Electronic Supplementary Information (ESI)

Tuning the color of thermally activated delayed fluorescent properties for spiro-acridine derivatives by structural modification on the acceptor fragment: A DFT study

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Contents

1. Computational method

At the first step, we optimized **ACRFLCN** structure with PBE0 functional in the description of charge-transfer transition. At the second step, the vibrational frequency calculations were performed to verify the optimized structure to be a true minimum on the potential energy surface at the same theoretical level. At the third step, the delayed emission wavelength (λ_{TADF}) was calculated by TD-DFT methods. On the basis of the optimized S_1 structure using TD-PBE0/6-31G (d) level, we have chosen different functionals for the computations of λ_{TADF}. The calculated λ_{TADF} data of ACRFLCN together with the experimental data (530 nm) are shown in Fig. 2. The λ_{TADF} calculated by the PBE0 functional (540 nm) is the most accurate among all the functionals.

2. Supplementary tables and figures

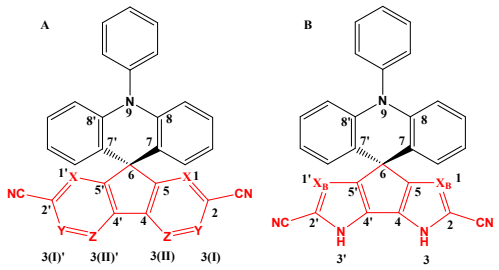


Table S1a Selected bond lengths (Å), bond angles (°), and dihedral angle (°) at optimized S_0, S_1 and T_1 geometries for the **ACRFLCN** and mono-substituted of "CH"/N derivative.

	ACRFLCN			**1a**			**1b**			**1c**		
	S_0	S_1	T_1	S_0	S_1	T_1	S_0	S_1	T_1	S_0	S_1	T_1
R(6,5)	1.529	1.539	1.532	1.526	1.536	1.537	1.529	1.547	1.547	1.532	1.561	1.562
R(6,5′)	1.529	1.539	1.532	1.532	1.541	1.541	1.527	1.530	1.530	1.519	1.519	1.518
R(6,7)	1.524	1.509	1.521	1.524	1.509	1.508	1.524	1.510	1.509	1.523	1.507	1.506
R(6,7′)	1.524	1.509	1.521	1.524	1.509	1.508	1.524	1.510	1.509	1.523	1.507	1.506
R(5,1)	1.382	1.366	1.361	1.379	1.363	1.363	1.382	1.363	1.363	1.317	1.295	1.295
R(5′,1′)	1.382	1.366	1.361	1.383	1.367	1.367	1.382	1.369	1.369	1.384	1.370	1.370
R(5,4)	1.404	1.426	1.445	1.404	1.425	1.425	1.400	1.423	1.424	1.408	1.416	1.416
R(5′,4′)	1.404	1.426	1.445	1.401	1.422	1.422	1.405	1.428	1.427	1.406	1.427	1.427
R[4,3(II)]	1.395	1.418	1.439	1.333	1.361	1.361	1.395	1.420	1.420	1.389	1.422	1.423
R[4′,3(II)′)	1.395	1.418	1.439	1.393	1.415	1.415	1.395	1.416	1.416	1.395	1.413	1.413
R[3(II),3(I)]	1.388	1.377	1.365	1.329	1.318	1.318	1.328	1.314	1.313	1.391	1.377	1.377
R[3(II)′,3(I)′]	1.388	1.377	1.365	1.387	1.378	1.378	1.388	1.378	1.378	1.387	1.380	1.380
R[3(I),2]	1.405	1.418	1.441	1.407	1.416	1.416	1.341	1.359	1.361	1.399	1.415	1.415
R(3(I)′,2′)	1.405	1.418	1.441	1.407	1.417	1.418	1.405	1.417	1.417	1.405	1.413	1.413
R(2,1)	1.403	1.425	1.432	1.404	1.431	1.431	1.401	1.423	1.421	1.343	1.377	1.378
R(2′,1′)	1.403	1.425	1.432	1.403	1.423	1.422	1.403	1.422	1.421	1.403	1.421	1.421
α(5,6,5′)	100.4	101.6	100.5	100.3	101.5	101.4	100.4	101.4	101.3	100.4	101.2	101.2
α(7,6,7′)	112.0	112.5	112.0	112.0	112.6	112.6	111.8	111.9	111.9	110.7	111.0	111.1
γ(8,9 6,5')	90.0	90.0	90.0	90.1	89.9	89.9	94.3	95.3	95.4	100.3	99.6	99.7

Table S1b Selected bond lengths (Å), bond angles (°), and dihedral angle (°) at optimized S_0, S_1 and T_1 geometries for the di-substituted of "CH"/N derivative.

	2a			**2b**			**2c**			**2d**			**2e**		
	S_0	S_1	T_1	S_0	S_1	T_1	S_0	S_1	T_1	S_0	S_1	T_1	S_0	S_1	T_1
R(6,5)	1.526	1.536	1.536	1.528	1.539	1.540	1.528	1.541	1.541	1.530	1.533	1.531	1.529	1.533	1.530
R(6,5′)	1.526	1.536	1.536	1.528	1.539	1.540	1.528	1.541	1.541	1.530	1.533	1.531	1.529	1.533	1.530
R(6,7)	1.524	1.509	1.509	1.523	1.510	1.510	1.520	1.504	1.504	1.524	1.511	1.522	1.522	1.508	1.517
R(6,7′)	1.524	1.509	1.509	1.523	1.510	1.510	1.520	1.504	1.504	1.524	1.511	1.522	1.522	1.508	1.517
R(5,1)	1.381	1.363	1.363	1.382	1.365	1.366	1.318	1.299	1.299	1.400	1.382	1.362	1.344	1.321	1.301
R(5′,1′)	1.381	1.363	1.363	1.382	1.365	1.366	1.318	1.299	1.299	1.400	1.382	1.362	1.344	1.321	1.301
R(5,4)	1.403	1.424	1.424	1.401	1.425	1.426	1.410	1.422	1.422	1.392	1.417	1.455	1.390	1.408	1.460
R(5′,4′)	1.403	1.424	1.424	1.401	1.425	1.426	1.410	1.422	1.422	1.392	1.417	1.455	1.390	1.408	1.460
R[4,3(II)]	1.332	1.358	1.358	1.396	1.419	1.419	1.390	1.418	1.418	1.352	1.368	1.381	1.355	1.369	1.376
R[4′,3(II)′)	1.332	1.358	1.358	1.396	1.419	1.419	1.390	1.418	1.418	1.352	1.368	1.381	1.355	1.369	1.376

R[3(II),3(I)]	1.327	1.318	1.318	1.328	1.315	1.315	1.390	1.380	1.380	-	-	-	-	-	-
R[3(II)′,3(I)′]	1.327	1.318	1.318	1.328	1.315	1.315	1.390	1.380	1.380	-	-	-	-	-	-
R[3(I),2]	1.409	1.415	1.415	1.341	1.357	1.358	1.401	1.411	1.411	1.388	1.415	1.404	1.383	1.415	1.411
R(3(I)′,2′)	1.409	1.415	1.415	1.341	1.357	1.358	1.401	1.411	1.411	1.388	1.415	1.404	1.383	1.415	1.411
R(2,1)	1.402	1.427	1.427	1.401	1.421	1.420	1.342	1.371	1.371	1.394	1.413	1.439	1.327	1.352	1.374
R(2′,1′)	1.402	1.427	1.427	1.401	1.421	1.420	1.342	1.371	1.371	1.394	1.413	1.439	1.327	1.352	1.374
α(5,6,5′)	100.2	101.3	101.3	100.2	101.1	101.0	100.1	101.0	101.0	98.9	100.3	98.7	97.4	98.6	97.4
α(7,6,7′)	112.1	112.6	112.6	112.2	112.5	112.5	112.6	113.2	113.2	112.0	112.4	112.1	112.5	112.9	112.8
γ(8,9 6,5’)	90.0	90.0	90.0	90.0	90.0	90.0	90.0	90.0	90.0	90.0	90.0	90.0	90.0	90.0	90.0

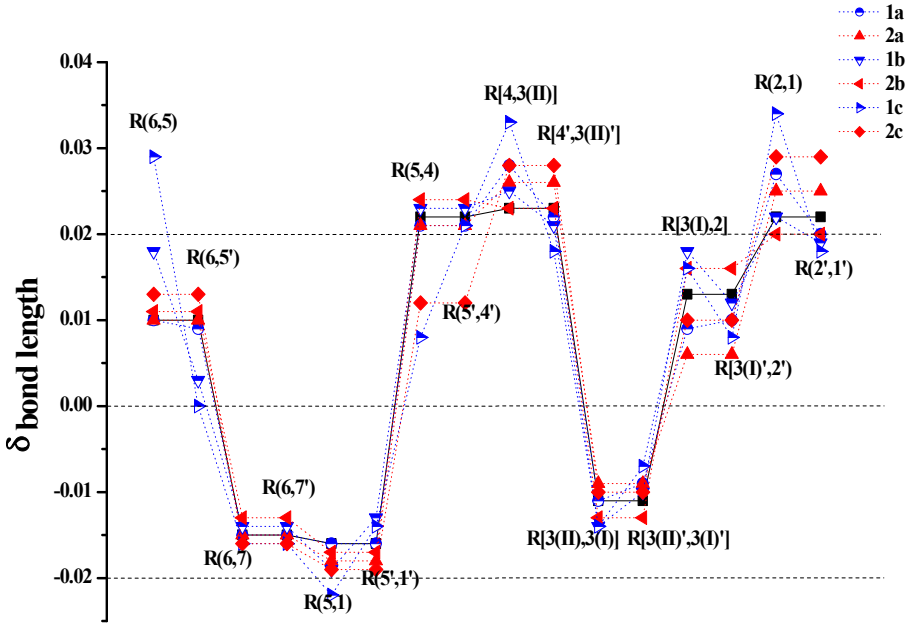


Fig. S1a The variations of calculated bond lengths at S_1 compared with S_0 for **a-c**.

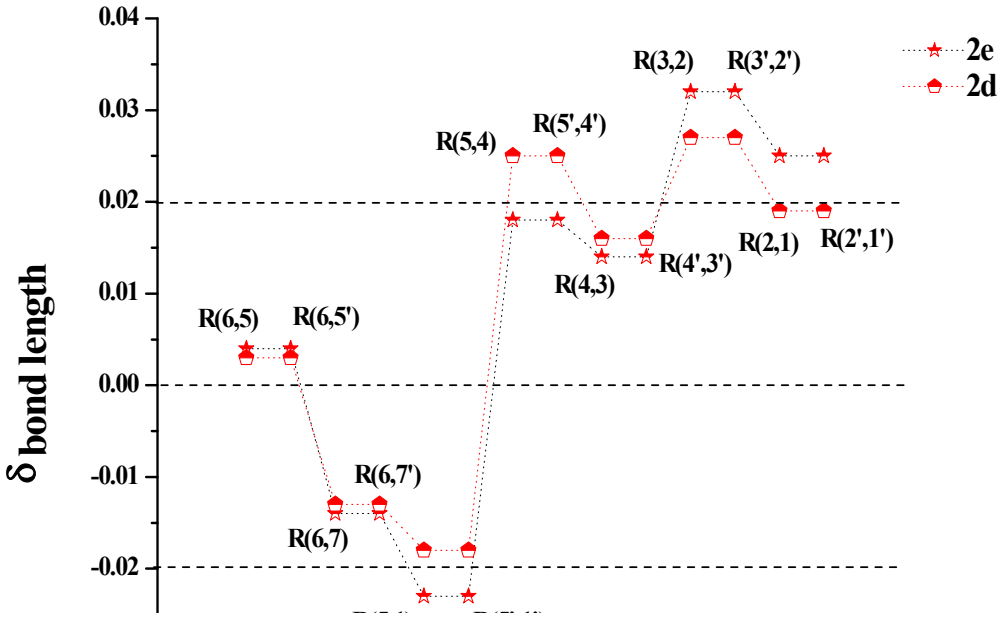
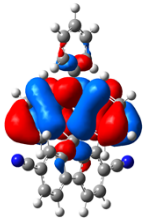
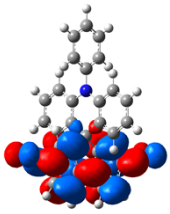


Fig. S1b The variations of calculated bond lengths at S_1 compared with S_0 for **2d** and **2e.**

ACRFLCN		
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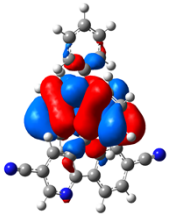
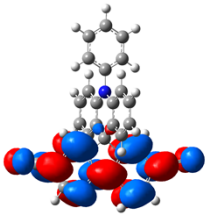
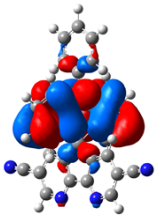
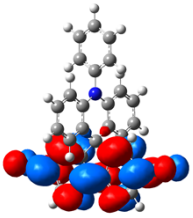
1a		
	96.1 : 3.9	1.0 : 99.0
2a		
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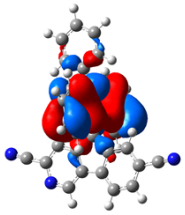
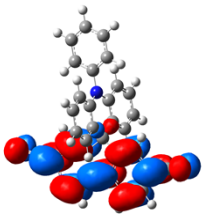
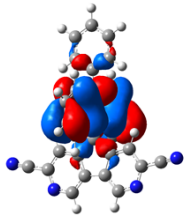
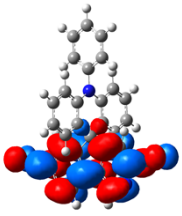
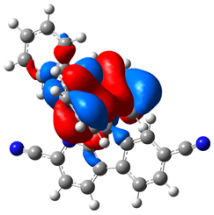
1b		
	96.5 : 3.5	1.5 : 98.5
2b		
	96.4 : 3.6	1.6 : 98.4
1c		
	96.8 : 3.2	1.3 : 98.7

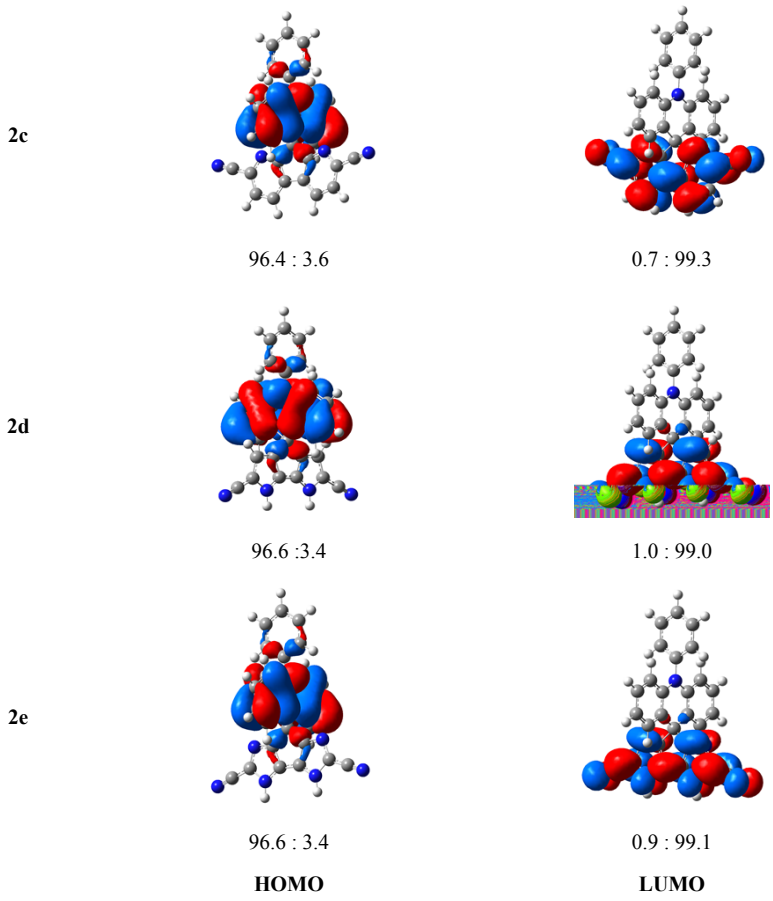
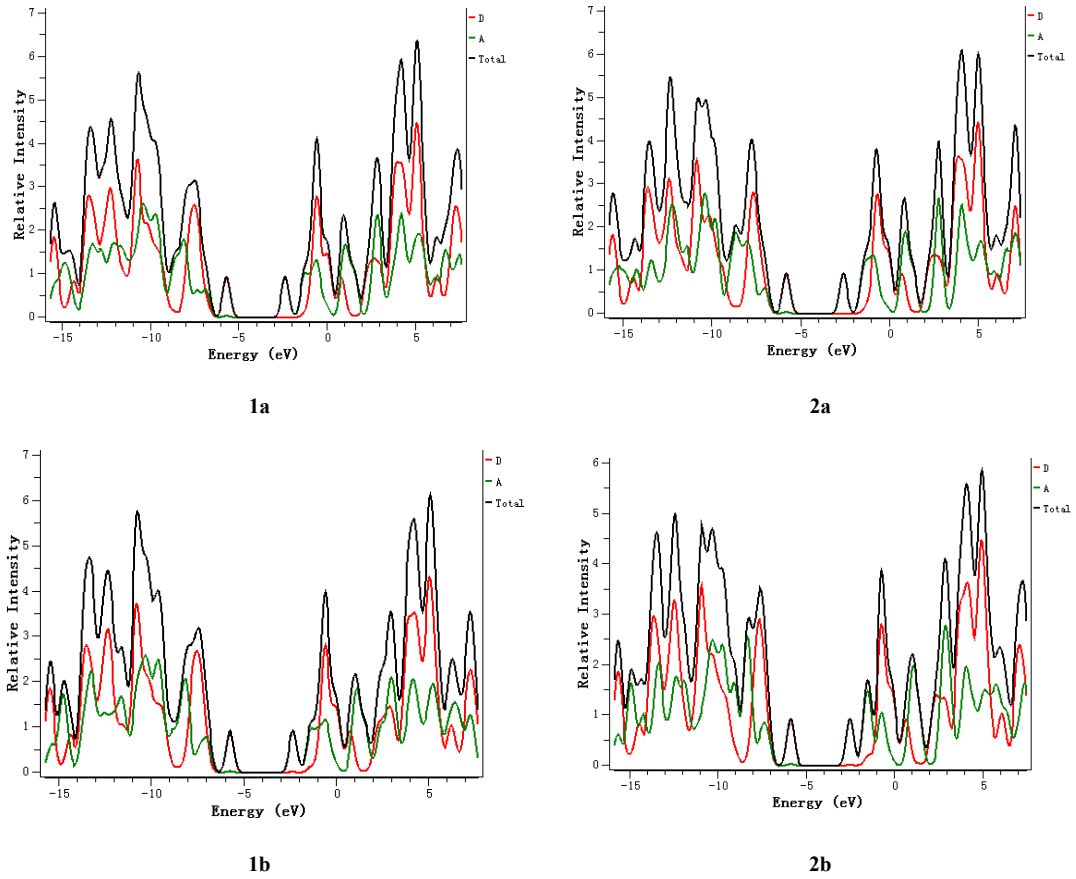
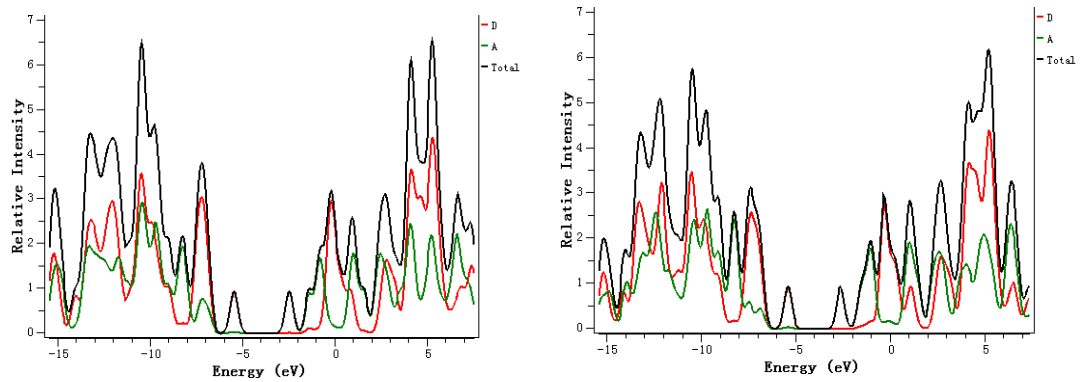
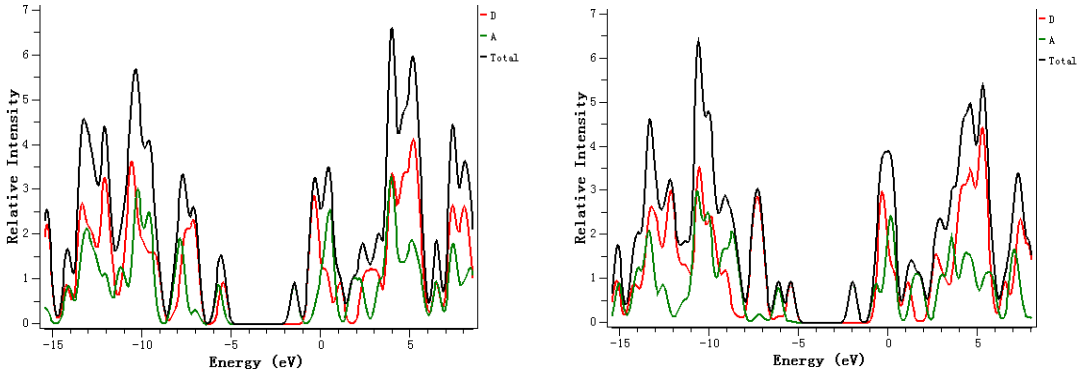


Fig. S2 The contour plots and donor/acceptor composition(%) of HOMO and LUMO of the studied compounds in S_0 states.



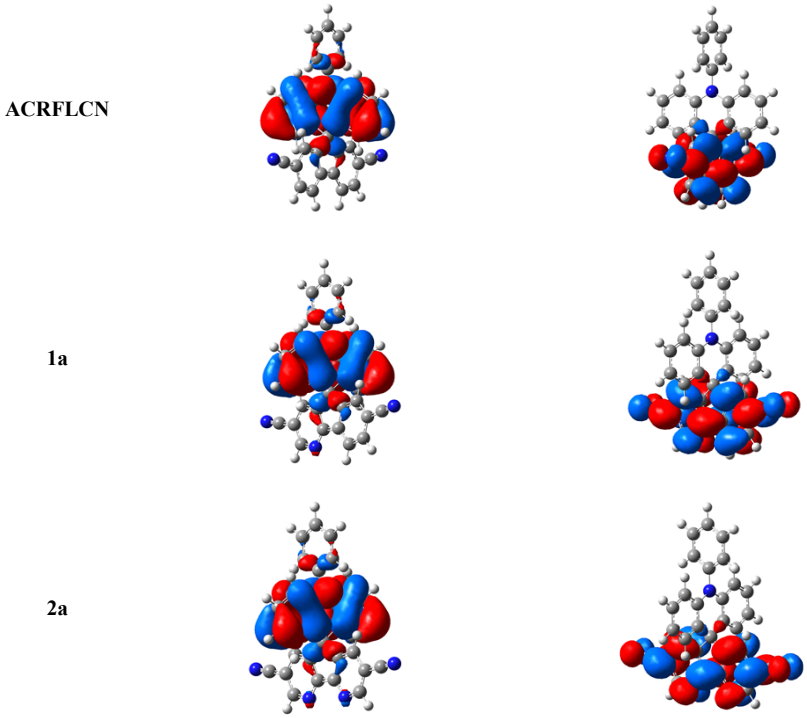


1c **2c**



2d **2e**

Fig. S3 the density of state (DOS) of the studied compounds in S_0 states.



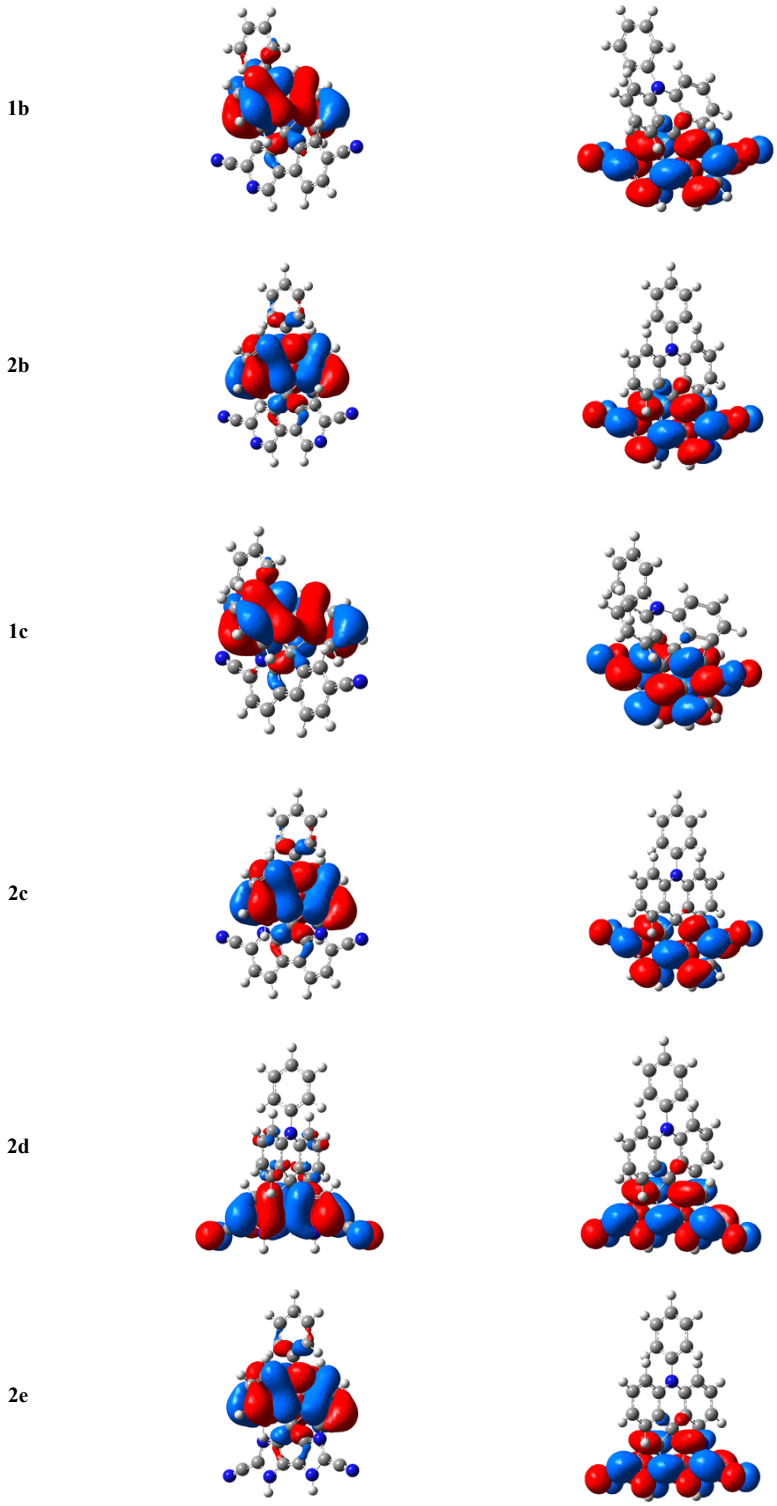


Fig. S4 The contour plots of occupied (left) and unoccupied (right) MOs of the studied compounds in T_1 state.

Table S2 The ΔE_{ST} values and donor/acceptor compositions (%) of LUMO for all these investigated TADF compounds.

	ACRFLCN	**1a**	**2a**	**1b**	**2b**	**1c**	**2c**	**2d**	**2e**
ΔE_{ST}	0.0102	0.0103	0.0109	0.0164	0.0168	0.0157	**0.0064**	0.0107	0.0099
D/A ratio	0.0111	0.0101	0.0101	0.0153	0.0163	0.0132	0.0070	0.0101	0.0091

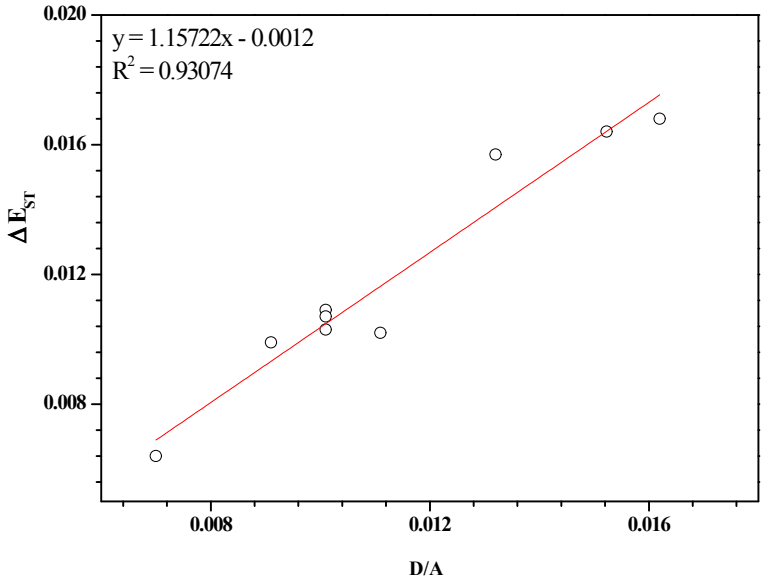
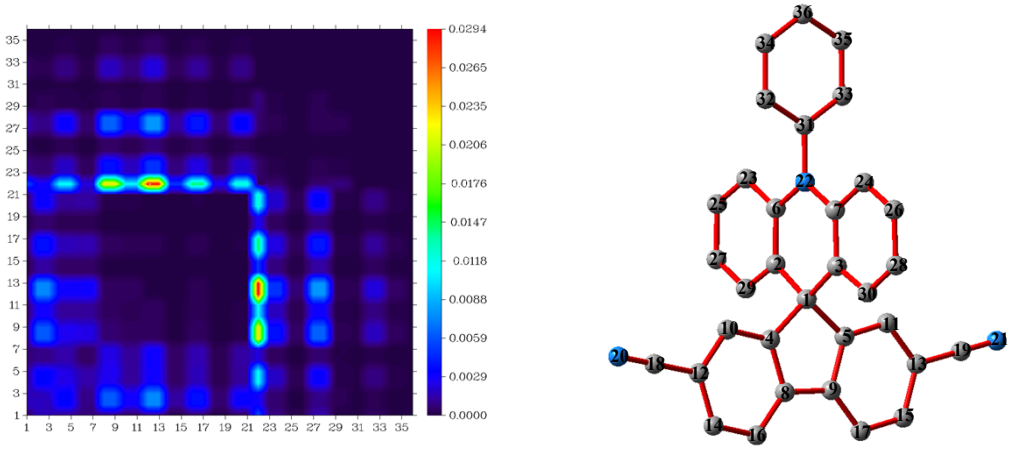
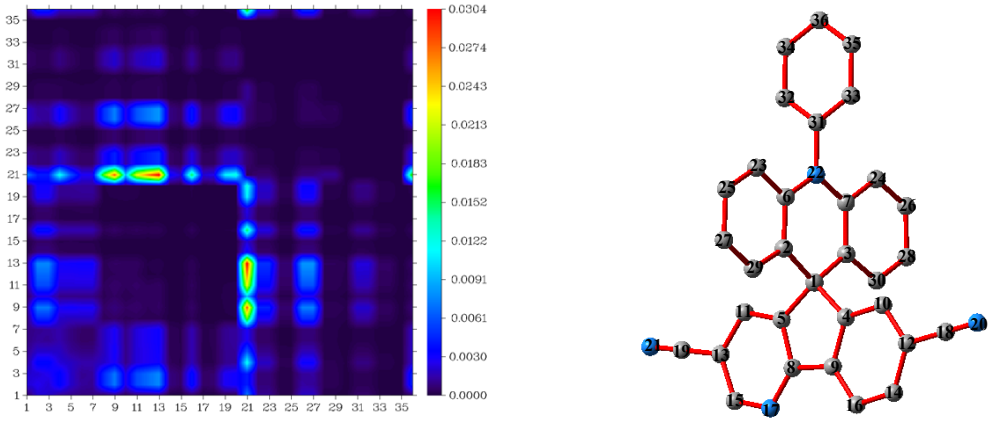


Fig. S5 The ΔE_{ST} values as a function of D/A ratio of LUMO.

The ΔE_{ST} values are plotted against the D/A ratio. A good linear relationship is found. It is indicated that the ΔE_{ST} values decrease with the low D/A ratio of LUMO.



ACRFLCN



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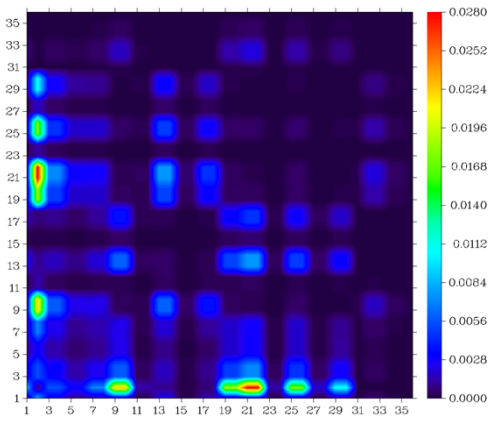
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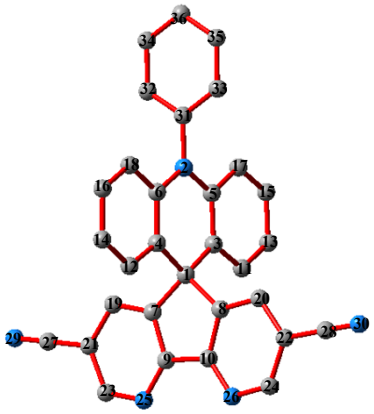
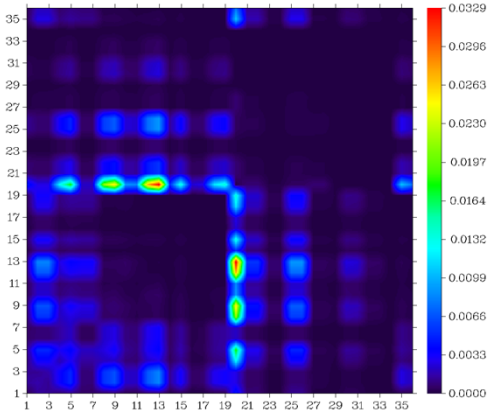


2a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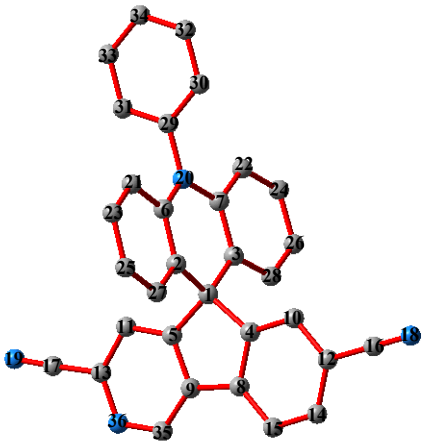
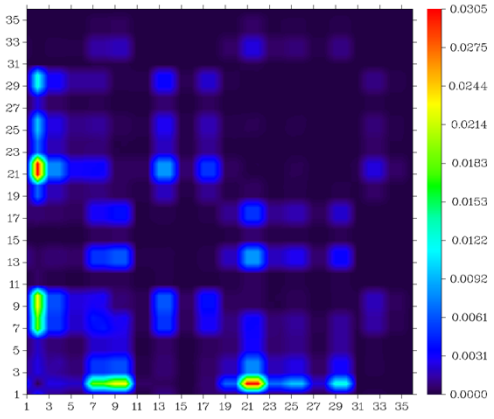


1b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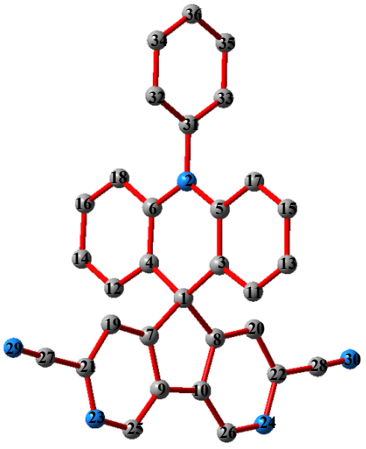
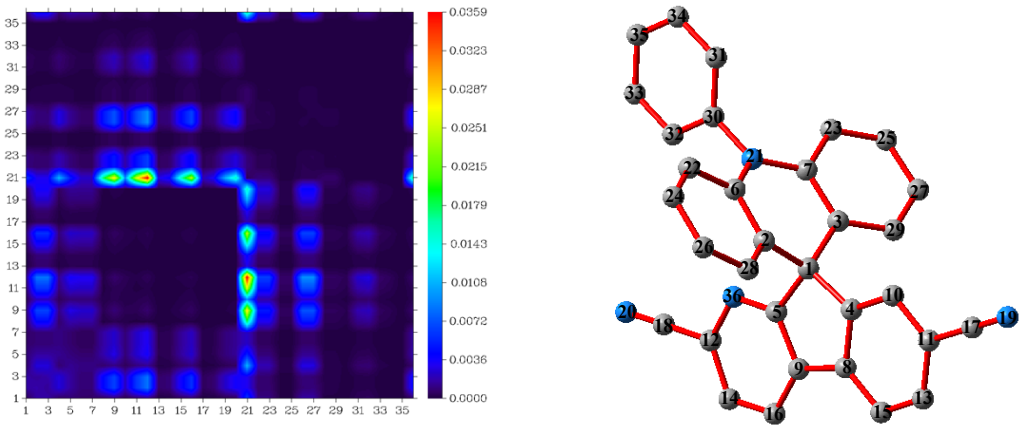


2b



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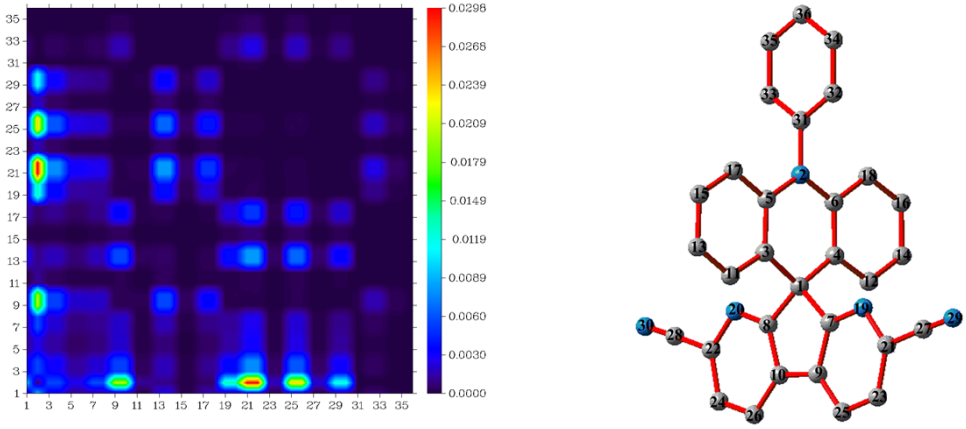

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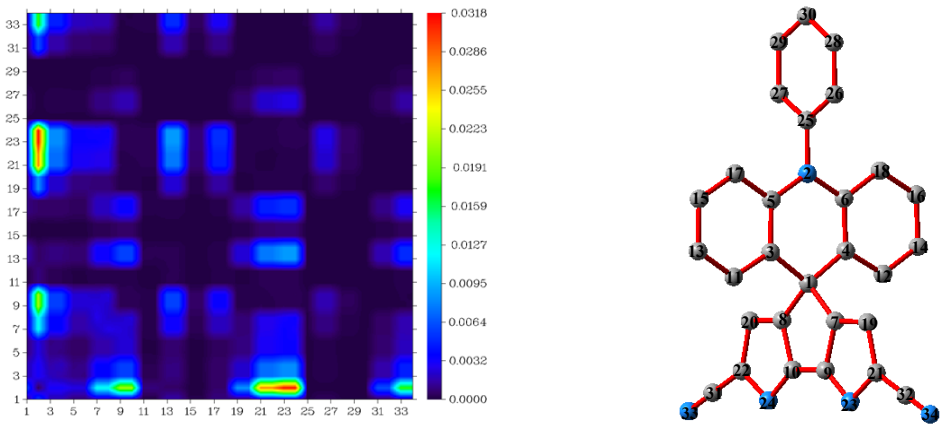

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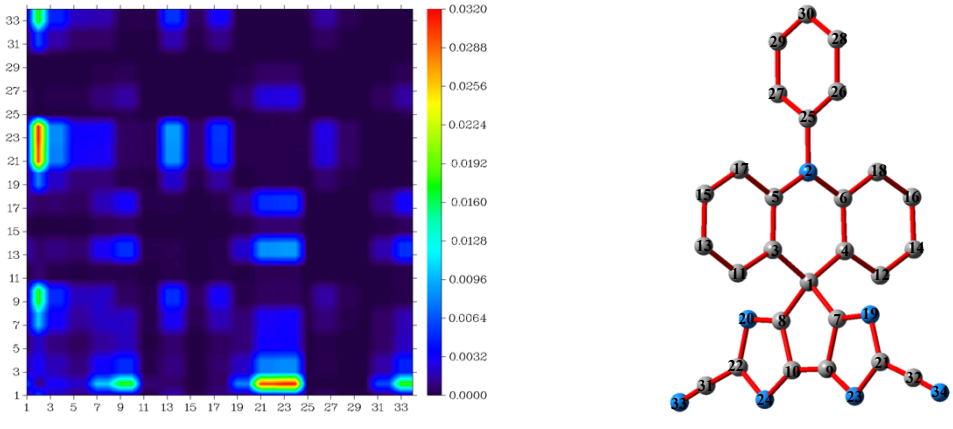


2e

Fig. S6 The transition density matrix pictures of these investigated compounds. Regions of higher transition density are shown in red and of lower transition density in black.

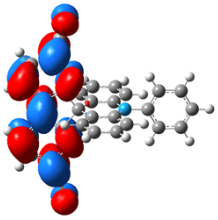
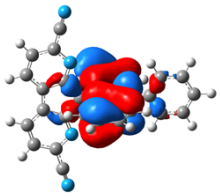
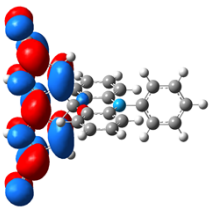
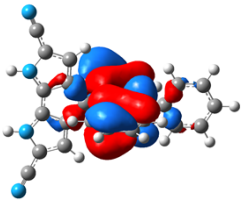
The transition density matrix (TDM) as a color-filled map is especially useful for visually studying the charge transfer patterns in detail, plotted by atom numbers on the horizontal and vertical axis. For 2e, the transition densities are mainly from the carbon atoms (labeled 21-22) and nitrogen atoms (labeled 23, and 24) of acceptor to nitrogen atom (labeled 2) of donor. The transition from carbon atoms (labeled 7-10) and nitrogen atoms (labeled 19-20, and 33-34) of acceptor to nitrogen atom (labeled 2) of donor is also given a non-ignorable contruibution for the ICT.

3. Constrained DFT calculation

Table S3 The calculated energies of **2d** using DFT and C-DFT with Mulliken population and Lowdin population.

2d	**E(DFT)** **hartree**	**E(C-DFT)** **hartree**	**E** **KJ/mol**
Mulliken population	-1387.43256	-1387.430320	5.8872
Lowdin population	-1387.43256	-1387.269194	428.9246

Table S4 The calculated lowest excitation energy of **2c** and **2d** using TD-DFT and Constrained DFT (C-DFT) method.

2c	1.618 [a] (1.824) [b]			CT
		LUMO → HOMO (100%)		
2d	2.870 (4.444)			CT
		LUMO → HOMO (100%)		

[a] the calculated emission energy using TD-DFT. [b] the calculated emission energy using C-DFT.

Our computational results predicted that **2c** and **2d** can be used as the high efficient red and blue emitting organic molecules, respectively, using TD-DFT calculation. As comparison, we used constrained density functional theory (C-DFT)[1] to calculate the excitation energies of the lowest charge transfer states in NWChem.[2] Energies are calculated using PBE0 functional and 6-31G (d) basis set, which is the same theoretical level with TD-DFT calculations. There are many different ways of defining the charge on atoms, and we have implemented two of them, i.e. Mulliken and Lowdin population. We find that Lowdin population gives reasonable results for this system. The calculated energy with Mulliken populations of **2d** only increases about 5.8872 KJ/mol once the constraint is established (Table S3), which underestimated the excitation energy.[1] Hereafter, we choose Lowdin population.

On the basis of the optimized structures, the corresponding excitation energies of charge transfer states using C-DFT method with Lowdin population for **2c** and **2d** are 1.824 eV and 4.444 eV, respectively, comparing to 1.618 eV and 2.870 eV calculated by TD-DFT calculations. The C-DFT calculations also give similar energies for these states to TD-DFT.

1. Wu, Q.; Van Voorhis, T., Direct optimization method to study constrained systems within density-functional theory. *physical review A* **2005,** *72* (2), 024502.

2. Valiev, M.; Bylaska, E. J.; Govind, N.; Kowalski, K.; Straatsma, T. P.; Van Dam, H. J. J.; Wang, D.; Nieplocha, J.; Apra, E.; Windus, T. L.; de Jong, W. A., NWChem: A comprehensive and scalable open-source solution for large scale molecular simulations. *Computer Physics Communications* **2010,** *181* (9), 1477-1489.

4. The optimized S_1 structures of these investigated compounds at the PBE0/6-31G (d) theoretical level

ACRFLCN

C	0.00000000	-0.80485700	0.00000000
C	-1.25462900	0.03332800	0.00000000
C	1.25462800	0.03332800	0.00000000
C	0.00000000	-1.77780500	1.19215600
C	0.00000000	-1.77780500	-1.19215600
C	-1.22019100	1.44619100	0.00000000
C	1.22019100	1.44619100	0.00000000
C	0.00000000	-3.12004500	0.70995900
C	0.00000000	-3.12004500	-0.70995900
C	0.00000000	-1.47061000	2.52354200
C	0.00000000	-1.47061000	-2.52354200
C	0.00000000	-2.52807200	3.47809000
C	0.00000000	-2.52807200	-3.47809000
C	0.00000000	-3.86689300	3.01021400
C	0.00000000	-3.86689300	-3.01021400
C	0.00000000	-4.16751900	1.66620200
C	0.00000000	-4.16751900	-1.66620200
H	0.00000000	-0.44229000	2.87492200
H	0.00000000	-0.44229000	-2.87492200
H	0.00000000	-4.66971600	3.74219100
H	0.00000000	-4.66971600	-3.74219100
H	0.00000000	-5.20481100	1.34273100
H	0.00000000	-5.20481100	-1.34273100
C	0.00000000	-2.23753200	4.86057600
C	0.00000000	-2.23753200	-4.86057600
N	0.00000000	-1.98085800	6.00052000
N	0.00000000	-1.98085800	-6.00052000
N	0.00000000	2.10690300	0.00000000
C	-2.41955900	2.19639500	0.00000000
C	2.41955900	2.19639500	0.00000000
C	-3.63367700	1.54611400	0.00000000
C	3.63367700	1.54611400	0.00000000
C	-3.67588200	0.14652900	0.00000000
C	3.67588200	0.14652900	0.00000000
C	-2.49706900	-0.58883500	0.00000000
C	2.49706900	-0.58883500	0.00000000

C	0.00000000	3.54809200	0.00000000
C	0.00000100	4.22756100	1.21453900
C	0.00000100	4.22756100	-1.21453900
C	0.00000100	5.61941600	-1.20765900
C	0.00000100	5.61941600	1.20765900
C	0.00000100	6.31354800	0.00000000
H	-2.38101300	3.27860300	0.00000000
H	2.38101300	3.27860300	0.00000000
H	-4.55275300	2.12305800	0.00000000
H	4.55275300	2.12305800	0.00000000
H	-4.63108600	-0.36889900	0.00000000
H	4.63108600	-0.36889800	0.00000000
H	-2.52822500	-1.67319700	0.00000000
H	2.52822500	-1.67319700	0.00000000
H	0.00000100	3.67016900	2.14663000
H	0.00000100	3.67016900	-2.14663000
H	0.00000100	6.15953100	2.14950400
H	0.00000100	6.15953100	-2.14950400
H	0.00000200	7.39943300	0.00000000

1a

C	0.78251600	0.00164800	-0.00000600
C	-0.05467800	-0.01509700	1.25520300
C	-0.05469800	-0.01509900	-1.25520100
C	1.73451700	1.21287800	-0.00001500
C	1.77693500	-1.16945700	-0.00001300
C	-1.46717000	-0.04572400	1.22014100
C	-1.46718900	-0.04572500	-1.22011700
C	3.08229400	0.75968800	-0.00002600
C	3.10714000	-0.65958300	-0.00002400
C	1.40745000	2.54037600	-0.00001400
C	1.54348500	-2.51226400	-0.00000800
C	2.45294900	3.50541900	-0.00002400
C	2.68902600	-3.37056200	-0.00001600
C	3.79864800	3.06118600	-0.00003500
C	3.96846900	-2.76393000	-0.00002800
C	4.11998700	1.72101000	-0.00003700
H	0.37487200	2.87888400	-0.00000500
H	0.54600700	-2.94171200	0.00000100
H	4.58873200	3.80684300	-0.00004300
H	4.84513700	-3.41147900	-0.00003500
H	5.15451800	1.39260500	-0.00004600
C	2.14085900	4.88525500	-0.00002300
C	2.55200600	-4.77490300	-0.00001200
N	1.86592900	6.02003100	-0.00002200
N	2.42474700	-5.93615900	-0.00000900
N	-2.12788300	-0.05822700	0.00001700

C	-2.21686600	-0.06139700	2.41963300
C	-2.21690400	-0.06139700	-2.41959700
C	-1.56675500	-0.04655600	3.63387600
C	-1.56681300	-0.04655600	-3.63385000
C	-0.16768300	-0.01467400	3.67640900
C	-0.16774200	-0.01467400	-3.67640600
C	0.56756700	0.00108700	2.49745900
C	0.56752700	0.00108600	-2.49746800
C	-3.56914200	-0.07644500	0.00002800
C	-4.26298600	1.12996100	0.00003500
C	-4.23402700	-1.29898100	0.00003100
C	-5.62589500	-1.30856400	0.00004200
C	-5.65462700	1.10659400	0.00004500
C	-6.33432700	-0.10924500	0.00004900
H	-3.29879700	-0.08525100	2.38108400
H	-3.29883500	-0.08525000	-2.38103000
H	-2.14363500	-0.05894400	4.55290200
H	-2.14370800	-0.05894300	-4.55286700
H	0.34770700	-0.00153200	4.63151400
H	0.34763200	-0.00153100	-4.63151900
H	1.65166500	0.02817800	2.52978300
H	1.65162500	0.02817700	-2.52980900
H	-3.71683200	2.06868000	0.00003200
H	-3.66575300	-2.22446300	0.00002600
H	-6.20585200	2.04197100	0.00005100
H	-6.15490600	-2.25667900	0.00004500
H	-7.42012000	-0.12216300	0.00005700
N	4.20253600	-1.46700300	-0.00003200

2a

C	-0.77082500	-0.00000700	-0.00000400
N	2.13984800	-0.00011800	0.00001100
C	0.06608900	-0.00002400	-1.25580000
C	0.06607600	-0.00010700	1.25580200
C	1.47889300	-0.00006100	-1.22004000
C	1.47888100	-0.00015500	1.22005500
C	-1.74422100	1.18789200	0.00003100
C	-1.74441500	-1.18774400	-0.00004800
C	-3.08612300	0.71207700	0.00001000
C	-3.08624000	-0.71171000	-0.00004000
C	-0.55643800	0.00001900	-2.49799200
C	-0.55646300	-0.00014200	2.49798700
C	0.17916800	0.00003200	-3.67705600
C	0.17913200	-0.00022800	3.67705800
C	1.57843200	0.00000700	-3.63405000
C	1.57839600	-0.00028600	3.63406600
C	2.22853700	-0.00003800	-2.41958300

C	2.22851300	-0.00025000	2.41960600
C	-1.47576400	2.52464200	0.00008000
C	-1.47617900	-2.52453800	-0.00009500
C	-2.59494100	3.41066600	0.00010800
C	-2.59550100	-3.41037800	-0.00013400
C	-3.88895500	2.83781700	0.00008200
C	-3.88942100	-2.83731700	-0.00012100
N	-4.15665800	1.54719000	0.00003500
N	-4.15691200	-1.54664500	-0.00007600
H	-0.46654200	2.92599200	0.00009800
H	-0.46702200	-2.92605400	-0.00010300
C	-2.41889900	4.81225000	0.00016000
C	-2.41969000	-4.81199100	-0.00018600
N	-2.25897500	5.96862000	0.00020300
N	-2.25995800	-5.96838700	-0.00022900
H	-4.74929000	3.50684300	0.00010200
H	-4.74986600	-3.50620100	-0.00015000
H	3.31072600	-0.00005400	-2.38090100
H	3.31070200	-0.00030000	2.38093400
H	2.15569400	0.00002500	-4.55291800
H	2.15564900	-0.00036000	4.55294000
H	-1.64093600	0.00004600	-2.53184300
H	-1.64096100	-0.00010200	2.53182700
C	3.58136900	-0.00014300	0.00001800
C	4.26080100	1.21442200	0.00012700
C	4.26076100	-1.21473100	-0.00008400
C	5.65265400	1.20749500	0.00013200
C	5.65261400	-1.20784900	-0.00007600
C	6.34673900	-0.00018800	0.00003200
H	3.70375800	2.14671600	0.00020400
H	3.70368700	-2.14700600	-0.00016700
H	6.19282800	2.14928500	0.00021500
H	6.19275800	-2.14965600	-0.00015300
H	7.43259400	-0.00020600	0.00003700
H	-0.33650600	0.00006600	-4.63207200
H	-0.33655200	-0.00025300	4.63206900

1b

C	0.85624000	-0.04685400	0.00000100
C	0.10039300	-0.42475800	-1.25130400
C	0.10039000	-0.42473600	1.25131200
C	2.30389000	-0.54242700	0.00000700
C	1.05830600	1.48645500	-0.00001200
C	-1.29571500	-0.65531400	-1.21858700
C	-1.29571800	-0.65529200	1.21859500
C	3.20006500	0.56894000	-0.00000200
C	2.45227100	1.77471100	-0.00001300

C	2.74390400	-1.83866100	0.00002000
C	0.13259900	2.48669200	-0.00002200
C	4.14206300	-2.09600800	0.00002400
C	0.61173300	3.82671500	-0.00003300
C	5.03903900	-0.99882300	0.00001500
C	4.59164400	0.30444700	0.00000200
H	2.05186100	-2.67653500	0.00002700
H	-0.93836000	2.30414800	-0.00002100
H	6.10602600	-1.20268200	0.00001800
H	5.30628600	1.12249000	-0.00000500
C	4.62088300	-3.42719200	0.00003700
C	-0.32280800	4.89439800	-0.00004300
N	5.00460100	-4.52983200	0.00004700
N	-1.14157700	5.72682300	-0.00005100
N	-1.95837500	-0.69015700	0.00000400
C	-2.01779400	-0.87357900	-2.41317200
C	-2.01780000	-0.87353300	2.41318300
C	-1.35393300	-0.88867400	-3.62155600
C	-1.35394200	-0.88860600	3.62156900
C	0.02957100	-0.68775300	-3.65917600
C	0.02956200	-0.68768700	3.65918900
C	0.73829900	-0.45733800	-2.48336600
C	0.73829300	-0.45729400	2.48337600
C	-3.39428900	-0.82146300	0.00000300
C	-3.96903100	-2.08957400	0.00001700
C	-4.17310800	0.33139700	-0.00001100
C	-5.55941900	0.20702500	-0.00001200
C	-5.35629800	-2.20000700	0.00001600
C	-6.14943500	-1.05459800	0.00000100
H	-3.08754800	-1.03777600	-2.37658000
H	-3.08755400	-1.03772900	2.37659200
H	-1.90905400	-1.06111400	-4.53784200
H	-1.90906600	-1.06102900	4.53785600
H	0.55611500	-0.70511000	-4.60820100
H	0.55610400	-0.70502700	4.60821500
H	1.80929300	-0.29070500	-2.51465100
H	1.80928700	-0.29066200	2.51466100
H	-3.33464800	-2.97124200	0.00002700
H	-3.69810700	1.30805600	-0.00002100
H	-5.81558800	-3.18386000	0.00002600
H	-6.17606000	1.10053100	-0.00002300
H	-7.23147000	-1.14591400	0.00000100
C	2.81044500	3.14864100	-0.00002600
H	3.86060700	3.44139700	-0.00002700
N	1.93679000	4.12992000	-0.00003500

2b

C	-0.78517100	-0.00001100	0.00000200
N	2.12762400	-0.00041200	0.00001800
C	0.05373000	-0.00023100	-1.25601700
C	0.05371500	-0.00020200	1.25603200
C	1.46661500	-0.00038600	-1.21994600
C	1.46660200	-0.00036200	1.21998100
C	-1.76263800	1.18916900	-0.00001500
C	-1.76330500	-1.18864000	0.00000700
C	-3.10493100	0.70973500	-0.00001900
C	-3.10532900	-0.70844900	-0.00000800
C	-0.56786600	-0.00022900	-2.49773800
C	-0.56790100	-0.00016500	2.49774200
C	0.16823900	-0.00036800	-3.67749100
C	0.16818200	-0.00028500	3.67750700
C	1.56680800	-0.00050600	-3.63408800
C	1.56675200	-0.00044800	3.63412900
C	2.21649400	-0.00051300	-2.41898700
C	2.21645900	-0.00048700	2.41903800
C	-1.49505400	2.52797000	-0.00002100
C	-1.49647900	-2.52759300	0.00001700
C	-2.60322700	3.41762700	-0.00002900
C	-2.60515800	-3.41662200	0.00001000
N	-3.89041900	2.98664700	-0.00003500
N	-3.89210600	-2.98491300	-0.00000200
C	-4.12774600	1.69350200	-0.00002900
C	-4.12870100	-1.69163500	-0.00001100
H	-0.48554700	2.92909000	-0.00001900
H	-0.48719900	-2.92928300	0.00002900
C	-2.37078900	4.81951900	-0.00003300
C	-2.37351400	-4.81864500	0.00001700
N	-2.12275100	5.95947400	-0.00003500
N	-2.12612500	-5.95874100	0.00002300
H	-5.17653400	1.39741700	-0.00003400
H	-5.17732200	-1.39495600	-0.00002100
H	3.29867200	-0.00061700	-2.37991900
H	3.29863700	-0.00062200	2.37999400
H	2.14451200	-0.00060600	-4.55265700
H	2.14443900	-0.00054800	4.55270700
H	-1.65222500	-0.00010900	-2.53277100
H	-1.65226100	-0.00003500	2.53275600
C	3.56936400	-0.00050200	0.00001000
C	4.24852100	1.21422300	0.00001700
C	4.24838000	-1.21530500	-0.00001700
C	5.64037300	1.20710800	0.00000700
C	5.64023300	-1.20835000	-0.00002300
C	6.33433400	-0.00066100	-0.00001100
H	3.69158700	2.14659500	0.00003100

H	3.69133900	-2.14761300	-0.00002500
H	6.18055300	2.14888700	0.00001500
H	6.18030600	-2.15019100	-0.00003800
H	7.42017800	-0.00072400	-0.00001800
H	-0.34728800	-0.00036300	-4.63255400
H	-0.34736100	-0.00025100	4.63256200

1c

C	-0.97838900	-0.12736600	0.00000100
C	-0.34511000	-0.69969200	1.24196600
C	-0.34511000	-0.69970100	-1.24196000
C	-2.49719500	-0.11051000	0.00000100
C	-0.65788000	1.40049600	-0.00000500
C	1.03381100	-1.02023500	1.21180600
C	1.03381100	-1.02024500	-1.21179900
C	-2.96957600	1.23605400	-0.00000400
C	-1.86886200	2.13454400	-0.00000800
C	-3.35371000	-1.17989600	0.00000600
C	-4.75552700	-0.94673400	0.00000500
C	0.67405100	3.23463600	-0.00001300
C	-5.22951700	0.38424400	0.00000000
C	-0.46122200	4.07928300	-0.00001700
C	-4.36482200	1.46005200	-0.00000500
C	-1.73237000	3.55044200	-0.00001400
H	-2.98496900	-2.20210700	0.00001000
H	-6.30262300	0.55309800	-0.00000100
H	-0.31110500	5.15482900	-0.00002100
H	-4.75858900	2.47241900	-0.00000900
H	-2.60233200	4.20045400	-0.00001700
C	-5.66013700	-2.03736500	0.00001000
C	1.99434100	3.74063600	-0.00001600
N	-6.39820000	-2.94071500	0.00001400
N	3.10108500	4.11843500	-0.00001800
N	1.70385800	-1.02830500	0.00000400
C	1.71892300	-1.36083100	2.39504300
C	1.71892100	-1.36085000	-2.39503300
C	1.02835100	-1.42732800	3.58923000
C	1.02834900	-1.42735600	-3.58921900
C	-0.33948000	-1.14777000	3.62012200
C	-0.33948200	-1.14779800	-3.62011200
C	-1.01075900	-0.77794600	2.45471800
C	-1.01076100	-0.77796500	-2.45471100
C	3.14545800	-0.99667600	0.00000300
C	3.88099500	-2.17855700	0.00000700
C	3.75734000	0.25346100	-0.00000200
C	5.14755000	0.31322600	-0.00000300
C	5.27129200	-2.10073100	0.00000700

C	5.90179500	-0.85811200	0.00000200
H	2.77858000	-1.58305400	2.35997300
H	2.77857800	-1.58307300	-2.35996300
H	1.55332100	-1.70092200	4.49876700
H	1.55331800	-1.70095700	-4.49875400
H	-0.88506100	-1.20486300	4.55693400
H	-0.88506400	-1.20489800	-4.55692400
H	-2.06648100	-0.53334500	2.48676400
H	-2.06648200	-0.53336400	-2.48675800
H	3.37115700	-3.13805700	0.00001100
H	3.14592800	1.15141100	-0.00000500
H	5.85947900	-3.01365900	0.00001000
H	5.63244500	1.28465800	-0.00000600
H	6.98659100	-0.80384300	0.00000100
N	0.55223300	1.86270200	-0.00000700

2c

C	-0.84142600	0.00000300	-0.00000100
N	2.05688600	-0.00007400	0.00000200
C	-0.01372900	-0.00025700	-1.25552000
C	-0.01373200	0.00018300	1.25552000
C	1.39788600	-0.00027400	-1.21916600
C	1.39788400	0.00014100	1.21916900
C	-1.82114800	1.18934200	-0.00021600
C	-1.82127900	-1.18922700	0.00021200
C	-3.16033300	0.71017900	-0.00013400
C	-3.16041200	-0.70991700	0.00012600
C	-0.63485900	-0.00047300	-2.49706800
C	-0.63486500	0.00040300	2.49706600
C	0.10076000	-0.00069600	-3.67641900
C	0.10075100	0.00057600	3.67641900
C	1.49879800	-0.00070600	-3.63291000
C	1.49878900	0.00052900	3.63291300
C	2.14752000	-0.00049700	-2.41738700
C	2.14751400	0.00031400	2.41739200
N	-1.42180100	2.42564200	-0.00044300
N	-1.42206900	-2.42557200	0.00043900
C	-2.41608200	3.37023000	-0.00062200
C	-2.41645400	-3.37004900	0.00061600
C	-3.78341400	3.02284000	-0.00056400
C	-3.78374800	-3.02250900	0.00055500
C	-4.17547700	1.70004200	-0.00032000
C	-4.17566500	-1.69966700	0.00031000
C	-2.01877000	4.73336000	-0.00087700
C	-2.01929400	-4.73322400	0.00087200
N	-1.71462700	5.85957500	-0.00108800
N	-1.71527900	-5.85947300	0.00108400

H	-4.52355200	3.81768100	-0.00071500
H	-4.52397300	-3.81726800	0.00070400
H	-5.22772000	1.43175600	-0.00027600
H	-5.22787900	-1.43126500	0.00026300
H	3.22957000	-0.00050400	-2.37792700
H	3.22956500	0.00027700	2.37793500
H	2.07697300	-0.00087700	-4.55118300
H	2.07696200	0.00066200	4.55118800
H	-1.71911700	-0.00046200	-2.53483600
H	-1.71912300	0.00043800	2.53483100
C	3.49786100	-0.00009700	0.00000400
C	4.17594700	1.21510200	-0.00015000
C	4.17591000	-1.21531700	0.00016000
C	5.56786100	1.20774800	-0.00014700
C	5.56782400	-1.20800600	0.00016100
C	6.26175400	-0.00014000	0.00000800
H	3.61663700	2.14613800	-0.00026900
H	3.61657100	-2.14633500	0.00027800
H	6.10821000	2.14949000	-0.00026600
H	6.10814300	-2.14976400	0.00028200
H	7.34770400	-0.00015600	0.00000900
H	-0.41448300	-0.00086200	-4.63167300
H	-0.41449400	0.00074600	4.63167100

2d

C	-0.76298100	-0.00001400	0.00000000
N	2.15080600	-0.00002900	0.00000100
C	0.07790000	-0.00021100	-1.25519700
C	0.07789900	0.00014800	1.25519800
C	1.49049500	-0.00018800	-1.22075000
C	1.49049400	0.00012300	1.22075300
C	-1.74516100	1.17637300	-0.00016900
C	-1.74522300	-1.17634800	0.00016800
C	-3.08010800	0.70121700	-0.00012900
C	-3.08014500	-0.70112200	0.00012800
C	-0.54411500	-0.00040000	-2.49733200
C	-0.54411800	0.00032100	2.49733200
C	0.19101800	-0.00054600	-3.67570300
C	0.19101300	0.00045200	3.67570400
C	1.59138500	-0.00049500	-3.63400700
C	1.59138000	0.00040200	3.63400900
C	2.24156500	-0.00031600	-2.42022300
C	2.24156300	0.00023700	2.42022700
C	-1.75522300	2.55858800	-0.00023700
C	-1.75535900	-2.55856300	0.00024100
C	-3.10773300	2.96635900	-0.00023600
C	-3.10789000	-2.96626300	0.00023500

N	-3.90126900	1.79507800	-0.00016300
N	-3.90136400	-1.79494000	0.00016100
H	3.32383600	-0.00026800	-2.38151800
H	3.32383300	0.00018800	2.38152300
H	2.16797300	-0.00059300	-4.55338800
H	2.16796700	0.00048900	4.55339100
H	-1.62837900	-0.00042200	-2.52303300
H	-1.62838200	0.00034400	2.52303100
C	3.59155500	-0.00002600	0.00000100
C	4.27171400	1.21407800	0.00001500
C	4.27172000	-1.21412700	-0.00001500
C	5.66355000	1.20747700	0.00001300
C	5.66355600	-1.20751900	-0.00001400
C	6.35788700	-0.00001900	0.00000000
H	3.71395700	2.14587300	0.00002500
H	3.71396800	-2.14592400	-0.00002500
H	6.20375300	2.14931300	0.00002100
H	6.20376400	-2.14935200	-0.00002200
H	7.44377300	-0.00001700	-0.00000100
H	-0.32416300	-0.00069200	-4.63111500
H	-0.32416900	0.00058700	4.63111500
H	-0.92046700	3.24643200	-0.00030300
H	-0.92063900	-3.24645100	0.00031000
C	-3.66093600	-4.24278100	0.00036800
C	-3.66071100	4.24290700	-0.00037200
N	-4.13382100	-5.31787600	0.00046900
N	-4.13353700	5.31802700	-0.00047300
H	-4.90618500	-1.80162500	0.00019100
H	-4.90608900	1.80181700	-0.00019400

2e

C	0.81021100	-0.00001100	0.00000000
N	-2.09477100	-0.00003100	0.00000300
C	-0.02363600	-0.00015900	1.25702700
C	-0.02363900	0.00010000	-1.25702600
C	-1.43545700	-0.00015100	1.22000500
C	-1.43545900	0.00008400	-1.22000200
C	1.81027100	1.16191400	0.00011800
C	1.81033600	-1.16188100	-0.00011800
C	3.14085900	0.70251100	0.00008500
C	3.14089800	-0.70240400	-0.00008900
C	0.59675600	-0.00029600	2.49837600
C	0.59675100	0.00022300	-2.49837600
C	-0.13930000	-0.00041400	3.67732900
C	-0.13930800	0.00032300	-3.67732800
C	-1.53795800	-0.00039300	3.63384400
C	-1.53796500	0.00029700	-3.63384000

C	-2.18630100	-0.00026100	2.41841600
C	-2.18630600	0.00017700	-2.41841000
N	1.70092000	2.47820300	0.00020100
N	1.70105700	-2.47817500	-0.00018700
C	2.97561900	2.92778900	0.00021200
C	2.97578100	-2.92769100	-0.00022500
N	3.88984600	1.84816700	0.00013500
N	3.88994900	-1.84801800	-0.00014300
H	-3.26837000	-0.00024100	2.37846600
H	-3.26837400	0.00015300	-2.37845800
H	-2.11612400	-0.00047800	4.55213300
H	-2.11613300	0.00036800	-4.55212800
H	1.68081900	-0.00030400	2.53094900
H	1.68081400	0.00023700	-2.53095200
C	-3.53563200	-0.00002900	0.00000400
C	-4.21438300	1.21481700	0.00004800
C	-4.21438600	-1.21487400	-0.00004000
C	-5.60626600	1.20771100	0.00005000
C	-5.60626900	-1.20776500	-0.00004000
C	-6.30033300	-0.00002600	0.00000600
H	-3.65546200	2.14602700	0.00008200
H	-3.65546700	-2.14608600	-0.00007500
H	-6.14660200	2.14946000	0.00008600
H	-6.14660700	-2.14951200	-0.00007500
H	-7.38625700	-0.00002500	0.00000600
H	0.37553100	-0.00052000	4.63281200
H	0.37552100	0.00041900	-4.63281200
C	3.39671900	-4.25668700	-0.00034000
C	3.39648200	4.25680800	0.00032200
N	3.79204900	-5.36080000	-0.00043000
N	3.79175000	5.36094400	0.00041200
H	4.89135200	-1.94003400	-0.00019400
H	4.89124400	1.94023900	0.00018400