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Visible light driven room temperature Pauson-Khand reaction

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_journal_name_full 'Dalton Trans.'

_journal_codен_Cambridge 0222

_publ_contact_author_name 'Mary Pryce'
_publ_contact_author_email MARY.PRYCE@DCU.IE

_publ_section_title
;
Visible Light Driven Room Temperature Pauson-Khand Reaction
;
loop_
_publ_author_name
'Mary Pryce'
'Wesley Browne'
'Anthony C. Coleman'
'Ben Feringa'
'Conor Long'
'Auke Meetsma'

Attachment 'q14241.cif'

CIF-file generated for C20H20FeO P-1 q1424

#=====

data_q14241.cif
_database_code_depnum_ccdc_archive 'CCDC 699252'

_chemical_name_systematic
;
;
_chemical_name_common ?
_chemical_melting_point ?
_chemical_formula_moiety 'C20 H20 Fe O'
Ex: 'C12 H16 N2 O6, H2 O' and '(Cd 2+)3, (C6 N6 Cr 3-)2, 2(H2 O)'
_chemical_formula_structural ?
_chemical_formula_sum 'C20 H20 Fe O'
_chemical_formula_iupac ?
_chemical_formula_weight 332.22
_chemical_compound_source 'see text'

loop_
_atom_type_symbol
_atom_type_description
_atom_type_scат_dispersiоn_real
_atom_type_scат_dispersiоn_imag
_atom_type_scат_source
O O 0.0106 0.0060 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Fe Fe 0.3463 0.8444 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
H H 0.0000 0.0000 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
C C 0.0033 0.0016 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

#=====

6. CRYSTAL DATA

_symmetry_cell_setting triclinic
_symmetry_space_group_name_Hall '-P 1'

_symmetry_space_group_name_H-M 'P -1'
_symmetry_Int_Tables_number 2

loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z

_cell_length_a 8.7216(12)
_cell_length_b 10.2643(14)
_cell_length_c 10.3445(14)
_cell_angle_alpha 60.6174(14)
_cell_angle_beta 88.8587(16)
_cell_angle_gamma 69.6825(15)
_cell_volume 743.79(18)
_cell_formula_units_Z 2

_cell_measurement_temperature 100(1)
_cell_measurement_reflns_used 3804
_cell_measurement_theta_min 2.47
_cell_measurement_theta_max 29.30
_cell_special_details

;

The final unit cell was obtained from the xyz centroids of
3804 reflections after integration using the SAINTPLUS
software package (Bruker, 2007).

Reduced cell calculations did not indicate any higher metric lattice symmetry
and examination of the final atomic coordinates of the structure did not
yield extra symmetry elements (Spek, 1988; Le Page 1987, 1988)

;

_exptl_crystal_description 'cut fragment'
_exptl_crystal_colour red
_exptl_crystal_size_max 0.47
_exptl_crystal_size_mid 0.39
_exptl_crystal_size_min 0.33
_exptl_crystal_size_rad ?
_exptl_crystal_density_meas ?
_exptl_crystal_density_diffn 1.483
_exptl_crystal_density_method 'not measured'
_exptl_crystal_F_000 348
_exptl_absorpt_coefficient_mu 1.012
_exptl_absorpt_correction_type multi-scan
_exptl_absorpt_process_details '(SADABS, (Bruker, 2007))'
_exptl_absorpt_correction_T_min 0.6114
_exptl_absorpt_correction_T_max 0.7160

#=====

7. EXPERIMENTAL DATA

_exptl_special_details
;
;
_diffrn_ambient_temperature 100(1)
_diffrn_radiation_wavelength 0.71073
_diffrn_radiation_type MoK α
_diffrn_radiation_source 'fine focus sealed Siemens Mo tube '
_diffrn_radiation_monochromator 'parallel mounted graphite'

```

_diffrn_radiation_detector
;
CCD area-detector
;
_diffrn_measurement_device_type
;
Bruker Smart Apex; CCD area detector
;
_diffrn_measurement_method      '\f and \w scans'
_diffrn_special_details
;
Crystal into the cold nitrogen stream of the low-temperature unit
(KRYOFLEX, (Bruker, 2006)).
;
_diffrn_detector_area_resol_mean 66.06

_diffrn_standards_number        0
_diffrn_standards_interval_count .
_diffrn_standards_interval_time .
_diffrn_standards_decay_%       0

loop_
_diffrn_standard_refl_index_h
_diffrn_standard_refl_index_k
_diffrn_standard_refl_index_l
? ? ?

# number of measured reflections (redundant set)
_diffrn_reflns_number           6709
_diffrn_reflns_av_R_equivalents 0.0215
_diffrn_reflns_av_sigmaI/netI   0.0346
_diffrn_reflns_limit_h_min      -11
_diffrn_reflns_limit_h_max      11
_diffrn_reflns_limit_k_min      -13
_diffrn_reflns_limit_k_max      13
_diffrn_reflns_limit_l_min      -13
_diffrn_reflns_limit_l_max      13
_diffrn_reflns_theta_min        2.47
_diffrn_reflns_theta_max        28.28
_diffrn_measured_fraction_theta_max 0.956
_diffrn_reflns_theta_full       25.00
_diffrn_measured_fraction_theta_full 0.978

_diffrn_reflns_reduction_process
;
Intensity data were corrected for Lorentz and polarization
effects, decay and absorption and reduced to  $F_o^2$ 
using SAINT-Plus & SADABS (Bruker, 2007).
;

# number of unique reflections
_reflns_number_total            3536
_reflns_number_gt               3182
_reflns_threshold_expression      $I > 2\sigma(I)$ 

_computing_data_collection      'SMART (Bruker, 2007)'
_computing_cell_refinement      'SAINT-Plus (Bruker, 2007)'
_computing_data_reduction       SAINT-Plus
_computing_structure_solution
;
DIRDIF-07 (Beurskens et al., 2007)

```

```

;
_computing_structure_refinement 'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
PLATON (Spek, 2003)
PLUTO (Meetsma, 2007)
;
_computing_publication_material 'PLATON (Spek, 2003)'

#=====

# 8. REFINEMENT DATA

_refine_special_details
;
Refinement of F2 against ALL reflections. The weighted R-factor wR and
goodness of fit S are based on F2, conventional R-factors R are based
on F, with F set to zero for negative F2. The threshold expression of
F2 > 2sigma(F2) is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on F2 are statistically about twice as large as those based on F, and R-
factors based on ALL data will be even larger.
;

_refine_ls_structure_factor_coef Fsqd
_refine_ls_matrix_type full
_refine_ls_weighting_scheme calc
_refine_ls_weighting_details
'calc w=1/[s2(Fo2)+(0.0468P)2+0.1640P] where P=(Fo2+2Fc2)/3'
_atom_sites_solution_primary heavy
_atom_sites_solution_secondary direct
_atom_sites_solution_hydrogens difmap
_refine_ls_hydrogen_treatment reffall
_refine_ls_extinction_method none
_refine_ls_extinction_coef ?
_refine_ls_abs_structure_details ?
_chemical_absolute_configuration .
_refine_ls_abs_structure_Flack ?
_refine_ls_number_reflns 3536
_refine_ls_number_parameters 279
_refine_ls_number_restraints 0
_refine_ls_number_constraints ?
_refine_ls_R_factor_all 0.0389
_refine_ls_R_factor_gt 0.0344
_refine_ls_wR_factor_ref 0.0874
_refine_ls_wR_factor_gt 0.0851
_refine_ls_goodness_of_fit_ref 1.107
_refine_ls_restrained_S_all 1.107
_refine_ls_shift/su_max 0.000
_refine_ls_shift/su_mean 0.000
_refine_diff_density_max 0.482
_refine_diff_density_min -0.388
_refine_diff_density_rms 0.077

_vrn_publ_code_number_frames 1800
_vrn_publ_code_frame_time_sec 5.0
_vrn_publ_code_meas_time_hour 5.4

#=====

# 9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

```

```

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_thermal_displace_type
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_U_iso_or_equiv
_atom_site_calc_flag
_atom_site_refinement_flags
Fe Fe Uani 1.15564(3) 0.22198(3) 0.42084(3) 1.000 0.0140(1) . .
O O Uani 0.66646(17) 0.31074(16) 0.42166(16) 1.000 0.0286(4) . .
C1 C Uani 1.2511(2) 0.3129(2) 0.5225(2) 1.000 0.0197(5) . .
C2 C Uani 1.3721(2) 0.1627(2) 0.5492(2) 1.000 0.0199(5) . .
C3 C Uani 1.3046(2) 0.0417(2) 0.6252(2) 1.000 0.0188(5) . .
C4 C Uani 1.1427(2) 0.1173(2) 0.64614(19) 1.000 0.0171(5) . .
C5 C Uani 1.1098(2) 0.2850(2) 0.58219(19) 1.000 0.0165(5) . .
C6 C Uani 1.0935(2) 0.3836(2) 0.1925(2) 1.000 0.0183(5) . .
C7 C Uani 1.2156(2) 0.2309(2) 0.2259(2) 1.000 0.0207(5) . .
C8 C Uani 1.1490(2) 0.1103(2) 0.3044(2) 1.000 0.0208(5) . .
C9 C Uani 0.9854(2) 0.1869(2) 0.3213(2) 1.000 0.0176(5) . .
C10 C Uani 0.9490(2) 0.3577(2) 0.25126(19) 1.000 0.0153(5) . .
C11 C Uani 0.7936(2) 0.4813(2) 0.24015(19) 1.000 0.0149(5) . .
C12 C Uani 0.6612(2) 0.4444(2) 0.3269(2) 1.000 0.0171(5) . .
C13 C Uani 0.5139(2) 0.6035(2) 0.2772(2) 1.000 0.0163(5) . .
C14 C Uani 0.5718(2) 0.7374(2) 0.16298(19) 1.000 0.0153(4) . .
C15 C Uani 0.7416(2) 0.6439(2) 0.15071(19) 1.000 0.0152(5) . .
C16 C Uani 0.3617(2) 0.6251(2) 0.1826(2) 1.000 0.0203(5) . .
C17 C Uani 0.2176(3) 0.7770(2) 0.1612(2) 1.000 0.0262(6) . .
C18 C Uani 0.2732(2) 0.9170(2) 0.0534(2) 1.000 0.0219(5) . .
C19 C Uani 0.4374(2) 0.8291(2) 0.0194(2) 1.000 0.0165(5) . .
C20 C Uani 0.4048(2) 0.6893(2) 0.0230(2) 1.000 0.0188(5) . .
H1 H Uiso 1.258(3) 0.417(3) 0.469(3) 1.000 0.032(6) . .
H2 H Uiso 1.479(3) 0.148(3) 0.518(2) 1.000 0.026(6) . .
H3 H Uiso 1.354(3) -0.073(3) 0.655(2) 1.000 0.024(6) . .
H4 H Uiso 1.068(3) 0.063(3) 0.693(2) 1.000 0.023(5) . .
H5 H Uiso 1.014(3) 0.360(3) 0.584(3) 1.000 0.030(6) . .
H6 H Uiso 1.105(3) 0.482(3) 0.142(2) 1.000 0.023(5) . .
H7 H Uiso 1.326(3) 0.213(3) 0.202(2) 1.000 0.024(6) . .
H8 H Uiso 1.206(3) -0.008(3) 0.347(3) 1.000 0.027(6) . .
H9 H Uiso 0.914(3) 0.134(3) 0.375(2) 1.000 0.021(5) . .
H13 H Uiso 0.488(3) 0.607(2) 0.364(2) 1.000 0.021(5) . .
H14 H Uiso 0.578(2) 0.809(2) 0.197(2) 1.000 0.011(5) . .
H15 H Uiso 0.803(2) 0.697(2) 0.082(2) 1.000 0.017(5) . .
H16 H Uiso 0.335(3) 0.529(2) 0.224(2) 1.000 0.020(5) . .
H17 H Uiso 0.200(3) 0.778(3) 0.254(3) 1.000 0.035(6) . .
H17' H Uiso 0.116(3) 0.783(3) 0.118(3) 1.000 0.033(6) . .
H18 H Uiso 0.288(3) 0.974(2) 0.099(2) 1.000 0.020(5) . .
H18' H Uiso 0.189(3) 0.990(3) -0.038(2) 1.000 0.023(5) . .
H19 H Uiso 0.471(2) 0.899(2) -0.069(2) 1.000 0.013(5) . .
H20 H Uiso 0.500(3) 0.615(3) 0.013(2) 1.000 0.017(5) . .
H20' H Uiso 0.316(3) 0.723(3) -0.053(3) 1.000 0.033(6) . .

```

```

loop_
_atom_site_aniso_label
_atom_site_aniso_U_11
_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_23

```

```

_atom_site_aniso_U_13
_atom_site_aniso_U_12
Fe 0.0130(1) 0.0159(1) 0.0113(1) -0.0066(1) 0.0011(1) -0.0040(1)
O 0.0232(7) 0.0171(6) 0.0293(8) -0.0014(6) 0.0085(6) -0.0067(5)
C1 0.0247(10) 0.0238(9) 0.0141(9) -0.0098(8) 0.0027(7) -0.0129(8)
C2 0.0145(9) 0.0313(10) 0.0142(9) -0.0126(8) 0.0013(7) -0.0077(7)
C3 0.0174(9) 0.0191(8) 0.0126(8) -0.0073(7) -0.0019(7) -0.0005(7)
C4 0.0187(9) 0.0189(8) 0.0119(8) -0.0069(7) 0.0027(7) -0.0069(7)
C5 0.0188(9) 0.0177(8) 0.0131(8) -0.0089(7) 0.0029(7) -0.0056(7)
C6 0.0179(9) 0.0207(8) 0.0109(8) -0.0053(7) 0.0001(7) -0.0060(7)
C7 0.0141(9) 0.0302(10) 0.0128(9) -0.0118(8) 0.0012(7) -0.0020(7)
C8 0.0199(9) 0.0208(8) 0.0183(9) -0.0126(8) -0.0033(7) 0.0000(7)
C9 0.0182(9) 0.0179(8) 0.0161(9) -0.0093(7) -0.0008(7) -0.0052(7)
C10 0.0141(8) 0.0166(8) 0.0116(8) -0.0062(7) -0.0009(6) -0.0035(6)
C11 0.0140(8) 0.0164(8) 0.0118(8) -0.0059(7) 0.0001(6) -0.0053(6)
C12 0.0156(8) 0.0169(8) 0.0147(8) -0.0055(7) 0.0012(7) -0.0059(7)
C13 0.0152(8) 0.0182(8) 0.0115(8) -0.0053(7) 0.0030(7) -0.0058(7)
C14 0.0164(8) 0.0137(7) 0.0130(8) -0.0058(7) 0.0011(7) -0.0044(6)
C15 0.0148(8) 0.0165(8) 0.0121(8) -0.0059(7) 0.0009(7) -0.0058(7)
C16 0.0162(9) 0.0199(8) 0.0202(9) -0.0078(8) 0.0023(7) -0.0060(7)
C17 0.0154(9) 0.0270(10) 0.0253(11) -0.0097(9) 0.0034(8) -0.0024(8)
C18 0.0183(9) 0.0183(8) 0.0200(10) -0.0086(8) 0.0009(8) 0.0009(7)
C19 0.0172(9) 0.0139(7) 0.0127(8) -0.0047(7) 0.0009(7) -0.0031(7)
C20 0.0166(9) 0.0198(8) 0.0191(9) -0.0109(8) -0.0001(7) -0.0046(7)

```

```
#=====
```

``` # 10. MOLECULAR GEOMETRY ```

```
_geom_special_details
```

```
;
```

Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

```
;
```

```
loop_
```

```
_geom_bond_atom_site_label_1
```

```
_geom_bond_atom_site_label_2
```

```
_geom_bond_distance
```

```
_geom_bond_site_symmetry_1
```

```
_geom_bond_site_symmetry_2
```

```
_geom_bond_publ_flag
```

```
Fe C1 2.051(2) . . yes
```

```
Fe C2 2.0510(19) . . yes
```

```
Fe C3 2.0451(19) . . yes
```

```
Fe C4 2.0532(17) . . yes
```

```
Fe C5 2.054(2) . . yes
```

```
Fe C6 2.0510(18) . . yes
```

```
Fe C7 2.0392(19) . . yes
```

```
Fe C8 2.043(2) . . yes
```

```
Fe C9 2.047(2) . . yes
```

```
Fe C10 2.0617(18) . . yes
```

```
O C12 1.218(3) . . yes
```

```
C1 C2 1.425(3) . . no
```

```
C1 C5 1.422(3) . . no
```

```
C2 C3 1.428(3) . . no
```

```
C3 C4 1.426(3) . . no
```

```
C4 C5 1.425(3) . . no
```

C6 C7 1.426(3) . . no
 C6 C10 1.440(3) . . no
 C7 C8 1.422(3) . . no
 C8 C9 1.425(3) . . no
 C9 C10 1.441(3) . . no
 C10 C11 1.459(3) . . no
 C11 C12 1.487(3) . . no
 C11 C15 1.350(3) . . no
 C12 C13 1.526(3) . . no
 C13 C14 1.551(3) . . no
 C13 C16 1.550(3) . . no
 C14 C15 1.502(3) . . no
 C14 C19 1.548(3) . . no
 C16 C17 1.540(3) . . no
 C16 C20 1.543(3) . . no
 C17 C18 1.560(3) . . no
 C18 C19 1.544(3) . . no
 C19 C20 1.540(3) . . no
 C1 H1 0.96(3) . . no
 C2 H2 0.97(3) . . no
 C3 H3 0.98(3) . . no
 C4 H4 0.97(3) . . no
 C5 H5 0.93(3) . . no
 C6 H6 0.92(3) . . no
 C7 H7 0.97(3) . . no
 C8 H8 0.99(3) . . no
 C9 H9 0.96(3) . . no
 C13 H13 0.94(2) . . no
 C14 H14 0.97(2) . . no
 C15 H15 0.947(19) . . no
 C16 H16 0.98(2) . . no
 C17 H17 0.97(3) . . no
 C17 H17' 0.97(3) . . no
 C18 H18 0.95(2) . . no
 C18 H18' 0.97(2) . . no
 C19 H19 0.964(18) . . no
 C20 H20 0.96(3) . . no
 C20 H20' 0.95(3) . . no

loop_
 _geom_angle_atom_site_label_1
 _geom_angle_atom_site_label_2
 _geom_angle_atom_site_label_3
 _geom_angle
 _geom_angle_site_symmetry_1
 _geom_angle_site_symmetry_2
 _geom_angle_site_symmetry_3
 _geom_angle_publ_flag
 C1 Fe C2 40.65(8) . . . yes
 C1 Fe C3 68.47(8) . . . yes
 C1 Fe C4 68.32(8) . . . yes
 C1 Fe C5 40.55(7) . . . yes
 C1 Fe C6 108.85(8) . . . yes
 C1 Fe C7 123.40(8) . . . yes
 C1 Fe C8 158.53(8) . . . yes
 C1 Fe C9 160.00(8) . . . yes
 C1 Fe C10 124.21(8) . . . yes
 C2 Fe C3 40.80(8) . . . yes
 C2 Fe C4 68.49(7) . . . yes
 C2 Fe C5 68.38(8) . . . yes
 C2 Fe C6 122.89(7) . . . yes

C2 Fe C7 106.63(8) . . . yes
C2 Fe C8 121.43(8) . . . yes
C2 Fe C9 157.49(9) . . . yes
C2 Fe C10 159.77(8) . . . yes
C3 Fe C4 40.74(8) . . . yes
C3 Fe C5 68.45(8) . . . yes
C3 Fe C6 158.02(8) . . . yes
C3 Fe C7 121.07(8) . . . yes
C3 Fe C8 105.40(8) . . . yes
C3 Fe C9 121.31(8) . . . yes
C3 Fe C10 158.58(8) . . . yes
C4 Fe C5 40.60(8) . . . yes
C4 Fe C6 160.39(8) . . . yes
C4 Fe C7 157.19(9) . . . yes
C4 Fe C8 121.29(8) . . . yes
C4 Fe C9 106.77(7) . . . yes
C4 Fe C10 123.33(7) . . . yes
C5 Fe C6 124.66(8) . . . yes
C5 Fe C7 160.29(8) . . . yes
C5 Fe C8 158.25(8) . . . yes
C5 Fe C9 123.24(8) . . . yes
C5 Fe C10 108.83(8) . . . yes
C6 Fe C7 40.81(8) . . . yes
C6 Fe C8 68.71(8) . . . yes
C6 Fe C9 68.89(8) . . . yes
C6 Fe C10 40.97(7) . . . yes
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Fe C10 C9 68.93(10) . . . yes

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 H5 H1 2.49(4) . 2_766 no
 H5 H5 2.44(4) . 2_766 no
 H6 C15 3.05(3) . . no
 H6 H16 2.47(4) . 1_655 no
 H7 H19 2.53(3) . 2_765 no
 H8 O 2.65(3) . 2_756 no
 H9 O 2.51(3) . . no
 H9 C12 2.98(3) . . no
 H9 Fe 3.48(3) . 2_756 no
 H9 C3 3.05(3) . 2_756 no
 H9 C4 2.90(3) . 2_756 no
 H9 C9 3.07(2) . 2_756 no
 H9 H4 2.40(4) . 2_756 no
 H13 H17 2.40(4) . . no
 H13 O 2.89(2) . 2_666 no
 H13 C1 3.10(3) . 2_766 no
 H13 H13 2.54(3) . 2_666 no
 H14 H18 2.40(3) . . no
 H14 C1 2.743(18) . 2_766 no
 H14 C2 2.837(19) . 2_766 no
 H14 H19 2.48(3) . 2_675 no
 H15 C6 2.99(2) . . no
 H15 C7 2.888(18) . 2_765 no
 H16 C1 3.05(2) . 1_455 no
 H16 C6 3.08(3) . 1_455 no
 H16 H1 2.41(3) . 1_455 no
 H16 H6 2.47(4) . 1_455 no
 H17 H13 2.40(4) . . no
 H17 H4 2.57(4) . 2_666 no
 H17' H20' 2.60(4) . . no
 H18 C8 3.10(2) . 1_465 no
 H18 H14 2.40(3) . . no

H18' C4 2.836(18) . 1_464 no
 H19 C3 2.901(18) . 1_464 no
 H19 H7 2.53(3) . 2_765 no
 H19 H14 2.48(3) . 2_675 no
 H20 C11 2.93(2) . . no
 H20 C12 2.912(19) . . no
 H20 C15 2.74(3) . . no
 H20 H20 2.50(4) . 2_665 no
 H20' H17' 2.60(4) . . no

loop_

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#

#D H A D - H H...A D...A D - H...A symm(A)

#

C2 H2 O 0.97(3) 2.58(3) 3.354(3) 137(2) 1_655 yes

C9 H9 O 0.96(3) 2.51(3) 3.026(3) 114(2) . yes

#===END of Crystallographic Information File