Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

ELECTRONIC SUPPORTING INFORMATION (ESI)

Intersystem crossing processes in the 2CzPN emitter: A DFT/MRCI study including vibrational spin–orbit interactions.

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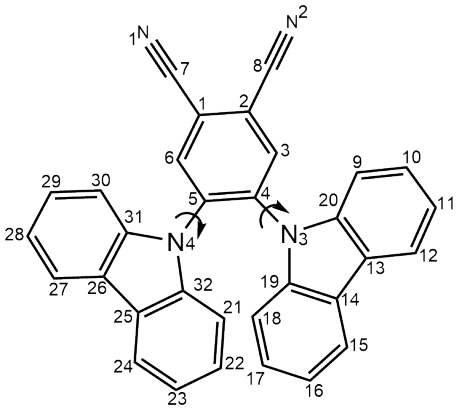
Table S1. Selected geometrical parameters (dihedrals, in degrees) of the ground state S_0 minimum of **2CzPN** optimized at the indicated level of theory.



Dihedral	Crystal* structure	Crystal* structure 2	PBE0/ def2-TZVP*	PBE0-D3(BJ)/ def2-TZVP	PBE0-D3(BJ)/ def-SV(P)
C3-C4-N3-C20	114.9	-123.8	129.8	-128.6	-130.7
C3-C4-N3-C19	-55.7	42.6	-57.1	55.6	59.5
C5-C4-N3-C20	-63.8	56.1	-20.3	51.5	49.7
C5-C4-N3-C19	125.6	-137.5	122.7	-124.3	-120.1
C4-C5-N4-C31	125.5	-131.3	122.7	-124.3	-120.0
C4-C5-N4-C32	-56.4	57.1	-50.3	51.3	49.7
C6-C5-N4-C31	-54.6	49.9	-57.1	55.6	59.5
C6-C5-N4-C32	123.5	-121.7	129.8	-128.8	-130.8
C4-N3-C20-C19	171.9	168.3	-174.1	-176.3	-171.1
C5-N4-C32-C31	178.4	172.8	-174.1	-176.2	-171.1
	B3LYP/ 6-31G*	**B3LYP-D3(BJ)/ def2-TZVP**	**BHLYP-D3(BJ)/ def2-TZVP**	**RI-ADC(2)/ def-SV(P)**	**RI-CC2/ defSV(P)**
C3-C4-N3-C20	-51.9	-129.3	-124.2	-137.7	-138.2
C3-C4-N3-C19	120.0	57.2	56.6	63.2	62.6
C5-C4-N3-C20	128.2	50.8	53.2	44.0	43.3
C5-C4-N3-C19	-59.9	-122.7	-123.1	-115.1	-115.8
C4-C5-N4-C31	128.2	-122.6	-123.0	-115.1	-115.8
C4-C5-N4-C32	-59.8	50.6	53.0	44.0	43.3
C6-C5-N4-C31	-51.9	57.1	56.6	63.2	62.6
C6-C5-N4-C32	120.1	-129.7	-127.4	-137.6	-138.2
C4-N3-C20-C19	173.2	-174.4	-176.8	-161.9	-162.0
C5-N4-C32-C31	173.2	-174.1	-176.6	-161.9	-162.0

*M. Y. Wong, S. Krotkus, G. Copley, W. Li, C. Murawski, David Hall, G. J. Hedley, M. Jaricot, D. B. Cordes, A. M. Z. Slawin, Y. Olivier, D. Beljonne, L. Muccioli, M. Moral, J.-C. Sancho-Garcia, M. C. Gather, I. D. W. Samuel, E. Zysman-Colman, Deep-blue oxadiazole-containing thermally activated delayed fluorescence emitters for organic light-emitting diodes, ACS Appl. Mater. Interfaces, 2018, 10, 33360−33372.

Table S2. Vertical excitation energies (ΔE_v, eV) of low-lying singlet (TD-DFT) and triplet states (TDA) of **2CzPN** calculated at the S_0 geometry optimized at the PBE0-D3(BJ)/def-SV(P) level of theory.

State	ΔE_v	Transition	%weight	f(*L*)	State	ΔE_v	Transition	%weight
S_0	0.00							
S_1	2.98	H→L	98.9%	0.061	T_1	2.68	H→L	84.5%
S_2	3.17	H-1→L	94.7%	0.102	T_2	2.92	H-1→L	94.8%
S_3	3.24	H-2→L	99.5%	0.013	T_3	3.15	H-2→L	81.2%
S_4	3.50	H-3→L	94.6%	0.000	T_4	3.32	H→L+1	82.2%
S_5	3.55	H→L+1	90.0%	0.125	T_5	3.35	H-3→L	31.0%
S_6	3.67	H-1→L+1	98.5%	0.003			H-2→L+2	23.6%
S_7	3.83	H-2→L+1	98.8%	0.011			H-3→L+3	17.1%
S_8	4.09	H-3→L+1	98.9%	0.000	T_6	3.42	H-1→L+1	78.1%
S_9	4.22	H→L+2	81.2%	0.039	T_7	3.45	H-2→L+3	34.6%
S_{10}	4.25	H→L+3	69.4%	0.006			H-3→L+2	28.5%
		H-1→L+1	19.5%		T_8	3.53	H-3→L	61.1%
							H-2→L+2	14.9%

Fig. S1 Kohn-Sham frontier molecular orbitals of **2CzPN** calculated at the S_0 geometry optimized at the PBE0-D3(BJ)/def-SV(P) level of theory.

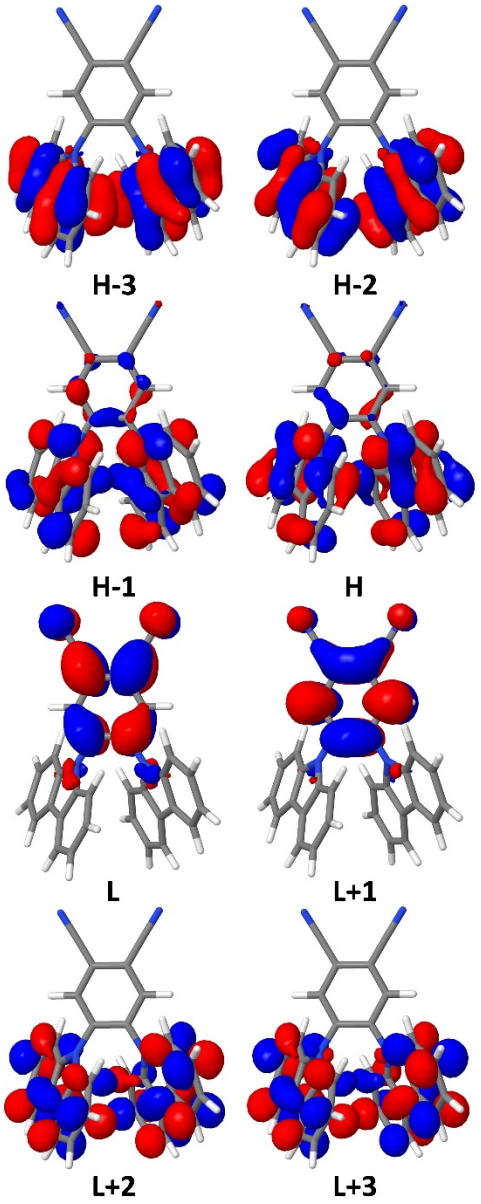
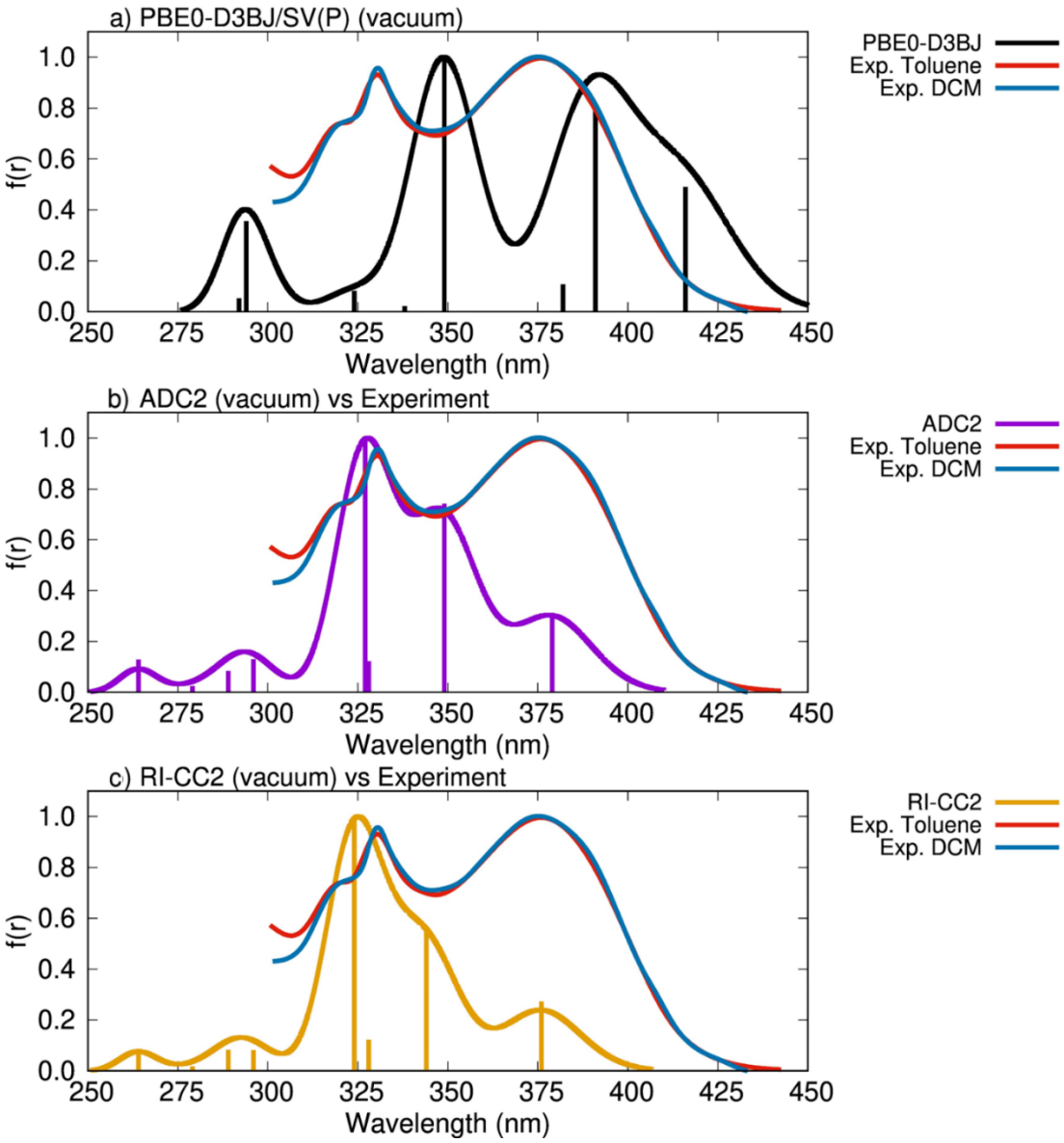


Table S3. Vertical excitation energies (ΔE_v, eV) of low-lying singlet and triplet states of **2CzPN** calculated at the S_0 geometry optimized at the indicated level of theory.

State	ΔE_v	Transition	%Weight	ΔE_v	Transition	%Weight
	RI-ADC2/def-SV(P)			**RI-CC2/def-SV(P)**		
S_1	3.27	H-1 → L	50.4%	3.30	H-1 → L	47.1%
		H → L	38.5%		H → L	41.9%
S_2	3.55	H-2 → L	63.3%	3.61	H-2 → L	61.0%
		H-3 → L	21.1%		H-3 → L	18.4%
S_3	3.78	H → L	55.6%	3.78	H → L	51.3%
		H-1 → L	39.2%		H-1 → L	43.1%
T_1	3.02	H-1 → L	52.8%	3.05	H-1 → L	51.5%
		H → L	22.1%		H → L	23.4%
		H-6 → L	15.2%		H-6 → L	15.1%
T_2	3.44	H-2 → L	60.2%	3.48	H-2 → L	60.7%
		H-3 → L	18.6%		H-3 → L	16.2%
T_3	3.54	H → L	28.3%	3.52	H → L	28.7%
		H → L+3	27.9%		H → L+2	27.3%
					H-1 → L	10.1%
	BHLYP-D3(BJ)/def2-TZVP			**B3LYP-D3(BJ)/def2-TZVP**		
S_1	3.81	H → L	91.1%	2.87	H → L	99.0%
S_2	3.98	H-1 → L	91.5%	3.02	H-1 → L	93.5%
S_3	4.28	H-2 → L	93.3%	3.11	H-2 → L	99.6%
T_1	2.58	H-6 → L	31.4%	2.53	H → L	83.6%
		H → L	27.3%			
		H-8 → L+1	16.3%			
T_2	2.77	H-2 → L+3	25.9%	2.78	H-1 → L	95.7%
		H-3 → L+2	24.9%			
T_3	2.78	H-2 → L+3	27.6%	3.00	H-2 → L	70.3%
		H-3 → L+3	24.2%			
T_4	3.43	H-1 → L	28.8%	3.11	H-2 → L+2	29.0%
					H-3 → L	26.4%
					H-3 → L+3	20.1%
T_5	3.51	H-1 → L+2	16.9%	3.14	H → L+1	89.6%
		H → L+3	16.4%			
T_6	3.67	H-1 → L	41.8%	3.21	H-1 → L+1	73.3%
		H → L+2	16.2%			
		H-1 → L+3	11.7%			
		H-8 → L	10.7%			
	PBE0-D3(BJ)/def2-TZVP			**PBE0-D3(BJ)/def-SV(P)**		
S_1	3.05	H → L	98.7%	2.98	H → L	98.9%
S_2	3.19	H-1 → L	93.8%	3.17	H-1 → L	94.7%
S_3	3.33	H-2 → L	99.5%	3.24	H-2 → L	99.5%
T_1	2.58	H → L	72.2%	2.68	H → L	84.5%
		H-6 → L	13.6%			
T_2	2.90	H-1 → L	92.1%	2.92	H-1 → L	94.8%
T_3	3.03	H-2 → L+3	26.5%	3.15	H-2 → L	81.2%
		H-3 → L+2	24.6%			
		H-2 → L	20.2%			
T_4	3.06	H-2 → L+2	34.1%	3.32	H → L+1	82.2%
		H-3→ L+3	26.2%			
T_5	3.27	H → L+1	86.4%	3.35	H-3 → L	31.0%
					H-2 → L+2	23.6%
					H-3 → L+3	17.1%
T_6	3.28	H-1 → L+1	52.0%	3.42	H-1 → L+1	78.1%
		H → L	16.6%			
		H-9 → L+1	13.0%			

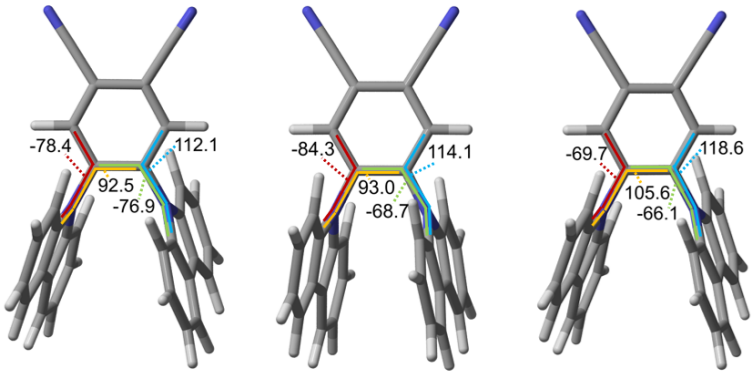
Fig. S2 a) PBE0-D3(BJ)/def-SV(P) and DFT/MRCI-R2016 absorption spectra calculated at the corresponding S_0 minimum. b) RI-ADC2/def-SV(P) and RI-CC2/def-SV(P) absorption spectra calculated at their corresponding S_0 minimum. The experimental absorption spectra of **2CzPN** in toluene* and DCM** is also presented.



*T. Hosokai, H. Matsuzaki, H. Nakanotani, K. Tokumaru, T. Tsutsui, A. Furube, K. Nasu, H. Nomura, M. Yahiro, C. Adachi, Evidence and mechanism of efficient thermally activated delayed fluorescence promoted by delocalized excited states, Sci. Adv. 2017, 3, e1603282(1-9).

**J. W. Sun, K.-H. Kim, C.-K. Moon, J.-H. Lee, J.-J. Kim, Highly efficient sky-blue fluorescent organic light emitting diode based on mixed cohost system for thermally activated delayed fluorescence emitter (2CzPN), ACS Appl. Mater. Interfaces, 2016, 8, 9806−9810.

Fig. S3 Selected geometrical parameters (dihedral angles) of the S_2', T_1' and T_2' excited state minima of **2CzPN** optimized at the PBE0-D3(BJ)/def-SV(P) level of theory. TDDFT was used for the optimization of the excited singlet states, while TDA approximation was used for the optimization of the triplet states.



a) S_2' b) T_1' c) T_2'

Table S4. Adiabatic excitation energies (ΔE^{ad}, eV) of low-lying singlet and triplet states of **2CzPN** calculated at its corresponding equilibrium geometry. Optimizations were performed at the PBE0-D3(BJ)/def-SV(P) level of theory: For the singlet states by using TDDFT and for the triplet states using TDA approximation.

State	ΔE(eV)	Transition	%DC	f(L)	ZPVE
S_1	2.43	H→L	99.4%	0.001	-0.09
S_1'	2.43	H→L	99.4%	0.001	-0.10
S_2	2.71	H-1→L	98.6%	0.010	-0.01
T_1	2.40	H→L	98.2%		-0.10
T_2	2.64	H-1→L	97.8%		-0.07

The ZPE values were scaled by 0.9944 to account for systematic errors of the PBE0 functional according to (M. K. Kesharwani, B. Brauer, J. M. L. Martin, J. Phys. Chem., A 119 (2015) 1701)

Fig. S4 Frontier molecular orbitals of **2CzPN** calculated at the corresponding excited state geometry optimized at the PBE0-D3(BJ)/def-SV(P) level of theory.

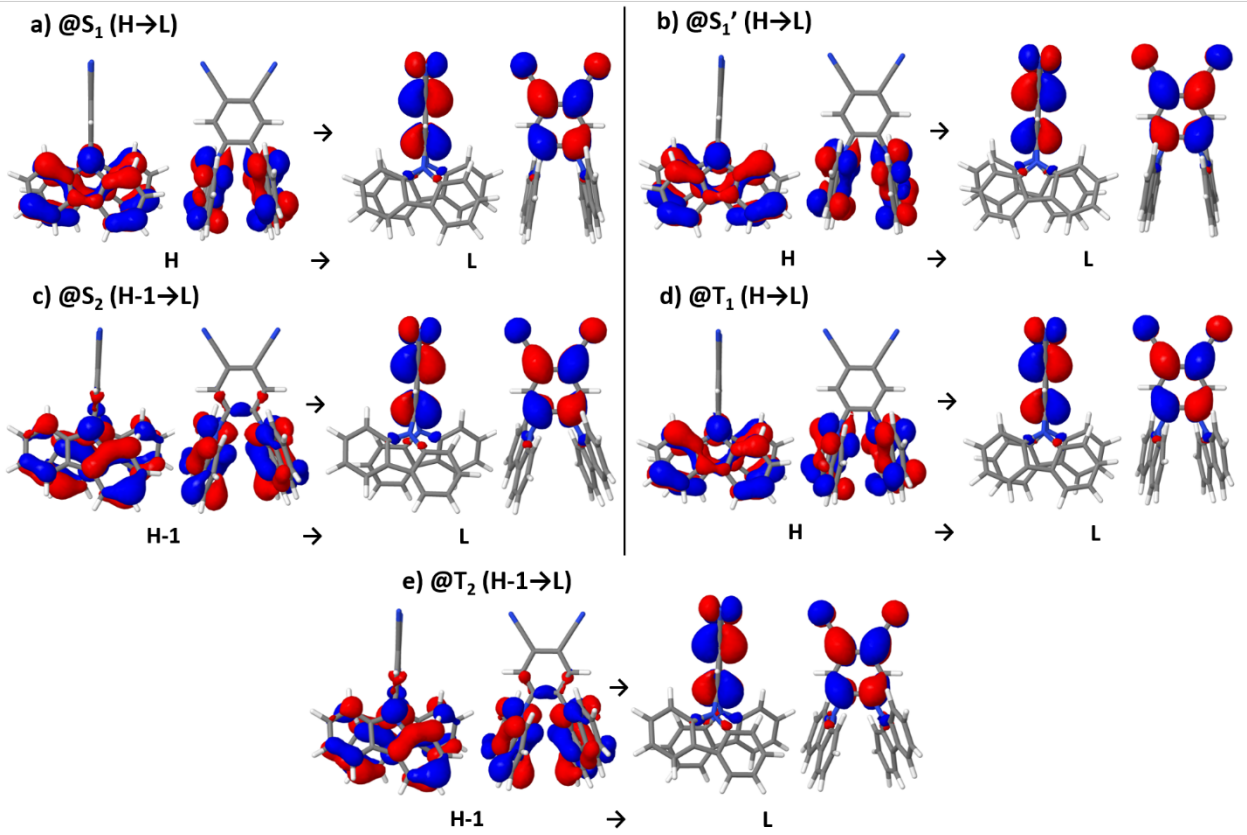


Fig. S5 BHLYP Frontier molecular orbitals of **2CzPN** calculated at the indicated excited state geometry.

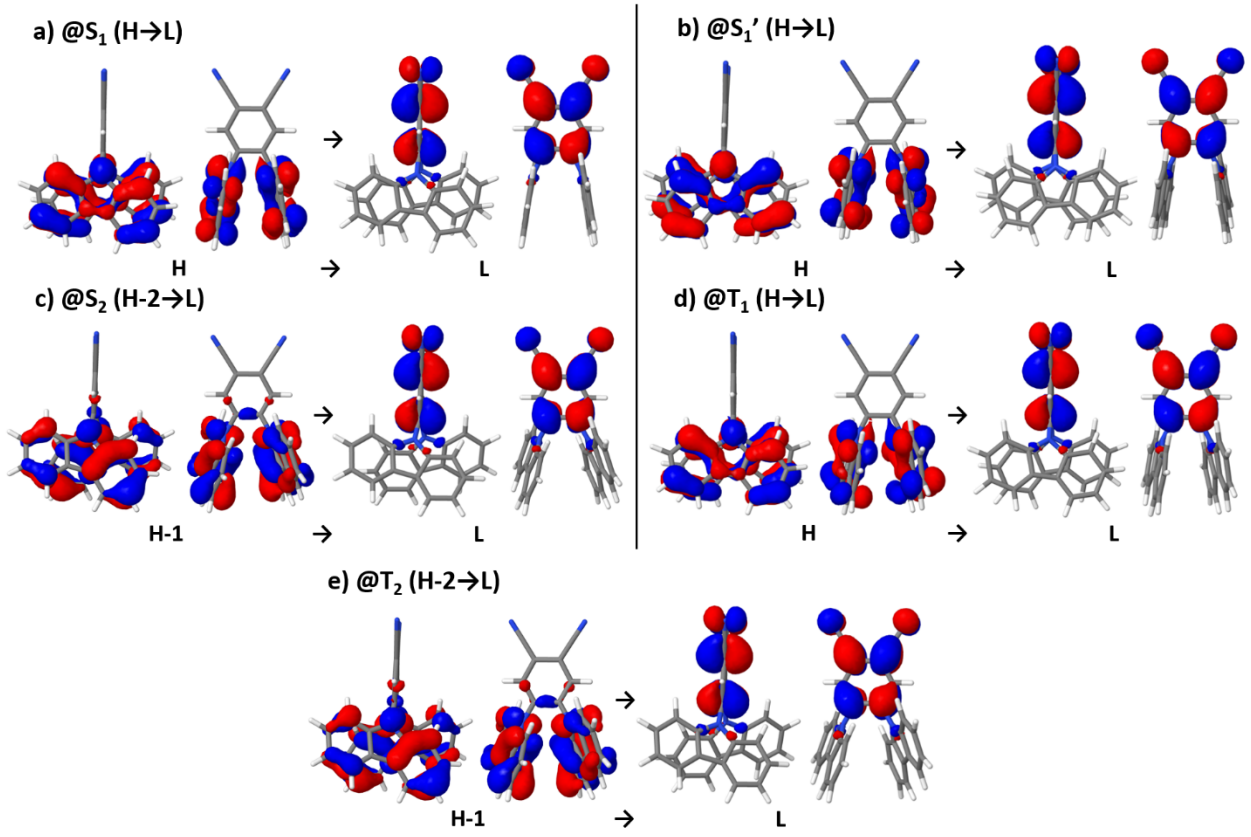


Table S5. DFT/MRCI excitation energies (ΔE, eV) of low-lying singlet and triplet states of **2CzPN** calculated at the S_1 minimum.

State	ΔE(eV)	Transition	%DC
S_0	0.48		
S_1	2.91	H → L	89.3%
S_2	3.42	H-3 → L	85.1%
S_3	3.45	H-1 → L	88.0%
S_4	3.72	H-2 → L	87.1%
T_1	2.83	H → L	87.5%
T_2	3.35	H-3 → L	84.4%
T_3	3.38	H-1 → L	87.3%
T_4	3.51	H-7 → L	60.3%
		H-2 → L	14.5%

Fig. S6 BH-LYP frontier molecular orbitals of **2CzPN** calculated at the S_1 minimum.

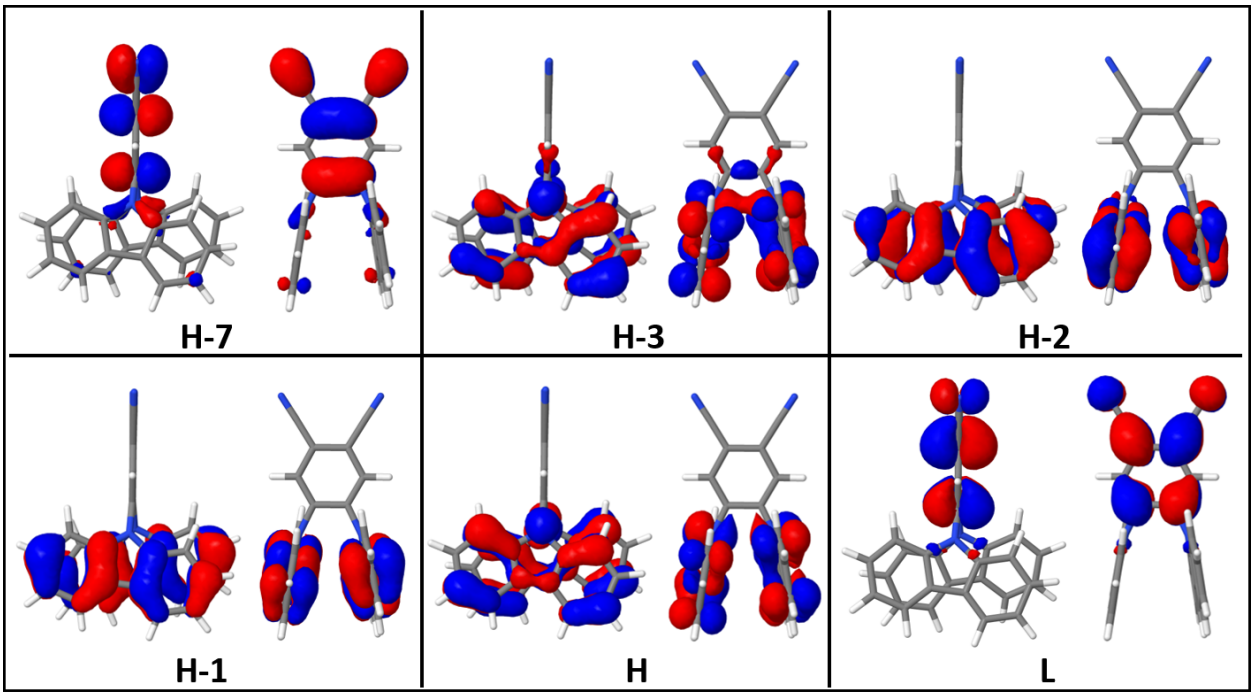


Table S6. DFT/MRCI excitation energies (ΔE, eV) of low-lying singlet and triplet states of **2CzPN** calculated at the S_1' minimum.

State	ΔE(eV)	Transition	%DC
S_0	0.48		
S_1	2.92	H → L	89.4%
S_2	3.41	H-2 → L	47.3%
		H-3→ L	39.3%
S_3	3.45	H-1 → L	87.7%
S_4	3.75	H-3→ L	48.5%
		H-2 → L	48.2%
T_1	2.83	H → L	87.4%
T_2	3.34	H-2 → L	47.0%
		H-3→ L	39.0%
T_3	3.39	H-1 → L	87.0%
T_4	3.52	H-7 → L	62.4%
		H-5→ L	8.1%

Fig. S7 BH-LYP frontier molecular orbitals of **2CzPN** calculated at the S_1' minimum.

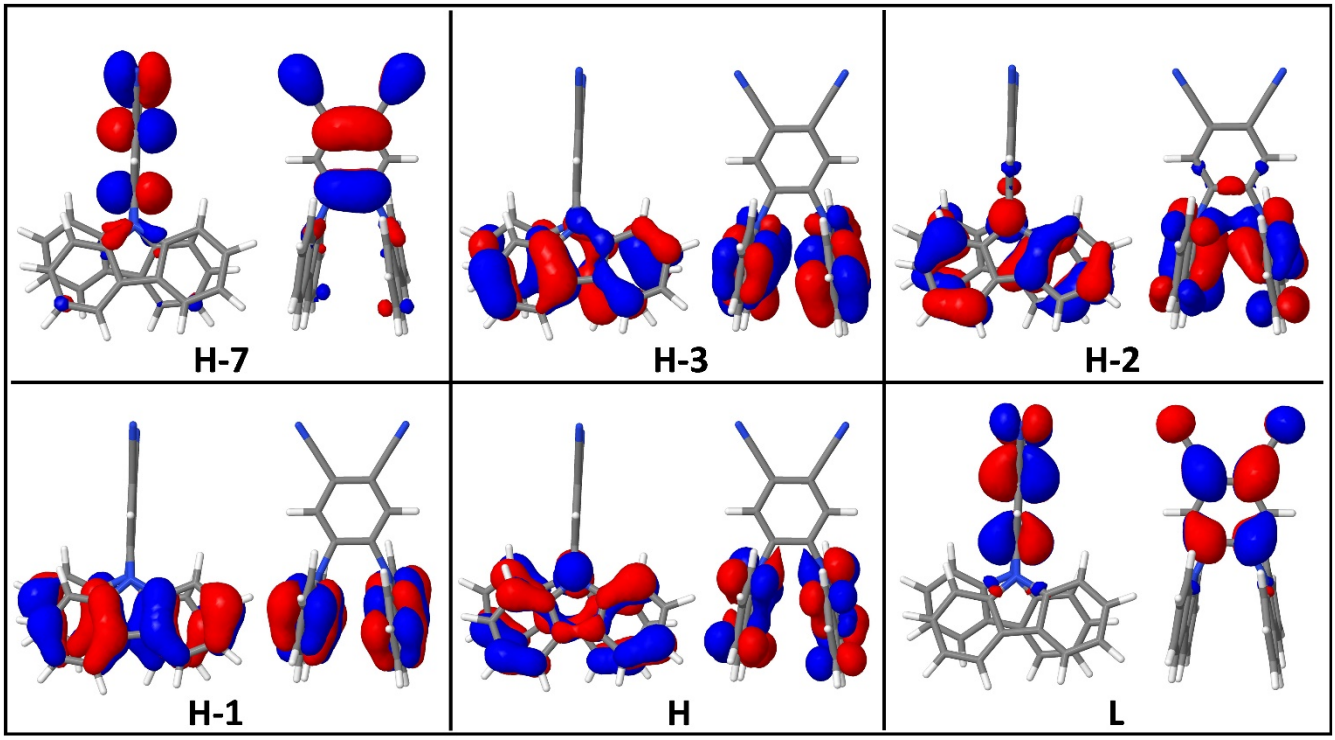


Table S7. DFT/MRCI excitation energies (ΔE, eV) of low-lying singlet and triplet states of **2CzPN** calculated at the T_1 minimum.

State	ΔE(eV)	Transition	%DC
S_0	0.43		
S_1	2.91	H → L	89.1%
S_2	3.39	H-3 → L	81.0%
S_3	3.48	H-1 → L	82.1%
S_4	3.66	H-2 → L	88.6%
T_1	2.79	H → L	84.7%
T_2	3.30	H-3 → L	80.6%
T_3	3.41	H-1 → L	81.9%
T_4	3.47	H-7 → L	50.2%
		H-2 → L	22.0%

Fig. S8 BH-LYP frontier molecular orbitals of **2CzPN** calculated at the T_1 minimum.

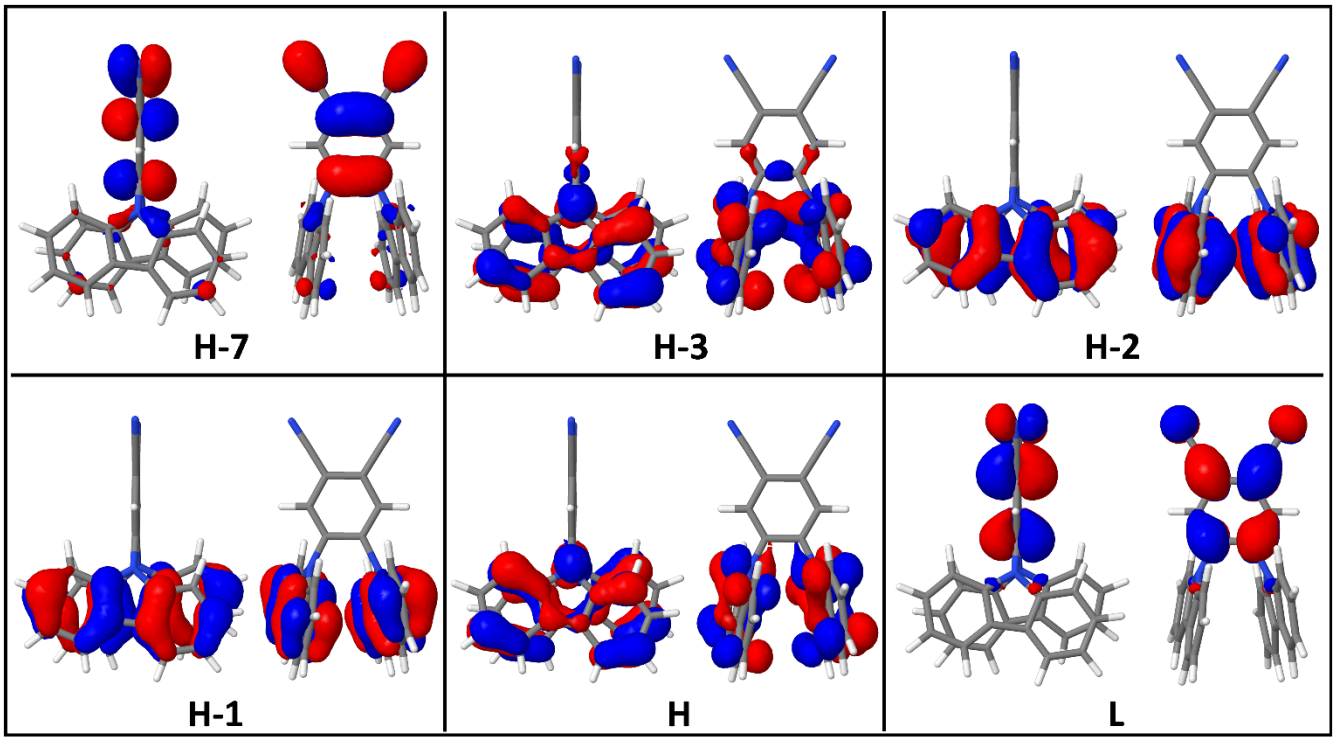


Table S8. DFT/MRCI excitation energies (ΔE, eV) of low-lying singlet and triplet states of **2CzPN** calculated at the T_2 minimum.

State	ΔE(eV)	Transition	%DC
S_0	0.32		
S_1	3.10	H → L	86.7%
S_2	3.12	H-1 → L	84.8%
S_3	3.45	H-2 → L	87.1%
S_4	3.71	H-3 → L	84.4%
T_1	2.84	H → L	69.4%
		H-6 → L	15.8%
T_2	3.01	H-1 → L	83.4%
T_3	3.36	H-2 → L	78.4%
T_4	3.59	H-3 → L	54.9%
		H-2→ L+3	13.7%

Fig. S9 BH-LYP frontier molecular orbitals of **2CzPN** calculated at the T_2 minimum.

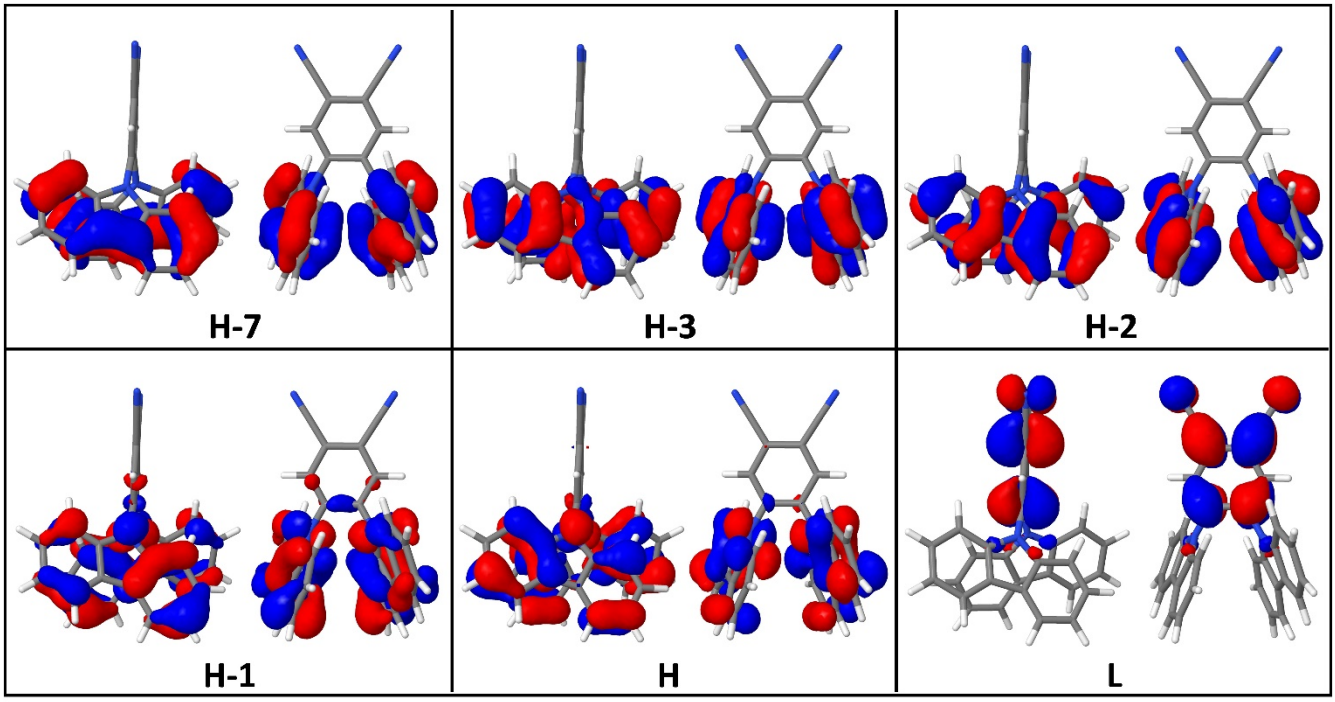
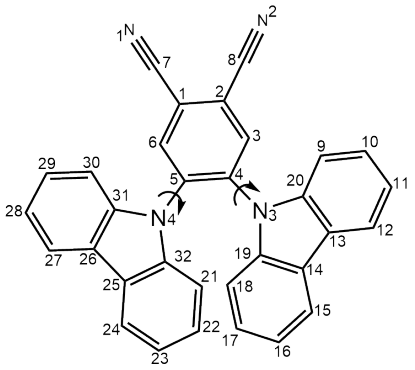


Table S9. Dihedral angles (in degrees) of the ground and excited state minima of **2CzPN** optimized at PBE0-D3(BJ)/def-SV(P) level of theory: For the singlet states by using TDDFT and for the triplet states using TDA approximation.



Dihedral	S_0	S_1	S_1'	S_2	T_1	T_2
C3-C4-N3-C20	-130.7	-109.9	-88.2	-111.8	-113.3	-117.8
C3-C4-N3-C19	59.5	88.7	110.0	78.2	85.2	70.1
C5-C4-N3-C20	49.7	74.9	87.3	77.1	69.5	67.3
C5-C4-N3-C19	-120.1	-86.5	-74.5	-92.8	-92.1	-104.8
C4-C5-N4-C31	-120.0	-86.6	-74.3	-92.9	-92.3	-104.7
C4-C5-N4-C32	49.7	75.0	87.0	77.2	69.7	67.1
C6-C5-N4-C31	59.5	88.7	110.0	78.1	84.8	70.3
C6-C5-N4-C32	-130.8	-109.8	-88.7	-111.8	-113.2	-117.9
C4-N3-C20-C19	-171.1	-163.8	-164.3	-171.3	-164.0	-173.2
C5-N4-C32-C31	-171.1	-163.9	-163.9	-171.4	-164.4	-172.9

Table S10. Harmonic frequencies (ν_i, cm^{-1}) and component-averaged ∂SOMEs (cm^{-1}) with respect to the corresponding (dimensionless) normal coordinates calculated at the S_1, S_1' and T_1 state minima of **2CzPN**.

Mode	ν_i@S_1	S_1-T_1	S_1-T_2	ν_i@S1'	S_1'-T_1	S_1'-T_2	ν_i@T_1	T_1-S_1
1	33.7	0.009	0.051	31.9	0.002	0.100	29.0	0.043
2	37.5	0.020	0.096	35.7	0.006	0.061	33.1	0.036
3	39.7	0.031	0.060	37.8	0.031	0.118	34.6	0.007
4	51.0	0.007	0.034	50.8	0.004	0.112	47.9	0.003
5	67.0	0.006	0.125	63.3	0.005	0.033	61.1	0.012
6	73.8	0.007	0.086	73.5	0.006	0.043	70.7	0.006
7	82.0	0.044	0.052	81.5	0.042	0.122	75.8	0.046
8	115.5	0.003	0.010	113.7	0.002	0.061	110.9	0.004
9	118.8	0.002	0.060	116.3	0.002	0.045	116.5	0.003
10	119.8	0.002	0.060	118.9	0.001	0.104	119.5	0.003
11	141.8	0.012	0.018	140.1	0.012	0.071	137.8	0.015
12	152.0	0.005	0.096	150.1	0.006	0.117	147.2	0.007
13	159.0	0.029	0.023	157.4	0.024	0.099	153.3	0.031
14	180.5	0.003	0.036	178.4	0.002	0.020	176.5	0.005
15	187.0	0.003	0.149	185.9	0.003	0.098	182.9	0.006
16	196.2	0.001	0.061	195.7	0.001	0.082	195.5	0.005
17	208.0	0.014	0.033	206.6	0.016	0.105	202.4	0.022
18	216.2	0.024	0.068	215.3	0.022	0.134	211.9	0.028
19	270.1	0.002	0.093	269.4	0.002	0.079	269.6	0.004
20	298.3	0.006	0.040	296.6	0.007	0.009	295.2	0.031
21	299.1	0.029	0.030	297.7	0.029	0.102	295.4	0.009
22	313.0	0.002	0.110	311.7	0.004	0.128	308.5	0.005
23	321.1	0.021	0.007	321.2	0.016	0.036	320.9	0.033
24	340.6	0.011	0.299	339.8	0.014	0.165	340.0	0.020
25	406.1	0.009	0.023	405.1	0.011	0.039	399.8	0.007
26	419.9	0.020	0.027	418.7	0.020	0.040	416.9	0.029
27	420.8	0.004	0.064	420.2	0.004	0.052	419.4	0.005
28	432.6	0.003	0.229	430.9	0.002	0.117	429.1	0.002
29	437.7	0.005	0.437	435.1	0.005	0.242	432.2	0.010
30	442.3	0.002	0.118	442.5	0.004	0.030	442.2	0.003
31	442.9	0.001	0.013	442.8	0.002	0.110	442.7	0.003
32	447.4	0.001	0.028	446.2	0.003	0.115	445.2	0.009
33	461.7	0.040	0.035	459.7	0.039	0.071	456.1	0.043
34	480.1	0.005	0.266	478.3	0.003	0.276	469.0	0.001
35	511.3	0.015	0.113	510.7	0.017	0.039	512.7	0.008
36	515.4	0.009	0.029	515.3	0.022	0.121	513.1	0.018
37	518.2	0.005	0.103	517.6	0.005	0.037	518.9	0.018
38	531.8	0.005	0.094	532.0	0.001	0.127	531.8	0.003
39	545.4	0.003	0.127	544.4	0.002	0.095	542.3	0.007
40	575.7	0.006	0.051	575.3	0.006	0.071	574.5	0.006
41	583.8	0.000	0.022	582.6	0.001	0.080	582.4	0.002
42	586.2	0.001	0.009	585.0	0.002	0.006	584.7	0.003
43	608.7	0.001	0.014	607.5	0.001	0.031	606.6	0.006

Mode	ν_i@S_1	S_1-T_1	S_1-T_2	ν_i@S1'	S_1'-T_1	S_1'-T_2	ν_i@T_1	T_1-S_1
44	613.6	0.008	0.170	613.0	0.007	0.128	612.3	0.015
45	617.3	0.009	0.099	617.3	0.007	0.015	617.9	0.012
46	619.7	0.005	0.043	619.7	0.006	0.118	620.0	0.005
47	636.8	0.002	0.051	636.7	0.005	0.079	635.5	0.004
48	642.0	0.002	0.015	641.5	0.003	0.126	641.4	0.004
49	665.7	0.007	0.029	664.8	0.004	0.052	663.6	0.008
50	685.8	0.007	0.040	685.2	0.007	0.004	685.2	0.013
51	703.7	0.002	0.078	703.4	0.003	0.042	703.3	0.004
52	722.1	0.026	0.038	721.7	0.029	0.116	720.7	0.038
53	729.6	0.002	0.029	727.7	0.006	0.035	725.1	0.009
54	742.6	0.024	0.009	742.2	0.025	0.047	741.8	0.028
55	750.1	0.003	0.053	748.6	0.003	0.028	747.6	0.005
56	757.2	0.000	0.011	755.5	0.000	0.021	754.4	0.002
57	768.1	0.001	0.083	768.0	0.002	0.049	767.3	0.008
58	770.7	0.009	0.021	768.9	0.012	0.046	767.9	0.003
59	774.9	0.001	0.059	772.9	0.003	0.105	771.7	0.002
60	778.6	0.010	0.040	778.8	0.012	0.073	778.6	0.006
61	801.1	0.007	0.024	799.7	0.007	0.010	797.8	0.011
62	804.3	0.004	0.007	802.9	0.008	0.010	801.3	0.013
63	806.0	0.016	0.015	804.5	0.015	0.071	803.8	0.019
64	810.0	0.002	0.178	808.9	0.003	0.142	807.5	0.003
65	873.7	0.001	0.014	873.4	0.001	0.017	873.9	0.002
66	889.8	0.009	0.033	888.8	0.009	0.005	888.0	0.012
67	894.2	0.010	0.022	893.2	0.007	0.023	892.7	0.015
68	905.6	0.009	0.015	904.7	0.010	0.078	903.3	0.010
69	907.9	0.003	0.050	906.6	0.005	0.094	905.6	0.005
70	923.1	0.008	0.001	921.7	0.009	0.030	922.8	0.012
71	925.8	0.004	0.018	924.3	0.006	0.097	923.7	0.003
72	958.5	0.003	0.293	956.8	0.001	0.134	957.5	0.004
73	960.9	0.013	0.055	959.5	0.019	0.118	959.3	0.011
74	968.5	0.003	0.050	967.2	0.001	0.124	966.3	0.001
75	970.0	0.002	0.082	969.4	0.003	0.065	968.5	0.005
76	972.4	0.002	0.029	971.5	0.005	0.116	970.5	0.007
77	974.7	0.002	0.124	973.9	0.003	0.020	973.6	0.004
78	975.5	0.002	0.057	974.4	0.002	0.102	974.1	0.003
79	1004.5	0.008	0.101	1003.5	0.010	0.009	1004.1	0.010
80	1009.2	0.002	0.022	1008.7	0.002	0.102	1007.8	0.006
81	1011.7	0.004	0.131	1011.2	0.006	0.027	1011.1	0.007
82	1013.0	0.006	0.046	1012.2	0.003	0.083	1011.9	0.008
83	1017.3	0.008	0.139	1016.9	0.010	0.037	1018.9	0.016
84	1025.9	0.006	0.057	1026.0	0.007	0.077	1026.3	0.006
85	1049.8	0.001	0.002	1049.3	0.002	0.016	1049.4	0.001
86	1052.3	0.014	0.030	1051.8	0.012	0.042	1052.0	0.020
87	1053.0	0.003	0.128	1052.3	0.003	0.004	1052.6	0.003
88	1053.1	0.003	0.029	1052.4	0.001	0.060	1053.1	0.004
89	1094.0	0.007	0.084	1093.6	0.007	0.052	1094.9	0.008
90	1102.5	0.012	0.095	1101.8	0.015	0.030	1107.2	0.020

Mode	ν_i@S_1	S_1-T_1	S_1-T_2	ν_i@S1'	S_1'-T_1	S_1'-T_2	ν_i@T_1	T_1-S_1
91	1123.6	0.009	0.045	1123.1	0.006	0.062	1122.0	0.015
92	1124.9	0.002	0.115	1124.4	0.004	0.119	1125.3	0.008
93	1143.5	0.002	0.073	1143.4	0.003	0.065	1144.6	0.003
94	1164.9	0.001	0.080	1164.4	0.002	0.003	1165.2	0.005
95	1168.6	0.001	0.073	1168.4	0.005	0.147	1168.0	0.001
96	1170.5	0.001	0.104	1170.0	0.001	0.012	1169.5	0.003
97	1170.8	0.002	0.036	1170.2	0.001	0.103	1169.6	0.001
98	1181.2	0.002	0.066	1180.2	0.007	0.108	1180.6	0.011
99	1181.6	0.004	0.133	1181.1	0.004	0.076	1181.5	0.008
100	1211.2	0.007	0.010	1210.0	0.007	0.014	1204.4	0.010
101	1244.3	0.017	0.133	1243.5	0.019	0.065	1246.5	0.032
102	1247.3	0.029	0.037	1246.7	0.026	0.114	1246.8	0.027
103	1259.8	0.001	0.087	1259.4	0.001	0.054	1260.1	0.004
104	1274.6	0.007	0.108	1274.3	0.009	0.085	1273.2	0.006
105	1302.3	0.001	0.027	1302.1	0.004	0.102	1302.0	0.007
106	1312.8	0.008	0.100	1312.1	0.009	0.027	1314.5	0.014
107	1340.3	0.013	0.067	1340.3	0.010	0.117	1339.5	0.016
108	1340.5	0.005	0.073	1340.4	0.002	0.007	1340.6	0.002
109	1345.7	0.012	0.169	1345.5	0.014	0.137	1343.2	0.010
110	1365.8	0.004	0.251	1365.6	0.004	0.207	1368.9	0.006
111	1390.2	0.003	0.081	1388.0	0.005	0.036	1392.9	0.007
112	1400.9	0.029	0.091	1398.6	0.034	0.125	1397.7	0.044
113	1407.0	0.006	0.167	1406.0	0.006	0.159	1403.5	0.002
114	1412.8	0.009	0.078	1412.2	0.009	0.092	1407.5	0.012
115	1423.1	0.038	0.021	1422.9	0.039	0.053	1422.3	0.055
116	1431.3	0.004	0.187	1429.8	0.003	0.089	1428.2	0.006
117	1457.6	0.012	0.050	1455.9	0.016	0.073	1454.1	0.026
118	1471.2	0.009	0.155	1469.9	0.011	0.026	1472.0	0.015
119	1478.5	0.009	0.075	1477.8	0.010	0.094	1478.2	0.014
120	1501.4	0.017	0.059	1500.9	0.020	0.077	1500.4	0.023
121	1509.0	0.001	0.115	1509.0	0.002	0.053	1506.9	0.003
122	1516.9	0.004	0.106	1516.6	0.004	0.078	1515.5	0.007
123	1525.3	0.010	0.049	1525.2	0.009	0.056	1523.6	0.056
124	1527.7	0.006	0.096	1528.4	0.005	0.135	1524.2	0.009
125	1531.3	0.048	0.124	1530.8	0.044	0.127	1525.4	0.076
126	1555.9	0.003	0.051	1555.3	0.003	0.077	1554.5	0.004
127	1567.2	0.063	0.146	1566.6	0.060	0.194	1559.4	0.079
128	1596.7	0.006	0.030	1596.1	0.009	0.033	1590.0	0.005
129	1639.6	0.007	0.108	1639.3	0.008	0.074	1641.1	0.012
130	1642.9	0.003	0.083	1642.2	0.003	0.008	1644.9	0.008
131	1649.5	0.003	0.061	1649.2	0.003	0.127	1650.3	0.014
132	1658.2	0.024	0.084	1657.9	0.019	0.096	1657.5	0.018
133	1659.7	0.004	0.103	1659.3	0.007	0.114	1659.9	0.012
134	1660.4	0.002	0.130	1660.3	0.003	0.050	1660.3	0.003
135	1678.9	0.002	0.054	1679.0	0.001	0.036	1677.8	0.001
136	1711.4	0.040	0.016	1711.1	0.048	0.059	1707.7	0.061
137	2295.4	0.003	0.038	2291.8	0.003	0.037	2294.2	0.003

Mode	ν_i@S_1	S_1-T_1	S_1-T_2	ν_i@S1'	S_1'-T_1	S_1'-T_2	ν_i@T_1	T_1-S_1
138	2325.5	0.054	0.024	2322.3	0.048	0.005	2324.4	0.043
139	3205.3	0.002	0.007	3205.9	0.001	0.005	3205.3	0.002
140	3205.6	0.002	0.006	3206.0	0.001	0.006	3205.5	0.002
141	3206.3	0.001	0.008	3206.6	0.001	0.001	3205.9	0.001
142	3206.8	0.001	0.004	3206.8	0.002	0.006	3206.5	0.001
143	3216.2	0.001	0.005	3216.4	0.001	0.017	3215.7	0.002
144	3216.6	0.001	0.009	3216.7	0.001	0.009	3216.3	0.002
145	3217.0	0.001	0.006	3217.4	0.001	0.016	3216.8	0.001
146	3217.7	0.004	0.011	3217.8	0.002	0.061	3217.4	0.002
147	3219.8	0.001	0.004	3221.9	0.001	0.003	3219.2	0.001
148	3221.9	0.005	0.004	3223.8	0.005	0.008	3221.2	0.006
149	3226.6	0.005	0.002	3226.6	0.001	0.003	3226.1	0.001
150	3227.4	0.002	0.002	3226.7	0.002	0.012	3226.5	0.001
151	3227.7	0.003	0.008	3227.5	0.001	0.003	3227.6	0.003
152	3228.5	0.001	0.012	3227.8	0.006	0.018	3227.9	0.003
153	3237.1	0.002	0.036	3237.9	0.001	0.024	3235.5	0.004
154	3238.2	0.004	0.008	3238.8	0.005	0.022	3236.7	0.010
155	3244.4	0.002	0.010	3244.1	0.001	0.015	3241.4	0.003
156	3245.3	0.001	0.008	3245.8	0.001	0.050	3242.5	0.006

Fig. S10 Fragment-based analysis for the low-lying singlet and triplet state DFT/MRCI-R2016 wavefunctions calculated at the S_1' and T_2 minima of **2CzPN**.

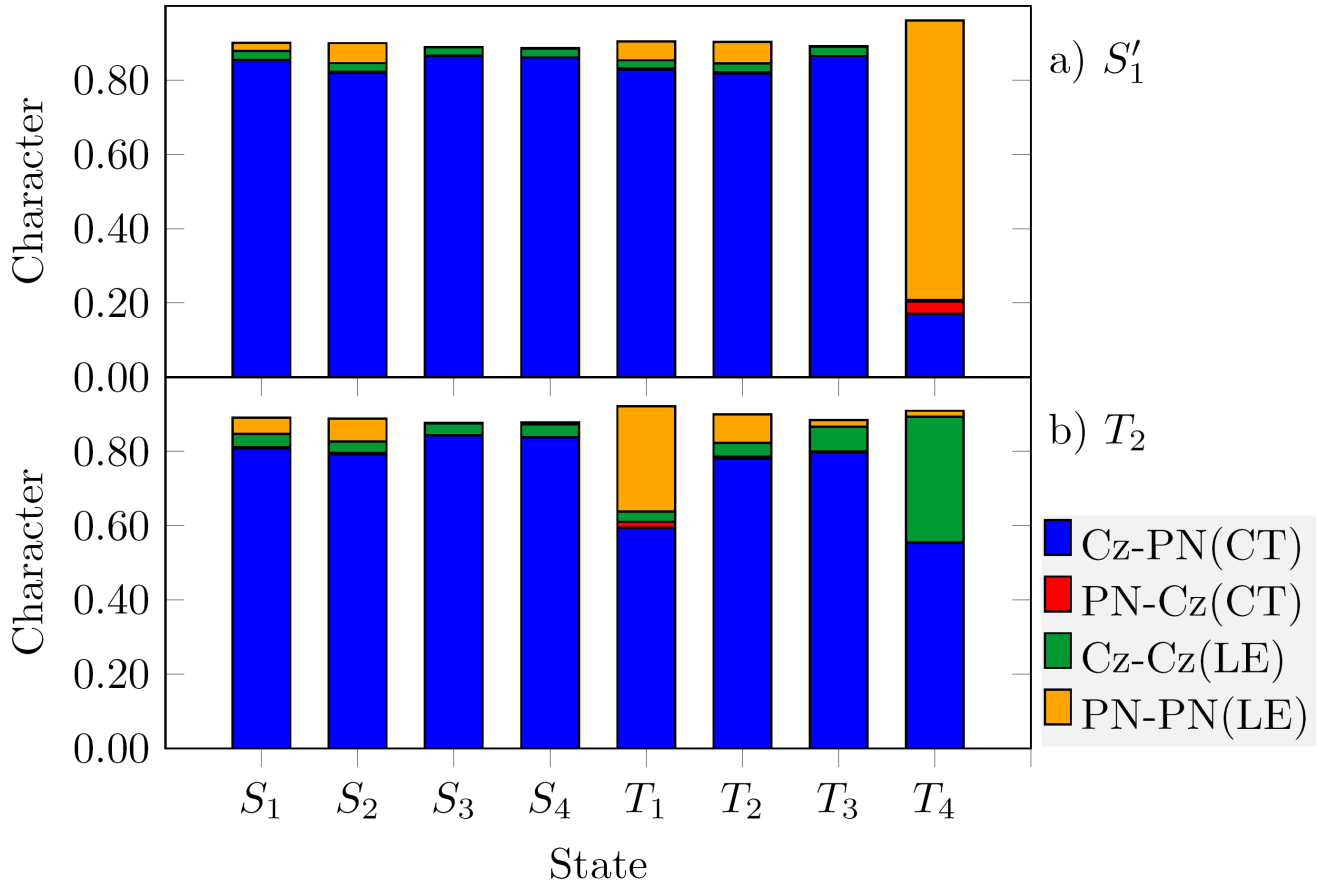
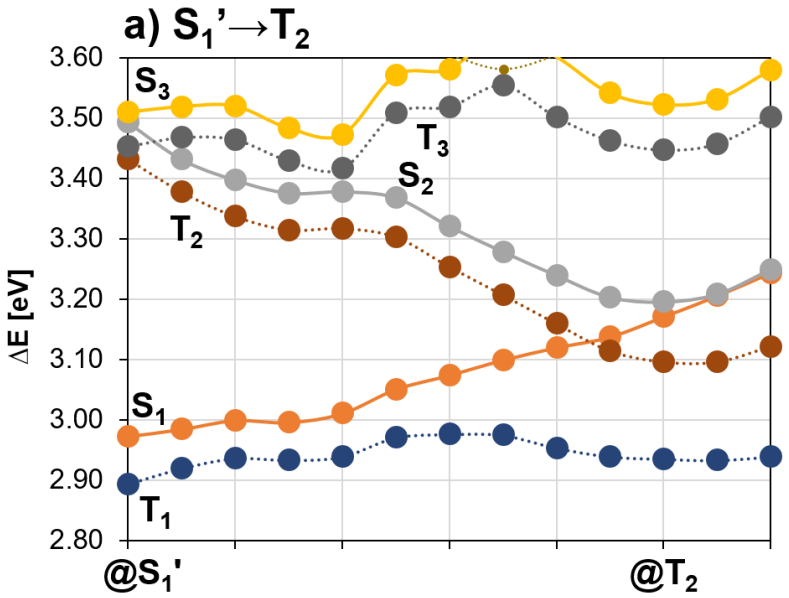


Fig. S11 DFT/MRCI-R2016 energies calculated at linear interpolated pathways (LIPs) between target electronic state minima of **2CzPN**. Dashed lines correspond to triplet state PESs while continuum lines correspond to singlet states. Excitation energies calculated relative to the S_0 state at its corresponding minimum.



Cartesian coordinates for the optimized structures

S_0

H	-1.2257387	0.1246830	-0.0481976
C	-0.4032055	0.0336602	0.6633205
C	1.7260656	-0.1213609	2.4405020
C	0.6542922	-0.8335650	0.3871090
C	-0.4166625	0.8296167	1.8113968
C	0.6617764	0.7367841	2.7280028
C	1.7431403	-0.9037309	1.2853726
H	2.5428169	-0.2039069	3.1597109
C	0.6308074	-1.6191586	-0.8075789
N	0.5913717	-2.2471982	-1.7806981
C	2.8475989	-1.7783555	1.0400550
N	3.7524441	-2.4796641	0.8602139
N	0.6924641	1.4862300	3.9063718
N	-1.4961556	1.6888287	2.0299134
C	-0.3414348	1.5902477	4.8404237
C	-2.0959952	2.1815983	6.8965180
C	-0.0212479	2.6099766	5.7643485
C	-1.5020497	0.8291131	4.9588971
C	-2.3799431	1.1486920	5.9904438
C	-0.9126617	2.9064817	6.7986217
H	-1.7245872	0.0093737	4.2739010
H	-3.3072166	0.5778926	6.0921521
H	-0.6810850	3.6953504	7.5198412
H	-2.8070377	2.4075351	7.6959940
C	1.6871641	2.4125430	4.2376809
C	3.2843075	4.4417452	5.2427558
C	1.2727982	3.1329535	5.3815794
C	2.8811921	2.7054118	3.5796686
C	3.6731308	3.7268538	4.1004965
C	2.0843038	4.1521694	5.8850237
H	3.1898445	2.1667732	2.6804785
H	4.6168196	3.9728154	3.6050942
H	1.7737006	4.7190638	6.7671478
H	3.9297922	5.2360450	5.6274353
C	-2.8290768	1.2811228	2.1495966
C	-5.5393909	0.9588229	2.6278782
C	-3.6020954	2.3812952	2.5870037
C	-3.3901239	0.0179578	1.9654304
C	-4.7549230	-0.1252520	2.2078593
C	-4.9683893	2.2128268	2.8227290
H	-2.7885745	-0.8389559	1.6527443
H	-5.2199123	-1.1051214	2.0663319
H	-5.5769486	3.0548580	3.1642678
H	-6.6081745	0.8135281	2.8071956
C	-1.4135307	3.0433858	2.3624095
C	-1.7663833	5.6833232	3.1118558
C	-0.3120978	3.8952165	2.3218941
C	-2.6991247	3.5038981	2.7245928
C	-2.8706365	4.8372046	3.1056372
C	-0.5043047	5.2164502	2.7147045
H	0.6700323	3.5500011	1.9948086
H	-3.8585619	5.2081076	3.3925982
H	0.3496088	5.8997280	2.7095891
H	-1.8836062	6.7274300	3.4149136

S_0'

H	-0.01688060	0.54647780	3.39174190
C	-0.48870760	1.00742570	2.52187820
C	-1.61469890	2.21869600	0.29699210
C	-1.30549550	2.12413960	2.69702860
C	-0.21801680	0.48036690	1.25380610
C	-0.80604330	1.09044490	0.11763960
C	-1.87147740	2.74812350	1.56139790
H	-2.08163230	2.67245170	-0.57927350
C	-1.53883540	2.62884850	4.01542290
N	-1.71574380	3.01819720	5.09261290
C	-2.71593960	3.89616480	1.68857380
N	-3.40056240	4.82799830	1.76732460
N	-0.61294940	0.60199560	-1.17942830
N	0.62998770	-0.62830140	1.15461160
C	-0.16790110	1.36374520	-2.26389450
C	0.71087240	2.40693100	-4.67936690
C	-0.13465970	0.54429030	-3.41490050
C	0.24958200	2.69558650	-2.30290120
C	0.68438910	3.20374000	-3.52525730
C	0.30722130	1.07646550	-4.62948990
H	0.24452960	3.32717240	-1.41079810
H	1.01157390	4.24618910	-3.58106870
H	0.33784330	0.45219480	-5.52722720
H	1.05597120	2.83649350	-5.62401100
C	-0.89239730	-0.69152640	-1.63128700
C	-1.32784080	-3.05478150	-3.01489390
C	-0.60018840	-0.76451190	-3.01216640
C	-1.43193720	-1.77667670	-0.94116210
C	-1.63767850	-2.95721070	-1.65001800
C	-0.81702860	-1.95998970	-3.70361030
H	-1.69515730	-1.71515500	0.11642170
H	-2.05208690	-3.82370140	-1.12643470
H	-0.59436190	-2.02872550	-4.77238860
H	-1.50038980	-3.99755120	-3.54165810
C	1.80707400	-0.71094960	0.40428470
C	4.20269160	-1.35188830	-0.83622920
C	2.39098460	-1.98123290	0.61163620
C	2.42443210	0.25527030	-0.38955670
C	3.62314330	-0.08610500	-1.01009630
C	3.59633090	-2.30075000	-0.02027610
H	1.99803040	1.25120120	-0.52318630
H	4.12033260	0.65371000	-1.64422660
H	4.05765190	-3.28075700	0.13232890
H	5.14471590	-1.58805310	-1.33912630
C	0.46861050	-1.82498090	1.85918840
C	0.56756470	-4.36693460	2.96548740
C	-0.55996870	-2.21966280	2.71701120
C	1.53600980	-2.69308700	1.53593880
C	1.58123150	-3.97195670	2.09825900
C	-0.49207710	-3.49842040	3.26623140
H	-1.39774510	-1.55887160	2.95399760
H	2.40198200	-4.65310840	1.85545490
H	-1.28429090	-3.82780500	3.94502980
H	0.59250650	-5.36373770	3.41464510

S_1

H	-0.4367595	-1.1876881	-3.3905492
C	0.2530677	-1.4511440	-2.5864127
C	2.0514475	-2.0895804	-0.5085810
C	1.2269214	-2.4456267	-2.8145028
C	0.1709539	-0.8022118	-1.3793565
C	1.0876281	-1.1309800	-0.3167529
C	2.1676151	-2.7702027	-1.7384257
H	2.7332155	-2.3421878	0.3057614
C	1.2741276	-3.0926863	-4.0654117
N	1.2974511	-3.6138488	-5.1094978
C	3.1737038	-3.7442069	-1.8961950
N	4.0121544	-4.5490666	-2.0034144
N	0.8643743	-0.4791853	0.9402775
N	-0.7358187	0.2781785	-1.1245471
C	0.0194135	-0.9621761	1.9163149
C	-1.6875776	-1.4688584	4.0245699
C	-0.2973949	0.0813026	2.8264468
C	-0.5004696	-2.2533110	2.0529780
C	-1.3522741	-2.4910298	3.1300848
C	-1.1667692	-0.1752747	3.8779620
H	-0.2307292	-3.0372237	1.3440598
H	-1.7664011	-3.4909358	3.2745792
H	-1.4396037	0.6118007	4.5842248
H	-2.3625589	-1.6826710	4.8558546
C	1.1511953	0.8417079	1.2144822
C	1.3345477	3.4575849	2.0775686
C	0.4268717	1.2525543	2.3650374
C	1.9915892	1.7133479	0.5149643
C	2.0677114	3.0285650	0.9650347
C	0.5182821	2.5715359	2.7923880
H	2.5747537	1.3585758	-0.3345962
H	2.7075355	3.7373713	0.4362627
H	-0.0392555	2.9161785	3.6660015
H	1.4123139	4.4970468	2.4026720
C	-1.8403218	0.2119015	-0.2997803
C	-3.9615031	0.5645558	1.4315538
C	-2.2368953	1.5259151	0.0638748
C	-2.5123960	-0.9225153	0.1645559
C	-3.5779324	-0.7227910	1.0381939
C	-3.3020676	1.6981036	0.9398998
H	-2.2177381	-1.9171956	-0.1695385
H	-4.1199614	-1.5875837	1.4251351
H	-3.6188439	2.6976970	1.2451424
H	-4.7991083	0.6871333	2.1211862
C	-0.4370108	1.6024538	-1.3601692
C	-0.1764482	4.3465795	-1.4949292
C	0.5779310	2.1339205	-2.1630695
C	-1.3340049	2.4274127	-0.6298288
C	-1.1897676	3.8069478	-0.6900427
C	0.6858009	3.5216759	-2.2258188
H	1.2437791	1.4755680	-2.7226342
H	-1.8539601	4.4648472	-0.1254878
H	1.4590314	3.9709913	-2.8522098
H	-0.0624161	5.4308404	-1.5563266

S_1'

H	-0.7583505	0.5843402	-0.4201523
C	-0.1081312	0.2789935	0.4030996
C	1.5318661	-0.5262716	2.5516938
C	0.8355783	-0.7470661	0.1875351
C	-0.2320179	0.8839248	1.6296235
C	0.6092158	0.4756968	2.7263485
C	1.6784764	-1.1744856	1.3074393
H	2.1756016	-0.8215004	3.3836395
C	0.9363631	-1.3348295	-1.0892261
N	1.0000037	-1.8080280	-2.1542543
C	2.6312096	-2.2041647	1.1736693
N	3.4283077	-3.0522335	1.0862081
N	0.4893419	1.2359308	3.9356083
N	-1.2403772	1.8570011	1.9308413
C	-0.5585561	1.1546834	4.8292408
C	-2.5566694	1.4743492	6.7087995
C	-0.5731094	2.3164141	5.6459879
C	-1.5096043	0.1386612	4.9656326
C	-2.5095525	0.3196237	5.9179209
C	-1.5842678	2.4757333	6.5862504
H	-1.4464781	-0.7658592	4.3593391
H	-3.2707902	-0.4540047	6.0471139
H	-1.6256960	3.3674317	7.2178294
H	-3.3566974	1.5885395	7.4451642
C	1.1971472	2.3916509	4.1860168
C	2.2558490	4.8089177	4.9960925
C	0.5703173	3.1128831	5.2368212
C	2.3477554	2.8606938	3.5434370
C	2.8726334	4.0781154	3.9740206
C	1.0996232	4.3341803	5.6324285
H	2.8138837	2.2790789	2.7455450
H	3.7786692	4.4682002	3.5027446
H	0.6299411	4.9178282	6.4288439
H	2.6855249	5.7646038	5.3084340
C	-2.4933313	1.5379680	2.4081308
C	-5.0056307	1.3515831	3.5370169
C	-3.0869900	2.6905640	2.9880103
C	-3.1430353	0.2994973	2.3801071
C	-4.4149921	0.2286441	2.9460975
C	-4.3457147	2.5889237	3.5654360
H	-2.6661380	-0.5670931	1.9178290
H	-4.9570816	-0.7205969	2.9298017
H	-4.8208651	3.4563858	4.0314332
H	-6.0015428	1.2649869	3.9798442
C	-1.0157210	3.2022447	2.1376896
C	-0.9623432	5.8681729	2.8567446
C	0.1012460	3.9636359	1.7796307
C	-2.1250636	3.7658903	2.8222694
C	-2.0909073	5.1064185	3.1876259
C	0.1093998	5.3053040	2.1527671
H	0.9176854	3.5176637	1.2102421
H	-2.9262926	5.5608542	3.7274274
H	0.9693095	5.9273641	1.8916037
H	-0.9243937	6.9238537	3.1385423

S_2

H	-0.7931883	0.6667337	-0.3434750
C	-0.1383779	0.3690719	0.4794047
C	1.4599632	-0.4559566	2.6275915
C	0.8033725	-0.6540941	0.2607800
C	-0.2976850	0.9697604	1.7075240
C	0.5608146	0.5697364	2.8115416
C	1.6095985	-1.1099692	1.3900147
H	2.1089934	-0.7451915	3.4580104
C	0.9204780	-1.2244533	-1.0237448
N	0.9972656	-1.6843525	-2.0930864
C	2.5452069	-2.1583397	1.2693354
N	3.3277783	-3.0199797	1.1913866
N	0.5853987	1.3653384	3.9893895
N	-1.4004791	1.8284606	1.9668870
C	-0.3707992	1.3797454	4.9657356
C	-2.1047716	1.8472114	7.0606633
C	-0.1144617	2.4573657	5.8661949
C	-1.4757612	0.5278829	5.1163805
C	-2.3374307	0.7799806	6.1716556
C	-0.9944543	2.6861867	6.9173533
H	-1.6438099	-0.2932407	4.4185043
H	-3.2141075	0.1426617	6.3134798
H	-0.8290201	3.5089815	7.6180137
H	-2.8069120	2.0218813	7.8804742
C	1.4912815	2.3980068	4.2319517
C	2.9851427	4.5547094	5.0925209
C	1.0927765	3.1037846	5.3903840
C	2.6314059	2.7358761	3.5088857
C	3.3711484	3.8321653	3.9567773
C	1.8473895	4.1933990	5.8207123
H	2.9261602	2.1634578	2.6265104
H	4.2719393	4.1265581	3.4110833
H	1.5588986	4.7559290	6.7130527
H	3.5878276	5.4060238	5.4201316
C	-2.6972953	1.3950229	2.2426770
C	-5.3478044	1.0106457	2.9142077
C	-3.4790981	2.4989153	2.6539361
C	-3.2192304	0.1088191	2.1413776
C	-4.5600143	-0.0664914	2.4895630
C	-4.8158053	2.3012796	2.9946299
H	-2.5974587	-0.7239556	1.8052313
H	-5.0023399	-1.0643833	2.4229607
H	-5.4407005	3.1390892	3.3164581
H	-6.3958287	0.8415407	3.1756929
C	-1.3335155	3.1778238	2.1742603
C	-1.6455868	5.8469128	2.8012858
C	-0.2282362	4.0292174	2.0241051
C	-2.6031571	3.6535456	2.6207497
C	-2.7502876	4.9991697	2.9360046
C	-0.4025590	5.3653257	2.3471314
H	0.7286542	3.6412235	1.6730435
H	-3.7081848	5.3907403	3.2885483
H	0.4398465	6.0553815	2.2518651
H	-1.7483838	6.9061712	3.0522832

T_1

H	-0.5081960	-1.2917378	-3.3462221
C	0.2246134	-1.5083175	-2.5652706
C	2.1009413	-2.0593690	-0.5335232
C	1.2191541	-2.4770133	-2.8074954
C	0.1616633	-0.8352636	-1.3688399
C	1.1192465	-1.1201124	-0.3275467
C	2.1925078	-2.7667970	-1.7491984
H	2.8258485	-2.2658284	0.2573706
C	1.2517531	-3.1360673	-4.0526104
N	1.2566500	-3.6697933	-5.0904621
C	3.2089123	-3.7289992	-1.9133921
N	4.0601016	-4.5193645	-2.0269131
N	1.0171666	-0.3427331	0.8685264
N	-0.8610491	0.1151990	-1.0597963
C	-0.0117350	-0.4392814	1.7855123
C	-1.9680637	-0.1577703	3.7141287
C	-0.0381278	0.7288870	2.5900785
C	-0.9263178	-1.4819768	1.9590857
C	-1.9069529	-1.3196104	2.9355469
C	-1.0284204	0.8692133	3.5556826
H	-0.8498989	-2.3930650	1.3638583
H	-2.6404341	-2.1145169	3.0931934
H	-1.0767469	1.7647166	4.1812322
H	-2.7515841	-0.0574338	4.4699256
C	1.7025054	0.8316880	1.0942459
C	2.6991204	3.2943501	1.8460416
C	1.0761732	1.5487923	2.1488438
C	2.8218497	1.3291454	0.4184707
C	3.3153838	2.5688695	0.8187460
C	1.5744781	2.7923252	2.5151800
H	3.2871176	0.7541791	-0.3847696
H	4.1953215	2.9825941	0.3189542
H	1.1012252	3.3730437	3.3115709
H	3.1045725	4.2682090	2.1337339
C	-2.0999960	-0.2127356	-0.5524062
C	-4.5756321	-0.4142051	0.6535310
C	-2.6992054	0.9437228	0.0147416
C	-2.7265707	-1.4630545	-0.5280052
C	-3.9791459	-1.5422283	0.0769384
C	-3.9394375	0.8346582	0.6299609
H	-2.2454825	-2.3345404	-0.9765192
H	-4.5013624	-2.5022634	0.1047117
H	-4.4154781	1.7052709	1.0889691
H	-5.5565780	-0.5082994	1.1272565
C	-0.6547118	1.4698251	-0.8861952
C	-0.6407573	4.1564731	-0.2470669
C	0.4371227	2.2423079	-1.2926883
C	-1.7596381	2.0307058	-0.1950904
C	-1.7460752	3.3823197	0.1294152
C	0.4265487	3.5947126	-0.9579648
H	1.2483855	1.7971226	-1.8704152
H	-2.5813232	3.8363090	0.6696717
H	1.2676480	4.2254224	-1.2568260
H	-0.6194062	5.2205146	0.0031982

T_2

H	-0.5470791	-1.2278405	-3.2780222
C	0.1879853	-1.4364253	-2.4966040
C	2.0401660	-1.9823610	-0.4749429
C	1.1833104	-2.4005668	-2.7450537
C	0.0913388	-0.7629102	-1.2996869
C	1.0729926	-1.0268698	-0.2573875
C	2.1410784	-2.6966977	-1.6838283
H	2.7694271	-2.1811314	0.3144404
C	1.2159773	-3.0571026	-3.9923040
N	1.2222609	-3.5916729	-5.0293151
C	3.1639045	-3.6546065	-1.8392289
N	4.0205329	-4.4391460	-1.9484242
N	1.0895690	-0.2300662	0.9167007
N	-1.0053149	0.0981003	-1.0356233
C	0.1113719	-0.2083368	1.8740382
C	-1.6605011	0.2693535	3.9331143
C	0.3745136	0.8457381	2.7972869
C	-1.0103538	-1.0414545	1.9910146
C	-1.8939538	-0.7816931	3.0280201
C	-0.5246923	1.0814048	3.8297413
H	-1.1743199	-1.8590173	1.2881743
H	-2.7849200	-1.4046167	3.1424534
H	-0.3542472	1.8870982	4.5488469
H	-2.3773781	0.4506551	4.7385968
C	2.0224261	0.7657181	1.2037925
C	3.5514319	2.8660042	2.1405188
C	1.6151077	1.4612886	2.3661948
C	3.1839801	1.0930751	0.5092200
C	3.9419497	2.1591833	0.9965767
C	2.3875423	2.5212907	2.8348775
H	3.4817210	0.5373583	-0.3826745
H	4.8600123	2.4428592	0.4747173
H	2.0912492	3.0761953	3.7293994
H	4.1688565	3.6939739	2.4989164
C	-2.3193724	-0.3120893	-0.8130049
C	-4.9951159	-0.6504694	-0.2182153
C	-3.0889963	0.8010964	-0.4014395
C	-2.8646339	-1.5866291	-0.9431192
C	-4.2180409	-1.7380137	-0.6355922
C	-4.4376698	0.6266905	-0.1003202
H	-2.2518927	-2.4302011	-1.2686542
H	-4.6782299	-2.7257212	-0.7271064
H	-5.0521630	1.4715012	0.2232328
H	-6.0533361	-0.8011807	0.0116824
C	-0.9171764	1.4439579	-0.8024490
C	-1.1873272	4.1045796	-0.1266843
C	0.2054182	2.2758766	-0.9201653
C	-2.1866878	1.9364043	-0.3794455
C	-2.3131443	3.2770879	-0.0377722
C	0.0525621	3.6088435	-0.5690761
H	1.1583634	1.8806513	-1.2736162
H	-3.2713673	3.6820080	0.2983589
H	0.9099226	4.2834663	-0.6379608
H	-1.2748576	5.1598597	0.1460012