Supplementary Material

Pyrazolium-sulfonates. Mesomeric betaines possessing iminium-sulfonate partial structures

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CIF FILE

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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
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 factors based on ALL data will be even larger.
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N1 N 0.7413(3) 0.2934(3) -0.18303(17) 0.0227(5) Uani 1 1 d . . .
N2 N 0.6913(3) 0.4331(3) -0.18021(18) 0.0238(5) Uani 1 1 d . . .
C3 C 0.6872(4) 0.4864(4) -0.0818(2) 0.0235(6) Uani 1 1 d . . .
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C5 C 0.7672(4) 0.2587(4) -0.0841(2) 0.0229(6) Uani 1 1 d . . .
S6 S 0.73419(10) 0.39658(10) 0.11819(5) 0.02310(18) Uani 1 1 d . . .
O7 O 0.8924(3) 0.3641(3) 0.15932(15) 0.0310(5) Uani 1 1 d . . .
O8 O 0.7571(3) 0.5779(3) 0.14654(17) 0.0361(5) Uani 1 1 d . . .
O9 O 0.5512(3) 0.2621(3) 0.13485(16) 0.0364(6) Uani 1 1 d . . .
C10 C 0.7538(4) 0.2025(4) -0.2793(2) 0.0228(6) Uani 1 1 d . . .
C11 C 0.8926(4) 0.2932(4) -0.3406(2) 0.0240(6) Uani 1 1 d . . .
C12 C 0.8974(4) 0.2025(4) -0.4330(2) 0.0249(6) Uani 1 1 d . . .
C13 C 0.7711(4) 0.0254(4) -0.4662(2) 0.0252(6) Uani 1 1 d . . .
C14 C 0.6372(4) -0.0605(4) -0.4016(2) 0.0243(6) Uani 1 1 d . . .
C15 C 0.6243(4) 0.0248(4) -0.3081(2) 0.0256(6) Uani 1 1 d . . .
C18 C 0.6603(5) 0.5111(5) -0.2726(2) 0.0320(7) Uani 1 1 d . . .
C19 C 0.8279(5) 0.1177(5) -0.0608(3) 0.0300(7) Uani 1 1 d . . .
C20 C 0.1779(7) 0.0114(6) -0.2385(4) 0.0536(11) Uani 1 1 d . . .
O21 O 0.2666(4) 0.1617(4) -0.2888(2) 0.0502(7) Uani 1 1 d . . .
H H 0.261(7) 0.247(7) -0.257(4) 0.076(17) Uiso 1 1 d . . .
H3 H 0.657(4) 0.581(4) -0.063(2) 0.023(8) Uiso 1 1 d . . .
H11 H 0.985(4) 0.416(4) -0.316(2) 0.022(8) Uiso 1 1 d . . .
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H13 H 0.765(4) -0.039(4) -0.529(2) 0.015(7) Uiso 1 1 d . . .
H15 H 0.543(5) -0.025(5) -0.266(3) 0.028(9) Uiso 1 1 d . . .
H18A H 0.776(6) 0.583(5) -0.296(3) 0.048(11) Uiso 1 1 d . . .
H18B H 0.607(5) 0.590(5) -0.252(3) 0.031(9) Uiso 1 1 d . . .
H18C H 0.592(5) 0.418(5) -0.328(3) 0.039(10) Uiso 1 1 d . . .
H19A H 0.866(7) 0.138(7) 0.006(4) 0.078(15) Uiso 1 1 d . . .
H19B H 0.738(7) 0.003(7) -0.081(4) 0.074(15) Uiso 1 1 d . . .
H19C H 0.929(7) 0.124(6) -0.097(4) 0.076(15) Uiso 1 1 d . . .
H20A H 0.046(8) -0.020(7) -0.236(4) 0.083(17) Uiso 1 1 d . . .
H20B H 0.247(6) 0.053(6) -0.167(4) 0.060(12) Uiso 1 1 d . . .
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N1 0.0255(12) 0.0242(13) 0.0168(11) 0.0009(10) 0.0034(9) 0.0094(10)
N2 0.0271(13) 0.0267(14) 0.0188(12) 0.0045(10) 0.0044(9) 0.0123(11)
C3 0.0226(15) 0.0250(16) 0.0219(14) 0.0006(12) 0.0052(11) 0.0093(13)
C4 0.0212(14) 0.0247(16) 0.0187(13) 0.0024(12) 0.0042(11) 0.0076(12)
C5 0.0207(14) 0.0249(16) 0.0188(13) 0.0032(12) 0.0041(11) 0.0056(12)
S6 0.0243(4) 0.0255(4) 0.0161(3) 0.0005(3) 0.0036(3) 0.0078(3)
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O7 0.0296(11) 0.0417(14) 0.0227(10) 0.0023(9) -0.0010(9) 0.0175(10)
O8 0.0505(14) 0.0324(13) 0.0253(11) -0.0034(9) 0.0041(10) 0.0192(11)
O9 0.0298(12) 0.0416(14) 0.0278(11) 0.0062(10) 0.0100(9) 0.0045(10)
C10 0.0243(14) 0.0264(16) 0.0177(13) -0.0001(11) 0.0005(10) 0.0119(12)
C11 0.0237(15) 0.0246(16) 0.0226(14) 0.0018(12) 0.0024(11) 0.0098(13)
C12 0.0279(15) 0.0288(16) 0.0214(14) 0.0063(12) 0.0049(11) 0.0147(13)
C13 0.0331(16) 0.0264(16) 0.0185(14) -0.0012(12) 0.0019(11) 0.0160(13)
C14 0.0284(16) 0.0219(15) 0.0219(14) 0.0003(12) -0.0031(11) 0.0118(13)
C15 0.0241(15) 0.0289(17) 0.0217(15) 0.0049(13) 0.0036(12) 0.0090(13)
C18 0.042(2) 0.042(2) 0.0206(16) 0.0089(15) 0.0082(14) 0.0244(18)
C19 0.0377(19) 0.0294(19) 0.0242(16) 0.0052(14) 0.0032(14) 0.0157(16)
C20 0.064(3) 0.047(3) 0.056(3) 0.011(2) 0.020(2) 0.026(2)
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 All esds (except the esd in the dihedral angle between two l.s. planes)
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N1 C10 1.437(4) . ?
N2 C3 1.325(4) . ?
N2 C18 1.464(4) . ?
C3 C4 1.388(4) . ?
C3 H3 0.94(3) . ?
C4 C5 1.391(4) . ?
C4 S6 1.771(3) . ?
C5 C19 1.485(4) . ?
S6 O7 1.444(2) . ?
S6 O9 1.444(2) . ?
S6 O8 1.454(2) . ?
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C10 C15 1.391(4) . ?
C11 C12 1.374(4) . ?
C11 H11 0.98(3) . ?
C12 C13 1.389(4) . ?
C13 C14 1.387(4) . ?
C13 H13 0.92(3) . ?
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C18 H18A 0.94(4) . ?
C18 H18B 0.95(4) . ?
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C18 H18C 0.95(4) . ?

C19 H19A 0.87(5) . ?

C19 H19B 0.91(5) . ?

C19 H19C 0.94(6) . ?

C20 O21 1.399(5) . ?

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N2 N1 C10 122.1(2) . . ?

C3 N2 N1 108.4(2) . . ?

C3 N2 C18 127.8(3) . . ?

N1 N2 C18 123.7(2) . . ?

N2 C3 C4 108.9(3) . . ?

N2 C3 H3 122.0(19) . . ?

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C3 C4 C5 106.8(3) . . ?
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C5 C4 S6 128.4(2) . . ?

N1 C5 C4 106.9(3) . . ?

N1 C5 C19 121.9(3) . . ?

C4 C5 C19 131.1(3) . . ?

O7 S6 O9 113.44(15) . . ?

O7 S6 O8 114.28(13) . . ?

O9 S6 O8 113.15(15) . . ?

O7 S6 C4 106.14(13) . . ?

O9 S6 C4 105.48(13) . . ?

O8 S6 C4 103.09(14) . . ?

C11 C10 C15 122.1(3) . . ?

C11 C10 N1 119.7(3) . . ?

C15 C10 N1 118.2(3) . . ?

C12 C11 C10 117.9(3) . . ?

C12 C11 H11 122.5(19) . . ?

C10 C11 H11 119.6(19) . . ?

C11 C12 C13 122.6(3) . . ?

C11 C12 Cl16 118.9(2) . . ?

C13 C12 Cl16 118.5(2) . . ?

C14 C13 C12 117.4(3) . . ?

C14 C13 H13 117.0(18) . . ?

C12 C13 H13 125.5(18) . . ?

C15 C14 C13 122.5(3) . . ?

C15 C14 Cl17 118.4(2) . . ?

C13 C14 Cl17 119.1(2) . . ?

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C14 C15 H15 125(2) . . ?
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C10 C15 H15 118(2) . . ?

N2 C18 H18A 111(2) . . ?

N2 C18 H18B 107(2) . . ?

H18A C18 H18B 106(3) . . ?

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H18B C18 H18C 118(3) . . ?

C5 C19 H19A 106(3) . . ?

C5 C19 H19B 115(3) . . ?

H19A C19 H19B 112(4) . . ?

C5 C19 H19C 111(3) . . ?

H19A C19 H19C 109(4) . . ?

H19B C19 H19C 103(4) . . ?

O21 C20 H20A 113(3) . . ?

O21 C20 H20B 102(3) . . ?

H20A C20 H20B 109(4) . . ?

O21 C20 H20C 107(3) . . ?

H20A C20 H20C 113(4) . . ?

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