $0.401 / -0.329$ CCDC number147940119170901919692	Final R indices $[I > 2\sigma(I)]^*$	$R_1 = 0.0650$	$R_1 = 0.0667$	$R_1 = 0.0604$
R indices (all data) $R_1 = 0.1830$, $R_1 = 0.1391$, $R_1 = 0.0991$, $WR_2 = 0.2091$ $WR_2 = 0.1999$ $WR_2 = 0.1665$ Largest diff. Peak and hole $0.530 / -0.437$ $0.312 / -0.266$ $0.401 / -0.329$ CCDC number 1479401 1917090 1919692 *Structure process of fine d on E 2 or D2		$wR_2 = 0.1458$	$wR_2 = 0.1589$	$wR_2 = 0.1438$
In a consist,In a consist,In a consist, $wR_2 = 0.2091$ $wR_2 = 0.1999$ $wR_2 = 0.1665$ Largest diff. Peak and hole $0.530 / -0.437$ $0.312 / -0.266$ $0.401 / -0.329$ CCDC number147940119170901919692* Streactore group of fined on E 2 or D2	R indices (all data)	$R_1 = 0.1830.$	$R_1 = 0.1391$	$R_1 = 0.0991$
Largest diff. Peak and hole $0.530/-0.437$ $0.312/-0.266$ $0.401/-0.329$ CCDC number 1479401 1917090 1919692 * Strencture encount fined on E 2 and		$wR_2 = 0.2091$	$wR_2 = 0.1999$	$wR_2 = 0.1665$
CCDC number 1479401 1917090 1919692 *Structure encount fine does E_{2}^{2} and	Largest diff. Peak and hole	0.530 /-0.437	0.312/-0.266	0.401/-0.329
*Structure and $E^2 = D^2 = D^2 = \sum_{i=1}^{n} (E^2 - E^2)^{i} (E^2 - E^2)^{i}$	CCDC number	1479401	1917090	1919692
NUCLURE was returned on $H_{2}^{(2)}$ with $J = 1 \times 1 \times (H_{2}^{(2)} - H_{2}^{(2)}) \times (H_{2}^{(2)})^{2} = 0$ where $W_{1}^{(1)} - 1 \times (H_{2}^{(2)}) + 0$	*Structure was refined on	$F^2 \cdot wR^2 - [\Sigma fw(F)]$	$(2 - F_{2}^{2})^{2} / \sum w (F_{2}^{2})^{2} ^{1/2}$ when	$w^{-1} - [\Sigma(F_{*}^{2})] +$

Table S1. Ci	rystal data and	structure refinem	ent details of co	ompounds 5d ,	6a and 6b.

Structure was refined on F_0^2 : wk2 = [$\sum [w(F_0^2 - F_c^2)^2]/$ ($aP)^2 + bP$] and P = [max(F_0^2 , 0) + 2 F_c^2]/3.

Table S2. Hydrogen bonds for compounds 5d and 6a (Å and $^{\circ}$).	

D-H A	d(D–H)	d(H A)	d(D A)	<(DHA)
5d				
C(19)–H(19B)F(1)	0.97	2.16	2.715(5)	116.0
C(23)–H(23)N(1)	0.98	2.43	3.281(6)	145.2
C(23)–H(23)N(2)	0.98	2.34	3.205(5)	147.2
6a				

N(1)-H(1)O(2) #1	0.86	2.10	2.902(6)	156.0
N(1)-H(1)N(2)	0.86	2.32	2.691(1)	106.0
C(5)–H(5)N(3)	0.93	2.62	2.927(9)	100.0
C(25)–H(25)O(2) #2	0.93	2.49	3.301(8)	146.0
C(42)–H(42A)O(1) #3	0.97	2.59	3.341(4)	135.0
6b				
N(1)–H(1)N(2)	0.87(3)	2.37(3)	2.700(3)	103(2)
				. ,
N(1)–H(1)O(2) #4	0.87(3)	2.38(3)	3.132(3)	146(2)
N(1)–H(1)O(2) #4 C(5)–H(5)N(4)	0.87(3) 0.93	2.38(3) 2.54	3.132(3) 2.868(3)	146(2) 101.0
N(1)–H(1)O(2) #4 C(5)–H(5)N(4) C(10)–H(10)O(3)	0.87(3) 0.93 0.93	2.38(3) 2.54 2.59	3.132(3) 2.868(3) 3.499(7)	146(2) 101.0 1.66.0

Symmetry code: #1 = x,1+y,z; #2 = 1-x,1-y,1-z; #3 = x,-1+y,z; #4 = -x,1-y,1-z

Table S3. C-X... π stacking interactions in compounds **5d**, **6b** and π ... π interaction in **6a**, **6b**.

$Y-X(I) \cdots Cg(J)$	X(I)•••Cg(J)	[Å]	X-Perp [/	Å]	γ [°]	$Y-X(I) \bullet \bullet Cg(J) [^{\circ}]$
5d						
Cg(1): N(2	2)-C(10)-C(9)-	C(8)-C(7)-C	C(11); Cg	(2): C(4)-C(5)	-C(6)-C(7)-C(11)-	C(12)
$C(24)-Cl(4)-Cg(1)^{\#1}$	3.882(2)	-3.6	19	21.20)	108.06(17)
$C(24)-Cl(5)-Cg(2)^{\#1}$	3.942(2)	-3.70	67	17.13	3	132.07(17)
6b						
	Cg(1	l): S(2)-C(3	1)-C(26)-	N(5)-C(37)-C	(32)	
$C(21)-H(21)-Cg(1)^{\#2}$	2.690	2.67	4	5.67		135.0
C(13)-N(3)-Cg(1)	3.180	-3.13	37	9.45	:	81.05
6a						
$Cg(I) \cdots Cg(J) \qquad Cg(I)$)•••Cg(J) [Å]	α[°]	β[°]	γ [°]	Cg(I)-Perp [Å]	Cg(J)-Perp [Å]
Cg(1): N(1)-C(12)-C(4)-	C(3)-C(2)-C	C(1); Cg(2)	2): N(2)-C(11)-	-C(7)-C(8)-C(9)-C	(10)
$Cg(1) \bullet Cg(2)^{\#3} = 3.887$	1	0.00	8.06	85.40	-4.773	-5.179
6b						
	Cg(2): C(20)-C(21)-C(22)-C(23)-C(24)-C(25)					
Cg(2)•••Cg(2) ^{#4} 3.779	01(14)	0.00	13.89	89.72	-5.068	-5.068
α = dihedral angle betwee	en $\overline{Cg(I)}$ and $\overline{Cg(I)}$	$Cg(\mathbf{J}); Cg(\mathbf{I})$	-Perp = P	erpendicular d	istance of $Cg(I)$ or	n ring J; Cg(J)-Perp

= perpendicular distance of Cg(I) and Cg(I), Cg(I) of Cg(I) reprint the interval distance of Cg(I) on ring I; β = angle $Cg(I) \rightarrow Cg(J)$ vector and normal to ring I; γ = angle $Cg(I) \rightarrow Cg(J)$ vector and normal to plane J

Symmetry code: #1 = 1-x, 2-y, -z; #2 = x, 3/2-y, -1/2+z; #3 = 1-x, 2-y, 1-z; #4 = -x, 1-y, -z

Table S4.	The experimental	¹ H chemical shifts	of compounds 4,	5 and 6 in CDC	2l3 (* in D2O/KOD).

	Aromatic	Others
4 a	7.71, 8.24, 9.06	_
4b	7.75, 7.77, 7.94, 9.02, 9.08	_
4c	7.85, 8.41, 9.12, 9.18	_
4d	7.69, 7.72, 8.04, 8.99, 9.00	3.15
4e	7.84, 8.88, 9.13, 9.19	_
4f*	6.47, 6.61, 7.69, 8.05, 8.28	_
4g	7.63, 8.24	2.93
4 h	7.67, 7.68, 7.86	2.97, 3.01

4i	7.63, 7.66, 8.27	2.92, 2.94
4j	7.63, 7.69, 8.58	2.93, 2.95
4k	7.62, 7.95	2.92, 2.96, 3.11
41	7.72, 7.73, 8.79	2.96, 2.99
4m	7.65, 8.31	1.43, 2.93, 2.94, 4.49
5a	6.69, 7.93, 8.72	2.03, 3.67
5b	6.67, 6.90, 7.92, 8.74	1.99, 2.07, 3.53, 3.70
5c	6.61, 7.90	2.04, 2.77, 3.68
5d	6.58, 6.65, 7.45	1.96, 2.01, 2.74, 2.76, 3.47, 3.61
5e	6.61, 6.85, 7.63	1.97, 2.03, 2.68, 2.76, 2.77, 3.35,
		3.68
5f	7.06, 7.28–7.36, 7.85, 8.15, 9.49	-
5g	7.03, 7.09, 7.30–7.43, 7.91, 8.18, 9.47, 9.54	_
5h	6.93, 7.10, 7.22, 7.29–7.40, 7.68, 7.80, 8.16, 8.18, 9.43	1.60
5i	6.10, 6.76, 6.82, 7.07, 7.88, 8.15, 9.50	_
5j	5.84, 6.17, 6.69, 6.75, 6.80, 6.85, 6.98, 7.08, 7.82, 7.87, 7.92, 9.47,	-
	9.52	
5k	5.80, 6.11, 6.65–6.85, 6.96, 7.07, 7.70, 7.83, 7.92, 9.45	2.91
5m	6.93, 7.07, 7.31-7.43, 7.88, 7.93, 8.05, 8.18, 9.55, 9.60	-
5n	5.67, 6.10, 6.67, 6.77, 6.82, 6.90, 6.98, 7.13, 7.89, 8.01, 8.76, 9.58,	-
	9.65	
6a	6.90, 7.14, 7.21, 7.29-7.45, 7.65, 7.83, 8.16-8.17, 9.27	11.24
6b	5.63, 6.63-6.58, 6.66, 6.77, 6.90-7.00, 7.12-7.18, 7.25, 7.84, 8.45,	11.11
	9.27	

9.27 For clarity the coupling constants are omitted. **51** purchased from Sigma–Aldrich

Table S5. The experimental ¹³ C{ ¹ H}	chemical shifts of compounds 4	, 5 and 6 in CDCl ₃ (* in D ₂ O/KOD).

	Aromatic	Others
4a	123.1, 123.9, 126.6, 142.8, 146.9, 150.2	_
4b	106.7, 119.9, 124.4, 126.3, 126.8, 140.3, 142.0, 144.7, 148.9, 149.7, 151.0,	-
4c	124.8, 124.9, 125.6, 126.4, 128.1, 130.7, 143.2, 143.3, 144.4, 147.3, 149.9, 150.4	_
4d	124.1, 124.9, 126.3, 126.5, 127.2, 134.9, 141.8, 143.1, 146.6, 148.7, 149.5, 149.6	26.5
4 e	108.1, 118.1, 124.2, 125.2, 125.3, 126.5, 135.4, 142.3, 143.6, 147.5, 148.1, 151.5, 153.4	-
4f*	111.5, 111.6, 114.8, 120.7, 125.1, 132.5, 138.1, 139.2, 140.7, 149.3, 173.8, 178.0, 179.7	-
4g	122.3, 124.4, 125.1, 143.0, 146.2, 160.1	26.0
4h	105.6, 118.0, 125.1, 126.1, 140.3, 142.8, 147.0, 154.9, 157.5, 159.1, 161.3	25.3, 25.5
4i	122.7, 124.5, 124.6, 125.0, 128.0, 129.0, 142.1, 142.3, 144.8, 147.6, 160.2, 160.3	25.3, 25.7
4j	116.2, 123.2, 125.0, 125.1, 127.8, 129.2, 142.1, 143.0, 145.0, 147.2, 160.0, 160.5	25.2, 25.8
4k	123.9, 124.5, 124.6, 125.4, 126.9, 133.8, 142.3, 143.1, 144.9, 147.2, 159.0, 159.1	25.2, 25.6, 26.3
41	106.9, 118.4, 122.6, 123.7, 125.6, 127.0, 134.3, 142.2, 143.7, 146.1, 146.8, 161.6, 163.8	25.6, 26.2
4m	122.1, 123.5, 123.8, 124.9, 126.0, 129.3, 141.7, 143.6, 146.3, 146.6, 160.5, 161.5, 169.0	14.1, 25.5, 25.9, 62.6
5a	105.6, 119.5, 119.6, 148.5, 149.4, 152.9	26.1, 52.4
5b	105.9, 107.9, 117.7, 118.5, 122.4, 124.1, 145.2, 147.7, 148.2, 148.9, 152.7, 153.9	25.1, 26.1, 52.1, 52.4

5c	105.7, 118.2, 119.0, 146.3, 158.4, 157.5	25.8, 26.0, 52.4
5d	102.9, 106.1, 109.9, 117.6, 144.5, 148.7, 152.1, 152.3, 152.9, 154.8, 157.1,	25.6, 25.6, 25.8, 25.9,
	158.7	25.9, 51.7, 51.8, 52.0
5e	105.8, 109.3, 117.9, 120.8, 122.4, 127.4, 145.1, 146.7, 153.2, 155.4, 156.7,	21.4, 24.4, 25.6, 25.7,
	157.5	26.0, 52.0, 52.3
5f	110.1, 120.7, 121.0, 123.0, 124.1, 126.5, 126.7, 141.3, 143.5, 148.8, 151.6	-
5g	106.5, 109.4, 110.0, 119.6, 120.7, 120.8, 121.0, 121.2, 121.4, 123.6, 124.1,	-
	125.1, 125.5, 126.56, 126.58, 141.1, 141.6, 141.7, 143.2, 146.1, 150.0, 150.9,	
	152.6, 154.2, 156.8	
5h	109.7, 110.1, 120.70, 120.73, 120.8, 121.0, 123.1, 123.7, 124.0, 124.5, 125.6,	21.1
	126.2, 126.5, 126.8, 128.2, 133.6, 141.4, 142.2, 142.4, 143.4, 148.0, 149.7,	
	150.9, 151.2	
5i	116.0, 121.1, 123.4, 123.5, 127.1, 127.3, 128.5, 142.9, 146.5, 149.5, 152.0	—
5j	106.5, 115.4, 119.8, 121.4, 122.4, 123.3, 127.0, 127.3, 128.2, 128.4, 142.8,	—
	144.3, 145.7, 147.3, 150.6, 151.1, 153.9, 154.7, 156.8	
5k	115.6, 116.0, 119.0, 120.9, 123.0, 123.3, 124.2, 126.8, 127.06, 127.1, 127.2,	23.6
	127.8, 129.0, 129.4, 134.5, 142.6, 142.8, 145.4, 146.4, 148.6, 151.0, 151.3,	
	151.7	
5m	107.1, 109.2, 109.6, 115.7, 121.0, 121.1, 121.3, 121.7, 123.8, 124.4, 124.5,	—
	125.2, 125.6, 125.8, 126.6, 126.9, 134.4, 141.2, 142.3, 143.1, 144.5, 148.8,	
	149.6, 153.1, 154.7	
5n	107.5, 115.1, 115.9, 117.6, 119.6, 121.7, 123.4, 124.1, 126.9, 127.1, 127.3,	—
	127.7, 128.6, 129.2, 135.0, 142.1, 142.8, 146.4, 147.4, 149.8, 150.7, 154.3,	
	155.1	
6a	100.8, 109.1, 110.0, 115.5, 115.7, 121.0, 121.2, 121.5, 121.7, 124.2, 124.4,	—
	124.5, 126.3, 126.7, 126.8, 126.9, 133.5, 139.0, 140.1, 140.5, 142.2, 143.6,	
	146.5, 151.8, 161.7	
6b	101.0, 115.1, 116.2, 116.7, 117.5, 119.8, 122.6, 123.5, 124.5, 127.0, 127.2,	—
	127.5, 127.9, 128.5, 129.7, 129.8 134.1, 139.6, 141.0, 141.9, 142.1, 146.9,	
	149.2, 153.0, 161.7	

For clarity the coupling constants are omitted. **51** purchased from Sigma–Aldrich

Table S6. The experimental CP/MAS ¹³ C chemical shifts of selected compounds 4 and	5.
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	Aromatic	Others
4g	121.7, 141.3, 143.8, 159.3	25.1
4k	122.5, 123.5, 131.0, 139.0, 143.3, 145.3, 158.3	25.0, 27.5
5c	104.7, 117.5, 147.3, 149.6, 154.6	26.0, 51.8
5f	109.4, 120.2, 122.0, 123.6, 124.8, 127.4, 139.4, 141.2, 147.5, 149.2, 150.3	-
5h	111.3, 116.6, 120.7, 123.3, 126.7, 128.2, 133.7, 136.6, 142.0, 147.4, 148.5, 150.3	23.4
5k	116.8, 123.4, 124.6, 127.2, 135.3, 141.5, 144.8, 147.1, 149.0, 152.6, 153.5, 155.6	25.9
51	101.4, 122.9, 130.5, 132.4, 140.8, 142.9, 145.4, 146.5, 152.7	_

Table S7. The experimental CP/MAS $^{\rm 15}N$ chemical shifts of selected compounds 4 and 5.

	Aromatic	Others
4g	-76.15	_
4k	-75.52	_
5c	-62.66	-291.94
5f	-73.05	-250.68
5h	-78.17, -54.38	-254.60, -249.48
5k	-62.21, -51.07	-273.57



 Table S8. Calculated HOMO and LUMO distribution of selected compounds 4.



 Table S9. Calculated HOMO and LUMO distribution of selected compounds 5.







Fig. S1. Natural atomic charges of compounds 5m (left) and 5n (right).[#]



5m	5n

Fig. S2. The plot of the electrostatic potential for compounds 5m (left) and 5n (right).#

[#] The calculations were done with the use of the density functional theory (DFT) and were carried out using the Gaussian09 program [1] on B3LYP/6-31g++ level [2, 3]. Molecular geometry of the singlet ground state of the compounds was optimized in the gas phase.

1. Gaussian 09, Revision A.02, Frisch M. J., Trucks G. W., Schlegel H. B., Scuseria G. E., Robb M. A., Cheeseman J. R., Scalmani G., Barone V., Petersson G. A., Nakatsuji H., Li X., Caricato M., Marenich A., Bloino J., Janesko B. G., Gomperts R., Mennucci B., Hratchian H. P., Ortiz J. V., Izmaylov A. F., Sonnenberg J. L., Williams-Young D., Ding F., Lipparini F., Egidi F., Goings J., Peng B., Petrone A., Henderson T., Ranasinghe D., Zakrzewski V. G., Gao J., Rega N., Zheng G., Liang W., Hada M., Ehara M., Toyota K., Fukuda R., Hasegawa J., Ishida M., Nakajima T., Honda Y., Kitao O., Nakai H., Vreven T., Throssell K., Montgomery J. A. Jr., Peralta J. E., Ogliaro F., Bearpark M., Heyd J. J., Brothers E., Kudin K. N., Staroverov V. N., Keith T., Kobayashi R., Normand J., Raghavachari K., Rendell A., Burant J. C., Iyengar S. S., Tomasi J., Cossi M., Millam J. M., Klene M., Adamo C., Cammi R., Ochterski J. W., Martin R. L., Morokuma K., Farkas O., Foresman J. B., and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

2. Becke A. D., J.Chem.Phys. 98, 1993 5648-5652.

3. Lee C., Yang W., Parr R.G., Phys. Rev. B 37, 1988, 785-789.



Fig. S1a. ¹H NMR (CDCl₃; 400.2 MHz) spectrum of **4a**.



Fig. S1b. ¹³C{¹H} NMR (CDCl₃; 100.5 MHz) spectrum of 4a.

Fig. S2a. ¹H NMR (CDCl₃; 600.2 MHz) spectrum of 4b.

Fig. S2b. ¹³C{¹H} NMR (CDCl₃; 150.0 MHz) spectrum of **4b**.

Fig. S2c. ¹⁹F NMR (CDCl₃; 470.5 MHz) spectrum of 4b.

Fig. S2d. $^{19}F\{^1H\}$ NMR (CDCl₃; 470.5 MHz) spectrum of 4b.

Fig. S2e. MS spectrum of 4b.

Fig. S3a. ¹H NMR (CDCl₃; 400.2 MHz) spectrum of 4c.

Fig. S3b. $^{13}C\{^{1}H\}$ NMR (CDCl₃; 100.5 MHz) spectrum of 4c.

Fig. S3c. MS spectrum of 4c.

Fig. S4a. ¹H NMR (CDCl₃; 600.1 MHz) spectrum of 4d.

Fig. S4b. ${}^{13}C{}^{1}H$ NMR (CDCl₃; 150.0 MHz) spectrum of 4d.

Fig. S4c. MS spectrum of 4d.

Fig. S5a. ¹H NMR (CDCl₃; 400.2 MHz) spectrum of 4e

Fig. S5b. $^{13}C\{^{1}H\}$ NMR (CDCl₃; 100.5 MHz) spectrum of 4e.

Fig. S6b. ¹H NMR (D₂O/D₂SO₄; 400.1 MHz) spectrum of 4f.

Fig. S6c. ¹³C{¹H} NMR (D₂O/KOD; 125.5 MHz) spectrum of 4f.

Fig. S6d. ¹H, ¹³C NMR HMQC in D₂O spectrum of 4f.

Fig. S6e. 1 H, 13 C NMR HSQC in D₂O spectrum of 4f.

Fig.S6e. MS spectrum of 4f.

Fig. S7a. ¹H NMR (CDCl₃; 400.2 MHz) spectrum of 4g.

Fig. S7b. ¹³C{¹H} NMR (CDCl₃; 100.5 MHz) spectrum of **4g**.

Fig. S7c. ¹³C CP/MAS NMR spectrum of 4g.

Fig. S7d. ¹⁵N CP/MAS NMR spectrum of 4g.

Fig. S8a. ¹H NMR (CDCl₃; 400.2 MHz) spectrum of **4h**.

Fig. S8b. ¹³C{¹H} NMR (CDCl₃; 100.5 MHz) spectrum of **4h**.

Fig. S8c. ¹⁹F NMR (CDCl₃; 470.5 MHz) spectrum of 4h.

Fig. S8d. ${}^{19}F{}^{1}H{}$ NMR (CDCl₃; 470.5 MHz) spectrum of 4h.

Fig. S8e. MS spectrum of 4h.

Fig. S9a. ¹H NMR (CDCl₃; 400.2 MHz) spectrum of 4i.

Fig. S9b. ¹³C{¹H} NMR (CDCl₃; 100.5 MHz) spectrum of **4i**.

Fig. S9c. MS spectrum of 4i.

Fig. S10a. ¹H NMR (CDCl₃; 400.2 MHz) spectrum of 4j.

Fig. S10b. $^{13}C{^{1}H}$ NMR (CDCl₃; 100.5 MHz) spectrum of 4j.

Fig. S10c. MS spectrum of 4j.

Fig. S11a. ¹H NMR (CDCl₃; 400.2 MHz) spectrum of 4k.

Fig. S11b. ¹³C{¹H} NMR (CDCl₃; 100.5 MHz) spectrum of 4k.

Fig. S11c. ¹³C CP/MAS NMR spectrum of 4k.

Fig. S11d. ¹⁵N CP/MAS NMR spectrum of 4k.

Fig. S11e. MS spectrum of 4k.

Fig. S12a. ¹H NMR (CDCl₃; 400.2 MHz) spectrum of 4l.

Fig. S12b. $^{13}C{^{1}H}$ NMR (CDCl₃; 125.8 MHz) spectrum of 4l.

Fig. S12c. MS spectrum of 4l.


Fig. S13a. ¹H NMR (CDCl₃; 400.2 MHz) spectrum of 4m.



Fig. S13b. ${}^{13}C{}^{1}H$ NMR (CDCl₃; 100.5 MHz) spectrum of 4m.



Fig. S13c. MS spectrum of 4m.



Fig. S14a. ¹H NMR (CDCl₃; 400.2 MHz) spectrum of 5a.



Fig. S14b. $^{13}C{^{1}H}$ NMR (CDCl₃; 100.5 MHz) spectrum of 5a.



Fig. S14c. MS spectrum of 5a.



Fig. S15a. ¹H NMR (CDCl₃; 400.2 MHz) spectrum of 5b.



Fig. S15b. $^{13}C{^{1}H}$ NMR (CDCl₃; 100.5 MHz) spectrum of 5b.



Fig. S15c. ¹H, ¹³C NMR HMQC in CDCl₃ spectrum of 5b.



Fig. S15d. MS spectrum of 5b.



Fig. S16a. ¹H NMR (CDCl₃; 500.2 MHz) spectrum of 5c.



Fig. S16b. $^{13}C{^{1}H}$ NMR (CDCl₃; 100.5 MHz) spectrum of 5c.



Fig. S16c. ¹³C CP/MAS NMR spectrum of 5c.



Fig. S16d. ¹⁵N CP/MAS NMR spectrum of 5c.



Fig. S16e. MS spectrum of 5c.



Fig. S17a. ¹H NMR (CDCl₃; 500.2 MHz) spectrum of 5d.



Fig. S17b. ${}^{13}C{}^{1}H$ NMR (CDCl₃; 100.5 MHz) spectrum of 5d.



Fig. S17c. ¹⁹F NMR (CDCl₃; 470.5 MHz) spectrum of 5d.



Fig. S17d. $^{19}F{^1H}$ NMR (CDCl₃; 470.5 MHz) spectrum of 5d.



Fig. S17e. MS spectrum of 5d.



Fig. S18a. ¹H NMR (CDCl₃; 400.2 MHz) spectrum of 5e.



Fig. S18b. $^{13}C{^{1}H}$ NMR (CDCl₃; 100.5 MHz) spectrum of 5e.



Fig. S18c. ¹H, ¹³C NMR HMQC in CDCl₃ spectrum of 5e.



Fig. S18d. MS spectrum of 5e



Fig. S19a. ¹H NMR (CDCl₃; 500.2 MHz) spectrum of 5f.



Fig. S19b. $^{13}C{^{1}H}$ NMR (CDCl₃; 125.8 MHz) spectrum of 5f.



Fig. S19c. ¹³C CP/MAS NMR spectrum of 5f.



Fig. S19d. ¹⁵N CP/MAS NMR spectrum of 5f.



Fig. S20a. ¹H NMR (CDCl₃; 400.2 MHz) spectrum of 5g.



Fig. S20b. $^{13}C{^{1}H}$ NMR (CDCl₃; 100.5 MHz) spectrum of 5g.



Fig. S20c. ¹⁹F NMR (CDCl₃; 470.5 MHz) spectrum of 5g.



Fig. S20d. ¹⁹F{¹H} NMR (CDCl₃; 470.5 MHz) spectrum of 5g.



Fig. S20e. ¹H, ¹³C NMR HMQC in CDCl₃ spectrum of 5g.



Fig. S20f. MS spectrum of 5g.



Fig. S21a. ¹H NMR (CDCl₃; 500.2 MHz) spectrum of 5h.



Fig. S21b. $^{13}C{^{1}H}$ NMR (CDCl₃; 100.5 MHz) spectrum of 5h.



Fig. S21c. 2D-COSY NMR in CDCl₃ spectrum of 5h.



Fig. S21d. ¹H, ¹³C NMR HMQC in CDCl₃ spectrum of 5h.



Fig. S21e. ¹³C CP/MAS NMR spectrum of 5h.



Fig. S21f. ¹⁵N CP/MAS NMR spectrum of 5h.



Fig. S21g. MS spectrum of 5h.



Fig. S22a. ¹H NMR (CDCl₃; 500.2 MHz) and spectrum of 5i.



Fig. S22b. $^{13}C{^{1}H}$ NMR (CDCl₃; 100.5 MHz) spectrum of 5i.



Fig. S22c. MS spectrum of 5i.



Fig. S23a. ¹H NMR (CDCl₃; 500.2 MHz) spectrum of 5j.



Fig. S23b. ¹³C{¹H} NMR (CDCl₃; 125.8 MHz) spectrum of **5**j.



Fig. S23c. ¹⁹F NMR (CDCl₃; 470.5 MHz) spectrum of 5j.



Fig. S23d. ¹⁹F{¹H} NMR (CDCl₃; 470.5 MHz) spectrum of 5j.



Fig. S23e. MS spectrum of 5j.



Fig. S24a. ¹H NMR (CDCl₃; 500.2 MHz) spectrum of 5k.



Fig. S24b. $^{13}C{^{1}H}$ NMR (CDCl₃; 100.5 MHz) spectrum of 5k.



Fig. S24c. ¹³C CP/MAS NMR spectrum of 5k.



Fig. S24d. ¹⁵N CP/MAS NMR spectrum of 5k.



Fig. S24e. MS spectrum of 5k.



Fig. S25b. ¹³C{¹H} NMR (CDCl₃; 125.8 MHz) spectrum of **5n**.



Fig. S25c. MS spectrum of 5n.



Fig. S26a. ¹H NMR (CDCl₃; 400.2 MHz) spectrum of 5m



Fig. S26b. $^{13}C{^{1}H}$ NMR (CDCl₃; 100.6 MHz) spectrum of 5m.





Fig. S26c. ¹H, ¹³C NMR HMQC in CDCl₃ spectrum of 5m.



Fig. S26d. MS spectrum of 5m.



Fig. S27a. ¹³C CP/MAS NMR spectrum of 5l.



Fig. S27b. ¹⁵N CP/MAS NMR spectrum of 5l.



Fig. S28a. ¹H NMR (CDCl₃; 400.2 MHz) spectrum of 6a.



Fig. S28b. $^{13}C{^{1}H}$ NMR (CDCl₃; 100.6 MHz) spectrum of 6a.




Fig. S29a. ¹H NMR (CDCl₃; 400.2 MHz) spectrum of 6b.



Fig. S29b. ${}^{13}C{}^{1}H$ NMR (CDCl₃; 100.6 MHz) spectrum of 6b.



Fig. S29c. ¹H, ¹³C NMR HMQC in CDCl₃ spectrum of **6**b.



Fig. S29d. MS spectrum of 6b.