Supplementary Material (ESI) for *Dalton Transactions*

Supplementary Information

for

Electronic Modification of an Aminotroponiminat Zinc Complex Leading to an Increased Reactivity in the Intramolecular Hydroamination of Alkenes

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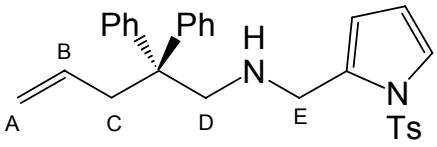
(9 pages)

S1 Characterisation of new cyclization educts

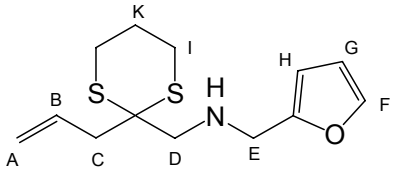
5a-6a and **8a-11a** have already been described previously.[i]

(2,2-Diphenylpent-4-enyl)-[1-(toluol-4-sulfonyl)-1*H*-pyrrol-2-ylmethyl]amine (7a)



^{1}H-NMR ($CDCl_3$, 500 MHz): δ(ppm) = 1.56 (bs, 1 H, NH); 2.41 (s, 3 H, CH_3 von Ts); 2.97 (d, *J* = 7.1 Hz, 2 H, H_C); 3.13 (s, 2 H, H_D); 3.73 (s, 2 H, H_E); 4.90-5.01 (m, 2 H, H_A); 5.35 (tdd, *J* = 7.1 Hz, *J* = 10.0 Hz, *J* = 17.0 Hz, 1 H, H_B); 5.99-6.01 (m, 1 H, H_{ar}); 6.19 (t, *J* = 3.3 Hz, 1 H, H_{ar}); 7.12-7.15 (m, 4 H, H_{ar}); 7.19 (tt, *J* = 2.0 Hz, *J* = 7.3 Hz, 2 H, H_{ar}); 7.23- 7.29 (m, 7 H, H_{ar}); 7.62 (d, *J* = 8.5 Hz, 2 H, H_{ar}).
^{13}C-NMR ($CDCl_3$, 125 MHz): δ(ppm) = 21.6; 41.6; 46.1; 50.0 (Cq); 54.8; 111.4; 113.8; 117.7; 122.9; 126.0; 126.7; 127.9; 128.0; 129.9; 133.9 (Cq); 134.9; 136.4 (Cq); 144.7 (Cq); 146.7 (Cq).
IR (ATR): □(cm^{-1}) = 3343 (w); 3058 (w); 1495 (m); 1476 (m); 1445 (m); 1366 (s); 1189 (s); 1175 (s); 1152 (s); 1110 (m); 1091 (s); 1110 (m); 1034 (w); 1018 (w); 1001 (w); 915 (m); 871 (w); 839 (w); 813 (m); 787 (w); 758 (m); 721 (m); 701 (s); 672 (s).
MS (EI, 70 eV): m/z (%) = 471 [M$^+$] (3); 315 (4); 263 (18); 236 (5); 235 (12); 234 (100); 165 85); 155 (15); 129 (9); 91 (38); 80 (22); 65 (4).
HRMS: $C_{29}H_{31}N_2O_2S$ calc.: 471.2106 found: 471.2111

(2-Allyl-[1.3]dithian-2-ylmethyl)-furan-2-ylmetyhlamine (12a)



^{1}H-NMR ($CDCl_3$, 400 MHz): δ(ppm) = 1.61 (s, 1 H, NH); 1.79-1.91 (m, 1 H, H_K); 1.95-2.04 (m, 1 H, $H_{K'}$); 2.62-2.69 (m, 2 H, H_I); 2.65 (d, *J* = 7.3 Hz, 2 H, H_C); 2.81

(ddd, *J* = 3.0 Hz, *J* = 10.6 Hz, *J* = 13.8 Hz, 2 H, $H_{I'}$); 2.96 (s, 2 H, H_D); 3.84 (s, 2 H, H_E); 5.10-5.18 (m, 2 H, H_A); 5.82-5.93 (m, 1 H, H_B); 6.18 (dd, *J* = 0.7 Hz, *J* = 3.1 Hz, 1 H, H_F); 6.32 (dd, *J* = 1.8 Hz, *J* = 3.1 Hz, 1 H, H_G); 7.36 (dd, *J* = 0.8 Hz, *J* = 1.8 Hz, 1 H, H_H).

^{13}C-NMR ($CDCl_3$, 100 MHz): δ(ppm) = 25.0; 25.9; 42.5; 46.0; 52.6 (C_q); 53.0; 107.0; 110.1; 118.7; 132.5; 141.7; 154.1 (C_q).

IR (ATR): n (cm^{-1}) = 2931 (m); 2907 (s); 2829 (m); 1638 (m); 1598 (w); 1505 (m); 1461 (m), 1425 (s); 1336 (m); 1276 (m); 1239 (m); 1218 (m); 1188 (m); 1147 (s); 1119 (m); 1110 (m); 1009 (s); 955 (m); 917 (s); 906 (s); 884 (m); 861 (w); 806 (m); 736 (s); 679 (m).

MS (EI, 70 eV): m/z (%) = 269 [M^+] (4); 159 (53); 110 (49); 85 (11); 81 (100); 53 (17).

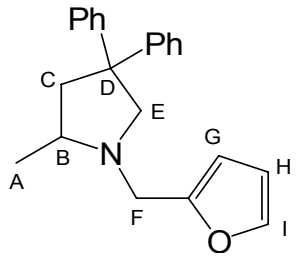
HRMS: $C_{13}H_{19}NOS_2$ calc.: 269.0908 found: 269.0903

Elemental analysis: calc.: C: 57.95 % H: 7.11 % N: 5.20 %
found: C: 57.83 % H: 6.68 % N: 5.12 %

S2 Characterisation of new cyclization products

1-Benzyl-2-methyl-4,4-diphenyl-pyrrolidine (**5b**) has already been described previously.[ii]

1-Furan-2-ylmethyl-2-methyl-4,4-diphenyl-pyrrolidine (6b)



^{1}H-NMR ($CDCl_3$, 400 MHz): δ (ppm) = 1.15 (d, *J* = 5.9 Hz, 3 H, H_A); 2.20 (dd, *J* = 7.6 Hz, *J* = 12.1 Hz, 1 H, H_C); 2.76-2.90 (m, 1 H, H_B); 2.86 (d, *J* = 12.1 Hz, 1 H, $H_{C'}$); 3.00 (d, *J* = 10.0 Hz, 1 H, H_E); 3.50 (d, *J* = 14.4 Hz, 1 H, H_F); 3.75 (d, *J* = 10.0 Hz, 1 H, $H_{E'}$); 3.96 (d, *J* = 14.4 Hz, 1 H, $H_{F'}$); 6.19 (d, *J* = 3.1 Hz, 1 H, H_G); 6.33 (dd, *J* = 1.8 Hz, *J* = 3.1 Hz, 1 H, H_H); 7.09-7.29 (m, 10 H, H_{ar}); 7.39 (dd, *J* =

0.7 Hz, *J* = 1.8 Hz, H_I).

^{13}C-NMR ($CDCl_3$, 100 MHz): δ (ppm) = 19.2; 47.9; 49.3; 52.5 (C_q); 58.8; 66.1; 107.8; 110.0; 125.5; 125.8; 127.2; 127.4; 128.0; 128.2; 141.8; 148.7 (C_q); 150.3 (C_q); 153.0 (C_q).

IR (ATR): □ (cm^{-1}) = 3084 (w); 3057 (w); 3025 (w); 2963 (m); 2925 (w); 2870 (w); 2797 (m); 1947 (w); 1872 (w); 1803 (w); 1741 (w); 1598 (m); 1493 (m); 1446 (m); 1376 (m); 1356 (m); 1336 (w); 1315 (w); 1268 (w); 1223 (w); 1188 (w); 1148 (m); 1107 (w); 1075 (w); 1033 (m); 1010 (m); 938 (w); 917 (w); 885 (w), 810 (w); 761 (m); 734 (m); 700 (s).

MS (EI, 70 eV): m/z (%) = 317 [M^+] (28); 302 (35); 165 (10); 137 (55); 81 (65); 56 (100).

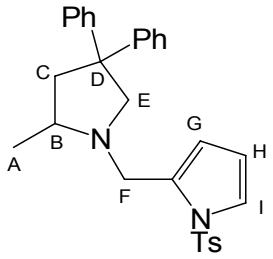
HRMS: $C_{22}H_{23}NO$ calc.: 317.1780 found: 317.1780

Elemental analysis: calc.: C: 83.24 % H: 7.30 % N: 4.41 %

found: C: 83.39 % H: 6.91 % N: 4.50 %

melting point: 69 °C

2-(2-Methyl-4,4-diphenylpyrrolidin-1-ylmethyl)-1-(toluene-4-sulfonyl)-1*H*-pyrrol (7b)



^{1}H-NMR ($CDCl_3$, 500 MHz): δ(ppm) = 1.06 (d, *J* = 5.5 Hz, 3 H, H_A); 2.20 (dd, *J* = 11.2 Hz, *J* = 15.2 Hz, 1 H, H_C); 2.79-2.83 (m, 1 H, H_B); 2.80 (d, *J* = 15.2 Hz, 1 H, $H_{C'}$); 2.83 (d, *J* = 10.1 Hz, 1 H, H_E); 3.33 (s, 3 H, CH_3 von Ts); 3.57 (d, *J* = 14.8 Hz, 1 H, H_F); 3.59 (d, *J* = 10.1 Hz, 1 H, $H_{E'}$); 4.10 (d, *J* = 14.8 Hz, 1 H, $H_{F'}$); 6.19 (s, 1 H, H_G); 6.22 (t, *J* = 3.2 Hz, 1 H, H_H); 7.12 (d, *J* = 8.2 Hz, 2 H, H_{ar} von Ts); 7.14-7.29 (m, 11 H, H_{ar}); 7.75 (d, *J* = 8.2 Hz, 2 H, H_{ar} von Ts).

^{13}C-NMR ($CDCl_3$, 125 MHz): δ(ppm) = 19.4; 21.7; 47.9; 50.1; 52.8 (C_q); 59.8; 66.5; 111.4; 114.3; 122.8; 125.6; 125.9; 127.2; 127.4; 128.0; 128.2; 129.8; 133.7 (C_q); 136.6 (C_q); 144.7 (C_q); 148.8 (C_q); 150.1 (C_q).

IR (ATR): □(cm^{-1}) = 1596 (m); 1494 (m); 1446 (m); 1399 (m); 1366 (s); 1307 (w); 1292 (w); 1230 (w); 1190 (m); 1175 (s); 1152 (s); 1127 (m); 1091 (m); 1054 (m); 1017 (w); 949 (w); 907 (w); 872 (w); 812 (m); 774 (w); 760 (w); 720 (m); 702 (s); 671 (s).

MS (EI, 70 eV): m/z (%) = 470 [M$^+$] (9); 456 (7); 455 (21); 290 (9); 236 (11); 235 (14); 234 (100); 155 (23); 93 (5); 91 (37); 56 (53).

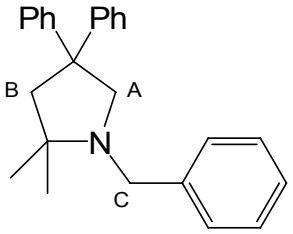
HRMS: $C_{29}H_{30}N_2O_2S$ calc.: 470.2028 found: 470.2022

Elemental analysis: calc.: C: 74.01 % H: 6.43 % N: 5.95 %

found: C: 74.07 % H: 6.59 % N: 6.13 %

melting point: 150 °C

1-Benzyl-2,2-dimethyl-4,4-diphenyl-pyrrolidine (8b)



^{1}H-NMR ($CDCl_3$, 400 MHz): δ (ppm) = 1.13 (s, 6 H, 2 × CH_3); 2.61 (s, 2 H, H_B); 3.28 (s, 2 H, H_A); 3.61 (s, 2 H, H_C); 7.09-7.39 (m, 15 H, H_{ar}).

^{13}C-NMR ($CDCl_3$, 100 MHz): δ (ppm) = 25.1; 51.6 (C_q); 52.4; 54.4; 60.5 (C_q); 63.1; 125.5; 126.7; 127.2; 127.8; 128.1; 128.5; 140.9 (C_q); 149.7 (C_q).

IR (ATR): □ (cm^{-1}) = 3085 (w); 3059 (m); 3026 (m); 2959 (m); 2924 (m); 2868 (w); 2795 (m); 2699 (w); 1946 (w); 1872 (w); 1805 8w); 1714 (w); 1599 (m); 1494 (m); 1453 (m); 1446 (m); 1380 (m); 1363 (m); 1334 (w); 1311 (w); 1291 (w); 1264 (w); 1222 (m); 1208 (w); 1191 (w); 1154 (m); 1123 (w); 1070 (w); 1050 (m); 1028 (m); 1002 (w); 962 (w); 952 (w); 907 (w); 865 (w); 826 (w); 775 (m); 760 (m); 747 (m); 730 (m); 697 (s); 654 (w).

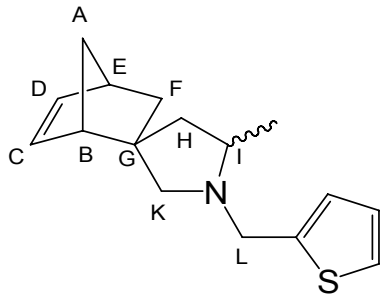
MS (EI, 70 eV): m/z (%) = 341 [M$^+$] (4); 327 (22); 326 (100); 207 (6); 161 (6); 129 (5); 92 (5); 91 (75); 70 (38); 65 (5); 55 (12).

HRMS: $C_{25}H_{27}N$ calc.: 341.2143 found: 341.2150

Elemental analysis: calc.: C: 87.93 % H: 7.97 % N : 4.10 %

found: C : 88.28 % H: 8.01 % N: 4.04 %

3-Methyl-2-thiophen-2-ylmethyl-2-aza-spiro[4.6]-bicylo[2.2.1]undecane (9b)



Diastereomer I:

^{1}H-NMR ($CDCl_3$, 400 MHz): δ (ppm) = 1.17 (d, *J* = 6.0 Hz, 3 H, CH_3); 1.37-1.40 (m, 3 H, H_A, H_F); 1.69 (dd, *J* = 8.8 Hz, *J* = 12.6 Hz, 1 H, H_H); 1.76 (dd, *J* = 3.8 Hz, *J* = 12.1 Hz, 1 $H_{F'}$); 1.96 (dd, *J* = 7.2 Hz, *J* = 12.6 Hz, 1 H, $H_{H'}$); 2.21 (d, *J* = 9.4 Hz, 1 H, H_K); 2.40 (bs, 1 H, H_B); 2.50-2.58 (m, 1 H, H_I); 2.56 (d, *J* = 9.4 Hz, 1 H, $H_{K'}$); 2.78 (bs, 1 H, H_E); 3.55 (d, *J* = 14.1 Hz, 1 H, H_L); 4.07 (dd, *J* = 0.7 Hz, *J* = 14.1 Hz, 1 H, $H_{L'}$); 6.00 (dd, *J* = 2.9 Hz, *J* = 5.4 Hz, 1 H, H_D); 6.07-6.11 (m, 1 H, H_C); 6.85-6.87 (m, 1 H, H_{ar}); 6.93 (m, 1 H, H_{ar}); 7.19 (m, 1 H, H_{ar}).

^{13}C-NMR ($CDCl_3$, 100 MHz): δ (ppm) = 19.1; 43.0; 45.7 (C_q); 47.6; 48.9; 49.7; 51.6; 51.8; 52.9; 59.3; 68.0; 125.1; 125.3; 134.5; 138.1; 142.9 (C_q).

Diastereomer II:

^{1}H-NMR ($CDCl_3$, 400 MHz): δ = (ppm) 1.03 (d, *J* = 11.6 Hz, 1 H, H_F); 1.17 (d, *J* = 6.0 Hz, 3 H, CH_3); 1.40-1.43 (m, 2 H, H_A); 1.56 (dd, *J* = 8.8 Hz, *J* = 12.4 Hz, 1 H, H_H); 1.66 (dd, *J* = 3.8 Hz, *J* = 11.6 Hz, 1 H, $H_{F'}$); 2.01 (dd, *J* = 7.4 Hz, *J* = 12.4 Hz, 1 H, $H_{H'}$); 2.03 (d, *J* = 9.9 Hz, 1 H, H_K); 2.50-2.58 (m, 1 H, H_I); 2.62 (bs, 1 H, H_B); 2.74 (bs, 1 H, H_E); 2.79 (d, *J* = 9.9 Hz, 1 H, $H_{K'}$); 3.49 (d, *J* = 14.1 Hz, 1 H, H_L); 4.06 (dd, *J* = 0.7 Hz, *J* = 14.1 Hz, 1 H, $H_{L'}$); 6.05 (dd, *J* = 2.8 Hz, *J* = 5.1 Hz, 1 H, H_D); 6.07-6.11 (m, 1 H, H_C); 6.85-6.87 (m, 1 H, H_{ar}); 6.93 (m, 1 H, H_{ar}); 7.19 (m, 1 H, H_{ar}).

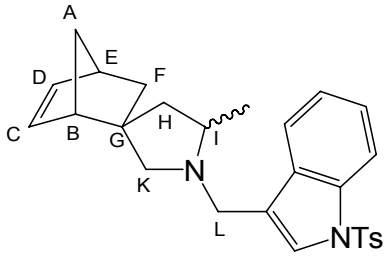
^{13}C-NMR ($CDCl_3$, 100 MHz): δ = (ppm) 19.3; 42.7; 44.6; 46.0 (C_q); 48.3; 50.1; 51.5; 52.0; 52.7; 58.6; 66.4; 124.4; 126.3; 135.2; 137.8; 142.5 (C_q).

IR (ATR): □ (cm^{-1}) = 3138 (w); 3104 (w); 3059 (w); 2960 (bs); 2937 (s); 2866 (m); 2781 (m); 2675 (w); 2583 (w); 1716 (w); 1694 (w); 1676 (w); 1589 (w); 1571 (w); 1538 (w); 1511 (w); 1458 (w); 1444 (w); 1375 (m); 1356 (m); 1332 (m); 1310 (m); 1273 (m); 1263 (m); 1211 (m); 1169 (m); 1142 (m); 1096 (m); 1077 (m); 1038 (w); 1025 (w); 971 (w); 954 (w); 938 (w); 907 (w); 853 (m); 823 (m); 801 (m); 713 (s); 695 (s).

MS (EI, 70 eV): m/z (%) = 259 [M^+] (13); 244 (38); 193 (10); 192 (20); 97 (100); 66 (11).

HRMS: $C_{16}H_{21}NS$ calc.: 259.1394 found: 259.1399

3-Methyl-2-[1-toluene-4-sulfonyl)-1*H*-indol -2-ylmethyl-2-aza-spiro[4.6]-bicylo[2.2.1]undecane (10b)



Diastereomer I:

^{1}H-NMR ($CDCl_3$, 400 MHz): δ(ppm) = 1.25 (dd, *J* = 2.4 Hz, *J* = 11.8 Hz, H_F); 1.20 (d, *J* = 6.0 Hz, 3 H, CH_3); 1.35-1.42 (m, X H, H_A); 1.64 (dd, *J* = 4.2 Hz, *J* = 12.7 Hz, H_H); 1.71 (dd, *J* = 3.7 Hz, *J* = 11.8Hz, 1 H, $H_{F'}$); 1.97 (dd, *J* = 7. 5 Hz, *J* = 12.7 Hz, 1 H, $H_{H'}$); 2.07 (d, *J* = 9.3 Hz, 1 H, H_K); 2.32 (s, 3 H, CH_3 of Ts); 2.37 (d, *J* = 9.3 Hz, 1 H, $H_{K'}$); 2.37 (bs, 1 H, H_B); 2.47-2.55 (m, 1 H, H_I); 2.72 (bs, 1 H, H_E); 3.25 (d, *J* = 13.9 Hz, 1 H, H_L); 3.99 (dd, *J* = 2.6 Hz, *J* = 13.8 Hz, 1 H, $H_{L'}$); 5.78 (dd, *J* = 3.0 Hz, *J* = 5.6 Hz, 1 H, H_D); 6.03 (dd, *J* = 3.0 Hz, *J* = 5.8 Hz, 1 H, H_C); 7.15-7.23 (m, 3 H, H_{ar}); 7.25-7.32 (m, 1 H, H_{ar}); 7.40 (s, 1 H, H_{ar}); 7.61-7.75 (m, 3 H, H_{ar}); 7.95 (dd, *J* = 3.8 Hz, *J* = 8.3 Hz, 1 H, H_{ar}).

^{13}C-NMR ($CDCl_3$, 100 MHz): δ(ppm) = 19.4; 21.5; 27.0; 42.6; 45.8 (C_q); 48.2; 48.8; 50.1; 52.9; 60.2; 66.9; 113.6; 120.4; 121.2 (C_q); 123.0; 124.0; 124.5 (C_q); 126.7; 129.7; 131.0 (C_q); 135.1; 135.3 (C_q); 135.5 (C_q); 137.7; 144.6 (C_q).

Diastereomer II:

^{1}H-NMR ($CDCl_3$, 400 MHz): δ(ppm) = 0.98 (dd, *J* = 2.0 Hz, *J* = 11.6 Hz, 1 H, H_F); 1.19 (d, *J* = 5.8 Hz, 3 H, CH_3); 1.35-1.42 (m, 2 H, H_A); 1.54 (dd, *J* = 8.8 Hz, *J* = 12.3 Hz, 1 H, H_H); 1.66 (dd, *J* = 3.6 Hz, *J* = 11.6 Hz, 1 H, $H_{F'}$); 1.87 (d, *J* = 9.9 Hz, 1 H, H_K); 2.03 (dd, *J* = 7.7 Hz, *J* = 12.6 Hz, 1 H, $H_{H'}$); 2.32 (s, 3 H, CH_3 of Ts); 2.47-2.55 (m, 1 H, H_I); 2.56 (bs, 1 H, H_B); 2.57 (d, *J* = 9.9 Hz, 1 H, $H_{K'}$); 2.75 (bs, 1 H, H_E); 3.28 (d, *J* = 13.9 Hz, 1 H, H_L); 4.00 (dd, *J* = 2.8 Hz, *J* = 13.9 Hz, 1 H, $H_{L'}$); 5.93 (dd, *J* = 3.0 Hz, *J* = 5.8 Hz, 1 H, H_D); 6.04 (dd, *J* = 3.0 Hz, *J* = 6.1 Hz, 1 H, H_C); 7.15-7.23 (m, 3 H, H_{ar}); 7.25-7.32 (m, 1 H, H_{ar}); 7.40 (s, 1 H, H_{ar}); 7.61-7.75

(m, 3 H, H_{ar}); 7.95 (dd, *J* = 3.8 Hz, *J* = 8.3 Hz, 1 H, H_{ar}).

^{13}C-NMR ($CDCl_3$, 100 MHz): δ (ppm) = 19.8; 21.5; 27.0; 42.9; 44.1; 46.1 (C_q); 47.5; 48.4; 49.8; 52.6; 59.1; 59.6; 65.1; 113.6; 121.4 (C_q); 123.0; 124.2; 124.6; 126.7; 129.7; 131.0 (C_q); 135.3 (C_q); 135.4 (C_q); 137.9; 144.6 (C_q).

IR (ATR): □ (cm^{-1}) = 3114 (w); 3056 (w); 2960 (m); 2936 (w); 2866 (w); 2786 (w); 1598 (w); 1570 (w); 1494 (w); 1446 (m); 1399 (w); 1372 (m); 1322 (w); 1306 (w); 1293 (w); 1276 (w); 1246 (w); 1206 (w); 1187 (m); 1174 (s); 1121 (m); 1106 (m); 1019 (w); 976 (m); 939 (w); 907 (w); 812 (m); 798 (w); 773 (w); 746 (m); 715 (w); 704 (w); 673 (m).

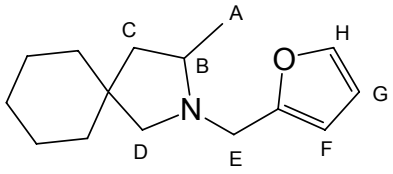
MS (EI, 70 eV): m/z (%) = 446 [M^+] [14); 285 (33); 284 (100); 225 (10); 162 (18); 155 (29); 130 (19); 129 (18); 91 (54); 66 (11).

HRMS: $C_{27}H_{30}N_2O_2S$ calc.: 446.2028 found: 446.2021

Elemental analysis: calc.: C: 72.61 % H: 6.77 % N: 6.27 %

found: C: 72.94 % H: 7.01 % N: 5.97 %

2-Furan-2-ylmethyl-3-methyl-2-aza-spiro[4.5]decanamine (11b)



^{1}H-NMR ($CDCl_3$, 400 MHz): δ (ppm) = 1.12 (d, *J* = 6.0 Hz, 3 H, H_A); 1.22-1.47 (m, 11 H, H_C, H_{Ring}); 1.72 (dd, *J* = 6.6 Hz, *J* = 12.4 Hz, 1 H, $H_{C'}$); 2.08 (d, *J* = 9.5 Hz, 1 H, H_D); 2.39-2.50 (m, 1 H, H_B); 2.85 (d, *J* = 9.5 Hz, 1 H, $H_{D'}$); 3.36 (d, *J* = 14.2 Hz, 1 H, H_E); 3.88 (d, *J* = 14.2 Hz, 1 H, $H_{E'}$); 6.15 (d, *J* = 3.1 Hz, 1 H, H_F); 6.30 (dd, *J* = 1.9 Hz, *J* = 3.1 Hz, 1 H, H_G); 7.35 (dd, *J* = 0.8 Hz, *J* = 1.9 Hz, 1 H, H_H).

^{13}C-NMR ($CDCl_3$, 100 MHz): δ (ppm) = 18.7; 23.5; 23.6; 26.0; 38.6; 39.1 (C_q); 39.3; 49.3; 58.1; 107.9; 109.9; 141.7; 152.9 (C_q).

IR (ATR): □ (cm^{-1}) = 3113 (w); 2959 (m); 2923 (vs); 2853 (m); 2784 (m); 2710 (w); 2670 (w); 1536 (w); 1506 (w); 1463 (w); 1448 (m); 1376 (m); 1148 (m); 1109 (w); 1075 (w); 1009 (m); 971 (w); 935 (w); 917 (w); 885 (w); 850 (w); 799 (w); 728 (m).

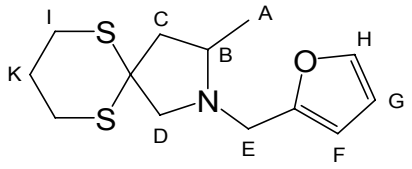
MS (EI, 70 eV): m/z (%) = 233 [M^+] (11); 232 (6); 219 (7); 218 (52); 82 (5); 81 (100); 56 (15); 53 (7).

HRMS: $C_{15}H_{23}NO$ calc.: 233.1780 found: 233.1780

Elemental analysis: calc.: C: 77.21 % H: 9.93 % N: 6.00 %

found: C: 76.42 % H: 9.60 % N: 5.86 %

1-Furan-2-ylmethyl-2-methyl-6,10-dithia-2-azaspiro[4.5]decane (12b)



^{1}H-NMR ($CDCl_3$, 400 MHz): δ (ppm) = 1.19 (d, *J* = 6.0 Hz, 3 H, H_A); 1.89 (dd, *J* = 9.4 Hz, *J* = 13.3 Hz, 1 H, H_C); 1.95-2.02 (m, 2 H, H_K); 2.41 (dd, *J* = 6.5 Hz, *J* = 13.3 Hz, 1 H, $H_{C'}$); 2.74-2.95 (m, 4 H, H_I); 2.86 (d, *J* = 10.5 Hz, 1 H, H_D); 3.51 (d, *J* = 10.5 Hz, 1 H, $H_{D'}$); 3.61 (d, *J* = 14.6 Hz, 1 H, H_E); 3.92 (d, *J* = 14.6 Hz, 1 H, $H_{E'}$); 6.18 (d, *J* = 3.1 Hz, 1 H, H_F); 6.31 (dd, *J* = 1.9 Hz, *J* = 3.1 Hz, 1 H, H_G); 7.36 (dd, *J* = 0.8 Hz, *J* = 1.9 Hz, 1 H, H_H).

^{13}C-NMR ($CDCl_3$, 100 MHz): δ (ppm) = 18.2; 25.2; 28.7; 29.1; 48.0; 50.3; 50.5 (C_q); 57.3; 68.0; 108.4; 110.1; 142.0; 151.9 (C_q).

IR (ATR): □ (cm^{-1}) = 3139 (w); 3111 (w); 2962 (s); 2929 (s); 2900 (s); 2813 (m); 2601 (w); 1738 (w); 1714 (w); 1598 (w); 1504 (m); 1463 (m); 1432 (s); 1423 (s); 1376 (s); 1356 (m); 1336 (m); 1312 (m), 1295 (w); 1275 (s); 1239 (m); 1223 (m); 1161 (s); 1147 (s); 1105 (m); 1073 (m); 1005 (s); 965 (w); 936 (m); 908 (m); 884 (m); 867 (w); 804 (m); 761 (s); 734 (vs); 673 (m).

MS (EI, 70 eV): m/z (%) = 269 [M^+] (20); 163 (11); 145 (12); 137 (66); 123 (16); 81 (88); 56 (100); 53 (18).

HRMS: $C_{13}H_{19}NOS_2$ calc.: 269.0908 found: 269.0910

Elemental analysis: calc.: C: 57.95 % H: 7.11 % N: 5.20 %

found: C: 57.74 % H: 7.03 % N: 5.22 %

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[i] (a) M. Dochnahl, J.-W. Pissarek, S. Blechert, K. Loehnwitz and P. W. Roesky, *Chem. Commun.* 2006, 3405-3407. (b) M. Dochnahl, K. Löhnwitz, J.-W. Pissarek, M. Biyikal, S. Schulz, S. Schön, N. Meyer, P. W. Roesky and S. Blechert *Chem. Eur. J.* 2007, *13*, 6654-6666.

[ii] C. F. Bender and R. A. Widenhoefer, *J. Am. Chem. Soc.,* 2005, **127**, 1070.