Kinetic Resolution of Chiral α-Olefins Using Optically Active *Ansa*-Zirconocene Polymerization Catalysts

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Supporting Information: X-ray data for (*S*)-**2**, (*S*)-**5**, (*S*)-**6**, and (*S*)-**7** (CIF) (68 pages). This material is available free of charge via the Internet at http://pubs.acs.org.

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 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and
is
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R-
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C20A C 0.5998(6) 0.1147(2) 0.5856(3) 0.0204(11) Uani 1 1 d . . .
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H20B H 0.6768 0.0812 0.6148 0.031 Uiso 1 1 calc R . .
H20C H 0.4958 0.1023 0.5910 0.031 Uiso 1 1 calc R . .
C21A C 1.3870(7) 0.3489(3) 0.6649(3) 0.0162(12) Uani 1 1 d . . .
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H25A H 1.2880 0.4683 0.3492 0.038 Uiso 1 1 calc R . .
H25B H 1.1006 0.4706 0.3240 0.038 Uiso 1 1 calc R . .
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H26B H 1.3242 0.2883 0.3455 0.038 Uiso 1 1 calc R . .
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Cl1B Cl 1.19746(17) 0.79500(7) 1.11294(7) 0.0199(3) Uani 1 1 d . . .
Cl2B Cl 1.09021(17) 0.79026(6) 0.87634(7) 0.0200(3) Uani 1 1 d . . .
Si1B Si 0.96004(19) 0.60742(7) 1.10468(8) 0.0158(3) Uani 1 1 d . . .
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Si2B Si 0.85050(18) 0.60615(7) 0.88658(8) 0.0142(3) Uani 1 1 d . . .
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C19B C 0.6010(6) 0.9604(2) 1.0160(3) 0.0252(12) Uani 1 1 d . . .
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H19F H 0.6496 0.9628 1.0764 0.038 Uiso 1 1 calc R . .
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H20F H 0.4058 0.8958 0.8848 0.037 Uiso 1 1 calc R . .
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Cl2A 0.0198(7) 0.0163(7) 0.0180(6) 0.0032(5) 0.0003(5) 0.0006(6)
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C7A 0.026(3) 0.002(2) 0.0062(19) -0.0018(16) -0.001(2) -0.003(2)
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C9A 0.017(3) 0.010(3) 0.020(3) 0.007(2) 0.013(2) 0.006(2)
C10A 0.028(3) 0.008(3) 0.011(2) -0.0019(19) 0.007(2) -0.002(2)
C11A 0.029(3) 0.024(3) 0.011(2) -0.0018(19) -0.001(2) -0.008(2)
C12A 0.021(3) 0.022(3) 0.024(3) 0.009(2) 0.002(2) 0.001(2)
C13A 0.028(3) 0.018(3) 0.019(2) -0.004(2) 0.007(2) -0.003(2)
```

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C14A 0.021(3) 0.027(3) 0.010(2) -0.0027(19) 0.005(2) -0.004(2)
C15A 0.024(3) 0.010(3) 0.008(2) -0.0013(17) 0.002(2) 0.003(2)
C16A 0.018(3) 0.011(2) 0.039(3) -0.0037(19) 0.005(2) -0.001(2)
C17A 0.017(3) 0.014(3) 0.020(3) -0.002(2) 0.002(2) 0.003(2)
C18A 0.016(3) 0.032(3) 0.029(3) 0.000(2) -0.002(2) -0.003(2)
C19A 0.031(4) 0.023(3) 0.041(3) -0.009(2) 0.017(3) -0.010(3)
C20A 0.022(3) 0.014(2) 0.024(2) 0.0039(19) 0.004(2) 0.000(2)
C21A 0.013(3) 0.018(3) 0.012(2) -0.0034(19) -0.007(2) 0.003(2)
C22A 0.024(3) 0.028(3) 0.014(2) 0.000(2) 0.001(2) -0.003(3)
C23A 0.013(3) 0.030(3) 0.020(3) 0.003(2) -0.003(2) 0.006(3)
C24A 0.018(3) 0.019(3) 0.010(2) -0.0043(19) 0.003(2) -0.001(2)
C25A 0.039(4) 0.023(3) 0.014(2) -0.003(2) 0.008(2) -0.001(3)
C26A 0.035(4) 0.027(3) 0.017(2) -0.001(2) 0.012(2) -0.005(3)
Zr1B 0.0141(3) 0.0130(3) 0.0100(2) 0.0002(2) 0.0026(2) -0.0010(2)
Cl1B 0.0180(7) 0.0229(7) 0.0174(6) -0.0058(5) 0.0024(5) -0.0029(6)
Cl2B 0.0273(8) 0.0169(7) 0.0179(6) 0.0048(5) 0.0098(5) -0.0001(5)
Si1B 0.0191(8) 0.0155(7) 0.0130(6) 0.0011(5) 0.0049(6) 0.0008(6)
Si2B 0.0153(8) 0.0153(7) 0.0107(6) 0.0010(5) 0.0011(6) -0.0026(6)
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C5B 0.014(3) 0.027(3) 0.011(2) -0.004(2) 0.004(2) -0.005(3)
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C11B 0.022(3) 0.024(3) 0.015(2) -0.001(2) 0.008(2) 0.008(3)
C12B 0.023(3) 0.021(3) 0.018(2) 0.001(2) 0.004(2) -0.002(2)
C13B 0.034(4) 0.032(3) 0.023(3) -0.010(2) 0.009(3) -0.014(3)
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C26B 0.032(4) 0.035(4) 0.018(3) 0.002(2) 0.002(3) 0.005(3)

_geom_special_details
;
 All esds (except the esd in the dihedral angle between two l.s. planes)
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 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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S1 S 0.30477(6) -0.09088(6) 0.048227(16) 0.02426(17) Uani 1 1 d . . .
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C1 C 0.5095(2) 0.11213(18) 0.01651(6) 0.0241(7) Uani 1 1 d . . .
C2 C 0.5971(2) 0.1254(2) 0.03527(6) 0.0242(7) Uani 1 1 d . . .
C3 C 0.5554(2) 0.1674(2) 0.06052(7) 0.0221(7) Uani 1 1 d . . .
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C4 C 0.4445(2) 0.1845(2) 0.05776(6) 0.0218(7) Uani 1 1 d . . .
C5 C 0.4178(2) 0.1471(2) 0.03096(6) 0.0225(7) Uani 1 1 d . . .
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C7 C 0.6489(2) -0.0825(2) 0.02773(6) 0.0228(7) Uani 1 1 d . . .
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H9 H 0.526(2) -0.2790(19) 0.0500(5) 0.027 Uiso 1 1 d . . .
C10 C 0.5015(2) -0.18508(19) 0.01656(5) 0.0183(6) Uani 1 1 d . . .
C11 C 0.3756(2) 0.0036(3) -0.02800(7) 0.0320(8) Uani 1 1 d . . .
H11A H 0.361(2) 0.064(2) -0.0362(6) 0.038 Uiso 1 1 d . . .
H11B H 0.324(2) -0.012(2) -0.0127(6) 0.038 Uiso 1 1 d . . .
H11C H 0.374(2) -0.048(2) -0.0408(6) 0.038 Uiso 1 1 d . . .
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C12 C 0.5973(3) 0.0601(3) -0.04343(7) 0.0402(9) Uani 1 1 d . . .
H12A H 0.596(2) 0.023(3) -0.0575(6) 0.048 Uiso 1 1 d . . .
H12B H 0.666(2) 0.080(2) -0.0379(6) 0.048 Uiso 1 1 d . . .
H12C H 0.578(2) 0.117(2) -0.0524(6) 0.048 Uiso 1 1 d . . .
C13 C 0.8181(3) 0.0789(3) 0.00434(9) 0.0420(10) Uani 1 1 d . . .
H13A H 0.834(3) 0.141(3) 0.0040(7) 0.050 Uiso 1 1 d . . .
H13B H 0.805(3) 0.063(3) -0.0138(7) 0.050 Uiso 1 1 d . . .
H13C H 0.884(3) 0.049(2) 0.0094(7) 0.050 Uiso 1 1 d . . .
C14 C 0.7926(3) 0.0604(3) 0.06637(8) 0.0378(9) Uani 1 1 d . . .
H14A H 0.850(2) 0.020(2) 0.0653(6) 0.045 Uiso 1 1 d . . .
H14B H 0.753(2) 0.042(2) 0.0815(6) 0.045 Uiso 1 1 d . . .
H14C H 0.807(2) 0.139(2) 0.0690(6) 0.045 Uiso 1 1 d . . .
C15 C 0.3727(2) 0.2425(2) 0.07774(6) 0.0229(7) Uani 1 1 d . . .
H15 H 0.304(2) 0.214(2) 0.0742(5) 0.027 Uiso 1 1 d . . .
C16 C 0.4033(3) 0.2261(3) 0.10790(7) 0.0329(8) Uani 1 1 d . . .
H16A H 0.403(2) 0.154(2) 0.1131(6) 0.039 Uiso 1 1 d . . .
H16B H 0.353(2) 0.259(2) 0.1211(6) 0.039 Uiso 1 1 d . . .
H16C H 0.468(2) 0.250(2) 0.1118(6) 0.039 Uiso 1 1 d . . .
C17 C 0.3625(2) 0.3631(2) 0.06973(6) 0.0255(7) Uani 1 1 d . . .
C18 C 0.3290(3) 0.3744(3) 0.03952(8) 0.0375(9) Uani 1 1 d . . .
H18A H 0.305(2) 0.442(2) 0.0348(6) 0.045 Uiso 1 1 d . . .
H18B H 0.270(2) 0.327(2) 0.0341(7) 0.045 Uiso 1 1 d . . .
H18C H 0.382(3) 0.359(2) 0.0274(7) 0.045 Uiso 1 1 d . . .
C19 C 0.2763(3) 0.4131(3) 0.08799(8) 0.0383(9) Uani 1 1 d . . .
H19A H 0.267(2) 0.481(2) 0.0823(6) 0.046 Uiso 1 1 d . . .
H19B H 0.299(2) 0.416(2) 0.1090(7) 0.046 Uiso 1 1 d . . .
H19C H 0.204(3) 0.376(2) 0.0854(6) 0.046 Uiso 1 1 d . . .
C20 C 0.4658(3) 0.4217(3) 0.07424(9) 0.0415(9) Uani 1 1 d . . .
H20A H 0.517(2) 0.390(2) 0.0640(7) 0.050 Uiso 1 1 d . . .
H20B H 0.489(3) 0.422(2) 0.0931(7) 0.050 Uiso 1 1 d . . .
H20C H 0.462(2) 0.496(2) 0.0680(6) 0.050 Uiso 1 1 d . . .
C21 C 0.7289(2) -0.2038(2) 0.06705(6) 0.0298(7) Uani 1 1 d . . .
H21 H 0.741(2) -0.149(2) 0.0820(6) 0.036 Uiso 1 1 d . . .
C22 C 0.8323(3) -0.2142(3) 0.05050(8) 0.0385(9) Uani 1 1 d . . .
H22A H 0.890(2) -0.238(2) 0.0638(7) 0.046 Uiso 1 1 d . . .
H22B H 0.856(2) -0.149(3) 0.0423(7) 0.046 Uiso 1 1 d . . .
H22C H 0.828(2) -0.256(2) 0.0350(7) 0.046 Uiso 1 1 d . . .
C23 C 0.7044(3) -0.3094(3) 0.08104(7) 0.0331(8) Uani 1 1 d . . .
H23A H 0.636(2) -0.306(2) 0.0937(6) 0.040 Uiso 1 1 d . . .
H23B H 0.762(2) -0.322(2) 0.0916(6) 0.040 Uiso 1 1 d . . .
H23C H 0.698(2) -0.366(2) 0.0671(6) 0.040 Uiso 1 1 d . . .
C24 C 0.4134(2) -0.2386(2) 0.00059(7) 0.0280(8) Uani 1 1 d . . .
H24 H 0.362(2) -0.194(2) -0.0022(6) 0.034 Uiso 1 1 d . . .
C25 C 0.4548(3) -0.2741(3) -0.02775(7) 0.0392(9) Uani 1 1 d . . .
H25A H 0.482(2) -0.217(2) -0.0397(6) 0.047 Uiso 1 1 d . . .
H25B H 0.395(2) -0.305(2) -0.0384(7) 0.047 Uiso 1 1 d . . .
H25C H 0.514(2) -0.321(2) -0.0249(6) 0.047 Uiso 1 1 d . . .
C26 C 0.3680(3) -0.3344(3) 0.01605(8) 0.0345(8) Uani 1 1 d . . .
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H26A H 0.426(2) -0.389(2) 0.0178(6) 0.041 Uiso 1 1 d . . .
H26B H 0.309(2) -0.358(2) 0.0060(6) 0.041 Uiso 1 1 d . . .
H26C H 0.346(2) -0.320(2) 0.0340(7) 0.041 Uiso 1 1 d . . .
C27 C 0.2198(2) 0.0047(2) 0.06358(6) 0.0256(6) Uani 1 1 d . . .
C28 C 0.1464(2) 0.0559(2) 0.04644(7) 0.0304(7) Uani 1 1 d . . .
H28 H 0.143(2) 0.038(2) 0.0263(6) 0.036 Uiso 1 1 d . . .
C29 C 0.0762(3) 0.1275(3) 0.05797(9) 0.0428(10) Uani 1 1 d . . .
H29 H 0.032(2) 0.164(2) 0.0462(6) 0.051 Uiso 1 1 d . . .
C30 C 0.0788(3) 0.1492(3) 0.08586(9) 0.0460(11) Uani 1 1 d . . .
H30 H 0.035(3) 0.193(2) 0.0940(7) 0.055 Uiso 1 1 d . . .
C31 C 0.1499(3) 0.0986(3) 0.10316(8) 0.0419(9) Uani 1 1 d . . .
H31 H 0.156(2) 0.112(3) 0.1219(7) 0.050 Uiso 1 1 d . . .
C32 C 0.2208(2) 0.0255(3) 0.09178(7) 0.0327(8) Uani 1 1 d . . .
H32 H 0.267(2) -0.005(2) 0.1028(6) 0.039 Uiso 1 1 d . . .
C33 C 0.5224(2) -0.1538(2) 0.11757(6) 0.0249(7) Uani 1 1 d . . .
C34 C 0.5962(3) -0.1836(2) 0.13771(6) 0.0294(7) Uani 1 1 d . . .
H34 H 0.653(2) -0.141(2) 0.1423(6) 0.035 Uiso 1 1 d . . .
C35 C 0.5903(3) -0.2824(3) 0.15008(7) 0.0363(9) Uani 1 1 d . . .
H35 H 0.646(2) -0.297(2) 0.1630(6) 0.044 Uiso 1 1 d . . .
C36 C 0.5109(3) -0.3518(2) 0.14320(7) 0.0372(8) Uani 1 1 d . . .
H36 H 0.507(2) -0.417(2) 0.1519(6) 0.045 Uiso 1 1 d . . .
C37 C 0.4362(3) -0.3224(3) 0.12363(7) 0.0341(8) Uani 1 1 d . . .
H37 H 0.385(2) -0.357(2) 0.1185(6) 0.041 Uiso 1 1 d . . .
C38 C 0.4406(2) -0.2230(2) 0.11085(7) 0.0288(8) Uani 1 1 d . . .
H38 H 0.395(2) -0.201(2) 0.0983(6) 0.035 Uiso 1 1 d . . .

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Si2 0.0218(4) 0.0254(5) 0.0363(5) -0.0005(4) 0.0055(4) 0.0003(4)
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C2 0.0233(16) 0.0189(16) 0.0304(17) 0.0034(14) 0.0046(14) -0.0007(11)
C3 0.0234(17) 0.0173(15) 0.0258(18) 0.0002(13) 0.0010(14) -0.0038(12)
C4 0.0251(16) 0.0163(15) 0.0239(17) 0.0088(12) 0.0040(13) 0.0003(12)
C5 0.0259(16) 0.0175(15) 0.0242(17) 0.0044(13) -0.0018(14) 0.0042(13)
C6 0.0275(16) 0.0223(15) 0.0163(15) -0.0004(12) 0.0045(12) 0.0048(11)
C7 0.0140(14) 0.0251(16) 0.0292(18) -0.0029(13) 0.0090(13) 0.0015(12)
C8 0.0238(16) 0.0213(15) 0.0251(16) -0.0047(13) 0.0010(13) 0.0073(11)
C9 0.0283(17) 0.0171(15) 0.0233(17) 0.0040(12) 0.0066(13) 0.0022(12)
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C10 0.0204(15) 0.0220(13) 0.0126(14) -0.0047(11) 0.0061(13) 0.0013(12)
C11 0.0435(18) 0.0295(19) 0.0229(18) -0.0005(15) -0.0108(15) 0.0087(17)
C12 0.059(2) 0.036(2) 0.0252(19) 0.0076(15) 0.0119(18) 0.0083(18)
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C14 0.0234(19) 0.035(2) 0.056(3) -0.0034(19) -0.0017(17) 0.0006(16)
C15 0.0217(17) 0.0218(17) 0.0251(18) -0.0032(13) 0.0016(13) -0.0008(13)
C16 0.039(2) 0.036(2) 0.0242(19) -0.0045(16) 0.0039(17) 0.0076(17)
C17 0.0290(17) 0.0214(16) 0.0261(19) -0.0029(14) 0.0052(14) 0.0023(14)
C18 0.049(2) 0.0245(19) 0.039(2) 0.0024(16) 0.0006(18) 0.0114(17)
C19 0.049(2) 0.0277(19) 0.038(2) -0.0041(17) 0.0064(19) 0.0074(17)
C20 0.038(2) 0.0253(19) 0.061(3) -0.0016(18) 0.001(2) -0.0031(17)
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C30 0.034(2) 0.031(2) 0.074(3) -0.008(2) 0.026(2) -0.0037(17)
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C34 0.0352(19) 0.0326(19) 0.0203(17) -0.0036(14) 0.0008(15) 0.0090(14)
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C37 0.032(2) 0.028(2) 0.042(2) 0.0020(16) 0.0081(17) -0.0025(15)
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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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PlnA . PlnB 75.76(9) . . ?
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 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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H12C H 0.6184 0.9247 1.1250 0.035 Uiso 1 1 calc R . .
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H13C H 0.2575 0.7520 0.9442 0.036 Uiso 1 1 calc R . .
C14 C 0.1932(3) 0.7702(2) 0.6814(2) 0.0246(7) Uani 1 1 d . . .
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H14B H 0.2341 0.7657 0.6258 0.037 Uiso 1 1 calc R . .
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H15B H 0.6699 1.0536 0.6133 0.021 Uiso 0.50 1 d PR A 2
C16A C 0.6540(3) 1.03794(19) 0.56919(18) 0.0236(13) Uani 0.50 1 d PR A 1
H16A H 0.7150 1.0730 0.5313 0.035 Uiso 0.50 1 calc PR A 1
H16B H 0.5659 1.0548 0.5521 0.035 Uiso 0.50 1 calc PR A 1
H16C H 0.6336 0.9594 0.5524 0.035 Uiso 0.50 1 calc PR A 1
C16B C 0.8719(6) 1.0736(5) 0.6874(5) 0.0279(15) Uani 0.50 1 d P A 2
H16D H 0.9373 1.1127 0.7531 0.042 Uiso 0.50 1 calc PR A 2
H16E H 0.9042 1.1064 0.6350 0.042 Uiso 0.50 1 calc PR A 2
H16F H 0.8680 0.9976 0.6772 0.042 Uiso 0.50 1 calc PR A 2
C17 C 0.7401(3) 1.2011(2) 0.7156(2) 0.0232(7) Uani 1 1 d . A .
C18 C 0.8335(4) 1.2467(2) 0.8239(2) 0.0450(10) Uani 1 1 d . . .
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H18B H 0.9264 1.2391 0.8299 0.068 Uiso 1 1 calc R . .
H18C H 0.7903 1.2068 0.8686 0.068 Uiso 1 1 calc R . .
C19 C 0.8071(3) 1.2677(2) 0.6473(2) 0.0306(8) Uani 1 1 d . . .
H19A H 0.7479 1.2400 0.5778 0.046 Uiso 1 1 calc R A .
H19B H 0.9007 1.2616 0.6527 0.046 Uiso 1 1 calc R . .
H19C H 0.8155 1.3438 0.6679 0.046 Uiso 1 1 calc R . .
C20 C 0.5963(4) 1.2128(3) 0.7065(2) 0.0339(8) Uani 1 1 d . . .
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H20B H 0.5533 1.1728 0.7512 0.051 Uiso 1 1 calc R . .
H20C H 0.5366 1.1837 0.6372 0.051 Uiso 1 1 calc R . .
C21 C 0.2971(3) 0.5507(2) 0.6368(2) 0.0170(6) Uani 1 1 d . . .
H21 H 0.2627 0.6049 0.6035 0.020 Uiso 1 1 calc R . .
C22 C 0.1818(3) 0.4884(2) 0.6792(2) 0.0232(7) Uani 1 1 d . . .
H22A H 0.1613 0.5411 0.7251 0.028 Uiso 1 1 calc R . .
H22B H 0.0949 0.4518 0.6233 0.028 Uiso 1 1 calc R . .
C23 C 0.2196(4) 0.4046(3) 0.7351(3) 0.0390(9) Uani 1 1 d . . .
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H23B H 0.1506 0.3791 0.7709 0.059 Uiso 1 1 calc R . .
H23C H 0.3134 0.4372 0.7832 0.059 Uiso 1 1 calc R . .
C24 C 0.3283(3) 0.4769(2) 0.5581(2) 0.0220(6) Uani 1 1 d . . .
H24A H 0.4073 0.5205 0.5373 0.026 Uiso 1 1 calc R . .
H24B H 0.3588 0.4207 0.5890 0.026 Uiso 1 1 calc R . .
C25 C 0.2035(3) 0.4216(3) 0.4657(2) 0.0316(8) Uani 1 1 d . . .
H25A H 0.1273 0.3736 0.4848 0.047 Uiso 1 1 calc R . .
H25B H 0.2319 0.3791 0.4172 0.047 Uiso 1 1 calc R . .
H25C H 0.1708 0.4765 0.4356 0.047 Uiso 1 1 calc R . .
C26 C 0.7767(3) 0.6306(2) 0.89542(19) 0.0157(6) Uani 1 1 d . . .
H26 H 0.8501 0.7035 0.9221 0.019 Uiso 1 1 calc R . .
C27 C 0.7531(3) 0.5809(2) 0.9860(2) 0.0205(6) Uani 1 1 d . . .
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H27B H 0.7186 0.6281 1.0269 0.025 Uiso 1 1 calc R . .
C28 C 0.6493(3) 0.4654(2) 0.9597(2) 0.0271(7) Uani 1 1 d . . .
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H28B H 0.6341 0.4432 1.0210 0.041 Uiso 1 1 calc R . .
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H29B H 0.8397 0.6005 0.7686 0.023 Uiso 1 1 calc R . .
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H30B H 1.0015 0.5155 0.8258 0.042 Uiso 1 1 calc R . .
H30C H 0.9553 0.5058 0.9256 0.042 Uiso 1 1 calc R . .
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H41B H -0.2295 -0.0135 0.3733 0.066 Uiso 0.50 1 d PR . .
H41C H -0.1421 -0.0827 0.3384 0.066 Uiso 0.50 1 d PR . .
C42 C -0.0506(6) 0.0024(5) 0.4822(5) 0.0286(14) Uani 0.50 1 d P . .
C43 C 0.0465(7) 0.0949(5) 0.4767(5) 0.0312(16) Uani 0.50 1 d P . .
H43A H 0.0318 0.1226 0.4165 0.037 Uiso 0.50 1 d PR . .
C44 C 0.1658(7) 0.1495(5) 0.5560(5) 0.0310(15) Uani 0.50 1 d P . .
H44A H 0.2368 0.2110 0.5494 0.037 Uiso 0.50 1 d PR . .
C45 C 0.1842(8) 0.1151(6) 0.6437(6) 0.0330(17) Uani 0.50 1 d P . .
H45A H 0.2635 0.1555 0.7002 0.040 Uiso 0.50 1 d PR . .
C46 C 0.0869(8) 0.0217(5) 0.6529(5) 0.0359(16) Uani 0.50 1 d P . .
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C9 0.0187(14) 0.0108(12) 0.0162(14) 0.0020(10) 0.0077(11) 0.0044(11)
C10 0.0171(14) 0.0109(12) 0.0160(13) 0.0053(10) 0.0067(11) 0.0024(11)
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