Supporting Information

Ammonium-Crown Ether Supramolecular Cation-Templated Assembly of an Unprecedented Heterobicluster-Metal Coordination Polymer with Enhanced NLO Properties

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Experimental Section:

The reaction and manipulations were conducted using standard Schlenk techniques under an atmosphere of argon. The starting material $[NH_4]_2WS_4$ was obtained according to the literature procedure.[S1] The solvents were carefully dried and distilled prior to use. Other chemicals were commercially available and used as received. Elemental analyses for carbon, hydrogen and nitrogen were performed on a Perkin-Elmer 240C elemental analyzer. Infrared spectra were recorded with a Nicolet FT-170SX Fourier transform spectrometer (KBr pellets). Thermogravimetric analyses were carried out on a TGA/1100SF thermal analyzer at a heating rate of 10 °C min^{-1} between 50 and 1000 °C under a dinitrogen atmosphere with a flow rate of 50 cm^3 min^{-1}. Powder X-ray diffraction (PXRD) patterns were recorded using Cu $K\alpha_1$ radiation on a Bruker D8 X-ray diffractometer.

Preparation of $^3_\infty${{[(NH$_4$)⊂(18-crown-6)]$_6$·5DMF·5CH$_3$CN·H$_2$O}⊂{[WS$_4$Cu$_3$(CN)$_2$]$_2$[WS$_4$Cu$_3$(CN)$_2$]$_2$[WS$_4$Cu$_4$(CN)$_3$][Cu(CN)$_{1.5}$]$_2$}} (HCM-CP 1). $[NH_4]_2WS_4$ (0.35 g, 1.00 mmol) and CuCN (0.27 g, 3.00 mmol) were added to 5 mL DMF and the resultant mixture was stirred for 20 min, affording a solution that was passed through a filter. The orange-red filtrate was carefully layered onto 0.5 mL DMF, and 10 mL of a solution of 18-crown-6 in CH_3CN (0.05 mol dm^{-3}) was in turn added on top. Several days later, HCM-CP **1** was obtained as orange block crystals (yield: 0.22 g, 21% based on W). Anal. Calcd. for $C_{111}H_{220}Cu_{18}N_{30}O_{42}S_{20}W_5$: C, 24.91; H, 4.14; N, 7.85%. Found: C, 25.13; H, 4.01; N, 7.67%. IR (KBr pellets, cm^{-1}): 2146.2(vs) (CN), 1652.8(s) (C=O in DMF), 433.8(s) (W-μ_3-S).

X-ray Structure Determination. A crystal of HCM-CP **1** suitable for a single-crystal X-ray diffraction study was obtained directly from the above preparation. All measurements were made on a Saturn 724+ CCD X-ray diffractometer by using graphite-monochromated Mo *Kα* (λ = 0.71070 Å) radiation. The single crystal of HCM-CP **1** was mounted with grease at the top of a glass fibre. Cell parameters were refined on all observed reflections by using the program *Crystalclear* (Rigaku Inc., 2007). The collected data were reduced by the program *Crystalclear* and an absorption correction (multiscan) was applied. The reflection data for HCM-CP **1** were also corrected for Lorentz and polarization effects. The crystal structure of HCM-CP **1** was solved by direct methods and refined on F^2 by full-matrix least-squares methods using the *SHELXTL* software package.[S2] All non-hydrogen atoms

except the disordered atoms were refined anisotropically. A summary of the key crystallographic information is listed in Table S1. More detailed crystallographic data have been given in the cif file. CCDC 967653.

Computational Details. Density functional theory (DFT) and time-dependent density functional theory (TD-DFT) calculations were performed to assign the experimental absorption spectra by using the Gaussian 03 program.[S3] A model compound of HCM-CP **1** was derived from the experimental single-crystal X-ray structure. The restricted singlet wave function for HCM-CP **1** in DMF solution (dielectric constant $\varepsilon = 36.71$) was shown to be stable within the framework of the polarized continuum model (PCM) at the B3LYP functional/LanL2DZ level of theory. Vertical electronic excitation energies of HCM-CP **1** in DMF solution were then obtained through TD-DFT/PCM calculations at the same level.

Nonlinear Optical Measurements. The third-order NLO properties of aniline, 18-crown-6, $[(NH_4)\subset(18\text{-crown-}6)]NO_3$[S4] and HCM-CP **1** were determined by performing *Z*-scan measurements.[S5] Aniline solvent and the aniline solutions of 18-crown-6, $[(NH_4)\subset(18\text{-crown-}6)]NO_3$ and HCM-CP **1** with concentrations of 1.37×10^{-3} mol dm^{-3}, 1.37×10^{-3} mol dm^{-3} and 2.28×10^{-4} mol dm^{-3}, respectively, were placed in a 5 mm quartz cuvette for the nonlinear optical measurements, which were performed with linearly polarized 5 ns pulses at 532 nm generated from a Q-switched frequency-doubled Nd:YAG laser. Aniline, 18-crown-6, $[(NH_4)\subset(18\text{-crown-}6)]NO_3$ and HCM-CP **1** are stable toward air and laser light under the experimental conditions. The spatial profiles of the optical pulses were of nearly Gaussian transverse mode. The pulsed laser was focused onto the sample cell with a 30 cm focal length mirror. The spot radius of the laser beam was measured to be 55 μm (half-width at $1/e^2$ maximum). The energy of the input and output pulses were measured simultaneously by precision laser detectors (Rjp-735 energy probes), which were linked to a computer by an IEEE interface,[S6] while the incident pulse energy was varied by a Newport Com. Attenuator. The interval between the laser pulses was chosen to be 1 Hz to avoid the influence of thermal and long-term effects. The samples were mounted on a translation stage that was controlled by computer to move along the axis of the incident laser beam (*Z*-direction) with respect to the focal point. To determine both the sign and magnitude of the nonlinear refraction, a 0.2 mm diameter aperture was placed in front of the transmission detector and the transmittance

recorded as a function of the sample position on the *Z*-axis (closed-aperture *Z*-scan). To measure the nonlinear absorption, the *Z*-dependent sample transmittance was taken without the aperture (open-aperture *Z*-scan).

Results and Discussion:

Synthetic Strategy. Although the heterobicluster-metal coordination polymer **1** is comprised of tetranuclear clusters ($[WS_4Cu_3]^+$), pentanuclear clusters ($[WS_4Cu_4]^{2+}$), and building metal ions (Cu^+), interconnected by ditopic anionic bridges (CN^-), an ammonium-crown ether host-guest supramolecular cation-templated assembly protocol has been demonstrated to be responsible for the construction of the heterobicluster-metal CP. The valence state and configuration (including size, geometry and structural rigidity) of cations have been shown to affect the formation of anionic skeletons of Mo(W)/S/Ag polymeric clusters.[S7] In our previous work, the univalent quaternary ammonium cation $[Et_4N]^+$ with a mean radius of 3.34 Å (Table S2) induced the formation of a 3-D anionic cyanide-bridged W/S/Cu cluster-based CP $\{[Et_4N]_2[WS_4Cu_4(CN)_4]\}_n$ (C-CP **2**) fabricated from pentanuclear $[WS_4Cu_4]^{2+}$ building clusters.[S8] When $[Et_4N]^+$ was replaced by $[n\text{-}Bu_4N]^+$, with a larger mean radius of 5.86 Å (Table S2), another 3-D anionic cyanide-bridged W/S/Cu cluster-based CP $\{[n\text{-}Bu_4N][WS_4Cu_3(CN)_2]\}_n$ (C-CP **3**) composed of tetranuclear $[WS_4Cu_3]^+$ building clusters was constructed.[S9] Compared with quaternary ammonium cations $[Et_4N]^+$ and $[n\text{-}Bu_4N]^+$, the host-guest supramolecular cation $[(NH_4)\subset(18\text{-crown-}6)]^+$ exhibits a distinct geometry and structural rigidity (Figure S3). The mean radius of $[(NH_4)\subset(18\text{-crown-}6)]^+$ (4.62 Å, Table S2) is very close to the average value (4.60 Å) of the radii of $[Et_4N]^+$ from **2** and $[n\text{-}Bu_4N]^+$ from **3**. The distinct radius afforded by supramolecular encapsulation of the ammonium ion may be a key reason that the supramolecular cation $[(NH_4)\subset(18\text{-crown-}6)]^+$ directs the formation of the novel 3-D anionic cyanide-bridged W/S/Cu cluster-based CP comprised of both pentanuclear $[WS_4Cu_4]^{2+}$ and tetranuclear $[WS_4Cu_3]^+$ building clusters. Judicious choice of supramolecular encapsulation may thereby offer a continuum of ammonium ion radii, and thereby greatly expand the palette of cations/radii for templating coordination polymer assembly.

TGA and PXRD Analyses. TGA measurements reveal that the anionic framework of **1** is stable to 540 °C, beyond which it begins to slowly decompose (Figure S4). The peak positions of the experimental and simulated PXRD patterns are in good agreement (Figure S5), which indicates that the crystal structure of **1** is truly representative of the bulk crystal product.

Initial Structure-Property Correlations. We note that C-CPs **2** and **3** were constructed from single building clusters; interactions therefore only exist between the same clusters. In contrast, HCM-CP **1** was constructed from tetranuclear $[WS_4Cu_3]^+$ and pentanuclear $[WS_4Cu_4]^{2+}$ building clusters, with consequent interactions between different clusters (tetranuclear cluster $[WS_4Cu_3]^+$ and pentanuclear cluster $[WS_4Cu_4]^{2+}$). Our TD-DFT calculations confirm that electron transitions occur between the tetranuclear clusters $[WS_4Cu_3]^+$ and the pentanuclear clusters $[WS_4Cu_4]^{2+}$ (Figure S6b), and we suggest that these intercluster transitions may be a key ingredient in its enhanced optical properties.

References:

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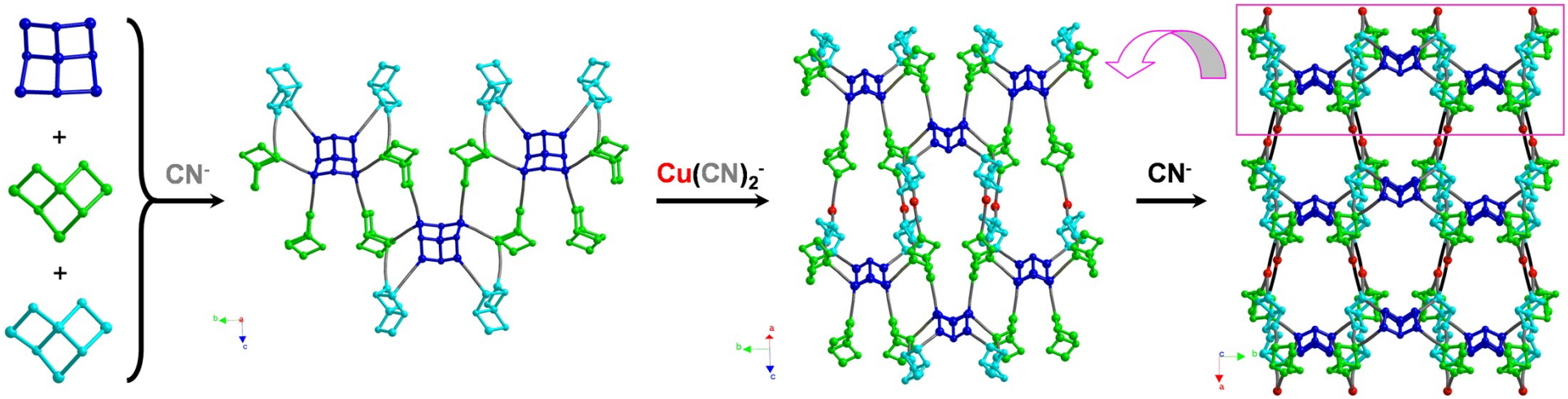
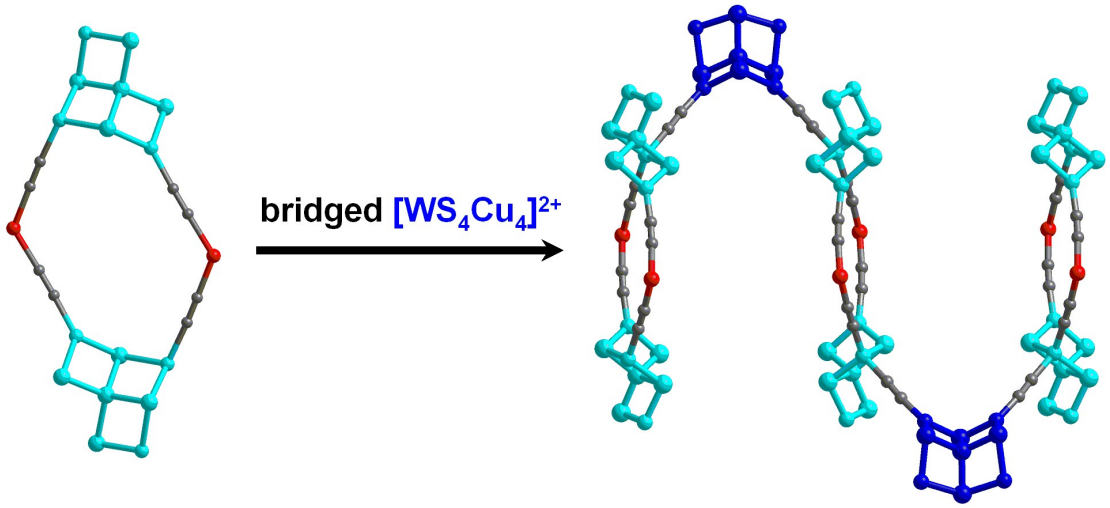
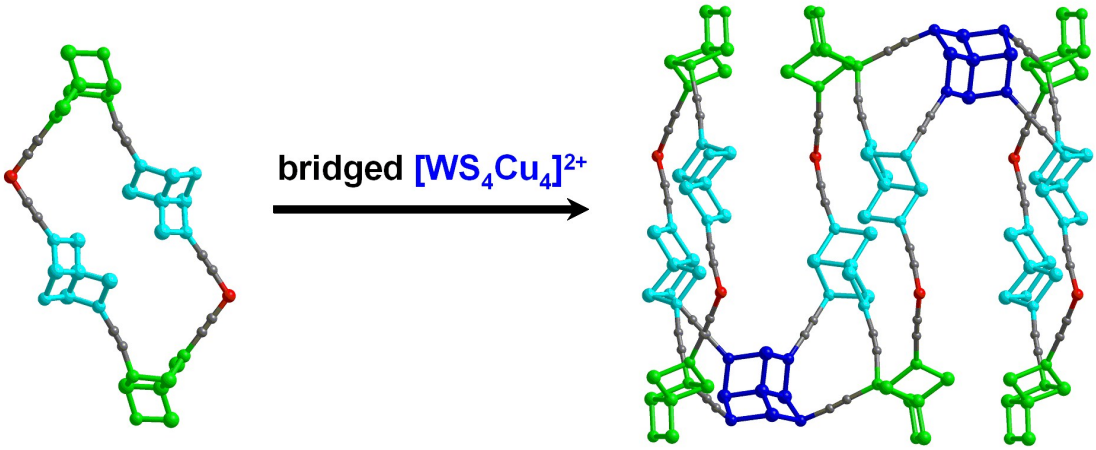


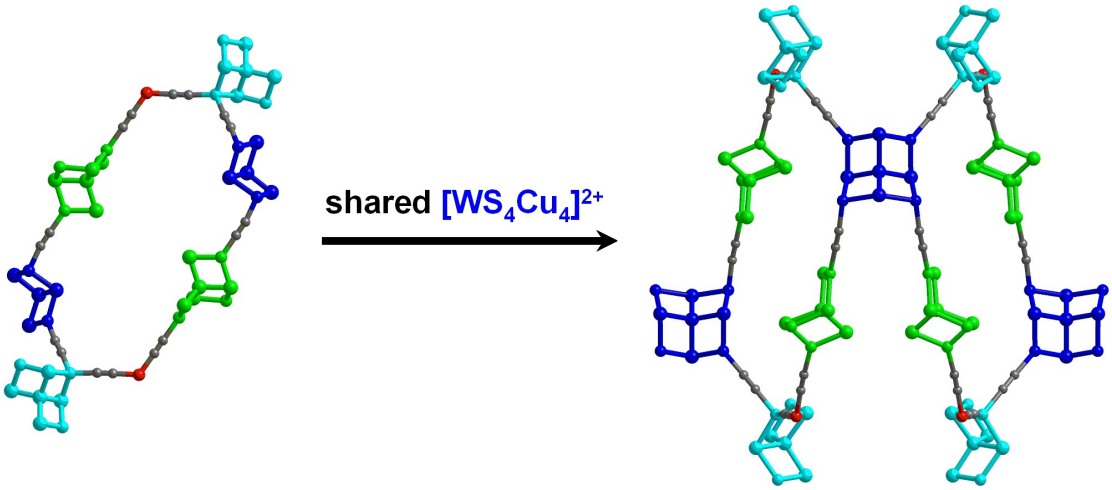
Scheme S1. Illustrative assembly of the anionic W/S/Cu-containing HCM-CP **1** (the W1-containing tetranuclear clusters, W2-containing tetranuclear clusters, pentanuclear clusters, and metal Cu ions are highlighted in green, cyanine, blue and red, respectively; the grey and black sticks represent the CN^- bridges).



Scheme S2. Four-membered rings connected through bridged planar 'open' $[WS_4Cu_4]^{2+}$ clusters (the dimensions of the four-membered ring are 6.591 Å × 8.300 Å).



Scheme S3. Six-membered rings connected through bridged planar 'open' $[WS_4Cu_4]^{2+}$ clusters (the dimensions of the six-membered rings are 7.057 Å × 16.388 Å).



Scheme S4. Eight-membered rings connected through shared planar 'open' $[WS_4Cu_4]^{2+}$ clusters (the dimensions of the eight-membered rings are 11.641 Å × 20.193 Å).

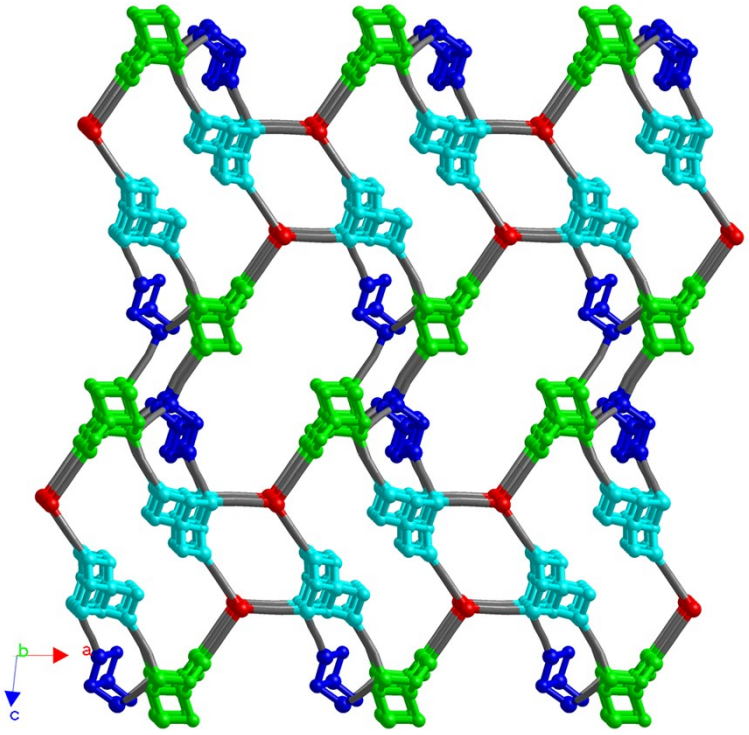


Figure S1. 3-D ball-and-stick packing diagram of the anionic HCM-CP **1** viewed approximately along the *b*-axis (the W1-containing tetranuclear clusters, W2-containing tetranuclear clusters, pentanuclear clusters, and metal Cu ions are highlighted in green, cyanine, blue, and red, respectively; the grey sticks represent the CN^- bridges).

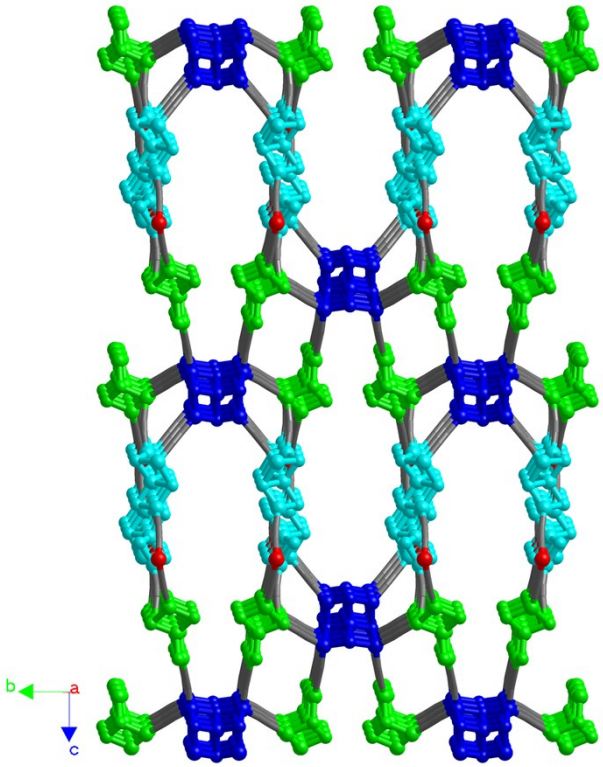


Figure S2. 3-D ball-and-stick packing diagram of the anionic HCM-CP **1** viewed approximately along the *a*-axis (the W1-containing tetranuclear clusters, W2-containing tetranuclear clusters, pentanuclear clusters, and metal Cu ions are highlighted in green, cyanine, blue, and red, respectively; the grey sticks represent the CN^- bridges).

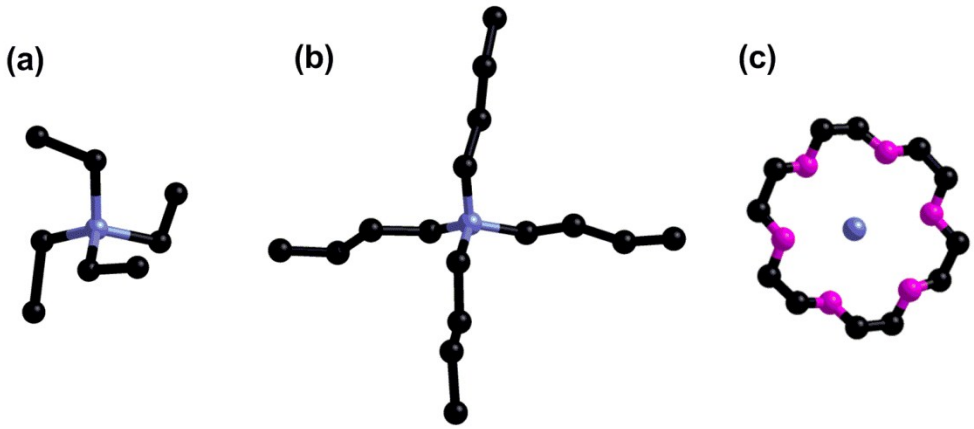


Figure S3. The configuration of the cation $[Et_4N]^+$ (a) from $\{[Et_4N]_2[WS_4Cu_4(CN)_4]\}_n$ (C-CP **2**), the cation $[Bu_4N]^+$ (b) from $\{[Bu_4N][WS_4Cu_3(CN)_2]\}_n$ (C-CP **3**), and the cation $[(NH_4)\subset(18\text{-crown-}6)]^+$ (c) from HCM-CP **1** (ball-and-stick representations, C black, O pink, N purple; all H atoms were omitted for clarity).

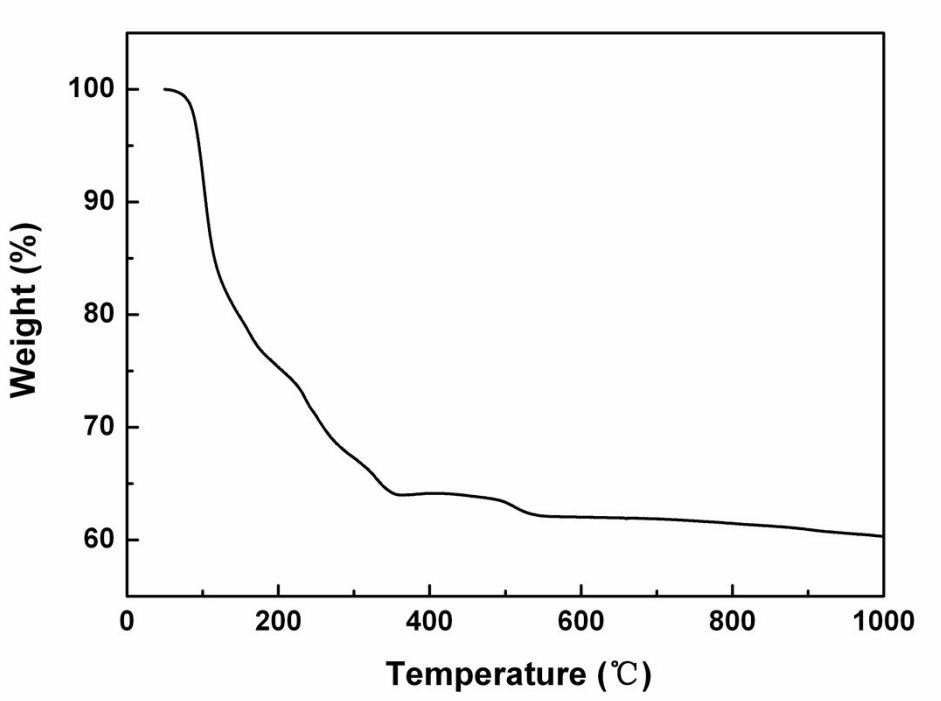


Figure S4. TGA curve for **1**.

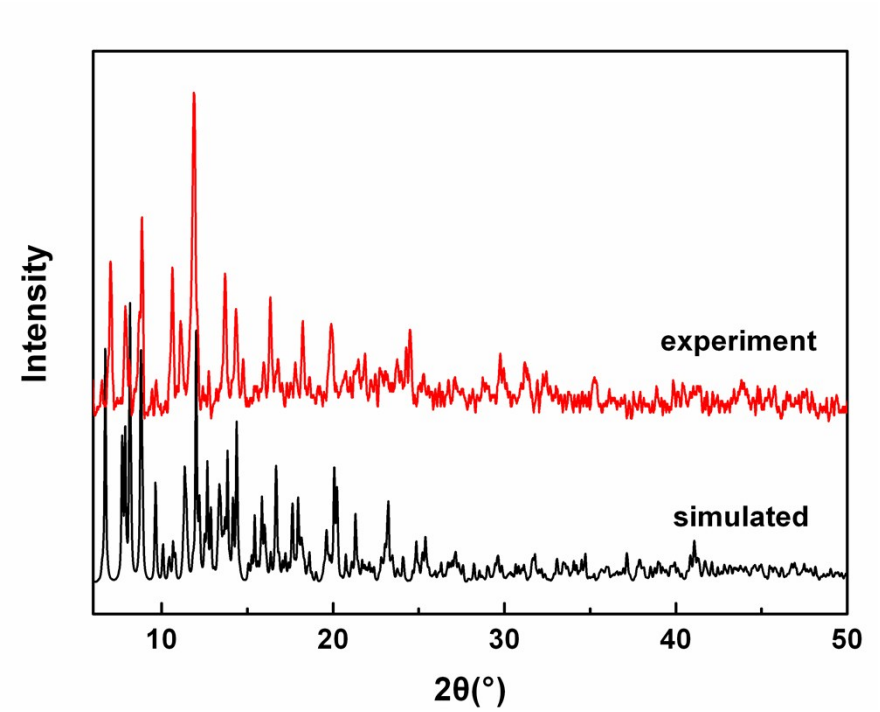


Figure S5. Comparison of the experimental and simulated PXRD patterns of **1**.

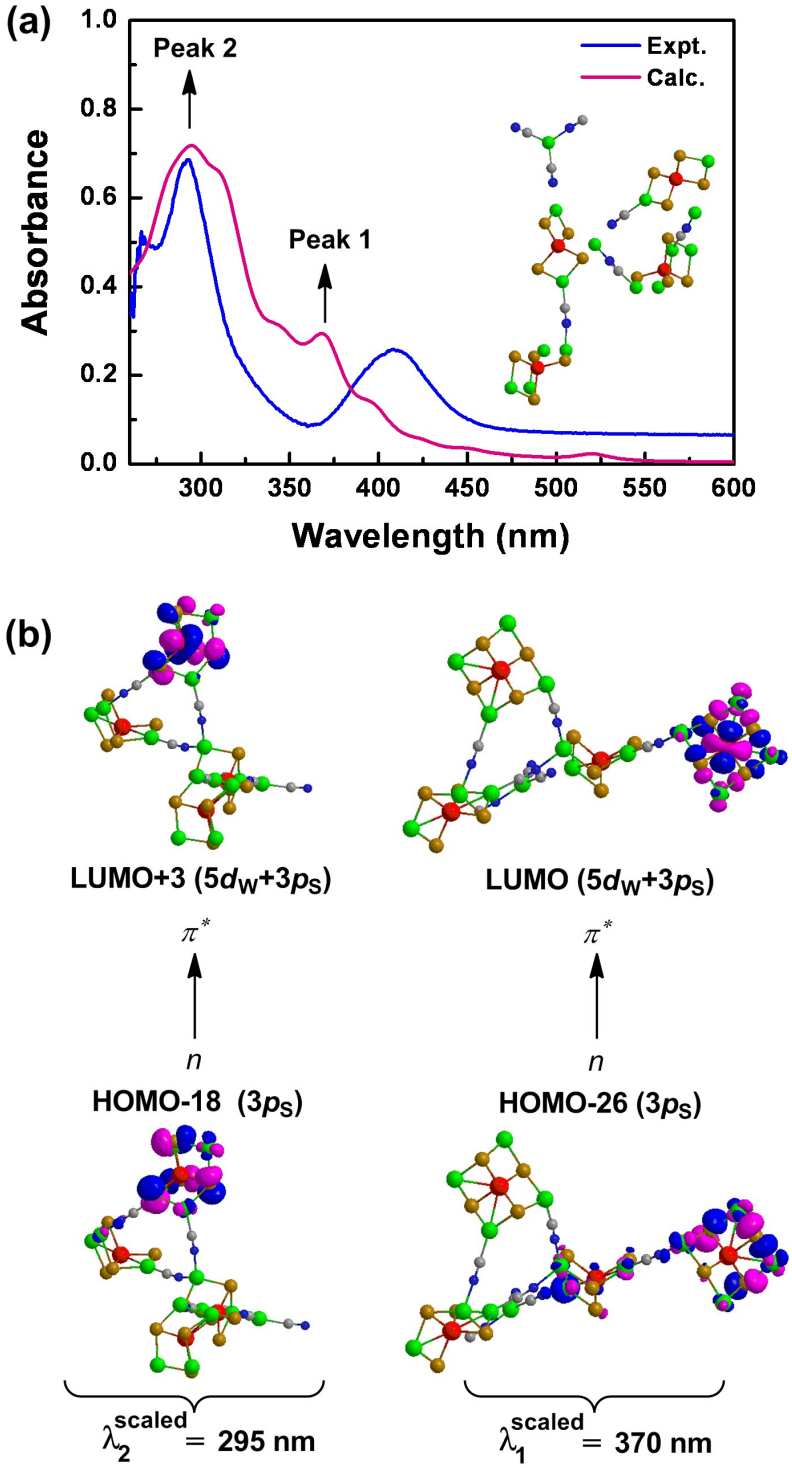


Figure S6. (a) Absorption spectra of **1** in DMF solution obtained from experimental observation (in blue line) and TD-DFT/PCM calculation (in red line). For the latter, a Lorentzian function has been employed with the spectral line width set to 60 nm. The theoretical spectrum is blue-shifted by 135 nm from that obtained from TD-DFT excitation energies. (b) Assignment of absorption peaks (Peak 1 and Peak 2) of **1** in DMF solution. The molecular orbitals are obtained through DFT/PCM calculations at the B3LYP/LanL2DZ level.

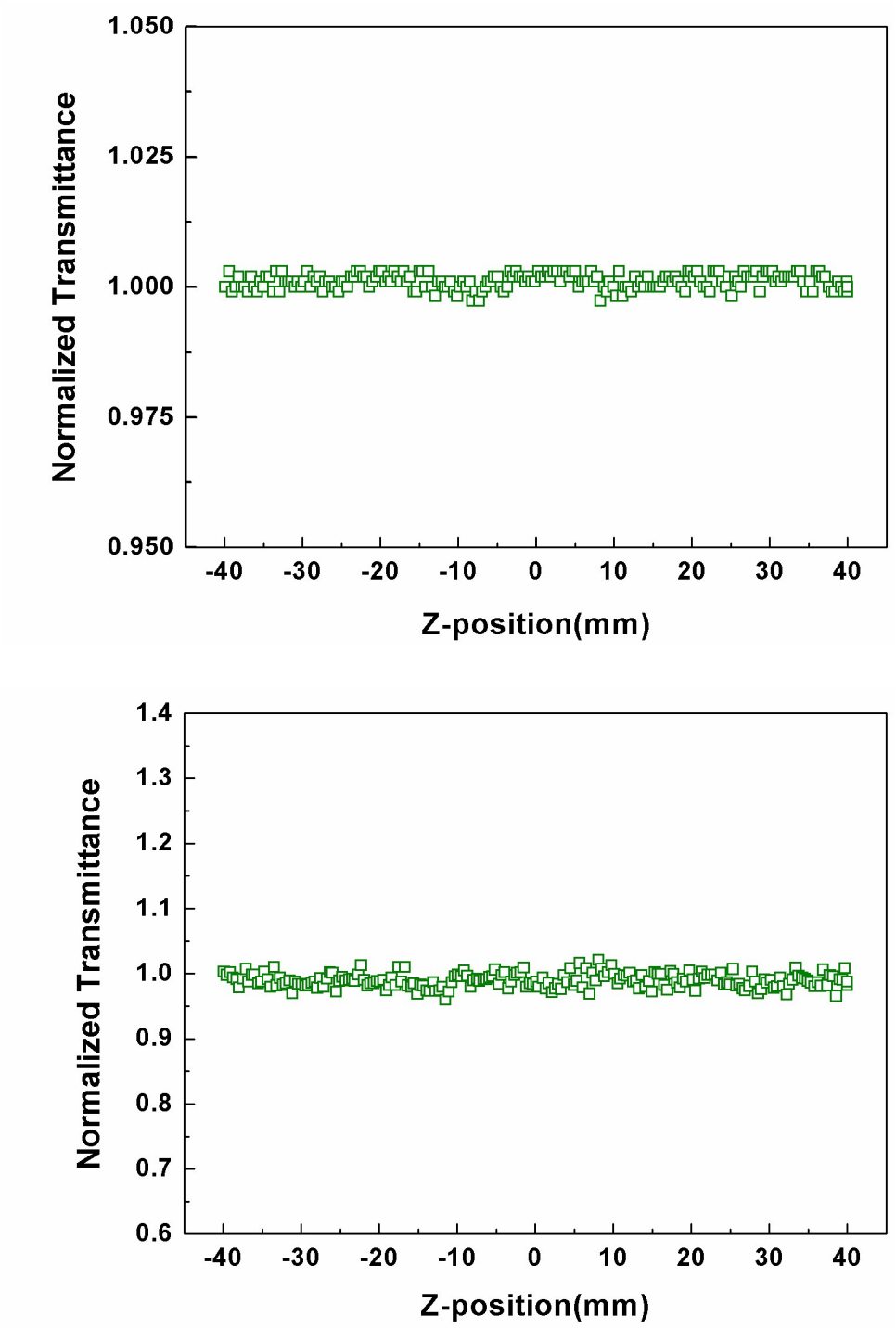


Figure S7. Normalized open-aperture (top) and closed-aperture (bottom) Z-scan curves showing negligible NLO absorption and refraction of aniline solvent, respectively, at 532 nm with 5 ns pulse durations.

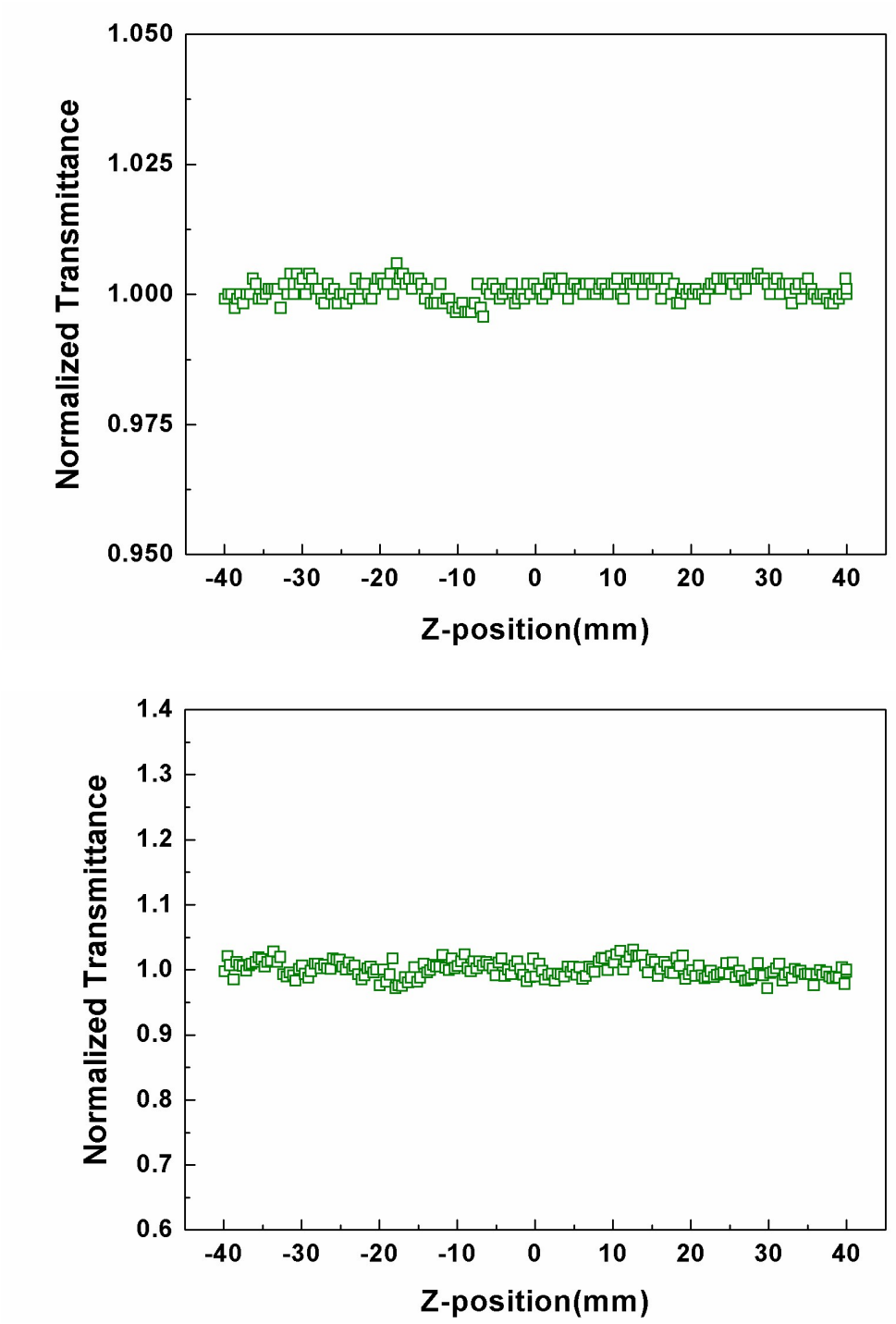


Figure S8. Normalized open-aperture (top) and closed-aperture (bottom) Z-scan curves showing negligible NLO absorption and refraction of 18-crown-6, respectively, at 532 nm with 5 ns pulse durations.

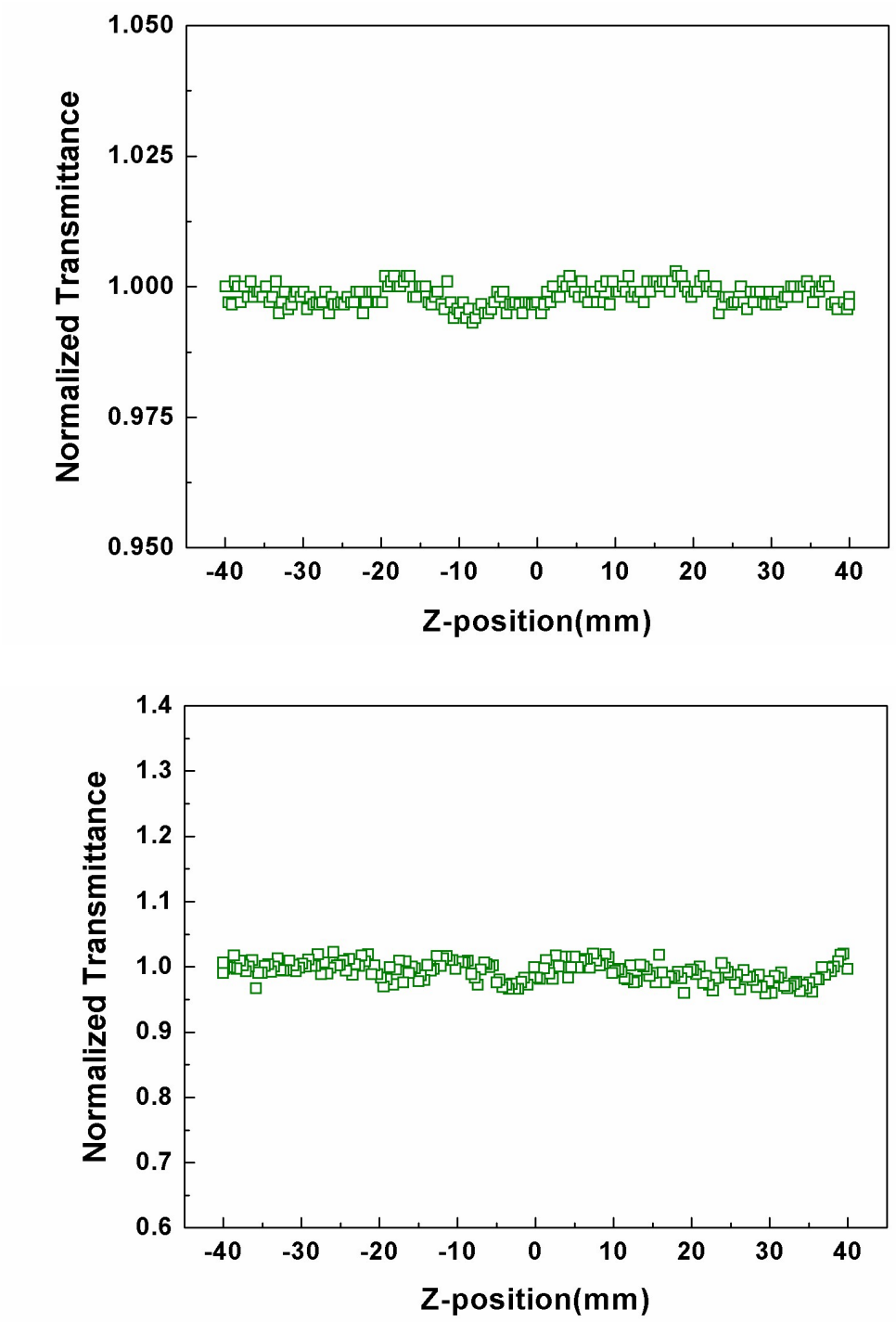


Figure S9. Normalized open-aperture (top) and closed-aperture (bottom) Z-scan curves showing negligible NLO absorption and refraction of $[(NH_4)\subset(18\text{-crown-}6)]NO_3$, respectively, at 532 nm with 5 ns pulse durations.

Table S1. Crystallographic and structural refinement data for HCM-CP **1**.

	HCM-CP 1
Molecular formula	$C_{111}H_{220}Cu_{18}N_{30}O_{42}S_{20}W_5$
Formula weight	5351.67
Temperature (K)	150(2) K
Wavelength (Å)	0.71073
Crystal system	monoclinic
Space group	$P2_1/m$
a (Å)	16.682(3)
b (Å)	21.662(4)
c (Å)	27.674(5)
α (°)	90
β (°)	96.49(3)
γ (°)	90
V (Å^3)	9936(3)
Z	2
ρ_{calc} (g cm^{-3})	1.789
μ (mm^{-1})	5.037
F (000)	5286
Reflections collected	38779
Unique reflections	16529
R_{int}	0.0390
No. parameters	919
GOF	0.998
R_1 [I > 2σ(I)]	0.0690
wR_2 [I > 2σ(I)]	0.1510
$\Delta\rho_{max}$ / $\Delta\rho_{min}$ (e Å^{-3})	1.538 / -1.892

Table S2. The mean radii of cations in some related W/S/Cu polymeric/discrete clusters and coordination polymers.

Molecular Formula	Mean radius of cation[a] (Å)	Reference
$\{[Et_4N]_2[WS_4Cu_4(CN)_4]\}_n$	3.34	[SS1]
$\{[Et_4N]_2[WS_4(CuNCSe)_4]\}_n$	3.38	[SS2]
$\{[Et_4N][WOS_3Cu_3\{S_2P(OMe)_2\}_2]\}_n$	3.36	[SS3]
$[Et_4N]_2[WS_4Cu_4(SCN)_4(2\text{-pic})_4]$	3.35	[SS4]
$\{[Et_4N][Fe(5\text{-ClL1})]_2[Fe(CN)_6]\}_n$	3.34	[SS5]
$\{[Et_4N][Cu_2(CN)_3]\}_n$	3.38	[SS6]
$\{[n\text{-}Bu_4N][WS_4Cu_3(CN)_2]\}_n$	5.86	[SS7]
$\{[n\text{-}Bu_4N]_2[W_2O_2S_6Cu_6Br_4(4,4'\text{-bipy})_3]\}_n$	5.84	[SS8]
$[n\text{-}Bu_4N)_4][W_4Cu_{10}S_{16.5}O_{2.5}]\cdot H_2O$	5.66	[SS9]
$[n\text{-}Bu_4N][WS_4Cu_3Br_2(dppm)_2]$	5.62	[SS10]
$\{[n\text{-}Bu_4N][Cu(CN)Br]\}_n$	5.72	[SS11]
$\{[n\text{-}Bu_4N][Cu_3(CN)_4]\cdot CH_3CN\}_n$	5.87	[SS11]
$\{[n\text{-}Bu_4N]_2[Eu(NO_3)_4Au(CN)_2]\}_n$	5.79	[SS12]
$^3{}_\infty\{\{[(NH_4)\subset(18\text{-crown-6})]_6\cdot 5DMF\cdot 5CH_3CN\cdot H_2O\}\subset\{[WS_4Cu_3(CN)_2]_2[WS_4Cu_3(CN)_2]_2[WS_4Cu_4(CN)_3][Cu(CN)_{1.5}]_2\}\}$	4.62	This work

[a] The mean radius of $[Et_4N]^+$ or $[n\text{-}Bu_4N]^+$ is defined as the average value of the longest distances between the central N and each H atom on every methyl; the mean radius of $[(NH_4)\subset(18\text{-crown-6})]^+$ is defined as the average value of the longest distances between the central N and each H atom on every methylene. All mean radii are calculated according to their CIFs from the CCDC.

[b] Abbreviation: dppm = bis(diphenylphosphino)methane; 4,4'-bipy = 4,4'-bipyridine; 5-ClL1H2 = N,N'-bis(5-chlorosalicylidenato)-2,2-dimethyl-1,3-diaminopropane.

Table S3. Nonlinear optical parameters (second hyperpolarizabilities) of some related Mo(W)/S/Cu polymeric/discrete heterothiometallic clusters and coordination polymers.

Molecular Formula	Skeleton Type	γ (esu)	λ (nm)	Reference
$[MoS_4Cu_4I_2(py)_6]$	Planar-Open Cluster	5.8×10^{-30}	532	[SS13]
$[WS_4Cu_4I_2(py)_6]$	Planar-Open Cluster	6.9×10^{-30}	532	[SS13]
$[MoS_4Cu_4Br_2(py)_6]$	Planar-Open Cluster	1.2×10^{-30}	532	[SS13]
$[WS_4Cu_4Br_2(py)_6]$	Planar-Open Cluster	1.3×10^{-30}	532	[SS13]
$[MoS_4Cu_4(SCN_2)(py)_6]$	Planar-Open Cluster	7.0×10^{-30} *b*	532	[SS14]
$[WS_4Cu_4(SCN_2)(py)_6]$	Planar-Open Cluster	7.4×10^{-30} *b*	532	[SS14]
$\{[Et_4N]_2[MoS_4Cu_4(CN)_4]\}_n$	3D Planar-Open Polymeric Cluster	1.2×10^{-29}	532	[SS1]
$\{[Et_4N]_2[WS_4Cu_4(CN)_4]\}_n$	3D Planar-Open Polymeric Cluster	1.3×10^{-29}	532	[SS1]
$\{[WS_4Cu_4(bipy)_4][WS_4Cu_4I_4(bipy)_2 \cdot 4H_2O]\}_n$	3D Planar-Open Polymeric Cluster	4.4×10^{-29} *b*	532	[SS15]
$\{[Bu_4N][WS_4Cu_3(CN)_2]\}_n$	3D T-Shaped Polymeric Cluster	3.4×10^{-30}	532	[SS7]
$\{[MoOS_3Cu_3(CN)(py)_3] \cdot 0.5C_6H_6\}_n$	1D Nest-Shaped Polymeric Cluster	1.9×10^{-29} b	532	[SS16]
$3_\infty\{[(NO_3)(NMe_4)_3] \subset [WOS_3Cu_3(CN)_3]\}$	3D Nest-Shaped Polymeric Cluster	3.3×10^{-30}	532	[SS17]
$3_\infty\{[(NH_4)(DMF)_2] \subset [W_2O_2S_6Cu_6(CN)_3(bipy)_4]\}$	3D Nest-Shaped Polymeric Cluster	4.9×10^{-29}	532	[SS17]
$3_\infty\{[(NH_4)(DMF)_2] \subset [W_2O_2S_6Cu_6(CN)_3(bpee)_4]\}$	3D Nest-Shaped Polymeric Cluster	3.6×10^{-29}	532	[SS17]
$\{[Tp^*WS_3Cu_3(\mu_3\text{-}DMF)\{Cu(CN)_3\}]_2 \cdot 2DMF \cdot MeCN\}_n$	2D Cubane-Like Polymeric Cluster	4.3×10^{-31}	800	[SS18]
$\{K[Tp^*WS_3Cu_3(\mu_3\text{-}DMF)\{Cu_2(CN)_{4.5}\}]_2 \cdot 4DMF \cdot 2MeCN\}_n$	3D Cubane-Like Polymeric Cluster	4.4×10^{-31}	800	[SS18]
$\{[MoOS_3Cu_3(bibp)_{2.5}](I)]\}_n$	2D Twin-Nest-Shaped Polymeric Cluster	2.3×10^{-29} *b*	532	[SS19]
$\{[WOS_3Cu_3Br(TIPA)] \cdot H_2O \cdot DMF\}_n$	3D Nest-Shaped Polymeric Cluster	1.9×10^{-29} *b*	532	[SS19]
$[Ag(1,3\text{-}\mu_2\text{-}SCN)(\mu_2\text{-}hmt)]_n$	2D Coordination Polymer	2.3×10^{-30}	532	[SS20]
$\{[Ag(1,1,3\text{-}\mu_3\text{-}SCN)]_2(\mu_2\text{-}hmt)\}_n$	2D Coordination Polymer	6.9×10^{-30}	532	[SS20]

$[Ag(1,1,3\text{-}\mu_3\text{-}SCN)(\mu_4\text{-}hmt)_{0.5}]_n$	3D Coordination Polymer	1.1×10^{-29}	532	[SS20]
$\{K{\cdot}Na{\cdot}[Ni_2(\mu_6\text{-}btc)(\mu_2\text{-}ox)(H_2O)_2]{\cdot}2H_2O\}_n$	3D Coordination Polymer	5.0×10^{-30}	532	[SS21]
$\{K{\cdot}Na{\cdot}[Co_2(\mu_6\text{-}btc)(\mu_2\text{-}ox)(H_2O)_2]{\cdot}2H_2O\}_n$	3D Coordination Polymer	3.0×10^{-30}	532	[SS21]
$[Fe_2(\mu_{10}\text{-}btc)_{0.5}(\mu_2\text{-}ox)_{0.5}(\mu_2\text{-}O)_{1.5}]_n$	3D Coordination Polymer	6.0×10^{-30}	532	[SS22]
$[Co(bbbt)_2(NCS)_2]_n$	2D Coordination Polymer	2.4×10^{-30}	532	[SS23]
$[Mn(bbbt)_2(NCS)_2]_n$	2D Coordination Polymer	1.5×10^{-30}	532	[SS23]
$[Cd(bbbt)_2(NCS)_2]_n$	2D Coordination Polymer	1.5×10^{-30}	532	[SS23]
$[Pb(bbbm)_2(NO_3)_2]_n$	2D Coordination Polymer	2.3×10^{-29} [b]	532	[SS24]
$[Zn(bbbt)(NCS)_2]_n$	1D Coordination Polymer	1.5×10^{-29} [b]	532	[SS24]
$[Zn(pbbt)(NCS)_2]_n$	1D Coordination Polymer	1.2×10^{-29} [b]	532	[SS24]
$\{[Cd(fcz)_2Cl_2]{\cdot}CH_3OH{\cdot}2H_2O\}_n$	2D Coordination Polymer	1.2×10^{-30}	532	[SS25]
$\{[Co(fcz)_2Cl_2]{\cdot}2CH_3OH\}_n$	2D Coordination Polymer	1.5×10^{-30}	532	[SS25]
$[AgCu_2(C_7H_2NO_5)(C_7H_3NO_5)]_n{\cdot}2nH_2O$	2D Coordination Polymer	1.3×10^{-29} [b]	532	[SS26]
$[Cu_3(C_7H_2NO_5)_2]_n{\cdot}3nH_2O$	3D Coordination Polymer	2.2×10^{-30} [b]	532	[SS27]
$[CuAg_2(C_7H_3NO_5)_2]_n$	2D Coordination Polymer	2.5×10^{-30} [b]	532	[SS27]
$^3{}_\infty\{\{[(NH_4)\subset(18\text{-crown-}6)]_6{\cdot}5DMF{\cdot}5CH_3CN{\cdot}H_2O\}$ $\subset\{[WS_4Cu_3(CN)_2]_2[WS_4Cu_3(CN)_2]_2[WS_4Cu_4(CN)_3][Cu(CN)_{1.5}]_2\}\}$	3D Planar-Open Cluster/T-Shaped Cluster/ Metal Polymeric Cluster	7.3×10^{-29}	532	This work

[a] Abbreviation: py = pyridine, bipy = 4,4'-bipyridine, bpee = 1,2-(*E*)-bis(4-pyridyl)ethene, bibp = 4,4'-di(1*H*-imidazol-1-yl)-1,1'-biphenyl, tipa = tris(4-(1*H*-imidazol-1-yl)phenyl)amine, hmt = hexamethylenetetramine, bbbt = 1,1'-(1,4-butanediyl)bis-1*H*-benzotriazole, $C_7H_5NO_5$ = 2,6-dicarboxy-4-hydroxypyridine, bbbm = 1,1'-(1,4-butanediyl)bis-1*H*-benzimidazole, pbbt = 1,1'-(1,3-propylene)bis-1*H*-benzotriazole, fcz = α-(2,4-difluorophenyl)-α-(1*H*-1,2,4-triazol-1-ylmethyl)-1*H*-1,2,4-triazole-1-ethanol, btc = 1,2,4,5-benzenetetracarboxylate, ox = oxalate.

[b] The hyperpolarizabilities γ are calculated based on nonlinear absorptive coefficients a_2 and nonlinear refractive indexes n_2 from the references.

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Table S4. Results of Time-dependent Density Functional Theory (TD-DFT) Calculations

1-B3LYP-LanL2DZ TD-PCM (200 states) in DMF (dielectric constant = 36.7) solution

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 0.6272 eV 1976.84 nm f = 0.0000
264 ->265 0.70709
This state for optimization and/or second-order correction.
Total Energy, E(RPA) = -4026.36864041
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 0.9190 eV 1349.14 nm f = 0.0000
264 ->266 0.70709

Excited State 3: Singlet-A 1.0488 eV 1182.11 nm f = 0.0000
264 ->267 0.70709

Excited State 4: Singlet-A 1.0516 eV 1178.98 nm f = 0.0000
263 ->265 0.70706

Excited State 5: Singlet-A 1.2662 eV 979.18 nm f = 0.0000
264 ->268 0.70706

Excited State 6: Singlet-A 1.3434 eV 922.90 nm f = 0.0000
263 ->266 0.70705

Excited State 7: Singlet-A 1.4668 eV 845.24 nm f = 0.0000
261 ->265 0.17830
262 ->265 0.68191

Excited State 8: Singlet-A 1.4738 eV 841.24 nm f = 0.0000
263 ->267 0.70706

Excited State 9: Singlet-A 1.4947 eV 829.47 nm f = 0.0000
259 ->265 0.10118
261 ->265 0.67748
262 ->265 -0.16915

Excited State 10: Singlet-A 1.6523 eV 750.36 nm f = 0.0001
259 ->265 0.65127
260 ->265 -0.22451

Excited State 11: Singlet-A 1.6912 eV 733.12 nm f = 0.0000
263 ->268 0.70703

Excited State 12: Singlet-A 1.7574 eV 705.49 nm f = 0.0000
261 ->266 0.17879
262 ->266 0.68162

Excited State 13:	Singlet-A	1.7794 eV	696.76 nm	f = 0.0000
264 ->271	0.70679			
Excited State 14:	Singlet-A	1.7855 eV	694.40 nm	f = 0.0000
259 ->266	0.10285			
261 ->266	0.67711			
262 ->266	-0.16935			
Excited State 15:	Singlet-A	1.7954 eV	690.55 nm	f = 0.0000
264 ->269	0.70633			
Excited State 16:	Singlet-A	1.7961 eV	690.29 nm	f = 0.0000
259 ->265	0.22891			
260 ->265	0.66821			
Excited State 17:	Singlet-A	1.8668 eV	664.15 nm	f = 0.0000
258 ->265	0.70447			
Excited State 18:	Singlet-A	1.8845 eV	657.93 nm	f = 0.0000
264 ->270	0.70694			
Excited State 19:	Singlet-A	1.8906 eV	655.79 nm	f = 0.0022
261 ->267	0.55403			
262 ->267	-0.42206			
Excited State 20:	Singlet-A	1.8975 eV	653.42 nm	f = 0.0004
261 ->267	0.43021			
262 ->267	0.55567			
Excited State 21:	Singlet-A	1.9004 eV	652.42 nm	f = 0.0000
264 ->272	0.70702			
Excited State 22:	Singlet-A	1.9425 eV	638.27 nm	f = 0.0001
259 ->266	0.65090			
260 ->266	-0.22431			
Excited State 23:	Singlet-A	1.9974 eV	620.72 nm	f = 0.0003
254 ->265	0.15345			
255 ->265	0.27015			
256 ->265	0.16343			
257 ->265	0.60501			
Excited State 24:	Singlet-A	2.0230 eV	612.89 nm	f = 0.0000
264 ->273	0.67092			
264 ->274	-0.22203			
Excited State 25:	Singlet-A	2.0282 eV	611.30 nm	f = 0.0000
255 ->265	0.11490			
256 ->265	0.65129			
257 ->265	-0.24138			
Excited State 26:	Singlet-A	2.0514 eV	604.38 nm	f = 0.0005

253 ->265 -0.10087
254 ->265 0.30110
255 ->265 0.51774
256 ->265 -0.21958
257 ->265 -0.25818

Excited State 27: Singlet-A 2.0879 eV 593.81 nm f = 0.0000
259 ->266 0.22906
260 ->266 0.66893

Excited State 28: Singlet-A 2.0955 eV 591.66 nm f = 0.0000
264 ->273 0.22201
264 ->274 0.67119

Excited State 29: Singlet-A 2.1064 eV 588.61 nm f = 0.0005
261 ->268 0.56083
262 ->268 -0.41360

Excited State 30: Singlet-A 2.1144 eV 586.37 nm f = 0.0009
261 ->268 0.41863
262 ->268 0.55938

Excited State 31: Singlet-A 2.1150 eV 586.22 nm f = 0.0002
252 ->265 -0.22145
253 ->265 0.59249
254 ->265 -0.16254
255 ->265 0.23660

Excited State 32: Singlet-A 2.1309 eV 581.85 nm f = 0.0006
259 ->267 0.65569
260 ->267 -0.23420

Excited State 33: Singlet-A 2.1578 eV 574.58 nm f = 0.0000
253 ->265 0.25853
254 ->265 0.58716
255 ->265 -0.29050

Excited State 34: Singlet-A 2.1586 eV 574.37 nm f = 0.0000
258 ->266 0.70444

Excited State 35: Singlet-A 2.1890 eV 566.40 nm f = 0.0000
264 ->275 0.70696

Excited State 36: Singlet-A 2.2054 eV 562.17 nm f = 0.0000
263 ->271 0.70676

Excited State 37: Singlet-A 2.2175 eV 559.12 nm f = 0.0000
259 ->267 0.23673
260 ->267 0.66621

Excited State 38: Singlet-A 2.2175 eV 559.11 nm f = 0.0026
237 ->265 0.13652
243 ->265 -0.26167

244 ->265 0.57892
245 ->265 -0.18060
253 ->265 -0.10508

Excited State 39: Singlet-A 2.2199 eV 558.52 nm f = 0.0000
263 ->269 0.70696

Excited State 40: Singlet-A 2.2435 eV 552.64 nm f = 0.0000
264 ->276 0.70673

Excited State 41: Singlet-A 2.2617 eV 548.19 nm f = 0.0000
252 ->265 0.66008
253 ->265 0.23558

Excited State 42: Singlet-A 2.2881 eV 541.86 nm f = 0.0000
258 ->267 0.70262

Excited State 43: Singlet-A 2.2888 eV 541.70 nm f = 0.0002
254 ->266 0.15562
255 ->266 0.27412
256 ->266 0.16369
257 ->266 0.60070

Excited State 44: Singlet-A 2.3089 eV 536.98 nm f = 0.0000
263 ->270 0.70689

Excited State 45: Singlet-A 2.3198 eV 534.47 nm f = 0.0000
255 ->266 0.11868
256 ->266 0.64388
257 ->266 -0.24990

Excited State 46: Singlet-A 2.3248 eV 533.31 nm f = 0.0000
263 ->272 0.70589

Excited State 47: Singlet-A 2.3263 eV 532.97 nm f = 0.0073
240 ->265 0.40028
241 ->265 -0.37331
248 ->267 -0.15004
249 ->267 0.17893
254 ->267 0.11739
255 ->267 0.15386
256 ->267 0.16185

Excited State 48: Singlet-A 2.3264 eV 532.95 nm f = 0.0014
240 ->265 -0.25254
241 ->265 0.23607
248 ->267 -0.23614
249 ->267 0.28180
251 ->267 0.12647
254 ->267 0.18509
255 ->267 0.24208
256 ->267 0.25436
257 ->267 0.12153

Excited State 49:	Singlet-A	2.3435 eV	529.07 nm	f = 0.0009
254 ->266	0.29684			
255 ->266	0.51614			
256 ->266	-0.21473			
257 ->266	-0.25153			
Excited State 50:	Singlet-A	2.3467 eV	528.32 nm	f = 0.0002
256 ->267	0.31592			
257 ->267	-0.11105			
259 ->268	0.56633			
260 ->268	-0.20212			
Excited State 51:	Singlet-A	2.3485 eV	527.94 nm	f = 0.0020
248 ->267	0.10073			
249 ->267	-0.11567			
255 ->267	-0.16673			
256 ->267	0.50919			
257 ->267	-0.21761			
259 ->268	-0.32791			
260 ->268	0.11730			
Excited State 52:	Singlet-A	2.4067 eV	515.17 nm	f = 0.0001
252 ->266	-0.22491			
253 ->266	0.60101			
254 ->266	-0.16635			
255 ->266	0.22936			
Excited State 53:	Singlet-A	2.4252 eV	511.23 nm	f = 0.0029
246 ->267	-0.28873			
248 ->267	0.11870			
253 ->267	0.33710			
254 ->267	0.14745			
255 ->267	-0.16984			
257 ->267	0.45657			
Excited State 54:	Singlet-A	2.4345 eV	509.27 nm	f = 0.0025
246 ->267	0.34421			
247 ->267	-0.12375			
249 ->267	-0.12840			
252 ->267	-0.21462			
253 ->267	0.17809			
254 ->267	-0.32273			
255 ->267	0.25700			
256 ->267	0.18014			
257 ->267	0.21326			
Excited State 55:	Singlet-A	2.4349 eV	509.21 nm	f = 0.0000
259 ->268	0.23656			
260 ->268	0.66614			
Excited State 56:	Singlet-A	2.4414 eV	507.84 nm	f = 0.0009
256 ->271	0.66329			

257 ->271 -0.15568

Excited State 57: Singlet-A 2.4474 eV 506.61 nm f = 0.0000
264 ->278 0.70377

Excited State 58: Singlet-A 2.4476 eV 506.56 nm f = 0.0047
246 ->267 -0.14323
247 ->267 -0.21541
249 ->267 0.14871
252 ->267 -0.14510
253 ->267 0.45677
257 ->267 -0.36161

Excited State 59: Singlet-A 2.4491 eV 506.25 nm f = 0.0000
263 ->273 0.67079
263 ->274 -0.22162

Excited State 60: Singlet-A 2.4494 eV 506.18 nm f = 0.0000
253 ->266 0.25511
254 ->266 0.58806
255 ->266 -0.29075

Excited State 61: Singlet-A 2.4571 eV 504.59 nm f = 0.0183
237 ->265 -0.28835
238 ->265 0.44005
240 ->265 0.13743
242 ->265 -0.10838
243 ->265 0.12936
245 ->265 -0.20192
248 ->265 -0.20387
249 ->265 -0.13741
251 ->265 -0.10672

Excited State 62: Singlet-A 2.4778 eV 500.37 nm f = 0.0053
264 ->277 0.48167
264 ->279 0.51430

Excited State 63: Singlet-A 2.4821 eV 499.52 nm f = 0.0006
246 ->267 -0.36317
247 ->267 0.20847
248 ->267 0.12110
251 ->267 -0.12623
252 ->267 0.12418
254 ->267 -0.22716
255 ->267 0.44188

Excited State 64: Singlet-A 2.5056 eV 494.82 nm f = 0.0000
258 ->268 0.70052

Excited State 65: Singlet-A 2.5122 eV 493.54 nm f = 0.0008
246 ->267 0.15627
248 ->267 0.13414
249 ->267 -0.16594

253 ->267 0.14354
254 ->267 0.42455
255 ->267 0.20227
257 ->267 -0.13781
264 ->277 0.25991
264 ->279 -0.24071

Excited State 66: Singlet-A 2.5123 eV 493.51 nm f = 0.0030
254 ->267 -0.24723
255 ->267 -0.11894
264 ->277 0.44593
264 ->279 -0.41751

Excited State 67: Singlet-A 2.5205 eV 491.90 nm f = 0.0000
263 ->273 0.22159
263 ->274 0.67102

Excited State 68: Singlet-A 2.5525 eV 485.73 nm f = 0.0002
252 ->266 0.64995
253 ->266 0.24770

Excited State 69: Singlet-A 2.5565 eV 484.98 nm f = 0.0057
246 ->267 0.19534
247 ->267 0.39469
248 ->267 -0.10805
249 ->267 0.12454
249 ->268 -0.10624
252 ->267 0.21902
253 ->267 0.30200
254 ->267 -0.12189
255 ->267 -0.14954
255 ->268 -0.12819
256 ->268 -0.11034

Excited State 70: Singlet-A 2.5673 eV 482.94 nm f = 0.0011
256 ->268 0.67218
257 ->268 -0.15714

Excited State 71: Singlet-A 2.5698 eV 482.47 nm f = 0.0021
235 ->265 -0.10605
237 ->265 -0.18940
238 ->265 0.18254
248 ->265 0.24440
249 ->265 0.35316
251 ->265 0.44863

Excited State 72: Singlet-A 2.5854 eV 479.56 nm f = 0.0038
252 ->271 -0.18074
254 ->271 0.44493
255 ->271 -0.25537
261 ->271 -0.39341

Excited State 73: Singlet-A 2.5899 eV 478.73 nm f = 0.0065

238 ->266 0.23086
243 ->266 -0.15220
244 ->266 0.51758
245 ->266 -0.24266
252 ->266 0.11326

Excited State 74: Singlet-A 2.5979 eV 477.24 nm f = 0.0024
246 ->267 0.12620
248 ->268 -0.11766
249 ->268 0.15030
252 ->267 0.35152
253 ->267 0.13065
254 ->268 0.19148
255 ->268 0.32617
257 ->268 0.34353

Excited State 75: Singlet-A 2.6140 eV 474.31 nm f = 0.0000
263 ->275 0.70678

Excited State 76: Singlet-A 2.6155 eV 474.03 nm f = 0.0041
247 ->267 -0.36238
252 ->267 0.46176
255 ->268 -0.17296
257 ->268 -0.24976

Excited State 77: Singlet-A 2.6336 eV 470.78 nm f = 0.0008
235 ->265 0.10099
237 ->265 0.12415
248 ->265 -0.29623
249 ->265 -0.23793
251 ->265 0.51672
262 ->269 -0.12054

Excited State 78: Singlet-A 2.6345 eV 470.61 nm f = 0.0001
261 ->269 0.18028
262 ->269 0.66966

Excited State 79: Singlet-A 2.6460 eV 468.57 nm f = 0.0011
247 ->267 -0.13919
247 ->268 -0.25890
252 ->268 -0.23110
253 ->268 0.50484
254 ->268 -0.13247
257 ->268 0.19077

Excited State 80: Singlet-A 2.6586 eV 466.35 nm f = 0.0004
248 ->265 -0.40056
249 ->265 0.45423
250 ->265 -0.29786

Excited State 81: Singlet-A 2.6625 eV 465.67 nm f = 0.0002
261 ->269 0.67596
262 ->269 -0.17362

Excited State 82:	Singlet-A	2.6630 eV	465.59 nm	f = 0.0000
248 ->265	-0.11465			
249 ->265	0.28651			
250 ->265	0.63136			
Excited State 83:	Singlet-A	2.6667 eV	464.94 nm	f = 0.0016
247 ->268	-0.12397			
254 ->268	-0.25580			
255 ->268	0.46341			
257 ->268	-0.39253			
Excited State 84:	Singlet-A	2.6685 eV	464.62 nm	f = 0.0000
263 ->276	0.70642			
Excited State 85:	Singlet-A	2.6900 eV	460.91 nm	f = 0.0021
247 ->268	-0.14582			
248 ->268	-0.10457			
249 ->268	0.14289			
253 ->268	0.20683			
254 ->268	0.51561			
255 ->268	-0.11558			
256 ->268	-0.10331			
257 ->268	-0.30053			
Excited State 86:	Singlet-A	2.7074 eV	457.95 nm	f = 0.0063
252 ->271	-0.26088			
253 ->271	-0.15551			
255 ->271	0.10144			
261 ->271	0.10495			
262 ->271	0.60057			
Excited State 87:	Singlet-A	2.7128 eV	457.03 nm	f = 0.0013
229 ->265	0.17061			
231 ->265	0.19680			
233 ->265	-0.13805			
235 ->265	0.18365			
237 ->265	0.15243			
238 ->266	-0.11363			
240 ->266	-0.22261			
241 ->266	0.15682			
245 ->265	-0.29337			
247 ->265	-0.15868			
248 ->265	0.31851			
Excited State 88:	Singlet-A	2.7194 eV	455.92 nm	f = 0.0088
252 ->271	0.39957			
253 ->271	0.22170			
254 ->273	0.11212			
261 ->271	-0.34293			
262 ->271	0.33387			
Excited State 89:	Singlet-A	2.7204 eV	455.75 nm	f = 0.0001

261 ->270 0.17660
262 ->270 0.67548

Excited State 90: Singlet-A 2.7347 eV 453.37 nm f = 0.0001
261 ->272 0.17735
262 ->272 0.66718

Excited State 91: Singlet-A 2.7396 eV 452.57 nm f = 0.0011
247 ->268 0.49880
251 ->268 -0.11559
252 ->268 0.10727
253 ->268 0.37975
255 ->268 0.12737

Excited State 92: Singlet-A 2.7474 eV 451.27 nm f = 0.0025
240 ->266 0.23385
241 ->266 -0.18523
247 ->265 -0.18484
261 ->270 0.55203
262 ->270 -0.12240

Excited State 93: Singlet-A 2.7525 eV 450.44 nm f = 0.0085
240 ->266 -0.28719
241 ->266 0.21809
245 ->265 0.11028
247 ->265 0.38802
261 ->270 0.37754
262 ->270 -0.11096

Excited State 94: Singlet-A 2.7625 eV 448.81 nm f = 0.0070
240 ->266 0.17561
241 ->266 -0.18076
245 ->265 -0.10039
247 ->265 0.39506
261 ->270 -0.10344
261 ->272 0.41671

Excited State 95: Singlet-A 2.7637 eV 448.62 nm f = 0.0038
240 ->266 -0.17035
241 ->266 0.13407
245 ->265 0.11748
247 ->265 -0.32413
261 ->272 0.50419
262 ->272 -0.13863

Excited State 96: Singlet-A 2.7711 eV 447.42 nm f = 0.0041
252 ->271 0.12060
254 ->271 0.12800
255 ->271 -0.10537
261 ->271 0.14424
261 ->278 0.46581
262 ->278 -0.33149
262 ->279 0.15933

Excited State 97:	Singlet-A	2.7743 eV	446.90 nm	f = 0.0018
248 ->268	-0.28337			
249 ->268	0.33717			
251 ->268	0.14039			
252 ->268	0.20019			
253 ->268	0.14190			
254 ->268	-0.27076			
255 ->268	-0.24923			
Excited State 98:	Singlet-A	2.7750 eV	446.80 nm	f = 0.0180
237 ->266	-0.26166			
238 ->266	0.34320			
241 ->266	0.15883			
243 ->266	0.23136			
244 ->266	-0.23080			
245 ->265	-0.10661			
247 ->265	0.10894			
248 ->266	-0.15329			
249 ->266	-0.11564			
261 ->272	0.12511			
Excited State 99:	Singlet-A	2.7809 eV	445.85 nm	f = 0.0037
252 ->271	0.18576			
253 ->271	0.15810			
254 ->271	0.29495			
255 ->271	-0.23324			
261 ->271	0.42221			
261 ->278	-0.20728			
262 ->278	0.19267			
Excited State 100:	Singlet-A	2.7947 eV	443.63 nm	f = 0.0028
261 ->279	0.22203			
262 ->278	0.25032			
262 ->279	0.57435			
Excited State 101:	Singlet-A	2.8059 eV	441.87 nm	f = 0.0062
246 ->268	-0.30601			
247 ->268	-0.21905			
252 ->268	0.54227			
Excited State 102:	Singlet-A	2.8127 eV	440.80 nm	f = 0.0000
264 ->280	0.70677			
Excited State 103:	Singlet-A	2.8176 eV	440.03 nm	f = 0.0001
246 ->265	0.69839			
Excited State 104:	Singlet-A	2.8204 eV	439.60 nm	f = 0.0005
259 ->269	0.65019			
260 ->269	-0.22417			
Excited State 105:	Singlet-A	2.8406 eV	436.48 nm	f = 0.0121
252 ->271	0.15257			

252 ->273	-0.19835			
253 ->273	-0.15289			
254 ->273	-0.26669			
255 ->273	0.20998			
256 ->273	0.23311			
261 ->273	0.34375			
261 ->274	-0.11327			
Excited State 106:	Singlet-A	2.8552 eV	434.23 nm	f = 0.0021
235 ->266	-0.11191			
237 ->266	-0.19544			
238 ->266	0.16926			
245 ->265	-0.12964			
248 ->266	0.27166			
249 ->266	0.34722			
251 ->266	0.41538			
Excited State 107:	Singlet-A	2.8605 eV	433.43 nm	f = 0.0108
239 ->267	0.33550			
240 ->267	0.10104			
242 ->267	-0.17128			
246 ->268	-0.23525			
249 ->268	0.16786			
251 ->267	0.33643			
252 ->268	-0.19309			
Excited State 108:	Singlet-A	2.8623 eV	433.16 nm	f = 0.0025
229 ->265	0.16712			
231 ->265	0.16810			
233 ->265	-0.11075			
235 ->265	0.14575			
242 ->265	-0.14166			
243 ->265	0.12873			
244 ->265	0.19558			
245 ->265	0.47919			
Excited State 109:	Singlet-A	2.8665 eV	432.52 nm	f = 0.0004
261 ->279	-0.20565			
263 ->278	0.65504			
Excited State 110:	Singlet-A	2.8800 eV	430.50 nm	f = 0.0176
239 ->267	0.11889			
246 ->268	0.45378			
247 ->268	-0.12172			
249 ->268	-0.13361			
251 ->267	0.34663			
251 ->268	0.10573			
252 ->268	0.19988			
Excited State 111:	Singlet-A	2.8909 eV	428.88 nm	f = 0.0020
261 ->279	0.22391			
263 ->277	0.34967			
263 ->279	0.55390			

Excited State 112:	Singlet-A	2.8975 eV	427.90 nm	f = 0.0000
264 ->281	0.70636			
Excited State 113:	Singlet-A	2.9012 eV	427.36 nm	f = 0.0133
251 ->271	-0.17132			
252 ->273	-0.11495			
254 ->273	0.19527			
255 ->273	-0.12622			
256 ->273	0.45786			
256 ->274	-0.16488			
261 ->273	-0.22398			
Excited State 114:	Singlet-A	2.9056 eV	426.71 nm	f = 0.0018
259 ->270	0.60991			
259 ->272	0.11861			
260 ->270	-0.21005			
261 ->279	-0.13261			
Excited State 115:	Singlet-A	2.9095 eV	426.14 nm	f = 0.0055
259 ->270	0.20623			
259 ->272	-0.13499			
259 ->278	-0.15231			
261 ->278	-0.13580			
261 ->279	0.46066			
262 ->279	-0.13792			
263 ->277	-0.17386			
263 ->278	0.21565			
263 ->279	-0.14032			
Excited State 116:	Singlet-A	2.9206 eV	424.52 nm	f = 0.0006
251 ->266	-0.18127			
259 ->272	0.58010			
260 ->272	-0.19967			
261 ->279	0.13127			
Excited State 117:	Singlet-A	2.9238 eV	424.05 nm	f = 0.0015
237 ->266	0.10292			
248 ->266	-0.29466			
249 ->266	-0.19625			
251 ->266	0.51019			
259 ->272	0.20999			
Excited State 118:	Singlet-A	2.9295 eV	423.23 nm	f = 0.0002
261 ->273	0.19458			
261 ->274	0.50528			
262 ->273	-0.17720			
262 ->274	-0.37046			
Excited State 119:	Singlet-A	2.9324 eV	422.81 nm	f = 0.0003
259 ->271	-0.10567			
263 ->277	0.57022			
263 ->279	-0.37075			

Excited State 120:	Singlet-A	2.9377 eV	422.04 nm	f = 0.0010
261 ->273	0.13354			
261 ->274	0.40143			
262 ->273	0.22130			
262 ->274	0.49450			
Excited State 121:	Singlet-A	2.9399 eV	421.73 nm	f = 0.0025
259 ->271	0.57392			
260 ->271	-0.32522			
262 ->274	-0.10016			
263 ->279	-0.10349			
Excited State 122:	Singlet-A	2.9485 eV	420.50 nm	f = 0.0021
236 ->267	-0.10235			
239 ->267	-0.31859			
240 ->267	-0.10599			
241 ->267	-0.10005			
242 ->267	0.16474			
246 ->267	-0.11101			
246 ->268	-0.10268			
249 ->267	-0.23920			
251 ->267	0.35193			
262 ->273	-0.26477			
Excited State 123:	Singlet-A	2.9494 eV	420.37 nm	f = 0.0001
259 ->271	0.33123			
260 ->271	0.62016			
Excited State 124:	Singlet-A	2.9500 eV	420.29 nm	f = 0.0015
248 ->266	-0.38869			
249 ->266	0.47462			
250 ->266	-0.28630			
Excited State 125:	Singlet-A	2.9515 eV	420.07 nm	f = 0.0075
239 ->267	-0.13883			
249 ->267	-0.10557			
251 ->267	0.15149			
261 ->273	-0.12463			
261 ->274	0.10976			
262 ->273	0.53061			
262 ->274	-0.25938			
Excited State 126:	Singlet-A	2.9548 eV	419.61 nm	f = 0.0000
248 ->266	-0.10205			
249 ->266	0.27842			
250 ->266	0.63789			
Excited State 127:	Singlet-A	2.9644 eV	418.25 nm	f = 0.0000
259 ->269	0.22917			
260 ->269	0.66885			
Excited State 128:	Singlet-A	2.9670 eV	417.88 nm	f = 0.0066

252 ->273	-0.15202			
259 ->271	-0.11376			
259 ->278	0.32336			
259 ->279	0.20247			
260 ->278	-0.10998			
261 ->273	-0.14279			
261 ->278	-0.29231			
262 ->278	-0.29488			
262 ->279	0.11480			
Excited State 129:	Singlet-A	2.9738 eV	416.92 nm	f = 0.0109
252 ->273	0.38056			
252 ->274	-0.13789			
253 ->273	0.23492			
256 ->273	0.15223			
259 ->278	0.14669			
261 ->273	0.25901			
261 ->274	-0.12215			
262 ->273	0.21693			
262 ->274	-0.10499			
Excited State 130:	Singlet-A	2.9765 eV	416.54 nm	f = 0.0000
264 ->282	0.70679			
Excited State 131:	Singlet-A	2.9931 eV	414.23 nm	f = 0.0003
229 ->265	-0.11574			
231 ->265	-0.12073			
238 ->265	-0.14769			
243 ->265	0.58500			
244 ->265	0.23574			
Excited State 132:	Singlet-A	3.0009 eV	413.16 nm	f = 0.0215
259 ->278	0.33888			
259 ->279	0.20307			
260 ->278	-0.11538			
261 ->278	0.22991			
261 ->279	0.18878			
262 ->278	0.31214			
262 ->279	-0.21992			
263 ->279	-0.10217			
Excited State 133:	Singlet-A	3.0104 eV	411.86 nm	f = 0.0013
231 ->266	0.10099			
239 ->267	-0.11255			
245 ->266	-0.18662			
247 ->266	-0.11150			
248 ->266	0.16342			
248 ->267	0.45163			
249 ->267	0.31773			
251 ->267	0.12316			
Excited State 134:	Singlet-A	3.0105 eV	411.84 nm	f = 0.0013
229 ->266	-0.13527			

231 ->266	-0.15773			
233 ->266	0.11161			
235 ->266	-0.14628			
237 ->266	-0.11450			
242 ->265	0.14172			
245 ->266	0.29170			
247 ->266	0.17492			
248 ->266	-0.25498			
248 ->267	0.28893			
249 ->267	0.20279			
Excited State 135:	Singlet-A	3.0193 eV	410.64 nm	f = 0.0000
258 ->271	0.70587			
Excited State 136:	Singlet-A	3.0255 eV	409.79 nm	f = 0.0006
229 ->265	0.12832			
231 ->265	0.15085			
238 ->265	0.17306			
239 ->265	0.16505			
240 ->265	-0.21662			
241 ->265	-0.18120			
242 ->265	0.49521			
245 ->266	-0.11682			
Excited State 137:	Singlet-A	3.0270 eV	409.59 nm	f = 0.0001
261 ->275	0.52849			
262 ->275	-0.43360			
Excited State 138:	Singlet-A	3.0346 eV	408.57 nm	f = 0.0032
252 ->273	0.17179			
254 ->273	-0.25236			
255 ->273	0.13571			
261 ->273	-0.27170			
261 ->274	0.10799			
261 ->275	0.24020			
262 ->275	0.41754			
Excited State 139:	Singlet-A	3.0351 eV	408.51 nm	f = 0.0000
258 ->269	0.70442			
Excited State 140:	Singlet-A	3.0378 eV	408.14 nm	f = 0.0039
252 ->273	-0.15054			
254 ->273	0.23629			
255 ->273	-0.12906			
261 ->273	0.25405			
261 ->275	0.38709			
262 ->275	0.34898			
Excited State 141:	Singlet-A	3.0524 eV	406.18 nm	f = 0.0000
264 ->283	0.70685			
Excited State 142:	Singlet-A	3.0525 eV	406.17 nm	f = 0.0006
245 ->266	-0.10217			

247 ->266	0.65512			
248 ->266	0.11817			
Excited State 143:	Singlet-A	3.0534 eV	406.05 nm	f = 0.0000
259 ->270	0.22900			
260 ->270	0.66823			
Excited State 144:	Singlet-A	3.0693 eV	403.95 nm	f = 0.0000
259 ->272	0.22878			
260 ->272	0.66895			
Excited State 145:	Singlet-A	3.0726 eV	403.52 nm	f = 0.0000
250 ->267	0.69946			
Excited State 146:	Singlet-A	3.0820 eV	402.28 nm	f = 0.0020
239 ->268	0.27706			
242 ->268	-0.13807			
251 ->268	0.29968			
261 ->276	0.41830			
262 ->276	-0.27031			
Excited State 147:	Singlet-A	3.0836 eV	402.07 nm	f = 0.0009
239 ->268	0.27309			
242 ->268	-0.13665			
247 ->268	0.10109			
251 ->268	0.30722			
261 ->276	-0.30735			
262 ->276	0.38762			
Excited State 148:	Singlet-A	3.0916 eV	401.04 nm	f = 0.0014
261 ->276	0.46374			
262 ->276	0.51115			
Excited State 149:	Singlet-A	3.1097 eV	398.70 nm	f = 0.0001
246 ->266	0.69832			
Excited State 150:	Singlet-A	3.1213 eV	397.22 nm	f = 0.0106
249 ->271	-0.21435			
251 ->271	0.54801			
252 ->273	-0.11234			
255 ->271	-0.16079			
256 ->273	0.13016			
Excited State 151:	Singlet-A	3.1238 eV	396.91 nm	f = 0.0000
237 ->265	-0.14423			
238 ->265	-0.17596			
239 ->265	-0.20435			
240 ->265	0.30420			
241 ->265	0.38221			
242 ->265	0.38749			
Excited State 152:	Singlet-A	3.1241 eV	396.86 nm	f = 0.0000
258 ->270	0.70409			

Excited State 153:	Singlet-A	3.1354 eV	395.44 nm	f = 0.0002
229 ->265	-0.11227			
231 ->265	-0.10552			
235 ->265	-0.12820			
237 ->265	0.47924			
238 ->265	0.33067			
240 ->265	0.15470			
241 ->265	0.17820			
242 ->265	0.13586			
Excited State 154:	Singlet-A	3.1400 eV	394.85 nm	f = 0.0000
258 ->272	0.70419			
Excited State 155:	Singlet-A	3.1523 eV	393.31 nm	f = 0.0011
229 ->266	0.16302			
231 ->266	0.16305			
233 ->266	-0.10754			
235 ->266	0.14040			
241 ->266	0.12833			
242 ->266	-0.14504			
243 ->266	0.12761			
244 ->266	0.20565			
245 ->266	0.48503			
Excited State 156:	Singlet-A	3.1595 eV	392.42 nm	f = 0.0081
236 ->268	-0.10527			
239 ->268	-0.33543			
240 ->268	-0.11292			
241 ->268	-0.10651			
242 ->268	0.17498			
246 ->268	-0.11671			
249 ->268	-0.24807			
251 ->268	0.44836			
Excited State 157:	Singlet-A	3.1657 eV	391.65 nm	f = 0.0001
254 ->269	0.15183			
255 ->269	0.26839			
256 ->269	0.16267			
257 ->269	0.60195			
Excited State 158:	Singlet-A	3.1676 eV	391.41 nm	f = 0.0133
253 ->278	0.14923			
257 ->271	-0.10081			
259 ->274	0.17533			
259 ->278	-0.29180			
259 ->279	0.47921			
260 ->279	-0.16257			
Excited State 159:	Singlet-A	3.1711 eV	390.98 nm	f = 0.0006
256 ->271	0.15600			
257 ->271	0.66118			

Excited State 160:	Singlet-A	3.1724 eV	390.83 nm	f = 0.0003
237 ->265	-0.10548			
239 ->265	0.60452			
240 ->265	0.17460			
241 ->265	0.18033			
259 ->274	-0.13572			
Excited State 161:	Singlet-A	3.1724 eV	390.82 nm	f = 0.0009
239 ->265	0.16428			
259 ->273	0.32368			
259 ->274	0.52092			
260 ->273	-0.12593			
260 ->274	-0.18197			
Excited State 162:	Singlet-A	3.1847 eV	389.31 nm	f = 0.0009
259 ->273	0.50718			
259 ->274	-0.30305			
260 ->273	-0.31187			
260 ->274	0.15171			
Excited State 163:	Singlet-A	3.1930 eV	388.30 nm	f = 0.0000
259 ->273	0.32962			
259 ->274	-0.12513			
260 ->273	0.58257			
260 ->274	-0.18661			
Excited State 164:	Singlet-A	3.1959 eV	387.94 nm	f = 0.0000
255 ->269	0.11274			
256 ->269	0.65216			
257 ->269	-0.24038			
Excited State 165:	Singlet-A	3.2131 eV	385.87 nm	f = 0.0007
202 ->265	-0.10442			
210 ->265	0.12607			
211 ->265	0.10023			
214 ->265	0.21519			
215 ->265	0.23714			
217 ->265	0.41940			
220 ->265	0.19490			
239 ->265	0.12247			
244 ->272	0.10478			
Excited State 166:	Singlet-A	3.2133 eV	385.85 nm	f = 0.0000
264 ->284	0.70486			
Excited State 167:	Singlet-A	3.2197 eV	385.08 nm	f = 0.0000
254 ->269	0.29959			
255 ->269	0.51791			
256 ->269	-0.21513			
257 ->269	-0.25820			
Excited State 168:	Singlet-A	3.2279 eV	384.11 nm	f = 0.0003
239 ->268	-0.12563			

248 ->268	0.54338			
249 ->268	0.37427			
251 ->268	0.13717			
Excited State 169:	Singlet-A	3.2376 eV	382.95 nm	f = 0.0000
263 ->280	0.70673			
Excited State 170:	Singlet-A	3.2535 eV	381.07 nm	f = 0.0002
254 ->270	0.16009			
255 ->270	0.28270			
256 ->270	0.16493			
257 ->270	0.59612			
Excited State 171:	Singlet-A	3.2628 eV	379.99 nm	f = 0.0000
258 ->273	0.66994			
258 ->274	-0.22169			
Excited State 172:	Singlet-A	3.2642 eV	379.83 nm	f = 0.0000
259 ->274	0.22336			
260 ->273	0.20879			
260 ->274	0.63199			
Excited State 173:	Singlet-A	3.2669 eV	379.51 nm	f = 0.0000
245 ->267	0.65913			
259 ->275	0.11300			
Excited State 174:	Singlet-A	3.2686 eV	379.31 nm	f = 0.0112
252 ->271	-0.12986			
253 ->271	0.39876			
254 ->271	0.26281			
255 ->271	0.46588			
257 ->271	-0.11883			
Excited State 175:	Singlet-A	3.2690 eV	379.27 nm	f = 0.0003
254 ->272	0.15084			
255 ->272	0.26592			
256 ->272	0.15319			
257 ->272	0.54902			
259 ->275	0.23530			
Excited State 176:	Singlet-A	3.2691 eV	379.27 nm	f = 0.0001
245 ->267	-0.11400			
255 ->272	-0.10468			
257 ->272	-0.21595			
259 ->275	0.59816			
260 ->275	-0.21339			
Excited State 177:	Singlet-A	3.2829 eV	377.67 nm	f = 0.0001
243 ->266	-0.24044			
252 ->269	-0.20428			
253 ->269	0.54595			
254 ->269	-0.15208			
255 ->269	0.21766			

Excited State 178:	Singlet-A	3.2847 eV	377.46 nm	f = 0.0003
229 ->266	-0.10358			
231 ->266	-0.10860			
238 ->266	-0.13585			
243 ->266	0.51887			
244 ->266	0.20642			
253 ->269	0.23974			
256 ->270	0.17145			
Excited State 179:	Singlet-A	3.2854 eV	377.38 nm	f = 0.0000
243 ->266	-0.15966			
255 ->270	0.11556			
256 ->270	0.62107			
257 ->270	-0.23755			
Excited State 180:	Singlet-A	3.2907 eV	376.77 nm	f = 0.0000
250 ->268	0.69954			
Excited State 181:	Singlet-A	3.3006 eV	375.64 nm	f = 0.0001
255 ->272	0.12307			
256 ->272	0.64085			
257 ->272	-0.25785			
Excited State 182:	Singlet-A	3.3021 eV	375.47 nm	f = 0.0020
251 ->271	-0.14154			
252 ->271	-0.32162			
253 ->271	0.43021			
254 ->271	-0.28501			
255 ->271	-0.27917			
Excited State 183:	Singlet-A	3.3071 eV	374.91 nm	f = 0.0003
254 ->270	0.29568			
255 ->270	0.50798			
256 ->270	-0.23533			
257 ->270	-0.26313			
Excited State 184:	Singlet-A	3.3086 eV	374.73 nm	f = 0.0002
221 ->267	0.16602			
239 ->267	0.11048			
240 ->267	-0.11057			
241 ->267	-0.14019			
242 ->267	0.26611			
243 ->267	0.41670			
244 ->267	0.29135			
245 ->267	0.12440			
259 ->276	0.13984			
Excited State 185:	Singlet-A	3.3110 eV	374.46 nm	f = 0.0000
236 ->265	0.69362			
Excited State 186:	Singlet-A	3.3134 eV	374.19 nm	f = 0.0005
229 ->266	0.12101			

231 ->266	0.14452			
238 ->266	0.16704			
239 ->266	0.17510			
240 ->266	-0.23363			
241 ->266	-0.19153			
242 ->266	0.51649			
Excited State 187:	Singlet-A	3.3218 eV	373.25 nm	f = 0.0009
253 ->272	-0.10438			
254 ->272	0.29130			
255 ->272	0.49581			
256 ->272	-0.24053			
257 ->272	-0.26907			
Excited State 188:	Singlet-A	3.3237 eV	373.03 nm	f = 0.0000
263 ->281	0.70631			
Excited State 189:	Singlet-A	3.3249 eV	372.90 nm	f = 0.0000
259 ->276	0.63837			
260 ->276	-0.22797			
Excited State 190:	Singlet-A	3.3255 eV	372.83 nm	f = 0.0000
253 ->269	0.25739			
254 ->269	0.58787			
255 ->269	-0.28951			
Excited State 191:	Singlet-A	3.3296 eV	372.37 nm	f = 0.0001
264 ->285	0.70338			
Excited State 192:	Singlet-A	3.3349 eV	371.77 nm	f = 0.0000
258 ->273	0.22072			
258 ->274	0.66778			
Excited State 193:	Singlet-A	3.3452 eV	370.63 nm	f = 0.0000
261 ->277	0.18937			
262 ->277	0.67190			
Excited State 194:	Singlet-A	3.3505 eV	370.04 nm	f = 0.0004
229 ->265	-0.16019			
231 ->265	-0.17195			
232 ->265	0.16510			
233 ->265	0.15909			
235 ->265	0.54595			
238 ->265	0.14775			
Excited State 195:	Singlet-A	3.3558 eV	369.46 nm	f = 0.0022
249 ->273	-0.21133			
251 ->271	0.10367			
251 ->273	0.53263			
251 ->274	-0.18924			
254 ->273	-0.12407			
255 ->273	-0.11929			

Excited State 196:	Singlet-A	3.3576 eV	369.26 nm	f = 0.0000
259 ->275	0.23644			
260 ->275	0.66621			
Excited State 197:	Singlet-A	3.3704 eV	367.86 nm	f = 0.0003
252 ->270	-0.22380			
253 ->270	0.59599			
254 ->270	-0.15751			
255 ->270	0.22801			
Excited State 198:	Singlet-A	3.3713 eV	367.77 nm	f = 0.0001
261 ->277	0.66148			
262 ->277	-0.17952			
Excited State 199:	Singlet-A	3.3786 eV	366.96 nm	f = 0.0009
221 ->267	-0.19755			
243 ->267	0.24085			
244 ->267	0.16894			
248 ->274	-0.21234			
249 ->274	0.23220			
251 ->274	0.13436			
254 ->274	0.14054			
255 ->273	0.10139			
255 ->274	0.26370			
257 ->274	0.15211			
Excited State 200:	Singlet-A	3.3835 eV	366.44 nm	f = 0.0013
252 ->272	-0.21037			
253 ->272	0.55880			
253 ->278	0.11579			
254 ->272	-0.13885			
255 ->272	0.22087			

Orbital coefficients of atoms corresponding to Peak 1 in the absorption spectrum of 1

Peak 1: 238 → 265

			238 (HOMO-26)
24	S	1S	0.00646
		2S	0.02232
		3PX	-0.09526
		3PY	0.15244
		3PZ	-0.09779
		4PX	-0.10099
		4PY	0.15328
27	S	1S	0.02383
		2S	0.03833
		3PX	-0.10996
		3PY	-0.16137
		3PZ	0.01627
		4PX	-0.10975
		4PY	-0.15991
		4PZ	0.00753
28	S	1S	-0.01106
		2S	-0.02854
		3PX	0.15470
		3PY	0.07661
		3PZ	0.04172
		4PX	0.15678
		4PY	0.07756
		4PZ	0.03960

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			265 (LUMO)
3	W	1S	-0.00229
		2S	-0.00512
		3S	-0.03402
		4PX	-0.01411
		4PY	0.00778
		4PZ	-0.00066
		5PX	0.03073
		5PY	-0.00246
		5PZ	-0.00001
		6PX	-0.01790
		6PY	0.03209
		6PZ	-0.01576
		7D 0	-0.22854
		7D+1	0.24812
		7D-1	0.45121
		7D+2	0.35356
		7D-2	-0.29010
		8D 0	-0.09704
		8D+1	0.09779
		8D-1	0.18557
		8D+2	0.15361
		8D-2	-0.12214

24	S	1S	-0.00746
		2S	-0.01600
		3PX	-0.05506
		3PY	0.07259
		3PZ	-0.09378
		4PX	-0.08178
		4PY	0.10416
		4PZ	-0.14200
27	S	1S	-0.02179
		2S	-0.04104
		3PX	0.11190
		3PY	0.07422
		3PZ	-0.05897
		4PX	0.16148
		4PY	0.11181
		4PZ	-0.07468
28	S	1S	-0.00513
		2S	-0.00587
		3PX	-0.10447
		3PY	-0.01617
		3PZ	0.07036
		4PX	-0.15710
		4PY	-0.02301
		4PZ	0.10543
29	S	1S	-0.01729
		2S	-0.03520
		3PX	0.03132
		3PY	-0.09702
		3PZ	0.06931
		4PX	0.04874
		4PY	-0.15452
		4PZ	0.10369

……

Orbital coefficients of atoms corresponding to Peak 2 in the absorption spectrum of 1

Peak 2: 246 → 268

			246 (HOMO-18)
23	S	1S	0.00840
		2S	0.02404
		3PX	0.00226
		3PY	-0.03477
		3PZ	-0.21235
		4PX	0.00144
		4PY	-0.03713
		4PZ	-0.21432
25	S	1S	-0.01364
		2S	-0.02842
		3PX	-0.06054
		3PY	-0.20156
		3PZ	-0.03661
		4PX	-0.06794
		4PY	-0.20460
		4PZ	-0.03660
26	S	1S	0.00703
		2S	0.01308
		3PX	-0.02044
		3PY	0.02352
		3PZ	0.22933
		4PX	-0.02202
		4PY	0.02962
		4PZ	0.23336
30	S	1S	-0.01259
		2S	-0.02306
		3PX	0.03702
		3PY	0.21889
		3PZ	-0.00600
		4PX	0.03320
		4PY	0.22124
		4PZ	-0.00659
		……	

			268 (LUMO+3)
2	W	1S	-0.00634
		2S	-0.01798
		3S	-0.09348
		4PX	-0.00467
		4PY	0.01779
		4PZ	-0.03081
		5PX	0.01640
		5PY	-0.02824
		5PZ	0.02325
		6PX	0.04564
		6PY	-0.07851
		6PZ	0.10040

		7D 0	0.01840
		7D+1	0.09248
		7D-1	0.66961
		7D+2	-0.26299
		7D-2	0.02472
		8D 0	-0.00216
		8D+1	0.03002
		8D-1	0.29643
		8D+2	-0.10430
		8D-2	0.00049
23	S	1S	-0.01030
		2S	-0.01779
		3PX	-0.03910
		3PY	0.03832
		3PZ	0.12933
		4PX	-0.06121
		4PY	0.07211
		4PZ	0.19250
25	S	1S	0.00068
		2S	0.00959
		3PX	-0.02179
		3PY	-0.16246
		3PZ	-0.03894
		4PX	-0.02993
		4PY	-0.23821
		4PZ	-0.07082
26	S	1S	-0.03400
		2S	-0.06177
		3PX	-0.04754
		3PY	-0.00564
		3PZ	-0.14085
		4PX	-0.07443
		4PY	-0.02465
		4PZ	-0.22911
30	S	1S	-0.02277
		2S	-0.04642
		3PX	0.09692
		3PY	0.12287
		3PZ	0.02258
		4PX	0.14965
		4PY	0.20636
		4PZ	0.03717

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Ground-to-excited-state transition electric dipole moments (a.u.):

state	X	Y	Z	Osc.
1	0.0161	0.0085	0.0064	0.0000
2	-0.0198	-0.0107	-0.0076	0.0000
3	-0.0014	0.0096	0.0015	0.0000
4	0.0066	0.0035	0.0027	0.0000
5	0.0005	-0.0046	-0.0005	0.0000
6	0.0023	0.0022	0.0007	0.0000
7	-0.0088	-0.0102	-0.0118	0.0000
8	0.0030	-0.0121	-0.0020	0.0000
9	0.0215	0.0153	0.0183	0.0000
10	0.0381	0.0180	0.0374	0.0001
11	-0.0006	0.0006	-0.0005	0.0000
12	-0.0062	-0.0020	0.0007	0.0000
13	0.0049	-0.0056	-0.0083	0.0000
14	-0.0098	-0.0002	-0.0089	0.0000
15	-0.0032	-0.0017	-0.0014	0.0000
16	0.0013	0.0006	0.0014	0.0000
17	-0.0039	-0.0014	-0.0027	0.0000
18	-0.0032	-0.0023	-0.0015	0.0000
19	0.1070	-0.1870	0.0037	0.0022
20	-0.0398	0.0827	-0.0291	0.0004
21	-0.0094	-0.0065	-0.0045	0.0000
22	-0.0379	0.0133	-0.0204	0.0001
23	0.0617	0.0270	0.0444	0.0003
24	-0.0028	0.0057	0.0084	0.0000
25	0.0194	0.0082	0.0123	0.0000
26	0.0743	0.0352	0.0587	0.0005
27	-0.0106	-0.0043	-0.0041	0.0000
28	-0.0002	-0.0053	-0.0011	0.0000
29	-0.0448	0.0791	-0.0369	0.0005
30	0.0467	-0.1165	0.0280	0.0009
31	-0.0332	-0.0348	-0.0481	0.0002
32	0.0543	-0.0888	-0.0056	0.0006
33	-0.0043	0.0013	0.0048	0.0000
34	0.0044	0.0001	0.0016	0.0000
35	0.0023	-0.0005	0.0012	0.0000
36	0.0031	-0.0035	-0.0053	0.0000
37	0.0018	-0.0013	0.0024	0.0000
38	0.0107	-0.0206	-0.2162	0.0026
39	0.0035	0.0007	-0.0020	0.0000
40	-0.0016	-0.0006	-0.0021	0.0000
41	0.0169	0.0098	-0.0077	0.0000
42	0.0076	-0.0226	0.0123	0.0000
43	-0.0495	-0.0106	-0.0306	0.0002
44	0.0056	0.0025	0.0025	0.0000
45	0.0052	-0.0109	-0.0083	0.0000
46	0.0111	-0.0094	-0.0003	0.0000
47	-0.2519	0.2481	-0.0497	0.0073
48	0.0608	0.1267	-0.0639	0.0014
49	-0.1141	0.0259	-0.0404	0.0009
50	-0.0224	-0.0296	0.0519	0.0002
51	-0.0004	-0.1391	0.1269	0.0020

52	0.0340	-0.0236	0.0198	0.0001
53	0.1598	-0.1459	-0.0417	0.0029
54	-0.0756	-0.1871	0.0347	0.0025
55	-0.0004	0.0021	-0.0016	0.0000
56	0.0484	-0.0026	-0.1112	0.0009
57	-0.0229	-0.0008	-0.0084	0.0000
58	0.1698	-0.1818	-0.1277	0.0047
59	-0.0003	0.0005	0.0029	0.0000
60	0.0070	0.0144	0.0089	0.0000
61	-0.3646	-0.3105	-0.2725	0.0183
62	-0.2111	-0.1742	-0.1146	0.0053
63	0.0332	0.0165	0.0963	0.0006
64	-0.0094	0.0174	-0.0068	0.0000
65	0.0257	0.0907	0.0671	0.0008
66	0.1766	0.1119	0.0696	0.0030
67	-0.0004	0.0009	0.0013	0.0000
68	-0.0427	0.0138	-0.0376	0.0002
69	-0.0371	0.2876	0.0785	0.0057
70	-0.0459	-0.0525	0.1148	0.0011
71	0.0310	-0.1689	-0.0608	0.0021
72	0.1549	0.1227	0.1454	0.0038
73	0.1434	-0.0617	0.2781	0.0065
74	-0.0214	-0.1302	0.1401	0.0024
75	-0.0015	0.0058	0.0050	0.0000
76	-0.0283	0.0252	-0.2495	0.0041
77	-0.0261	0.0959	0.0418	0.0008
78	-0.0308	0.0139	-0.0015	0.0001
79	0.0005	-0.0164	-0.1313	0.0011
80	-0.0327	0.0638	0.0202	0.0004
81	0.0452	0.0054	0.0163	0.0002
82	-0.0069	0.0132	0.0050	0.0000
83	-0.0874	-0.0798	0.1000	0.0016
84	0.0018	0.0000	-0.0027	0.0000
85	0.0794	-0.1129	0.1107	0.0021
86	0.1222	0.1872	-0.2131	0.0063
87	0.0982	0.0722	0.0693	0.0013
88	0.2396	-0.2722	-0.0005	0.0088
89	-0.0129	-0.0314	-0.0174	0.0001
90	0.0319	0.0254	0.0112	0.0001
91	0.0739	0.0914	-0.0558	0.0011
92	-0.1750	0.0803	0.0079	0.0025
93	0.3426	-0.0726	0.0547	0.0085
94	-0.3188	-0.0276	0.0370	0.0070
95	0.2066	-0.1062	0.0445	0.0038
96	0.1043	-0.1166	0.1901	0.0041
97	-0.0050	0.0110	0.1624	0.0018
98	0.2678	0.3246	-0.2970	0.0180
99	0.1551	-0.1009	0.1440	0.0037
100	0.0474	0.1913	-0.0395	0.0028
101	0.2516	-0.1445	-0.0792	0.0062
102	-0.0021	-0.0067	-0.0021	0.0000
103	-0.0241	0.0278	-0.0091	0.0001
104	0.0763	0.0333	0.0020	0.0005

105	-0.1289	-0.3504	0.1849	0.0121
106	-0.1290	0.0883	-0.0731	0.0021
107	-0.0522	-0.3483	0.1715	0.0108
108	-0.1225	0.1285	-0.0665	0.0025
109	-0.0015	0.0397	-0.0605	0.0004
110	-0.4984	0.0210	0.0339	0.0176
111	-0.0817	-0.1132	0.0971	0.0020
112	-0.0079	0.0027	0.0066	0.0000
113	-0.3189	0.1284	0.2637	0.0133
114	0.1037	0.1117	0.0396	0.0018
115	0.0773	-0.2452	0.1039	0.0055
116	-0.0832	-0.0302	-0.0085	0.0006
117	0.1283	-0.0564	0.0347	0.0015
118	-0.0278	-0.0326	-0.0280	0.0002
119	0.0532	-0.0141	-0.0324	0.0003
120	-0.0138	-0.1186	0.0003	0.0010
121	-0.1441	-0.0084	0.1207	0.0025
122	0.0714	-0.0493	0.1465	0.0021
123	-0.0155	-0.0029	0.0323	0.0001
124	0.1351	-0.0336	0.0387	0.0015
125	0.3170	0.0369	0.0477	0.0075
126	0.0252	-0.0035	0.0057	0.0000
127	0.0018	0.0010	0.0010	0.0000
128	-0.1755	-0.1448	-0.1965	0.0066
129	-0.3641	-0.1293	-0.0055	0.0109
130	-0.0075	-0.0058	-0.0039	0.0000
131	-0.0154	-0.0658	-0.0128	0.0003
132	0.3850	0.0760	0.3713	0.0215
133	0.1288	0.0075	-0.0230	0.0013
134	-0.0817	0.0956	0.0356	0.0013
135	0.0012	0.0020	0.0206	0.0000
136	0.0861	0.0331	0.0060	0.0006
137	-0.0157	0.0049	0.0375	0.0001
138	-0.1599	-0.1295	0.0237	0.0032
139	-0.0032	-0.0003	-0.0001	0.0000
140	0.0539	0.2208	0.0182	0.0039
141	-0.0035	0.0108	0.0166	0.0000
142	0.0854	-0.0238	0.0016	0.0006
143	0.0057	-0.0017	0.0001	0.0000
144	-0.0033	-0.0020	-0.0027	0.0000
145	0.0014	0.0012	-0.0036	0.0000
146	0.0690	-0.1391	0.0488	0.0020
147	0.0820	-0.0593	0.0444	0.0009
148	-0.1044	0.0809	-0.0353	0.0014
149	0.0245	-0.0119	-0.0041	0.0001
150	-0.1556	0.1977	0.2750	0.0106
151	-0.0156	0.0098	-0.0074	0.0000
152	-0.0037	-0.0007	-0.0020	0.0000
153	0.0188	-0.0441	-0.0011	0.0002
154	0.0019	-0.0008	0.0005	0.0000
155	0.0999	-0.0641	-0.0194	0.0011
156	-0.1725	-0.1885	0.1992	0.0081
157	0.0379	-0.0128	-0.0130	0.0001

158	-0.2617	0.2740	0.1656	0.0133
159	0.0757	0.0223	-0.0296	0.0006
160	-0.0435	0.0354	0.0225	0.0003
161	0.0872	-0.0443	-0.0450	0.0009
162	-0.0728	0.0691	0.0329	0.0009
163	-0.0135	0.0102	0.0051	0.0000
164	0.0039	0.0012	-0.0024	0.0000
165	0.0863	-0.0356	-0.0197	0.0007
166	0.0031	-0.0011	-0.0016	0.0000
167	0.0110	0.0077	-0.0097	0.0000
168	0.0146	0.0306	-0.0501	0.0003
169	-0.0027	0.0080	0.0000	0.0000
170	0.0503	-0.0031	0.0139	0.0002
171	0.0038	0.0014	-0.0014	0.0000
172	0.0022	-0.0034	-0.0001	0.0000
173	-0.0077	0.0022	-0.0049	0.0000
174	0.3265	-0.0645	-0.1698	0.0112
175	-0.0419	-0.0123	-0.0397	0.0003
176	0.0134	0.0334	0.0027	0.0001
177	-0.0335	-0.0216	-0.0028	0.0001
178	0.0328	0.0359	0.0313	0.0003
179	0.0031	-0.0122	-0.0059	0.0000
180	0.0033	0.0094	-0.0037	0.0000
181	-0.0241	-0.0048	-0.0065	0.0001
182	0.1000	-0.0398	-0.1120	0.0020
183	0.0535	-0.0066	0.0148	0.0003
184	0.0350	-0.0145	0.0271	0.0002
185	-0.0107	0.0047	-0.0055	0.0000
186	-0.0642	-0.0336	-0.0380	0.0005
187	-0.0871	-0.0253	-0.0505	0.0009
188	0.0014	-0.0022	-0.0015	0.0000
189	-0.0072	-0.0084	-0.0030	0.0000
190	0.0040	-0.0004	0.0010	0.0000
191	0.0207	0.0248	0.0027	0.0001
192	0.0032	-0.0053	-0.0061	0.0000
193	0.0105	0.0029	0.0028	0.0000
194	-0.0623	0.0083	-0.0180	0.0004
195	-0.1063	-0.0748	-0.0985	0.0022
196	0.0011	0.0015	0.0007	0.0000
197	-0.0536	-0.0178	-0.0107	0.0003
198	-0.0074	-0.0314	-0.0095	0.0001
199	-0.0568	0.0505	0.0723	0.0009
200	0.0617	-0.1015	0.0436	0.0013