Isomerism in rhodium(I) $N,S$-donor heteroscorpionates: 
ring substituent and ancillary ligand effects

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Figure S1  Molecular structure of $[\text{Rh(CO)}(\text{PCy}_3)\{\text{HB(taz)}_2(\text{pz}^\text{Me}_2)\}]$ 17

Figure S2  Molecular structure of $[\text{Rh(CO)}_2\{\text{HB(taz)}_2(\text{pz}^\text{Me}_2)\}]$ 10
Figure S3  Variable temperature $^1$H NMR spectra of [Rh(CO)(PPh$_3$)$_2$HB(taz)$_2$(pz)$_2$]$_2$, showing two isomers († and ‡), residual CH$_2$Cl$_2$/CHDCl$_2$ (*) and trace (CH$_3$)$_2$CO (¶)
Table S1 Proton NMR spectroscopic data for 6, 7 and 21 at low temperatures, showing multiple isomers († and ‡)

<table>
<thead>
<tr>
<th>Complex</th>
<th>6</th>
<th>7</th>
<th>21</th>
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<tr>
<td>[Rh(cod){HB(taz)2(pzMe2)}]</td>
<td>5.82 (s, 1H, pz 4-H)†, 5.71 (s, 1H, pz 4-H)‡, 4.95-3.93 (br m, 8H+8H, taz 4-C2H2CH3 &amp; cod C2H2), 2.78-1.36 (br m, 8H+8H, cod C2H2), 2.47-2.25 (m, 12H+12H, pz 3/5-C3H3 &amp; taz 3-C3H3), 1.24 (t, 3H, 3JHH 7.0, taz 4-CH2C2H), 1.15 (br t, 3H+6H, 3JHH 7.0, taz 4-CH2C2H)</td>
<td>8.73-7.88 (m, 5H+5H, pz 3-Ph), 8.48 (d, 1H, 3JIII 2.2, pz 5-H)†, 8.36 (d, 1H, 3JIII 2.4, pz 5-H)‡, 6.73 (d, 1H, 3JIII 2.2, pz 4-H)†, 6.49 (d, 1H, 3JIII 2.4, pz 4-H)‡, 4.43-3.72 (br m, 8H+8H, taz 4-C2H2CH3 &amp; cod C2H2), 3.58-1.42 (br m, 8H+8H, cod C2H2), 2.54 (s, 3H, taz 3-C3H3), 2.37 (s, 6H, taz 3-C3H3), 2.32 (s, 3H, taz 3-C3H3), 1.37 (t, 3H, 3JIII 7.0, taz 4-C2H2CH3)†, 1.31 (t, 3H, 3JIII 7.4, taz 4-C2H2CH3)‡</td>
<td>8.03-7.12 (m, 20H+20H, PPh3 &amp; pz 3-Ph), 6.72 (d, 1H, 3JIII 2.2 pz 4-H)†, 6.02 (d, 1H, 3JIII 2.6 pz 4-H)‡, 4.37 (q, 1H, 3JIII 7.3; taz 4-CHHCH3), 4.32 (q, 1H, 3JIII 7.0, taz 4-CHHCH3), 4.15 (q, 1H, 3JIII 7.3, taz 4-CHHCH3), 3.96 (m, 3H, taz 4-CHHCH3), 3.40 (q, 1H, 3JIII 6.9, taz 4-CHHCH3)‡, 3.17 (q, 1H, 3JIII 7.3, taz 4-CHHCH3)‡, 2.50 (s, 3H, taz 3-C3H3), 2.42 (s, 3H, taz 3-C3H3), 2.32 (s, 3H, taz 3-C3H3)‡, 2.16 (s, 3H, taz 3-C3H3)‡, 1.39 (s, 6H+3H, 3JIII 7.0, taz 4-C2H2CH3)†, 0.91 (t, 3H, 3JIII 7.2, taz 4-C2H2CH3)‡</td>
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a Chemical shift (δ) in ppm, J values in Hz, spectra in CD2Cl2. b At –80 °C. c At –60 °C.