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LLNL-TR-414987

Crystallographic Information File of 1,1,tetraphenyl-1,3-butadiene

J.-H. Park Klepeis, W. Evans, N. Zaitseva, E. Schwegler, S. Teat

July 22, 2009

Disclaimer

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

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2009-07-16 # Formatted by publCIF
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_contact_author_name          'Jae-Hyun Park Klepeis'
_contact_author_address
;Lawrence Livermore National Laboratory
7000 East Avenue
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_contact_author_email         klepeis2@llnl.gov
_contact_author_phone         '1-925-422-2466'
_contact_author_fax           '1-925-422-6594'
_publ_requested_journal  'the data not intended for publication elsewhere'
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July 20, 2009

Please consider this CIF submission for data deposition at Cambridge
Structure Database.

The CIF has passed the Chester CHECKCIF routines.  VRF responses are
at the start of the _d6ata_I section of the CIF.

Jae-Hyun Park Klepeis
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# 2. PROCESSING SUMMARY (IUCr OFFICE Use Only)
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# 3. TITLE AND AUTHOR LIST

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1,1,4,4-tetraphenyl-1,3-butadiene
;

loop_
_publ_author_name
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'Jae-Hyun Park Klepeis'
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Lawrence Livermore National Laboratory
7000 East Avenue
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'Natalia Zaitseva'
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USA
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#=============================================================================
;
_publ_section_acknowledgements
;
This work was supported by the Laboratory Directed Research and Development
program office (07-ERD-045) at LLNL and performed under the auspices of the US
Department of Energy by Lawrence Livermore National Laboratory under Contract
DE-AC57097NA27344. The ALS is supported by the Director, Office of Science,
Office of Basic Energy Sciences (OBES), and the OBES Division of Chemical
Sciences, Geosciences, and Biosciences of the US Department of Energy at LBNL
under Contract No. DE-AC02-05CH11231.
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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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H14 H -0.0422(19) 0.1927(18) 0.2997(17) 0.052(5) Uiso 1 1 d . . .
H15 H 0.0290(18) 0.2504(17) 0.1137(17) 0.047(4) Uiso 1 1 d . . .
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H22 H 0.7586(15) 0.4458(15) 0.5083(14) 0.031(3) Uiso 1 1 d . . .
H23 H 0.9339(18) 0.3191(17) 0.5980(16) 0.046(4) Uiso 1 1 d . . .
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H25 H 0.6555(16) -0.0354(17) 0.4338(16) 0.041(4) Uiso 1 1 d . . .
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C3 C41 1.4837(14) . ?
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C21 C22 H22 120.3(8) . . ?
C22 C23 C24 120.20(11) . . ?
C22 C23 H23 119.5(10) . . ?
C24 C23 H23 120.3(10) . . ?
C25 C24 C23 119.65(10) . . ?
C25 C24 H24 119.5(10) . . ?
C23 C24 H24 120.9(10) . . ?
C24 C25 C26 120.27(11) . . ?
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C24 C25 H25 120.0(9) . . ?
C26 C25 H25 119.8(9) . . ?
C25 C26 C21 120.84(11) . . ?
C25 C26 H26 119.2(9) . . ?
C21 C26 H26 120.0(9) . . ?
C32 C31 C36 118.01(10) . . ?
C32 C31 C3 120.06(9) . . ?
C36 C31 C3 121.94(9) . . ?
C33 C32 C31 120.79(10) . . ?
C33 C32 H32 118.8(9) . . ?
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C34 C33 H33 121.0(9) . . ?
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C31 C36 H36 120.6(9) . . ?
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C42 C41 C3 120.84(9) . . ?
C46 C41 C3 120.81(9) . . ?
C43 C42 C41 120.73(10) . . ?
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C41 C42 H42 119.4(9) . . ?
C42 C43 C44 120.13(11) . . ?
C42 C43 H43 119.3(9) . . ?
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C45 C46 H46 120.0(9) . . ?
C41 C46 H46 119.1(9) . . ?

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C2 C1 C3 C41 -173.84(9) . . . . ?
C1 C2 C4 C21 -175.75(10) . . . . ?
C1 C2 C4 C11 5.69(18) . . . . ?
C2 C4 C11 C12 -136.93(11) . . . . ?
C21 C4 C11 C12 44.51(13) . . . . ?
C2 C4 C11 C16 43.72(15) . . . . ?
C21 C4 C11 C16 -134.84(10) . . . . ?
C16 C11 C12 C13 -2.03(16) . . . . ?
C4 C11 C12 C13 178.60(10) . . . . ?
C11 C12 C13 C14 1.17(17) . . . . ?
C12 C13 C14 C15 0.32(18) . . . . ?
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C14 C15 C16 C11 -0.01(18) . . . . ?
C12 C11 C16 C15 1.45(16) . . . . ?
C4 C11 C16 C15 -179.20(10) . . . . ?
C2 C4 C21 C26 -142.78(11) . . . . ?
C11 C4 C21 C26 35.87(14) . . . . ?
C2 C4 C21 C22 34.69(15) . . . . ?
C11 C4 C21 C22 -146.66(10) . . . . ?
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C4 C21 C22 C23 -174.93(10) . . . . ?
C21 C22 C23 C24 -1.16(17) . . . . ?
C22 C23 C24 C25 -0.76(18) . . . . ?
C23 C24 C25 C26 1.18(18) . . . . ?
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C22 C21 C26 C25 -2.18(16) . . . . ?
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C41 C3 C31 C36 -136.04(10) . . . . ?
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C3 C41 C46 C45 176.94(10) . . . . ?

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_refine_diff_density_max    0.392
_refine_diff_density_min   -0.211
_refine_diff_density_rms    0.051

#########################################################
#=======================================================================
#start validation form
_vrf_DIFF020_I
;
PROBLEM: _diffrn_standards_interval_count and
RESPONSE: data were collected at synchrotron with CCD and proper
attenuators to prevent saturation of the diffraction spots.
;
_vrf_PLAT092_4
;
PROBLEM:  _check wavelength given is not Cu, Mo, or Ag Ka
RESPONSE: synchrotron radation with lamda=0.7749 Ang.
;
_vrf_PLAT154_1
;
PROBLEM: _The su's on the cell angles are equal(x10000) 200 Deg.
RESPONSE: the standard deviation ofthe cell angle is 2x10\^-3 degree.
```

```
;
#end of validation form
#================================================================================
```