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Electronic Supplementary Information

Simple aliphatic oximes as nonconventional luminogens with aggregation-induced emission characteristics

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Supporting Figures

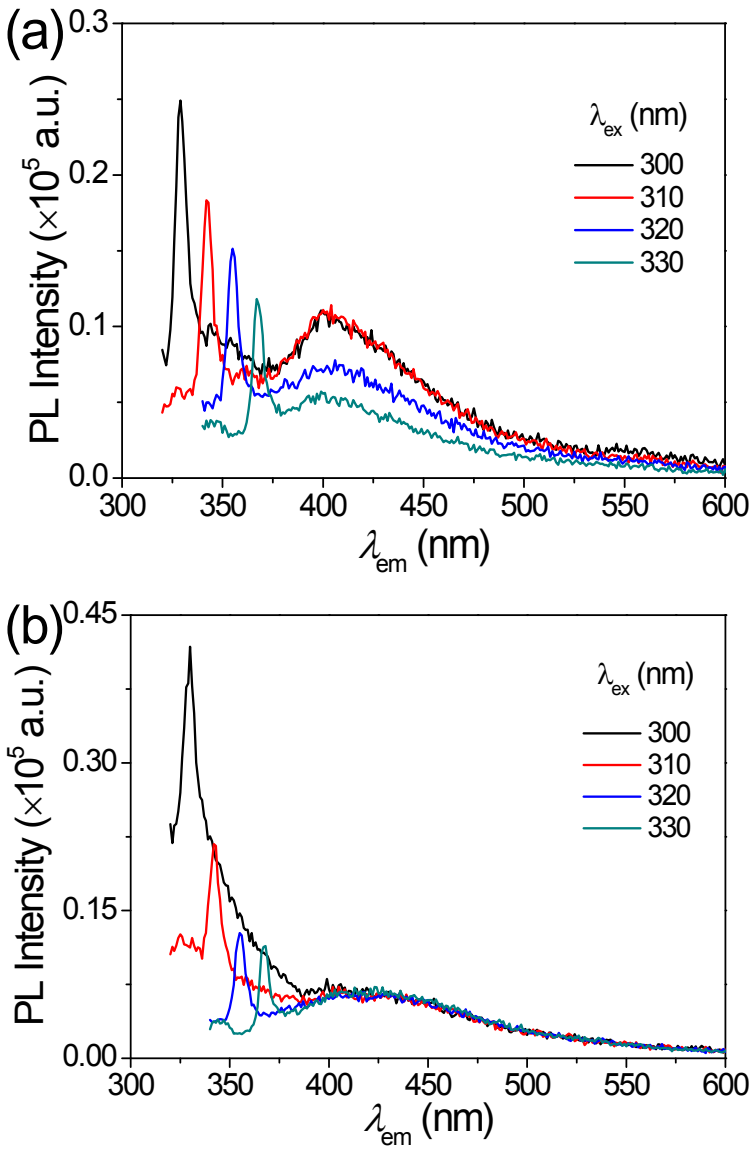

Fig. S1. Fluorescence emission spectra of HA (a) and EBA (b) in ethanol solutions (5 vol.%) under different excitation wavelengths.

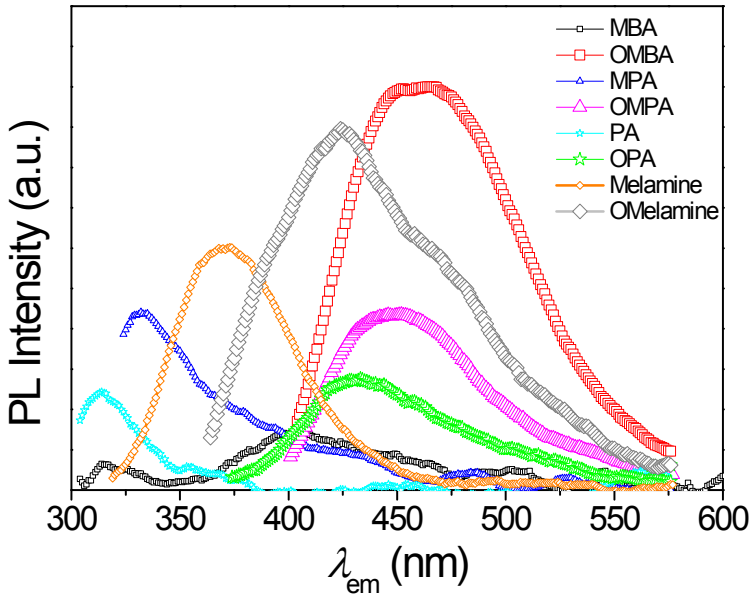

Fig. S2. Fluorescence emission spectra of the ethanol solutions of *N*-methylbutanamine (MBA) (0.3 mol L^{-1}), *N*-methylpentanamine (MPA) (0.7 mol L^{-1}) and propanamine (PA) (0.7 mol L^{-1}), melamine glycerol solution (0.1 mol L^{-1}) and their oxidized products.

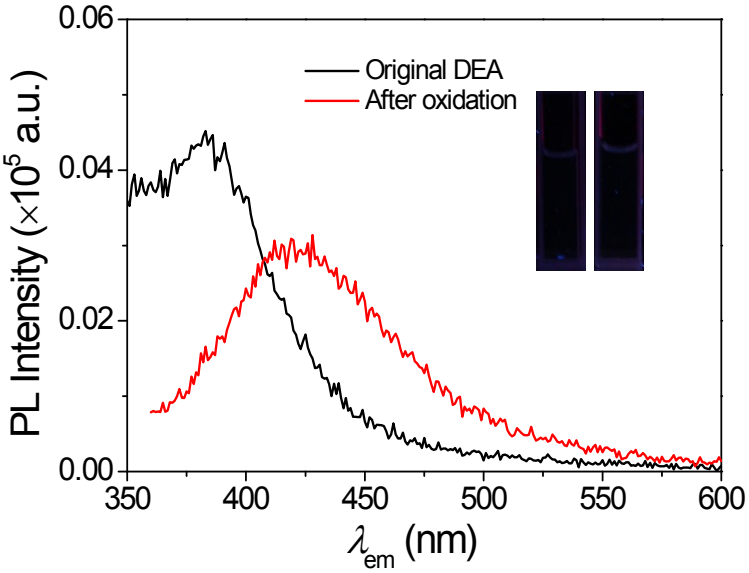

Fig. S3. Fluorescence emission spectra of *N*, *N*-diethylethanamine (DEA) and its product after reaction with H_2O_2. The insets show the photographs of the solutions of DEA before (left) and after the reaction (right) under UV light.

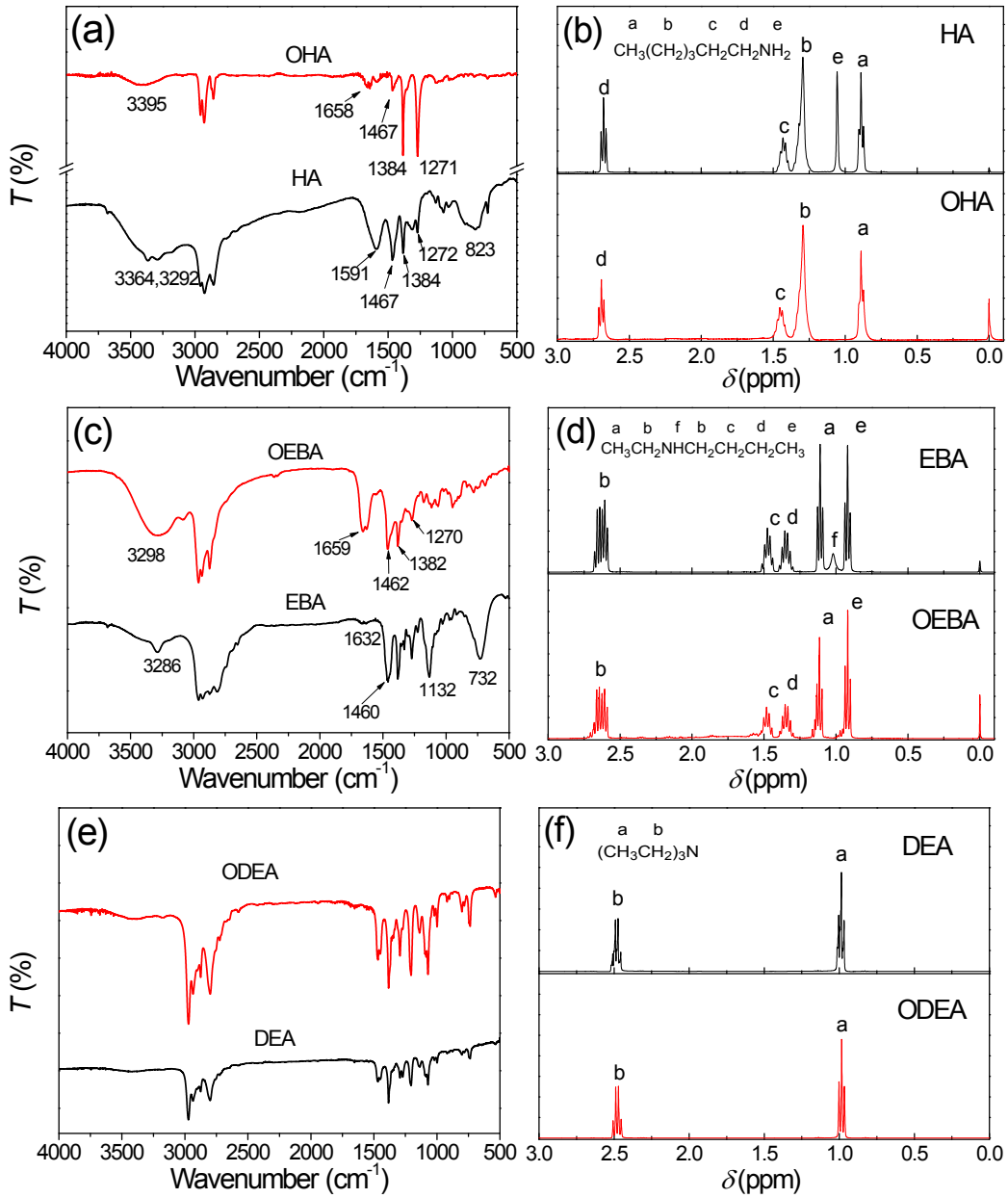

Fig. S4. FTIR spectra (a, c, e) and ^{1}H NMR spectra (b, d, f) of HA, EBA and DEA as well as their products after reaction with H_2O_2. OHA, OEBA and ODEA represent the products of HA, EBA and DEA, respectively.

The FTIR spectrum of HA shows the characteristic –NH_2 absorption bands at 3364, 3292, 1591 and 832 cm^{-1} (Fig. S4a), and that of EBA shows the –NH– absorption bands at 3286, 1632 and 732 cm^{-1} (Fig. S4c), respectively. These characteristic bands disappear in the spectra of the oxidized products (OHA and OEBA). Absorption bands of –OH group are found at 3395 and 3298 cm^{-1} for OHA and OEBA, respectively (Fig. S4a, c). Fig. 4b and 4d show that the chemical shifts corresponding to the H in –NH_2 or –NH– appear at 1.03 ppm in the ^{1}HNMR spectra of both HA and EBA, but they disappear in the spectra of OHA and OEBA. While for the tertiary amine DEA, no obvious changes are found in the FTIR and ^{1}HNMR spectra of the oxidized product (ODEA) with comparison to those of the original DEA (Fig. S4e, f).

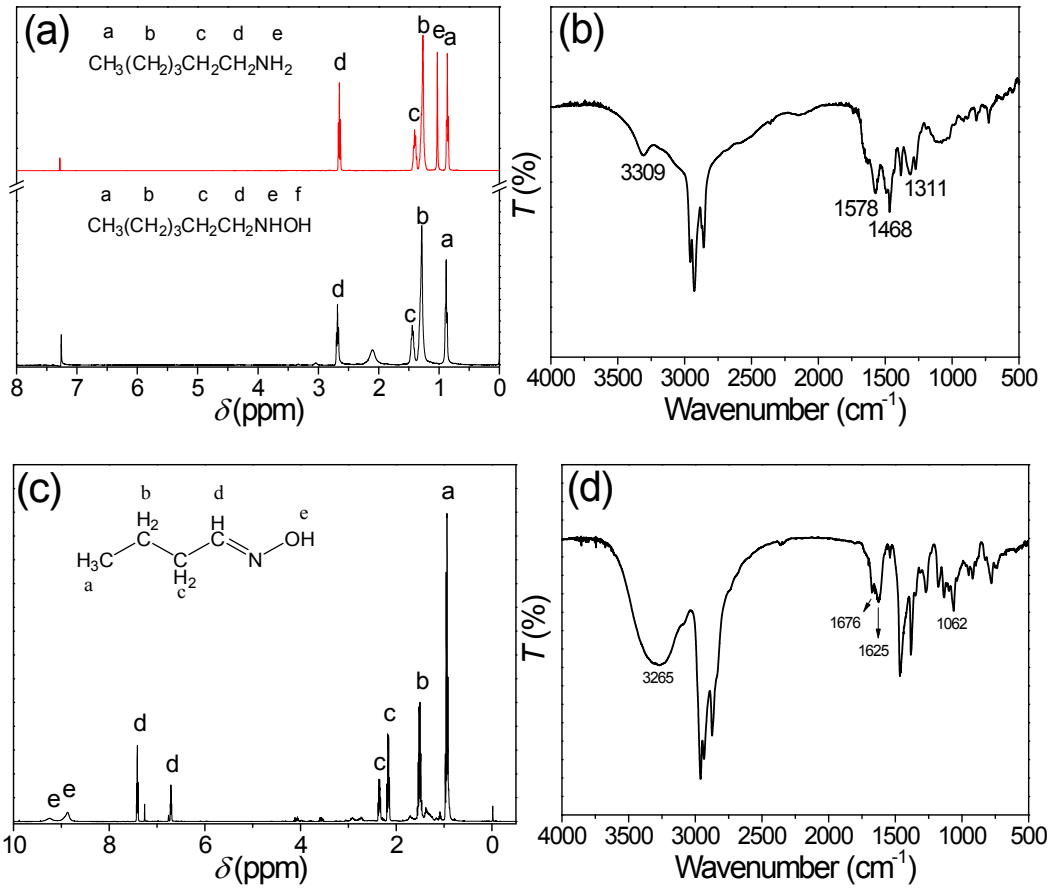

Fig. S5. ^{1}HNMR spectra and FTIR spectra of *N*-hexylhydroxylamine (a, b) and butanal oxime (c, d).

Chemical shifts of the H atoms in HA and *N*-hexylhydroxylamine are as follows: ^{1}HNMR (400MHz, TMS, $CDCl_3$): HA: δ 0.82-0.85 (3H, t), 1.01 (2H, s), 1.24-1.30 (6H, m), 1.35-1.40 (2H, m), 2.61-2.65 (2H, t); *N*-hexylhydroxylamine: 0.87-0.88 (3H, t), 1.29 (6H, m), 1.43-1.44 (2H, m), 2.67-2.70 (2H, t).

The ^{1}HNMR and FTIR spectra of butanal oxime are shown in Figure S5c,d. ^{1}HNMR (400MHz, TMS, $CDCl_3$): δ 8.87 and 9.25 (1H, s), 7.41 and 6.71 (1H, t), 2.36 and 2.17 (2H, q), 1.50-1.56 (2H, m), 0.92-0.97 (3H, m). FTIR spectrum shows the characteristic –OH absorption band at 3265 cm^{-1} and the C=N absorption band at 1676 cm^{-1} (Figure S5d).

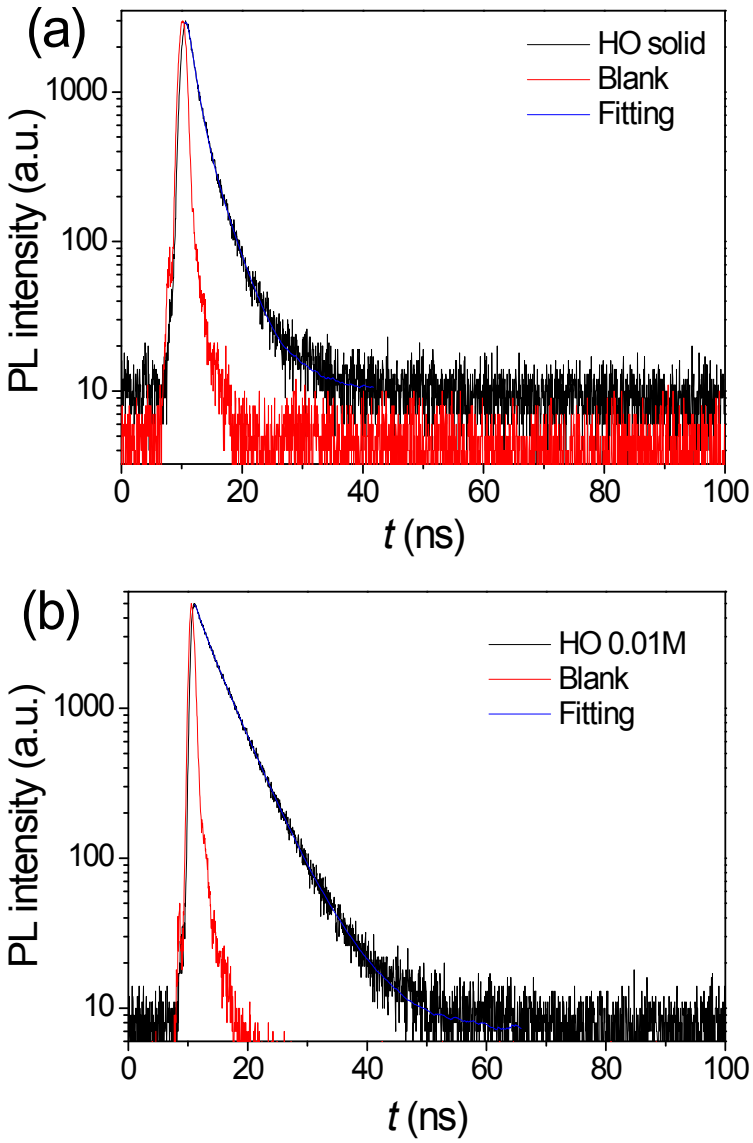

Fig. S6. Fluorescence lifetime measurements of hexanal oxime in both solid state and in an ethanol solution (0.01 M).

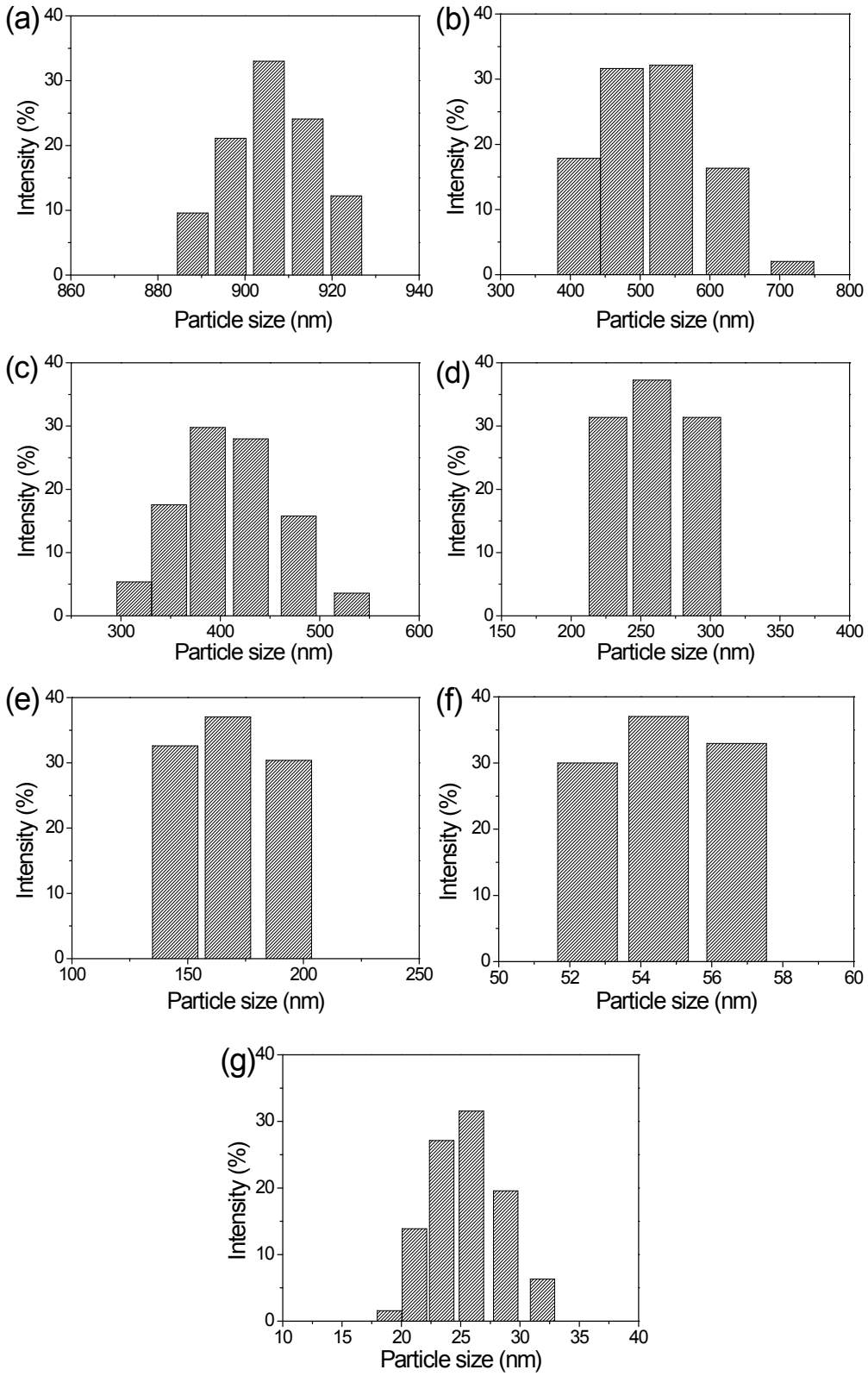

Fig. S7. Particle size distributions of hexanal oxime in ethanol solutions with the hexanal oxime concentration of 0.02 M (a), 0.01 M (b), 5×10^{-3} M (c), 2.5×10^{-3} M (d), 1.25×10^{-3} M (e), 1.25×10^{-4} M (f) and 1.25×10^{-5} M (g).

Table S1. Crystallographic data of hexanal oxime single crystals.

Formula	$C_6H_{13}NO$	***V*(Å^3)**	708.14
Formula weight	115.17	***Z***	4
Radiation	Cu *Kα*	**ρ_{calc} g/cm^3**	1.080
Crystal system	Monoclinic	**Absorption coefficient (mm^{-1})**	0.579
Space group	$P2_1/c$	***F* (0 0 0)**	256.0
***a*(Å)**	5.55642(18)	**Goodness-of-fit**	1.061
***b*(Å)**	4.79489(14)	**R_1, R_w**	0.0357, 0.0962
***c*(Å)**	26.6236(9)	**Temperature(K)**	100.00
α(°)	90	**CCDC**	1533695
β(°)	93.307(3)		
γ(°)	90		