

**Novel molecular descriptor for highly efficient ($\phi_{TADF} > 90\%$)
transition metal TADF Au(III) complexes**

Yu Wang,^a Qian Peng,^{*b} Qi Ou,^a Shiyun Lin,^a Zhigang Shuai,^{*a}

^a MOE Key Laboratory of Organic OptoElectronics and Molecular Engineering, Department of Chemistry, Tsinghua University, Beijing 100084, P. R. China

^b CAS Key Laboratory of Organic Solids, Institute of Chemistry, Beijing National Laboratory for Molecular Sciences, Chinese Academy of Sciences, Beijing 100190, P. R. China

Computational details

Under the time-dependent thermal vibration correlation function (TVCF) formalism based on the Fermi's golden rule (FGR) and the Franck-Condon approximation, the emission spectra $\sigma_{em}(\omega, T)$ can be expressed as

$$\sigma_{em}^{FC}(\omega, T) = \frac{2\omega^3}{3\pi\hbar c^3} |\mu_{fi}|^2 \int_{-\infty}^{\infty} e^{-i(\omega - \omega_{if})t} \rho_{em,0}^{FC}(t, T) dt \quad (1)$$

Here, μ_{fi} is the electronic transition dipole moment between final and initial electronic states; $\rho_{em,0}^{FC}(t, T)$ is the TVCFs and can be formulated as $Z_i^{-1} Tr[e^{-i\tau_f \hat{H}_f} e^{-i\tau_i \hat{H}_i}]$ that can be analytically solved by multidimensional Gaussian integrations; $\tau_i = -i\beta - t/\hbar$, $\tau_f = t/\hbar$, $\beta = (k_B T)^{-1}$ and $\hat{H}_f$ ($\hat{H}_i$) is the harmonic oscillator Hamiltonian of the final (initial) electronic states.

The radiative decay rate constant is the integration over the whole emission spectrum

$$k_r(T) = \int \sigma_{em}^{FC}(\omega, T) d\omega \quad (2)$$

The internal conversion (IC) rate between two electronic states can be written based on the first-order perturbation theory

$$k_{ic} \equiv \frac{1}{\hbar^2} R_{kl} \int_{-\infty}^{\infty} e^{i\omega_{if}t} \rho_{fi}^{ic}(t, T) dt \quad (3)$$

here $R_{kl} = \langle \Phi_f | \hat{p}_{fk} | \Phi_i \rangle \langle \Phi_i | \hat{p}_{fl} | \Phi_f \rangle$ is the nonadiabatic electronic coupling between two electronic states, where $\hat{p}_{fk} = -i\hbar \partial / \partial Q_{fl}$ is the normal mode momentum operator; $\rho_{fi}^{ic}(t, T) = Z_i^{-1} Tr[\hat{p}_{fk} e^{-i\tau_f \hat{H}_f} e^{-i\tau_i \hat{H}_i}]$ is the TVCFs in the IC processes.

The intersystem crossing (ISC) rate between two electronic states can be recast based on the second-order perturbation theory as

$$k_{isc} = k_{isc}^{(0)} + k_{isc}^{(1)} + k_{isc}^{(2)} \quad (4)$$

where

$$k_{isc}^{(0)} \equiv \frac{1}{\hbar^2} |H_{fi}^{SO}|^2 \int_{-\infty}^{\infty} e^{i\omega_{if}t} \rho_{fi}^{(0)}(t) dt \quad (5)$$

$$k_{isc}^{(1)} \equiv \text{Re} \left[\frac{2}{\hbar^2} \sum_k H_{fi}^{SO} T_{if,k} \int_{-\infty}^{\infty} e^{i\omega_{if}t} \rho_{fi}^{(1)}(t) dt \right] \quad (6)$$

$$k_{isc}^{(2)} \equiv \frac{1}{\hbar^2} \sum_{k,l} T_{if,k} T_{fi,l} \int_{-\infty}^{\infty} e^{i\omega_{if}t} \rho_{fi}^{(2)}(t) dt \quad (7)$$

$T_{if,k(l)}$ is the mixed spin-orbit and nonradiative couplings between two electronic states for the $k(l)$ th normal mode; $\rho_{fi}^{(0)}(t)$ is the same with $\rho_{em,0}^{FC}(t,T)$; $\rho_{fi}^{(1)}(t)$ and $\rho_{fi}^{(2)}(t)$ are $Z_i^{-1} \text{Tr} \left[\hat{p}_{fk} e^{-i\tau_f \hat{H}_f} e^{-i\tau_i \hat{H}_i} \right]$ and $Z_i^{-1} \text{Tr} \left[\hat{p}_{fk} e^{-i\tau_f \hat{H}_f} \hat{p}_{fl} e^{-i\tau_i \hat{H}_i} \right]$ respectively. Detail solutions can be found in our previous works.^{1,2,3}

All of the density functional theory (DFT) and time-dependent DFT (TDDFT) were calculated with *Gaussian16* software.⁴ Geometry optimizations were performed for the S_0 , S_1 , and T_1 minimum with the hybrid Perdew, Burke, and Ernzerhof functional (PBE0)^{5,6} and TD-PBE0 (within the Tamm-Dancoff approximation (TDA)) methods. Basis set combining with Stuttgart Dresden ECP (SDD)⁷ was chosen for heavy atom Au(III), and 6-31G(d, p) basis set was adopted for light atoms. The polarizable continuum model (PCM)⁸ for toluene solvent was adopted in order to account for the solvent effect. Vibrational frequency calculations

at the same level of the theory were conducted to affirm the nature of stationary points of geometries. In the calculation of spectral properties, different methods have been employed, as shown in Table S3. Through comparing with experimental results, PBE0 method was chosen in this study.

Spin-orbit coupling (SOC) of singlet and triplet states calculations were carried out with ORCA program⁹ based on the PBE0 functional with DKH-def2-TZVP triplet- ζ basis set for light elements and SARC-DKH-TZVP all-electron relativistically contracted basis set for atom Au.¹⁰ It is demonstrated that $T_1 \rightarrow S_0$ transition dipole moment calculated by ORCA is inaccurate,¹¹ therefore, in consideration of the precision on the $T_1 \rightarrow S_0$ transition dipole in transition metal complexes, Dalton program was employed^{12,13} for calculations at B3LYP^{14,15}/6-31g(d, p)/SDD theoretical level. Natural transition orbitals (NTO) and molecular orbital composition analysis which are calculated by Becke method¹⁶ were conducted with Multiwfn software.¹⁷ All the interconversion rates were calculated using TVCF formalisms in MOMAP package.¹⁸

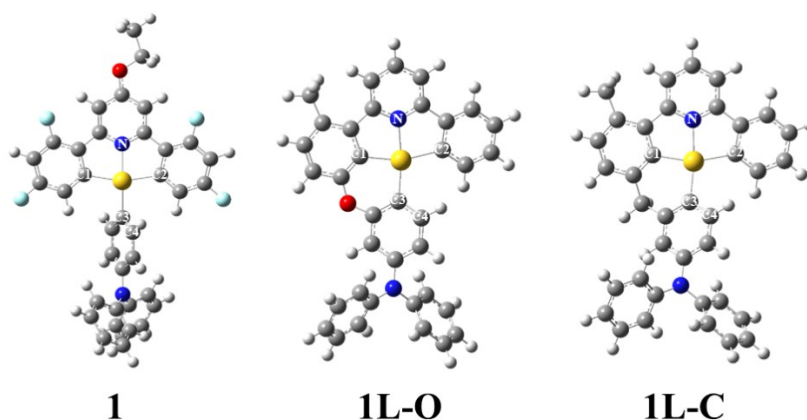


Figure S1. Chemical structures of complexes **1**, **1L-O**, and **1L-C** with corresponding atomic numbers.

Table S1. Calculated and X-ray crystal data of main geometry parameters of complex **1**, and absolute errors are also listed.

	Exp. ^a	Calc.	Abs. Err.
Selected bond lengths (Å)			
Au-N	2.0223	2.0453	0.0230
Au-C1	2.0738	2.0727	0.0011
Au-C2	2.0607	2.0738	0.0131
Au-C3	2.0196	2.0167	0.0029
Selected bond angles (°)			
N-Au-C3	176.05	179.96	3.91
C1-Au-C2	161.54	161.27	0.27
N-Au-C1	80.92	80.69	0.23
C1-Au-C3	99.16	99.33	0.17
Selected dihedral angles (°)			
C2-Au-C3-C4	53.57	58.84	5.27

^a From Ref.¹⁹

Table S2. Calculated main geometry parameters of complexes **1**, **1L-O**, and **1L-C** at their S₀, S₁, and T₁ optimized structures.

	S ₀	S ₁	T ₁	S ₀	S ₁	T ₁
	1	1L-O				
Selected bond lengths (Å)						
Au-N	2.0453	1.9976	1.9986	2.0473	2.0009	1.9954
Au-C1	2.0727	2.0693	2.0699	2.0221	2.0215	2.0213
Au-C2	2.0738	2.0590	2.0612	2.1011	2.0960	2.0935
Au-C3	2.0167	2.0036	2.0021	2.0117	2.0218	2.0097
Selected bond angles (°)						
N-Au-C3	179.96	179.72	179.85	170.39	170.30	170.22
C1-Au-C2	161.27	161.61	161.53	160.51	160.97	160.99
N-Au-C1	80.69	80.65	80.28	80.57	80.92	80.55
C1-Au-C3	99.33	99.61	99.51	91.93	92.01	92.13
Selected dihedral angles (°)						
C2-Au-C3-C4	58.84	96.28	65.92	16.63	19.15	19.11
1L-C						
Selected bond lengths (Å)						
Au-N	2.0515	2.0007	1.9968			
Au-C1	2.0405	2.0369	2.0374			
Au-C2	2.0958	2.0894	2.0881			
Au-C3	2.0199	2.0239	2.0106			
Selected bond angles (°)						
N-Au-C3	168.81	167.80	167.68			
C1-Au-C2	160.42	160.96	161.01			
N-Au-C1	80.12	80.31	80.31			
C1-Au-C3	94.01	93.50	93.55			
Selected dihedral angles (°)						
C2-Au-C3-C4	27.70	30.99	30.13			

Table S3. Calculated emission wavelength of phosphorescence ($\lambda_{em(phos.)}/nm$) and of fluorescence ($\lambda_{em(fluor.)}/nm$) via different methods and corresponding experimental results of complexes **1** and **1L-O** at their optimized T₁ and S₁ geometries^a.

	Method	$\lambda_{em(phos.)}/nm$	$\lambda_{em(fluor.)}/nm$	$\lambda_{em,exp.}(fluor.)/nm$
1	PBE0	529	522	524
	M06	515	509	
	B3LYP	579	572	
1L-O	PBE0	555	528	533
	M06	534	513	
	B3LYP	604	576	

^a Because of a little structural alterations between S₁ and T₁ minimum geometries (reorganization energy is less than 0.045 eV) for complex **1**, the emission properties are all evaluated at its optimized T₁ structures.

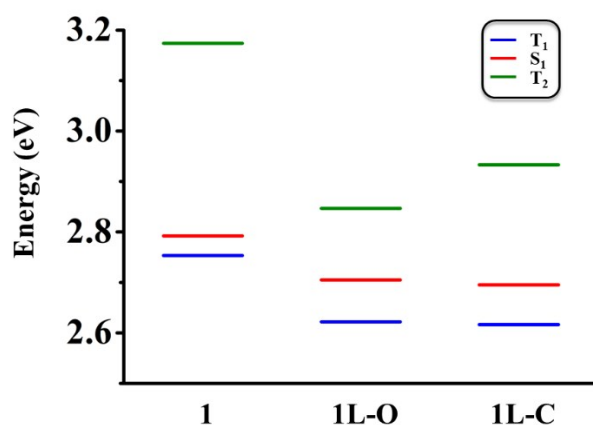


Figure S2. Energies of T₁, S₁ and T₂ excited states of complexes **1**, **1L-O** and **1L-C** at their optimized S₀ geometries.

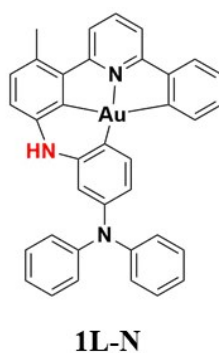


Chart S1. Chemical structure of complex **1L-N**.

Table S4. Calculated energy gap between S₁ and T₁ states ($\Delta E_{S_1-T_1}$) and interconversion rates (s⁻¹), as well as TADF quantum efficiency (ϕ_{TADF}) for **1L-N**.

	$\Delta E_{S_1-T_1}$ (eV)	k_r^S ($\times 10^7$)	k_{nr}^S ($\times 10^4$)	k_r^T ($\times 10^3$)	k_{nr}^T ($\times 10^4$)	k_{isc} ($\times 10^8$)	k_{risc} ($\times 10^8$)	$k_{ravr.}$ ($\times 10^5$)	ϕ_{TADF}
1L-N	0.28	1.97	43.40	4.44	8.16	57.71	0.00023	0.046	0.0009

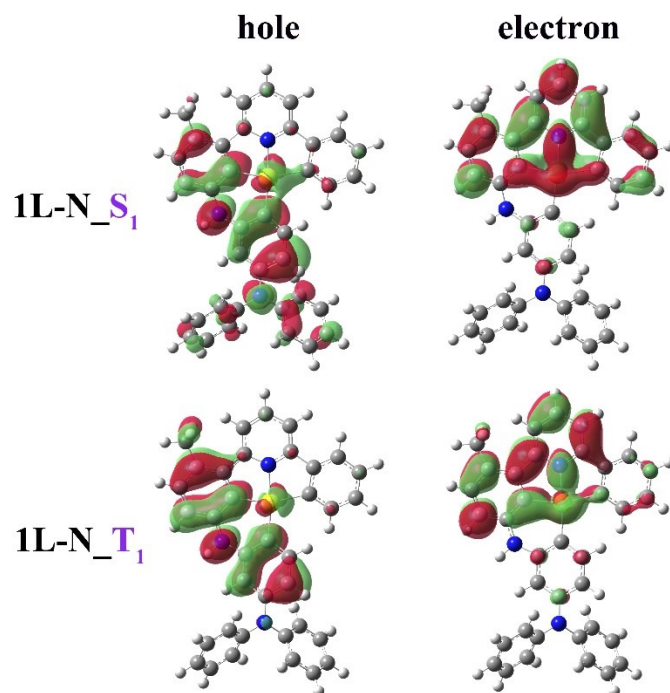


Figure S3. The hole and electron pairs for $S_1 \rightarrow S_0$ and $T_1 \rightarrow S_0$ transitions obtained by natural transition orbital (NTO) analysis at optimized S_1 and T_1 geometries of complex **1L-N**.

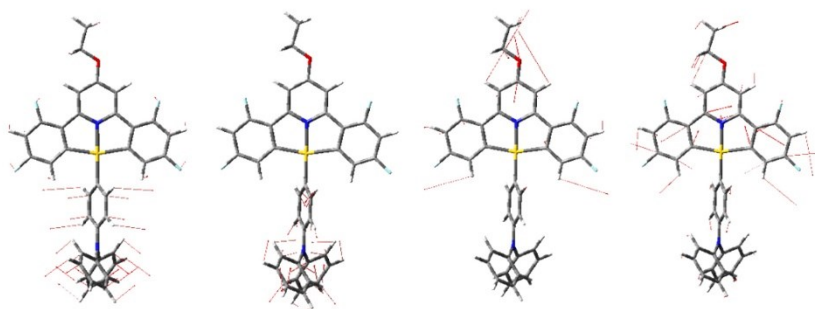
Table S5. The first singlet (S_1) excited states for complexes **1**, **1L-O**, and **1L-C** calculated by TDDFT/PCM calculations (Toluene) at their S_1 optimized geometries. (H = HOMO, L = LUMO)

	Excitation (S_1)	f (S_1)	λ_{em}/nm (S_1)	Assignment (S_1)
1	$H \rightarrow L$ (99%)	0.0419	522	$^1LLCT/^1LMCT$
1L-O	$H \rightarrow L$ (99%)	0.1469	528	$^1LLCT/^1LMCT$
1L-C	$H \rightarrow L$ (99%)	0.1492	527	$^1LLCT/^1LMCT$

Table S6. The first singlet (S_1) and triplet (T_1) excited states with main orbital transitions for complexes **1**, **1L-O**, and **1L-C** calculated by TDDFT/PCM method (Toluene) at their T_1 optimized geometries. And the calculated proportion of atom Au in relevant orbitals as well. (H = HOMO, L = LUMO)

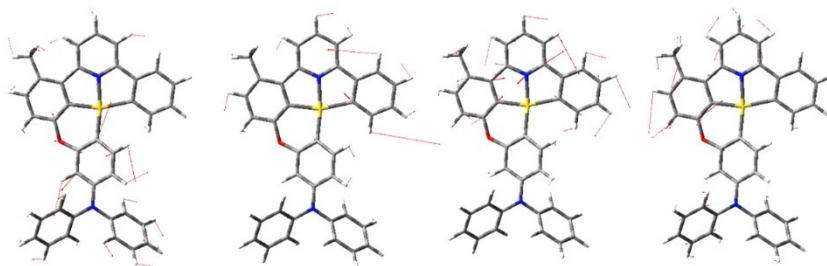
	Excitation (S_1)	Excitation (T_1)	Orbitals	Au%
1	$H \rightarrow L$ (98.7%)	$H \rightarrow L$ (97.4%)	$H - 2$	9.69
		$H - 2 \rightarrow L$ (1.4%)	H	2.66
			L	11.71
1L-O	$H \rightarrow L$ (98.4%)	$H \rightarrow L$ (94.8%)	$H - 1$	4.07
		$H - 1 \rightarrow L$ (2.5%)	H	3.12
			L	9.09
1L-C	$H \rightarrow L$ (98.7%)	$H \rightarrow L$ (95.6%)	$H - 3$	8.62
		$H - 3 \rightarrow L$ (1.1%)	H	3.16
			L	10.21

a)



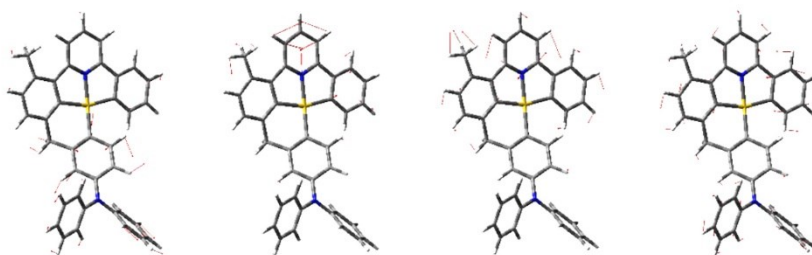
$$\begin{array}{cccc} \omega = 102.69 \text{ cm}^{-1} & \omega = 316.64 \text{ cm}^{-1} & \omega = 1256.87 \text{ cm}^{-1} & \omega = 1515.66 \text{ cm}^{-1} \\ \lambda = 107.81 \text{ cm}^{-1} & \lambda = 89.40 \text{ cm}^{-1} & \lambda = 127.86 \text{ cm}^{-1} & \lambda = 218.17 \text{ cm}^{-1} \end{array}$$

b)



$$\begin{array}{cccc} \omega = 1070.56 \text{ cm}^{-1} & \omega = 1288.96 \text{ cm}^{-1} & \omega = 1425.72 \text{ cm}^{-1} & \omega = 1661.82 \text{ cm}^{-1} \\ \lambda = 66.08 \text{ cm}^{-1} & \lambda = 60.79 \text{ cm}^{-1} & \lambda = 177.80 \text{ cm}^{-1} & \lambda = 82.26 \text{ cm}^{-1} \end{array}$$

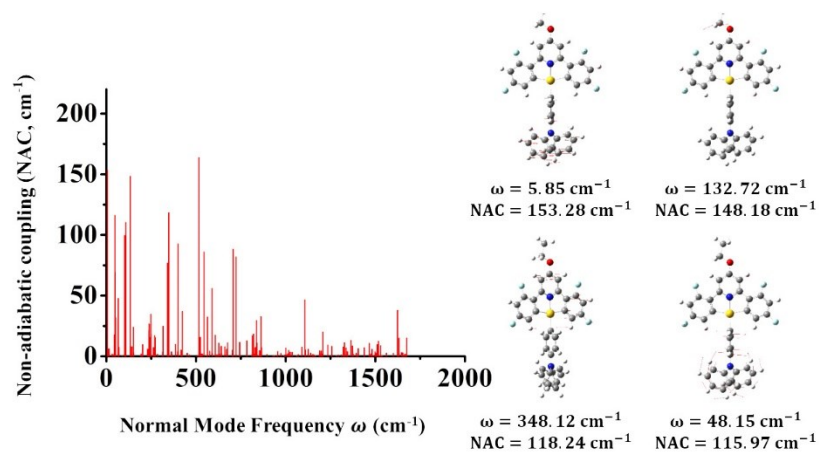
c)



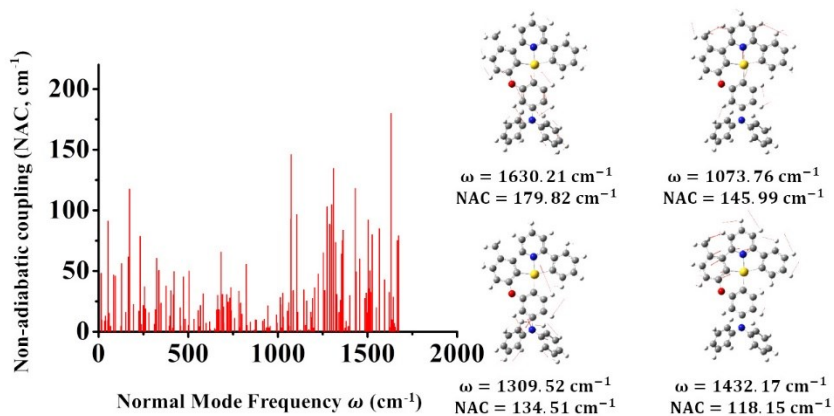
$$\begin{array}{cccc} \omega = 1066.82 \text{ cm}^{-1} & \omega = 1071.80 \text{ cm}^{-1} & \omega = 1414.32 \text{ cm}^{-1} & \omega = 1653.57 \text{ cm}^{-1} \\ \lambda = 54.19 \text{ cm}^{-1} & \lambda = 95.37 \text{ cm}^{-1} & \lambda = 94.76 \text{ cm}^{-1} & \lambda = 57.95 \text{ cm}^{-1} \end{array}$$

Figure S4. Displacement vectors of important vibration modes for complexes **1** (a), **1L-O** (b) and **1L-C** (c) of $T_1 \rightarrow S_0$ transitions.

a)



b)



c)

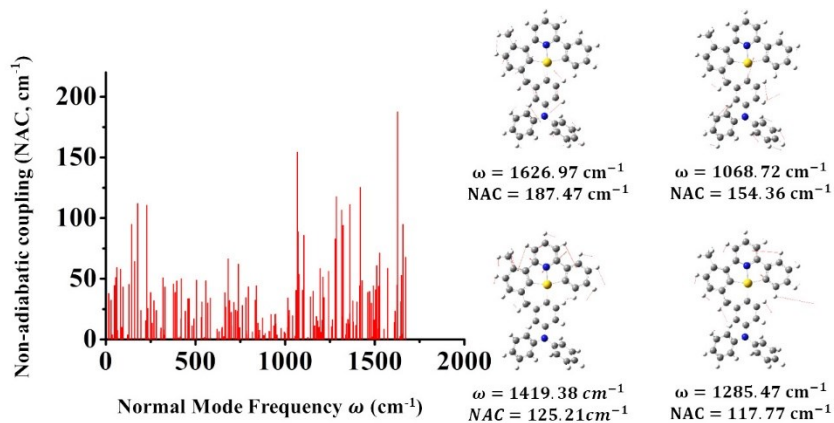


Figure S5. Relationships of non-adiabatic couplings (NAC) and normal modes for complexes **1** (a), **1L-O** (b) and **1L-C** (c) of $S_1 \rightarrow S_0$ transitions, as well as displacement vectors of main vibration modes.

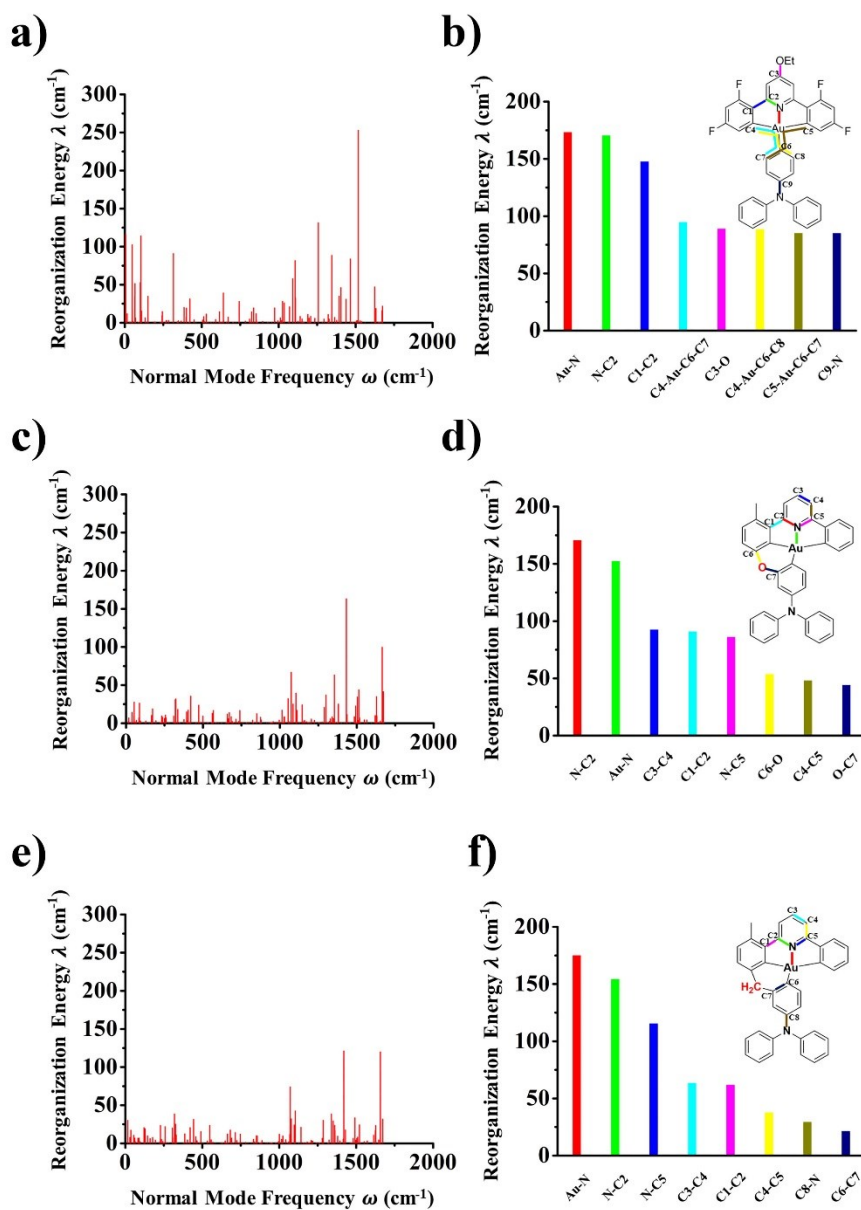
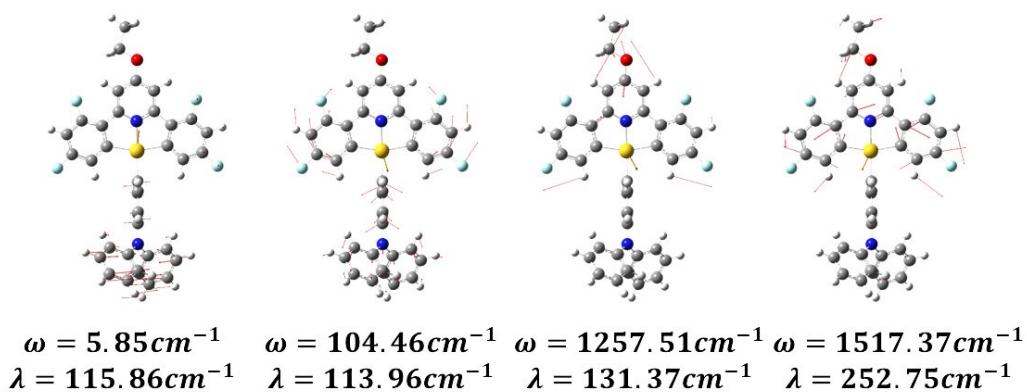
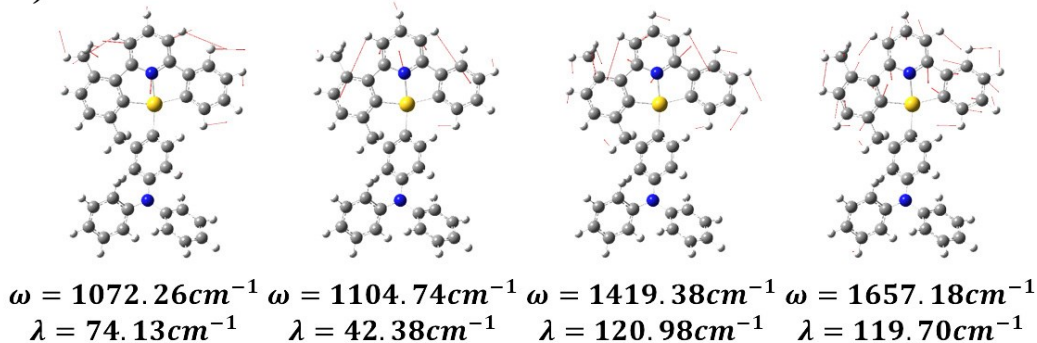


Figure S6. The relationship between normal mode frequencies and reorganization energies of $S_1 \rightarrow S_0$ for complexes **1** (a), **1L-O** (c), **1L-C** (e); the projection of the $S_1 \rightarrow S_0$ reorganization energies onto the internal coordinates for complexes **1** (b), **1L-O** (d), **1L-C** (f).

a)



b)



c)

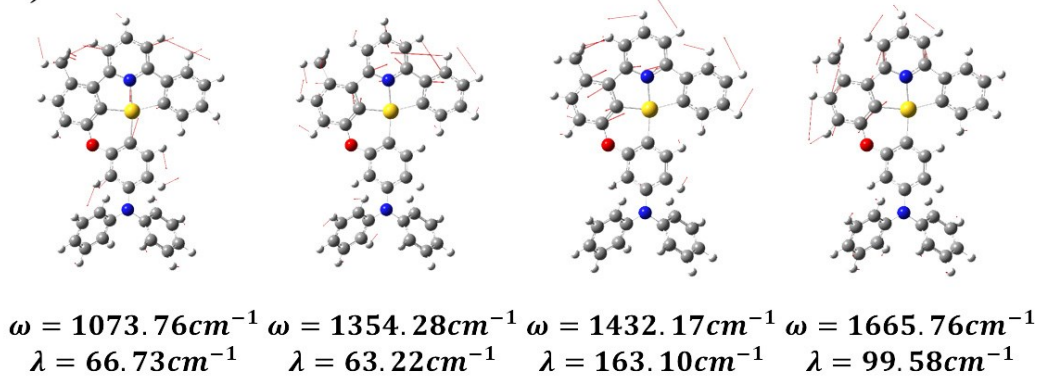


Figure S7. Displacement vectors of important vibration modes for complexes **1** (a), **1L-O** (b) and **1L-C** (c) of $S_1 \rightarrow S_0$ transitions.

Table S7. The first singlet (S_1) excited states for complexes **1L-O1** ~ **1L-O8** calculated by TDDFT/PCM calculations (Toluene) at their S_1 optimized geometries. (H = HOMO, L = LUMO)

	Excitation (S_1)	f (S_1)	λ_{em}/nm (S_1)	Assignment (S_1)
1L-O1	$H \rightarrow L$ (99%)	0.1545	498	$^1LLCT/^1LMCT$
1L-O2	$H \rightarrow L$ (99%)	0.1246	561	$^1LLCT/^1LMCT$
1L-O3	$H \rightarrow L$ (99%)	0.1108	585	$^1LLCT/^1LMCT$
1L-O4	$H \rightarrow L$ (99%)	0.1033	618	$^1LLCT/^1LMCT$
1L-O5	$H \rightarrow L$ (99%)	0.0824	540	$^1LLCT/^1LMCT$
1L-O6	$H \rightarrow L$ (99%)	0.0774	534	$^1LLCT/^1LMCT$
1L-O7	$H \rightarrow L$ (99%)	0.0660	564	$^1LLCT/^1LMCT$
1L-O8	$H \rightarrow L$ (99%)	0.0701	568	$^1LLCT/^1LMCT$

Table S8. Calculated interconversion rates (s^{-1}) among S_0 , S_1 , and T_1 states, and TADF quantum efficiency (ϕ_{TADF}) for complexes **1L-O1** ~ **1L-O8**.

	k_r^S ($\times 10^7$)	k_{nr}^S ($\times 10^4$)	k_r^T ($\times 10^3$)	k_{nr}^T ($\times 10^4$)	k_{isc} ($\times 10^8$)	k_{risc} ($\times 10^8$)	$k_{r_{avr.}}$ ($\times 10^5$)	ϕ_{TADF}
1L-O1	3.67	1.75	2.41	0.34	6.65	0.16	3.70	0.94
1L-O2	2.46	13.40	1.06	3.08	27.00	2.87	4.96	0.97
1L-O3	2.04	4.35	0.69	0.64	13.35	2.20	5.64	0.98
1L-O4	1.67	45.07	0.61	8.52	53.04	9.47	4.93	0.94
1L-O5	1.71	0.49	1.29	2.05	27.63	3.14	4.73	0.98
1L-O6	1.66	2.49	3.53	1.98	49.52	3.15	4.79	0.97
1L-O7	1.30	7.77	2.18	2.86	112	20.54	6.03	0.98
1L-O8	1.35	1.60	0.96	1.41	32.14	7.65	6.28	0.99

Table S9. Calculated energy gap between S_1 and T_1 states ($\Delta E_{S_1T_1}$), energy barrier of $T_1 \rightarrow S_1$ ($\Delta G_{S_1T_1}$), SOC between S_1/S_0 and T_1 states calculated at optimized T_1 geometries, and reorganization energies (λ) between S_1/S_0 and T_1 states for complexes **1L-O1** ~ **1L-O8**.

	$SOC_{S_0T_1}$ (cm^{-1})	$\lambda_{S_0T_1}$ (cm^{-1})	$\Delta E_{S_1T_1}$ (eV)	$SOC_{S_1T_1}$ (cm^{-1})	$\lambda_{S_1T_1}$ (cm^{-1})	$\Delta G_{S_1T_1}$ (eV)
1L-O1	56	1516	0.09	3	142	0.16
1L-O2	71	1556	0.07	3	157	0.11
1L-O3	45	1632	0.06	1	127	0.10
1L-O4	58	1956	0.06	3	127	0.09
1L-O5	107	1999	0.06	6	61	0.17
1L-O6	99	2434	0.06	10	52	0.18
1L-O7	78	2362	0.05	7	54	0.12
1L-O8	82	1920	0.05	4	86	0.08

Table S10. The first singlet (S_1) and triplet (T_1) excited states with main orbital transitions for complexes **1L-O1** ~ **1L-O8** calculated by TDDFT/PCM method (Toluene) at their T_1 optimized geometries. And the calculated proportion of atom Au in relevant orbitals as well. (H = HOMO, L = LUMO)

	Excitation (S_1)	Excitation (T_1)	Orbitals	Au%
1L-O1	$H \rightarrow L$ (98.6%)	$H \rightarrow L$ (94.6%)	$H - 1$	3.14
		$H - 1 \rightarrow L$ (1.2%)	H	2.69
			L	11.77
1L-O2	$H \rightarrow L$ (98.9%)	$H \rightarrow L$ (96.7%)	$H - 1$	4.35
		$H - 1 \rightarrow L$ (1.1%)	H	2.25
			L	9.05
1L-O3	$H \rightarrow L$ (99.2%)	$H \rightarrow L$ (97.6%)	H	1.78
			L	10.22
1L-O4	$H \rightarrow L$ (99.1%)	$H \rightarrow L$ (97.8%)	$H - 1$	4.61
		$H - 1 \rightarrow L$ (0.6%)	H	1.99
			L	7.78
1L-O5	$H \rightarrow L$ (98.6%)	$H \rightarrow L$ (96.0%)	$H - 1$	2.68
		$H - 1 \rightarrow L$ (1.1%)	H	3.23
			L	7.38
1L-O6	$H \rightarrow L$ (98.9%)	$H \rightarrow L$ (96.8%)	$H - 3$	15.52
		$H - 3 \rightarrow L$ (1.2%)	H	2.76
			L	7.03
1L-O7	$H \rightarrow L$ (99.1%)	$H \rightarrow L$ (97.6%)	$H - 3$	13.01
		$H - 3 \rightarrow L$ (0.9%)	H	2.11
			L	6.98
1L-O8	$H \rightarrow L$ (98.9%)	$H \rightarrow L$ (97.0%)	$H - 3$	11.74
		$H - 3 \rightarrow L$ (0.8%)	H	2.40
			L	7.32

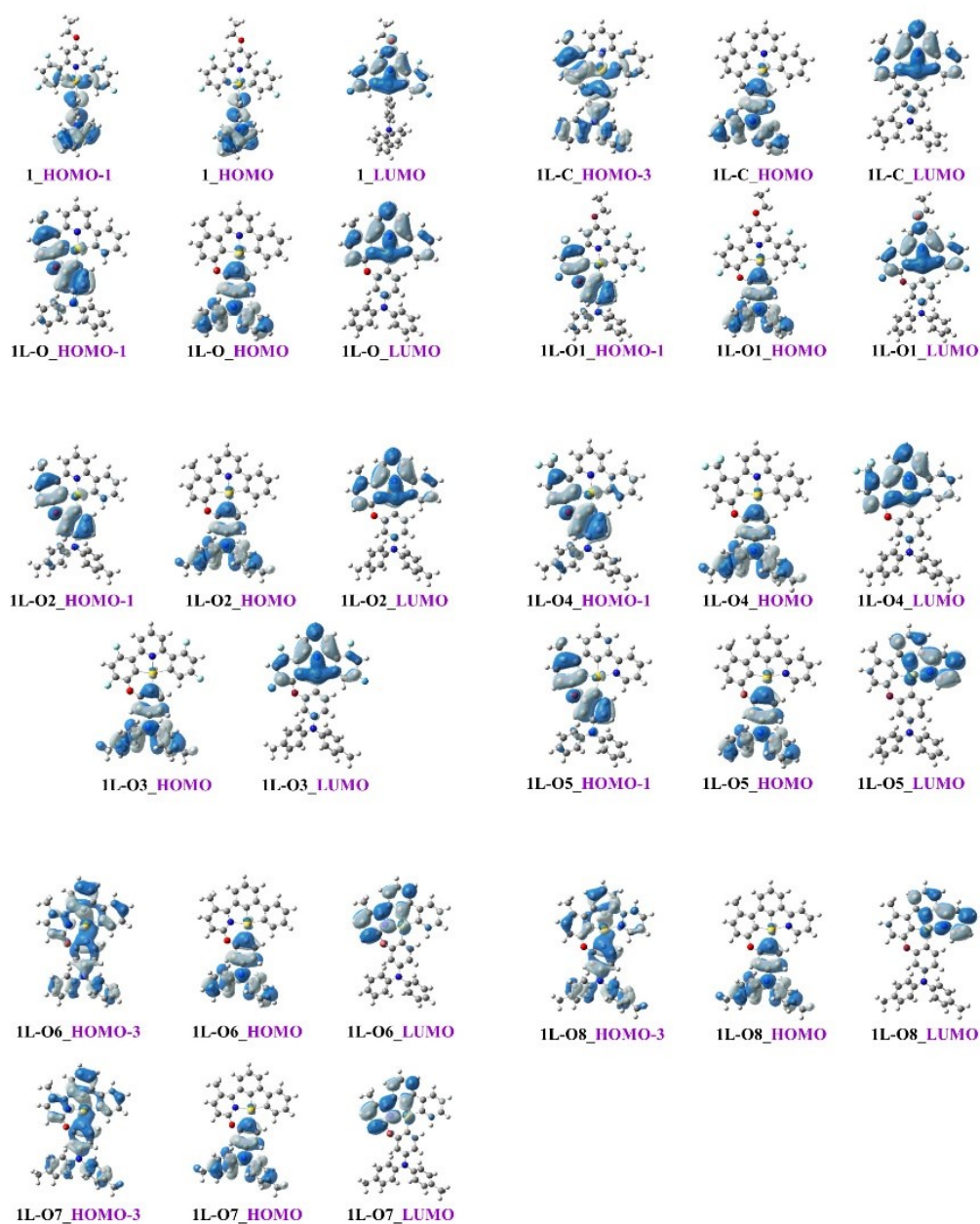


Figure S8. Profiles of the selected frontier orbitals of all Au(III)-TADF complexes investigated in this study at their optimized T_1 geometries.

Coordinates

1L-C: S₀

Au	0.01617700	-0.40911300	-0.21653900
C	-0.00304900	-1.34407400	1.65904300
N	1.94246700	-0.01193600	0.36672500
C	0.71587600	0.49113600	-1.90876300
C	-1.90473000	-0.41034700	-0.84108400
C	-0.94492500	-2.15165300	2.29545700
H	-1.90168500	-2.34095000	1.81554600
C	-0.69154100	-2.73763900	3.53779000
C	0.52847000	-2.53156000	4.17594400
H	0.72766200	-2.98583900	5.14204800
C	1.50057500	-1.75081300	3.56144000
H	2.45956600	-1.61240200	4.05389100
C	1.24941000	-1.16752600	2.31492800
H	-1.44916300	-3.36083200	4.00634400
C	2.27693100	-0.36993200	1.61848600
C	3.51328800	0.04493200	2.11754200
H	3.82763300	-0.22067000	3.11963400
C	4.31864500	0.83022400	1.30468500
C	3.91748000	1.20343500	0.02324000
H	4.56031500	1.83547700	-0.56804300
C	2.68083000	0.76456900	-0.46111500
H	5.27894400	1.17516000	1.67681400
C	2.03301900	1.01509800	-1.77378400
C	2.64160900	1.66255800	-2.87457000
C	1.91376200	1.73409200	-4.06615500
C	0.65631600	1.16241100	-4.20485400
H	0.15027700	1.20813000	-5.16712500
C	0.04704600	0.51894000	-3.12492000
H	2.36469300	2.23638200	-4.91824500
C	-2.25033700	-0.23895300	-2.19632900
C	-2.93781500	-0.40852500	0.10594800
H	-2.69374500	-0.49130800	1.15994100
C	-4.27327900	-0.26377300	-0.25130600
H	-5.04695000	-0.24958400	0.51046700
C	-4.61822800	-0.12840700	-1.59750800
C	-3.59643900	-0.12011700	-2.55083800
H	-3.86280200	-0.00871500	-3.59882200
C	4.01887000	2.26885500	-2.87039200
H	4.10681700	3.09482800	-2.15553700
H	4.79396900	1.53266100	-2.63050300
H	4.25072800	2.67277900	-3.85872100

N	-5.97017600	0.00946800	-1.99072300
C	-6.32176000	0.94506900	-2.98751100
C	-5.70417900	2.20219200	-3.03170100
C	-7.28994500	0.63100800	-3.95077400
C	-6.04470700	3.11647400	-4.02200400
H	-4.95643600	2.45400700	-2.28605200
C	-7.63614800	1.55924600	-4.92609700
H	-7.76746500	-0.34362900	-3.92781700
C	-7.01476300	2.80554300	-4.97283100
H	-5.55526400	4.08637100	-4.03980000
H	-8.38893400	1.29765400	-5.66469000
H	-7.28285400	3.52512500	-5.74048600
C	-6.96293800	-0.78505500	-1.37856300
C	-8.21775100	-0.24467300	-1.06612600
C	-6.70756700	-2.12790900	-1.06948800
C	-9.19316400	-1.03504800	-0.46910600
H	-8.42104000	0.79690100	-1.29452800
C	-7.68385000	-2.90467700	-0.45631600
H	-5.73964500	-2.55498900	-1.31275600
C	-8.93407300	-2.36780800	-0.15575700
H	-10.15975400	-0.59800100	-0.23389600
H	-7.46727200	-3.94397500	-0.22487900
H	-9.69621300	-2.97978500	0.31704500
C	-1.24484000	-0.23807900	-3.32476900
H	-1.73455300	0.12204300	-4.23548000
H	-0.97032600	-1.28377600	-3.53512600
1L-O1: S ₀			
Au	0.02852300	-0.35901000	-0.28297000
C	0.10659100	-1.32303100	1.58379400
N	2.02688800	-0.19672700	0.11787800
C	0.63301200	0.49887900	-2.00682600
C	-1.90307300	-0.23504400	-0.85007600
C	-0.85921400	-2.03769200	2.28325100
H	-1.86626600	-2.16281300	1.90163400
C	-0.54785200	-2.64018300	3.49735100
C	0.71327800	-2.56767800	4.06209600
H	0.94516000	-3.03724800	5.01002200
C	1.68128400	-1.88009500	3.35074400
C	1.43217700	-1.26287800	2.12177300
C	2.47693200	-0.60530700	1.31580200
C	3.81611400	-0.38997600	1.64153600
H	4.19611600	-0.71037000	2.59809000
C	4.63574400	0.24743700	0.70179800
C	4.12209100	0.66511700	-0.53716100

H	4.77143000	1.16032500	-1.24477400
C	2.78560300	0.43359500	-0.81135600
C	2.02612200	0.78280000	-2.02329000
C	2.56560400	1.31506700	-3.19069400
C	1.78831600	1.55130600	-4.31811500
C	0.44271800	1.24274300	-4.27367100
C	-0.15201500	0.71175600	-3.11654900
H	2.22912700	1.96400300	-5.21750500
O	-1.47339400	0.42975800	-3.21329300
C	-2.29181700	0.12967200	-2.15046700
C	-2.95041200	-0.42407900	0.06686800
H	-2.70342600	-0.62614500	1.10242500
C	-4.28951800	-0.31897900	-0.27058600
H	-5.05663400	-0.46015100	0.48355200
C	-4.65109800	-0.02042500	-1.59199800
C	-3.63805900	0.20285600	-2.52024300
H	-3.87194200	0.45892600	-3.54781800
N	-6.00577600	0.07461000	-1.96613700
C	-6.42044800	1.04407700	-2.90903200
C	-5.92475500	2.35246000	-2.84816100
C	-7.33815900	0.70909000	-3.91205800
C	-6.33395500	3.29978000	-3.77970900
H	-5.21741000	2.61852600	-2.06873700
C	-7.75547100	1.66845700	-4.82796600
H	-7.72092800	-0.30534700	-3.96627800
C	-7.25411400	2.96708000	-4.77190900
H	-5.93914300	4.31009500	-3.71910800
H	-8.46789200	1.39208400	-5.60025600
H	-7.57627300	3.71160400	-5.49359000
C	-6.95573000	-0.81421200	-1.41376100
C	-8.22459600	-0.35196000	-1.04180000
C	-6.64512400	-2.16817900	-1.23411900
C	-9.16155900	-1.23008200	-0.50925300
H	-8.46881400	0.69744400	-1.17445300
C	-7.58290600	-3.03458500	-0.68354200
H	-5.66653200	-2.53431900	-1.52886600
C	-8.84733200	-2.57461900	-0.32163600
H	-10.14094200	-0.85462400	-0.22594900
H	-7.32535800	-4.08173900	-0.55118800
H	-9.57939500	-3.25595600	0.10117300
F	2.91040900	-1.83502800	3.89731900
F	-1.49914000	-3.31833300	4.14894700
F	-0.31224500	1.45291900	-5.35176200
F	3.87459100	1.60784900	-3.26764200

O	5.93169200	0.50831700	0.89885600
C	6.54017700	0.12342700	2.13350900
H	6.02102000	0.61779900	2.96431800
H	6.44399900	-0.96190200	2.26356000
C	7.98966400	0.53958100	2.07039400
H	8.07667600	1.62112100	1.93892400
H	8.49403800	0.26197600	2.99976800
H	8.49863700	0.04499100	1.23917400
1L-O2: S ₀			
Au	-0.01686300	-0.22274300	-0.08137900
C	-0.00979600	-1.17560900	1.79131300
N	1.95748200	0.01653200	0.40587400
C	0.65165600	0.64412200	-1.78145300
C	-1.92316400	-0.16344500	-0.72035700
C	-0.96068300	-1.93283600	2.47520900
H	-1.94057700	-2.09487900	2.03562600
C	-0.69005700	-2.51705400	3.71453600
C	0.55999000	-2.36301800	4.30649100
H	0.77229000	-2.81287700	5.27178900
C	1.54554500	-1.64416300	3.64138300
H	2.52951600	-1.55023800	4.09305400
C	1.27678200	-1.06544900	2.39628100
H	-1.45955900	-3.09848200	4.21606400
C	2.32878200	-0.36222000	1.64030400
C	3.62876500	-0.06915200	2.05857800
H	3.97408000	-0.35303900	3.04527200
C	4.46268000	0.61293500	1.18419400
C	4.03135800	0.99508400	-0.08513000
H	4.70116000	1.54091900	-0.73025700
C	2.73029100	0.67992600	-0.48663600
H	5.47290700	0.86304500	1.49461500
C	2.03801800	0.97344400	-1.76617800
C	2.65375400	1.48775000	-2.92706800
C	1.85224900	1.64903700	-4.06647700
C	0.50885300	1.32010300	-4.09002700
H	-0.08694900	1.44574200	-4.98902300
C	-0.08903100	0.81046900	-2.93354300
H	2.31128900	2.04127500	-4.96997400
O	-1.40452800	0.48449200	-3.06466900
C	-2.26236200	0.17768100	-2.04003800
C	-3.00270600	-0.37485900	0.15324400
H	-2.79234300	-0.56682300	1.19893600
C	-4.32851500	-0.30956000	-0.24283000
H	-5.12405600	-0.46671000	0.47803300

C	-4.64030400	-0.03144800	-1.58161800
C	-3.59373500	0.21070000	-2.46746700
H	-3.79095600	0.44965100	-3.50685300
C	4.10800800	1.85454200	-3.04864600
H	4.37491600	2.71129700	-2.41899600
H	4.76966300	1.02318800	-2.78290900
H	4.33598000	2.13336800	-4.08014300
N	-5.97938400	0.02281800	-2.01485200
C	-6.37656500	0.96038000	-2.99640000
C	-5.92584700	2.28489700	-2.94475500
C	-7.24009900	0.58705700	-4.03180100
C	-6.32216800	3.19981400	-3.91172300
H	-5.26381300	2.59200000	-2.14082200
C	-7.64334800	1.51868400	-4.98130800
H	-7.59926900	-0.43622800	-4.08395300
C	-7.18913700	2.83990900	-4.94855400
H	-5.96084700	4.22385700	-3.84906100
H	-8.31855900	1.20560000	-5.77444900
C	-6.93081500	-0.87939300	-1.48705700
C	-8.22490200	-0.44796200	-1.17385500
C	-6.60463600	-2.22445000	-1.27625800
C	-9.16164900	-1.34229100	-0.67039200
H	-8.49362100	0.59176500	-1.33378400
C	-7.54642700	-3.10243200	-0.75419900
H	-5.60902600	-2.57774600	-1.52691600
C	-8.84342500	-2.68421000	-0.44153800
H	-10.16197200	-0.98365400	-0.43839300
H	-7.26998100	-4.14342700	-0.60223400
C	-7.59536300	3.83203100	-6.00195700
H	-6.86538800	3.86423600	-6.82008400
H	-8.56396300	3.57568600	-6.44057800
H	-7.66584200	4.84406200	-5.59207900
C	-9.84920000	-3.63628200	0.14240200
H	-9.78834000	-3.65681100	1.23748100
H	-10.87149200	-3.34907500	-0.12015200
H	-9.68314400	-4.65863800	-0.20993600
1L-O3: S ₀			
Au	-0.01384800	-0.20932200	-0.06674700
C	0.00645800	-1.17564900	1.79866800
N	1.96322400	0.02446400	0.42738000
C	0.63615600	0.67158300	-1.76169000
C	-1.91934400	-0.14956600	-0.72034900
C	-0.96482300	-1.92749200	2.44954300
H	-1.94757500	-2.08742000	2.02056900

C	-0.68911300	-2.52335200	3.67571200
C	0.54053600	-2.40836200	4.29983400
H	0.74404200	-2.87349100	5.25642600
C	1.51589700	-1.68378800	3.63695300
C	1.30179600	-1.07082800	2.39887300
C	2.36138800	-0.37593900	1.64881200
C	3.68134700	-0.10811400	2.02651100
H	4.04652300	-0.40844700	2.99740100
C	4.50927100	0.55397900	1.12581600
C	4.05625200	0.95521800	-0.12787600
H	4.70449400	1.47289200	-0.82070100
C	2.73264400	0.67867000	-0.47001400
H	5.53551100	0.76636600	1.41048400
C	2.01817200	1.00232900	-1.71422900
C	2.59264700	1.55409200	-2.85614500
C	1.86024400	1.76545000	-4.01795300
C	0.52515600	1.41178800	-4.03486900
C	-0.10404000	0.85932800	-2.90574400
H	2.32751400	2.19392500	-4.89634900
O	-1.40877800	0.53415700	-3.06207400
C	-2.26296200	0.20387900	-2.03648600
C	-2.99965700	-0.37563600	0.14899800
H	-2.79267600	-0.56921000	1.19485000
C	-4.32463400	-0.31730700	-0.24786200
H	-5.11807000	-0.48555000	0.47251700
C	-4.63974400	-0.02903200	-1.58473600
C	-3.59275100	0.23193300	-2.46574200
H	-3.78793700	0.48194700	-3.50269500
N	-5.97592100	0.01904500	-2.01678300
C	-6.37402800	0.92995300	-3.02475000
C	-5.94316800	2.26128300	-2.99705400
C	-7.22214000	0.52035700	-4.05855000
C	-6.34246900	3.14857400	-3.98836900
H	-5.29458000	2.59598700	-2.19308400
C	-7.62911200	1.42442800	-5.03272700
H	-7.56625900	-0.50896000	-4.08987200
C	-7.19347400	2.75237400	-5.02512600
H	-5.99676100	4.17892400	-3.94560900
H	-8.29226400	1.08443300	-5.82485800
C	-6.93415700	-0.86346100	-1.46488600
C	-8.21740600	-0.40742300	-1.14404700
C	-6.62598200	-2.21051000	-1.24285900
C	-9.16246300	-1.28087800	-0.61990900
H	-8.47107600	0.63440400	-1.31474100

C	-7.57543400	-3.06754800	-0.70000300
H	-5.63910800	-2.58242200	-1.50130700
C	-8.86203000	-2.62475800	-0.37835000
H	-10.15474800	-0.90441300	-0.38203900
H	-7.31402300	-4.11096200	-0.53883300
F	2.71553500	-1.59634500	4.23772300
F	-1.64514200	-3.23775600	4.27962000
F	-0.18622300	1.59825300	-5.14591000
F	3.89330100	1.89085600	-2.87383700
C	-7.60240700	3.71423300	-6.10506900
H	-6.86704500	3.73255700	-6.91870600
H	-8.56549300	3.43771200	-6.54344100
H	-7.68474700	4.73529900	-5.72081900
C	-9.87604000	-3.55380000	0.22781400
H	-9.80689800	-3.55713600	1.32253500
H	-10.89628200	-3.25699700	-0.03183200
H	-9.72600400	-4.58372600	-0.10905300
1L-O4: S ₀			
Au	-0.00301800	-0.24342700	-0.09339400
C	0.00407600	-1.22727700	1.75490100
N	1.96412200	0.02130400	0.40528600
C	0.66255400	0.65827700	-1.77989100
C	-1.91210500	-0.18901700	-0.71859900
C	-0.93491400	-2.02506000	2.40696600
H	-1.90290200	-2.20541800	1.94855800
C	-0.66342700	-2.62639000	3.63806400
C	0.57302800	-2.44692100	4.25088400
H	0.78544000	-2.91101300	5.20932500
C	1.54623400	-1.68463800	3.61611800
H	2.52067900	-1.57164900	4.08367500
C	1.27799000	-1.08931700	2.37914700
H	-1.42137300	-3.24142600	4.11635100
C	2.31597500	-0.33662700	1.65219000
C	3.58128300	0.03318700	2.11248900
H	3.91048600	-0.23264300	3.10973100
C	4.39243500	0.78183700	1.27305500
C	3.97896200	1.14671300	-0.00747000
H	4.62564900	1.75686000	-0.61610000
C	2.72541500	0.73259100	-0.45791400
H	5.36910900	1.10481000	1.62075500
C	2.04415800	0.98718500	-1.76333700
C	2.63954300	1.45937100	-2.95485600
C	1.84883500	1.61867200	-4.09716100
C	0.50237000	1.30739400	-4.10242300

H	-0.09866800	1.42588500	-4.99809000
C	-0.08438800	0.81146800	-2.93629400
H	2.31001700	1.98114500	-5.00749000
O	-1.39304300	0.48191600	-3.05699000
C	-2.25418600	0.16888100	-2.03127900
C	-2.98965700	-0.40996600	0.15453500
H	-2.77850200	-0.61691200	1.19728500
C	-4.31560400	-0.33590000	-0.23973600
H	-5.10995100	-0.50119200	0.48050800
C	-4.63052100	-0.03724700	-1.57364300
C	-3.58365600	0.21410000	-2.45830700
H	-3.78085700	0.46689300	-3.49429000
C	4.10134700	1.76944200	-3.11579400
N	-5.96824700	0.02736100	-2.00315100
C	-6.36070400	0.96306600	-2.98946900
C	-5.91057200	2.28753900	-2.93893700
C	-7.22069600	0.58633900	-4.02629000
C	-6.30353100	3.19989400	-3.90986300
H	-5.25246900	2.59717700	-2.13268100
C	-7.62071700	1.51525500	-4.97973700
H	-7.57970500	-0.43713700	-4.07616000
C	-7.16657600	2.83666700	-4.94874900
H	-5.94324500	4.22433800	-3.84848900
H	-8.29344500	1.20027200	-5.77416700
C	-6.92949400	-0.86144100	-1.46817400
C	-8.21287800	-0.40868300	-1.14246500
C	-6.62410200	-2.21240600	-1.26619600
C	-9.16042900	-1.28880300	-0.63426800
H	-8.46473300	0.63613000	-1.29672400
C	-7.57620700	-3.07635400	-0.73921000
H	-5.63711300	-2.58174400	-1.52780400
C	-8.86292200	-2.63689800	-0.41352500
H	-10.15253700	-0.91434100	-0.39242700
H	-7.31670600	-4.12262900	-0.59408400
F	4.47831500	2.86388500	-2.41454800
F	4.43037900	2.01654900	-4.39160300
F	4.88732700	0.75620200	-2.70714300
C	-7.56938800	3.82566400	-6.00632200
H	-6.84032500	3.84982800	-6.82550900
H	-8.53980300	3.57199800	-6.44239900
H	-7.63398800	4.83996100	-5.60129400
C	-9.87993800	-3.57379500	0.17534500
H	-9.81629100	-3.59202200	1.27027600
H	-10.89891900	-3.27334100	-0.08516200

H	-9.72856200	-4.59911400	-0.17476900
1L-O5: S ₀			
Au	0.01250400	-0.19933900	-0.07183900
C	0.68436200	0.58678700	-1.77784000
C	-1.96059600	-0.14103200	-0.69901000
C	-0.87805800	-1.78687200	2.57085100
H	-1.82373400	-1.86813600	2.04788700
C	-0.70191000	-2.35446200	3.82378100
C	0.54154500	-2.22670700	4.43425900
H	0.72089100	-2.65068000	5.41756400
C	1.55978100	-1.56444900	3.76478200
H	2.54317000	-1.47472500	4.21189300
C	1.32918600	-1.02321200	2.49838800
H	-1.52178200	-2.88070000	4.29876200
C	2.35963700	-0.36622100	1.68169200
C	3.68740900	-0.11421300	2.06049500
H	4.06545500	-0.38738300	3.04190600
C	4.53104300	0.50986800	1.14986300
C	4.09775700	0.88883700	-0.12780100
H	4.80831400	1.38052700	-0.77930900
C	2.77781900	0.64059900	-0.52658200
H	5.55881600	0.71553600	1.43467900
C	2.07321000	0.93160900	-1.79941200
C	2.63820600	1.44430100	-2.97877000
C	1.80880800	1.58016000	-4.10261700
C	0.47499900	1.22634600	-4.08684600
H	-0.15014900	1.33133900	-4.96805400
C	-0.10012200	0.72180500	-2.91190100
H	2.23762200	1.97337900	-5.02088700
O	-1.41074100	0.38546700	-3.04521100
C	-2.29966300	0.13670900	-2.02823900
C	-3.05674900	-0.29980900	0.16905200
H	-2.87511300	-0.43662100	1.23201800
C	-4.38125100	-0.24347600	-0.24111400
H	-5.18863600	-0.35909100	0.47514000
C	-4.67520600	-0.02791900	-1.59375400
C	-3.62164600	0.16320500	-2.48289600
H	-3.80989500	0.35551100	-3.53400600
C	4.08355300	1.83737200	-3.11344000
H	4.35199900	2.65902000	-2.43989800
H	4.75852600	1.00105100	-2.90046300
H	4.28940100	2.17238100	-4.13325700
N	-6.01548400	0.01740300	-2.04262500
C	-6.41295800	0.99034300	-2.98589300

C	-5.92854300	2.30226200	-2.90004700
C	-7.29584300	0.65954400	-4.02222200
C	-6.31584100	3.25518500	-3.83503500
H	-5.24585600	2.56603700	-2.09831600
C	-7.69120400	1.62458100	-4.94171900
H	-7.66864000	-0.35698900	-4.10031900
C	-7.20246500	2.92662200	-4.85867000
H	-5.92931300	4.26726800	-3.75274500
H	-8.37626400	1.34939700	-5.73894400
H	-7.50744300	3.67558100	-5.58324300
C	-6.94839600	-0.92080300	-1.55294100
C	-8.26596100	-0.53593500	-1.26926300
C	-6.57090300	-2.25322900	-1.33784800
C	-9.18153500	-1.46650200	-0.79165500
H	-8.56486100	0.49573800	-1.42635700
C	-7.48974900	-3.17190800	-0.84337700
H	-5.55418100	-2.56041700	-1.56216800
C	-8.80138300	-2.78881400	-0.57063100
H	-10.19828400	-1.14881700	-0.57729400
H	-7.17860700	-4.20088200	-0.68489000
H	-9.51802800	-3.51108300	-0.19155700
N	0.09104400	-1.12309600	1.93256200
C	1.94590700	0.00955900	0.40913500
1L-O6: S ₀			
Au	0.02506800	-0.33293300	0.00198200
C	0.11962300	-1.19014500	1.84966800
C	-1.96710300	-0.34487900	-0.58141700
C	-0.85373900	-1.95442700	2.48027900
H	-1.79799800	-2.15358700	1.98485900
C	-0.62493000	-2.49323000	3.75159300
C	0.58676200	-2.27548700	4.39639500
H	0.76196000	-2.68974400	5.38524100
C	1.58859200	-1.54185900	3.76336400
H	2.54648300	-1.40026100	4.25801700
C	1.37878700	-1.00794000	2.49250800
H	-1.39981000	-3.08563800	4.23063200
C	2.39330900	-0.29051100	1.70121100
C	3.68974300	0.09141600	2.04964300
H	4.09940700	-0.12663600	3.03274300
C	4.46649200	0.78245500	1.11643700
C	3.99357600	1.09983100	-0.15589000
H	4.64493200	1.65485000	-0.81617800
C	2.69265100	0.71336100	-0.53517500
H	5.47131900	1.09169600	1.38956600

C	1.99793600	0.94198400	-1.82342100
C	2.55138500	1.44664900	-3.00453400
C	1.71694300	1.51747000	-4.13340600
C	0.40707500	1.10340400	-4.10436900
H	-0.24365600	1.14542300	-4.96896500
C	-0.09366000	0.60683700	-2.89431300
H	2.12984700	1.90661400	-5.06016400
O	-1.35241000	0.17030200	-2.93703900
C	-2.27798500	-0.03289400	-1.90777800
C	-3.08781200	-0.48180600	0.25693500
H	-2.92809800	-0.65991500	1.31595400
C	-4.39836900	-0.36653600	-0.18407400
H	-5.22430800	-0.47212000	0.51243100
C	-4.66053700	-0.10600500	-1.53543600
C	-3.57986700	0.06130100	-2.39905700
H	-3.73598900	0.27663600	-3.45064600
C	3.97941000	1.88736300	-3.15133200
H	4.20109600	2.77099400	-2.54382100
H	4.68130100	1.09811100	-2.86526300
H	4.18180000	2.14843100	-4.19254500
N	-5.98539700	0.00078400	-2.01105200
C	-6.31824800	0.98772300	-2.96535600
C	-5.79116200	2.28174800	-2.86231800
C	-7.18065500	0.68812700	-4.02783100
C	-6.11566300	3.24792300	-3.80768300
H	-5.12776000	2.52199100	-2.03719900
C	-7.51320100	1.66653700	-4.95803600
H	-7.58770200	-0.31429100	-4.11680100
C	-6.98106600	2.95035200	-4.85863300
H	-5.69870400	4.24660500	-3.71124700
H	-8.18381900	1.41636100	-5.77545800
H	-7.23800000	3.70987800	-5.59078400
C	-6.97390000	-0.89259800	-1.54237200
C	-8.27232900	-0.43915800	-1.27502100
C	-6.67053500	-2.24465200	-1.33599400
C	-9.24365400	-1.32361100	-0.82027900
H	-8.51232900	0.60871500	-1.42599800
C	-7.64441900	-3.11718300	-0.86356900
H	-5.66818600	-2.60410300	-1.54714200
C	-8.93742500	-2.66613900	-0.60675800
H	-10.24509900	-0.95420000	-0.61744600
H	-7.39101200	-4.16233900	-0.70902500
H	-9.69700300	-3.35214400	-0.24437200
C	1.94033500	0.02435000	0.42079700

N	0.67167600	0.54855400	-1.81125400
1L-O7: S ₀			
Au	0.03517800	-0.33403100	-0.00619700
C	-1.95841000	-0.35425300	-0.58210700
C	-0.81876300	-2.00940700	2.44491900
H	-1.76351100	-2.20708200	1.94986100
C	-0.57963100	-2.57026900	3.70471400
C	0.63295400	-2.35415300	4.34843800
H	0.81618400	-2.78564000	5.32843300
C	1.62539400	-1.59964300	3.72527900
H	2.58412900	-1.45881100	4.21852000
C	1.40532500	-1.04353100	2.46570100
H	-1.34719100	-3.17848600	4.17568700
C	2.41013000	-0.30205500	1.68417100
C	3.70443900	0.08516300	2.03467900
H	4.12022600	-0.14766200	3.01182800
C	4.47087000	0.80116900	1.11177200
C	3.98992100	1.13796700	-0.15254000
H	4.63331200	1.71174300	-0.80458900
C	2.69123300	0.74620300	-0.53411900
H	5.47380700	1.11478700	1.38689500
C	1.98936100	0.99170700	-1.81538500
C	2.53395300	1.52173900	-2.98941900
C	1.69447000	1.60552700	-4.11369700
C	0.38825200	1.18018200	-4.08690700
H	-0.26624600	1.23204000	-4.94812400
C	-0.10384100	0.65787800	-2.88396400
H	2.10045700	2.01436900	-5.03502700
O	-1.35883500	0.21225000	-2.92989800
C	-2.27852600	-0.02013500	-1.90074300
C	-3.07537700	-0.51792700	0.25663100
H	-2.91064100	-0.71407900	1.31174400
C	-4.38842400	-0.40770200	-0.17729100
H	-5.20969500	-0.53463900	0.52100500
C	-4.66038200	-0.12389100	-1.52299200
C	-3.58274600	0.07113500	-2.38587000
H	-3.74327200	0.30508500	-3.43269000
C	3.95785000	1.97639300	-3.13398000
H	4.17473000	2.85188600	-2.51309600
H	4.66711800	1.18836700	-2.86311200
H	4.15437200	2.25588100	-4.17154700
N	-5.98575000	-0.02223700	-1.99027700
C	-6.32513300	0.93894200	-2.96966700
C	-5.82237100	2.24372600	-2.89632300

C	-7.18091700	0.61044300	-4.02683100
C	-6.16066000	3.18247300	-3.86264900
H	-5.16760200	2.51738000	-2.07448000
C	-7.52552100	1.56595100	-4.97557400
H	-7.58063700	-0.39664100	-4.09618800
C	-7.01904500	2.86742900	-4.92091500
H	-5.76079400	4.19082800	-3.78164200
H	-8.19623500	1.28760300	-5.78532600
C	-6.97831000	-0.89830200	-1.49486700
C	-8.26561300	-0.42906300	-1.20929900
C	-6.69889100	-2.25423600	-1.28734700
C	-9.24135500	-1.29769600	-0.73584500
H	-8.49809900	0.61980600	-1.36629900
C	-7.67963400	-3.10647700	-0.79518700
H	-5.70859900	-2.63630100	-1.51597100
C	-8.97026800	-2.65052800	-0.51036200
H	-10.23535500	-0.90987700	-0.52461600
H	-7.43901900	-4.15649600	-0.64454500
C	-7.36324000	3.88444900	-5.97269300
H	-6.61882200	3.89123700	-6.77838100
H	-8.33435200	3.67398900	-6.42973100
H	-7.39692600	4.89538700	-5.55555700
C	-10.01862500	-3.57496400	0.04218000
H	-9.98825900	-3.60040100	1.13840400
H	-11.02469200	-3.25758900	-0.24697800
H	-9.87236800	-4.60059300	-0.30932500
C	1.94898600	0.03264200	0.41167600
C	0.14504200	-1.22476300	1.82463600
N	0.66649900	0.58669800	-1.80508600

1L-O8: S₀

Au	0.01971900	-0.20214800	-0.07215500
C	0.68661800	0.60922600	-1.76819500
C	-1.95391500	-0.14156400	-0.69553500
C	-0.86194800	-1.82706000	2.55126000
H	-1.80847400	-1.90335800	2.02910500
C	-0.68204500	-2.41101300	3.79612200
C	0.56231800	-2.28863100	4.40587100
H	0.74456700	-2.72528200	5.38308300
C	1.57768300	-1.61513200	3.74332500
H	2.56177000	-1.52906700	4.18964800
C	1.34335400	-1.05754700	2.48468500
H	-1.49983200	-2.94542400	4.26555200
C	2.37079600	-0.38744100	1.67495200
C	3.69886200	-0.13812000	2.05453400

H	4.07938000	-0.42395400	3.03138100
C	4.53950700	0.49976100	1.15075000
C	4.10285400	0.89516700	-0.12080700
H	4.81126500	1.39684900	-0.76702100
C	2.78255300	0.64993800	-0.52024700
H	5.56750900	0.70344300	1.43620200
C	2.07482900	0.95700100	-1.78758300
C	2.63672900	1.48719700	-2.96069700
C	1.80498200	1.63725700	-4.08095100
C	0.47182400	1.28096700	-4.06750200
H	-0.15522100	1.39724000	-4.94595300
C	-0.10049500	0.75900400	-2.89871900
H	2.23135200	2.04403200	-4.99446200
O	-1.41050900	0.42278600	-3.03445700
C	-2.29706900	0.15540800	-2.01944900
C	-3.04897700	-0.31842700	0.17058500
H	-2.86599900	-0.47075200	1.23125600
C	-4.37405900	-0.26142900	-0.23674100
H	-5.17905500	-0.39150700	0.47959200
C	-4.67284600	-0.02506700	-1.58572800
C	-3.61948500	0.18485700	-2.47199300
H	-3.80849900	0.39329100	-3.51977400
C	4.08105200	1.88502200	-3.09255800
H	4.34917200	2.69778600	-2.40817500
H	4.75818400	1.04724600	-2.89251900
H	4.28427200	2.23461400	-4.10801500
N	-6.01170100	0.02210200	-2.03082300
C	-6.40563000	0.97203900	-3.00014800
C	-5.93968400	2.29115200	-2.93919100
C	-7.27671900	0.61852000	-4.03675100
C	-6.32939000	3.21930700	-3.89613400
H	-5.26996400	2.58337700	-2.13614600
C	-7.67292800	1.56347400	-4.97591500
H	-7.64703700	-0.40021300	-4.09851800
C	-7.20425200	2.87934400	-4.93293700
H	-5.95529400	4.23827600	-3.82566300
H	-8.35386100	1.26484300	-5.76981400
C	-6.95503800	-0.89565300	-1.51999100
C	-8.26378000	-0.49112900	-1.23003000
C	-6.60571000	-2.23344800	-1.29735300
C	-9.19026300	-1.40323500	-0.73974900
H	-8.55208300	0.54206400	-1.39771300
C	-7.53823100	-3.12916000	-0.78906200
H	-5.59883500	-2.56670100	-1.52959700

C	-8.84908900	-2.73770800	-0.50063000
H	-10.20163800	-1.06430900	-0.52650700
H	-7.24298100	-4.16393300	-0.62940100
C	-7.60265000	3.88545000	-5.97606400
H	-6.87492700	3.91734700	-6.79625000
H	-8.57538000	3.64382600	-6.41400500
H	-7.66082600	4.89447200	-5.55684000
C	-9.84545400	-3.70879800	0.06812200
H	-9.80664800	-3.72381700	1.16438000
H	-10.86831400	-3.44505300	-0.21609000
H	-9.65072300	-4.72883400	-0.27634900
N	0.10432900	-1.15260600	1.91995300
C	1.95358600	0.00473300	0.40846900

Reference

- 1 Y. Niu, Q. Peng and Z. Shuai, *Sci. China Ser. B Chem.*, 2008, **51**, 1153–1158.
- 2 Q. Peng, Y. Niu, C. Deng and Z. Shuai, *Chem. Phys.*, 2010, **370**, 215–222.
- 3 Q. Peng, Y. Niu, Q. Shi, X. Gao and Z. Shuai, *J. Chem. Theory Comput.*, 2013, **9**, 1132–1143.
- 4 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L.

- Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, 2016.
- 5 J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.*, 1996, **77**, 3865–3868.
 - 6 J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.*, 1997, **78**, 1396.
 - 7 D. Andrae, U. Häußermann, M. Dolg, H. Stoll and H. Preuß, *Theor Chim Acta*, 1990, **77**, 123–141.
 - 8 M. Caricato, B. Mennucci, J. Tomasi, F. Ingrosso, R. Cammi, S. Corni and G. Scalmani, *J. Chem. Phys.*, 2006, **124**, 124520.
 - 9 F. Neese, *WIREs Comput. Mol. Sci.*, 2012, **2**, 73–78.
 - 10 F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.*, 2005, **7**, 3297–3305.
 - 11 Web site:, <http://sobereva.com/462>.
 - 12 K. Aidas, C. Angeli, K. L. Bak, V. Bakken, R. Bast, L. Boman, O. Christiansen, R. Cimiraglia, S. Coriani, P. Dahle, E. K. Dalskov, U. Ekström, T. Enevoldsen, J. J. Eriksen, P. Ettenhuber, B. Fernández, L. Ferrighi, H. Fliegl, L. Frediani, K. Hald, A. Halkier, C. Hättig, H. Heiberg, T. Helgaker, A. C. Hennum, H. Hettema, E. Hjertenæs, S. Høst, I.-M. Høyvik, M. F. Iozzi, B. Jansík, H. J. A. Jensen, D. Jonsson, P. Jørgensen, J. Kauczor, S. Kirpekar, T. Kjærgaard, W. Klopper, S. Knecht, R. Kobayashi, H. Koch, J. Kongsted, A. Krapp,

- K. Kristensen, A. Ligabue, O. B. Lutnæs, J. I. Melo, K. V. Mikkelsen, R. H. Myhre, C. Neiss, C. B. Nielsen, P. Norman, J. Olsen, J. M. H. Olsen, A. Osted, M. J. Packer, F. Pawłowski, T. B. Pedersen, P. F. Provasi, S. Reine, Z. Rinkevicius, T. A. Ruden, K. Ruud, V. V. Rybkin, P. Sałek, C. C. M. Samson, A. S. de Merás, T. Saue, S. P. A. Sauer, B. Schimmelpfennig, K. Sneskov, A. H. Steindal, K. O. Sylvester-Hvid, P. R. Taylor, A. M. Teale, E. I. Tellgren, D. P. Tew, A. J. Thorvaldsen, L. Thøgersen, O. Vahtras, M. A. Watson, D. J. D. Wilson, M. Ziolkowski and H. Ågren, *WIREs Comput. Mol. Sci.*, 2014, **4**, 269–284.
- 13 Dalton, , a Molecular Electronic Structure Program, Release V2017.Alpha (2017), See [Http://Daltonprogram.Org](http://Daltonprogram.Org).
 - 14 A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648–5652.
 - 15 C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785–789.
 - 16 A. D. Becke, *J. Chem. Phys.*, 1988, **88**, 2547–2553.
 - 17 T. Lu and F. Chen, *J. Comput. Chem.*, 2012, **33**, 580–592.
 - 18 Y. Niu, W. Li, Q. Peng, H. Geng, Y. Yi, L. Wang, G. Nan, D. Wang and Z. Shuai, *Mol. Phys.*, 2018, **116**, 1078–1090.
 - 19 W.-P. To, D. Zhou, G. S. M. Tong, G. Cheng, C. Yang and C.-M. Che, *Angew. Chemie Int. Ed.*, 2017, **56**, 14036–14041.