Supplementary Information for ***Acta Phys. -Chim. Sin.*****, 2009, 25(12): 2493-2500**

四苯基卟啉锌 J-聚集体的光谱与晶体结构分析

李　晔*　　韩伟伟　　廖明霞

(北京科技大学应用科学学院化学系，北京　100083)

Spectroscopic and Crystal Structural Analyses of Zinc (II) Tetraphenylporphyrin J-aggregates

LI Ye* HAN Wei-Wei LIAO Ming-Xia

(*Department of Chemistry, School of Applied Science, University of Science and Technology Beijing, Beijing 100083, P. R. China*)

*Corresponding author. Email: liye@sas.ustb.edu.cn; Tel: +86-10-62332689.

Table S1 Crystallographic experimental details and a summary of crystal data of ZnTPP in C_2H_5OH (A) and CH_3CN (B)

(A)

A. Crystal Data

formula	$C_{46}H_{31}N_5Zn$
formula weight	719.13
crystal dimensions (mm)	0.23 × 0.22 × 0.10
crystal system	monoclinic
space group	$P2_1/n$ (an alternate setting of $P2_1/c$ [No. 14])
unit cell parameters[a]	
a (Å)	10.0557 (6)
b (Å)	16.2590 (9)
c (Å)	21.2433 (13)
β (deg)	93.7280 (10)
V (Å^3)	3465.8 (4)
Z	4
ρ_{calcd} (g cm^{-3})	1.378
μ (mm^{-1})	0.751

B. Data Collection and Refinement Conditions

diffractometer	Bruker PLATFORM/SMART 1000 CCD[b]
radiation (λ [Å])	graphite-monochromated Mo Kα (0.71073)
temperature (°C)	–80
scan type	ω scans (0.2°) (25 s exposures)
data collection 2θ limit (deg)	52.76
total data collected	17054 (–12 ≤ h ≤ 12, –20 ≤ k ≤ 19, –26 ≤ l ≤ 13)
independent reflections	7102 (R_{int} = 0.0382)
number of observed reflections (*NO*)	5372 [$F_o^2 \geq 2\sigma(F_o^2)$]
structure solution method	Patterson search/structure expansion (*DIRDIF–99*[c])
refinement method	full-matrix least-squares on F^2 (*SHELXL–93*[d])
absorption correction method	multi-scan (*SADABS*)
range of transmission factors	0.9287–0.8462
data/restraints/parameters	7102 [$F_o^2 \geq -3\sigma(F_o^2)$] / 0 / 470
goodness-of-fit (S)[e]	1.016 [$F_o^2 \geq -3\sigma(F_o^2)$]
final R indices[f]	

$R1$ [$F_o^2 \geq 2\sigma(F_o^2)$]	0.0382
$wR2$ [$F_o^2 \geq -3\sigma(F_o^2)$]	0.0933
largest difference peak and hole	0.415 and –0.329 e Å^{-3}

[a]Obtained from least-squares refinement of 5819 reflections with 4.59° < 2θ < 52.50°.

[b]Programs for diffractometer operation, data collection, data reduction and absorption correction were those supplied by Bruker.

[c]Beurskens, P. T.; Beurskens, G.; de Gelder, R.; Garcia-Granda, S.; Israel, R.; Gould, R. O.; Smits, J. M. M. (1999). The *DIRDIF-99* program system. Crystallography Laboratory, University of Nijmegen, The Netherlands.

[d]Sheldrick, G. M. *SHELXL-93*. Program for crystal structure determination. University of Göttingen, Germany, 1993. Refinement on F_o^2 for all reflections (all of these having $F_o^2 \geq -3\sigma(F_o^2)$). Weighted *R*-factors $wR2$ and all goodnesses of fit *S* are based on F_o^2; conventional *R*-factors $R1$ are based on F_o, with F_o set to zero for negative F_o^2. The observed criterion of $F_o^2 > 2\sigma(F_o^2)$ is used only for calculating $R1$, and is not relevant to the choice of reflections for refinement. *R*-factors based on F_o^2 are statistically about twice as large as those based on F_o, and *R*-factors based on ALL data will be even larger.

[e]$S = [\Sigma w(F_o^2 - F_c^2)^2/(n-p)]^{1/2}$ (n = number of data; p = number of parameters varied; $w = [\sigma^2(F_o^2) + (0.0459P)^2 + 0.5314P]^{-1}$ where $P = [\mathrm{Max}(F_o^2, 0) + 2F_c^2]/3$).

[f]$R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^4)]^{1/2}$.

Table 2 (B)

A. Crystal Data

formula	$C_{45}H_{32}N_4OZn$
formula weight	710.12
crystal dimensions (mm)	0.26 × 0.13 × 0.11
crystal system	triclinic
space group	$P\bar{1}$ (No. 2)
unit cell parameters[a]	
a (Å)	9.6388 (11)
b (Å)	11.0200 (13)

c (Å)	17.894 (2)
α (deg)	99.597 (2)
β (deg)	105.290 (2)
γ (deg)	99.907 (2)
V (Å^3)	1760.5 (4)
Z	2
ρcalcd (g cm^{-3})	1.340
μ (mm^{-1})	0.739

B. Data Collection and Refinement Conditions

diffractometer	Bruker PLATFORM/SMART 1000 CCD[b]
radiation (λ [Å])	graphite-monochromated Mo Kα (0.71073)
temperature (°C)	–80
scan type	ω scans (0.3°) (25 s exposures)
data collection 2θ limit (deg)	52.80
total data collected	13667 (-12 ≤ h ≤ 12, -13 ≤ k ≤ 13, -22 ≤ l ≤ 22)
independent reflections	7162 (R_{int} = 0.0610)
number of observed reflections (*NO*)	4689 [$F_o^2 \geq 2\sigma(F_o^2)$]
structure solution method (*DIRDIF–99*[c])	Patterson search/structure expansion
refinement method (*SHELXL–93*[d])	full-matrix least-squares on F^2
absorption correction method	Gaussian integration (face-indexed)
range of transmission factors	0.9231–0.8310
data/restraints/parameters	7162 [$F_o^2 \geq -3\sigma(F_o^2)$] / 0 / 460
goodness-of-fit (S)[e]	1.005 [$F_o^2 \geq -3\sigma(F_o^2)$]
final R indices[f]	
$R1$ [$F_o^2 \geq 2\sigma(F_o^2)$]	0.0601
$wR2$ [$F_o^2 \geq -3\sigma(F_o^2)$]	0.1365
largest difference peak and hole	0.770 and –0.592 e Å^{-3}

[a]Obtained from least-squares refinement of 2820 reflections with 4.50° < 2θ < 46.62°.

[b]Programs for diffractometer operation, data collection, data reduction and absorption correction were those supplied by Bruker.

[c]Beurskens, P. T.; Beurskens, G.; de Gelder, R.; Garcia-Granda, S.; Israel, R.; Gould, R. O.; Smits, J. M. M. (1999). The *DIRDIF-99* program system. Crystallography Laboratory, University of Nijmegen, The Netherlands.

[d]Sheldrick, G. M. *SHELXL-93*. Program for crystal structure determination. University of Göttingen, Germany, 1993. Refinement on F_o^2 for all reflections (all of these having $F_o^2 \geq -3\sigma(F_o^2)$). Weighted R-factors $wR2$ and all

goodnesses of fit S are based on F_o^2; conventional R-factors R_1 are based on F_o, with F_o set to zero for negative F_o^2. The observed criterion of $F_o^2 > 2\sigma(F_o^2)$ is used only for calculating R_1, and is not relevant to the choice of reflections for refinement. R-factors based on F_o^2 are statistically about twice as large as those based on F_o, and R-factors based on ALL data will be even larger.

[e] $S = [\Sigma w(F_o^2 - F_c^2)^2/(n - p)]^{1/2}$ (n = number of data; p = number of parameters varied; $w = [\sigma^2(F_o^2) + (0.0609P)^2]^{-1}$ where $P = [\text{Max}(F_o^2, 0) + 2F_c^2]/3$).

[f] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^4)]^{1/2}$.