# A new type of solid-state luminescent 2-phenylbenzo[g]furo [2,3-B]quinoxaline derivatives: synthesis, photophysical characterization and transporting properties

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**Electronic Supplementary Information**

**Contents**

## Section 1: Computational details and Results of theoretical calculations

Singlet ground state ($S_0$) geometries of 3a were fully optimized by using M06 method of density functional theory (DFT). The standard 6-311G(d,p) basis set on non-metal atoms and the relativistic effective core potential (ECP) LANL2DZ on Ir atom were taken in our calculations. The solvent effects were evaluated with the self-consistent reaction field (SCRF) based on the integral equation formalism of the polarizable continuum model (IEFPCM) in $CH_2Cl_2$ solvent (ε=8.93). The vertical excitation calculations in $CH_2Cl_2$ for the simulation of absorption spectra were used by the time-dependent (TD) DFT method. To gain the features of emission processes of the 3a compounds, the first triplet state ($T_1$) geometries were located by the M05-2x functional combined with the same basis set as mentioned above. The suitability of M05-2x functional for the emission spectra of a series of iridium compounds has been well-documented.[S1, S2] Based on $T_1$ optimized structures, the single-point energy calculations were conducted at their $S_0$ states. In this way, the positions of the first phosphorescence bands of all iridium compounds were estimated by the $S_0$-$T_1$ gap of electronic energies including solvent effects. All calculations were carried out with the Gaussian 09 program package.[S3]

## Section 2: Supplementary Tables

**Table S1.** The photophysical data for 5a in different states, including maximum emission wavelength (nm), fluorescence quantum yields $\Phi_F$, fluorescence lifetimes $\tau_F$, and rate constants for radiative $k_r$, calculated via $\Phi_F = k_r \bullet \tau_F$.

| | system | $\lambda_{em}$ /nm | $\Phi_F$/ % | $\tau_F$/ ns | $k_r$/ $ns^{-1}$ |
|---|---|---|---|---|---|
| solution | $CH_2Cl_2$ | 515 | 9.19 | 3.58 | 0.026 |
| | THF | 512 | 9.79 | 3.06 | 0.032 |
| | doped in PS film(1%) | 505 | 9.28 | 2.78 | 0.033 |
| Solid state | powders | 597 | 22.14 | 11.39 | 0.019 |
| | NPs in THF:$H_2O$ (1:1) | 545 | 19.73 | 10.37 | 0.019 |

**Table S2** The semiconductor character data of 3a, 3b deposited on different substrate.

| | Substrate | μ($cm^2 \cdot V^{-1} \cdot s^{-1}$) | $V_T$ (V) | $I_{on}/I_{off}$ |
|---|---|---|---|---|
| 3a | OTS | $5.7\times10^{-3}$ | -26 | $1.4\times10^{5}$ |
| | $SiO_2$ | $8.2\times10^{-5}$ | -33 | $1.5\times10^{3}$ |
| 3b | OTS | $1.1\times10^{-4}$ | -34 | $2.0\times10^{3}$ |
| | $SiO_2$ | $3.6\times10^{-5}$ | -44 | $2.5\times10^{2}$ |
| 5c | OTS | no mobility | -- | -- |

| | | | | |
|---|---|---|---|---|
| | $SiO_2$ | no mobility | -- | -- |

## Section 3: Supplementary Figures S1-6

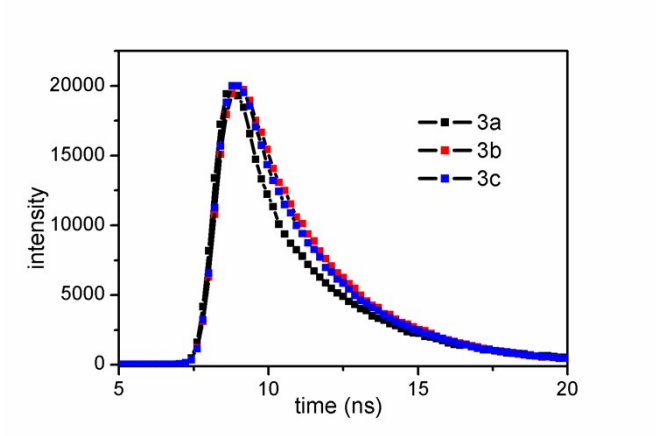



**Fig. S1** The fluorescence decay of 3a-3c in $CH_2Cl_2$ solution.

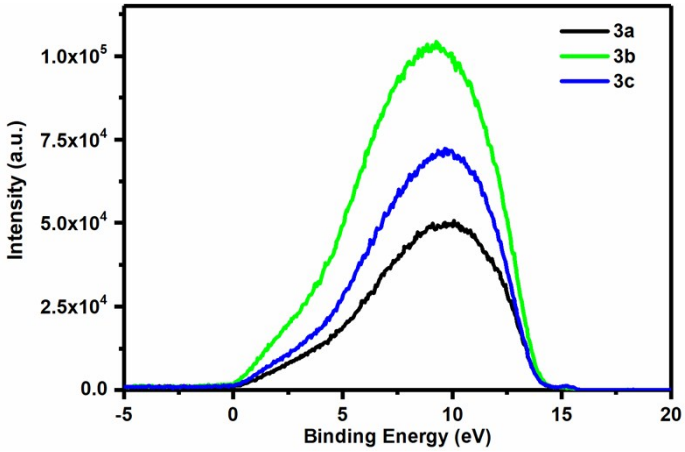



**Fig. S2** UPS energy distribution curves of 3a-3c.

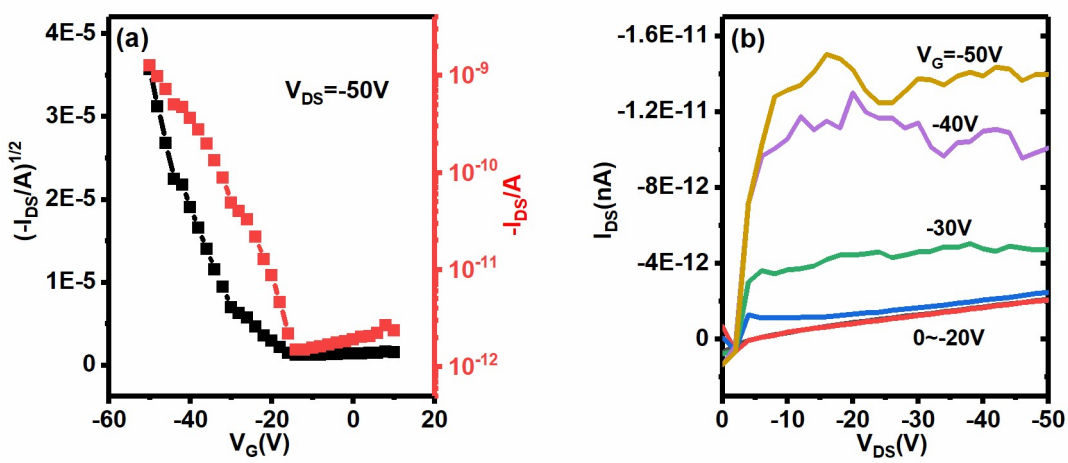



**Fig. S3** (a) Transfer and (b) output curves of the field-effect transistors with 5b thin film deposited on OTS/SiO2/Si

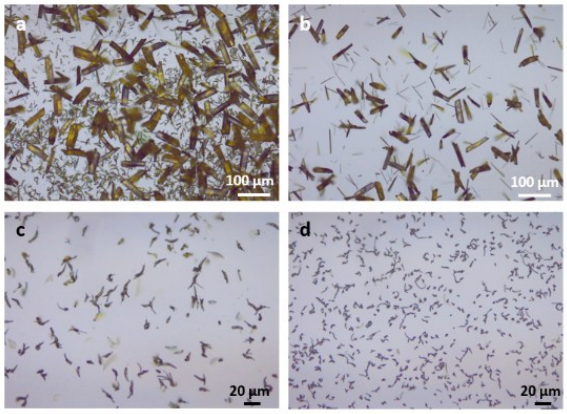



**Fig. S4** Optical micrographs of 3a crystals with PVD technology in different zone

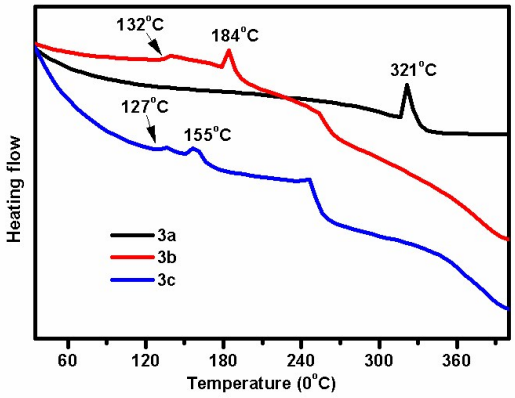



**Fig. S5** DSC curves of 3a-3c with the melting temperature and glass transition temperature indicated by arrows

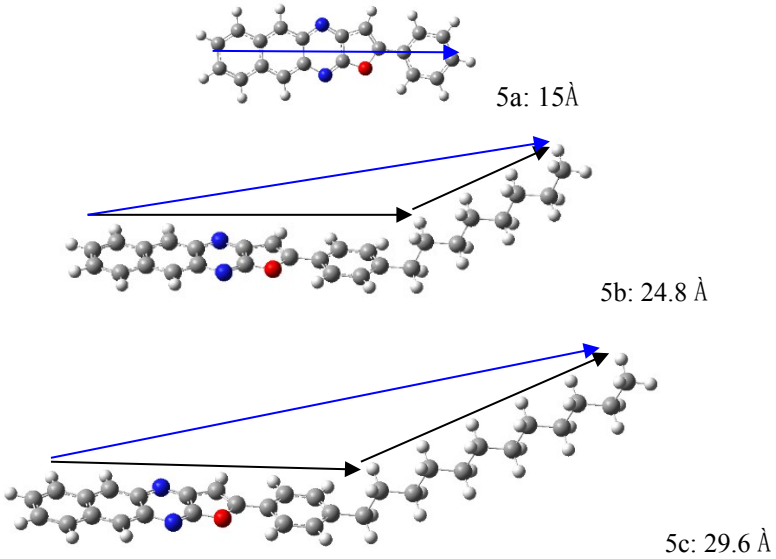
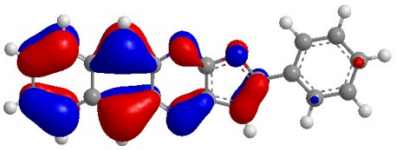
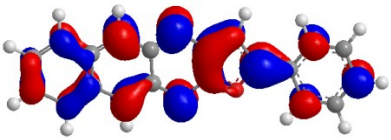



**Fig. S6** The calculated molecular length (blue line) of 5a-5c



**LUMO**

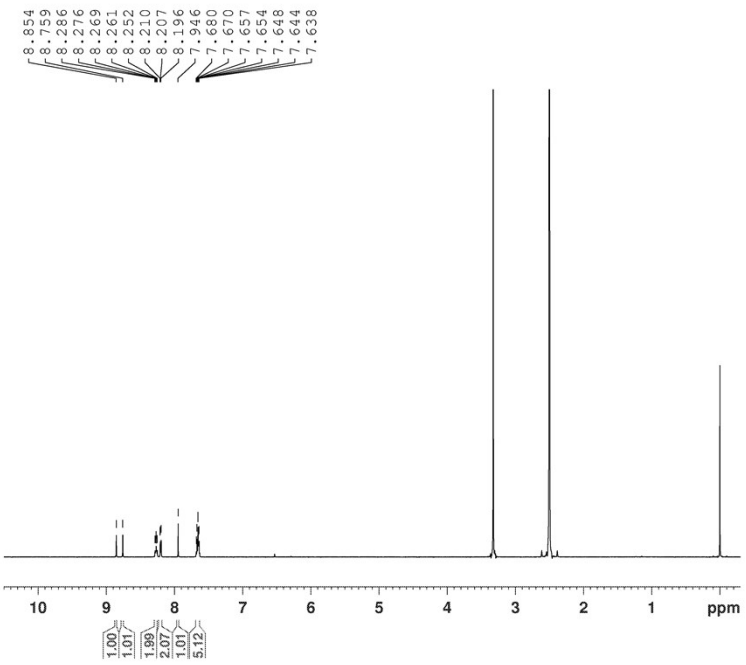


**HOMO**

twist angle: 0°

**Fig. S7** The calculated contours of the HOMOs and LUMOs orbitals of 3a with twist angle of 0° between the phenyl face and benzo [g] furo [2,3-B] quinoxaline

## Section 4: $^{1}H$ NMR and $^{13}C$ NMR spectra.

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RG                     11.16
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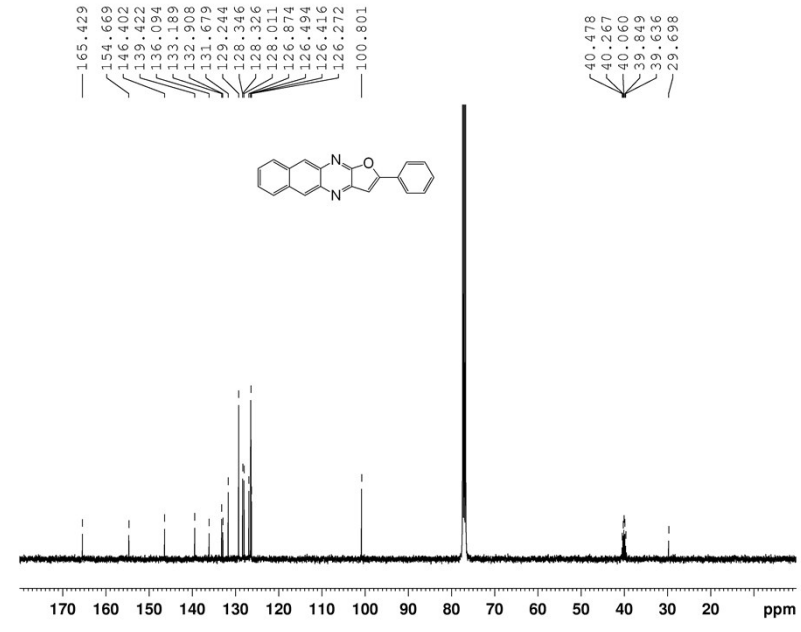


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RG                       203
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TE                    297.8 K
D1                 2.00000000 se
D11                0.03000000 se
TD0                        1

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NUC1                      13C
P1                     8.90 us
PL1                   -3.00 dB
PL1W              66.65790558 W
SFO1             100.6228298 MH

======== CHANNEL f2 ======
CPDPRG2               waltz16
NUC2                      1H
PCPD2                 80.00 us
PL2                   -3.00 dB
PL12                  12.20 dB
PL13                  13.00 dB
PL2W              17.09048462 W
PL12W              0.51612443 W
PL13W              0.42929357 W
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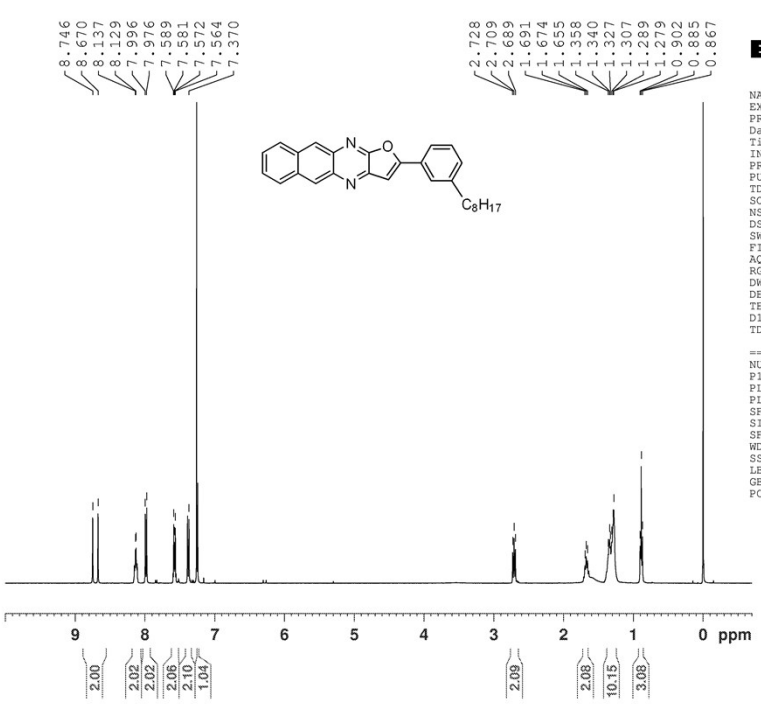


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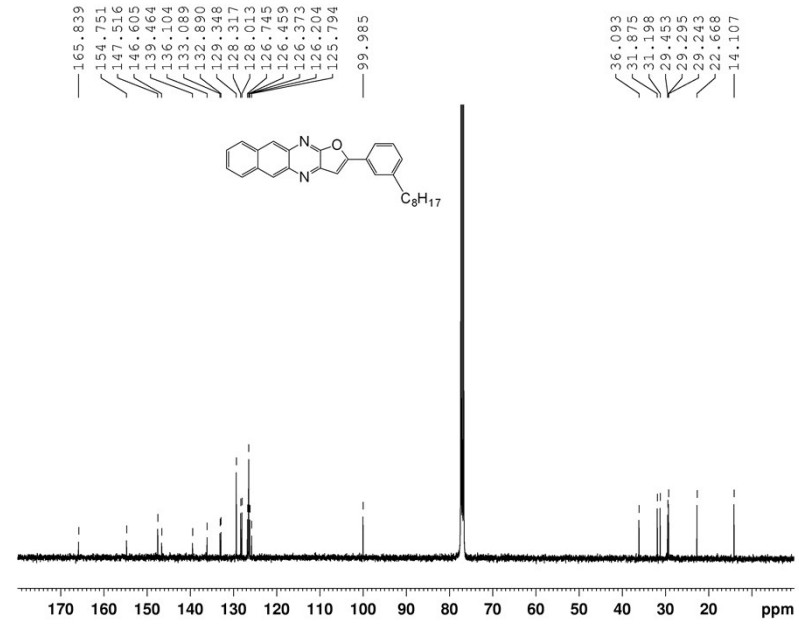


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D1                    2.00000000 se
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P1                          8.90 us
PL1                        -3.00 dB
PL1W                66.65790558 W
SFO1                100.6228298 MH

======== CHANNEL f2 ========
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NUC2                           1H
PCPD2                      80.00 us
PL2                        -3.00 dB
PL12                       12.20 dB
PL13                       13.00 dB
PL2W                17.09048462 W
PL12W                0.51612443 W
PL13W                0.42929357 W
SFO2                400.1316005 MH
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SF                  100.6127690 MH
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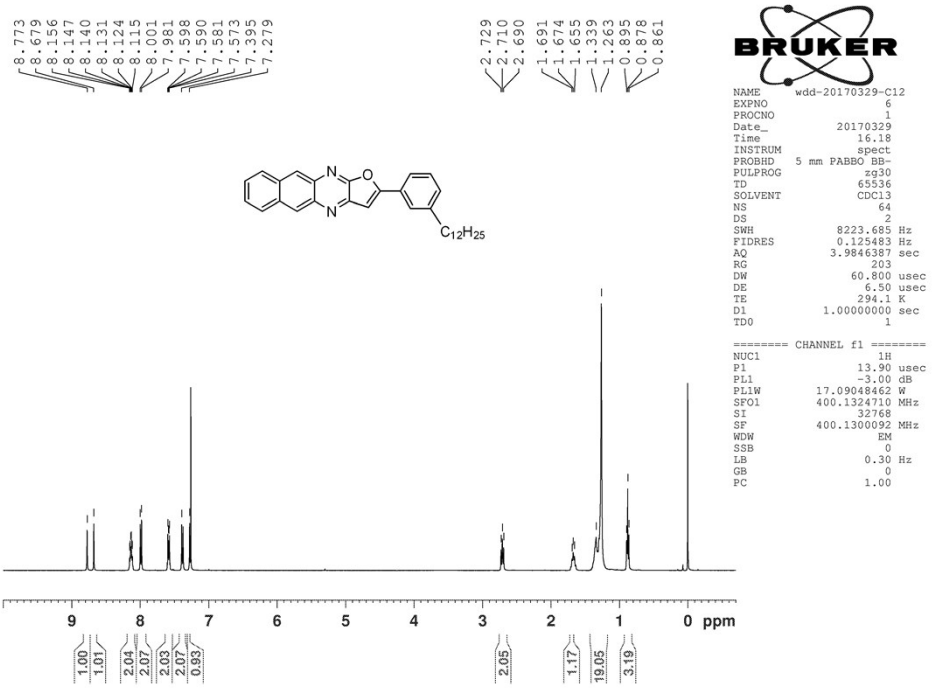


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TE                    294.1 K
D1                 1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
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P1                      13.90 usec
PL1                     -3.00 dB
PL1W               17.09048462 W
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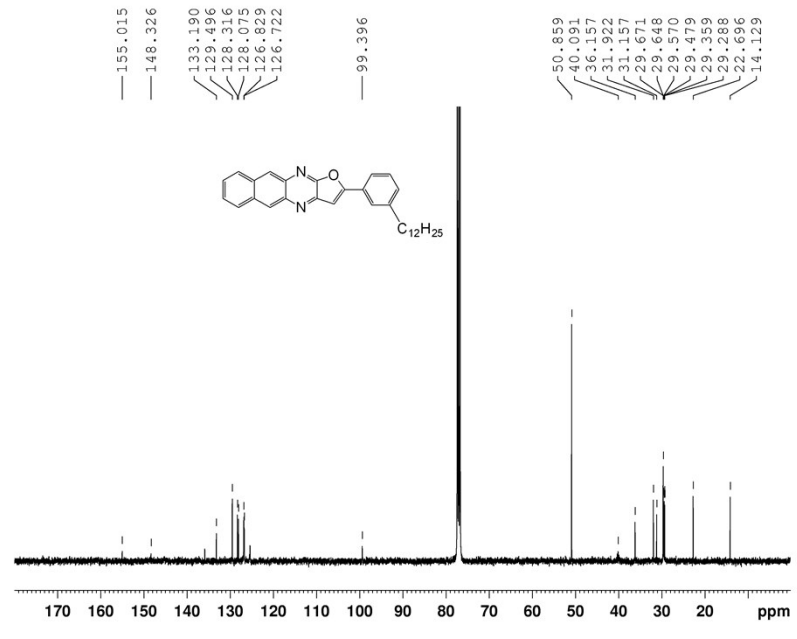


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SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631988 se
RG                       203
DW                    20.800 us
DE                     6.50 us
TE                    2961.0 K
D1                 2.00000000 se
D11                0.03000000 se
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======== CHANNEL f1 ========
NUC1                      13C
P1                      8.90 us
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CPDPRG2                waltz16
NUC2                       1H
PCPD2                  80.00 us
PL2                     -3.00 dB
PL12                    12.20 dB
PL13                    13.00 dB
PL2W               17.09048462 W
PL12W               0.51612443 W
PL13W               0.42929357 W
SFO2               400.1316005 MH
SI                       32768
SF                 100.6127690 MH
WDW                        EM
SSB                         0
LB                       1.00 Hz
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**REFERENCE**

(S1) K. Swiderek, P. Paneth, *J. Phys. Org. Chem.*, 2009, **22**, 845.

(S2) E. Baranoff, B. F. E. Curchod, F. Monti, et al. *Inorg. Chem.* 2012, **51**, 799.

(S3) Gaussian 09, Revision **B.02**, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.