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Crystal structure and Hirshfeld surface analysis of 1-[(benzyldimethylsilyl)methyl]-1-ethylpiperidin-1-ium ethanesulfonate. Corrigendum

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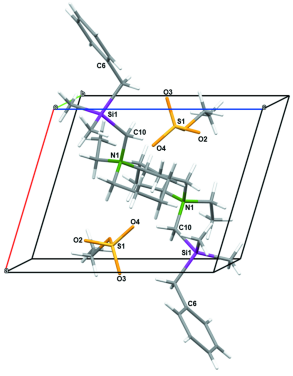
Supporting information: this article has supporting information at journals.iucr.org/e

In the paper by Kirchhoff *et al.* [*Acta Cryst.* (2022), E**78**, 135–139], there was an error in the chemical name of the title compound.

The chemical name of the title compound in the paper by Kirchhoff *et al.* (2022) is incorrect and should be '1-[(benzyldimethylsilyl)methyl]-1-ethylpiperidin-1-ium ethanesulfate'. The original article has been updated and is available as supporting information. Specifically, the title and the occurrence of the chemical name in the *Chemical context* section have been updated. The chemical scheme and Fig. 5 have been modified to show the correct structure.

References

Kirchhoff, J.-L., Koller, S. G., Louven, K. & Strohmann, C. (2022). *Acta Cryst.* E**78**, 135–139.



supporting information

Acta Cryst. (2025). E**81**, 782 [https://doi.org/10.1107/S2056989025006012]

Crystal structure and Hirshfeld surface analysis of 1-[(benzyldimethylsilyl)methyl]-1-ethylpiperidin-1-ium ethanesulfonate. Corrigendum

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1-[(Benzyldimethylsilyl)methyl]-1-ethylpiperidin-1-ium ethanesulfate

Crystal data

$C_{17}H_{30}NSi^{+}\cdot C_2H_5O_4S^{-}$
M_r = 401.63
Monoclinic, $P2_1$
a = 8.4627 (8) Å
b = 12.8187 (11) Å
c = 10.3926 (9) Å
β = 107.033 (3)°
V = 1077.95 (17) Å^3
Z = 2
$F(000)$ = 436
D_x = 1.237 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9642 reflections
θ = 3.0–30.6°
μ = 0.23 mm^{-1}
T = 100 K
Block, colourless
0.82 × 0.44 × 0.38 mm

Data collection

Bruker D8 VENTURE diffractometer
Radiation source: microfocus sealed X-ray tube
HELIOS mirror optics monochromator
Detector resolution: 10.4167 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (SADABS; Bruker, 2021)
T_{min} = 0.699, T_{max} = 0.747
68418 measured reflections
8122 independent reflections
7987 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 33.0°, θ_{min} = 2.5°
h = −12→12
k = −19→19
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.065
S = 1.05
8122 reflections
375 parameters
1 restraint
Primary atom site location: iterative
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.039P)^2 + 0.1456P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}
Absolute structure: Flack x determined using 3811 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: −0.005 (6)

Special details

Geometry. 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.88614 (3)	0.62026 (2)	0.40720 (3)	0.01913 (6)
Si1	0.05612 (4)	0.31084 (3)	0.20000 (3)	0.01987 (7)
O3	1.05747 (10)	0.61067 (7)	0.48491 (8)	0.01886 (15)
O1	0.85485 (10)	0.74269 (6)	0.37242 (10)	0.01822 (15)
O4	0.77064 (16)	0.60053 (10)	0.4817 (2)	0.0533 (5)
O2	0.85245 (18)	0.56667 (8)	0.27863 (13)	0.0439 (4)
N1	0.35820 (12)	0.43767 (7)	0.34820 (11)	0.01724 (16)
C10	0.19151 (13)	0.39252 (8)	0.34376 (12)	0.01601 (18)
C14	0.53245 (16)	0.29189 (10)	0.48490 (16)	0.0253 (2)
C17	0.41837 (15)	0.50777 (10)	0.47118 (15)	0.0230 (2)
C6	−0.27742 (13)	0.25033 (8)	0.16162 (10)	0.01469 (17)
C5	−0.31035 (14)	0.14496 (9)	0.17585 (11)	0.01782 (18)
C13	0.48527 (15)	0.35320 (9)	0.35398 (14)	0.0211 (2)
C7	−0.13320 (13)	0.30314 (9)	0.25953 (11)	0.01589 (17)
C1	−0.38217 (16)	0.30517 (11)	0.05336 (13)	0.0247 (2)
C15	0.59552 (18)	0.36517 (13)	0.60478 (17)	0.0298 (3)
C18	0.96437 (15)	0.78813 (9)	0.30464 (13)	0.0206 (2)
C4	−0.44312 (17)	0.09575 (11)	0.08387 (14)	0.0258 (2)
C3	−0.54609 (16)	0.15050 (14)	−0.02339 (13)	0.0295 (3)
C16	0.46575 (16)	0.44744 (12)	0.60249 (15)	0.0276 (3)
C11	0.35005 (16)	0.50178 (10)	0.22355 (15)	0.0245 (2)
C19	0.93127 (16)	0.90390 (9)	0.29232 (12)	0.0202 (2)
C12	0.23198 (19)	0.59372 (11)	0.19959 (18)	0.0306 (3)
C8	0.0020 (3)	0.3761 (2)	0.03268 (16)	0.0472 (5)
C2	−0.51474 (18)	0.25531 (15)	−0.03823 (14)	0.0316 (3)
C9	0.1422 (2)	0.17830 (15)	0.1885 (3)	0.0455 (5)
H13A	0.442 (2)	0.3078 (18)	0.274 (2)	0.024 (4)*
H3	−0.638 (3)	0.121 (2)	−0.085 (3)	0.043 (6)*
H13B	0.583 (3)	0.3899 (17)	0.346 (2)	0.025 (5)*
H5	−0.241 (2)	0.1076 (17)	0.250 (2)	0.024 (4)*
H11A	0.318 (2)	0.4547 (16)	0.1467 (19)	0.017 (4)*
H12A	0.122 (3)	0.5740 (19)	0.193 (2)	0.029 (5)*
H10A	0.128 (3)	0.4494 (18)	0.358 (2)	0.026 (5)*
H7A	−0.108 (3)	0.2671 (17)	0.343 (2)	0.023 (4)*
H16A	0.368 (3)	0.4130 (18)	0.614 (2)	0.032 (5)*
H7B	−0.162 (3)	0.369 (2)	0.277 (3)	0.041 (6)*
H8A	−0.071 (4)	0.332 (3)	−0.020 (3)	0.056 (8)*
H18A	1.077 (3)	0.7716 (19)	0.355 (2)	0.037 (6)*
H17A	0.512 (3)	0.5403 (16)	0.456 (2)	0.023 (5)*
H16B	0.512 (3)	0.504 (2)	0.676 (3)	0.040 (6)*
H17B	0.331 (3)	0.5512 (18)	0.475 (2)	0.032 (5)*
H12B	0.233 (3)	0.630 (2)	0.106 (3)	0.043 (6)*
H2	−0.586 (3)	0.296 (2)	−0.110 (2)	0.041 (6)*
H11B	0.454 (3)	0.525 (2)	0.235 (2)	0.033 (6)*
H14A	0.439 (3)	0.2515 (19)	0.494 (2)	0.030 (5)*

H14B	0.617 (3)	0.2459 (19)	0.477 (2)	0.033 (6)*
H19A	0.825 (3)	0.916 (2)	0.235 (3)	0.040 (6)*
H19B	0.945 (3)	0.933 (2)	0.382 (2)	0.037 (6)*
H9A	0.058 (3)	0.133 (2)	0.123 (3)	0.048 (7)*
H19C	1.009 (3)	0.943 (2)	0.251 (2)	0.031 (5)*
H1	−0.362 (3)	0.379 (2)	0.045 (3)	0.041 (6)*
H10B	0.205 (3)	0.3469 (18)	0.418 (2)	0.027 (5)*
H9B	0.231 (5)	0.175 (4)	0.154 (4)	0.090 (13)*
H4	−0.477 (3)	0.018 (2)	0.093 (3)	0.037 (6)*
H8B	0.103 (6)	0.397 (4)	0.005 (4)	0.095 (14)*
H18B	0.945 (3)	0.751 (2)	0.216 (2)	0.037 (6)*
H15A	0.700 (4)	0.397 (2)	0.597 (3)	0.058 (8)*
H12C	0.274 (3)	0.647 (2)	0.270 (3)	0.046 (7)*
H15B	0.623 (4)	0.327 (2)	0.686 (3)	0.051 (7)*
H8C	−0.044 (5)	0.439 (4)	0.038 (4)	0.078 (11)*
H9C	0.167 (5)	0.140 (4)	0.293 (4)	0.092 (12)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.01109 (10)	0.01196 (10)	0.03141 (13)	0.00019 (8)	0.00167 (8)	0.00310 (9)
Si1	0.01993 (14)	0.02043 (14)	0.02339 (14)	−0.00530 (11)	0.01279 (11)	−0.00846 (11)
O3	0.0134 (3)	0.0214 (4)	0.0193 (3)	0.0031 (3)	0.0009 (3)	0.0034 (3)
O1	0.0140 (3)	0.0118 (3)	0.0301 (4)	0.0013 (3)	0.0084 (3)	0.0021 (3)
O4	0.0297 (5)	0.0335 (7)	0.1128 (13)	0.0101 (5)	0.0458 (7)	0.0345 (7)
O2	0.0507 (7)	0.0172 (4)	0.0404 (6)	0.0058 (4)	−0.0234 (5)	−0.0085 (4)
N1	0.0133 (4)	0.0120 (4)	0.0294 (5)	−0.0001 (3)	0.0109 (3)	−0.0006 (3)
C10	0.0127 (4)	0.0146 (4)	0.0237 (5)	−0.0019 (3)	0.0099 (3)	−0.0023 (3)
C14	0.0194 (5)	0.0169 (5)	0.0405 (7)	0.0031 (4)	0.0104 (5)	0.0045 (4)
C17	0.0145 (4)	0.0161 (5)	0.0387 (6)	−0.0020 (4)	0.0082 (4)	−0.0083 (4)
C6	0.0134 (4)	0.0151 (4)	0.0158 (4)	0.0024 (3)	0.0045 (3)	−0.0004 (3)
C5	0.0185 (4)	0.0157 (4)	0.0178 (4)	−0.0026 (3)	0.0030 (3)	−0.0012 (3)
C13	0.0168 (4)	0.0148 (4)	0.0361 (6)	0.0035 (4)	0.0148 (4)	−0.0004 (4)
C7	0.0156 (4)	0.0146 (4)	0.0185 (4)	−0.0018 (3)	0.0066 (3)	−0.0030 (3)
C1	0.0215 (5)	0.0259 (5)	0.0243 (5)	0.0078 (4)	0.0032 (4)	0.0072 (5)
C15	0.0190 (5)	0.0313 (7)	0.0367 (7)	0.0027 (5)	0.0047 (5)	0.0017 (5)
C18	0.0222 (5)	0.0148 (4)	0.0282 (5)	0.0033 (4)	0.0129 (4)	0.0036 (4)
C4	0.0235 (5)	0.0286 (6)	0.0240 (5)	−0.0094 (4)	0.0052 (4)	−0.0081 (4)
C3	0.0162 (5)	0.0506 (8)	0.0197 (5)	−0.0043 (5)	0.0022 (4)	−0.0102 (5)
C16	0.0177 (5)	0.0326 (6)	0.0321 (6)	−0.0019 (5)	0.0064 (4)	−0.0093 (5)
C11	0.0217 (5)	0.0200 (5)	0.0367 (6)	0.0007 (4)	0.0163 (5)	0.0072 (5)
C19	0.0250 (5)	0.0131 (4)	0.0230 (5)	−0.0009 (4)	0.0081 (4)	−0.0012 (4)
C12	0.0283 (6)	0.0195 (5)	0.0444 (8)	0.0042 (4)	0.0115 (6)	0.0082 (5)
C8	0.0582 (11)	0.0667 (13)	0.0200 (6)	−0.0352 (11)	0.0163 (7)	−0.0063 (7)
C2	0.0201 (5)	0.0496 (9)	0.0211 (5)	0.0105 (6)	−0.0004 (4)	0.0041 (5)
C9	0.0296 (7)	0.0320 (7)	0.0824 (14)	−0.0062 (6)	0.0279 (9)	−0.0332 (9)

Geometric parameters (Å, º)

S1—O3	1.4435 (8)	C1—C2	1.396 (2)
S1—O1	1.6149 (9)	C1—H1	0.98 (3)
S1—O4	1.4364 (12)	C15—C16	1.518 (2)
S1—O2	1.4545 (13)	C15—H15A	1.00 (3)
Si1—C7	1.8814 (11)	C15—H15B	0.95 (3)
Si1—C8	1.862 (2)	C18—C19	1.5086 (16)
Si1—C9	1.8662 (18)	C18—H18A	0.97 (3)
Si1—C10	1.9075 (12)	C18—H18B	1.00 (3)
O1—C18	1.4412 (14)	C4—C3	1.388 (2)
N1—C10	1.5130 (14)	C4—H4	1.05 (3)
N1—C17	1.5227 (17)	C3—C2	1.387 (3)
N1—C13	1.5148 (15)	C3—H3	0.93 (3)
N1—C11	1.5186 (17)	C16—H16A	0.98 (2)
C10—H10A	0.94 (2)	C16—H16B	1.04 (3)
C10—H10B	0.95 (2)	C11—C12	1.5177 (19)
C14—C13	1.5199 (19)	C11—H11A	0.97 (2)
C14—C15	1.526 (2)	C11—H11B	0.91 (2)
C14—H14A	0.97 (2)	C19—H19A	0.94 (3)
C14—H14B	0.95 (2)	C19—H19B	0.99 (2)
C17—C16	1.517 (2)	C19—H19C	1.01 (2)
C17—H17A	0.95 (2)	C12—H12A	0.94 (2)
C17—H17B	0.93 (2)	C12—H12B	1.08 (3)
C6—C5	1.3957 (15)	C12—H12C	0.99 (3)
C6—C7	1.5019 (15)	C8—H8A	0.89 (3)
C6—C1	1.4005 (16)	C8—H8B	1.01 (5)
C5—C4	1.3946 (16)	C8—H8C	0.91 (4)
C5—H5	0.95 (2)	C2—H2	0.96 (3)
C13—H13A	0.99 (2)	C9—H9A	1.01 (3)
C13—H13B	0.97 (2)	C9—H9B	0.92 (4)
C7—H7A	0.95 (2)	C9—H9C	1.15 (4)
C7—H7B	0.91 (3)		
O3—S1—O1	106.26 (5)	C14—C15—H15A	106.7 (18)
O3—S1—O2	111.61 (7)	C14—C15—H15B	110.4 (18)
O4—S1—O3	114.45 (8)	C16—C15—C14	109.66 (11)
O4—S1—O1	101.47 (6)	C16—C15—H15A	111.9 (18)
O4—S1—O2	115.54 (11)	C16—C15—H15B	111.2 (18)
O2—S1—O1	106.15 (6)	H15A—C15—H15B	107 (3)
C7—Si1—C10	98.35 (5)	O1—C18—C19	108.00 (9)
C8—Si1—C10	114.32 (7)	O1—C18—H18A	108.5 (14)
C8—Si1—C7	109.31 (9)	O1—C18—H18B	107.5 (15)
C8—Si1—C9	110.06 (12)	C19—C18—H18A	112.9 (15)
C9—Si1—C10	113.19 (8)	C19—C18—H18B	114.0 (15)
C9—Si1—C7	111.06 (7)	H18A—C18—H18B	106 (2)
C18—O1—S1	114.55 (7)	C5—C4—H4	123.5 (14)
C10—N1—C17	109.32 (9)	C3—C4—C5	120.81 (13)

C10—N1—C13	111.87 (9)	C3—C4—H4	115.5 (14)
C10—N1—C11	111.84 (9)	C4—C3—H3	123.5 (18)
C13—N1—C17	109.24 (10)	C2—C3—C4	118.93 (12)
C13—N1—C11	105.96 (9)	C2—C3—H3	117.5 (18)
C11—N1—C17	108.49 (10)	C17—C16—C15	111.58 (12)
Si1—C10—H10A	107.8 (13)	C17—C16—H16A	109.3 (13)
Si1—C10—H10B	101.7 (14)	C17—C16—H16B	104.1 (15)
N1—C10—Si1	125.08 (8)	C15—C16—H16A	108.7 (14)
N1—C10—H10A	105.8 (14)	C15—C16—H16B	110.8 (15)
N1—C10—H10B	108.7 (13)	H16A—C16—H16B	112.3 (19)
H10A—C10—H10B	106.6 (18)	N1—C11—H11A	107.2 (12)
C13—C14—C15	110.47 (11)	N1—C11—H11B	105.7 (15)
C13—C14—H14A	110.8 (14)	C12—C11—N1	115.05 (11)
C13—C14—H14B	104.5 (14)	C12—C11—H11A	109.7 (12)
C15—C14—H14A	110.4 (14)	C12—C11—H11B	109.4 (16)
C15—C14—H14B	111.0 (15)	H11A—C11—H11B	109.7 (19)
H14A—C14—H14B	110 (2)	C18—C19—H19A	109.5 (16)
N1—C17—H17A	101.9 (12)	C18—C19—H19B	109.3 (15)
N1—C17—H17B	108.3 (14)	C18—C19—H19C	113.5 (14)
C16—C17—N1	112.92 (10)	H19A—C19—H19B	111 (2)
C16—C17—H17A	111.3 (13)	H19A—C19—H19C	106 (2)
C16—C17—H17B	105.7 (14)	H19B—C19—H19C	107 (2)
H17A—C17—H17B	117 (2)	C11—C12—H12A	112.9 (14)
C5—C6—C7	120.82 (10)	C11—C12—H12B	107.8 (14)
C5—C6—C1	118.15 (11)	C11—C12—H12C	109.8 (16)
C1—C6—C7	121.03 (10)	H12A—C12—H12B	108.6 (19)
C6—C5—H5	118.5 (13)	H12A—C12—H12C	112 (2)
C4—C5—C6	120.72 (11)	H12B—C12—H12C	106 (2)
C4—C5—H5	120.8 (13)	Si1—C8—H8A	103 (2)
N1—C13—C14	113.73 (10)	Si1—C8—H8B	113 (3)
N1—C13—H13A	107.5 (12)	Si1—C8—H8C	110 (2)
N1—C13—H13B	105.1 (13)	H8A—C8—H8B	118 (3)
C14—C13—H13A	112.5 (13)	H8A—C8—H8C	112 (3)
C14—C13—H13B	108.6 (13)	H8B—C8—H8C	101 (3)
H13A—C13—H13B	109.1 (17)	C1—C2—H2	118.4 (17)
Si1—C7—H7A	109.8 (13)	C3—C2—C1	120.64 (13)
Si1—C7—H7B	108.6 (17)	C3—C2—H2	121.0 (17)
C6—C7—Si1	113.71 (7)	Si1—C9—H9A	110.7 (16)
C6—C7—H7A	108.8 (13)	Si1—C9—H9B	116 (3)
C6—C7—H7B	109.9 (17)	Si1—C9—H9C	107 (2)
H7A—C7—H7B	106 (2)	H9A—C9—H9B	102 (3)
C6—C1—H1	118.4 (16)	H9A—C9—H9C	107 (3)
C2—C1—C6	120.75 (13)	H9B—C9—H9C	114 (3)
C2—C1—H1	120.8 (16)		

S1—O1—C18—C19	−174.27 (8)	C5—C4—C3—C2	0.2 (2)
O3—S1—O1—C18	55.64 (10)	C13—N1—C10—Si1	−65.17 (13)
O4—S1—O1—C18	175.59 (11)	C13—N1—C17—C16	−52.78 (12)

O2—S1—O1—C18	−63.30 (11)	C13—N1—C11—C12	−178.50 (12)
N1—C17—C16—C15	56.11 (14)	C13—C14—C15—C16	56.25 (15)
C10—Si1—C7—C6	174.81 (8)	C7—C6—C5—C4	−179.20 (11)
C10—N1—C17—C16	69.94 (12)	C7—C6—C1—C2	179.19 (11)
C10—N1—C13—C14	−67.70 (13)	C1—C6—C5—C4	0.58 (17)
C10—N1—C11—C12	59.35 (15)	C1—C6—C7—Si1	−82.81 (12)
C14—C15—C16—C17	−56.65 (16)	C15—C14—C13—N1	−56.46 (14)
C17—N1—C10—Si1	173.69 (8)	C4—C3—C2—C1	−0.2 (2)
C17—N1—C13—C14	53.48 (13)	C11—N1—C10—Si1	53.52 (12)
C17—N1—C11—C12	−61.30 (14)	C11—N1—C17—C16	−167.85 (10)
C6—C5—C4—C3	−0.40 (19)	C11—N1—C13—C14	170.17 (10)
C6—C1—C2—C3	0.4 (2)	C8—Si1—C7—C6	55.31 (11)
C5—C6—C7—Si1	96.96 (11)	C9—Si1—C7—C6	−66.31 (12)
C5—C6—C1—C2	−0.59 (19)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O2^{i}	0.93 (3)	2.39 (3)	3.2990 (17)	167 (2)
C7—H7*B*···O2^{ii}	0.91 (3)	2.54 (3)	3.3881 (16)	156 (2)
C17—H17*A*···O4	0.95 (2)	2.26 (2)	3.1815 (16)	162.8 (17)
C17—H17*B*···O3^{ii}	0.93 (2)	2.47 (2)	3.3680 (15)	161.3 (19)

Symmetry codes: (i) −*x*, *y*−1/2, −*z*; (ii) *x*−1, *y*, *z*.