Supporting Information

Alumazene Adducts with Pyridines: Synthesis, Structure, and Stability Studies

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[2,6-(*i*-Pr)$_2$C$_6$H$_3$NAlMe]$_3$(C$_5$H$_5$N)$_2$ (**2**)

IR (KBr pellet, cm^{-1}): ν 3047 vw, 3004 vw, 2961 vs, 2866 w, 1613 m, 1586 vw, 1575 vw, 1495 vw, 1462 w, 1448 s, 1421 vs, 1381 vw, 1360 vw, 1308 w, 1253 vw, 1229 m, 1179 vs, 1157 vw, 1143 vw, 1107 w, 1070 w, 1049 w, 1039 w, 1018 vw, 955 vw, 930 vw, 898 vs, 879 m, 858 s, 832 w, 791 vs, 761 w, 743 w, 735 w, 728 w, 715 m, 701 m, 648 m, 618 vw, 603 vw, 579 vw, 569 vw, 535 vw, 465 vw, 446 w.

[2,6-(*i*-Pr)$_2$C$_6$H$_3$NAlMe]$_3$(dmap)$_2$ (**4**)

IR (KBr pellet, cm^{-1}): ν 3044 vw, 2961 m, 2928 m, 2903 w, 2868 w, 2829 vw, 1631 vs, 1584 vw, 1545 m, 1496 vw, 1458 w, 1445 w, 1421 m, 1392 w, 1356 vw, 1311 w, 1253 w, 1231 s, 1178 s, 1144 vw, 1117 vw, 1105 w, 1068 w, 1037 w, 1020 s, 950 vw, 929 vw, 901 m, 857 m, 813 w, 789 s, 767 w, 732 w, 713 w, 652 w, 645 w, 606 vw, 577 vw, 534 vw, 438 vw.

[2,6-(*i*-Pr)$_2$C$_6$H$_3$NAlMe]$_3$(C$_5$H$_5$N)(dmap) (**5**)

^{13}C{^{1}H} NMR (125.77 MHz, chloroform-d_1, 223 K): δ –12.04, –11.98, –11.91 (3×s, Al*C*H$_3$), –9.7, –7.82, –5.73 (br s, base-A*C* H$_3$), 22.98, 23.00, 23.18, 23.24, 23.30, 23.51, 23.77, 24.01, 24.69, 24.75, 24.88, 24.93, 25.06, 25.15, 25.17, 25.28, 25.32, 25.40, 25.48 (19×s, CH(*C*H$_3$)$_2$), 26.75, 27.02, 27.06, 27.11, 27.13, 27.18, 27.25, 27.41, 27.45, 27.57, 27.75, 27.80 (12×s, *C*H(CH$_3$)$_2$), 39.37 and 39.43 (2×s, N(*C*H$_3$)$_2$), 106.43 and 106.46 (2×s, C-3, dmap), 118.02, 118.45, 118.91, 119.06, 119.38, 119.72, 122.29, 122.35, 122.42, 122.48, 122.52, 122.59, 122.61, 122.69, 122.86, 124.77, 140.24, 143.46, 143.61, 143.93, 143.99, 144.07, 144.18, 144.26, 144.38, 144.79, 144.85, 145.11, 146.97, 147.15, 148.08, 148.22, 148.25, 148.33, 149.19, 149.28, 151.70, 152.59, 153.39, 154.18, 154.37 (s).

IR (KBr pellet, cm^{-1}): ν 3047 vw, 2961 vs, 2866 w, 1632 s, 1586 vw, 1547 w, 1494 vw, 1448 w, 1421 s, 1395 vw, 1381 vw, 1359 vw, 1309 w, 1253 vw, 1231 s, 1179 vs, 1108 w, 1069 vw, 1049 vw, 1040 vw, 1020 m, 950 vw, 899 s, 857 s, 812 vw, 790 vs, 732 w, 714 m, 648 w, 60 vw, 578 vw, 535 vw.

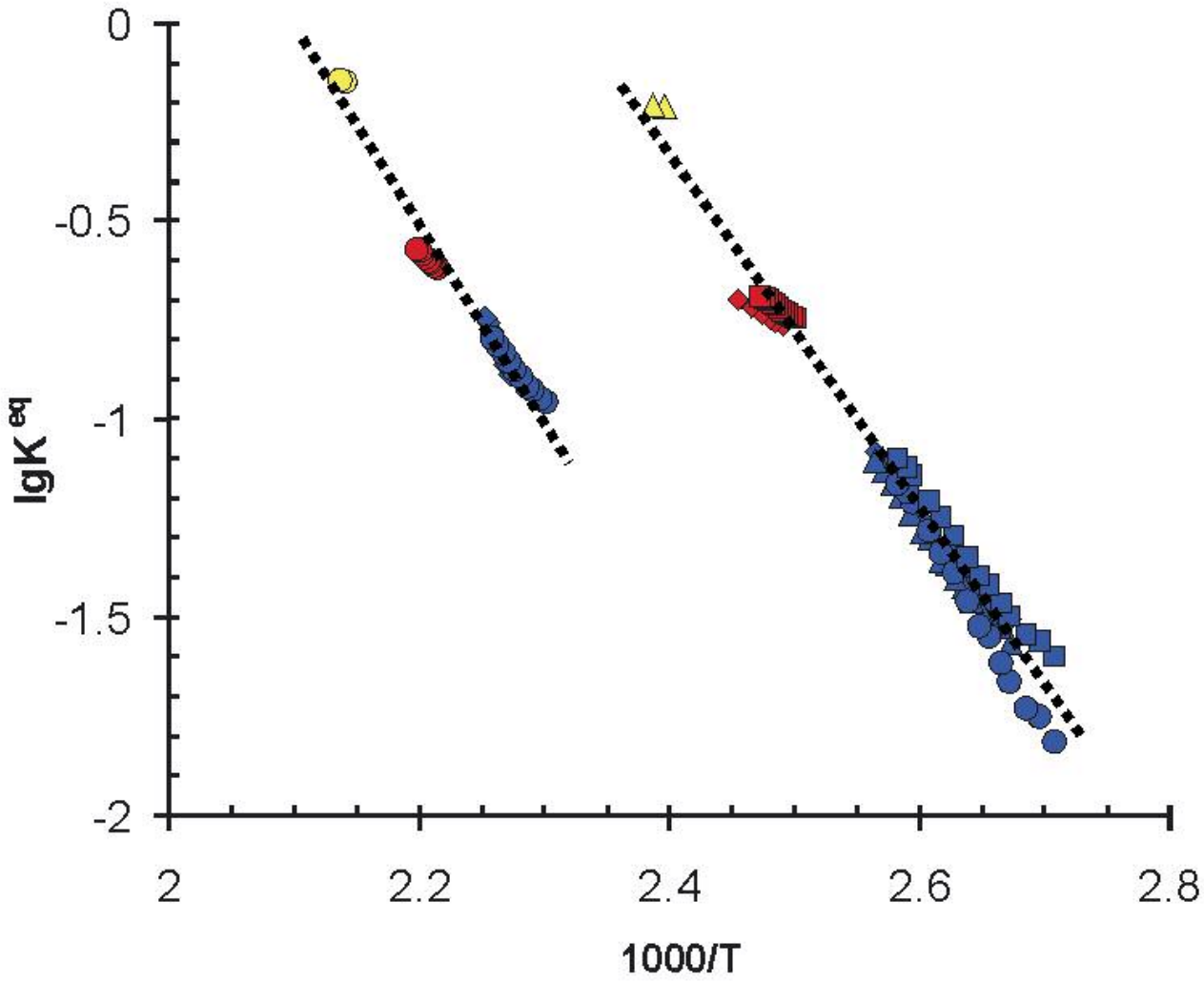
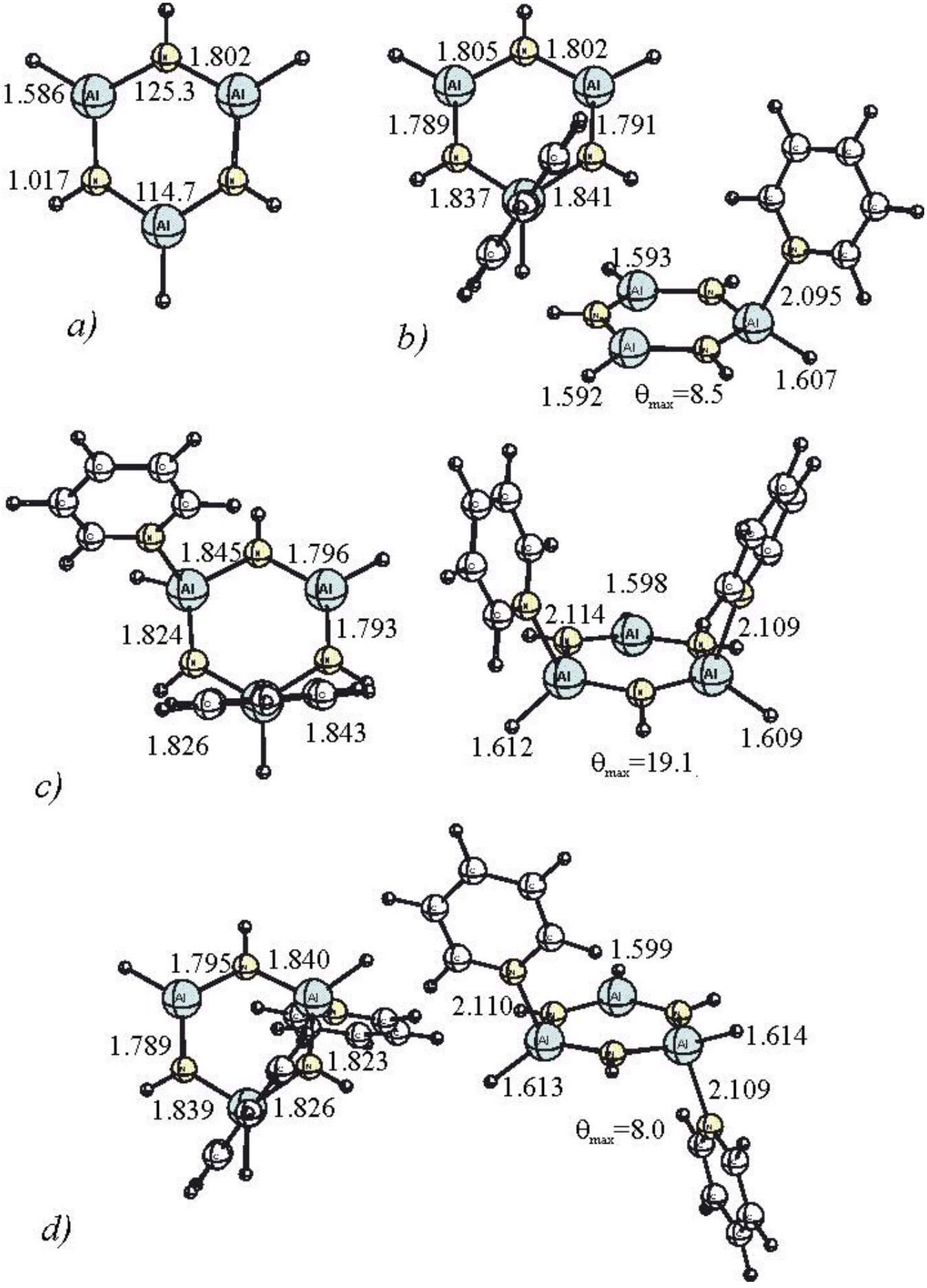


Figure 6S. Logarithm of the equilibrium constant versus inverse temperature. Yellow points – data of the first series, blue points – second series, red points – third series.


1.802
1.586
125.3
1.017
114.7
a)
1.805
1.802
1.789
1.791
1.837
1.841
1.593
2.095
1.592
θmax=8.5
1.607
b)
1.845
1.796
1.824
1.793
1.826
1.843
c)
1.598
2.114
2.109
1.612
1.609
θmax=19.1
1.795
1.840
1.789
1.823
1.839
1.826
d)
1.599
2.110
1.614
1.613
2.109
θmax=8.0

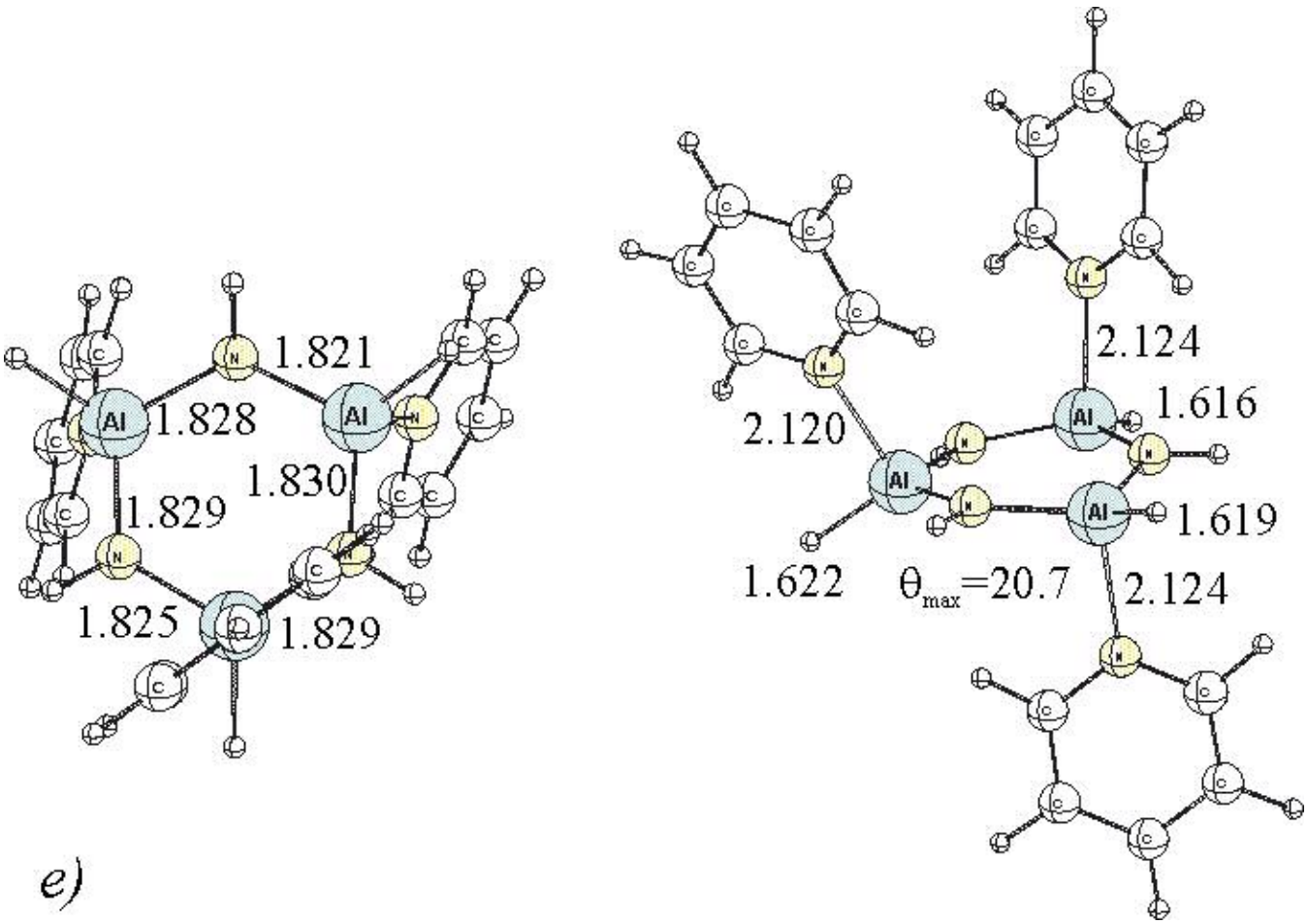


Figure 7S. Optimized structures of the model compounds: a) $[HAlNH]_3$; b) $[HAlNH]_3(py)$; c) cis-$[HAlNH]_3(py)_2$; d) trans-$[HAlNH]_3(py)_2$ e) trans-$[HAlNH]_3(py)_3$. All distances in angstroms, all angles in degrees.

References

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