Supporting Information

Crystalline Confinement Leads to Broadening of Absorption Spectra through Activated Spin-Forbidden Transitions in Alq_3-$Irppy_2acac$ Engineered Crystals

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Theoretical Background

Photoexcitation is a quantum transition described by the Fermi Golden rule as[1-3]

$$\sigma_{\mathrm{ex}}(\omega) = \frac{4\pi^2\omega}{3c}\sum_{v,u} P_{iv}(T)\left|\left\langle \Phi_f\middle|\hat{\mu}_{\mathrm{fi}}\middle|\Phi_i\right\rangle\right|^2\left|\left\langle \Theta_{fu}\middle|\,\Theta_{iv}\right\rangle\right|^2 \delta\left(\hbar\omega - E_{fi} - E_{fu} + E_{iv}\right), \tag{1}$$

where, the Φ and Θ are the electronic and vibrational wavefunctions, and indices i and f represent the initial and final states, respectively; ω is the circular frequency, the c is the speed of light in vacuum, the E_{fi} is the electronic energy difference between the initial and the final states, the E_{iv} is the vibrational energy level of the initial state and the E_{fu} is the vibrational energy level of the final state. This equation describes both electronic and vibrational transitions. The electronic transition is characterized by the matrix element $\left\langle \Phi_f\middle|\hat{\mu}_{fi}\middle|\Phi_i\right\rangle$ called TDM, which is spin-allowed if Φ_i and Φ_f have a same spin state. When the spin states of Φ_i and Φ_f are different, the value of the TDM is zero and the transition is spin-forbidden.

To allow a spin-forbidden transition, between the pure singlet, S, and triplet, T, the states have to mix with an intermediate state through the SOC as [4-6]

$$|S'\rangle = |S\rangle + \sum_{n}^{7}\sum_{m=-1}^{1}\frac{\left\langle {}^3T_{n,m}\middle|\hat{H}_{\mathrm{SO}}\middle|S\right\rangle}{{}^1E_S - {}^3E_n}\left|{}^3T_{n,m}\right\rangle, \tag{2}$$

$$|T_m'\rangle = |T_m\rangle + \sum_{n}^{\{\mathrm{singlets}\}}\frac{\left\langle {}^1S_n\middle|\hat{H}_{\mathrm{SO}}\middle|{}^3T_m\right\rangle}{{}^3E_T - {}^1E_n}\left|{}^1S_n\right\rangle, \tag{3}$$

where *S*' and *T*' are the mixed states and S_n and T_n are the intermediate states. The index *n* is for the intermediates, *m* is the magnetic spin quantum number (*m* = -1, 0, 1), and $\hat{H}_{SO}$ is the SOC Hamiltonian operator.

In this mixing, the TDM and SOC interplay to generate a new spin-forbidden TDM (TDM_{SF}). There are two processes that result in non-zero TDM_{SF}. When the intermediate state is a singlet (S_n), the TDM_{SF} from the S_0 state to the T_k state (final state) is expressed as

$$TDM_{SF} = \frac{\left\langle \Phi_{S_n} | \hat{\mu} | \Phi_{S_0} \right\rangle \left\langle \Phi_{T_k} | \hat{H}_{SO} | \Phi_{S_n} \right\rangle}{E_{T_k} - E_{S_n}} \quad . \tag{4}$$

It involves two parts: the spin-allowed part, naming $TDM = \left\langle \Phi_{S_n} | \hat{\mu} | \Phi_{S_0} \right\rangle$ and the spin-forbidden part, naming $SOC = \left\langle \Phi_{T_k} | \hat{H}_{SO} | \Phi_{S_n} \right\rangle$.

The spin-forbidden TDM through a triplet mixed intermediate (T_n) is expressed as

$$TDM_{SF} = \frac{\left\langle \Phi_{T_k} | \hat{\mu} | \Phi_{T_n} \right\rangle \left\langle \Phi_{T_n} | \hat{H}_{SO} | \Phi_{S_0} \right\rangle}{E_{T_n} - E_{S_0}} \quad . \tag{5}$$

The schematic graphic of the spin-forbidden excitation transition is shown in Figure 1(a). To sum up, a strong TDM_{SF} requires both strong spin-allowed TDM and SOC.

Calculation Formulas for the Photophysical Parameters:

$$k_r = \frac{\Phi p}{\tau p} \quad . \tag{6}$$

$$k_{nr} = \frac{1 - \Phi p}{\tau p} \tag{7}$$

Where Φp is the prompt phosphorescence component of Φ_{PL};τp is the lifetime of prompt phosphorescence; k_r is the rate constant of radiative transition from T_1 to S_0; k_{nr} is the non-radiative decay rate constant from T_1 to S_0.

Experimental methods:

(1) Fabrication of engineered crystals

(2,4-pentanedionyl) bis (2-phenylpyridine) iridium ($Irppy_2acac$, 99%) (CAS:337526-85-9) and tris(8-hydroxyquinoline) aluminum (Alq_3, 98%) (CAS: 2085-33-8) were purchased from Bide

Pharmatech Ltd. To take double-film annealing method get high-quality engineering organic crystal (fig. S1). Firstly, $Irppy_2acac$ (90%) and Alq_3 (10%) were mixed and deposited on a quartz substrate in a vacuum evaporator. The thickness of the deposited film was 120 nm. Secondly, another quartz substrate is horizontally stacked face to face and then heated at 523k for 7 minutes. The temperature control precision is ±0.2 K. (Heating at a temperature of 523K, according to TGA data, provided in **figure S4**, the sample is safe and has not undergone decomposition). Then the heating was stopped and the double substrates were naturally cooled. By comparing the crystal morphology of different doping ratios, the optimal crystal morphology was found at the ratio of $Irppy_2acac$ (90): Alq_3 (10), while crystals with other doping ratios are shown in the **figure S2**. The content of Ir and Al elements in the sample was determined by inductively coupled plasma mass spectrometry (ICP-MS), and the results showed that the content of Alq_3 in the crystal was 4.2%.

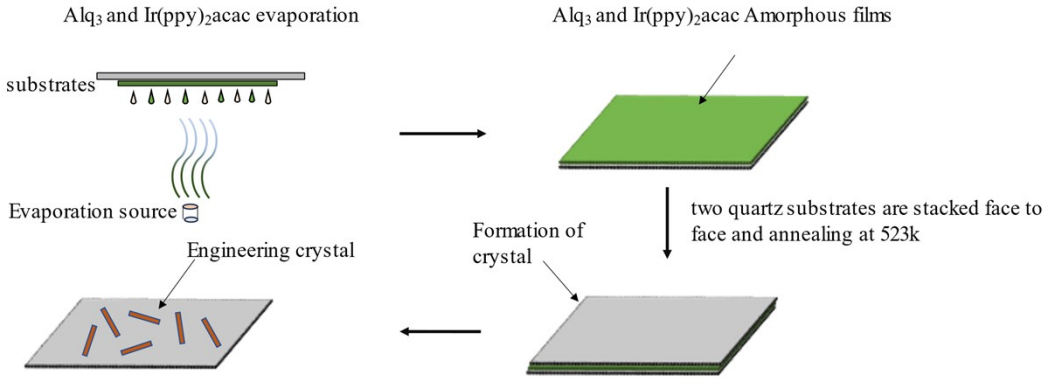

Figure S1. The process to fabricate engineered crystals.

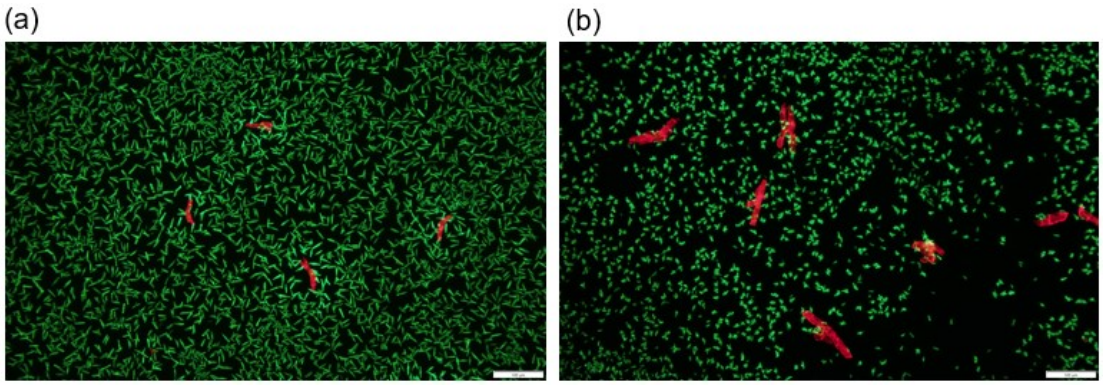

Figure S2. (a) Crystal morphology of $Irpy_2acac$ (30): Alq_3 (70), (b) Crystal morphology of $Irpy_2acac$ (60): Alq_3 (40).

Crystals doped with more proportions of host and guest were presented. The images of the morphology of some proportions of crystals are show in **Figure S2**. When the ratio between $Irppy_2acac$ and Alq_3 is 3:7 or 6:4 a lot of green crystals can be observed. When the proportion of

Irppy$_2$acac is increased the size of the red crystals tend to be lager and the green crystals tend to be smaller. When the ratio is raised to 9:1, as shown in Figure 1 in the main text, all the crystals convert to red.

Two crystallization phases with green and yellow luminescent colors were prepared. As shown in **Figure S3 (a)** green luminescent crystals were obtain under 523 K and yellow crystals were obtained when the temperature was increased to 543 K, as shown in **Figure S3 (b)**. The luminescent spectrum of the yellow crystals excited at 405 nm were measured as shown in **Figure S4**. Two peaks were observed. One is at 541 nm and the other is at about 592 nm. The spectrum of the green crystallization phase as shown in **Figure 1(c)** has two peaks. One peak is at 518 nm and the other peak is at 541 nm. And there is also a shoulder peak at about 585 nm that is close to the peak at 592 nm of the yellow crystallization phase. Therefore, this strong peak at 592 nm should be one of the vibronic peak of Irppy$_2$acac. In some certain crystallization phase, the vibronic coupling can be significantly enhanced. The thermal gravimetric analyzer (TGA) curves of Irppy$_2$acac was also measured as shown in **Figure S5**. Below 613 K no significant weight loss was observed. The annealing at 543 K should be safe.

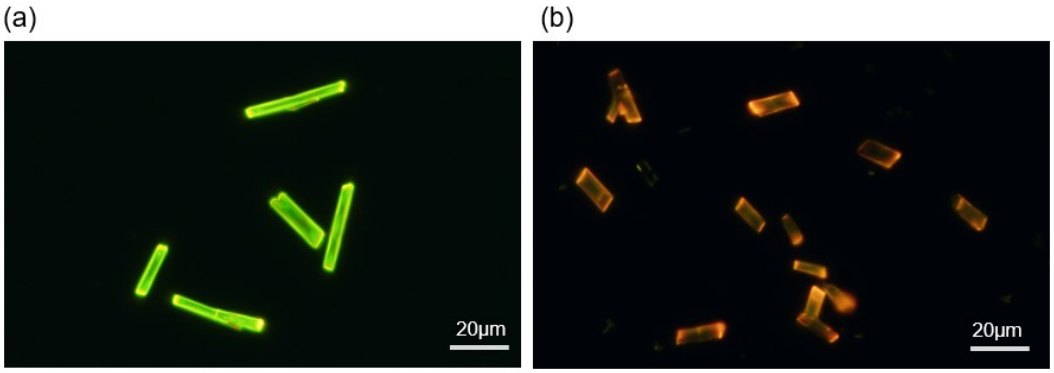

Figure S3. The different luminescent colors of Irpy$_2$acac crystals (a) yellow green (heating temperature: 250℃); (b) Orange light (heating temperature: 270℃).

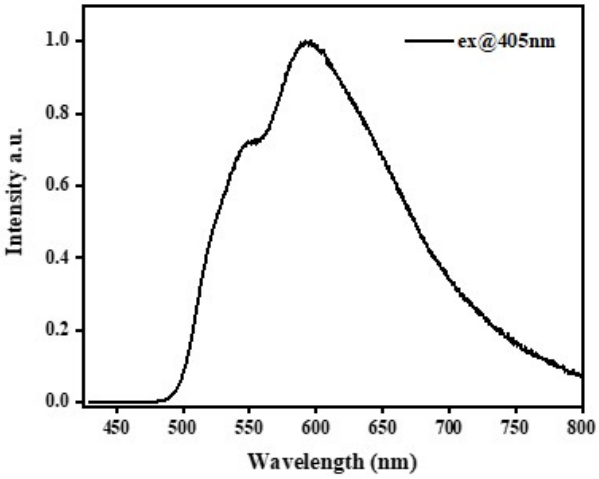

Figure S4. The luminescence spectrum of $Irppy_2acac$ orange single crystals.

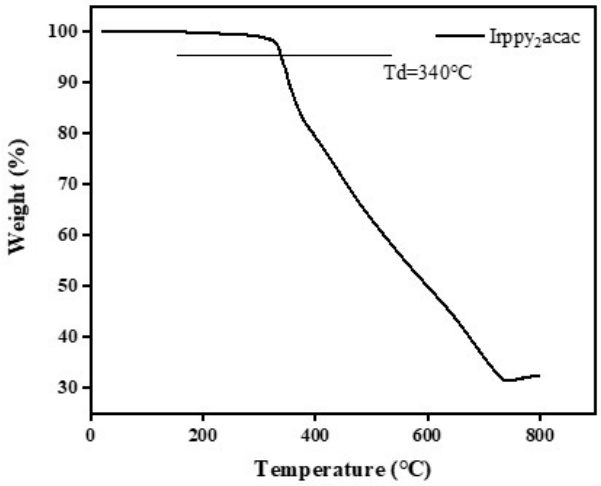

Figure S5. The thermal gravimetric analyzer (TGA) curves of $Irppy_2acac$.

(2) Observation and spectrum measurement

The observation of morphology was performed using an Olympus fluorescence microscope with UV light source and a Thermo Scientific Prisma E SEM. The photoluminescence spectrums were measured by a Renishaw microscope. The excitation light sources are 405 nm, 589 nm, and 632 nm laser. The photoluminescence lifetimes of the long wavelength phosphorescence were measured by an Edinburgh spectrophotometer using a μs pulse flash lamp. XRD diffraction spectra were measured by a Bruker D8 Advance instrument. The transient absorption spectra were measured by a Helios Fire automated femtosecond Transient Absorption Spectrometer with a 390 nm excitation, and the time window is 8 ns.

Computational details:

Geometry optimizations and single point computations of a ground state were performed by a

DFT method. A hybrid functional M06L[8] was applied with D3 correction[9], and the basis set was def2-SVP[10-11] and the auxiliary basis is def2/J. The spin-orbital coupling (SOC) matrix elements and the transition dipole moment (TDM) were calculated by TDA. For the computation of SOC, the DKH method was adopted. The basis set was DKH-def2-TZVP[12-13] a version for DKH method[14] (the auxiliary basis is SARC/J[12-13]). To well describe the SOC matrix elements, no effective core potential for Ir was adopted. All the methods above were provided by ORCA 5.0.4[15-16] and the grid size was set as high as "DEFGRID3"[17].

The calculation of transition dipole moments between excited states was performed by Multiwfn 3.7[18-22] based on the computational results from ORCA. Based on the computations of SOC and TDM, the spin-forbidden TDMs (TDM_{SF}s) can be calculated, and 30 intermediate states were considered. The conformer searching of the two-molecular system was performed by Crest module in XTB program[23-27]. The conformer searching depends on the initial geometry sent into the program. In this work, the initial geometries of a dimer were created by joining the two molecules in the direction of $\pm x$, $\pm y$, and $\pm z$ (shown in Figure S6). To avoid calculating conformers of extreme close geometries, e.g., the only difference between two conformers is the rotation of a methyl group, the minimum energy difference between two conformers was set 0.5 kcal mol^{-1}. To cover different possible conformers in lattice confinements, five conformers with the lowest energies were selected as shown in Figure S7. The coordinates optimized in ground state were listed in Table S4-S8. Conformer 1 as the most stable one was studied emphatically. And the excitation spectra of all the five conformers were calculated and overlapped to create an excitation spectrum for the engineered crystal.

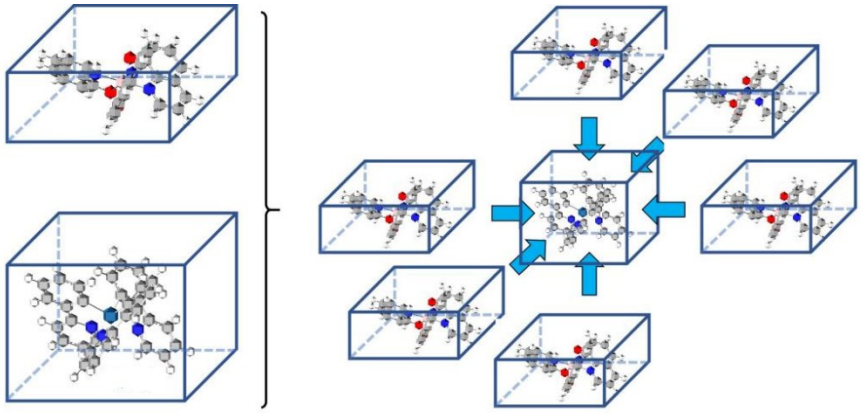

Figure S6. The generation of initial geometries for conformer searching. The initial geometries of two-molecule-systems were created by joining the two molecules in the direction of $\pm x$, $\pm y$, and $\pm z$.

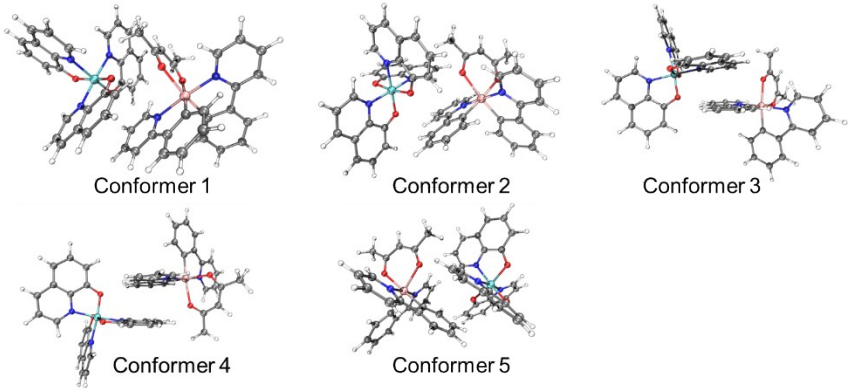

Figure S7. The graph of the five searched conformers with the lowest energies. From Confirmer 1 to 5 the energy raises. The coordinates were shown in Table S4 to S8.

Supplementary data:

Table S1. The luminescence lifetimes and the proportions at different temperatures of the engineered crystals excited at 633 nm, 405 nm, and 590 nm.

Ex@633 Em@702	Temperature /K	Lifetimes /μs	χ^2	Ex@405 Em@609	Temperature /K	Lifetimes /μs	χ^2
	77k	1.27	1.07		77k	12.59	1.06
		12.07				20.34	
	127k	1.27	1.16		127k	10.29	1.05
		11.88				18.89	
	177k	1.31	1.04		177k	9.54	1.09
		11.58				18.09	
	227k	1.40	1.19		227k	9.11	1.12
		12.00				17.56	
	298k	1.44	1.04		298k	6.04	1.12
		12.78				14.98	
	350k	1.33	1.10		350k	3.89	1.05
		12.36				11.67	
	400k	1.25	1.07		400k	3.32	1.11
		10.61				8.59	

Ex@590 Em@670	Temperature /K	Lifetimes /μs	χ^2
	77K	18.3	0.98
		26.9	
	127K	17.3	1.08
		27.2	
	177K	17.5	1.17
		32.4	
	227K	16.7	1.06
		29.5	
	298K	15.5	0.86
		29.6	
	350K	13.2	0.79
		19.0	
	400K	10.6	0.98
		10.0	

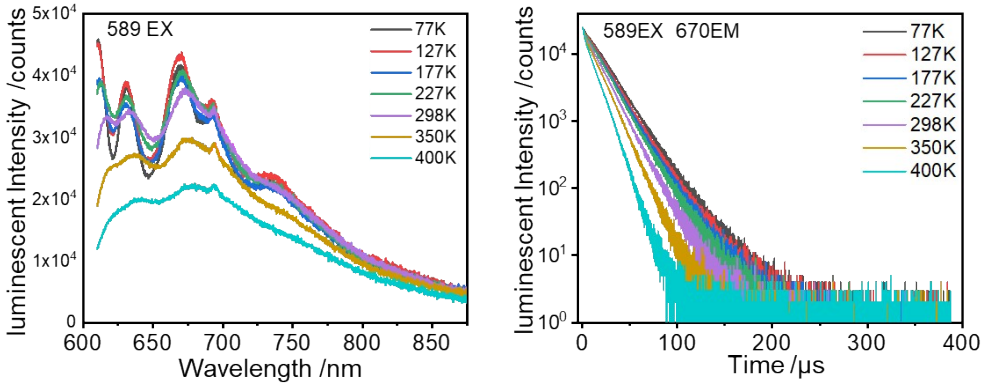

Figure S8. (a) the spectra excited at 589 nm, (b) the lifetime measurements at 670 nm excited at 590 nm.

For the luminescent spectrum excited at 589 nm, the maximum luminescent intensity is found at 127 K. The luminescent intensities below 227 K are close. Higher than 227 K the luminescent intensity becomes lower when the temperature increases. This behavior is in between the spectra excited at 405 nm and 633 nm. The change of the lifetime with the temperature is similar with that excited at 405 nm. The emission at 670 nm contains some component of the phosphorescence of $Irppy_2acac$ as shown in Figure 1 (c) and the excitation at 589 nm also involves some component of spin-allowed excitation. These two reasons lead to the results that the luminescent behavior excited at 589 nm is to some extend different from the excitation at 633 nm.

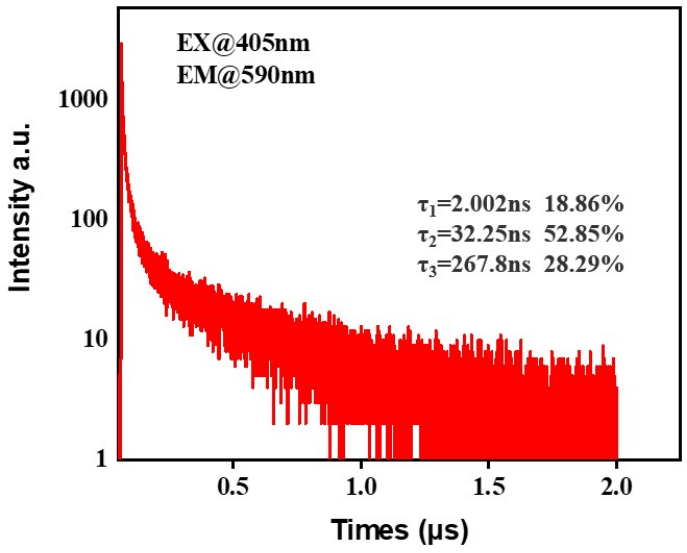

Figure S9. luminescent lifetimes of the activated emission peak excited at 405 nm about $Ir(ppy)_2acac$.

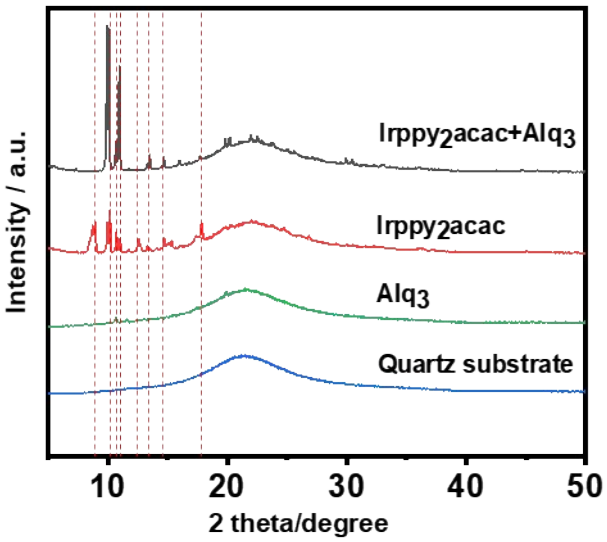

Figure S10. X-ray diffraction spectra of the engineered crystal and the single-component crystals.

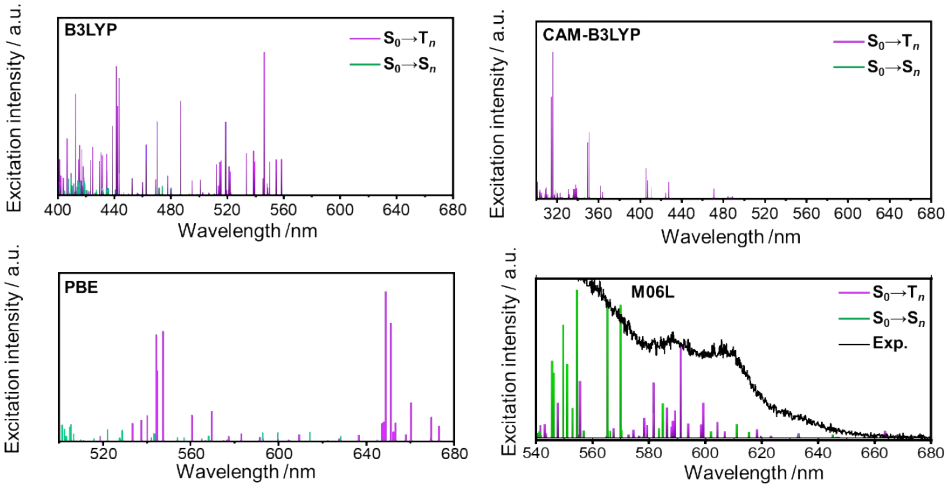

Figure S11. Calculated excitations using different functionals

Four functionals B3LYP (hybrid functional), CAM-B3LYP (range-separated hybrid functional), PBE (pure GGA), and M06L (meta-GGA) were tested to calculate the containing spin-allowed and spin-forbidden excitations. For B3LYP and cam-B3LYP the excitation energies are overestimated. The excitations are shorter than 560 nm. The intensities of the spin-forbidden excitations are overestimated. For PBE, the excitation energies are underestimated and the wavelength of the strongest excitation extends to over 640 nm, which is away from the experimental observation that the maximum absorption is at about 588 nm. The intensities of the spin-forbidden excitations are also overestimated. On the whole, M06L is a proper functional to give a best performance in reproducing the experimental spectrum. This may because M06L does not contain

166 the Hartree Fock component as a Meta-GGA functional and thus the low excitation energies are not
167 overestimated. But it can approximately describe the dispersion which is difficult for other pure
168 GGA functionals like PBE to describe. It also contains the complicated computation of electron
169 kinetic energy density which may also help reproduce the excitation intensity.

170 **s**

171 **Table S1**. The original TDM elements between S_0 and S_n calculated at M06L/def2-svp level.

States		TDM elements between S_0 and S_n /debye				
S_0	S_n	Conformer 1	Conformer 2	Conformer 3	Conformer 4	Conformer 5
0	1	0.44	0.17	0.47	0.52	0.12
0	2	0.39	0.22	0.17	0.26	0.27
0	3	0.68	0.23	0.52	0.36	0.08
0	4	0.07	0.10	0.03	0.18	0.38
0	5	0.35	0.37	0.81	1.57	1.59
0	6	0.11	1.15	1.64	1.08	0.07
0	7	0.43	0.12	0.73	1.17	0.17
0	8	0.36	0.14	0.31	0.34	0.37
0	9	1.43	1.26	0.08	0.62	0.49
0	10	0.40	0.85	0.12	0.09	0.70
0	11	0.42	0.41	1.22	1.23	0.50
0	12	0.18	0.36	0.43	0.47	0.08
0	13	0.93	0.88	0.08	0.20	0.79
0	14	0.90	1.44	0.74	0.75	0.17
0	15	0.62	0.84	0.54	1.32	0.79
0	16	1.04	0.56	1.26	0.45	0.51
0	17	0.29	0.14	1.78	1.16	0.43
0	18	1.23	0.15	0.38	1.78	0.34
0	19	0.50	0.82	0.92	1.10	0.78
0	20	0.17	0.34	0.30	0.16	0.15
0	21	0.70	1.37	0.31	0.47	0.33
0	22	0.73	1.36	1.66	0.09	0.45
0	23	1.23	0.42	0.82	0.36	1.61
0	24	0.68	0.42	0.23	1.21	1.46
0	25	0.37	0.28	0.61	0.50	0.34
0	26	0.90	1.01	0.38	1.99	0.38
0	27	1.35	0.27	2.09	0.83	0.39
0	28	0.98	1.74	0.97	1.09	0.49
0	29	0.79	0.91	0.35	0.28	0.68
0	30	0.73	1.29	0.90	0.18	0.10

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Table S2. The original TDM elements between T_i and T_j calculated at M06L/def2-svp level.

States		TDM elements between T_i and T_j /debye				
T_i	T_j	Conformer 1	Conformer 2	Conformer 3	Conformer 4	Conformer 5
1	1	0.00	0.00	0.00	0.00	0.00
1	2	5.30	4.11	2.94	2.84	1.30
1	3	8.61	8.28	2.28	1.08	9.66
1	4	0.34	0.37	3.40	0.38	0.36
1	5	0.00	0.36	2.77	4.43	0.18
1	6	0.46	0.92	0.38	0.18	0.15
1	7	0.62	0.37	0.12	0.11	0.48
1	8	0.44	0.85	0.27	0.36	0.26
1	9	0.33	0.68	0.37	0.36	0.33
1	10	0.82	0.26	0.58	0.36	0.32
1	11	0.31	0.00	1.19	0.17	1.45
1	12	0.90	0.96	0.13	0.24	0.00
1	13	0.72	0.10	0.37	0.12	0.20
1	14	0.24	0.13	1.42	1.37	0.00
1	15	0.31	0.59	0.04	0.01	0.00
1	16	0.07	0.00	0.15	0.05	0.82
1	17	0.00	0.61	0.00	0.00	1.22
1	18	0.00	0.16	0.00	0.00	0.94
1	19	0.08	0.19	0.02	0.00	0.05
1	20	0.18	0.04	0.00	0.00	0.47
1	21	3.23	0.00	0.52	0.05	0.06
1	22	4.56	0.33	5.82	0.02	0.00
1	23	0.05	0.57	0.33	0.00	0.00
1	24	0.85	0.51	0.26	5.82	0.00
1	25	2.53	0.35	0.13	0.00	0.26
1	26	0.83	0.00	0.47	0.55	0.00
1	27	0.55	6.03	0.00	0.00	0.00
1	28	0.08	0.00	0.05	0.09	0.00
1	29	0.11	0.00	0.00	0.11	6.24
1	30	0.39	0.00	0.00	0.27	0.00
2	2	0.00	0.00	0.00	0.00	0.00
2	3	11.03	8.30	0.00	0.00	0.00
2	4	0.00	0.00	2.42	0.34	0.00
2	5	0.34	0.20	1.71	3.00	1.28
2	6	0.12	0.25	0.09	0.66	7.25
2	7	0.18	0.22	1.49	0.42	0.00
2	8	0.82	0.09	0.00	0.56	5.55
2	9	0.63	1.46	0.89	0.67	4.88
2	10	0.54	0.33	1.11	0.29	0.48
2	11	0.22	0.87	0.56	0.30	0.31

2	12	0.19	0.52	0.37	0.19	0.40
2	13	1.48	0.00	1.32	1.12	2.32
2	14	0.87	0.62	0.00	0.00	0.50
2	15	0.68	0.05	0.03	0.02	0.00
2	16	0.18	1.18	0.13	0.14	0.00
2	17	0.00	0.21	0.00	0.35	0.47
2	18	0.43	0.00	1.42	0.97	0.31
2	19	0.29	0.07	0.02	0.93	0.11
2	20	0.16	0.12	0.40	0.00	0.00
2	21	0.16	0.61	0.35	0.07	0.00
2	22	0.11	0.08	0.00	0.04	0.00
2	23	0.03	0.14	0.24	0.00	0.00
2	24	0.55	0.12	0.19	0.00	1.08
2	25	0.00	0.42	0.06	0.00	0.00
2	26	0.00	0.00	0.25	0.27	0.00
2	27	1.29	0.00	0.00	0.00	0.00
2	28	5.36	0.00	0.04	0.15	0.00
2	29	1.08	0.00	0.00	0.19	0.59
2	30	0.53	0.00	0.00	0.47	0.00
3	3	0.00	0.00	0.00	0.00	0.00
3	4	0.00	0.06	0.32	0.02	0.99
3	5	0.00	1.12	0.64	2.66	0.22
3	6	0.40	0.49	2.67	11.51	1.12
3	7	0.31	0.23	4.12	1.11	1.63
3	8	0.85	0.00	0.69	3.48	0.45
3	9	0.18	1.82	16.72	5.81	0.67
3	10	0.20	0.66	16.12	18.09	0.00
3	11	0.10	0.00	0.00	20.15	2.44
3	12	0.30	0.62	1.32	0.00	0.00
3	13	1.47	0.83	15.12	10.51	0.32
3	14	0.44	0.37	0.79	2.36	0.00
3	15	0.39	0.19	0.21	0.17	0.33
3	16	0.89	0.22	0.11	0.03	0.94
3	17	0.00	0.24	6.22	14.39	0.52
3	18	0.63	0.32	0.00	0.32	0.61
3	19	0.84	0.08	0.31	0.16	0.18
3	20	0.28	0.83	0.00	0.14	0.57
3	21	0.02	0.00	0.00	0.13	0.07
3	32	0.00	0.36	4.22	0.33	0.00
3	23	0.19	0.57	0.39	4.90	0.00
3	24	1.28	0.86	5.71	1.05	0.00
3	25	0.00	0.58	1.26	0.05	0.65
3	26	0.00	0.59	0.00	0.00	1.38
3	27	1.35	0.00	0.92	0.09	0.00

3	28	0.19	0.00	0.15	0.14	0.00
3	29	0.26	0.00	0.10	0.25	0.00
3	30	0.89	0.00	0.00	0.07	0.00
4	4	0.00	0.00	0.00	0.00	0.00
4	5	5.25	0.00	12.68	0.43	0.00
4	6	7.55	10.71	18.27	11.24	0.00
4	7	4.63	22.95	0.21	0.00	10.99
4	8	0.00	4.12	0.00	0.00	0.00
4	9	0.87	0.00	1.44	0.02	0.24
4	10	0.84	4.88	0.64	0.12	0.00
4	11	0.23	0.10	4.45	0.15	1.46
4	12	1.71	7.16	0.00	3.29	1.29
4	13	0.00	0.29	0.85	0.07	0.00
4	14	0.58	1.39	0.00	0.00	0.00
4	15	0.74	0.54	0.41	0.64	0.04
4	16	0.18	2.20	1.40	3.31	1.64
4	17	0.43	0.00	1.41	0.08	1.08
4	18	0.00	4.97	0.00	0.03	1.33
4	19	0.20	0.00	0.26	0.02	0.00
4	20	0.00	21.16	0.00	1.21	2.12
4	21	1.45	0.00	1.70	1.00	0.31
4	42	2.05	0.04	0.00	0.57	0.35
4	23	0.10	0.03	1.44	0.03	0.23
4	24	0.00	0.02	0.78	0.00	0.00
4	25	4.70	0.02	0.47	0.73	1.08
4	26	1.90	0.17	1.06	0.07	0.00
4	27	0.00	0.41	0.93	1.17	0.00
4	28	0.00	0.48	0.38	0.32	0.00
4	29	0.09	0.06	0.98	0.18	0.00
4	30	0.00	0.09	0.36	0.78	1.27
5	5	0.00	0.00	0.00	0.00	0.00
5	6	8.29	0.00	18.92	4.29	1.96
5	7	6.82	0.00	0.10	8.38	0.00
5	8	0.00	0.00	0.01	18.84	4.80
5	9	35.13	1.63	0.96	0.90	6.54
5	10	1.28	0.00	0.30	1.10	12.52
5	11	0.59	0.00	5.64	1.49	0.09
5	12	0.45	0.00	0.53	1.71	0.13
5	13	0.00	0.00	0.42	0.74	3.16
5	14	1.37	0.00	0.23	0.48	0.24
5	15	0.79	0.00	0.97	0.22	0.22
5	16	0.43	0.00	2.96	1.31	0.00
5	17	0.80	3.51	1.65	1.26	0.27
5	18	1.31	0.00	0.00	0.41	0.18

5	19	0.89	1.13	0.82	0.21	4.99
5	20	0.00	0.00	0.00	0.24	0.00
5	21	0.32	0.00	0.97	0.65	0.03
5	22	0.23	0.55	0.36	0.26	0.19
5	23	0.07	0.67	0.49	0.17	0.08
5	24	0.00	0.71	0.21	0.34	0.22
5	25	0.43	0.82	0.45	0.05	0.00
5	26	1.33	0.00	0.79	1.02	0.26
5	27	0.27	0.00	0.26	0.06	0.00
5	28	2.42	0.29	1.18	1.31	0.26
5	29	0.62	0.99	0.52	1.09	0.94
5	30	0.00	0.21	0.71	3.78	0.00
6	6	0.00	0.00	0.00	0.00	0.00
6	7	15.56	4.87	0.13	3.42	0.00
6	8	0.00	9.86	0.03	24.42	7.60
6	9	19.04	0.00	0.48	22.43	15.40
6	10	10.07	11.22	0.58	9.39	5.97
6	11	29.55	0.49	0.83	3.55	9.43
6	12	9.36	11.56	2.89	0.37	5.78
6	13	0.00	11.35	0.47	24.19	8.66
6	14	21.00	20.05	1.28	22.10	6.06
6	15	11.17	12.98	1.74	0.23	0.65
6	16	7.68	17.33	1.05	0.36	0.00
6	17	0.62	0.02	1.16	3.54	0.60
6	18	9.88	23.11	0.00	0.47	0.40
6	19	2.78	0.05	3.54	0.45	4.91
6	20	0.00	6.80	0.00	0.23	0.00
6	21	0.30	0.81	0.15	0.14	0.06
6	22	1.70	0.32	1.96	0.58	0.37
6	23	1.42	0.23	0.32	0.40	0.13
6	24	0.00	0.10	0.04	1.48	1.42
6	25	1.23	0.12	0.41	0.09	0.00
6	26	0.76	1.10	0.05	0.23	0.54
6	27	0.05	1.86	0.72	0.09	0.06
6	28	0.32	0.00	0.27	0.36	0.58
6	29	0.10	0.32	0.74	0.26	0.15
6	30	0.00	0.98	0.13	0.82	0.00
7	7	0.00	0.00	0.00	0.00	0.00
7	8	33.48	11.46	9.93	4.88	0.00
7	9	13.86	0.00	4.61	5.89	0.41
7	10	34.43	9.20	10.41	6.38	0.00
7	11	25.67	2.73	0.00	39.16	2.62
7	12	23.52	2.97	5.07	0.00	0.00
7	13	0.71	0.89	9.85	9.16	0.00

7	14	5.18	5.69	0.26	1.25	1.28
7	15	10.78	10.73	0.13	0.05	0.00
7	16	27.41	4.40	0.07	0.01	3.08
7	17	0.55	0.02	3.86	0.47	1.70
7	18	7.67	16.63	0.75	1.31	1.99
7	19	29.00	0.03	0.20	3.09	0.00
7	20	0.37	10.17	1.38	0.07	2.87
7	21	0.83	1.67	0.00	0.03	0.20
7	22	2.21	0.19	0.29	0.29	0.05
7	23	0.47	0.14	0.37	1.12	0.00
7	24	0.03	0.11	3.38	0.34	0.00
7	25	1.16	0.07	1.60	0.14	1.16
7	26	1.26	0.84	0.00	0.00	0.00
7	27	0.09	0.47	0.83	0.10	0.00
7	28	0.30	0.08	0.09	0.15	0.34
7	29	0.16	0.29	0.06	0.35	0.00
7	30	0.05	1.15	0.23	0.22	0.10
8	8	0.00	0.00	0.00	0.00	0.00
8	9	0.00	0.00	0.37	12.27	4.87
8	10	0.00	19.08	2.25	15.06	14.60
8	11	0.00	7.17	0.00	11.16	17.66
8	12	0.00	12.56	10.16	0.00	10.12
8	13	5.87	7.82	2.14	11.29	9.51
8	14	0.00	8.69	2.31	3.95	10.29
8	15	0.00	2.45	0.00	0.06	0.52
8	16	0.00	6.19	0.00	0.01	0.00
8	17	0.21	0.10	0.00	0.98	1.00
8	18	0.00	0.22	0.00	1.19	0.67
8	19	0.00	0.30	0.00	0.68	0.60
8	20	3.11	3.99	2.82	0.13	0.00
8	21	0.00	0.20	0.00	0.02	0.10
8	22	0.00	0.24	0.94	0.55	0.60
8	23	0.00	0.34	0.21	1.84	0.23
8	24	0.28	0.43	0.49	0.65	1.28
8	25	0.00	0.20	0.55	0.11	0.00
8	26	0.17	0.14	0.00	0.00	0.77
8	27	0.63	1.26	0.17	0.11	0.12
8	28	0.20	0.00	0.03	0.18	0.91
8	29	1.02	0.03	0.00	0.21	0.20
8	30	0.44	0.18	0.19	0.14	0.00
9	9	0.00	0.00	0.00	0.00	0.00
9	10	19.52	0.00	5.61	13.25	31.99
9	11	9.14	0.00	0.23	22.14	10.83
9	12	15.07	0.00	16.60	0.00	1.73

9	13	0.00	0.00	22.64	5.24	28.85
9	14	9.50	0.00	0.13	10.86	1.08
9	15	5.00	0.00	8.44	0.35	1.59
9	16	18.62	0.00	0.50	0.07	0.28
9	17	0.12	3.22	3.49	17.31	0.46
9	18	8.23	0.00	0.79	1.96	0.09
9	19	9.85	1.01	1.72	0.95	0.41
9	20	0.00	0.00	1.31	0.29	0.59
9	21	4.48	0.00	0.00	0.12	0.06
9	22	0.23	0.62	0.68	0.81	0.44
9	23	17.16	1.05	13.15	4.66	0.20
9	24	0.00	2.18	15.49	0.57	1.40
9	25	0.48	2.59	13.70	0.14	0.10
9	26	0.11	0.16	0.00	0.00	0.22
9	27	0.25	0.00	15.98	0.13	0.43
9	28	2.67	0.00	3.44	0.17	0.49
9	29	0.54	0.17	0.63	0.21	0.36
9	30	0.00	0.82	0.73	0.08	0.07
10	10	0.00	0.00	0.00	0.00	0.00
10	11	5.45	0.58	0.00	11.40	0.00
10	12	10.26	7.43	35.49	0.00	0.00
10	13	0.00	16.49	15.70	3.71	11.57
10	14	6.54	2.60	1.44	10.19	0.00
10	15	10.82	10.73	0.22	0.95	9.37
10	16	5.90	0.97	0.22	0.28	0.22
10	17	0.06	0.00	11.96	4.53	0.93
10	18	11.40	32.40	0.57	16.76	0.86
10	19	21.12	0.00	0.62	8.56	2.51
10	20	0.00	8.54	0.84	1.80	0.05
10	21	0.84	1.17	0.00	0.29	0.44
10	22	0.77	0.57	1.40	1.69	0.04
10	23	0.65	0.50	0.62	6.07	0.00
10	24	0.00	0.17	13.33	0.57	0.00
10	25	1.06	0.18	2.80	0.25	0.00
10	26	0.25	1.44	0.00	0.00	0.00
10	27	0.19	0.38	1.55	0.51	1.46
10	28	2.09	0.07	0.19	0.97	0.05
10	29	0.59	0.24	0.20	1.93	2.42
10	30	0.00	0.82	0.73	0.48	0.15
11	11	0.00	0.00	0.00	0.00	0.00
11	12	12.09	14.32	0.00	0.00	5.22
11	13	0.00	8.13	0.00	35.28	0.00
11	14	5.77	14.86	0.00	1.35	5.26
11	15	8.50	1.26	0.83	1.22	0.00

11	16	5.91	11.73	3.23	0.34	1.49
11	17	0.02	0.06	0.00	11.47	0.82
11	18	9.10	0.28	0.00	17.92	0.97
11	19	22.22	0.16	0.44	8.80	0.00
11	20	0.00	6.96	0.00	2.14	2.77
11	21	8.72	1.54	2.92	0.33	0.34
11	22	1.24	0.47	0.00	1.53	0.00
11	23	3.53	0.73	1.69	2.99	0.00
11	24	0.00	0.92	1.30	0.27	0.42
11	25	0.69	0.42	0.79	0.12	0.49
11	26	0.21	0.30	0.46	0.00	0.00
11	27	0.07	0.00	1.44	0.78	0.29
11	28	0.81	0.00	0.62	1.23	0.00
11	29	0.17	0.04	0.28	2.28	0.00
11	30	0.00	0.26	0.00	0.61	0.00
12	12	0.00	0.00	0.00	0.00	0.00
12	13	0.00	17.22	34.70	0.00	0.00
12	14	28.48	20.27	0.26	0.00	11.80
12	15	6.37	7.38	1.32	0.60	0.03
12	16	6.82	12.64	0.68	3.92	0.18
12	17	0.01	0.00	0.58	0.00	0.11
12	18	10.79	11.66	1.14	0.00	0.19
12	19	14.54	0.00	2.31	0.00	0.00
12	20	0.00	11.49	0.31	0.00	0.00
12	21	1.89	1.34	0.00	2.84	0.50
12	22	2.43	0.55	0.30	1.77	3.87
12	23	12.94	0.48	0.37	0.16	1.85
12	24	0.00	0.16	0.67	0.00	2.45
12	25	1.42	0.17	0.65	0.12	0.00
12	26	0.45	1.34	0.00	0.25	0.00
12	27	0.08	1.66	0.52	0.55	0.04
12	28	0.84	0.09	0.08	1.41	0.00
12	29	0.19	0.52	0.34	0.81	0.00
12	30	0.00	1.19	0.23	1.98	0.52
13	13	0.00	0.00	0.00	0.00	0.00
13	14	0.00	12.96	0.92	36.39	0.00
13	15	0.00	3.59	0.47	0.65	1.27
13	16	0.00	8.92	0.21	0.18	0.00
13	17	0.00	0.32	15.96	7.53	0.77
13	18	0.00	7.14	1.22	4.53	0.52
13	19	0.00	0.79	0.62	3.42	2.65
13	20	3.58	11.52	1.77	1.12	0.00
13	21	0.00	0.69	0.00	0.19	0.10
13	22	0.00	0.63	0.89	4.19	0.62

13	23	0.00	1.04	1.74	18.35	0.17
13	24	1.95	1.23	13.26	0.10	0.00
13	25	0.10	0.61	4.16	0.20	0.00
13	26	0.34	1.09	0.00	0.00	1.38
13	27	2.68	0.18	1.71	0.23	0.00
13	28	0.34	0.00	0.34	0.61	1.09
13	29	0.48	0.13	0.31	1.31	0.17
13	30	1.14	0.21	0.73	0.34	0.00
14	14	0.00	0.00	0.00	0.00	0.00
14	15	12.27	12.03	0.15	0.05	0.00
14	16	17.65	14.55	0.00	0.00	0.00
14	17	0.12	0.04	0.00	0.73	0.00
14	18	7.36	16.53	2.91	2.11	0.00
14	19	4.74	0.10	0.14	1.71	0.00
14	20	0.00	9.58	0.00	0.05	0.03
14	21	1.47	2.19	0.00	0.00	0.27
14	22	1.50	0.35	0.49	0.04	0.05
14	23	6.57	0.19	0.52	0.00	0.00
14	24	0.00	0.15	0.49	0.46	3.94
14	25	0.38	0.19	0.80	0.37	0.00
14	26	0.14	1.80	0.00	0.00	0.00
14	27	0.11	0.22	1.58	0.49	0.04
14	28	0.53	0.16	1.63	0.82	3.80
14	29	0.67	0.14	3.34	3.92	0.00
14	30	0.00	0.39	0.14	1.14	0.09
15	15	0.00	0.00	0.00	0.00	0.00
15	16	3.54	15.00	1.79	12.26	14.33
15	17	0.02	0.05	5.76	3.05	8.44
15	18	17.14	6.64	0.08	0.49	15.13
15	19	4.57	0.10	5.85	0.25	0.20
15	20	0.00	11.27	0.00	7.30	0.31
15	21	1.24	3.94	1.30	1.35	2.38
15	22	1.66	0.05	0.00	3.86	0.56
15	23	7.82	0.79	0.54	0.75	0.08
15	24	0.00	0.87	1.48	0.00	0.00
15	25	0.49	0.99	4.92	12.27	0.00
15	26	0.27	7.97	0.34	0.11	1.12
15	27	0.10	1.05	8.14	5.51	2.33
15	28	0.73	0.04	1.39	13.65	0.00
15	29	0.15	0.23	2.75	9.11	0.00
15	30	0.00	0.26	6.02	13.60	0.96
16	16	0.00	0.00	0.00	0.00	0.00
16	17	0.10	0.00	20.17	0.22	20.68
16	18	29.84	13.21	0.00	0.00	6.26

16	19	17.47	0.00	4.97	0.00	0.00
16	20	0.00	17.37	0.00	26.02	7.85
16	21	0.88	3.04	5.05	0.88	6.97
16	22	0.72	0.21	0.00	0.53	1.71
16	23	0.16	0.18	3.78	0.07	0.41
16	24	0.00	0.06	2.77	0.00	0.98
16	25	0.11	0.06	0.92	0.92	2.68
16	26	0.19	0.48	1.31	0.71	0.00
16	27	0.17	0.00	3.11	0.65	0.92
16	28	0.52	0.09	5.65	1.12	0.00
16	29	0.55	0.07	0.94	1.59	0.00
16	30	0.00	0.32	0.06	4.10	2.79
17	17	0.00	0.00	0.00	0.00	0.00
17	18	0.00	0.00	0.00	19.26	17.91
17	19	0.02	6.68	29.35	7.02	0.11
17	20	0.00	0.00	0.00	1.53	5.23
17	21	0.00	0.00	0.00	0.53	2.94
17	22	0.00	10.60	0.00	39.96	1.01
17	23	0.00	2.86	1.83	11.37	0.24
17	24	0.00	1.19	7.48	0.00	0.54
17	25	1.71	6.01	2.82	0.89	1.48
17	26	5.92	0.10	0.00	0.00	7.95
17	27	8.25	0.00	5.91	0.69	0.54
17	28	5.55	0.46	4.08	1.00	0.05
17	29	8.13	11.54	0.80	1.87	0.37
17	30	0.00	0.06	6.65	0.66	1.52
18	18	0.00	0.00	0.00	0.00	0.00
18	19	20.75	0.00	0.07	20.85	0.07
18	20	0.00	24.66	2.59	0.62	6.42
18	21	2.65	0.00	0.00	0.07	5.54
18	22	1.93	0.17	0.00	10.02	1.80
18	23	1.45	0.10	0.36	7.79	0.43
18	24	0.00	0.09	0.34	0.00	0.64
18	25	0.00	0.09	0.62	0.17	1.74
18	26	0.08	0.75	0.00	0.00	5.34
18	27	0.14	0.16	1.16	0.29	0.97
18	28	1.23	1.04	1.03	0.50	0.03
18	29	0.30	0.05	2.29	1.97	0.25
18	30	0.00	0.33	0.07	0.65	3.04
19	19	0.00	0.00	0.00	0.00	0.00
19	20	0.00	0.00	0.00	0.32	0.00
19	21	0.87	0.04	0.66	0.03	0.05
19	22	0.55	18.16	0.00	5.08	0.32
19	23	3.40	15.27	5.60	3.95	0.99

19	24	0.00	21.30	0.73	0.00	0.00
19	25	0.12	8.45	15.49	0.08	0.00
19	26	0.07	7.06	0.17	0.00	0.65
19	27	0.09	0.00	6.68	0.11	0.00
19	28	0.97	1.35	8.31	0.23	0.52
19	29	0.14	3.16	18.29	1.28	0.25
19	30	0.00	6.93	5.05	0.29	0.00
20	20	0.00	0.00	0.00	0.00	0.00
20	21	0.00	0.27	0.00	0.39	3.54
20	22	0.00	0.33	0.00	7.15	3.86
20	23	0.00	0.19	0.00	0.60	0.00
20	24	5.28	0.38	0.00	0.00	0.00
20	25	0.00	0.40	0.00	15.43	3.80
20	26	0.00	3.20	0.00	0.00	0.00
20	27	6.86	0.08	0.00	5.61	0.31
20	28	0.98	0.12	0.00	16.30	0.17
20	29	1.32	0.52	0.00	9.88	0.00
20	30	1.29	0.89	0.00	13.92	7.65
21	21	0.00	0.00	0.00	0.00	0.00
21	22	30.91	0.00	0.00	18.59	2.60
21	23	13.04	0.95	6.68	39.66	1.52
21	24	0.00	1.06	25.98	0.00	0.00
21	25	1.91	1.01	7.05	14.53	0.47
21	26	0.62	8.05	17.57	2.94	0.31
21	27	0.31	0.00	0.00	4.35	2.45
21	28	2.83	0.00	5.84	5.34	1.70
21	29	0.50	0.14	0.00	1.38	0.00
21	30	0.00	0.03	0.00	20.18	3.60
22	22	0.00	0.00	0.00	0.00	0.00
22	23	27.08	15.14	0.00	7.46	9.04
22	24	0.00	7.93	0.00	0.00	0.00
22	25	2.69	5.83	0.00	7.08	0.00
22	26	0.88	17.09	0.00	1.53	0.00
22	27	0.48	0.00	0.00	19.43	0.43
22	28	4.31	4.18	0.00	10.25	10.89
22	29	0.77	6.49	0.00	6.58	0.00
22	30	0.00	2.03	0.00	22.27	11.36
23	23	0.00	0.00	0.00	0.00	0.00
23	24	0.00	13.24	19.57	0.00	0.00
23	25	0.22	16.92	10.47	6.44	0.00
23	26	0.07	1.91	1.11	0.00	0.00
23	27	0.01	0.00	5.61	0.90	0.00
23	28	0.06	2.56	8.25	7.42	0.00
23	29	0.01	3.60	12.26	2.92	0.00

23	30	0.00	2.86	1.83	13.07	1.02
24	24	0.00	0.00	0.00	0.00	0.00
24	25	0.00	9.63	14.78	0.00	0.00
24	26	0.00	2.39	9.57	0.00	0.00
24	27	4.62	0.00	21.42	0.00	0.00
24	28	0.71	0.00	8.98	0.00	0.00
24	29	0.95	0.41	25.28	0.00	0.00
24	30	8.17	2.76	4.10	0.00	0.00
25	25	0.00	0.00	0.00	0.00	0.00
25	26	18.47	17.43	43.07	0.00	0.00
25	27	0.00	0.00	5.74	7.81	0.00
25	28	0.00	0.00	10.13	11.31	0.00
25	29	17.83	0.27	7.39	6.16	0.00
25	30	0.00	1.26	9.86	32.72	0.00
26	26	0.00	0.00	0.00	0.00	0.00
26	27	10.45	0.00	0.00	0.00	0.00
26	28	7.03	0.00	16.67	0.92	0.20
26	29	10.70	0.67	0.00	1.12	0.00
26	30	0.00	1.03	0.00	2.77	0.91
27	27	0.00	0.00	0.00	0.00	0.00
27	28	2.95	0.00	2.84	19.07	0.00
27	29	14.44	0.00	10.90	12.00	0.00
27	30	5.16	0.00	12.02	5.68	0.85
28	28	0.00	0.00	0.00	0.00	0.00
28	29	11.78	4.47	8.27	15.56	0.00
28	30	12.70	0.97	4.99	14.26	1.55
29	29	0.00	0.00	0.00	0.00	0.00
29	30	17.06	3.22	0.71	10.48	0.00
30	30	0.00	0.00	0.00	0.00	0.00

174 **Table S3**. The original SOC elements between T_i and S_j calculated at M06L/def2-svp level.

States		SOC elements between T_i and S_j /cm^{-1}				
T_i	S_j	Conformer 1	Conformer 2	Conformer 3	Conformer 4	Conformer 5
1	0	18.78	14.55	10.23	7.31	13.62
1	1	1.50	0.27	0.31	0.63	0.39
1	2	1.55	0.58	0.71	1.13	7.28
1	3	4.58	0.64	78.38	395.62	1.42
1	4	642.53	675.49	676.77	563.40	2.23
1	5	5.84	70.40	4.31	11.58	9.45
1	6	22.65	5.99	2.10	24.39	671.42
1	7	689.33	5.34	2.23	11.29	0.84
1	8	373.85	86.56	34.68	113.26	1.41
1	9	4.34	22.25	3.12	20.33	9.00

1	10	44.79	84.26	753.12	742.48	41.65
1	11	11.23	138.31	0.98	1.84	3.83
1	12	6.66	727.82	0.51	1.85	6.90
1	13	8.20	76.99	1.28	1.98	62.99
1	14	8.11	9.01	4.26	3.59	743.31
1	15	9.46	17.64	1.52	2.48	2.06
1	16	18.29	1.96	3.93	2.08	8.16
1	17	122.84	2.87	14.48	3.26	0.70
1	18	2.23	0.35	130.61	14.29	9.11
1	19	8.76	2.97	1.76	8.57	0.78
1	20	1.59	1.10	2.12	114.45	0.56
1	21	352.99	2.08	1.11	2.45	2.45
1	22	250.03	43.72	11.36	0.49	5.42
1	23	10.82	138.09	2.20	0.30	9.17
1	24	5.56	3.18	1.90	2.53	36.29
1	25	1.66	1.61	2.13	2.64	7.69
1	26	11.76	5.07	3.04	1.16	5.19
1	27	37.07	0.77	2.64	2.13	90.87
1	28	24.39	3.54	135.52	17.29	76.90
1	29	127.50	1.10	156.05	9.87	8.36
1	30	19.62	39.43	83.79	246.02	0.52
2	0	40.28	33.67	7.30	7.74	1.43
2	1	2.57	0.88	1.00	0.43	6.30
2	2	2.92	1.15	0.09	0.35	0.09
2	3	4.59	0.40	0.62	2.19	0.31
2	4	3.96	1.68	1.33	0.55	0.98
2	5	643.29	3.66	1.63	2.92	0.28
2	6	11.22	10.25	17.52	405.48	36.23
2	7	5.08	676.26	84.59	129.47	2.64
2	8	12.89	35.17	37.02	151.64	2.72
2	9	7.36	46.24	674.98	525.23	0.67
2	10	98.48	32.63	2.17	7.21	3.41
2	11	761.61	10.38	11.80	4.71	2.04
2	12	40.18	7.10	19.69	19.46	3.32
2	13	129.06	16.92	751.82	741.97	3.36
2	14	37.75	35.21	28.85	52.16	41.50
2	15	61.22	25.58	1.38	74.51	0.04
2	16	2.11	16.40	43.25	2.70	0.62
2	17	4.33	751.35	4.67	4.72	0.09
2	18	6.21	1.24	1.53	6.02	0.58
2	19	7.92	2.19	2.51	2.77	1.97
2	20	1.15	9.17	1.04	1.49	0.10
2	21	4.24	4.09	1.00	1.37	3.42
2	22	3.56	16.95	5.56	0.04	0.20

2	23	109.76	4.47	3.29	0.27	1.50
2	24	18.17	4.66	0.80	2.25	2.00
2	25	14.37	9.19	1.97	7.66	0.70
2	26	114.13	8.71	6.00	13.83	0.35
2	27	84.83	2.36	10.36	2.52	4.60
2	28	77.32	28.86	59.41	3.56	4.00
2	29	34.03	15.62	98.53	1.15	1.22
2	30	15.88	15.71	41.76	2.30	0.19
3	0	15.84	38.57	10.16	2.60	34.59
3	1	1.77	1.52	57.45	320.73	0.88
3	2	0.86	1.13	0.97	3.38	0.24
3	3	3.00	0.48	2.54	8.39	0.67
3	4	4.37	0.73	63.69	85.51	8.17
3	5	12.33	1.72	3.45	14.52	10.13
3	6	641.80	5.92	1.78	10.61	0.42
3	7	31.71	8.10	0.36	4.32	3.83
3	8	25.37	5.07	4.02	49.38	3.96
3	9	7.02	76.65	4.57	9.69	14.14
3	10	34.36	32.75	99.20	330.77	5.88
3	11	0.41	657.19	8.26	5.32	4.45
3	12	707.04	110.35	4.74	8.90	669.16
3	13	82.33	69.12	6.39	4.19	33.93
3	14	24.73	9.17	38.90	22.30	2.86
3	15	321.52	57.99	1.13	0.76	1.44
3	16	12.57	5.60	0.39	1.15	26.34
3	17	4.11	11.05	3.03	2.94	5.95
3	18	2.22	7.42	13.04	4.88	11.96
3	19	3.68	187.09	5.54	5.08	14.43
3	20	1.05	725.10	1.81	34.50	6.31
3	21	2.58	20.62	0.67	0.95	729.75
3	32	2.48	2.86	2.35	0.36	36.94
3	23	32.95	8.80	4.93	0.71	124.09
3	24	5.04	4.05	4.29	4.41	51.38
3	25	2.30	9.03	4.60	20.62	1.98
3	26	80.57	36.65	39.12	9.36	8.87
3	27	65.63	2.94	1.01	1.90	17.17
3	28	38.25	25.57	4.98	9.77	2.13
3	29	17.38	17.22	9.26	4.20	22.58
3	30	95.12	48.34	7.42	63.44	4.61
4	0	23.06	8.44	304.22	350.42	390.23
4	1	639.73	35.10	3.76	23.49	7.40
4	2	5.62	0.56	1.19	4.93	0.09
4	3	10.47	3.81	1.40	3.47	9.78
4	4	1.74	18.31	2.60	0.93	4.46

4	5	4.81	1.94	12.15	18.82	77.23
4	6	21.06	3.62	70.42	36.60	1.43
4	7	616.05	1.15	14.55	126.52	34.28
4	8	311.60	3.62	1.39	4.46	46.51
4	9	1.82	1.77	7.93	3.19	131.34
4	10	17.44	4.39	5.42	21.21	17.28
4	11	6.89	19.18	153.21	111.19	12.32
4	12	4.42	38.14	66.78	277.43	31.48
4	13	1.26	3.93	28.49	3.44	4.40
4	14	7.93	0.85	529.50	73.56	15.19
4	15	5.60	1.01	74.88	3.72	104.88
4	16	4.26	5.34	5.51	214.36	543.56
4	17	58.59	1.35	84.14	20.25	33.98
4	18	1.09	1.75	8.03	394.45	310.96
4	19	4.83	10.48	346.55	392.97	27.84
4	20	1.44	16.70	48.01	18.43	26.90
4	21	52.69	16.89	15.46	60.64	3.52
4	42	37.05	1.80	7.42	10.50	220.59
4	23	4.03	8.27	67.34	135.54	125.32
4	24	2.78	2.32	34.14	52.89	16.48
4	25	0.71	2.53	71.04	25.27	59.51
4	26	7.47	1.32	581.93	13.26	45.69
4	27	26.17	1.13	22.77	142.12	16.61
4	28	18.85	1.21	38.83	58.24	21.85
4	29	145.67	1.07	7.59	18.14	31.79
4	30	16.31	1.78	95.40	18.54	9.18
5	0	35.28	319.09	245.45	82.07	0.74
5	1	7.38	2.81	126.73	144.40	3.04
5	2	625.18	6.47	2.90	6.25	1.09
5	3	11.72	3.98	11.08	17.93	1.72
5	4	1.24	1.74	2.17	10.27	0.18
5	5	15.68	0.68	7.59	15.24	0.11
5	6	1.37	135.83	78.92	7.38	8.11
5	7	3.36	8.40	16.94	11.52	0.57
5	8	11.97	0.53	4.50	20.00	0.90
5	9	10.05	69.89	4.50	3.59	0.33
5	10	83.37	0.44	135.50	156.27	0.48
5	11	660.98	9.28	54.93	97.68	0.33
5	12	51.30	5.21	32.40	298.47	10.75
5	13	71.19	5.66	12.84	48.81	1.60
5	14	27.28	0.84	363.52	560.52	7.34
5	15	42.72	2.63	192.03	16.37	0.16
5	16	1.46	182.55	1.94	24.90	0.46
5	17	3.29	7.99	67.98	100.13	1.93

5	18	4.18	66.56	18.94	58.04	0.12
5	19	9.34	273.74	509.18	52.95	0.42
5	20	2.81	55.87	73.28	13.25	3.53
5	21	2.48	574.02	11.88	10.99	12.88
5	22	3.89	59.95	11.33	2.51	0.81
5	23	41.68	5.63	29.81	12.76	1.99
5	24	7.34	72.50	149.28	35.70	1.42
5	25	6.65	74.85	39.40	586.42	0.60
5	26	46.47	11.96	302.98	271.60	0.28
5	27	21.59	28.24	4.77	48.57	1.26
5	28	21.30	30.79	20.79	196.06	0.98
5	29	4.91	22.32	26.53	63.64	0.58
5	30	2.77	95.44	202.30	55.64	1.68
6	0	16.65	5.61	51.04	11.62	2.61
6	1	130.22	39.06	667.54	571.14	13.08
6	2	16.61	6.00	2.20	11.53	1.62
6	3	479.54	4.75	59.78	82.60	3.32
6	4	101.92	25.36	1.83	17.44	0.78
6	5	9.75	3.85	7.83	8.37	0.08
6	6	12.54	1.17	12.26	15.26	6.97
6	7	67.72	7.39	2.38	8.00	3.26
6	8	51.79	4.34	24.18	76.04	4.59
6	9	3.06	4.30	2.60	18.60	0.57
6	10	7.20	5.53	724.56	610.39	1.59
6	11	11.60	24.04	8.27	20.85	2.17
6	12	473.71	49.20	5.50	77.35	43.23
6	13	56.35	6.41	2.65	16.79	2.10
6	14	16.65	1.16	70.20	123.72	11.84
6	15	199.52	2.76	35.71	3.75	0.96
6	16	0.66	1.28	2.97	2.48	1.53
6	17	22.75	13.90	23.06	22.48	0.78
6	18	1.02	3.11	79.69	16.09	2.13
6	19	16.87	6.44	92.58	8.26	1.57
6	20	3.54	26.41	14.14	59.52	1.19
6	21	42.89	3.31	1.82	3.64	48.57
6	22	22.86	3.15	9.61	0.42	6.78
6	23	10.55	11.99	5.49	1.56	8.74
6	24	3.14	0.75	29.07	7.60	4.24
6	25	2.03	1.60	6.66	135.31	8.51
6	26	15.04	1.86	58.60	60.83	1.00
6	27	12.00	1.27	2.01	16.45	1.10
6	28	10.23	1.90	91.43	51.01	1.51
6	29	38.44	0.52	101.93	17.43	2.30
6	30	38.50	2.59	75.75	124.30	0.67

7	0	36.90	1.78	10.10	4.66	267.61
7	1	253.72	79.93	5.06	44.37	2.84
7	2	10.86	22.90	28.19	56.44	0.26
7	3	408.31	4.41	0.65	5.91	5.25
7	4	223.26	8.47	1.47	1.68	1.28
7	5	14.05	1.15	2.98	2.83	10.59
7	6	7.99	0.52	1.34	6.96	3.12
7	7	65.77	9.72	3.17	1.98	21.82
7	8	77.07	9.02	1.75	4.09	23.58
7	9	12.62	1.93	47.54	21.46	87.80
7	10	24.49	8.40	5.79	47.72	10.02
7	11	18.53	20.55	6.10	3.44	11.34
7	12	398.38	83.97	3.27	11.89	16.07
7	13	51.55	9.50	56.28	54.83	4.61
7	14	29.46	1.96	41.98	21.95	4.20
7	15	174.48	1.48	7.18	5.96	73.58
7	16	5.75	0.69	2.83	1.10	110.92
7	17	49.75	33.07	1.84	3.95	20.24
7	18	2.25	3.30	0.58	3.22	187.73
7	19	64.22	4.25	12.44	2.14	31.75
7	20	11.37	15.95	3.05	4.57	26.96
7	21	77.62	0.66	0.27	0.34	75.92
7	22	80.51	3.68	0.69	0.26	525.33
7	23	7.27	12.76	2.45	0.81	237.39
7	24	15.39	1.06	8.86	1.20	28.38
7	25	6.16	0.89	4.55	21.29	125.25
7	26	19.00	1.53	42.24	10.91	115.65
7	27	32.15	1.05	1.47	1.65	33.27
7	28	21.47	2.16	4.65	7.07	31.52
7	29	63.53	1.21	5.80	2.54	6.80
7	30	26.25	3.38	16.03	11.23	14.03
8	0	363.04	14.25	0.78	3.97	6.24
8	1	10.61	672.01	17.64	142.51	45.25
8	2	9.11	6.88	2.50	80.10	1.68
8	3	51.16	2.38	3.36	28.30	7.48
8	4	10.53	2.66	21.91	7.16	0.74
8	5	6.51	19.43	0.88	7.19	0.74
8	6	2.79	0.97	0.12	4.89	13.58
8	7	9.61	5.64	0.17	1.01	2.39
8	8	7.62	70.34	1.56	21.44	4.19
8	9	123.65	24.17	4.62	25.03	2.42
8	10	2.51	78.72	9.30	150.17	2.80
8	11	6.14	133.03	0.17	6.45	3.07
8	12	57.17	693.18	0.32	23.97	5.22

8	13	30.62	76.25	5.76	78.88	4.32
8	14	142.95	9.92	2.04	38.86	47.13
8	15	48.52	18.30	0.23	8.35	1.23
8	16	3.36	4.02	0.66	0.98	4.41
8	17	11.82	9.08	0.60	7.34	0.48
8	18	21.02	0.85	2.85	3.45	3.67
8	19	524.68	2.26	0.21	3.43	1.72
8	20	93.10	0.66	0.18	15.56	0.59
8	21	162.58	6.08	0.11	0.88	6.59
8	22	239.63	32.41	0.33	0.34	4.98
8	23	4.62	123.44	0.14	0.45	2.64
8	24	142.88	2.29	0.40	2.85	4.32
8	25	56.03	0.78	0.37	41.39	33.32
8	26	11.23	2.85	2.36	20.33	2.25
8	27	26.66	0.60	0.24	4.33	4.12
8	28	24.17	2.22	2.20	15.29	4.68
8	29	18.55	1.95	3.14	6.16	2.41
8	30	9.80	26.57	1.34	31.60	1.20
9	0	10.68	348.43	43.25	7.72	4.82
9	1	346.54	5.05	15.52	84.32	98.45
9	2	136.53	12.37	29.66	350.50	5.36
9	3	44.52	5.07	1.30	43.21	4.20
9	4	307.86	3.41	13.27	51.94	0.59
9	5	65.51	2.01	20.58	21.02	2.15
9	6	20.29	81.26	2.73	4.61	5.40
9	7	48.40	14.52	0.88	2.96	2.54
9	8	36.08	1.07	1.33	1.58	4.29
9	9	3.90	131.63	19.95	77.95	3.84
9	10	8.45	3.97	14.49	45.68	5.05
9	11	138.73	48.04	22.43	2.02	4.27
9	12	30.43	22.61	6.58	11.71	6.70
9	13	24.23	16.07	44.62	369.84	9.68
9	14	7.09	8.00	93.05	25.87	107.15
9	15	19.74	6.63	11.12	36.83	1.54
9	16	4.79	30.08	2.06	1.05	4.61
9	17	74.57	26.66	8.33	4.04	1.07
9	18	1.69	3.86	3.53	4.97	4.27
9	19	7.06	37.37	11.45	1.35	1.97
9	20	1.24	35.21	7.88	11.51	0.32
9	21	116.10	33.00	1.79	0.45	8.34
9	22	79.57	11.40	1.85	0.48	9.58
9	23	9.05	1.36	7.12	1.30	7.14
9	24	2.33	7.84	22.25	1.87	21.37
9	25	1.74	234.29	13.50	14.74	105.10

9	26	8.55	21.19	101.53	13.64	5.47
9	27	21.77	24.88	4.05	3.02	8.97
9	28	15.16	133.81	11.95	6.72	6.99
9	29	78.81	93.20	6.54	2.45	5.26
9	30	12.28	432.16	45.02	12.98	1.04
10	0	12.29	1.51	21.54	8.81	19.58
10	1	609.02	43.23	16.25	27.67	662.67
10	2	104.19	26.62	74.03	168.48	33.13
10	3	65.66	8.80	1.97	14.97	2.70
10	4	541.82	20.87	8.15	16.55	1.67
10	5	68.03	2.29	8.43	64.02	3.76
10	6	12.15	0.28	2.33	3.38	2.52
10	7	59.23	6.57	2.90	4.01	0.76
10	8	73.98	2.24	0.80	1.16	1.06
10	9	2.01	1.76	26.81	34.99	10.05
10	10	46.43	3.26	27.27	14.08	34.53
10	11	79.18	18.30	9.20	5.66	4.32
10	12	78.92	31.32	2.23	25.68	8.16
10	13	17.34	4.47	88.42	180.57	62.70
10	14	17.95	1.74	32.34	44.10	721.62
10	15	16.56	3.27	4.44	18.50	3.31
10	16	8.83	0.66	4.47	2.16	5.85
10	17	130.56	32.19	2.77	10.21	0.44
10	18	1.64	1.31	4.05	4.68	7.19
10	19	16.83	5.41	5.18	4.55	0.99
10	20	2.92	20.68	3.83	4.70	0.48
10	21	201.83	1.22	0.83	1.39	5.10
10	22	138.31	2.06	0.39	0.97	7.62
10	23	25.78	10.25	3.17	4.81	6.12
10	24	8.06	1.48	10.75	8.52	22.33
10	25	3.56	1.55	5.27	69.05	18.68
10	26	14.12	0.87	38.05	34.09	5.24
10	27	38.76	2.26	2.20	8.07	55.60
10	28	26.02	1.64	9.67	23.75	46.42
10	29	142.16	0.88	8.47	7.85	5.36
10	30	23.96	3.94	23.41	4.42	0.48
11	0	5.56	23.93	260.05	9.43	39.11
11	1	134.79	6.21	10.90	99.61	0.62
11	2	46.39	677.39	34.54	416.44	0.37
11	3	44.68	14.51	1.90	54.36	0.98
11	4	117.03	5.30	8.01	71.82	0.62
11	5	22.54	1.95	9.46	78.93	6.78
11	6	5.12	3.95	27.94	39.36	1.98
11	7	24.81	1.47	3.75	10.60	4.10

11	8	10.70	6.64	0.55	12.61	5.91
11	9	1.93	31.91	5.27	48.87	8.27
11	10	2.97	27.50	4.16	33.61	1.13
11	11	48.49	7.26	83.01	6.48	3.89
11	12	40.26	6.82	5.90	28.41	4.62
11	13	11.83	15.67	37.05	442.83	0.74
11	14	2.83	35.51	123.96	65.73	2.74
11	15	19.74	20.01	25.47	44.64	6.98
11	16	1.55	16.98	2.42	3.52	6.96
11	17	29.69	721.35	13.49	11.69	0.69
11	18	0.69	1.87	1.22	8.22	9.81
11	19	2.50	3.54	57.75	4.60	10.80
11	20	0.33	15.93	33.57	13.76	2.26
11	21	42.58	8.34	7.32	2.75	8.50
11	22	29.25	16.78	16.79	1.61	121.07
11	23	2.34	4.28	15.96	2.23	56.44
11	24	1.15	3.79	116.31	17.52	119.51
11	25	0.63	7.60	26.05	86.74	629.30
11	26	2.92	7.67	277.66	31.99	36.55
11	27	7.65	2.24	37.39	21.03	4.82
11	28	5.35	27.24	135.99	26.28	2.02
11	29	31.51	14.14	1.82	8.17	23.40
11	30	6.83	10.58	493.47	17.18	3.20
12	0	3.68	2.57	21.04	307.35	15.58
12	1	172.24	84.72	8.46	15.15	0.68
12	2	55.55	26.31	658.80	18.82	3.65
12	3	79.02	12.18	2.15	7.45	0.43
12	4	143.95	72.92	6.58	10.06	5.68
12	5	51.67	6.71	6.14	26.57	6.82
12	6	30.78	0.90	13.04	13.79	0.21
12	7	51.72	12.38	57.79	40.30	0.35
12	8	4.79	0.99	6.76	1.35	1.97
12	9	0.60	1.86	8.19	2.57	0.78
12	10	14.48	2.45	8.06	2.90	0.57
12	11	10.18	17.09	14.53	113.41	44.26
12	12	75.06	29.32	18.59	14.06	0.08
12	13	3.37	5.17	713.61	17.72	1.01
12	14	4.55	1.02	26.42	40.17	0.70
12	15	37.68	2.10	3.12	3.04	3.57
12	16	3.22	0.65	38.13	31.67	20.93
12	17	38.37	29.14	1.91	6.28	2.56
12	18	0.63	3.07	1.20	47.09	12.94
12	19	2.54	4.96	6.05	36.03	10.13
12	20	0.81	19.11	1.73	8.95	1.42

12	21	50.73	0.55	0.77	5.41	2.23
12	22	34.98	4.87	3.80	23.11	6.55
12	23	11.13	17.42	2.98	20.53	10.50
12	24	0.55	0.99	5.73	191.52	3.19
12	25	1.52	0.34	3.26	104.10	27.92
12	26	6.97	0.84	26.62	34.58	1.42
12	27	13.45	2.16	6.07	509.58	0.70
12	28	8.88	0.49	36.29	88.30	0.39
12	29	39.20	0.32	58.29	14.51	15.85
12	30	1.27	3.39	44.02	74.24	3.00
13	0	292.27	21.63	12.74	14.33	0.54
13	1	4.28	128.28	26.87	85.73	39.89
13	2	35.61	15.53	150.59	382.19	2.59
13	3	27.33	664.76	2.87	47.32	32.91
13	4	5.94	123.65	21.01	68.00	2.15
13	5	35.65	14.73	14.16	56.45	0.78
13	6	21.09	3.73	6.05	90.00	36.79
13	7	8.27	4.99	16.63	29.32	0.86
13	8	5.88	9.27	3.45	24.08	0.79
13	9	18.90	49.03	25.69	26.41	0.78
13	10	3.00	10.35	21.79	7.05	1.11
13	11	17.33	9.09	5.75	3.57	0.27
13	12	9.31	5.34	6.07	11.46	15.00
13	13	11.98	10.56	168.97	397.34	1.38
13	14	109.88	7.39	53.71	24.17	10.27
13	15	36.54	12.18	4.13	41.77	0.17
13	16	5.57	9.58	9.43	1.25	0.56
13	17	4.69	16.44	5.48	8.44	5.34
13	18	3.28	5.43	5.39	5.08	0.41
13	19	59.39	172.48	4.20	2.94	0.88
13	20	10.77	685.54	1.96	12.55	1.91
13	21	39.28	29.71	0.25	0.39	33.18
13	22	59.06	12.66	2.84	0.68	1.66
13	23	60.06	23.97	4.78	0.71	5.53
13	24	511.28	6.23	9.75	2.45	3.62
13	25	296.70	9.87	6.12	43.39	1.01
13	26	12.51	37.59	62.30	26.83	0.57
13	27	34.37	2.45	4.36	2.08	4.77
13	28	94.27	26.32	14.60	15.63	4.08
13	29	21.49	14.77	20.65	5.06	1.27
13	30	13.34	39.29	49.37	14.14	0.36
14	0	28.97	2.93	5.98	12.94	11.08
14	1	22.51	161.53	753.56	736.14	1.50
14	2	576.93	36.72	2.56	16.38	1.94

14	3	141.86	60.95	112.96	408.79	1.95
14	4	5.25	154.12	734.52	596.03	1.84
14	5	520.31	13.53	10.47	26.57	2.73
14	6	104.70	1.60	0.46	9.64	1.31
14	7	15.52	15.58	3.78	4.41	29.47
14	8	17.46	8.37	36.35	56.60	34.23
14	9	4.13	2.69	1.84	1.58	6.48
14	10	26.61	2.58	0.65	0.77	0.88
14	11	23.03	9.54	3.79	4.61	2.37
14	12	50.69	3.09	0.23	3.13	0.51
14	13	85.41	3.26	1.58	17.79	0.29
14	14	24.74	2.52	4.21	6.37	0.39
14	15	47.99	1.21	1.00	2.93	1.29
14	16	2.96	0.72	3.22	1.04	3.26
14	17	2.73	32.52	16.14	3.32	0.73
14	18	3.92	0.95	121.46	13.22	6.31
14	19	4.86	17.24	1.29	8.62	27.63
14	20	2.11	64.86	1.09	108.04	1.10
14	21	1.97	1.63	1.08	1.95	5.26
14	22	4.01	9.31	11.50	0.29	18.74
14	23	109.39	25.29	1.64	0.39	18.27
14	24	29.78	3.18	1.68	4.03	3.73
14	25	11.27	0.38	2.14	16.60	6.07
14	26	65.77	4.17	6.12	9.72	2.78
14	27	42.56	0.79	1.66	6.58	1.87
14	28	34.74	3.43	61.24	10.72	1.87
14	29	27.38	2.17	72.11	5.53	14.45
14	30	12.99	6.22	41.69	113.03	3.31
15	0	19.76	12.40	178.03	229.76	27.16
15	1	24.02	720.55	5.12	3.22	1.67
15	2	506.63	6.54	11.95	4.34	2.42
15	3	85.10	105.63	3.61	2.47	666.18
15	4	1.78	691.90	4.07	4.34	40.34
15	5	445.74	60.60	371.96	17.44	86.21
15	6	73.20	7.79	575.87	200.04	0.85
15	7	23.39	2.23	102.92	646.36	5.18
15	8	15.57	37.09	2.59	9.86	4.59
15	9	9.63	6.68	9.50	4.79	20.00
15	10	27.95	6.19	5.02	2.54	5.05
15	11	57.57	3.83	74.90	34.61	1.89
15	12	62.88	2.66	62.38	126.12	1.19
15	13	54.63	10.51	6.66	4.86	5.45
15	14	28.05	2.91	40.94	67.61	2.45
15	15	35.44	3.16	40.09	1.45	8.41

15	16	1.20	1.43	0.84	32.43	22.54
15	17	4.11	6.05	27.26	18.19	7.80
15	18	3.45	1.21	6.28	218.09	15.47
15	19	3.62	30.17	305.15	221.85	13.93
15	20	1.58	106.07	41.44	14.12	9.32
15	21	2.58	3.55	14.96	34.92	716.76
15	22	1.08	37.54	4.08	8.52	6.34
15	23	103.12	112.80	51.94	71.20	102.96
15	24	26.75	2.59	64.21	19.87	55.32
15	25	9.39	1.56	39.13	64.85	11.34
15	26	42.18	7.88	403.85	48.09	11.28
15	27	24.89	0.88	17.24	163.09	18.68
15	28	24.98	2.68	51.31	32.35	0.81
15	29	9.12	2.48	3.08	11.20	19.76
15	30	13.20	20.13	88.08	17.44	6.25
16	0	25.50	1.06	164.90	167.69	130.75
16	1	13.93	16.13	4.19	2.73	72.32
16	2	64.72	58.30	12.53	5.29	3.69
16	3	724.41	6.94	1.38	1.20	50.99
16	4	5.00	15.82	1.97	1.36	42.49
16	5	37.95	1.48	161.49	15.38	462.85
16	6	648.56	1.07	52.38	14.86	72.30
16	7	40.51	53.21	7.21	44.14	31.72
16	8	20.93	2.15	0.79	1.13	64.28
16	9	6.32	5.12	11.54	4.23	111.65
16	10	33.80	0.51	2.08	0.88	15.24
16	11	10.85	7.31	84.27	58.10	12.67
16	12	31.01	1.58	5.56	19.69	2.81
16	13	26.44	0.54	2.58	0.48	4.66
16	14	22.17	0.41	34.49	13.21	5.02
16	15	78.92	0.51	21.01	0.59	14.26
16	16	11.75	0.79	0.87	15.52	86.20
16	17	4.45	30.59	3.77	2.86	15.20
16	18	1.60	0.29	1.37	35.50	109.04
16	19	5.61	1.26	54.13	37.19	3.60
16	20	1.29	6.30	11.33	2.72	20.69
16	21	2.60	1.32	6.54	18.10	30.02
16	22	3.39	1.50	3.61	1.79	208.89
16	23	41.06	2.82	15.21	17.44	119.40
16	24	13.76	2.22	39.19	40.73	7.79
16	25	6.05	0.49	22.18	3.74	60.87
16	26	93.63	1.37	169.86	3.78	30.14
16	27	84.73	3.33	5.35	58.88	10.25
16	28	50.24	3.43	21.88	36.30	13.71

16	29	17.89	1.68	3.39	10.19	25.95
16	30	99.28	0.66	65.75	19.27	5.48
17	0	198.48	136.37	34.44	69.58	109.59
17	1	2.64	1.47	1.32	12.21	616.62
17	2	11.54	2.94	24.27	199.12	32.04
17	3	0.79	7.30	2.58	3.70	31.70
17	4	4.15	2.16	0.52	8.07	24.56
17	5	9.04	3.74	143.56	650.95	252.36
17	6	9.80	274.87	60.66	121.75	605.82
17	7	1.21	2.30	11.82	41.11	11.98
17	8	5.01	0.27	1.48	45.50	15.80
17	9	694.66	36.95	23.79	142.94	53.26
17	10	6.22	0.71	1.12	5.04	22.93
17	11	8.76	3.90	13.36	46.91	3.78
17	12	2.62	4.36	9.76	17.67	3.91
17	13	13.38	2.20	1.13	2.93	5.03
17	14	47.65	1.13	11.99	11.54	1.02
17	15	11.23	1.12	8.58	2.01	13.12
17	16	2.62	15.42	0.92	17.96	38.15
17	17	3.60	4.02	20.92	57.87	8.90
17	18	8.21	12.98	2.32	42.77	31.41
17	19	218.74	39.20	53.20	49.14	1.87
17	20	47.83	12.83	6.21	6.62	10.97
17	21	114.04	143.60	3.23	13.19	20.15
17	22	173.37	20.57	3.03	4.16	134.31
17	23	5.04	4.44	41.87	2.85	71.07
17	24	199.26	20.33	6.73	36.74	31.64
17	25	95.97	40.77	12.61	567.24	26.35
17	26	9.81	4.27	142.85	256.27	25.32
17	27	24.91	20.19	3.21	32.00	75.08
17	28	31.47	9.55	26.12	189.28	64.87
17	29	14.96	12.40	4.60	62.69	14.86
17	30	5.37	55.45	32.94	27.94	5.17
18	0	13.21	13.45	23.54	18.81	180.01
18	1	3.50	7.12	2.76	2.96	413.96
18	2	45.38	5.47	748.80	574.50	21.51
18	3	211.35	42.98	2.33	1.88	52.68
18	4	0.99	8.56	0.99	2.09	42.31
18	5	13.00	0.84	31.52	163.92	463.77
18	6	174.03	35.11	45.49	327.21	407.53
18	7	5.30	4.57	120.81	104.37	16.21
18	8	9.80	1.16	41.24	123.69	33.50
18	9	21.10	8.73	728.40	430.71	69.71
18	10	4.89	0.72	1.37	4.63	10.46

18	11	47.66	12.32	14.70	8.16	5.16
18	12	78.41	4.49	4.92	5.70	6.04
18	13	6.16	2.11	0.73	3.70	3.43
18	14	6.60	0.48	10.67	2.51	0.78
18	15	3.85	0.54	1.65	7.05	20.29
18	16	3.49	2.81	9.75	3.89	74.42
18	17	0.95	1.25	7.19	14.41	15.64
18	18	1.20	2.40	0.55	9.93	62.24
18	19	6.74	2.54	26.54	12.62	3.93
18	20	1.48	37.13	6.58	2.14	19.68
18	21	3.69	20.95	1.78	3.01	32.86
18	22	5.77	2.50	8.65	1.01	226.04
18	23	6.34	1.44	4.99	0.73	127.51
18	24	4.77	6.70	10.16	9.25	26.28
18	25	1.45	4.97	5.84	141.68	50.15
18	26	26.57	1.73	25.91	64.00	33.65
18	27	23.34	1.51	32.62	10.31	49.90
18	28	14.33	0.76	58.66	48.24	37.99
18	29	5.81	0.95	90.95	16.42	21.16
18	30	29.57	2.20	39.60	7.73	7.93
19	0	8.14	289.29	219.02	10.41	0.52
19	1	8.00	1.96	4.96	2.07	0.25
19	2	50.84	5.68	60.15	434.48	0.29
19	3	134.93	10.93	3.21	1.49	15.04
19	4	1.58	9.39	1.22	0.99	1.14
19	5	27.31	10.44	527.86	78.71	0.75
19	6	116.69	655.68	400.57	247.96	1.96
19	7	4.50	5.78	76.53	78.75	0.16
19	8	9.95	0.61	3.71	93.81	0.18
19	9	5.24	72.90	57.36	327.75	0.14
19	10	12.88	4.10	2.11	3.83	0.15
19	11	48.60	14.20	114.85	3.08	0.07
19	12	14.11	4.33	44.64	3.89	12.33
19	13	5.66	7.29	3.25	8.52	0.59
19	14	8.40	2.81	63.03	1.83	2.41
19	15	12.18	1.85	13.92	3.90	0.10
19	16	2.51	37.98	2.24	1.61	0.14
19	17	0.69	5.56	55.52	6.90	1.04
19	18	0.30	39.33	6.77	5.16	0.21
19	19	1.72	166.36	236.20	7.43	0.20
19	20	0.76	23.73	67.21	1.37	3.61
19	21	1.38	359.83	14.56	1.59	12.25
19	22	2.24	47.42	16.37	0.46	1.03
19	23	1.90	4.62	7.76	0.66	2.37

19	24	1.44	49.90	123.72	4.59	1.16
19	25	2.56	74.11	66.13	67.28	0.15
19	26	21.90	9.46	486.49	30.85	0.17
19	27	16.96	28.84	2.43	5.93	0.51
19	28	10.38	21.09	17.11	23.44	0.30
19	29	5.57	26.93	12.21	7.00	0.65
19	30	19.20	56.73	208.42	3.87	1.45
20	0	167.81	3.64	2.13	102.39	80.51
20	1	4.53	6.33	1.25	0.68	5.23
20	2	2.50	5.41	58.67	7.88	0.23
20	3	3.90	60.47	0.22	1.40	3.55
20	4	0.97	6.69	0.90	2.89	2.02
20	5	0.80	1.46	1.08	28.61	24.67
20	6	2.68	4.78	1.69	89.52	3.65
20	7	3.09	4.80	8.40	292.05	25.97
20	8	1.61	0.70	2.97	5.25	26.55
20	9	29.29	7.33	53.92	6.26	103.45
20	10	0.76	2.48	0.71	1.72	11.41
20	11	1.26	44.52	0.62	25.81	7.00
20	12	2.81	8.98	0.36	103.33	3.70
20	13	19.76	4.74	10.23	1.59	0.92
20	14	79.87	0.65	0.75	39.56	0.97
20	15	15.49	3.06	0.09	0.86	13.88
20	16	1.93	1.11	0.09	51.40	30.84
20	17	4.67	1.47	0.40	5.49	1.39
20	18	2.11	3.06	0.11	165.87	36.61
20	19	38.22	10.00	0.22	166.56	4.34
20	20	7.79	35.80	0.13	7.26	2.61
20	21	25.69	1.86	0.16	24.06	5.05
20	22	38.23	0.26	1.17	3.05	15.68
20	23	4.12	0.95	0.33	54.29	6.94
20	24	35.17	0.71	0.41	46.31	5.55
20	25	37.05	1.04	0.25	6.79	23.30
20	26	6.13	3.30	0.77	6.11	16.13
20	27	3.31	3.87	2.73	77.19	2.18
20	28	16.73	2.22	4.51	15.55	3.21
20	29	2.21	0.80	7.14	8.51	6.32
20	30	8.20	3.46	2.52	9.87	1.63
21	0	11.51	35.30	92.87	245.71	419.78
21	1	70.94	4.93	7.78	2.40	4.19
21	2	4.01	748.37	0.62	1.46	0.49
21	3	6.67	19.02	0.54	1.39	26.14
21	4	33.57	4.05	5.86	2.02	24.86
21	5	3.09	5.47	21.11	16.77	248.79

21	6	4.19	12.65	15.53	11.61	5.24
21	7	86.87	716.79	2.87	39.08	154.17
21	8	48.05	35.24	0.40	0.85	155.40
21	9	3.66	96.06	1.09	3.65	592.65
21	10	3.24	26.51	8.52	1.12	65.59
21	11	2.49	21.14	57.60	290.20	49.06
21	12	6.88	5.48	4.30	30.72	24.46
21	13	3.11	7.19	1.70	1.82	2.58
21	14	12.59	19.12	16.71	31.76	2.53
21	15	3.69	11.50	12.43	2.64	31.74
21	16	0.87	9.04	0.58	36.66	235.54
21	17	0.52	4.93	11.60	1.46	8.58
21	18	0.40	1.70	1.48	28.70	245.34
21	19	2.27	6.72	10.58	29.42	22.49
21	20	0.69	6.74	16.44	3.19	5.19
21	21	18.44	9.54	11.63	16.91	6.79
21	22	12.77	5.35	3.69	2.96	120.24
21	23	0.76	2.32	16.28	9.91	68.24
21	24	4.65	1.86	23.16	38.11	16.51
21	25	2.93	9.49	4.22	12.35	42.33
21	26	1.49	4.32	31.59	5.95	86.56
21	27	2.63	2.57	2.49	123.37	21.76
21	28	1.56	18.80	5.47	30.33	28.23
21	29	9.44	9.34	1.14	6.09	2.60
21	30	1.95	32.80	17.33	21.31	3.44
22	0	16.89	127.72	6.54	246.00	75.21
22	1	98.91	3.53	131.41	5.45	0.32
22	2	5.63	31.88	0.78	7.29	0.05
22	3	2.81	56.10	13.49	3.84	3.83
22	4	48.45	3.29	82.72	4.51	2.21
22	5	4.57	3.27	4.72	82.45	19.61
22	6	2.62	54.87	2.14	35.17	0.70
22	7	116.88	41.53	0.64	106.52	28.55
22	8	64.56	2.75	7.28	2.29	31.10
22	9	4.93	255.78	0.81	8.02	102.86
22	10	4.87	13.02	123.70	4.59	16.15
22	11	3.38	63.84	5.11	488.11	8.58
22	12	1.63	17.36	1.50	44.21	4.63
22	13	4.57	14.11	0.74	5.06	0.78
22	14	15.77	5.78	2.99	91.65	0.79
22	15	3.20	9.44	0.54	4.99	7.14
22	16	1.98	36.50	0.33	44.88	15.88
22	17	1.08	7.73	0.84	4.38	0.32
22	18	0.33	5.89	0.40	60.25	27.79

22	19	2.76	22.61	1.37	55.95	1.71
22	20	0.67	7.90	1.92	4.78	1.38
22	21	25.68	48.13	1.26	48.93	3.10
22	22	17.89	8.41	1.40	7.34	11.33
22	23	1.74	1.71	1.35	24.27	11.16
22	24	6.45	6.37	1.10	40.67	9.61
22	25	3.82	21.29	0.21	33.24	3.45
22	26	1.70	42.66	4.81	14.73	14.75
22	27	3.51	6.50	0.59	190.97	27.31
22	28	2.40	24.93	13.35	56.13	27.16
22	29	13.53	10.76	15.33	10.39	3.21
22	30	2.02	107.91	8.89	40.01	1.24
23	0	2.12	206.47	209.64	92.48	21.35
23	1	13.80	4.75	2.63	1.78	0.17
23	2	3.44	45.04	4.57	1.26	0.05
23	3	13.52	79.71	0.75	0.91	0.91
23	4	2.07	4.79	1.54	1.36	4.11
23	5	1.35	3.27	97.37	59.95	41.06
23	6	9.18	51.83	45.63	6.10	0.24
23	7	8.64	60.79	8.70	16.20	7.74
23	8	4.77	6.12	0.74	0.65	10.62
23	9	0.32	396.13	3.68	2.58	27.16
23	10	0.87	15.48	1.11	1.35	4.60
23	11	5.09	92.55	241.05	183.27	2.30
23	12	6.94	26.27	27.26	28.45	0.25
23	13	1.86	21.20	3.68	3.95	0.82
23	14	1.40	10.12	98.83	46.44	1.08
23	15	2.61	6.82	44.41	2.08	6.24
23	16	0.68	56.00	0.65	17.05	24.54
23	17	1.14	12.28	8.05	2.17	1.80
23	18	0.43	8.33	1.37	13.68	10.65
23	19	0.15	23.71	44.47	11.61	1.08
23	20	0.09	16.29	11.13	1.77	0.42
23	21	0.24	55.82	4.96	13.47	0.35
23	22	0.34	7.53	4.18	2.23	3.36
23	23	0.46	2.71	11.04	9.29	2.69
23	24	0.32	8.91	19.82	12.82	6.48
23	25	0.70	31.32	3.21	25.08	1.39
23	26	1.38	31.79	45.99	11.22	1.74
23	27	1.16	12.31	5.68	74.23	2.03
23	28	0.79	25.36	25.89	24.17	1.41
23	29	3.73	19.22	1.15	5.71	8.39
23	30	1.24	172.67	121.00	15.48	44.31
24	0	19.77	176.52	113.46	7.34	11.58

24	1	1.47	6.92	5.69	115.91	0.32
24	2	0.65	46.43	2.96	0.70	1.90
24	3	0.45	88.82	1.13	43.13	4.55
24	4	0.45	8.80	3.35	59.95	1.99
24	5	1.12	3.51	71.40	4.82	4.01
24	6	0.63	59.42	80.86	4.01	0.48
24	7	1.35	61.46	15.47	7.47	10.56
24	8	0.66	5.99	0.95	16.00	8.73
24	9	4.90	457.38	4.31	3.19	6.27
24	10	0.17	18.96	4.73	111.03	0.34
24	11	1.45	107.31	77.54	12.43	31.12
24	12	0.50	29.97	24.28	1.40	4.39
24	13	1.11	25.12	2.33	0.70	0.88
24	14	5.69	10.39	59.44	3.17	0.47
24	15	1.39	10.00	22.66	0.32	8.72
24	16	0.57	46.66	0.65	1.77	3.06
24	17	0.37	14.10	10.02	0.47	0.58
24	18	0.12	6.90	2.02	3.05	3.34
24	19	3.39	28.56	56.60	3.07	1.08
24	20	0.73	27.53	24.75	0.48	0.07
24	21	1.55	44.66	14.26	1.67	0.19
24	22	1.45	9.91	3.66	0.27	1.80
24	23	1.32	1.46	9.41	1.23	3.10
24	24	11.92	4.06	13.24	1.48	1.17
24	25	9.07	18.51	6.58	4.27	0.55
24	26	2.59	5.04	28.06	1.79	1.74
24	27	5.05	9.62	4.36	5.64	0.75
24	28	6.81	26.90	16.73	3.17	0.60
24	29	2.91	16.14	0.78	1.05	7.48
24	30	1.34	193.78	60.46	15.66	2.30
25	0	132.31	163.07	169.72	161.96	193.64
25	1	412.19	5.91	2.76	1.79	3.65
25	2	6.07	18.22	5.94	1.20	0.13
25	3	6.18	89.33	1.75	0.94	46.63
25	4	62.86	6.94	3.05	1.32	4.47
25	5	3.29	2.23	208.71	84.14	57.29
25	6	6.09	53.46	145.43	136.70	3.07
25	7	269.91	21.43	26.12	447.16	27.75
25	8	130.89	2.60	1.58	6.46	30.20
25	9	55.56	154.45	6.72	5.54	84.06
25	10	7.41	5.23	2.58	3.13	9.25
25	11	7.65	90.69	283.81	61.57	6.73
25	12	7.51	17.52	29.91	169.92	44.89
25	13	46.53	12.14	6.73	2.49	3.27

25	14	194.58	3.71	191.31	6.91	1.87
25	15	39.07	6.05	19.44	2.62	31.79
25	16	6.24	18.48	1.47	131.61	32.82
25	17	35.42	4.72	24.82	20.94	3.78
25	18	1.77	5.17	2.97	223.78	49.51
25	19	48.23	16.96	116.06	220.51	2.46
25	20	8.07	13.23	38.05	8.14	3.21
25	21	20.84	25.74	20.46	45.23	4.43
25	22	31.11	2.86	5.54	4.80	33.94
25	23	6.67	1.57	19.97	82.90	13.63
25	24	49.62	2.40	11.67	14.38	3.26
25	25	44.28	3.08	8.94	12.34	5.09
25	26	10.32	13.68	48.46	3.99	46.72
25	27	17.57	4.15	4.94	6.35	5.75
25	28	10.56	10.67	34.61	8.18	10.15
25	29	109.08	4.87	1.08	9.49	2.48
25	30	6.78	85.99	162.20	3.90	2.42
26	0	371.26	62.64	56.59	27.90	32.15
26	1	138.25	2.84	0.53	0.53	0.28
26	2	14.08	6.37	0.78	0.26	2.55
26	3	15.31	734.77	0.38	0.21	743.99
26	4	16.26	2.10	0.83	0.28	39.84
26	5	14.72	8.87	34.09	5.69	29.05
26	6	9.03	24.87	51.44	2.10	0.34
26	7	93.04	9.84	9.51	6.49	13.09
26	8	46.12	8.55	0.34	0.28	13.11
26	9	170.95	186.93	1.21	0.44	36.22
26	10	4.88	37.19	0.69	0.65	4.92
26	11	24.08	680.69	13.02	6.36	5.89
26	12	19.26	113.36	7.09	4.64	730.10
26	13	142.46	66.87	1.39	0.37	37.16
26	14	591.05	6.34	29.64	5.38	2.63
26	15	119.59	47.21	16.22	0.35	7.91
26	16	13.99	7.81	0.72	2.51	23.71
26	17	29.51	2.09	7.00	1.35	2.30
26	18	4.41	3.05	1.01	5.59	9.84
26	19	147.94	6.57	35.88	4.76	2.26
26	20	26.72	4.72	10.48	0.29	0.48
26	21	64.86	14.03	5.07	4.12	2.05
26	22	96.19	4.26	1.29	0.19	7.44
26	23	11.43	2.35	4.83	1.80	1.45
26	24	156.16	2.40	6.49	4.70	7.84
26	25	132.60	3.34	2.94	4.04	1.94
26	26	16.27	10.66	6.13	1.69	4.16

26	27	15.82	3.11	1.00	3.89	3.07
26	28	68.78	10.49	3.27	3.49	2.08
26	29	25.04	4.34	0.28	0.91	2.11
26	30	25.04	46.43	17.23	1.01	1.77
27	0	123.67	5.77	245.90	172.42	25.79
27	1	3.56	144.63	4.45	1.22	1.51
27	2	13.96	1.61	7.97	1.20	0.27
27	3	6.54	12.34	3.35	0.61	10.30
27	4	1.14	129.58	4.15	2.70	5.57
27	5	6.93	11.08	315.69	113.44	61.99
27	6	4.06	1.38	324.75	130.86	1.63
27	7	1.83	1.36	57.48	428.56	453.91
27	8	1.29	19.93	2.55	6.92	442.12
27	9	169.56	6.11	7.76	5.63	215.97
27	10	3.24	15.01	4.15	3.37	19.79
27	11	17.17	21.29	314.82	139.93	27.52
27	12	5.95	121.56	68.04	173.24	10.91
27	13	14.16	12.65	11.86	4.74	4.48
27	14	44.94	1.40	297.15	23.44	2.51
27	15	5.25	2.79	50.33	2.68	30.71
27	16	1.53	0.64	3.11	117.11	34.59
27	17	3.81	1.26	53.80	13.41	2.60
27	18	4.58	0.38	4.78	205.02	40.68
27	19	122.39	1.43	253.06	197.93	11.07
27	20	16.02	1.38	48.77	7.90	0.95
27	21	26.66	1.75	18.79	42.89	2.27
27	22	41.83	1.46	5.55	5.04	9.05
27	23	3.61	0.28	35.42	77.62	9.26
27	24	18.11	0.74	38.84	11.55	6.67
27	25	4.16	1.13	20.60	19.18	7.10
27	26	9.78	0.67	41.50	7.68	5.60
27	27	3.60	0.44	4.40	30.95	2.15
27	28	6.04	1.03	36.12	9.67	0.72
27	29	3.59	0.70	1.45	8.77	13.28
27	30	2.97	3.78	200.27	7.87	1.68
28	0	37.92	6.43	213.06	164.52	22.28
28	1	5.87	0.05	2.54	3.23	11.56
28	2	121.88	0.18	4.26	2.75	0.54
28	3	7.29	0.08	0.48	0.46	10.36
28	4	3.88	0.32	2.00	2.58	4.42
28	5	56.20	0.38	228.50	151.82	40.90
28	6	3.06	19.89	625.42	63.33	7.84
28	7	5.31	0.27	116.72	215.56	33.82
28	8	4.19	1.32	0.73	3.20	37.27

28	9	106.27	2.55	4.44	5.77	107.81
28	10	21.02	2.10	2.16	1.15	12.88
28	11	171.91	0.43	247.93	309.28	11.12
28	12	12.86	0.95	86.03	124.60	9.02
28	13	28.11	4.59	6.10	9.85	2.06
28	14	24.04	3.65	273.24	132.96	10.95
28	15	10.89	1.28	206.51	6.50	17.65
28	16	0.85	3.58	3.11	103.48	9.97
28	17	1.09	0.16	69.53	19.21	46.60
28	18	2.86	2.82	3.87	95.71	24.41
28	19	78.39	8.06	448.27	97.67	4.89
28	20	11.93	1.67	74.74	1.84	4.54
28	21	18.49	16.69	37.03	29.14	11.57
28	22	32.03	4.22	3.40	4.24	78.10
28	23	7.45	1.24	28.66	36.19	35.12
28	24	9.78	1.89	65.34	30.03	3.54
28	25	2.65	1.23	30.68	12.94	16.75
28	26	7.28	0.94	15.46	6.08	12.32
28	27	8.07	1.79	12.87	51.06	4.54
28	28	5.86	1.91	24.44	14.06	4.26
28	29	2.79	1.61	1.32	8.33	2.68
28	30	2.38	14.34	103.30	14.43	2.48
29	0	241.08	184.77	221.34	107.88	7.37
29	1	2.72	2.55	7.73	14.12	124.20
29	2	24.95	9.41	5.85	11.65	5.86
29	3	5.85	25.72	4.34	7.82	1.59
29	4	1.27	7.70	5.22	11.18	1.89
29	5	5.39	8.26	585.98	687.86	18.58
29	6	2.33	606.20	39.84	49.73	77.61
29	7	3.51	4.34	3.01	109.42	5.93
29	8	4.68	1.78	2.90	4.85	6.37
29	9	682.54	70.22	5.37	8.59	2.85
29	10	6.77	2.84	3.98	4.28	7.00
29	11	31.95	24.08	476.10	147.94	0.59
29	12	13.61	4.80	44.53	296.61	2.36
29	13	51.71	9.15	27.65	46.99	10.49
29	14	211.71	2.33	516.56	569.52	123.57
29	15	44.02	5.35	26.65	15.79	2.89
29	16	3.41	144.20	2.57	30.55	14.18
29	17	12.37	2.52	37.43	81.42	4.25
29	18	19.00	58.81	7.82	68.09	8.49
29	19	469.31	205.38	39.20	63.27	0.72
29	20	74.18	41.88	10.49	10.42	0.28
29	21	114.05	385.14	11.29	27.05	1.01

29	22	172.20	32.79	7.53	4.79	2.26
29	23	9.75	2.59	24.91	14.68	0.74
29	24	74.62	40.51	36.68	29.10	0.60
29	25	49.61	28.11	13.55	27.67	2.42
29	26	2.53	6.40	46.78	14.50	3.99
29	27	8.56	36.99	11.43	19.97	0.43
29	28	11.09	4.61	26.19	30.35	0.98
29	29	2.43	4.44	1.86	10.07	0.51
29	30	6.24	19.25	72.41	7.02	0.30
30	0	42.82	36.40	36.84	164.60	284.64
30	1	1.24	1.09	0.30	4.44	2.21
30	2	5.01	1.75	0.47	3.81	0.79
30	3	6.79	2.11	0.21	2.36	36.71
30	4	1.52	2.21	0.39	3.82	65.82
30	5	1.13	1.48	7.78	203.88	682.68
30	6	3.03	120.04	67.52	55.68	2.06
30	7	2.28	2.93	12.65	163.73	33.95
30	8	0.81	0.66	1.51	3.33	82.91
30	9	31.97	48.37	0.64	4.01	262.25
30	10	1.06	2.20	0.52	3.77	31.67
30	11	7.05	5.83	34.94	146.50	25.53
30	12	7.55	2.47	10.49	54.43	46.18
30	13	1.90	2.14	0.34	15.20	4.59
30	14	6.68	1.00	12.95	190.38	17.51
30	15	4.13	1.04	24.57	4.42	99.16
30	16	0.63	32.33	0.42	40.19	486.44
30	17	0.96	2.58	9.23	24.90	28.31
30	18	1.62	51.95	0.50	94.62	260.92
30	19	22.18	44.69	58.14	92.49	20.73
30	20	4.14	7.63	8.35	4.24	11.80
30	21	8.34	79.33	4.15	31.69	4.07
30	22	10.95	7.31	0.80	2.43	43.83
30	23	4.19	0.55	6.62	30.27	20.82
30	24	9.94	8.23	9.81	23.52	4.70
30	25	4.89	14.78	4.12	23.20	8.08
30	26	3.06	3.29	1.37	11.78	51.38
30	27	3.98	7.40	3.24	28.75	12.72
30	28	2.48	6.21	7.52	17.16	16.44
30	29	2.13	4.98	0.91	4.94	3.19
30	30	2.73	22.18	13.53	6.06	7.56

Table S4. Coordinate of Conformer 1.

Element	X /Bohr	Y /Bohr	Z /Bohr

Ir	-2.608552	-0.038520	0.161827
O	-1.992924	-2.042790	-0.520425
O	-1.030308	-0.293498	1.703937
C	-1.154334	-2.814900	0.030110
C	-0.301769	-1.315987	1.878102
C	-0.331071	-2.512174	1.133658
C	-1.068922	-4.187428	-0.575927
C	0.672464	-1.219440	3.020157
H	0.190841	-0.758041	3.893448
H	1.099384	-2.188965	3.308332
H	1.492060	-0.553801	2.711055
H	-0.337765	-4.839230	-0.082036
H	-2.059412	-4.662865	-0.534666
H	-0.809115	-4.106961	-1.640896
H	0.349919	-3.302046	1.460234
C	-2.420323	2.842436	-0.063431
C	-2.653326	4.202320	0.190395
C	-3.531245	4.585907	1.196883
C	-4.181500	3.602707	1.950704
C	-3.959689	2.249714	1.699391
H	-3.712424	5.644647	1.395572
H	-2.134412	4.967770	-0.395115
H	-4.875955	3.899009	2.742411
H	-4.494235	1.506183	2.299361
C	-1.482568	2.363049	-1.065670
C	-0.750906	3.156199	-1.955834
C	0.143478	2.563331	-2.837049
H	-0.888583	4.238365	-1.944032
C	-0.446127	0.434394	-1.917546
C	0.313250	1.179416	-2.810058
H	0.720013	3.178901	-3.532557
H	-0.363152	-0.653451	-1.853789
H	1.035724	0.671341	-3.447372
C	-5.202856	-1.256788	0.702034
C	-6.213423	-1.938742	1.393689
C	-6.012290	-2.340342	2.705956
C	-4.794951	-2.052881	3.328038
C	-3.824040	-1.380057	2.601722
H	-6.800260	-2.870610	3.245399
H	-7.158541	-2.144589	0.889521
H	-4.595841	-2.343482	4.360008
H	-2.853081	-1.113796	3.026901
C	-5.285155	-0.747762	-0.656858
C	-6.419876	-0.899734	-1.469399

C	-6.440876	-0.361595	-2.749006
H	-7.294731	-1.442235	-1.098892
C	-4.190642	0.489633	-2.418893
C	-5.321966	0.335830	-3.217399
H	-7.323395	-0.479702	-3.381457
H	-3.334248	1.040241	-2.820265
H	-5.334988	0.765928	-4.223118
C	-4.134645	-0.051917	-1.124875
C	-3.074391	1.830976	0.693274
N	-4.016391	-0.999332	1.329162
N	-1.330916	1.004408	-1.085830
Al	3.337926	-0.151932	-0.511591
N	4.536705	0.331080	1.147274
N	3.143629	-2.092224	0.129314
C	4.209202	0.770668	2.354102
C	5.840437	0.109482	0.847084
N	3.358341	1.802135	-1.094533
O	1.854598	0.403858	0.482037
O	2.482474	-0.787674	-2.031062
O	5.028721	-0.487681	-1.260382
C	3.456437	-2.688149	1.268759
C	2.654159	-2.830340	-0.899591
C	5.182006	1.007347	3.343519
H	3.145554	0.940609	2.544213
C	6.897998	0.314588	1.778549
C	6.068850	-0.349031	-0.494195
C	4.137284	2.432537	-1.960222
C	2.446380	2.497649	-0.370241
C	1.638329	1.692491	0.500227
C	2.308505	-2.075549	-2.072108
C	3.311622	-4.076119	1.445777
H	3.839543	-2.053333	2.073833
C	2.498660	-4.243684	-0.830284
C	6.513590	0.777964	3.059506
H	4.869392	1.370121	4.323705
C	8.220991	0.046617	1.358630
C	7.394673	-0.599098	-0.858381
C	4.045431	3.824070	-2.147514
H	4.853826	1.813793	-2.508028
C	2.302928	3.910417	-0.461007
C	0.710947	2.357281	1.305278
C	1.806300	-2.792722	-3.160690
C	2.846240	-4.848407	0.400508
H	3.580021	-4.524602	2.403478

C	2.011814	-4.923633	-1.970212
C	8.437442	-0.399664	0.064806
H	7.604050	-0.952081	-1.869853
C	3.144818	4.556323	-1.396329
H	4.698359	4.311091	-2.873283
C	1.346221	4.537227	0.371815
C	0.588339	3.758585	1.231526
H	0.056610	1.768051	1.952612
C	1.679116	-4.192663	-3.097789
H	1.530742	-2.249741	-4.067325
H	9.461333	-0.607024	-0.258269
H	-0.155923	4.241849	1.870939
H	1.294144	-4.717945	-3.976236
H	1.888854	-6.008202	-1.942015
H	1.217488	5.621184	0.328675
H	9.050924	0.194055	2.052366
H	7.280985	0.954804	3.818477
H	2.740272	-5.931142	0.514729
H	3.076274	5.641201	-1.519183

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178 **Table S5**. Coordinate of Conformer 2.

Element	X /Bohr	Y /Bohr	Z /Bohr
Ir	-2.600548	-0.718232	-0.563740
O	-3.123146	-1.846751	-2.402740
O	-0.672877	-1.816528	-0.699985
C	-2.433897	-2.737125	-2.978763
C	-0.363525	-2.729887	-1.524591
C	-1.146815	-3.183089	-2.604602
C	-3.080564	-3.362783	-4.184474
C	0.971211	-3.380081	-1.283483
H	1.757486	-2.614221	-1.199377
H	0.958462	-3.895693	-0.310298
H	1.253931	-4.099507	-2.061187
H	-3.325986	-2.583159	-4.919648
H	-2.458706	-4.124707	-4.668637
H	-4.038580	-3.815918	-3.893350
H	-0.712937	-3.977302	-3.215433
C	-1.167590	1.489986	0.620520
C	-0.589782	2.314828	1.595337
C	-0.798486	2.056702	2.942361
C	-1.607276	0.978219	3.316608
C	-2.190456	0.154983	2.353010
H	-0.336372	2.695979	3.699159

H	0.036845	3.157480	1.297134
H	-1.787945	0.778583	4.377101
H	-2.824673	-0.676123	2.679331
C	-1.018617	1.721289	-0.804255
C	-0.265709	2.741180	-1.405305
C	-0.266533	2.880548	-2.784861
H	0.341816	3.393765	-0.777589
C	-1.724944	0.988156	-2.925052
C	-1.025827	2.001502	-3.562986
H	0.325481	3.668971	-3.255559
H	-2.322661	0.253150	-3.471451
H	-1.063242	2.084535	-4.649953
C	-4.846824	-2.051016	0.732669
C	-5.558847	-3.026824	1.443552
C	-4.900333	-4.133684	1.958579
C	-3.522424	-4.260596	1.763688
C	-2.862442	-3.274701	1.046201
H	-5.454237	-4.892357	2.515831
H	-6.631764	-2.899401	1.593842
H	-2.963385	-5.109176	2.159515
H	-1.784853	-3.306205	0.862894
C	-5.383671	-0.815223	0.189936
C	-6.734737	-0.446617	0.290187
C	-7.164309	0.775529	-0.208745
H	-7.455667	-1.119112	0.764649
C	-4.894908	1.281043	-0.909783
C	-6.236662	1.639296	-0.803006
H	-8.215096	1.062581	-0.130955
H	-4.191927	1.980788	-1.372170
H	-6.569075	2.608735	-1.185384
C	-4.434053	0.043973	-0.433073
C	-1.970060	0.374208	0.984467
N	-3.502976	-2.209674	0.538169
N	-1.710000	0.840691	-1.590207
Al	3.309094	1.171778	0.482778
N	4.158628	-0.715084	0.756079
N	3.969173	1.794384	2.323515
C	5.369782	-1.166410	0.466205
C	3.243520	-1.547219	1.314506
N	2.762356	0.660639	-1.400828
O	4.883895	1.741683	-0.366246
O	2.475920	2.840045	0.445237
O	1.828388	0.306654	1.228906
C	4.722604	1.206846	3.239506

C	3.437187	3.017950	2.576569
C	5.739530	-2.499537	0.729138
H	6.062426	-0.446231	0.020531
C	3.522023	-2.910054	1.623454
C	1.967208	-0.940540	1.564771
C	1.678869	0.032132	-1.830853
C	3.726157	1.039696	-2.276059
C	4.875856	1.648482	-1.666551
C	2.636176	3.561852	1.514541
C	4.992176	1.812615	4.479822
H	5.130249	0.222525	2.991629
C	3.650898	3.712623	3.801270
C	4.825311	-3.361102	1.303658
H	6.746100	-2.835787	0.475931
C	2.495005	-3.682922	2.210896
C	0.982659	-1.748805	2.140690
C	1.499176	-0.257429	-3.197767
H	0.943361	-0.263504	-1.075120
C	3.619722	0.821622	-3.676698
C	5.895959	2.062682	-2.525889
C	2.076409	4.824138	1.729886
C	4.459199	3.054536	4.758137
H	5.617512	1.291047	5.205680
C	3.052484	4.982559	3.969856
C	1.263716	-3.089576	2.453659
H	-0.003849	-1.317443	2.323436
C	2.453651	0.144280	-4.110880
H	0.604340	-0.799827	-3.511999
C	4.680670	1.263272	-4.502090
C	5.779451	1.869784	-3.916050
H	6.783516	2.535993	-2.101425
C	2.288656	5.507201	2.941034
H	1.469239	5.272419	0.940197
H	0.468869	-3.690497	2.906930
H	6.599243	2.209103	-4.555428
H	1.828323	6.490570	3.069517
H	3.201849	5.531855	4.901328
H	4.626278	1.114514	-5.582409
H	2.680105	-4.728625	2.465213
H	5.100443	-4.398358	1.515585
H	4.655963	3.540707	5.717784
H	2.324356	-0.067291	-5.176411

Table S6. Coordinate of Conformer 3.

Element	X /Bohr	Y /Bohr	Z /Bohr
Ir	-3.051723	0.166898	1.433172
O	-2.026977	-1.532295	2.450417
O	-4.792949	-1.208605	1.367379
C	-2.539462	-2.646547	2.777871
C	-4.883334	-2.362620	1.874647
C	-3.858249	-3.073706	2.536774
C	-1.615050	-3.576082	3.519424
C	-6.230375	-3.018027	1.735549
H	-6.511186	-3.065985	0.674033
H	-6.272169	-4.026975	2.161976
H	-6.992667	-2.393469	2.222313
H	-2.078721	-4.533512	3.783760
H	-0.714696	-3.774391	2.919753
H	-1.263226	-3.090130	4.441871
H	-4.118821	-4.067923	2.904579
C	-4.914482	2.360089	1.678182
C	-5.779575	3.402532	1.309216
C	-5.894824	3.776709	-0.022701
C	-5.137397	3.108190	-0.990799
C	-4.277965	2.071165	-0.634369
H	-6.567029	4.587990	-0.310057
H	-6.366542	3.926996	2.068971
H	-5.219297	3.404169	-2.040620
H	-3.698858	1.573045	-1.417811
C	-4.715805	1.934056	3.053092
C	-5.319137	2.492160	4.188547
C	-5.010797	2.008893	5.451443
H	-6.027064	3.312908	4.066286
C	-3.524321	0.442534	4.423519
C	-4.091344	0.964519	5.576104
H	-5.478952	2.445332	6.336471
H	-2.790682	-0.367109	4.449349
H	-3.813954	0.557999	6.549121
C	-1.155962	0.258712	-0.792386
C	-0.556619	-0.052031	-2.021539
C	-1.086081	-1.062164	-2.810883
C	-2.217965	-1.754910	-2.370722
C	-2.779206	-1.402212	-1.152382
H	-0.606744	-1.317106	-3.759155
H	0.351272	0.475230	-2.325859
H	-2.665689	-2.556507	-2.959393
H	-3.672956	-1.892004	-0.758068
C	-0.679744	1.242946	0.163151

C	0.473394	2.017693	-0.040903
C	0.901174	2.894535	0.948533
H	1.057532	1.910174	-0.960050
C	-0.974942	2.236111	2.344049
C	0.177143	2.995723	2.140239
H	1.807764	3.485720	0.799242
H	-1.526955	2.352192	3.282522
H	0.518495	3.679296	2.923688
C	-1.433998	1.341483	1.365502
C	-4.149087	1.662295	0.701999
N	-2.265921	-0.427091	-0.384281
N	-3.828311	0.905231	3.200865
Al	3.718204	-0.271165	-1.884116
N	2.542404	-0.812209	-0.320344
N	5.083111	-1.783734	-1.480872
C	1.528673	-1.664089	-0.251563
C	2.872908	-0.070129	0.768966
N	4.917044	0.486253	-3.381394
O	2.519203	1.018590	-2.497130
O	2.993944	-1.600203	-3.000942
O	4.553981	0.806355	-0.606709
C	6.130599	-1.796821	-0.669932
C	4.765128	-2.893050	-2.192196
C	0.755901	-1.796047	0.913049
H	1.311999	-2.236636	-1.157823
C	2.162310	-0.148063	1.997264
C	3.985027	0.813351	0.571501
C	6.137178	0.169342	-3.784312
C	4.243208	1.484046	-4.010346
C	2.930018	1.748130	-3.494030
C	3.604476	-2.747802	-3.025713
C	6.935194	-2.943469	-0.530125
H	6.333620	-0.869330	-0.126558
C	5.514928	-4.100602	-2.119891
C	1.058852	-1.032845	2.024545
H	-0.107269	-2.463451	0.914834
C	2.589654	0.672143	3.067947
C	4.373351	1.592523	1.661803
C	6.764624	0.835068	-4.852782
H	6.644063	-0.638472	-3.248288
C	4.791430	2.218126	-5.100913
C	2.198006	2.767778	-4.105227
C	3.230311	-3.861585	-3.782271
C	6.630706	-4.083096	-1.248708

H	7.790434	-2.917972	0.146755
C	5.093077	-5.196905	-2.906747
C	3.675341	1.509566	2.883329
H	5.219076	2.273927	1.547871
C	6.096381	1.850658	-5.505679
H	7.771335	0.538976	-5.150900
C	4.008161	3.239267	-5.686420
C	2.743205	3.490353	-5.181872
H	1.197042	2.995722	-3.732054
C	3.973281	-5.054562	-3.710572
H	2.353199	-3.788303	-4.428291
H	4.003555	2.143833	3.711683
H	2.139101	4.281422	-5.634281
H	3.648049	-5.903765	-4.317913
H	5.648275	-6.136229	-2.871982
H	4.408100	3.815050	-6.523268
H	2.048984	0.644183	4.016188
H	0.426909	-1.099642	2.914267
H	7.247355	-4.980994	-1.149739
H	6.567846	2.379670	-6.338648

Table S7. Coordinate of Conformer 4.

Element	X /Bohr	Y /Bohr	Z /Bohr
Ir	-3.408430	0.065717	0.552295
O	-4.772809	-1.198217	1.758097
O	-2.531222	0.624138	2.527146
C	-4.832920	-1.283892	3.017789
C	-2.951182	0.272330	3.672771
C	-4.007032	-0.615361	3.948204
C	-5.902275	-2.201622	3.544281
C	-2.230805	0.903153	4.835647
H	-2.619087	0.588086	5.811134
H	-1.156620	0.668966	4.794049
H	-2.305046	1.998661	4.765182
H	-6.883394	-1.871475	3.175308
H	-5.751870	-3.213153	3.140980
H	-5.931919	-2.256507	4.638623
H	-4.216730	-0.803316	5.002853
C	-0.933750	0.305436	-0.934002
C	0.082135	0.862514	-1.724813
C	0.011116	2.199514	-2.099845
C	-1.076234	2.976798	-1.687186

C	-2.096093	2.422757	-0.913039
H	0.805090	2.635531	-2.711227
H	0.949127	0.265140	-2.024438
H	-1.135518	4.028303	-1.984569
H	-2.944756	3.051909	-0.625371
C	-0.922354	-1.075481	-0.481295
C	0.075506	-2.019983	-0.755462
C	-0.058840	-3.318041	-0.286254
H	0.959796	-1.715539	-1.321253
C	-2.135341	-2.685249	0.723260
C	-1.186860	-3.662717	0.462143
H	0.720278	-4.055200	-0.493850
H	-3.042426	-2.890374	1.297124
H	-1.332379	-4.672823	0.847083
C	-5.784060	1.516553	-0.319412
C	-6.820952	2.459736	-0.319042
C	-6.875331	3.437315	0.663147
C	-5.882685	3.471752	1.645741
C	-4.880532	2.514187	1.606495
H	-7.682048	4.173606	0.662556
H	-7.578649	2.418036	-1.102517
H	-5.880444	4.227154	2.432116
H	-4.068613	2.489363	2.337627
C	-5.580653	0.468512	-1.305396
C	-6.433765	0.261239	-2.401216
C	-6.154167	-0.734998	-3.326724
H	-7.322436	0.885273	-2.534245
C	-4.160469	-1.328805	-2.074522
C	-5.011178	-1.524780	-3.160029
H	-6.817610	-0.895288	-4.179212
H	-3.273945	-1.962787	-1.978710
H	-4.781312	-2.304512	-3.891882
C	-4.425299	-0.340083	-1.113869
C	-2.056017	1.076543	-0.518496
N	-4.833306	1.561654	0.661914
N	-2.008275	-1.428409	0.269621
Al	4.280861	-0.216600	-0.629620
N	5.771683	0.367240	0.675264
N	5.599927	-1.344097	-1.738589
C	6.211970	-0.213258	1.781872
C	6.327524	1.529594	0.253651
N	2.816982	0.681304	0.446528
O	3.901959	-1.684391	0.471047
O	3.075407	-0.703927	-1.973306

O	4.778877	1.379654	-1.488857
C	6.880954	-1.629564	-1.567694
C	4.939554	-1.846459	-2.814160
C	7.258214	0.348882	2.537315
H	5.722435	-1.149826	2.063884
C	7.390550	2.175002	0.945950
C	5.753174	2.053219	-0.954066
C	2.332130	1.913267	0.396154
C	2.207235	-0.252165	1.224882
C	2.839911	-1.540477	1.220069
C	3.555322	-1.473533	-2.906351
C	7.589339	-2.442183	-2.471268
H	7.372700	-1.205867	-0.687021
C	5.566600	-2.682295	-3.782385
C	7.842550	1.529915	2.122400
H	7.595795	-0.156613	3.443302
C	7.897845	3.381920	0.412367
C	6.292310	3.248092	-1.439044
C	1.183236	2.282784	1.116803
H	2.855974	2.615240	-0.259241
C	1.027893	0.020218	1.966975
C	2.269750	-2.529520	2.021592
C	2.833495	-1.974488	-3.992260
C	6.936498	-2.964544	-3.568966
H	8.645184	-2.648930	-2.291103
C	4.791185	-3.160533	-4.863383
C	7.343884	3.884908	-0.754287
H	5.883215	3.676110	-2.356081
C	0.518224	1.340169	1.875304
H	0.800478	3.300433	1.025996
C	0.456453	-1.035729	2.718423
C	1.089960	-2.265896	2.744052
H	2.734995	-3.517389	2.050375
C	3.456345	-2.800979	-4.944696
H	1.779728	-1.705957	-4.094518
H	7.737627	4.818512	-1.165527
H	0.648377	-3.075218	3.332830
H	2.857352	-3.169601	-5.781859
H	5.251677	-3.801923	-5.617295
H	-0.479399	-0.870794	3.253608
H	8.712765	3.900921	0.920595
H	8.657629	1.976901	2.698734
H	7.469793	-3.599576	-4.281936
H	-0.418266	1.583219	2.385109

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185 **Table S8**. Coordinate of Conformer 5.

Element	X /Bohr	Y /Bohr	Z /Bohr
Ir	-2.452346	-1.232898	0.365948
O	-3.253220	-2.265146	2.160152
O	-0.500183	-2.095811	1.018078
C	-2.596938	-2.868358	3.057155
C	-0.273413	-2.778138	2.064111
C	-1.208526	-3.129202	3.056085
C	-3.412246	-3.359820	4.221999
C	1.149326	-3.243079	2.225447
H	1.840940	-2.390891	2.147687
H	1.333954	-3.760809	3.174264
H	1.411861	-3.924308	1.402391
H	-2.822565	-3.898846	4.972499
H	-3.910626	-2.507470	4.704907
H	-4.217057	-4.015549	3.861109
H	-0.822391	-3.696197	3.905353
C	-1.779223	-1.266938	-2.452120
C	-1.296575	-0.828203	-3.695859
C	-0.688093	0.414589	-3.809200
C	-0.552098	1.220087	-2.672984
C	-1.060561	0.806178	-1.442592
H	-0.285120	0.744305	-4.769607
H	-1.366809	-1.475373	-4.576273
H	-0.031502	2.180146	-2.740232
H	-0.928360	1.463264	-0.578918
C	-2.314818	-2.594114	-2.217266
C	-2.453175	-3.614798	-3.168816
C	-2.954067	-4.853502	-2.796228
H	-2.163772	-3.419059	-4.202565
C	-3.160006	-4.033254	-0.558591
C	-3.314938	-5.072279	-1.463989
H	-3.064662	-5.647367	-3.538229
H	-3.435000	-4.131985	0.494545
H	-3.712732	-6.030089	-1.127655
C	-3.371066	1.316479	1.462665
C	-3.341313	2.521618	2.179025
C	-2.230322	2.854950	2.938945
C	-1.147613	1.973274	2.985354
C	-1.227272	0.791999	2.263351
H	-2.201287	3.797798	3.489635
H	-4.197927	3.194577	2.123490
H	-0.251451	2.202144	3.564689

H	-0.417814	0.058071	2.247436
C	-4.450419	0.846851	0.612868
C	-5.656994	1.542817	0.439047
C	-6.639730	1.037774	-0.401252
H	-5.829893	2.485865	0.965851
C	-5.216887	-0.864176	-0.908322
C	-6.411837	-0.167165	-1.074974
H	-7.579067	1.577797	-0.536894
H	-5.073452	-1.800789	-1.455774
H	-7.180119	-0.566486	-1.743305
C	-4.208839	-0.385250	-0.056951
C	-1.691671	-0.436755	-1.300894
N	-2.297654	0.473332	1.521345
N	-2.676938	-2.834184	-0.919014
Al	3.304516	1.538954	-0.699290
N	3.188829	0.783665	1.258026
N	2.467286	-0.141514	-1.469199
C	2.211533	0.859992	2.147388
C	4.321913	0.107704	1.561849
N	3.959504	3.334717	0.023883
O	1.613930	2.317100	-0.409592
O	3.545626	2.010919	-2.471109
O	5.015127	0.760482	-0.569964
C	1.819706	-1.149937	-0.909079
C	2.665542	-0.133527	-2.813927
C	2.314002	0.247624	3.411388
H	1.324871	1.418724	1.835860
C	4.524601	-0.546817	2.810812
C	5.306883	0.113308	0.516797
C	5.191648	3.782313	0.203902
C	2.899500	4.116590	0.346683
C	1.619306	3.517628	0.089489
C	3.254175	1.072197	-3.326327
C	1.374084	-2.253007	-1.658730
H	1.613335	-1.091833	0.162585
C	2.272508	-1.210891	-3.653093
C	3.460618	-0.449407	3.739515
H	1.483944	0.323051	4.117601
C	5.746792	-1.226295	3.016669
C	6.497633	-0.573181	0.772766
C	5.434580	5.063814	0.732486
H	6.000320	3.104038	-0.082602
C	3.040817	5.420721	0.895358
C	0.490342	4.273964	0.416248

C	3.439260	1.144454	-4.709065
C	1.622220	-2.293706	-3.014230
H	0.812808	-3.039768	-1.151589
C	2.500166	-1.094918	-5.043771
C	6.693883	-1.224574	2.004285
H	7.269049	-0.594548	0.000758
C	4.369954	5.873067	1.077761
H	6.463208	5.402311	0.864694
C	1.866082	6.145211	1.207333
C	0.632547	5.563018	0.964627
H	-0.501503	3.854016	0.231173
C	3.069821	0.067749	-5.536630
H	3.873948	2.051413	-5.133353
H	7.638766	-1.750956	2.165510
H	-0.274217	6.126889	1.202205
H	3.235310	0.161905	-6.613669
H	2.209604	-1.910069	-5.710201
H	1.943828	7.149677	1.627976
H	5.931032	-1.739278	3.962569
H	3.553997	-0.933595	4.715866
H	1.279871	-3.142303	-3.615331
H	4.544439	6.869917	1.492597

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