Unprecedented reactivity of an aluminium hydride complex with ArNH2BH3

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S.Harder
J.Speilmann

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R.H. Blessing, Acta Cryst. (1995) A51 33-38
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goodness of fit S are based on F^2^, conventional R-factors R are based
on F, with F set to zero for negative F^2^. The threshold expression of
F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on F^2^ are statistically about twice as large as those based on F, and R-
factors based on ALL data will be even larger.
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C1 C 0.3580(4) 0.1816(3) 0.3883(2) 0.0292(8) Uani 1 1 d . . .
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C3 C 0.3008(4) 0.3931(3) 0.39469(18) 0.0225(7) Uani 1 1 d . . .
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C4 C 0.2940(4) 0.5131(3) 0.37085(17) 0.0201(6) Uani 1 1 d . . .
C5 C 0.1448(4) 0.6033(3) 0.4058(2) 0.0300(8) Uani 1 1 d . . .
H5A H 0.1706 0.6105 0.4531 0.045 Uiso 1 1 calc R . .
H5B H 0.0440 0.5770 0.4151 0.045 Uiso 1 1 calc R . .
H5C H 0.1229 0.6810 0.3719 0.045 Uiso 1 1 calc R . .
C6 C 0.6132(4) 0.1984(3) 0.27036(18) 0.0197(6) Uani 1 1 d . . .
C7 C 0.5583(4) 0.2012(3) 0.20293(18) 0.0229(7) Uani 1 1 d . . .
C8 C 0.6305(5) 0.1007(3) 0.1704(2) 0.0297(8) Uani 1 1 d . . .
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C10 C 0.8138(4) 0.0034(3) 0.2649(2) 0.0276(7) Uani 1 1 d . . .
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C11 C 0.7419(4) 0.1009(3) 0.30160(18) 0.0213(6) Uani 1 1 d . . .
C12 C 0.4218(5) 0.3074(3) 0.1668(2) 0.0287(8) Uani 1 1 d . . .
H12 H 0.4252 0.3802 0.1815 0.034 Uiso 1 1 calc R . .
C13 C 0.2447(5) 0.2964(4) 0.1946(3) 0.0450(10) Uani 1 1 d . . .
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H13B H 0.1607 0.3644 0.1685 0.067 Uiso 1 1 calc R . .
H13C H 0.2193 0.2956 0.2483 0.067 Uiso 1 1 calc R . .
C14 C 0.4552(6) 0.3259(4) 0.0816(2) 0.0439(10) Uani 1 1 d . . .
H14A H 0.4337 0.2625 0.0650 0.066 Uiso 1 1 calc R . .
H14B H 0.5738 0.3235 0.0650 0.066 Uiso 1 1 calc R . .
H14C H 0.3796 0.4037 0.0603 0.066 Uiso 1 1 calc R . .
C15 C 0.8102(4) 0.0953(3) 0.37247(19) 0.0234(7) Uani 1 1 d . . .
H15 H 0.7360 0.1659 0.3949 0.028 Uiso 1 1 calc R . .
C16 C 0.9918(4) 0.1033(4) 0.3543(2) 0.0342(8) Uani 1 1 d . . .
H16A H 1.0691 0.0309 0.3370 0.051 Uiso 1 1 calc R . .
H16B H 1.0278 0.1108 0.3992 0.051 Uiso 1 1 calc R . .
H16C H 0.9945 0.1732 0.3151 0.051 Uiso 1 1 calc R . .
C17 C 0.8071(5) -0.0178(3) 0.4305(2) 0.0330(8) Uani 1 1 d . . .
H17A H 0.6923 -0.0249 0.4399 0.049 Uiso 1 1 calc R . .
H17B H 0.8390 -0.0130 0.4771 0.049 Uiso 1 1 calc R . .
H17C H 0.8878 -0.0879 0.4117 0.049 Uiso 1 1 calc R . .
C18 C 0.3793(4) 0.6736(3) 0.28580(17) 0.0202(6) Uani 1 1 d . . .
C19 C 0.4254(4) 0.7505(3) 0.31674(19) 0.0228(7) Uani 1 1 d . . .
C20 C 0.3982(5) 0.8685(3) 0.2787(2) 0.0291(8) Uani 1 1 d . . .
H20 H 0.4309 0.9215 0.2982 0.038 Uiso 1 1 calc R . .
C21 C 0.3253(5) 0.9096(3) 0.2136(2) 0.0328(8) Uani 1 1 d . . .
H21 H 0.3084 0.9900 0.1884 0.043 Uiso 1 1 calc R . .
C22 C 0.2767(5) 0.8331(3) 0.1850(2) 0.0288(8) Uani 1 1 d . . .
H22 H 0.2237 0.8627 0.1408 0.038 Uiso 1 1 calc R . .
C23 C 0.3035(4) 0.7143(3) 0.21929(18) 0.0232(7) Uani 1 1 d . . .
C24 C 0.4971(4) 0.7140(3) 0.39035(19) 0.0258(7) Uani 1 1 d . . .
H24 H 0.5094 0.6277 0.4101 0.031 Uiso 1 1 calc R . .
C25 C 0.6722(5) 0.7305(4) 0.3805(2) 0.0357(9) Uani 1 1 d . . .
H25A H 0.7489 0.6854 0.3432 0.054 Uiso 1 1 calc R . .
H25B H 0.7185 0.7012 0.4282 0.054 Uiso 1 1 calc R . .
H25C H 0.6614 0.8154 0.3637 0.054 Uiso 1 1 calc R . .
C26 C 0.3773(5) 0.7869(4) 0.4482(2) 0.0389(9) Uani 1 1 d . . .
H26A H 0.3699 0.8712 0.4312 0.058 Uiso 1 1 calc R . .
H26B H 0.4219 0.7571 0.4963 0.058 Uiso 1 1 calc R . .
H26C H 0.2639 0.7787 0.4539 0.058 Uiso 1 1 calc R . .
C27 C 0.2430(5) 0.6343(3) 0.1869(2) 0.0288(8) Uani 1 1 d . . .
H27 H 0.3029 0.5497 0.2088 0.035 Uiso 1 1 calc R . .
C28 C 0.0533(6) 0.6553(5) 0.2094(3) 0.0515(12) Uani 1 1 d . . .
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H28B H 0.0279 0.6428 0.2639 0.077 Uiso 1 1 calc R . .
H28C H 0.0190 0.5993 0.1908 0.077 Uiso 1 1 calc R . .
C29 C 0.2871(7) 0.6491(5) 0.1027(3) 0.0532(12) Uani 1 1 d . . .
H29A H 0.2208 0.7288 0.0793 0.080 Uiso 1 1 calc R . .
H29B H 0.2601 0.5885 0.0854 0.080 Uiso 1 1 calc R . .
H29C H 0.4087 0.6394 0.0891 0.080 Uiso 1 1 calc R . .
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N2 N 0.4124(3) 0.5474(2) 0.31995(14) 0.0187(5) Uani 1 1 d . . .
Al1 Al 0.61828(11) 0.43203(8) 0.29007(5) 0.0175(2) Uani 1 1 d . . .
C32 C 0.6939(8) 0.8747(5) 0.0479(3) 0.0625(14) Uani 1 1 d . . .
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C31 C 0.7494(10) 0.7557(6) 0.0512(4) 0.080(2) Uani 1 1 d . . .
H31 H 0.6896 0.7068 0.0849 0.119 Uiso 1 1 calc R . .
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H201 H 0.743(5) 0.504(3) 0.314(2) 0.027(10) Uiso 1 1 d . . .
H101 H 0.625(6) 0.517(4) 0.198(2) 0.042(12) Uiso 1 1 d . . .
H102 H 0.787(6) 0.370(4) 0.226(3) 0.044(12) Uiso 1 1 d . . .
H204 H 0.759(5) 0.458(4) 0.418(2) 0.038(11) Uiso 1 1 d . . .
H202 H 0.736(6) 0.354(4) 0.368(3) 0.051(13) Uiso 1 1 d . . .
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C6 0.0187(14) 0.0176(15) 0.0238(15) -0.0046(12) 0.0024(12) -0.0092(12)
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C8 0.037(2) 0.0275(19) 0.0285(18) -0.0103(15) -0.0030(15) -0.0120(16)
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C19 0.0163(14) 0.0231(17) 0.0267(16) -0.0075(13) 0.0016(12) -0.0040(13)
C20 0.0332(19) 0.0202(17) 0.0356(19) -0.0097(15) -0.0013(15) -0.0092(15)
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C26 0.041(2) 0.042(2) 0.034(2) -0.0177(18) -0.0005(17) -0.0087(18)
C27 0.0315(18) 0.0234(18) 0.0310(18) -0.0081(14) -0.0124(15) -0.0011(15)
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C29 0.065(3) 0.068(3) 0.037(2) -0.017(2) -0.011(2) -0.026(3)
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N2 0.0178(12) 0.0184(13) 0.0198(13) -0.0044(10) -0.0023(10) -0.0050(10)
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C33 0.093(4) 0.048(3) 0.057(3) -0.005(3) 0.027(3) -0.009(3)
C31 0.092(5) 0.057(4) 0.107(5) 0.015(4) -0.066(4) -0.036(4)
C34 0.070(4) 0.070(4) 0.039(3) 0.008(2) 0.007(2) 0.007(3)
C35 0.064(4) 0.103(6) 0.089(5) -0.059(4) -0.046(4) 0.037(4)
C30 0.115(7) 0.047(4) 0.198(10) -0.027(5) -0.119(7) 0.003(4)

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are estimated using the full covariance matrix. The cell esds are taken
into account individually in the estimation of esds in distances, angles
and torsion angles; correlations between esds in cell parameters are only
used when they are defined by crystal symmetry. An approximate (isotropic)
treatment of cell esds is used for estimating esds involving l.s. planes.
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B1 H104 1.12(5) . ?
B2 Al1 2.232(4) . ?
B2 H201 1.18(4) . ?
B2 H204 1.13(4) . ?
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C1 C2 1.508(4) . ?
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C1 H1B 0.9800 . ?
C1 H1C 0.9800 . ?
C2 N1 1.344(4) . ?
C2 C3 1.394(5) . ?
C3 C4 1.401(5) . ?
C3 H3 0.9500 . ?
C4 N2 1.337(4) . ?
C4 C5 1.508(5) . ?
C5 H5A 0.9800 . ?
C5 H5B 0.9800 . ?
C5 H5C 0.9800 . ?
C6 C11 1.398(4) . ?
C6 C7 1.414(4) . ?
C6 N1 1.468(4) . ?
C7 C8 1.388(5) . ?
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C17 H17C 0.9800 . ?
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C21 C22 1.381(5) . ?
C21 H21 0.9500 . ?
C22 C23 1.389(5) . ?
C22 H22 0.9500 . ?
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C28 H28C 0.9800 . ?
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C29 H29B 0.9800 . ?
C29 H29C 0.9800 . ?
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Al1 H101 1.77(4) . ?
Al1 H102 1.75(4) . ?
Al1 H202 1.81(5) . ?
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C31 H31 0.9500 . ?
C34 C35 1.371(10) . ?
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H202 B2 H203 111(3) . . ?
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C6 N1 Al1 123.16(19) . . ?
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