10.1071/CH11227_AC
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_publ_contact_author_address
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University of New South Wales
Sydney
NSW 2052
Australia
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_publ_contact_author_email       m.cole@unsw.edu.au
_publ_contact_author_phone       '+61 (0)2 93854678'
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H8A3 H 0.8779 -0.2056 0.4011 0.086 Uiso 0.679(17) 1 calc PR A 1
C5B C 0.711(4) -0.0605(19) 0.518(3) 0.014(7) Uani 0.321(17) 1 d PU A 2
H5B1 H 0.6931 -0.0824 0.6031 0.017 Uiso 0.321(17) 1 calc PR A 2
H5B2 H 0.6173 -0.0639 0.4672 0.017 Uiso 0.321(17) 1 calc PR A 2
C6B C 0.846(4) -0.097(2) 0.457(4) 0.042(9) Uani 0.321(17) 1 d PU A 2
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O2 0.068(6) 0.048(5) 0.060(6) -0.015(5) -0.001(5) 0.015(5)
O3 0.060(6) 0.042(5) 0.148(10) -0.041(6) -0.018(6) 0.002(5)
O4 0.043(5) 0.047(5) 0.096(7) -0.038(5) -0.005(5) 0.007(4)
O5 0.078(6) 0.060(5) 0.025(4) 0.011(4) 0.029(4) 0.042(5)
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C4 0.130(13) 0.023(5) 0.033(7) -0.006(5) 0.000(7) 0.007(7)
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C10 0.057(8) 0.036(6) 0.026(6) -0.003(5) -0.007(5) 0.006(6)
C11 0.040(6) 0.036(6) 0.045(7) -0.013(5) -0.014(5) 0.016(6)
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O3 C11 1.118(13) . ?
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School of Chemistry
University of New South Wales
Sydney
NSW 2052
Australia
;
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;
 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 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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Cl1 Cl 0.60371(14) 0.81028(10) 0.72304(10) 0.0254(2) Uani 1 1 d . . .
N1 N 1.0427(5) 0.8160(3) 0.9902(3) 0.0199(6) Uani 1 1 d . . .
N2 N 1.0961(5) 0.7393(3) 0.8166(3) 0.0214(7) Uani 1 1 d . . .
C1 C 0.9560(5) 0.7323(4) 0.8687(4) 0.0184(7) Uani 1 1 d . . .
C2 C 1.2361(6) 0.8750(4) 1.0148(4) 0.0255(9) Uani 1 1 d . . .
H2 H 1.3266 0.9372 1.0933 0.031 Uiso 1 1 calc R . .
C3 C 1.2696(6) 0.8267(4) 0.9058(4) 0.0257(8) Uani 1 1 d . . .
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C4 C 0.9490(6) 0.8421(5) 1.0849(4) 0.0276(9) Uani 1 1 d . . .
H4A H 0.8229 0.8410 1.0418 0.041 Uiso 1 1 calc R . .
H4B H 1.0221 0.9383 1.1462 0.041 Uiso 1 1 calc R . .
H4C H 0.9390 0.7647 1.1308 0.041 Uiso 1 1 calc R . .
C5 C 1.0702(6) 0.6842(4) 0.6802(4) 0.0250(8) Uani 1 1 d . . .
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C6 C 1.1079(6) 0.8103(5) 0.6169(4) 0.0275(9) Uani 1 1 d . . .
H6A H 1.0041 0.8505 0.6095 0.033 Uiso 1 1 calc R . .
H6B H 1.2257 0.8899 0.6722 0.033 Uiso 1 1 calc R . .
C7 C 1.1253(6) 0.7638(5) 0.4851(4) 0.0266(9) Uani 1 1 d . . .
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H8A H 1.1105 0.9503 0.4279 0.055 Uiso 1 1 calc R . .
H8B H 1.2039 0.8594 0.3471 0.055 Uiso 1 1 calc R . .
H8C H 1.3222 0.9581 0.4900 0.055 Uiso 1 1 calc R . .
C9 C 0.6854(6) 0.4389(4) 0.8763(4) 0.0239(8) Uani 1 1 d . . .
H9 H 0.7814 0.4927 0.9552 0.029 Uiso 1 1 calc R . .
C10 C 0.7089(6) 0.4049(4) 0.7549(4) 0.0232(8) Uani 1 1 d . . .
H10 H 0.8236 0.4304 0.7351 0.028 Uiso 1 1 calc R . .
C11 C 0.5089(6) 0.3173(4) 0.6601(4) 0.0251(8) Uani 1 1 d . . .
H11 H 0.4995 0.2588 0.5744 0.030 Uiso 1 1 calc R . .
C12 C 0.4192(6) 0.4368(4) 0.6616(4) 0.0229(8) Uani 1 1 d . . .
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C14 C 0.4730(6) 0.3713(4) 0.8561(4) 0.0248(8) Uani 1 1 d . . .
H14 H 0.4339 0.3582 0.9336 0.030 Uiso 1 1 calc R . .
C15 C 0.4184(6) 0.2319(4) 0.7466(4) 0.0291(9) Uani 1 1 d . . .
H15A H 0.2806 0.1824 0.7081 0.035 Uiso 1 1 calc R . .
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N1 0.0092(16) 0.0221(15) 0.0246(16) 0.0045(12) 0.0037(12) 0.0022(12)
N2 0.0120(16) 0.0237(16) 0.0296(17) 0.0077(13) 0.0095(13) 0.0050(13)
C1 0.0120(18) 0.0206(17) 0.0249(18) 0.0089(14) 0.0066(14) 0.0064(14)
C2 0.0082(18) 0.028(2) 0.034(2) 0.0082(17) 0.0016(15) 0.0010(15)
C3 0.0101(19) 0.028(2) 0.037(2) 0.0102(17) 0.0065(16) 0.0050(15)
C4 0.021(2) 0.033(2) 0.025(2) 0.0030(16) 0.0086(16) 0.0046(17)
C5 0.019(2) 0.029(2) 0.030(2) 0.0053(16) 0.0125(16) 0.0098(16)
C6 0.025(2) 0.028(2) 0.035(2) 0.0076(17) 0.0131(18) 0.0141(17)
C7 0.018(2) 0.030(2) 0.029(2) 0.0070(17) 0.0069(16) 0.0070(17)
C8 0.041(3) 0.040(3) 0.041(3) 0.020(2) 0.019(2) 0.021(2)
C9 0.016(2) 0.0202(18) 0.0258(19) 0.0050(15) -0.0017(15) 0.0003(15)
C10 0.0130(19) 0.0205(18) 0.033(2) 0.0055(15) 0.0049(16) 0.0036(14)
C11 0.014(2) 0.0209(18) 0.033(2) -0.0023(15) 0.0053(16) 0.0024(15)
C12 0.0108(18) 0.0231(18) 0.0255(19) 0.0016(15) -0.0014(15) 0.0007(14)
C13 0.0065(18) 0.0215(18) 0.034(2) 0.0017(15) 0.0055(15) -0.0016(14)
C14 0.014(2) 0.0235(19) 0.032(2) 0.0067(16) 0.0077(16) 0.0002(15)
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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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C7 C8 1.515(6) . ?
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C1 N1 C2 111.3(3) . . ?
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C1 N2 C5 125.2(3) . . ?
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C9 C10 C11 105.8(4) . . ?
C9 C10 Rh1 70.9(2) . . ?
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C10 C11 C15 100.4(3) . . ?
C13 C12 C11 106.7(4) . . ?
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C11 C12 Rh1 93.9(2) . . ?
C12 C13 C14 107.0(4) . . ?
C12 C13 Rh1 71.3(2) . . ?
C14 C13 Rh1 94.4(2) . . ?
C13 C14 C9 100.7(3) . . ?
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;
School of Chemistry
University of New South Wales
Sydney
NSW 2052
Australia
;
_publ_contact_author_email       m.cole@unsw.edu.au
_publ_contact_author_phone       '+61 (0)2 93854678'
_publ_contact_author_fax         '+61 (0)2 93856141'

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_refine_special_details
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 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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Cl1 Cl 0.19929(5) 0.47242(4) 0.26842(5) 0.03061(15) Uani 1 1 d . . .
N1 N 0.02441(16) 0.38706(13) 0.02902(16) 0.0217(4) Uani 1 1 d . . .
N2 N 0.15248(16) 0.41154(12) -0.00367(16) 0.0206(4) Uani 1 1 d . . .
C1 C 0.12343(19) 0.38183(14) 0.06876(18) 0.0190(5) Uani 1 1 d . . .
C2 C -0.0074(2) 0.42054(15) -0.06573(19) 0.0247(5) Uani 1 1 d . . .
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C3 C 0.0731(2) 0.43574(15) -0.08604(19) 0.0243(5) Uani 1 1 d . . .
H3 H 0.0750 0.4587 -0.1456 0.029 Uiso 1 1 calc R . .
C4 C -0.0395(2) 0.36088(18) 0.0802(2) 0.0308(6) Uani 1 1 d . . .
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H4B H -0.0910 0.3998 0.0710 0.046 Uiso 1 1 calc R . .
H4C H -0.0010 0.3545 0.1521 0.046 Uiso 1 1 calc R . .
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H5B H 0.2952 0.3808 0.0539 0.034 Uiso 1 1 calc R . .
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H6A H 0.2888 0.5089 0.1138 0.043 Uiso 1 1 calc R . .
H6B H 0.2562 0.5417 0.0016 0.043 Uiso 1 1 calc R . .
C7 C 0.4019(3) 0.5104(4) 0.0615(4) 0.0832(18) Uani 1 1 d . . .
H7A H 0.4365 0.4675 0.1072 0.100 Uiso 1 1 calc R A 1
H7B H 0.4044 0.4971 -0.0048 0.100 Uiso 1 1 calc R A 1
C8A C 0.4583(5) 0.5700(4) 0.0916(5) 0.0459(19) Uani 0.542(8) 1 d P B 1
H8A1 H 0.4642 0.5837 0.1600 0.069 Uiso 0.542(8) 1 calc PR B 1
H8A2 H 0.4305 0.6143 0.0467 0.069 Uiso 0.542(8) 1 calc PR B 1
H8A3 H 0.5232 0.5576 0.0910 0.069 Uiso 0.542(8) 1 calc PR B 1
C8B C 0.4674(5) 0.4690(5) 0.1520(6) 0.046(2) Uani 0.458(8) 1 d P B 2
H8B1 H 0.5345 0.4883 0.1699 0.069 Uiso 0.458(8) 1 calc PR B 2
H8B2 H 0.4656 0.4128 0.1383 0.069 Uiso 0.458(8) 1 calc PR B 2
H8B3 H 0.4455 0.4784 0.2079 0.069 Uiso 0.458(8) 1 calc PR B 2
C9 C 0.1664(2) 0.22840(16) 0.1663(2) 0.0284(6) Uani 1 1 d . . .
H9 H 0.1085 0.2484 0.1163 0.034 Uiso 1 1 calc R . .
C10 C 0.2568(2) 0.24438(15) 0.1554(2) 0.0284(6) Uani 1 1 d . . .
H10 H 0.2558 0.2759 0.1005 0.034 Uiso 1 1 calc R . .
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C11 C 0.3548(2) 0.21393(18) 0.2266(2) 0.0326(6) Uani 1 1 d . . .
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H11B H 0.3447 0.1635 0.2553 0.039 Uiso 1 1 calc R . .
C12 C 0.4063(2) 0.27098(18) 0.3126(2) 0.0309(6) Uani 1 1 d . . .
H12A H 0.4479 0.2409 0.3720 0.037 Uiso 1 1 calc R . .
H12B H 0.4496 0.3057 0.2922 0.037 Uiso 1 1 calc R . .
C13 C 0.3359(2) 0.32067(17) 0.3416(2) 0.0254(6) Uani 1 1 d . . .
H13 H 0.3482 0.3753 0.3488 0.030 Uiso 1 1 calc R . .
C14 C 0.2548(2) 0.29273(17) 0.35846(19) 0.0256(6) Uani 1 1 d . . .
H14 H 0.2134 0.3294 0.3732 0.031 Uiso 1 1 calc R . .
C15 C 0.2288(2) 0.20684(18) 0.3546(2) 0.0339(7) Uani 1 1 d . . .
H15A H 0.2007 0.1959 0.4063 0.041 Uiso 1 1 calc R . .
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C16 C 0.1552(2) 0.18181(18) 0.2515(3) 0.0366(7) Uani 1 1 d . . .
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C9 0.0352(15) 0.0183(12) 0.0270(14) 0.0020(11) 0.0061(12) 0.0018(11)
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Cl1 Cl 0.4562(4) 0.6041(4) 0.2291(2) 0.0772(10) Uani 1 1 d . . .
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N3 N 0.3980(10) 0.1459(10) 0.1567(5) 0.0408(19) Uani 1 1 d . . .
N4 N 0.2943(13) 0.1252(12) 0.2574(5) 0.057(2) Uani 1 1 d . B .
C1 C 0.0678(12) 0.5350(11) 0.1406(6) 0.040(2) Uani 1 1 d . . .
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C15A C -0.035(4) 0.097(3) 0.3930(12) 0.075(8) Uani 0.532(15) 1 d P B 1
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H15D H 0.3947 0.1543 0.4334 0.158 Uiso 0.468(15) 1 calc PR B 2
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H16E H 0.6722 0.4345 0.5071 0.235 Uiso 0.468(15) 1 calc PR B 2
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C17 C 0.380(4) 0.031(3) 0.5412(13) 0.082(9) Uani 0.56(2) 1 d P . 3
H17 H 0.2994 0.0465 0.5713 0.098 Uiso 0.56(2) 1 calc PR . 3
C18 C 0.566(5) 0.162(4) 0.5490(14) 0.089(9) Uani 0.56(2) 1 d P . 3
H18 H 0.6094 0.2741 0.5789 0.107 Uiso 0.56(2) 1 calc PR . 3
C19 C 0.682(4) 0.120(4) 0.5115(17) 0.090(9) Uani 0.56(2) 1 d P . 3
C20 C 0.877(11) 0.285(9) 0.569(2) 0.14(3) Uani 0.30 1 d P C 3
H20A H 0.9048 0.2471 0.6171 0.211 Uiso 0.30 1 calc PR C 3
H20B H 0.8534 0.3892 0.5788 0.211 Uiso 0.30 1 calc PR C 3
H20C H 0.9855 0.3151 0.5454 0.211 Uiso 0.30 1 calc PR C 3

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Pd1 0.0344(4) 0.0238(4) 0.0473(4) 0.0083(3) 0.0098(3) 0.0197(3)
Cl1 0.0652(19) 0.057(2) 0.116(3) 0.0072(19) -0.0004(18) 0.0419(17)
Cl2 0.0707(19) 0.0441(16) 0.082(2) 0.0098(15) 0.0023(15) 0.0334(15)
N1 0.045(5) 0.025(4) 0.062(5) 0.013(4) 0.002(4) 0.018(4)
N2 0.034(4) 0.031(4) 0.068(6) -0.007(4) -0.007(4) 0.023(4)
N3 0.035(4) 0.031(4) 0.057(5) -0.006(4) 0.001(4) 0.021(4)
N4 0.074(6) 0.056(6) 0.071(6) 0.033(5) 0.031(5) 0.049(5)
C1 0.028(5) 0.023(5) 0.065(6) -0.005(5) -0.006(4) 0.015(4)
C2 0.056(7) 0.030(6) 0.081(8) 0.009(6) -0.014(6) 0.023(5)
C3 0.046(6) 0.034(6) 0.091(9) -0.022(6) -0.028(6) 0.031(5)
C4 0.058(7) 0.032(6) 0.064(7) 0.006(5) 0.003(6) 0.014(5)
C5 0.040(6) 0.042(6) 0.069(7) -0.008(6) 0.005(5) 0.022(5)
C6 0.098(12) 0.130(15) 0.064(9) -0.006(10) 0.037(9) 0.013(11)
C7 0.084(13) 0.24(3) 0.128(17) -0.027(19) 0.016(12) 0.051(17)
C8 0.30(4) 0.33(5) 0.29(4) 0.04(4) 0.08(3) 0.26(4)
C9 0.036(5) 0.026(5) 0.061(6) 0.011(5) 0.006(5) 0.016(4)
C10 0.045(6) 0.027(5) 0.078(8) 0.000(5) -0.001(5) 0.027(5)
C11 0.069(8) 0.043(7) 0.094(9) 0.027(7) 0.000(7) 0.036(6)
C12 0.048(6) 0.065(8) 0.060(7) -0.003(6) 0.002(5) 0.034(6)
C13 0.120(14) 0.123(15) 0.126(15) 0.078(12) 0.076(12) 0.088(13)
C14A 0.074(17) 0.053(15) 0.061(14) -0.010(11) -0.015(12) 0.032(14)
C14B 0.28(7) 0.32(8) 0.04(2) -0.01(3) 0.04(3) 0.23(7)
C15A 0.11(2) 0.080(19) 0.054(14) 0.023(13) 0.029(13) 0.056(17)
C15B 0.10(3) 0.13(4) 0.17(5) 0.05(4) 0.03(3) 0.04(3)
C16A 0.041(14) 0.15(3) 0.12(2) -0.07(2) -0.004(14) 0.051(17)
C16B 0.16(4) 0.17(5) 0.14(4) -0.04(4) -0.04(3) 0.11(4)
C17 0.12(2) 0.060(16) 0.062(15) 0.000(13) -0.007(14) 0.042(17)
C18 0.11(2) 0.067(18) 0.073(17) -0.017(14) -0.005(15) 0.035(19)
C19 0.076(18) 0.10(2) 0.09(2) 0.028(18) -0.003(15) 0.045(18)
C20 0.28(9) 0.19(7) 0.02(2) 0.01(3) 0.01(3) 0.17(7)

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 All esds (except the esd in the dihedral angle between two l.s. planes)
 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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Pd1 C9 2.039(8) . ?
Pd1 Cl1 2.304(4) . ?
Pd1 Cl2 2.320(3) . ?
N1 C1 1.351(12) . ?
N1 C2 1.373(12) . ?
N1 C4 1.417(13) . ?
N2 C1 1.358(11) . ?
N2 C3 1.403(12) . ?
N2 C5 1.441(13) . ?
N3 C9 1.334(11) . ?
N3 C10 1.391(11) . ?
N3 C12 1.409(13) . ?
N4 C9 1.335(12) . ?
N4 C11 1.385(12) . ?
N4 C13 1.490(17) . ?
C2 C3 1.329(16) . ?
C5 C6 1.499(17) . ?
C6 C7 1.47(3) . ?
C7 C8 1.42(3) . ?
C10 C11 1.330(16) . ?
C13 C14A 1.31(3) . ?
C13 C14B 1.40(5) . ?
C14A C15A 1.55(3) . ?
C14B C15B 1.24(5) . ?
C15A C16A 1.54(3) . ?
C15B C16B 1.53(5) . ?
C17 C19 1.39(4) 2_656 ?
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C1 Pd1 Cl1 88.7(3) . . ?
C9 Pd1 Cl1 90.1(3) . . ?
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C9 Pd1 Cl2 90.1(3) . . ?
Cl1 Pd1 Cl2 179.72(12) . . ?
C1 N1 C2 110.2(9) . . ?
C1 N1 C4 124.2(8) . . ?
C2 N1 C4 125.6(9) . . ?
C1 N2 C3 108.3(9) . . ?
C1 N2 C5 124.7(7) . . ?
C3 N2 C5 126.9(9) . . ?
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C9 N3 C10 110.4(9) . . ?
C9 N3 C12 124.7(8) . . ?
C10 N3 C12 124.9(8) . . ?
C9 N4 C11 110.2(9) . . ?
C9 N4 C13 125.3(9) . . ?
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N1 C1 N2 106.4(7) . . ?
N1 C1 Pd1 127.1(7) . . ?
N2 C1 Pd1 126.5(7) . . ?
C3 C2 N1 107.5(9) . . ?
C2 C3 N2 107.7(9) . . ?
N2 C5 C6 112.5(10) . . ?
C7 C6 C5 114.3(14) . . ?
C8 C7 C6 117(3) . . ?
N3 C9 N4 105.9(7) . . ?
N3 C9 Pd1 126.8(7) . . ?
N4 C9 Pd1 127.4(7) . . ?
C11 C10 N3 106.3(8) . . ?
C10 C11 N4 107.1(9) . . ?
C14A C13 C14B 121(3) . . ?
C14A C13 N4 119(2) . . ?
C14B C13 N4 120(3) . . ?
C13 C14A C15A 118(2) . . ?
C15B C14B C13 110(5) . . ?
C16A C15A C14A 120(2) . . ?
C14B C15B C16B 105(4) . . ?
C19 C17 C18 118(3) 2_656 . ?
C19 C18 C17 117(3) . . ?
C18 C19 C17 124(3) . 2_656 ?
C18 C19 C20 91(3) . . ?
C17 C19 C20 144(3) 2_656 . ?

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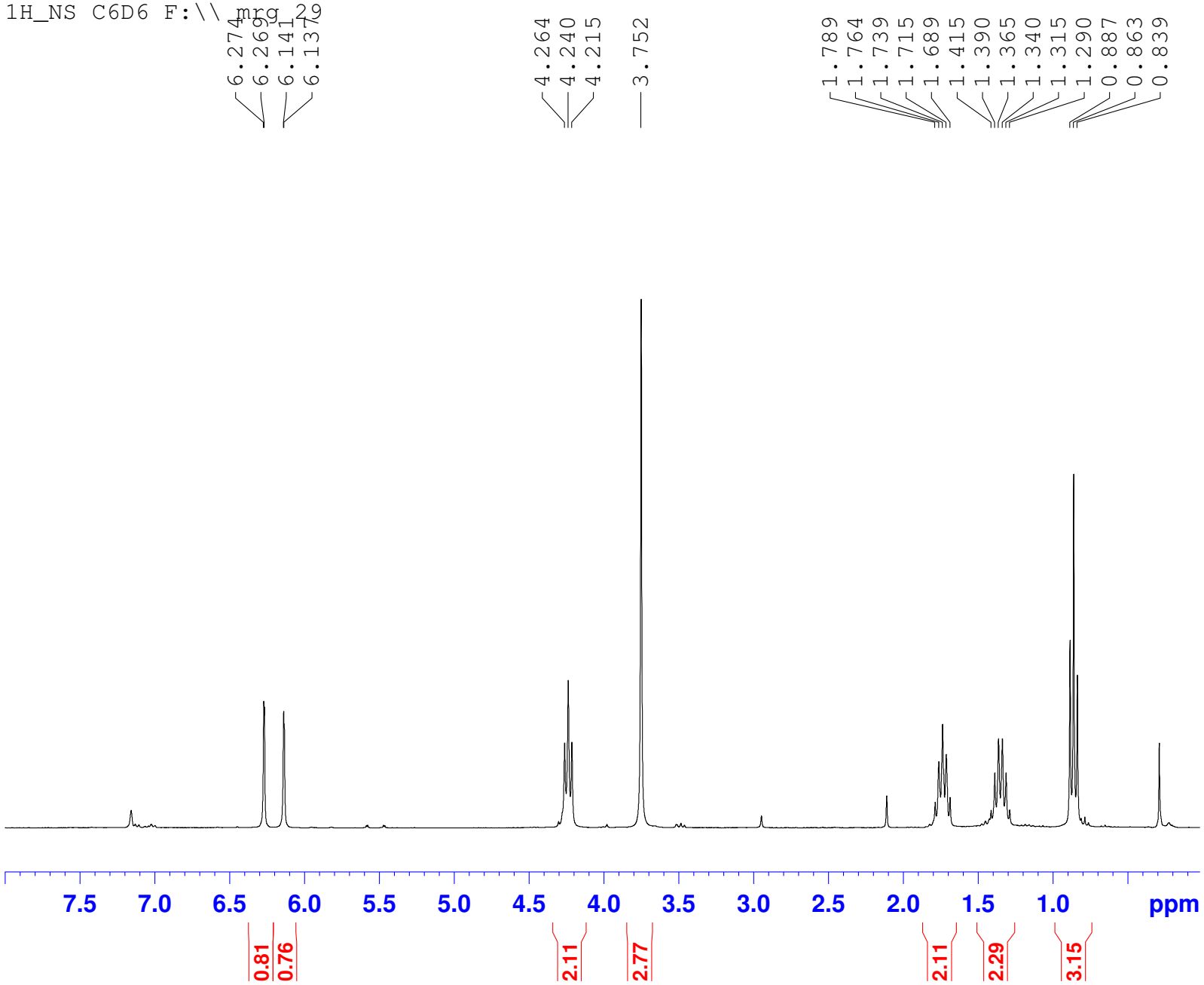
Supervisor Cole
IBuMe
1H_NS C6D6 F:\\ mrg 29



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PROCNO	1
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Time	9.16
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PULPROG	zg
TD	32768
SOLVENT	C6D6
NS	16
DS	4
SWH	6172.839 Hz
FIDRES	0.188380 Hz
AQ	2.6542580 sec
RG	128
DW	81.000 usec
DE	12.00 usec
TE	298.1 K
D1	2.00000000 sec
TD0	1

======== CHANNEL f1 ========	
NUC1	1H
P1	14.90 usec
PL1	2.50 dB
SFO1	300.1318537 MHz
SI	65536
SF	300.1300325 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00