

**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  $F^2 > 2\sigma(F^2)$  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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loop\_

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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 . . .  
C4 C 0.7331(4) 0.3803(4) -0.0187(2) 0.0223(6) Uani 1 1 d . . .  
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 . . .

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 . . .  
H20C H 0.200(7) -0.086(7) -0.274(4) 0.080(16) Uiso 1 1 d . . .

loop\_

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\_atom\_site\_aniso\_U\_22

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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)



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)  
O21 0.0681(19) 0.0410(17) 0.0448(15) 0.0022(13) 0.0183(13) 0.0254(15)

\_geom\_special\_details

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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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loop\_

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N1 N2 1.373(3) . ?  
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) . ?  
C10 C11 1.391(4) . ?  
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) . ?  
C14 C15 1.387(4) . ?  
C15 H15 0.87(4) . ?  
C18 H18A 0.94(4) . ?  
C18 H18B 0.95(4) . ?

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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C20 H20B 0.99(5) . ?

C20 H20C 0.99(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) . . ?

C4 C3 H3 129.1(19) . . ?

C3 C4 C5 106.8(3) . . ?

C3 C4 S6 124.6(2) . . ?  
C5 C4 S6 128.4(2) . . ?  
N1 C5 C4 106.9(3) . . ?  
N1 C5 C19 121.9(3) . . ?  
C4 C5 C19 131.1(3) . . ?  
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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) . . ?  
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C11 C12 C116 118.9(2) . . ?  
C13 C12 C116 118.5(2) . . ?  
C14 C13 C12 117.4(3) . . ?  
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C10 C15 H15 118(2) . . ?  
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C5 C19 H19A 106(3) . . ?  
C5 C19 H19B 115(3) . . ?  
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C20 O21 H 109(4) . . ?

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