Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information for

Theoretical perspective for luminescent mechanism of thermally activated delayed fluorescence emitter with excited-state intramolecular proton transfer

Guanyu Jiang, Feiyan Li, Jianzhong Fan, Yuzhi Song, Chuan-Kui Wang*, Lili Lin*

Shandong Key Laboratory of Medical Physics and Image Processing & Shandong Provincial Engineering and Technical Center of Light Manipulations, School of Physics and Electronics, Shandong Normal University, Jinan 250358, China

*Author to whom correspondence should be addressed.
E-mail: ckwang@sdnu.edu.cn and linll@sdnu.edu.cn

1. Independent gradient model (IGM) method

IGM method is convenient for visualization of the weak interaction. The δg function method of the subtraction between the initial molecular density gradient and the independent gradient density is adopted .The δg formula is written as

$$\delta g(r) = g^{IGM}(r) - g(r) \quad (1)$$

$$g(r) = \left| \sum_i \nabla \rho_i(r) \right| \quad (2)$$

$$g^{IGM}(r) = \left| \sum_i abs\left[\nabla \rho_i(r) \right] \right| \quad (3)$$

Where i is the atomic ordinal number, $\nabla\rho$ (r) is the gradient vector, $abs(\nabla\rho)$(r) represents every component of $\nabla\rho$ (r) vector takes absolute value.

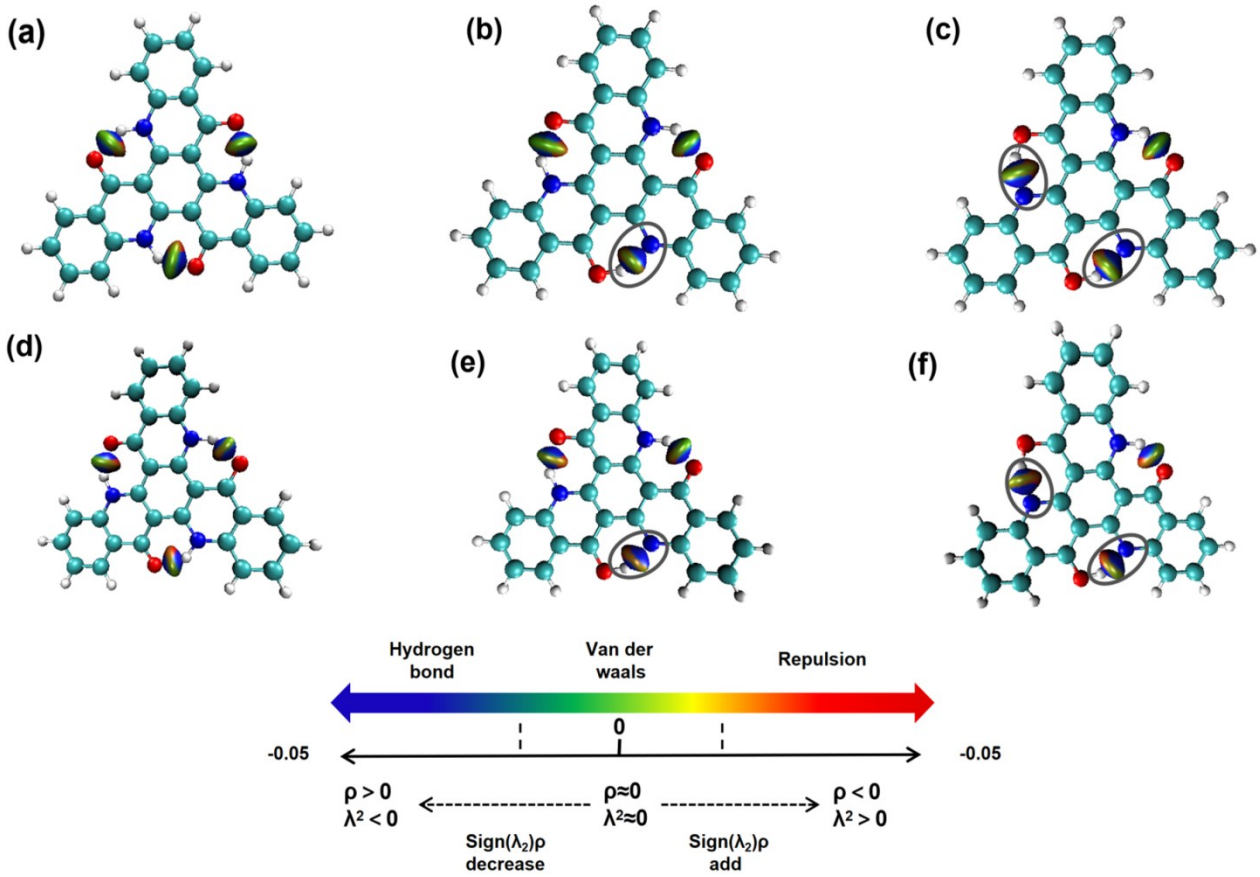
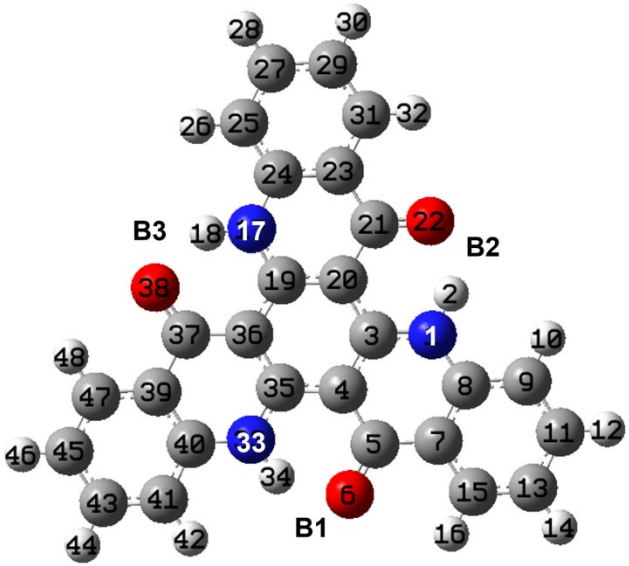


Figure S1 Visualization of intramolecular hydrogen bond of the molecule in S_1 state. ρ and λ2 represents the electron density and eigenvalue of the electron-density Hessian (second derivative) matrix, respectively. (a) TQB-TA, (b) TQB-TB and (c) TQB-TC in DMF; (d) TQB-TA, (e) TQB-TB and (f) TQB-TC in solid phase.



B1: 34-6	θ1: 33-34-6	α1: 33-34-6-5
B2: 22-2	θ2: 38-18-17	α2: 38-18-17-19
B3: 38-18	θ3: 22-2-1	α3: 1-2-22-21

Figure S2 Atomic labels of TQB.

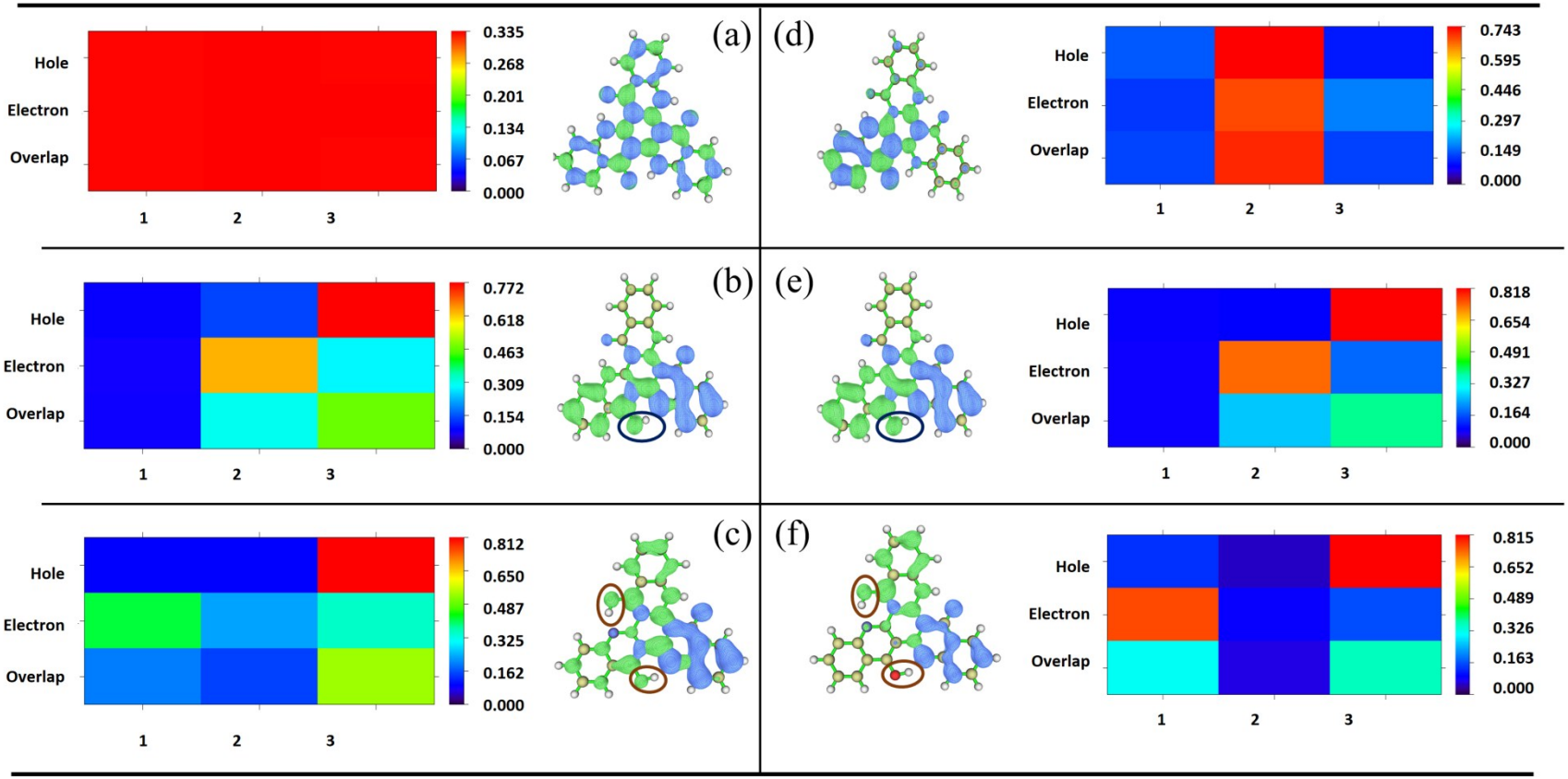


Figure S3. Isosurface of hole and electron distribution and heat map of molecules at T_1 state. (a) TQB-TA, (b) TQB-TB and (c) TQB-TC in DMF; (d) TQB-TA, (e) TQB-TB and (f) TQB-TC in solid phase.

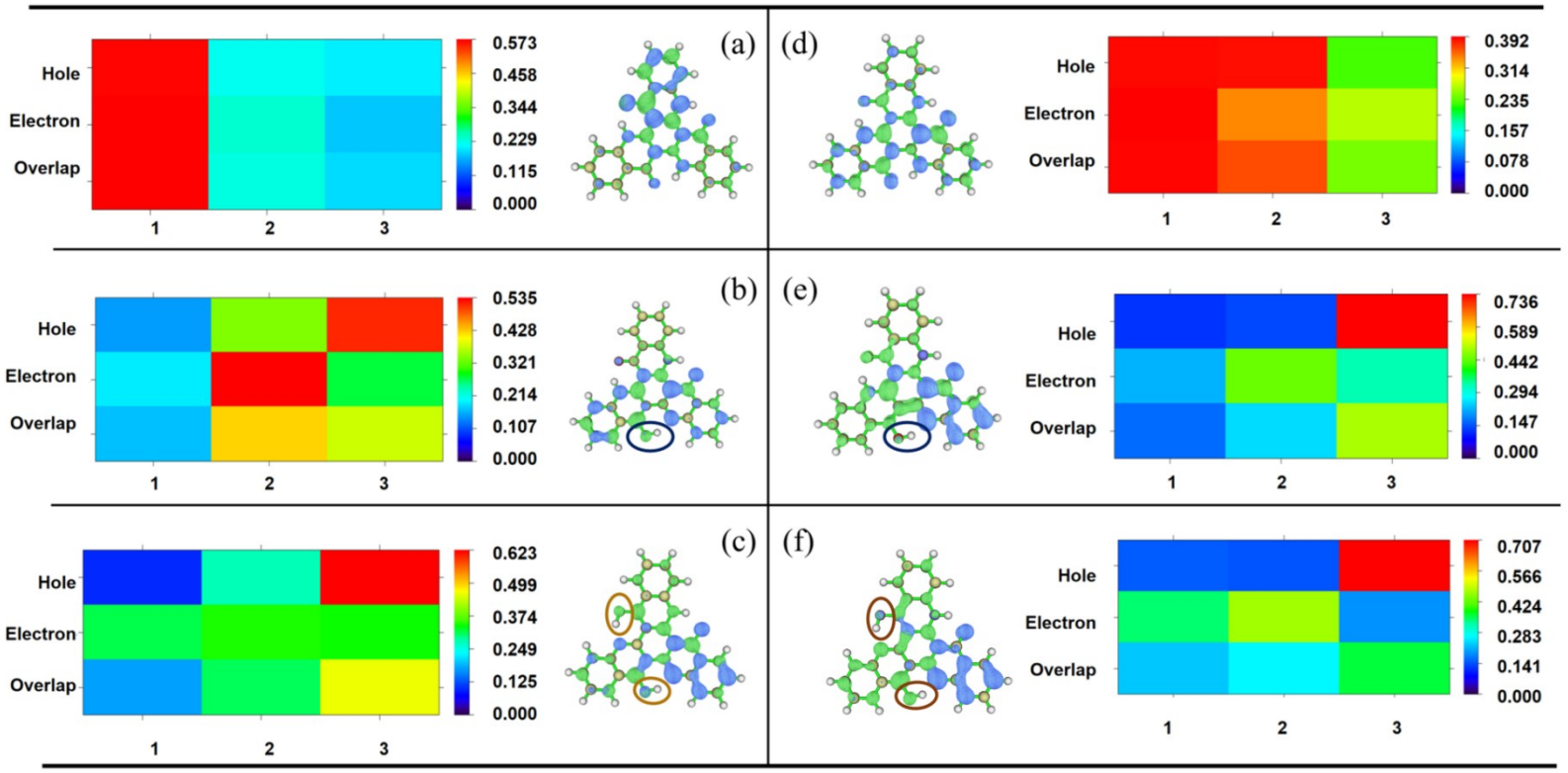


Figure S4. Isosurface of hole and electron distribution and heat map of molecules at T_2 state. (a) TQB-TA, (b) TQB-TB and (c) TQB-TC in DMF; (d) TQB-TA, (e) TQB-TB and (f) TQB-TC in solid phase.

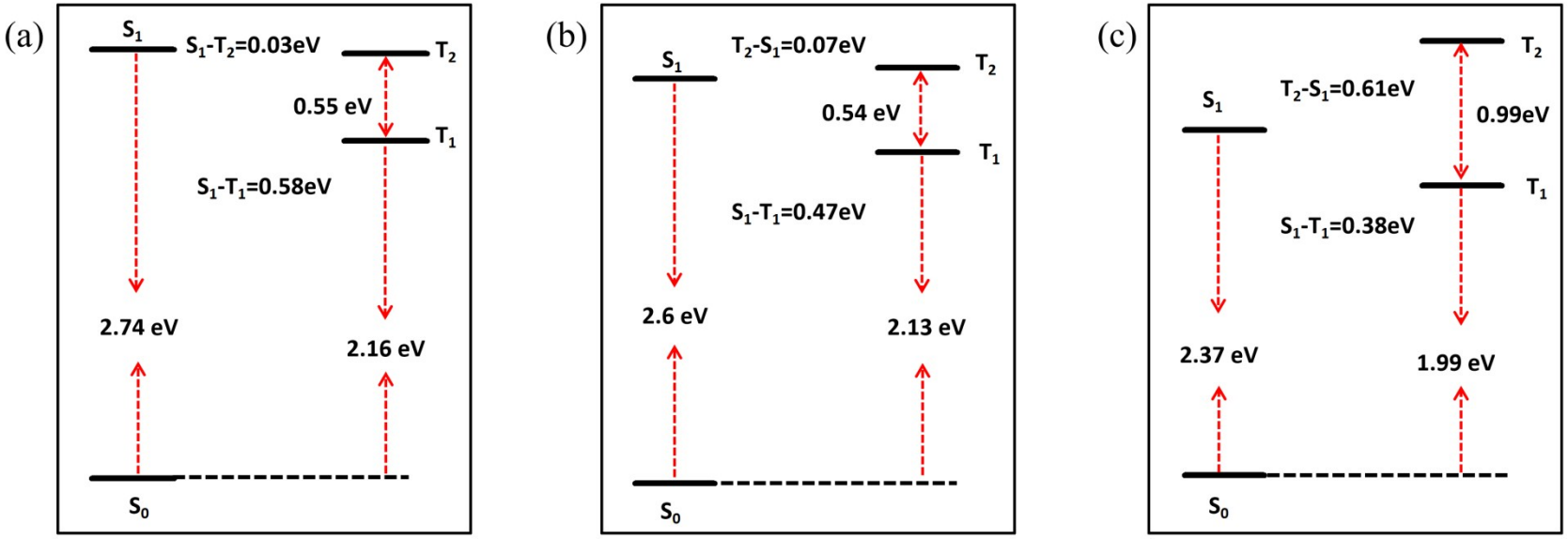


Figure S5. Excitation energies for TQB**-TA (a), TQB**-TB (b) and TQB*-TA (c) in toluene.

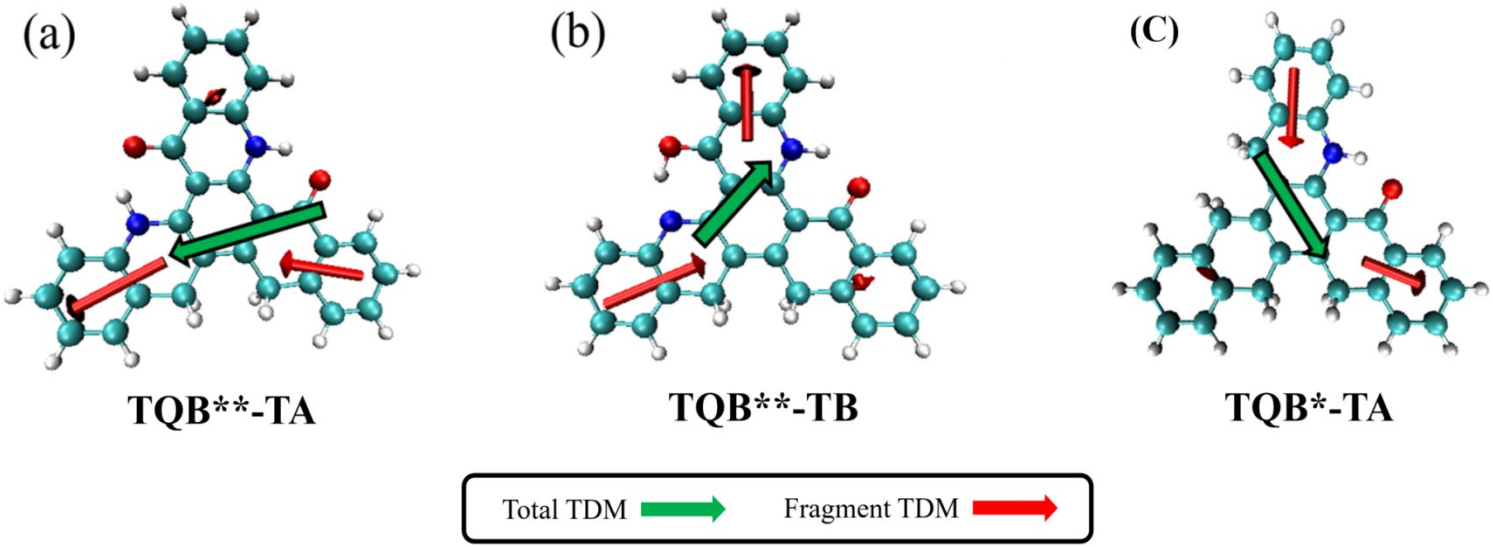


Figure S6. Transition dipole moment (TDM): (a) TQB**-TA, (b) TQB**-TB and (c) TQB*-TA in toluene.

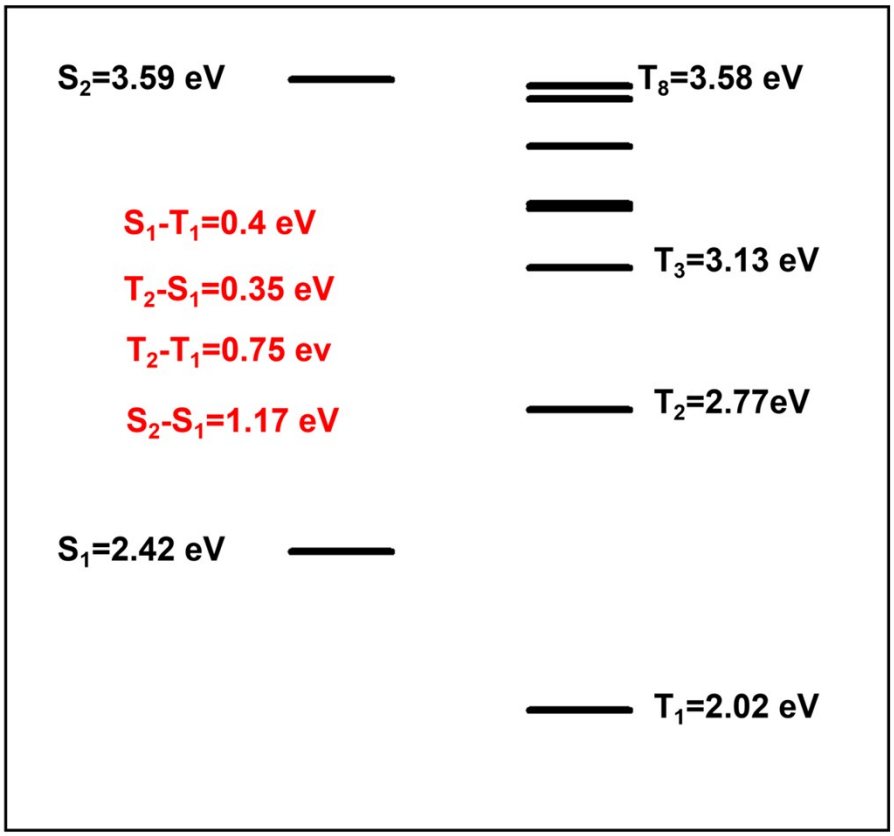


Figure S7. Vertical excitation energies for TQB*-TA in toluene

Table S1. Geometry parameters of S_1 states for TQB-TA, TQB-TB and TQB-TC in DMF and in solid phase. Bond lengths (B1, B2, B3), bond angles (θ1, θ2,θ3) and dihedral angles (α1, α2, α3) are marked in Fig. S2.

	DMF			**Solid**		
	TQB-TA	**TQB-TB**	**TQB-TC**	**TQB-TA**	**TQB-TB**	**TQB-TC**
B1	1.73	1.00	1.01	1.71	1.01	1.01
B2	1.73	1.77	1.80	1.73	1.76	1.79
B3	1.73	1.79	1.01	1.71	1.75	1.01
θ1	139.85	147.81	150.23	139.91	146.49	150.72
θ2	139.76	135.58	137.72	140.07	138.29	137.98
θ3	139.79	137.52	148.51	139.85	138.02	149.16
α1	-0.01	-0.03	0	4.64	1.69	2.64
α2	0.02	0	0	-0.04	2.73	-12.98
α3	0	-0.01	0	0.43	1.48	-0.12