Altered coordinates for palmitic acid, phase C.

The coordinates original reported for palmitic acid, phase C[1] were altered based upon the NMR refinement at the H1 position. New coordinates are listed below and differ from the original coordinates ONLY in the H1 position.

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loop_
   _atom_site_type_symbol
   _atom_site_label
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_U_iso_or_equiv
   _atom_site_adp_type
   _atom_site_calc_flag
   _atom_site_refinement_flags
   _atom_site_occupancy
   _atom_site_disorder_assembly
   _atom_site_disorder_group

   O O1 0.49465(7) 0.2631(5) -0.3717(2) 0.0577(7) Uani d . 1 . .
   H H1 0.518556(3) 0.330487(4) -0.463162(4) 0.19(3) Uiso d . 1 . .
   O O2 0.45853(6) 0.6125(5) -0.4249(2) 0.0552(7) Uani d . 1 . .
   C C1 0.46616(8) 0.4111(6) -0.3504(3) 0.0428(8) Uani d . 1 . .
   C C2 0.44219(9) 0.3338(6) -0.2281(3) 0.0471(8) Uani d . 1 . .
   H H2A 0.4573(4) 0.3431(6) -0.143(2) 0.093(14) Uiso d R 1 . .
   H H2B 0.4347(2) 0.148(5) -0.2405(4) 0.060(10) Uiso d R 1 . .
   C C3 0.40732(9) 0.4999(7) -0.2052(4) 0.0505(9) Uani d . 1 . .
   H H3A 0.3914(4) 0.4857(7) -0.287(2) 0.072(11) Uiso d R 1 . .
   H H3B 0.41416(18) 0.685(5) -0.1940(4) 0.062(10) Uiso d R 1 . .
   C C4 0.38612(9) 0.4074(8) -0.0753(4) 0.0556(9) Uani d . 1 . .
   H H4A 0.38142(16) 0.208(6) -0.0840(4) 0.106(16) Uiso d R 1 . .
   H H4B 0.4025(5) 0.4361(10) 0.011(3) 0.095(14) Uiso d R 1 . .
   C C5 0.34925(9) 0.5460(7) -0.0504(4) 0.0566(9) Uani d . 1 . .
   H H5A 0.3339(4) 0.5213(9) -0.130(2) 0.071(12) Uiso d R 1 . .
   H H5B 0.35342(14) 0.730(5) -0.0401(4) 0.064(11) Uiso d R 1 . .
   C C6 0.32914(10) 0.4419(8) 0.0799(4) 0.0594(10) Uani d . 1 . .
   H H6A 0.32613(12) 0.234(6) 0.0703(4) 0.096(14) Uiso d R 1 . .
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H H6B 0.3460(5) 0.4782(12) 0.168(3) 0.104(15) Uiso d R 1 . .
C C7 0.29103(9) 0.5629(8) 0.1063(4) 0.0591(10) Uani d . 1 . .
H H7A 0.2754(5) 0.5328(10) 0.024(2) 0.079(13) Uiso d R 1 . .
H H7B 0.29374(11) 0.755(6) 0.1182(5) 0.076(12) Uiso d R 1 . .
C C8 0.27149(10) 0.4491(8) 0.2348(4) 0.0606(10) Uani d . 1 . .
H H8A 0.26916(11) 0.248(7) 0.2229(5) 0.090(14) Uiso d R 1 . .
H H8B 0.2877(5) 0.4828(12) 0.321(3) 0.108(16) Uiso d R 1 . .
C C9 0.23303(10) 0.5634(8) 0.2624(4) 0.0616(10) Uani d . 1 . .
H H9A 0.2170(5) 0.5321(11) 0.177(3) 0.084(13) Uiso d R 1 . .
H H9B 0.23533(11) 0.762(6) 0.2756(5) 0.088(13) Uiso d R 1 . .
C C10 0.21355(10) 0.4461(8) 0.3900(4) 0.0633(10) Uani d . 1 . .
H H10A 0.2302(5) 0.4786(11) 0.478(3) 0.098(15) Uiso d R 1 . .
H H10B 0.21120(11) 0.240(6) 0.3762(5) 0.093(14) Uiso d R 1 . .
C C11 0.17498(10) 0.5601(8) 0.4183(4) 0.0659(11) Uani d . 1 . .
H H11A 0.17731(12) 0.762(7) 0.4322(6) 0.107(16) Uiso d R 1 . .
H H11B 0.1587(5) 0.5290(12) 0.331(3) 0.105(16) Uiso d R 1 . .
C C12 0.15543(10) 0.4424(8) 0.5454(5) 0.0685(11) Uani d . 1 . .
H H12A 0.1728(5) 0.4767(12) 0.639(3) 0.086(13) Uiso d R 1 . .
H H12B 0.15302(11) 0.226(6) 0.5309(6) 0.117(17) Uiso d R 1 . .
C C13 0.11678(11) 0.5566(9) 0.5726(5) 0.0733(12) Uani d . 1 . .
H H13A 0.11902(12) 0.753(7) 0.5851(6) 0.14(2) Uiso d R 1 . .
H H13B 0.1011(6) 0.5250(13) 0.488(3) 0.103(17) Uiso d R 1 . .
C C14 0.09692(11) 0.4418(9) 0.6993(5) 0.0745(12) Uani d . 1 . .
H H14A 0.1143(5) 0.4824(13) 0.796(3) 0.092(14) Uiso d R 1 . .
H H14B 0.09483(12) 0.218(6) 0.6865(5) 0.122(17) Uiso d R 1 . .
C C15 0.05804(13) 0.5541(11) 0.7226(6) 0.0937(16) Uani d . 1 . .
H H15A 0.05982(14) 0.760(9) 0.7311(6) 0.16(2) Uiso d R 1 . .
H H15B 0.0418(7) 0.5112(19) 0.635(4) 0.18(3) Uiso d R 1 . .
C C16 0.03875(14) 0.4452(13) 0.8519(6) 0.112(2) Uani d . 1 . .
H H16A 0.0379(7) 0.221(6) 0.8466(15) 0.16(3) Uiso d R 1 . .
H H16B 0.0096(8) 0.525(5) 0.8564(18) 0.089(13) Uiso d R 1 . .

H H16C 0.0545(6) 0.509(5) 0.949(2) 0.18(3) Uiso d R 1 . .

1. E. Moreno, R. Cordobilla, T. Calvet, F. Lahoz and A. I. Balana, *Acta Crystallogr. Sect. C*, 2006, **62**, o129.