Electronic Supplementary Information

Dinuclear osmium complexes as mitochondrion-targeting antitumor photothermal agents in vivo

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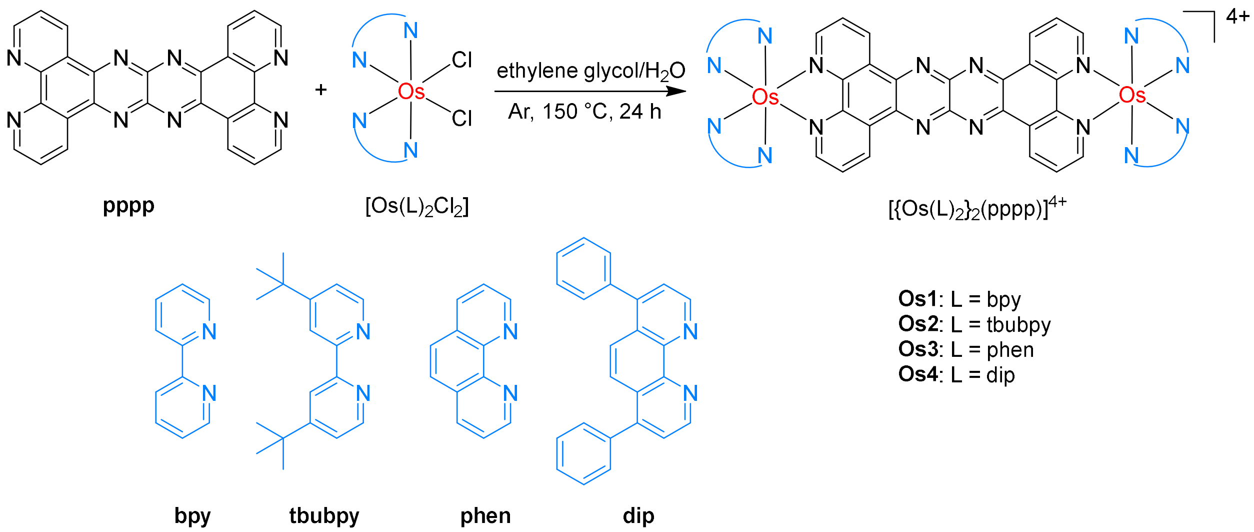
1. General

Instruments. ^1H NMR spectra were recorded on a Bruker Avance 300 spectrometer at 400 MHz. All chemical shifts are given relative to tetramethylsilane (TMS). Electron Spray ionization mass spectra (ESI-MS) were recorded on AB QSTAR Pulsar mass spectrometer. UV−Vis spectra were recorded on a Perkin-Elmer Lambda 365 spectrophotometer equipped with a temperature controller accessory and circulating water system. Fluorescence spectra were recorded on a Hitachi F-4700 fluorescence spectrophotometer. FT-IR spectra were recorded on a Nicolet iS 10 FTIR spectrometer.

Materials. The compounds 1,10-phenanthroline-5,6-dione and *cis*-[Os(L)$_2$Cl$_2$] (L = bpy, tbubpy, phen, dip, where bpy = 2,2'-bipyridine, tbubpy = 4,4'-di-*tert*-butyl-2,2'-bipyridine, phen = 1,10-phenanthroline, dip = 4,7-diphenyl-1,10-phenanthroline) were synthesized according to the literature methods.[1,2] The bridging ligand **pppp** ([1,10]phenanthrolino[5'',6'':5',6']pyrazino[2',3':5,6]pyrazino [2,3-*f*][1,10]phenanthroline) were prepared according a 6-step method previously designed by us.[3] Potassium phthalimide, 3,4-dichloro-1,2,5-thiadiazole, acetonitrile (MeCN) and methylamine hydrochloride were purchased from Adamas-beta. DMSO-d_6 were purchased from Energy Chemical. Alumina (200−300 mesh), ammonium hydroxide, tetrahydrofuran (THF), N,N-dimethylformamide (DMF), ethanol (EtOH), trichloromethane ($CHCl_3$), acetone and toluene were purchased from Greagent.



Scheme S1. Synthetic route to the dinuclear Os(II) complexes (DOCs).

2. Synthesis and Characterization

The ligand **pppp** (34 mg, 0.08 mmol) was stirred with *cis*-[Os(L)$_2$Cl$_2$] (0.17 mmol, 2.1 eq.), 1 mL water and 6 mL ethylene glycol under Ar at 150 °C for 24 h. The black solution was cooled to 20 °C and poured into water (20 mL). Upon addition of NH_4PF_6 (1 g, 6.2 mmol) in water (5 mL), the dinuclear Os(II) complexes precipitated as black solid, which was isolated by suction filtration, washed by small amount of water, EtOH and diethyl ether (3 × 10 mL), and dried in vacuo. The crude product was purified by flash column chromatography on alumina (200–300 mesh) with MeCN/Tol (1:2) as eluent.

Os1 (L = bpy): ^{1}H NMR (400 MHz, DMSO-d_6): 9.55 (d, J = 8.0 Hz, 4H), 8.91 (d, J = 8.0 Hz, 4H), 8.88 (d, J = 8.0 Hz, 4H), 8.30 (d, J = 4.0 Hz, 4H), 8.07 (t, J = 8.0 Hz, 4H), 8.01 (d, J = 8.0 Hz, 4H), 7.99 (t, J = 8.0 Hz, 4H), 7.76 (d, J = 8.0 Hz, 4H), 7.71 (d, J = 4.0 Hz, 4H), 7.54 (t, J = 4.0 Hz, 4H), 7.33 (t, J = 4.0 Hz, 4H); MS (ESI) calcd for $C_{66}H_{44}N_{16}Os_2$ [M–4PF$_6$]$^{4+}$: 360.5784; Found: 360.5747. FTIR (KBr) ν_{max} (cm^{-1}): 2963 (CH, aryl), 2924 (CH, aryl), 1631 (C=C, aryl), 1464 (C=C, aryl), 1424 (CH, aryl),1384 (CN, pyridyl), 1357 (CN, pyridyl), 1312 (CN, pyridyl), 1161 (CN, pyrazine), 1118 (CN, pyrazine), 845 (PF), 765 (C=C, aryl), 725 (C=C, aryl), 558 (PF).

Os2 (L = tbubpy): ^{1}H NMR (400 MHz, DMSO-d_6): 9.51 (d, J = 8.0 Hz, 4H), 8.89 (d, J = 12.0 Hz, 8H), 8.25 (d, J = 8.0 Hz, 4H), 8.01 (t, J = 8.0 Hz, 4H), 7.57 (s, 8H), 7.56 (d, J = 4.0 Hz, 4H), 7.32 (d, J = 8.0 Hz, 4H), 1.44 (s, 36H), 1.36 (s, 36H); MS (ESI) calcd for $C_{98}H_{107}N_{16}Os_2$ [M–H–4PF$_6$]$^{4+}$: 472.7024; Found: 472.7000. FTIR (KBr) ν_{max} (cm^{-1}): 2964 (CH, aryl), 2925 (CH, aryl), 1618 (C=C, aryl), 1481 (C=C, aryl), 1417 (CH, aryl), 1384 (CN, pyridyl), 1160 (CN, pyridyl), 1116 (CN, imidazolyl), 839 (PF), 719, (C=C, aryl), 558 (PF).

Os3 (L = phen): ^{1}H NMR (400 MHz, DMSO-d_6): 9.51 (d, J = 8.0 Hz, 4H), 8.62 (d, J = 8.0 Hz, 4H), 8.60 (d, J = 8.0 Hz, 4H), 8.43 (s, 8H), 8.23 (d, J = 8.0 Hz, 8H), 7.99 (d, J = 4.0 Hz, 4H), 7.88 (dd, J = 8.0, 4.0 Hz, 4H), 7.79 (dd, J = 8.0, 4.0 Hz, 4H), 7.74 (dd, J = 8.0, 4.0 Hz, 4H); MS (ESI) calcd for $C_{74}H_{44}N_{16}Os_2$ [M–4PF$_6$]$^{4+}$: 384.5784; Found: 384.5742. FTIR (KBr) ν_{max} (cm^{-1}): 2962 (CH, aryl), 2925 (CH, aryl),1618 (C=C, aryl), 1481 (C=C, aryl),1417 (CH, aryl), 1384 (CN, pyridyl), 1356 (CN, pyridyl), 1313 (CN, pyridyl), 1160 (CN, pyrazine), 1116 (CN, pyrazine), 840 (PF), 719 (C=C, aryl), 558 (PF).

Os4 (L = dip): ^{1}H NMR (400 MHz, DMSO-d_6): 9.59 (d, J = 8.0 Hz, 4H), 8.40 (d, J = 4.0 Hz, 4H), 8.36 (d, J = 4.0 Hz, 4H), 8.32 (s, 8H), 8.27 (d, J = 4.0 Hz, 4H), 8.00 (t, J = 4.0 Hz, 4H), 7.79 (d, J = 4.0 Hz, 8H), 7.68 (dd, 24H). 7.65 (s, 8H), 7.62 (m, 8H); MS (ESI) calcd for $C_{122}H_{75}N_{16}Os_2$ [M–H–4PF$_6$]$^{4+}$: 536.6398; Found: 536.6368. FTIR (KBr) ν_{max} (cm^{-1}): 2925 (CH, aryl), 2854 (CH, aryl), 1629 (C=C, aryl), 1384 (CN, pyridyl) ,1117 (CN, imidazolyl), 839 (PF), 703 (C=C, aryl), 558 (PF).

For spectra, please see "**6. ^{1}H NMR, Mass, and FT-IR Spectra of DOCs Os1–4**" (page 34–38).

3. Experimental Procedures

1) DFT Calculations.

The density functional theory (DFT) calculations were carried out with the Gaussian16 quantum chemistry program package.[4] MN15,[5] a Kohn–Sham global-hybrid exchange-correlation density functional with simultaneous accuracy for photochemistry application, was selected because the theoretical data calculated by this functional were much closer to the experimental data than the other tested density functions, such as Becke's three-parameter hybrid functional (B3LYP), CAM-B3LYP,[6] global-hybrid meta-GGA (generalized gradient approximation) M06,[7] and MN15-L.[8] For the same reason, Lanl2DZ basis set (a double-zeta basis set containing effective core potential) for all atoms was selected from a number of benchmarks, including SDD (Stuttgart/Dresden effective core potential) for all atoms, def2TZVP (Coulomb-fitting basis set) for all atoms, Lanl2DZ for Os/6-31G(d) for the others, Lanl2DZ for Os/6-311G(d,p) for the others, SDD for Os/6-31G(d) for the others, and SDD for Os/6-311G(d,p) for the others. The benchmark data is available to specialists in theoretical calculation upon request. DFT-D3 dispersion correction[9] containing Becke-Johnson (BJ) damping[10] was used in all calculations to improve accuracy. The full geometry optimization was carried out for the DOCs in aqueous solution, using the conductor polarized continuum model (CPCM)[11]. The stability of the optimized conformation of the DOCs was confirmed by the frequency analysis, which shows no imaginary frequency for each energy minimum. For absorption spectral calculations, 80 lowest singlet excited states (ESs) were calculated using the analytical time-dependent DFT (TDDFT) theory to reproduce the experimental spectra. The discrete optical transitions with their corresponding oscillator strength were broadened by a Gaussian function with the full width at half maxima (FWHM) of 2200 cm^{-1} to represent an experimental inhomogeneous spectral broadening. For fluorescence emission spectral calculations, the lowest singlet excited states (S1) were structurally optimized for the lowest 5 states and the theoretical spectra were generated as described for absorption spectra above. The structures of the excited triplet states were also optimized to reveal their transition properties. A compact representation of an ES *via* photoexcited hole–electron pair, which fits for chemical intuition, can be obtained using natural transition orbital (NTO) analysis.[12] By performing NTO calculations, a hole–electron pair transition from a ground state to an ES could be realized through unitary transformation of transition density matrix. NTO pairs contributing to the most important optical transitions were visualized for plotting excited charge densities (isovalue = 0.02).

2) Electrochemistry.

Cyclic voltammetry (CV) measurements were performed with a CH Instruments 840D electrochemical workstation. Samples were dissolved in MeCN (water ≤ 30 ppm by Karl Fischer) with 0.1 M tetrabutylammonium hexafluorophosphate ($TBAPF_6$) as a supporting electrolyte and the ferrocenium/ferrocene couple (Fc^+/Fc) used as an internal standard. A 3 mm diameter platinum-plate working electrode, a $Ag^+/AgCl$ (0.1 M $AgNO_3$ in MeCN) reference electrode, and a platinum-wire counter electrode were used. All potentials are reported relative to Fc^+/Fc.

3) DNA-binding Experiments.

Calf thymus DNA (CT-DNA) was obtained from the Sigma Company. The preparation of DNA stock solution, determination of the DNA concentration and DNA-binding experiments of the DOCs, including absorption spectral titration, calculation of instinct binding constants, and thermal denaturation studies, were performed as described previously.[13]

4) Topoisomerase Inhibition Assay.

DNA Topoisomerase I (TopoI) was purchased from Invitrogen. The reaction mixture (20 μL) contained 50 mM Tris HCl (pH 7.5), 50 mM KCl, 10 mM $MgCl_2$, 0.5 mM DTT (dithiothreitol), 0.1 mM EDTA, 30 μg/mL BSA, 0.1 μg pBR322 DNA, 2 Unit of Topo, and different concentrations of DOC. The reaction mixtures were incubated for 30 min at 37°C. The samples were electrophoresed through 1% agarose gel (Sangon) in TBE at 90 V for 30 min. The gel was stained with 4S Red Plus Nucleic Acid Stain (Sangon), photographed and quantified on a FluorChem FC3 imaging system (ProteinSimple). The concentrations of DOC that prevented 50% of the supercoiled DNA from being converted into relaxed DNA (IC_{50}) were calculated by the midpoint concentration for DOC-induced DNA unwinding.

5) Singlet Oxygen Generation.

Singlet oxygen ($^1O_2$) generation in air-saturated water was examined by monitoring the photo-oxidation of 9,10-anthracenediyl-bis(methylene)dimalonic acid (ABDA) induced by the DOCs at specific time intervals, under irradiation by 450, 520 and 600 nm light emitting diode (LED) array and 808 nm low-power laser (LPL) with external air-cooling devices. In air-saturated water, the absorbance of ABDA was adjusted to 0.4 at 378 nm, while the absorbance of DOCs was adjusted to 0.1 at 400 nm. The irradiances of LED array light sources were measured by an optical power meter (PM100D, Thorlabs) equipped with a thermal power sensor (S425C, Thorlabs), using the standard 5-point method, and unified to 50 mW cm^{-2} by adjusting the distance between light source and sample. The power of

808 nm LPL was modified by a tunable controller, until the output irradiance reached 0.1 W cm^{-2}, as indicated by the optical power meter. ABDA without DOCs and ABDA with $[Os(bpy)_3]^{2+}$ (**Os0**) were tested as controls.

6) Photothermal Effect Measurement.

The temperature changes of **Os1−4** aqueous solution (1 mL) at different concentrations under 450, 520 and 600 nm LED (50 mW cm^{-2}) and 808 nm LPL (100 mW cm^{-2}) irradiation were monitored using an IR camera for living body (HIKvision). The photothermal conversion efficiencies (η) of DOCs were calculated.[14]

7) Two-photon Absorption Cross-section (TPACS) Measurement

TPACSs of **Os4** (100 μM) in dry THF (water ≤ 30 ppm by Karl Fischer) were measured by the well-established method involving two-photon-induced fluorescence.[15] Two-photon photoluminescence spectra were recorded on a SpectroPro300i instrument, and the pump laser beam came from a Ti:sapphire laser system (pulse duration, 200 fs; repetition rate, 76 MHz; Coherent Mira900-D).

8) Oil and Water Distribution Coefficient (Lipophilicity).

Aqueous solution of DOC (5 mL, 10 μM) was mixed thoroughly with *n*-octanol (5 mL) in a 15 mL centrifuge tube. The tube was wrapped in aluminum foil, shaken for 24 h in an incubator equipped with a thermostatic shaker, and allowed to settle until the two phases were fully separated. The oil and water distribution coefficient (log $P_{o/w}$) was calculated using the relative concentrations of DOC in the two phases.[16]

9) Cell Line and Culture Conditions.

Human malignant melanoma A375 cell lines (STR authentication, Animal Research and Resource Center, Yunnan University) were cultured in Roswell Park Memorial Institute 1640 medium (RPMI 1640, Adamas Life) supplemented with 10% (v/v) fetal bovine serum (FBS, Gibco BRL) at 37 °C in a CO_2 incubator with a humidified atmosphere (95% air and 5% CO_2). The tumor cells were routinely sub-cultured twice per week by trypsin-EDTA treatment. The cells in an exponential growth phase were harvested and counted for tumor inoculation.[3]

10) Subcellular Colocalization Studied by Confocal Laser Scanning Microscope.

A375 cells were grown on 8-Chamber Glass Slides (Thermo Fisher Scientific) at a density of 6×10^4 cell mL^{-1} and incubated for 1 h with the DOCs at 2.5 μM. The cells were washed with PBS (pH 7.4) twice. Nuclei and mitochondria were counterstained with Hoechst33342 (Invitrogen) and MitoTracker Green (MTG, Invitrogen), respectively. Fluorescence images were collected on a Leica TCS SP8 DIVE two-photon CLSM at three detection channels and processed by LAS X (Leica) software.[3]

11) ICP-MS assay.

Exponentially growing A375 cells were harvested, and the resulting single-cell suspension was plated into 100 mm tissue culture plates (Adamas) in 1×10^5 cells per plate. After 24 h at 37 °C, the cells were incubated with 5 μM **Os4** for 2 h at 37 °C in either medium with serum or medium without serum. The cells were rinsed with PBS, detached with trypsin, counted and divided into three portions: (1) in portion 1, the nuclei were extracted using a nucleus extraction kit (Thermo); (2) in portion 2, the cytoplasm was extracted using a cytoplasm extraction kit (Thermo); (3) in portion 3, the mitochondria were extracted using a mitochondrial extraction kit (Thermo). All extraction procedures followed the manufacturer's protocols. The samples were digested with 60% HNO_3 at room temperature for one day. Each sample was diluted with water to obtain 2% HNO_3 sample solutions. The osmium content was measured using PlasmaQuant PQ9000 inductively coupled plasma mass spectrometry (ICP-MS) using $(NH_4)_2OsCl_6$ (99.99% trace metals basis, Sigma) as standard.

12) In vitro Cell Viability Test (CCK-8 assay).

The cell viability was determined by the CCK-8 assay. Exponentially growing cells (1×10^5 cells per well) were seeded in 96-well plates, followed by a 24-hour incubation for attachment. Cells were incubated with different concentrations of DOCs or cisplatin. For phototoxicity studies, after 12 h of incubation, supernatant was replaced with fresh culture medium and cells were subjected to irradiation by the 808 nm LPL (100 mW cm^{-2}, light dose = 30.0 J cm^{-2}), and incubated for an additional 48 h. Cells without irradiation were replaced with fresh culture medium and maintained in the dark. Then 10 uL of CCK-8 (Adamas Life) working solution was added and incubated for 1 h. Absorbance at 450 nm was measured on an iMark (Bio-rad) microplate reader, before and after CCK-8 incubation. Data were reported as the mean ± standard deviation (n = 3). IC_{50} values were determined by plotting the percentage of viability versus concentration on a logarithmic graph.[3]

13) Flow Cytometry Analysis.

Cell apoptosis was measured by Annexin V-FITC (fluorescein isothiocyanate) and propidium iodide (PI) based on the manufacturer's manual (Beyotime). DOC-treated human melanoma cells A375 at a density of 1×10^5 cell mL^{-1} in 1 mL of RPMI 1640 medium containing 10% FBS and 1×10^3 units penicillin/streptomycin were incubated at 37 °C (5% CO_2) for 2 h. The DOC-containing medium were replaced with fresh DOC-free medium. Cells were irradiated by the 808 nm LPL, or away from the light, for 5 min at room temperature, stained with Annexin V-FITC and PI, and immediately examined with a BD FACSCalibur flow cytometer.[17]

14) In vivo photothermal therapy (PTT).

All animal experiments were reviewed and approved by the Institutional Animal Care and Use Committee (IACUC) at Yunnan University, Kunming, China (Approval No: YNU20220269). BALB/c female nude mice aged 6−8 weeks (body weight 18−20 g) were purchased from GemPharmatech. The mice were kept in individually ventilated cage (IVC) systems at constant temperature (20−26 ºC) and humidity (40−70%) with five animals in each cage. Each mouse was inoculated subcutaneously at the posterior right flank region with A375 tumor cells (5×10^6) in 0.1 ml of PBS for tumor development. The drug treatments were started when the mean tumor size reached 66 mm^3. The mice were randomly allocated into four groups (5 mice for each group): group 1, PBS injection only; group 2, PBS injection and subsequent irradiation with 808 nm laser (100 mW cm^{-2}, light dose = 30.0 J cm^{-2}); group 3, **Os4** (20 μL, 10 μM) injection only; group 4, **Os4** (20 μL, 10 μM) injection and subsequent irradiation with 808 nm laser (100 mW cm^{-2}, light dose = 30.0 J cm^{-2}). The temperature changes and photothermal imaging of tumor sites were monitored using an IR camera for living body (Hikvision). The body weight and tumor volume data were recorded every 2 or 3 days in the therapeutic regimen. Tumor volumes were expressed in mm^3 using the formula: $V = 0.5\, a \times b^2$, where a and b are the long and short diameters of the tumor, respectively. Tumor weight was measured at study termination. The entire procedure of dosing, as well as tumor and bodyweight measurement, were conducted in a Laminar Flow Cabinet. The relative tumor volume is calculated by V/V_0 (V is the tumor volume on the day when data were recorded, V_0 is the tumor volume on the day when treatment was started). After 14 days of therapy, the mice were sacrificed, and the tumors and primary organs (heart, lung, kidney, spleen, liver, intestine and brain) were obtained for histological analysis by hematoxylin-eosin (H&E) staining.[3]

4. Supplementary Figures

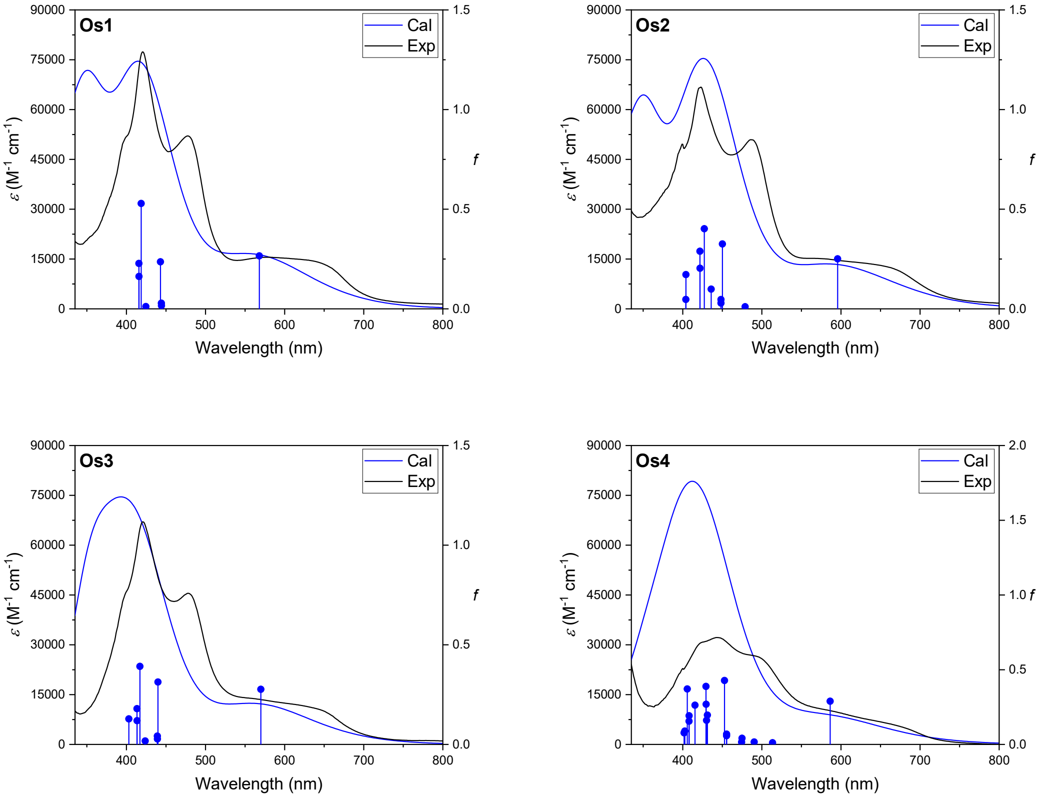


Fig. S1. Calculated (Cal, by Mn15/Lanl2dz/CPCM method) and experimental (Exp) UV-Vis absorption spectra and oscillator strengths (blue spikes) of **Os1**−**4**.

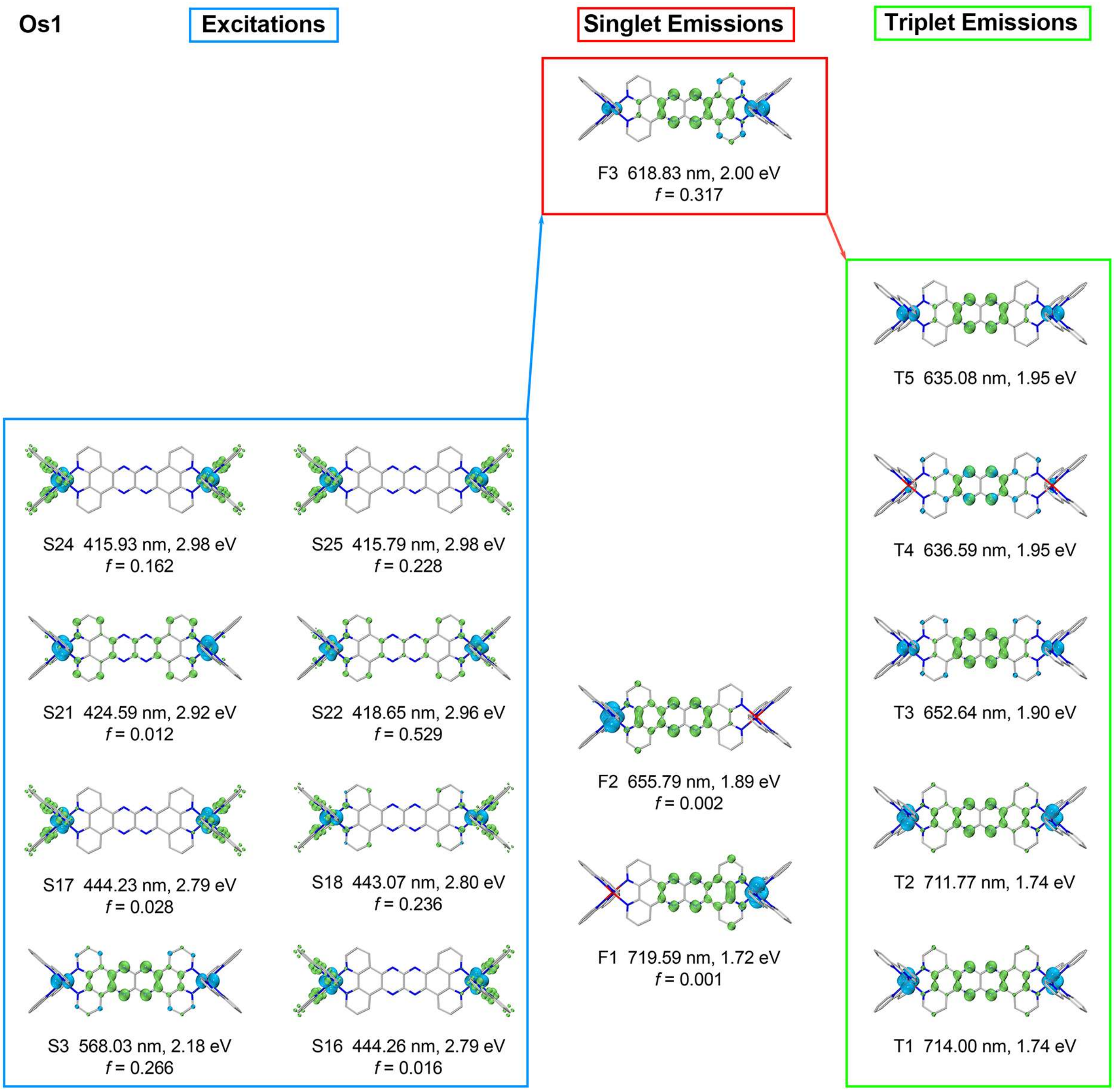


Fig. S2. Real space representation of hole (blue) and electron (green) distributions of **Os1** for ground, excited singlet and triplet states. Excitation wavelength (nm), excitation energy (eV), and oscillator strength (*f*) for each hole-to-electron transition are presented.

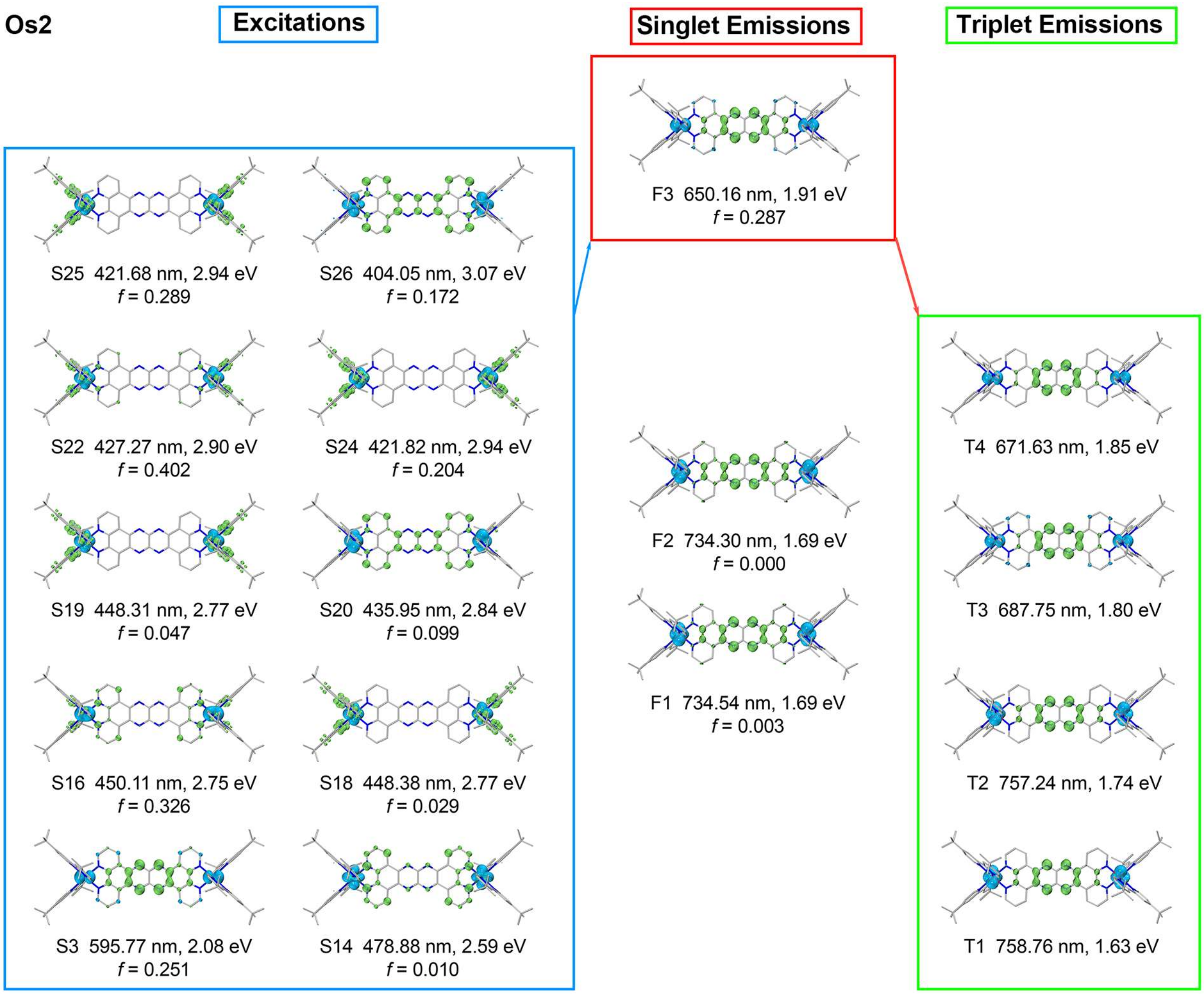


Fig. S3. Real space representation of hole (blue) and electron (green) distributions of **Os2** for ground, excited singlet and triplet states. Excitation wavelength (nm), excitation energy (eV), and oscillator strength (*f*) for each hole-to-electron transition are presented.

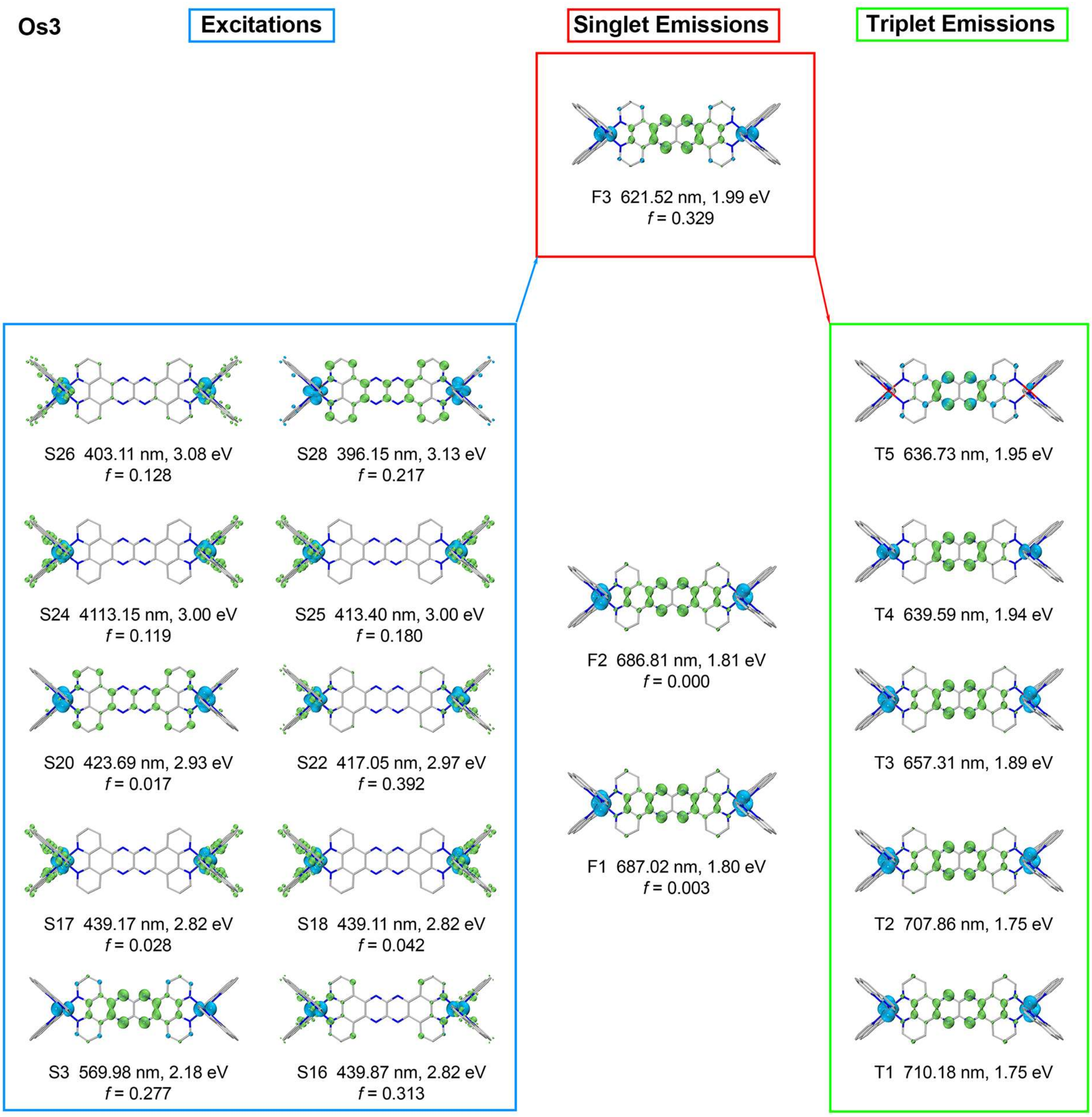


Fig. S4. Real space representation of hole (blue) and electron (green) distributions of **Os3** for ground, excited singlet and triplet states. Excitation wavelength (nm), excitation energy (eV), and oscillator strength (*f*) for each hole-to-electron transition are presented.

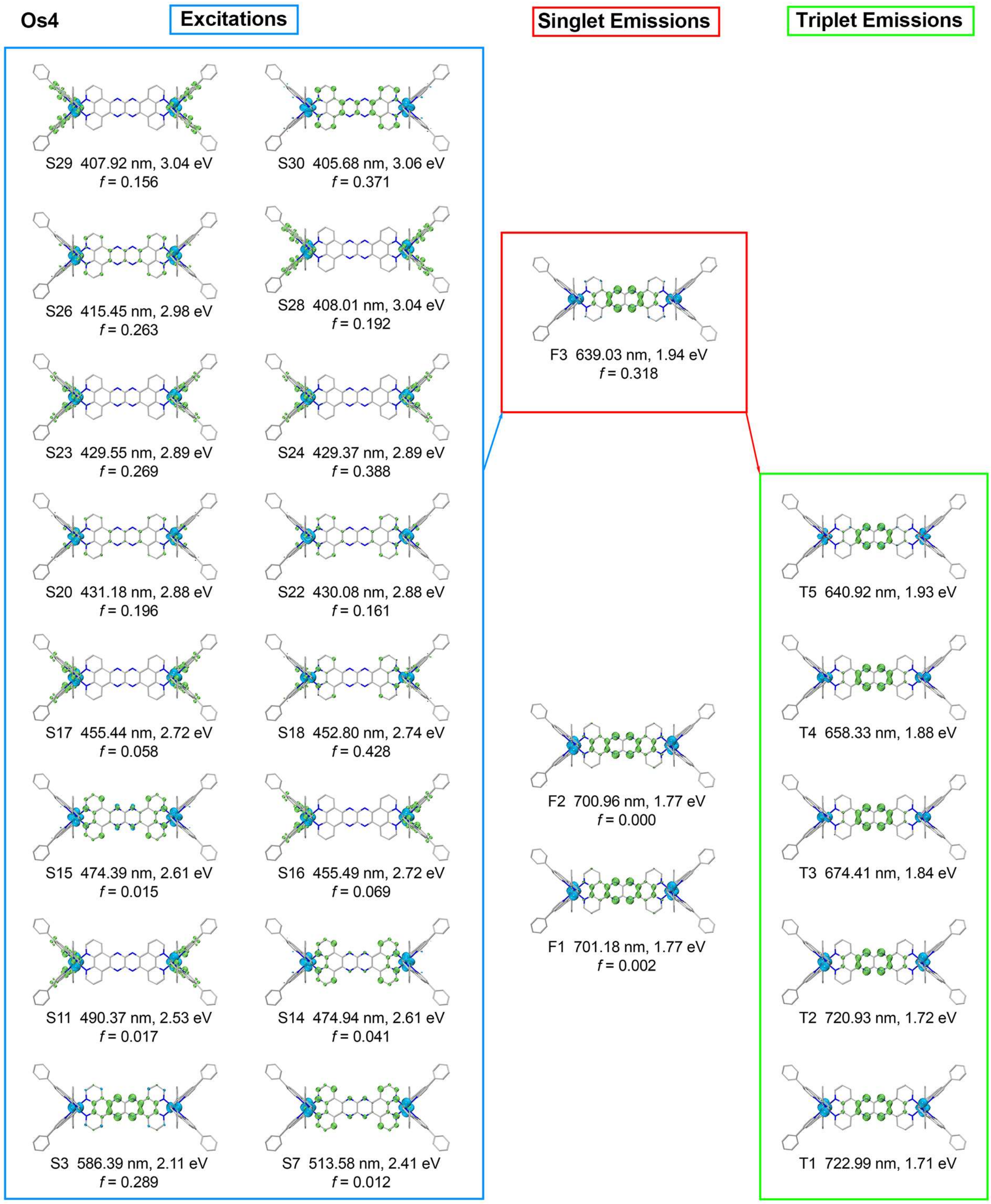


Fig. S5. Real space representation of hole (blue) and electron (green) distributions of **Os4** for ground, excited singlet and triplet states. Excitation wavelength (nm), excitation energy (eV), and oscillator strength (*f*) for each hole-to-electron transition are presented.

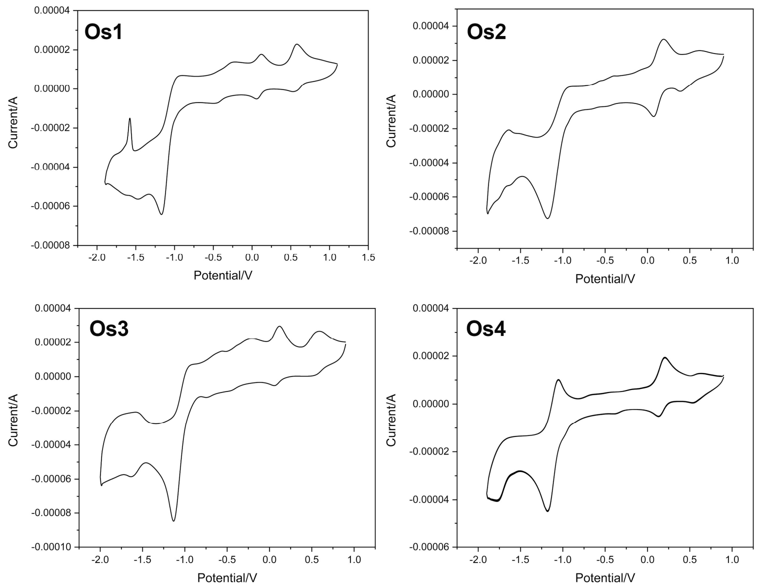


Fig. S6. Cyclic voltammetry of DOCs **Os1–4** in argon-saturated MeCN with ferrocenium/ferrocene couple (Fc^+/Fc) used as an internal reference.

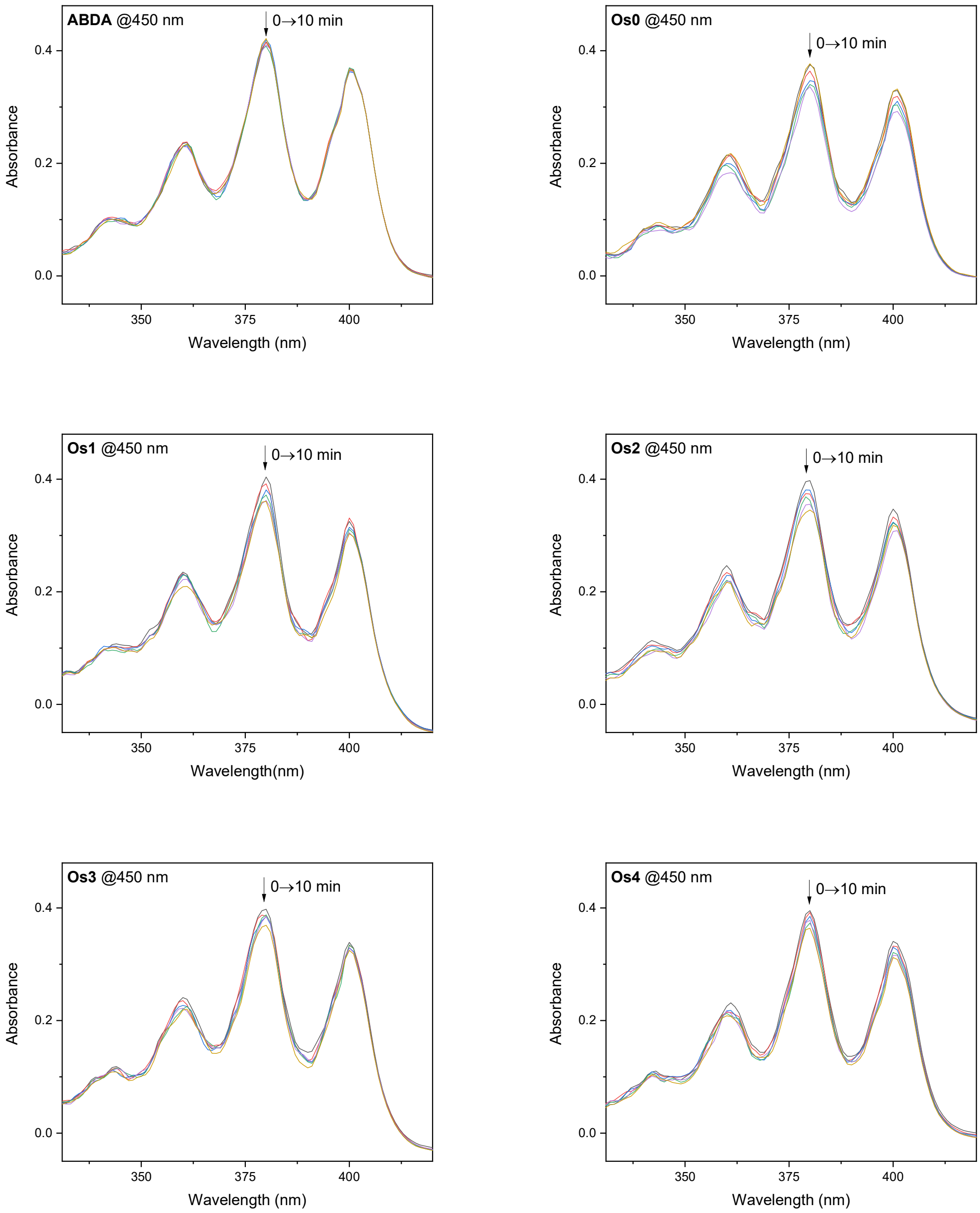


Fig. S7. Absorption spectral changes of ABDA in aqueous solution upon 450 nm LED (50 mW cm^{-2}) irradiation in the absence and presence of DOCs **Os1−4** and $[Os(bpy)_3]^{2+}$ (**Os0**).

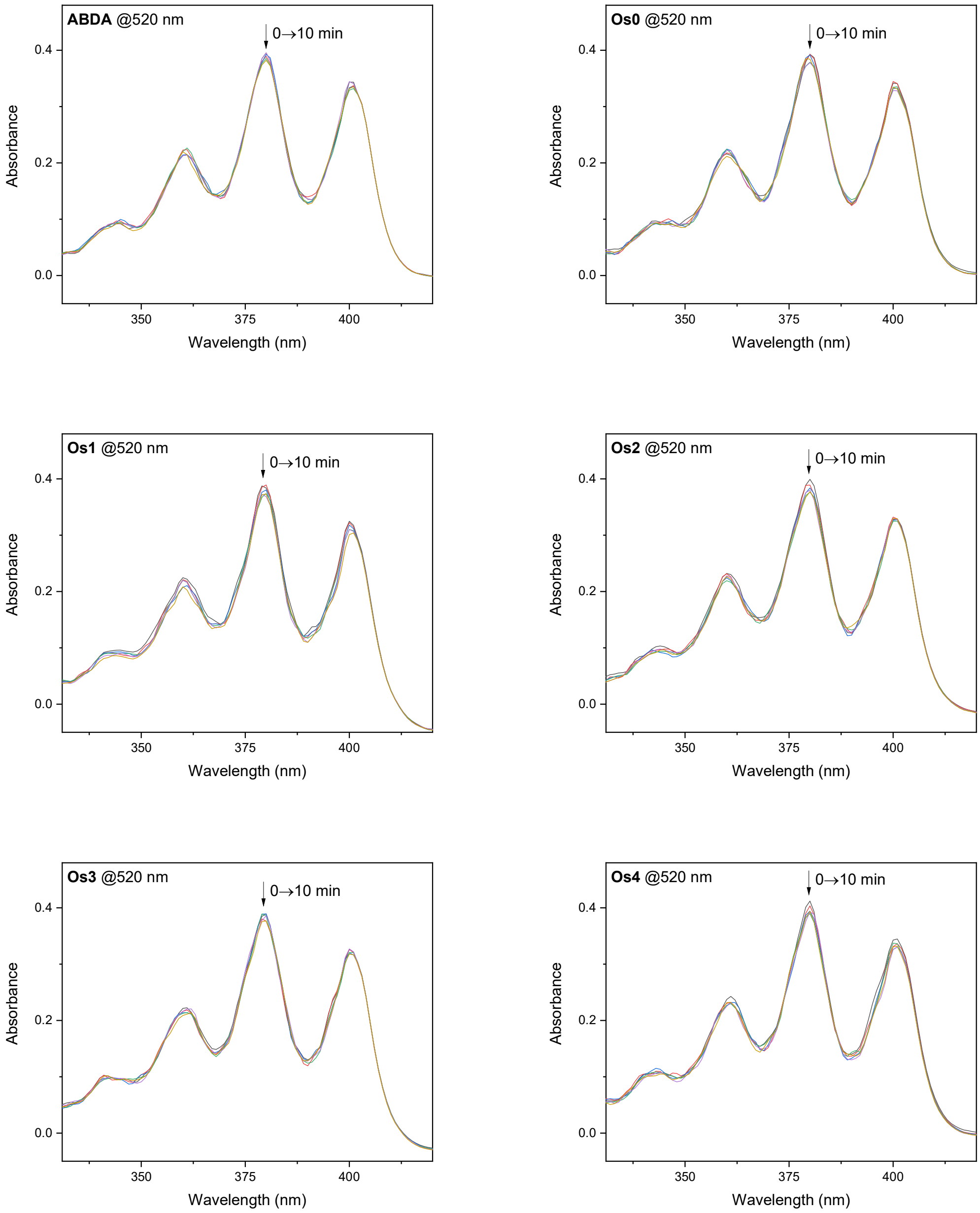


Fig. S8. Absorption spectral changes of ABDA in aqueous solution upon 520 nm LED (50 mW cm^{-2}) irradiation in the absence and presence of DOCs **Os1−4** and $[Os(bpy)_3]^{2+}$ (**Os0**).

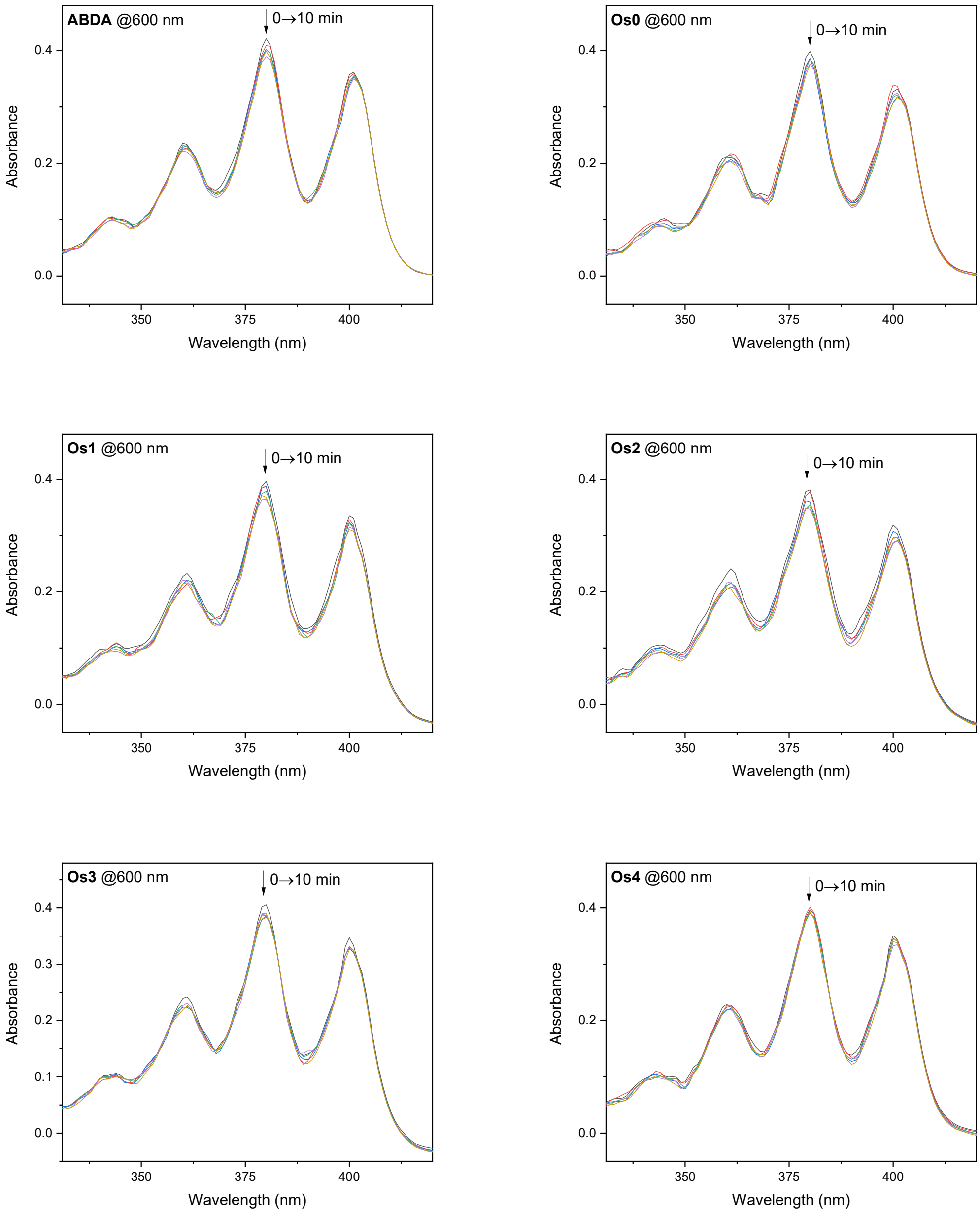


Fig. S9. Absorption spectral changes of ABDA in aqueous solution upon 600 nm LED (50 mW cm^{-2}) irradiation in the absence and presence of DOCs **Os1−4** and $[Os(bpy)_3]^{2+}$ (**Os0**).

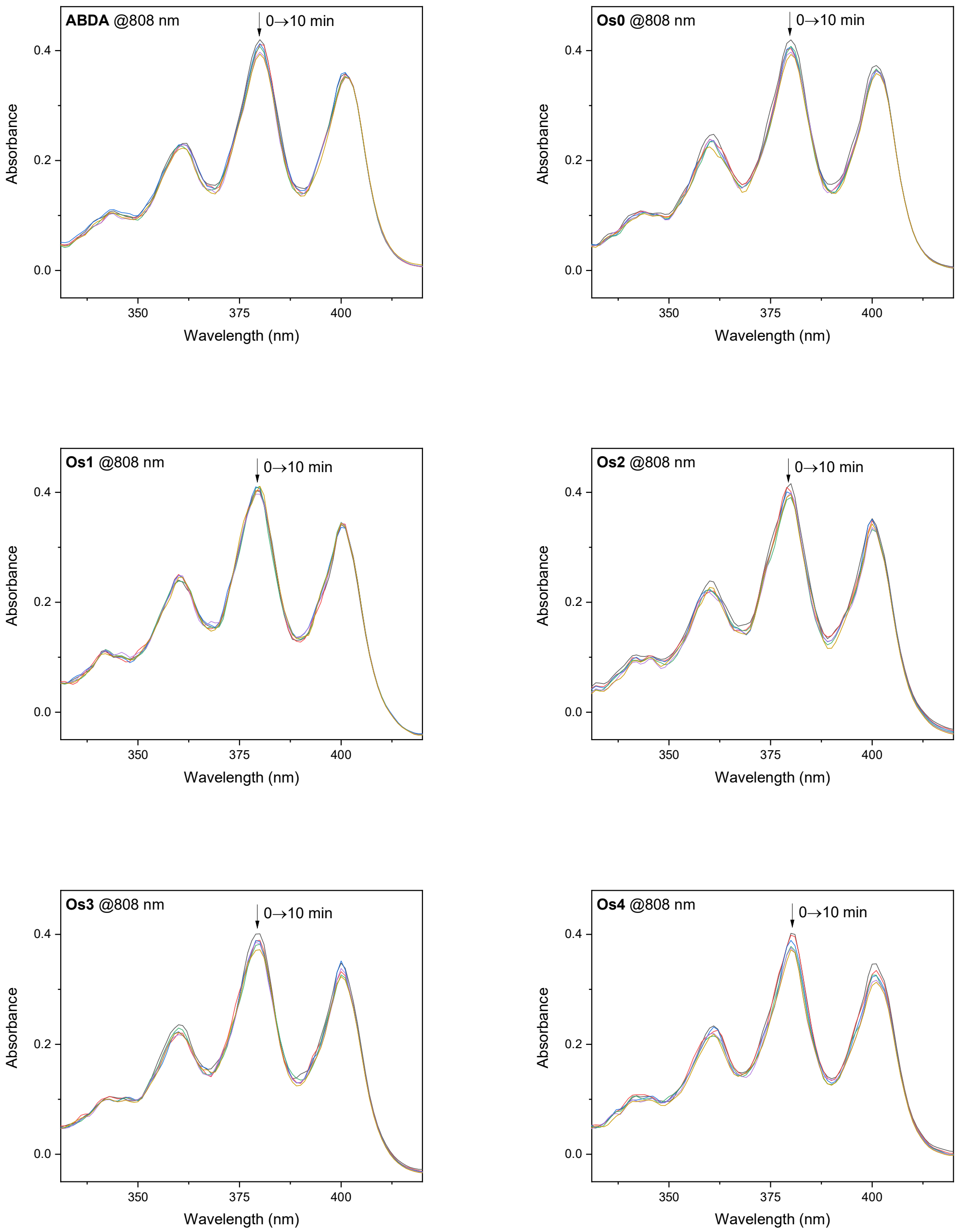


Fig. S10. Absorption spectral changes of ABDA in aqueous solution upon 808 nm LPL (100 mW cm^{-2}) irradiation in the absence and presence of DOCs **Os1−4** and $[Os(bpy)_3]^{2+}$ (**Os0**).

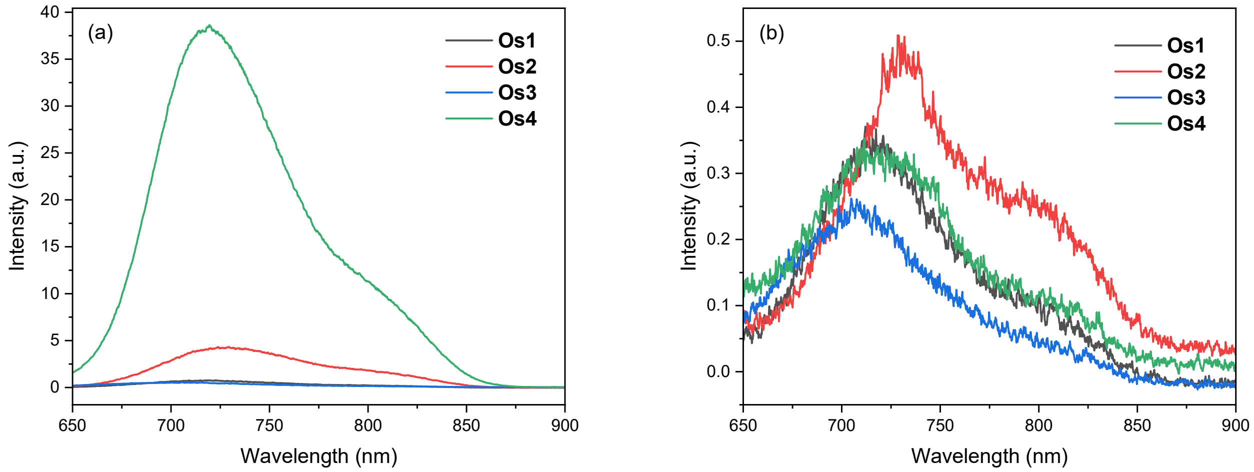


Fig. S11. Emission spectra of **Os1−4** (10 μM) in acetonitrile (a) and aqueous (b) solution.

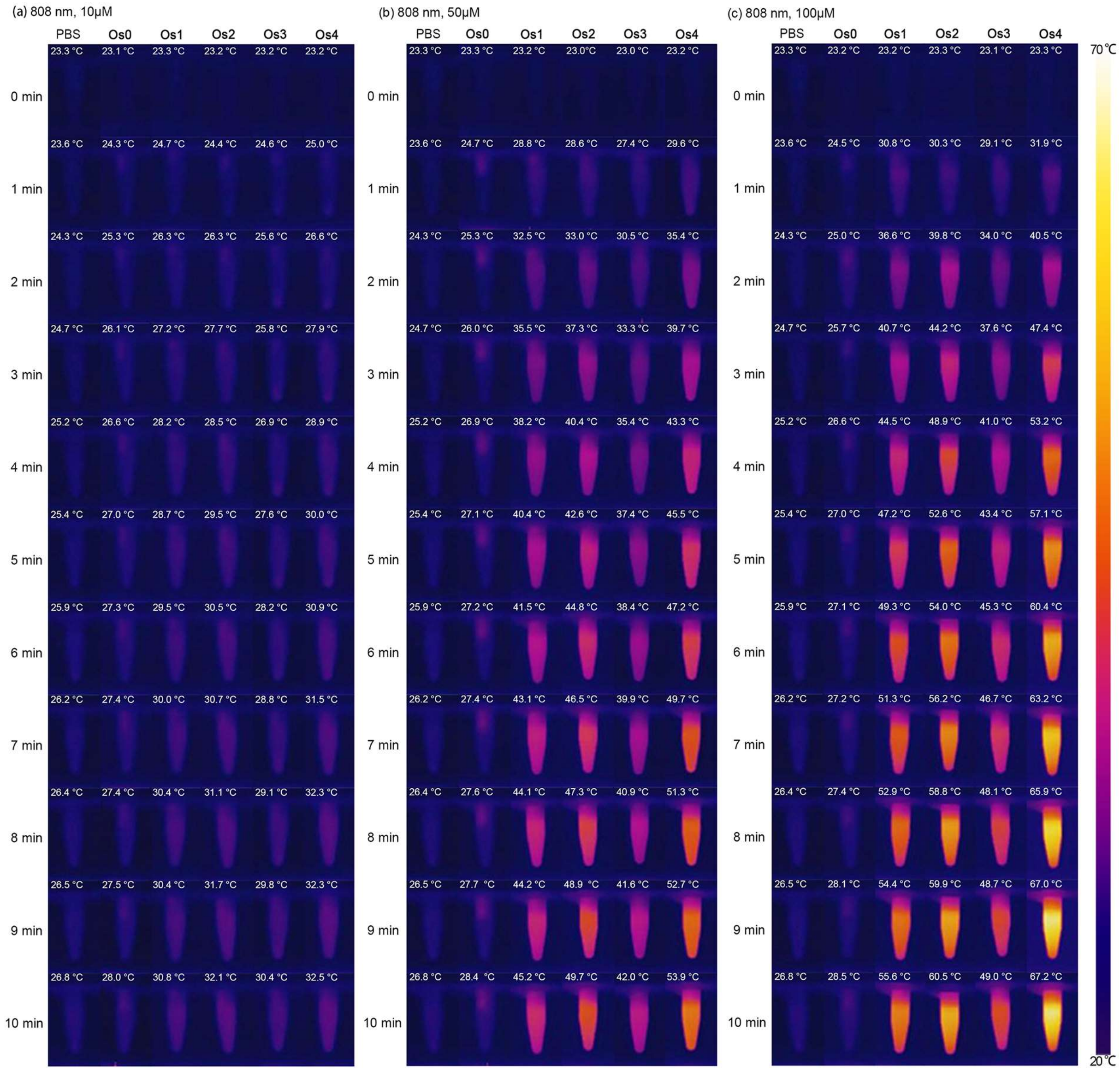


Fig. S12. Thermal images of PBS, **Os1−4** and $[Os(bpy)_3]^{2+}$ (**Os0**) at different concentrations in aqueous solution upon 808 nm LPL (100 mW cm^{-2}) irradiation for 10 min at 1 min intervals. (a) 10 μM; (b) 50 μM; (c) 100 μM.

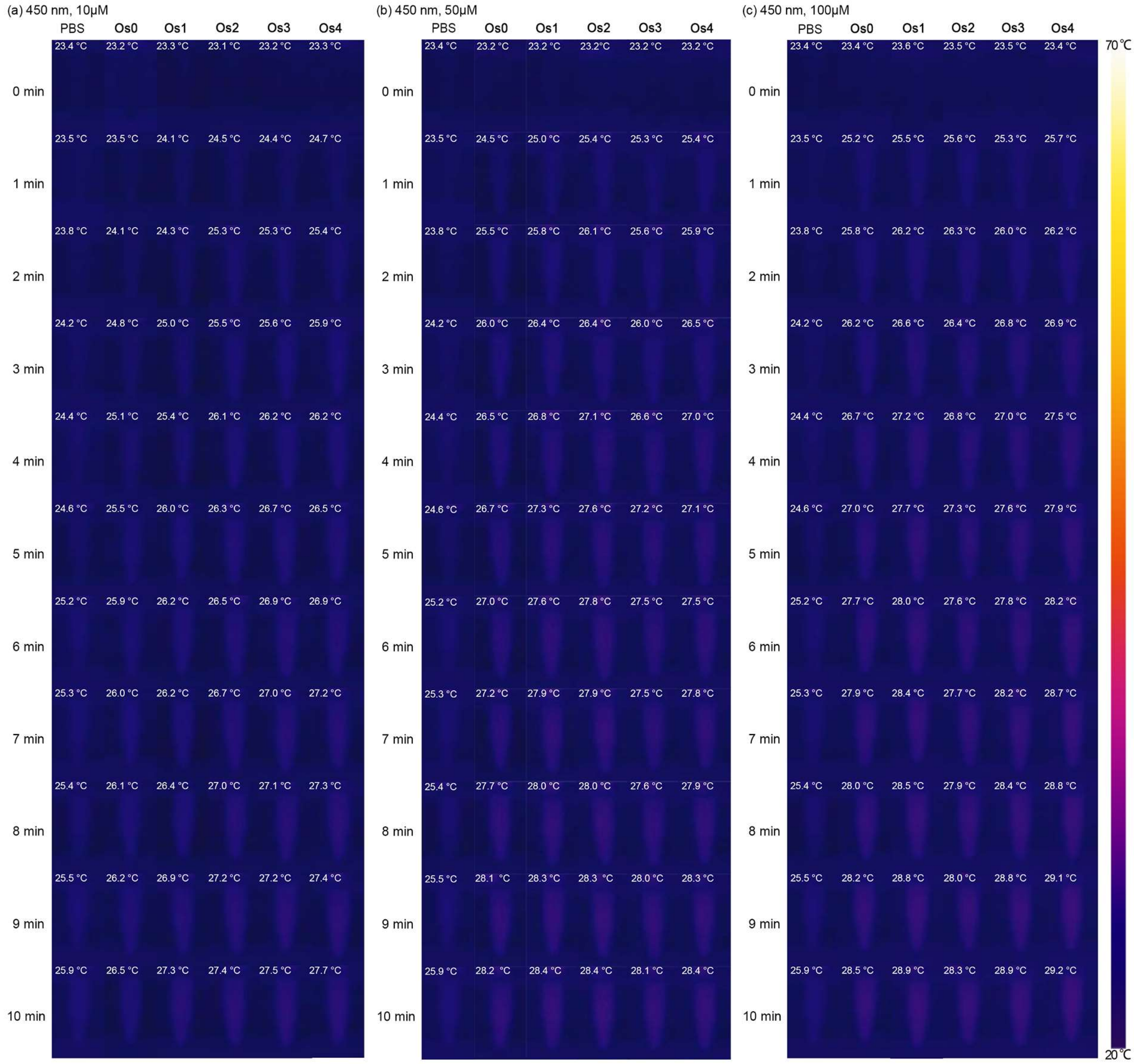


Fig. S13. Thermal images of PBS, **Os1−4** and $[Os(bpy)_3]^{2+}$ (**Os0**) at different concentrations in aqueous solution upon 450 nm LED (50 mW cm^{-2}) irradiation for 10 min at 1 min intervals. (a) 10 μM; (b) 50 μM; (c) 100 μM.

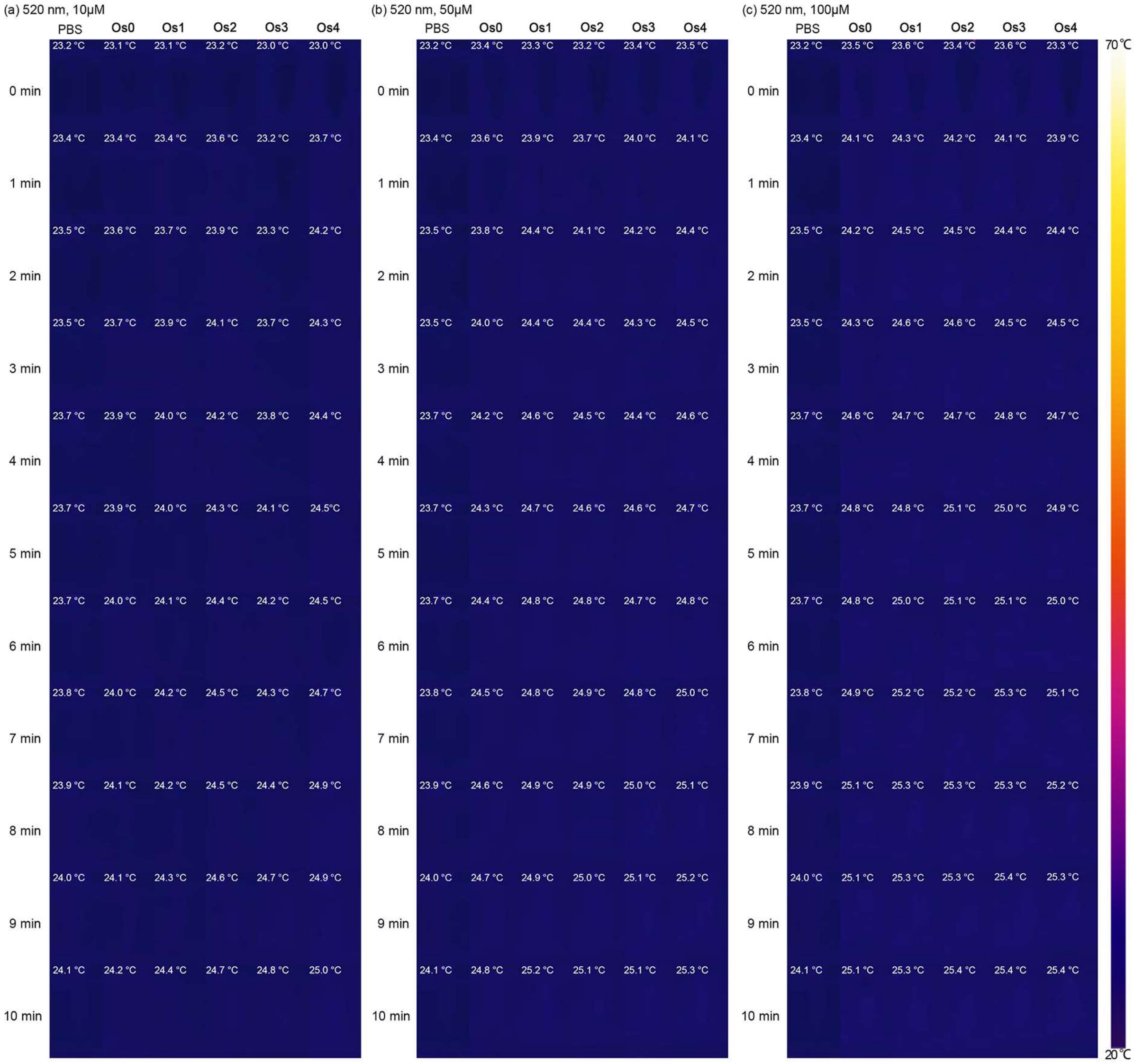


Fig. S14. Thermal images of PBS, **Os1−4** and $[Os(bpy)_3]^{2+}$ (**Os0**) at different concentrations in aqueous solution upon 520 nm LED (50 mW cm^{-2}) irradiation for 10 min at 1 min intervals. (a) 10 μM; (b) 50 μM; (c) 100 μM.

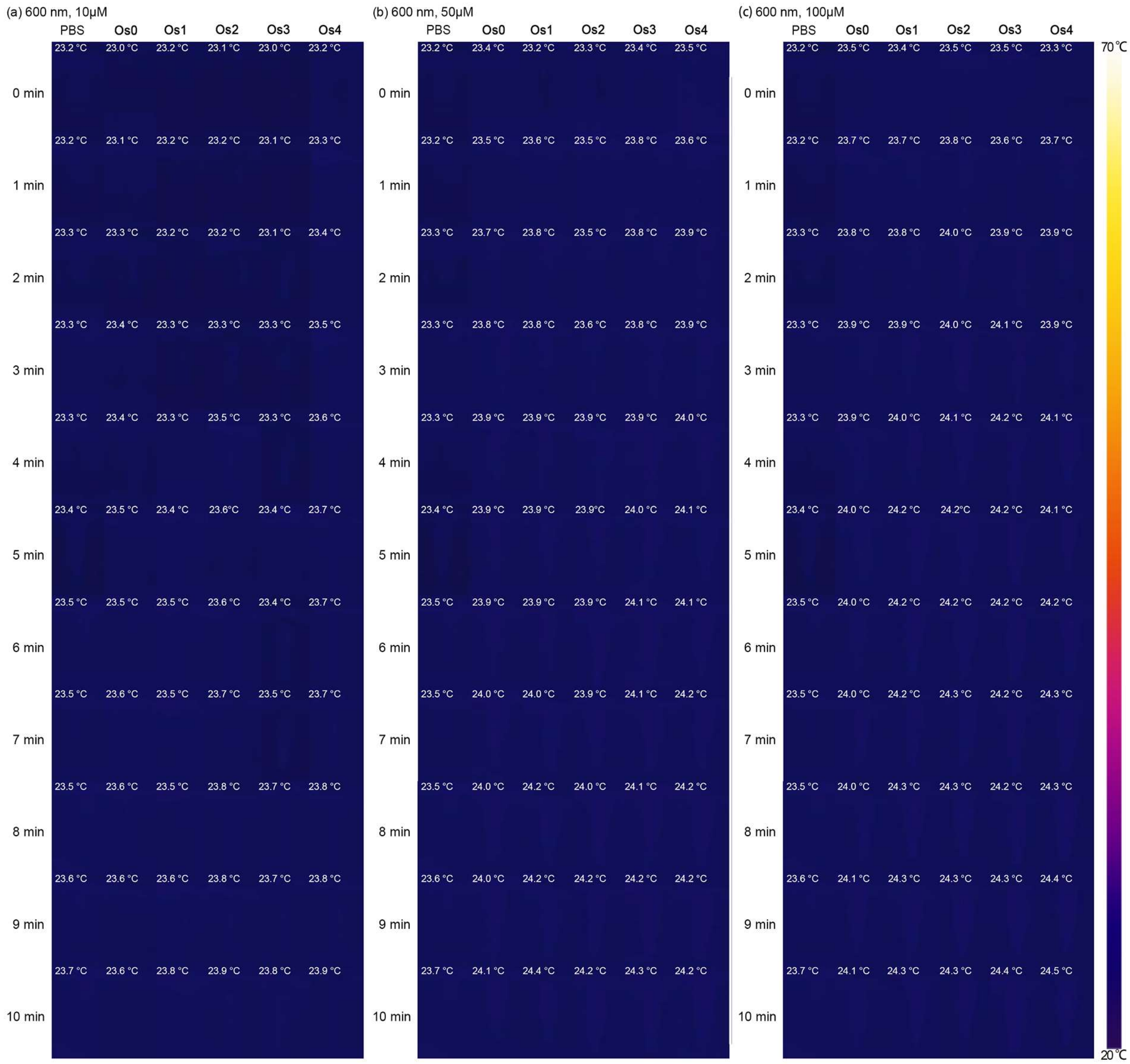


Fig. S15. Thermal images of PBS, **Os1−4** and $[Os(bpy)_3]^{2+}$ (**Os0**) at different concentrations in aqueous solution upon 600 nm LED (50 mW cm^{-2}) irradiation for 10 min at 1 min intervals. (a) 10 μM; (b) 50 μM; (c) 100 μM.

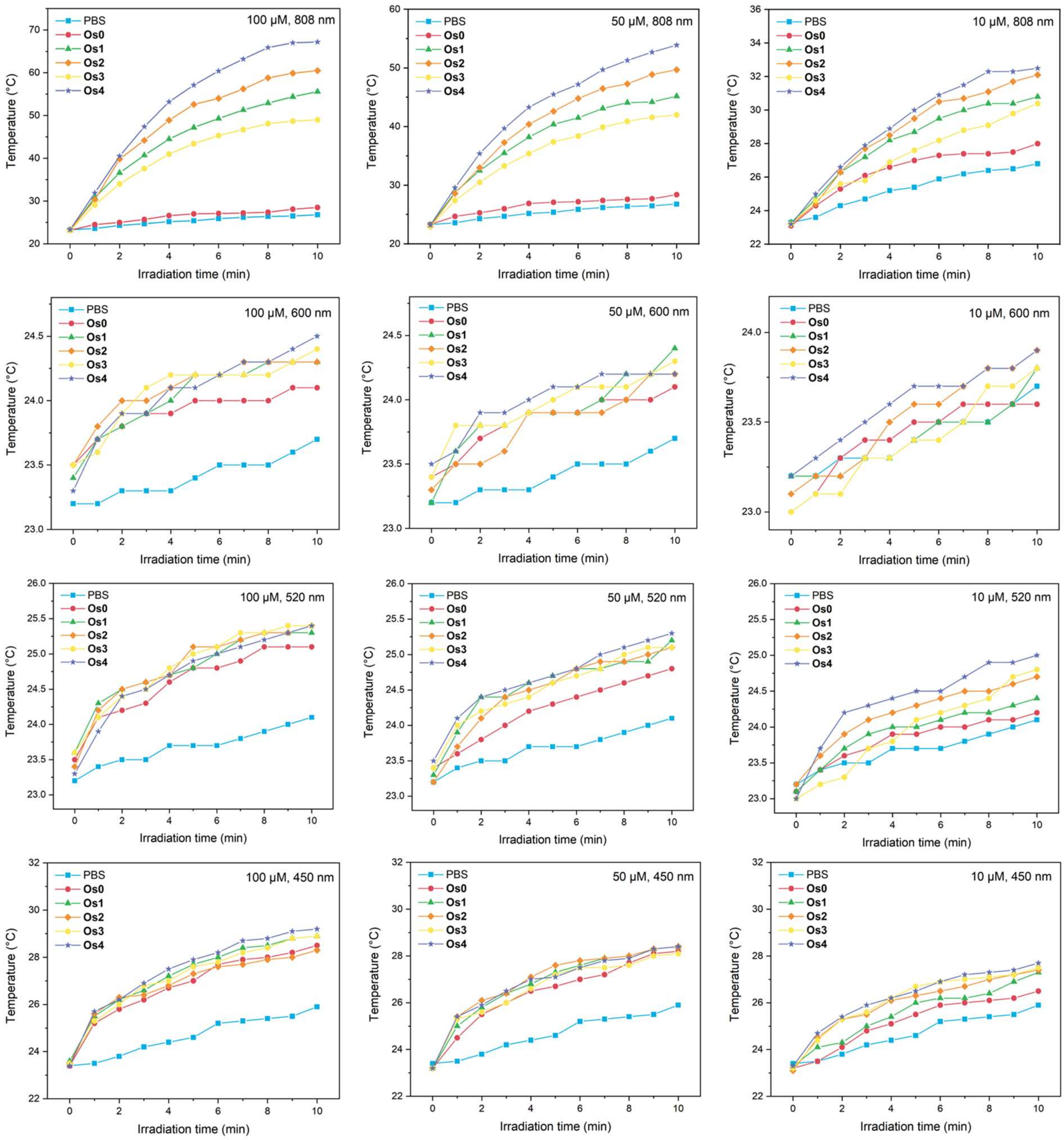


Fig. S16. The temperature-rising curves of PBS, **Os1**−**4** and $[Os(bpy)_3]^{2+}$ (**Os0**) aqueous solution (100 μM, 50 μM, and 10 μM) upon irradiation of 450, 520, and 600 nm LED (50 mW cm^{-2}) and 808 nm LPL (100 mW cm^{-2}) for 10 min at 1 min intervals.

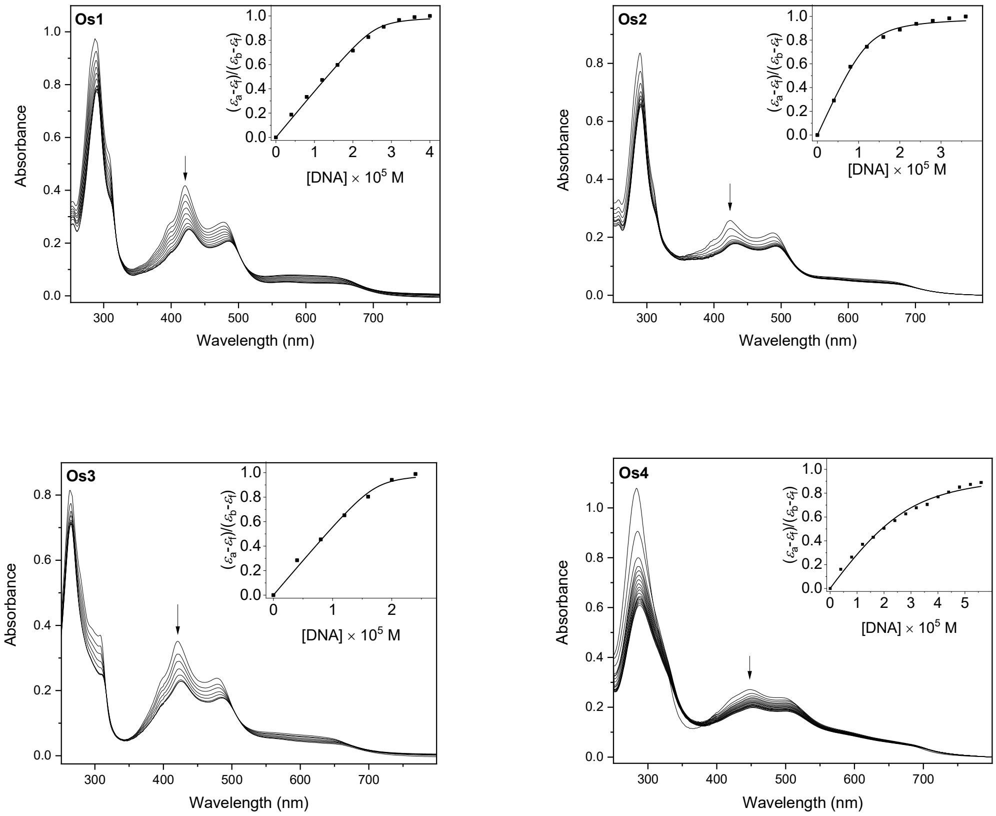


Fig. S17. Absorption spectra of **Os1−4** in 5 mM Tris–HCl and 50 mM NaCl buffer (pH 7.0) in the presence of increasing amounts of CT-DNA. Insets show the nonlinear fitting by which the binding constants K_b were calculated. The binding sizes s for **Os1−4** are 1.25 ± 0.03, 2.03 ± 0.11, 1.66 ± 0.07, and 2.71 ± 0.14, respectively.

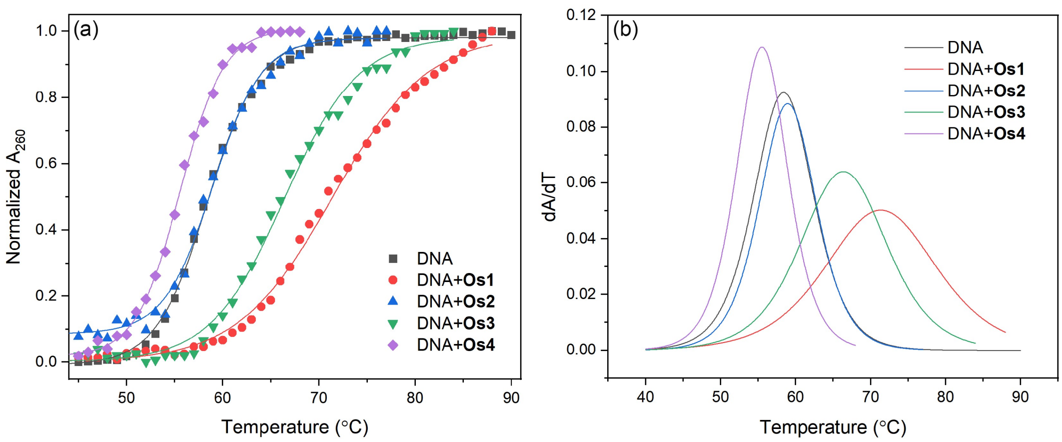


Fig. S18. The melting curves of CT-DNA (100 μM) at 260 nm in the absence and the presence of **Os1−4** (10 μM) in PBS (a) and first derivative of melting curves (b).

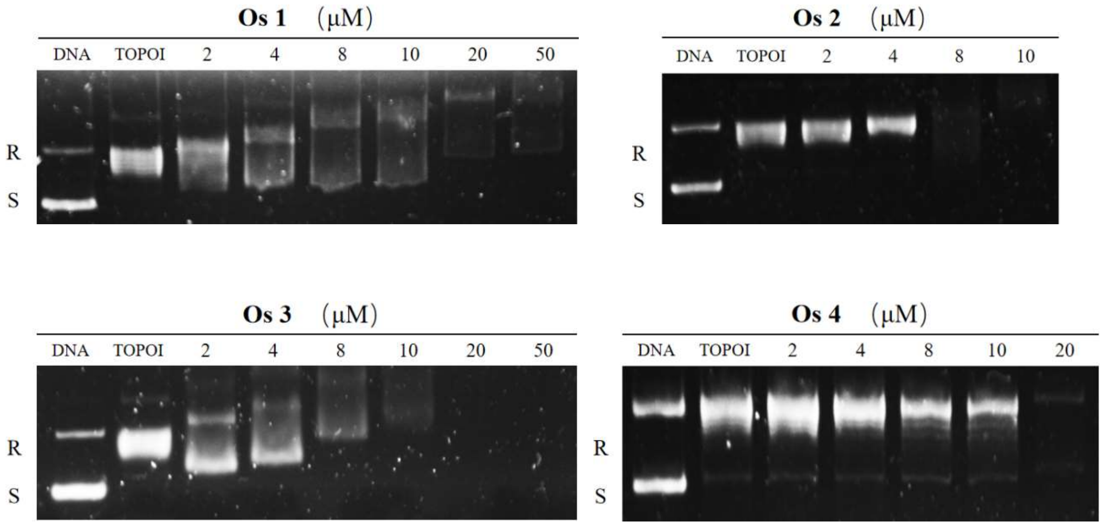


Fig. S19. Effects of different concentration of **Os1−4** on the activity of DNA topoisomerase I (TopoI).

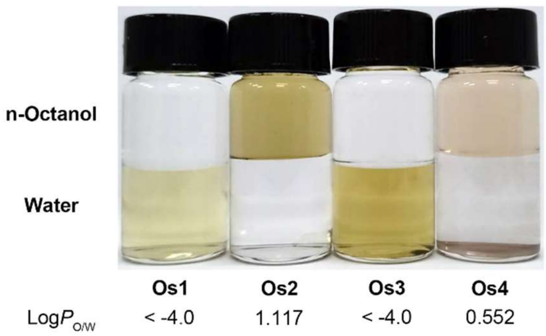


Fig. S20. Octanol/water partition coefficients (log $P_{o/w}$) of **Os1−4** (10 μM in total) at 25 ºC.

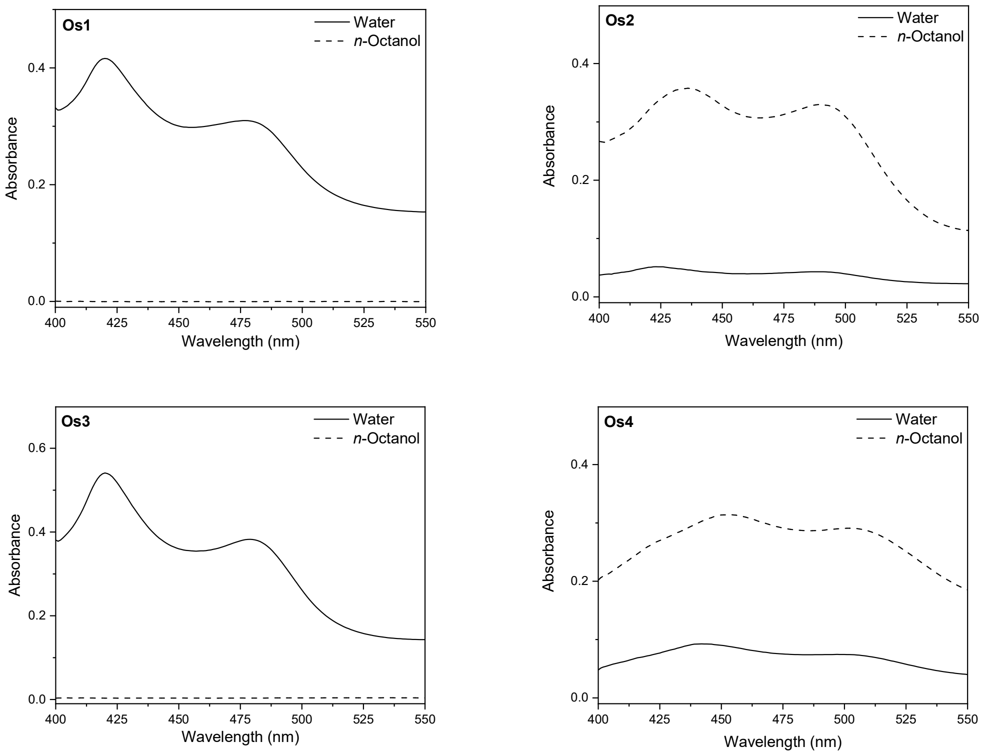


Fig. S21. Absorption spectra of **Os1−4** in the *n*-octanol and water phase (10 μM in total), by which the partition coefficients (log $P_{o/w}$) were calculated.

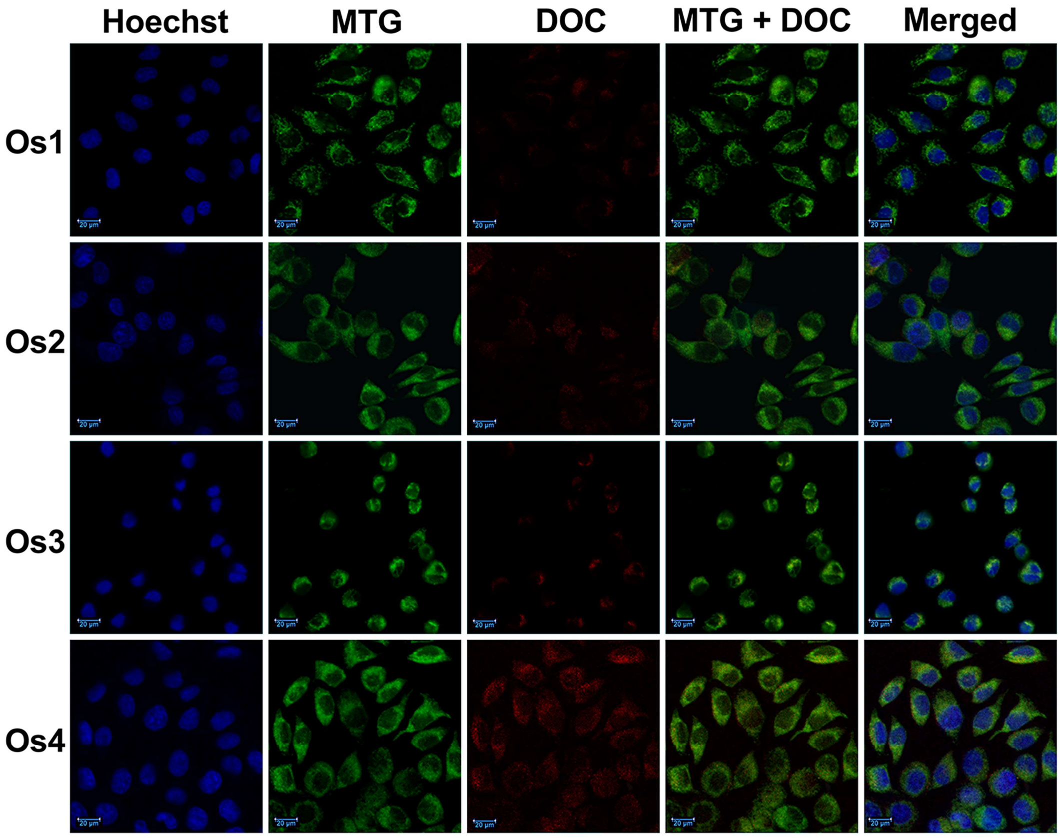


Fig. S22. Cellular colocalization of **Os4** with Hoechst 33342 (Hoechst) and MitoTracker Green (MTG) in A375 cells by CLSM.

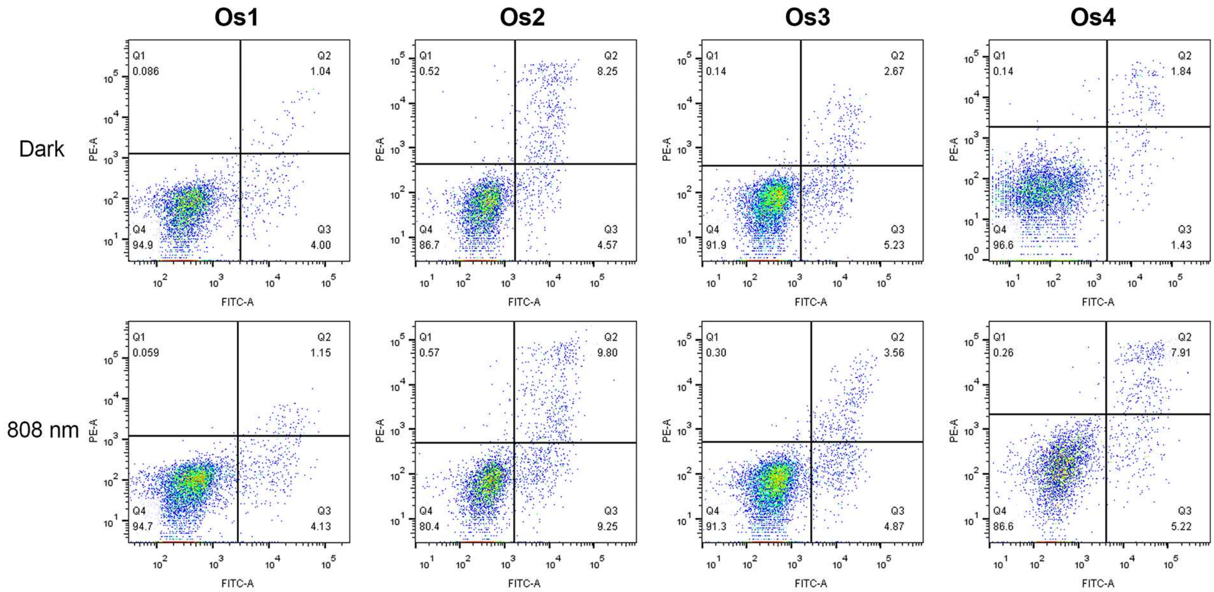


Fig. S23. Cytotoxicity of **Os1−4** towards A375 cell lines in the dark and under irradiation of 808 nm LPL (100 mW cm^{-2}) tested by flow cytometry. The cell numbers and light doses (30 J cm^{-2}) were consistent with the CCK-8 experiment.

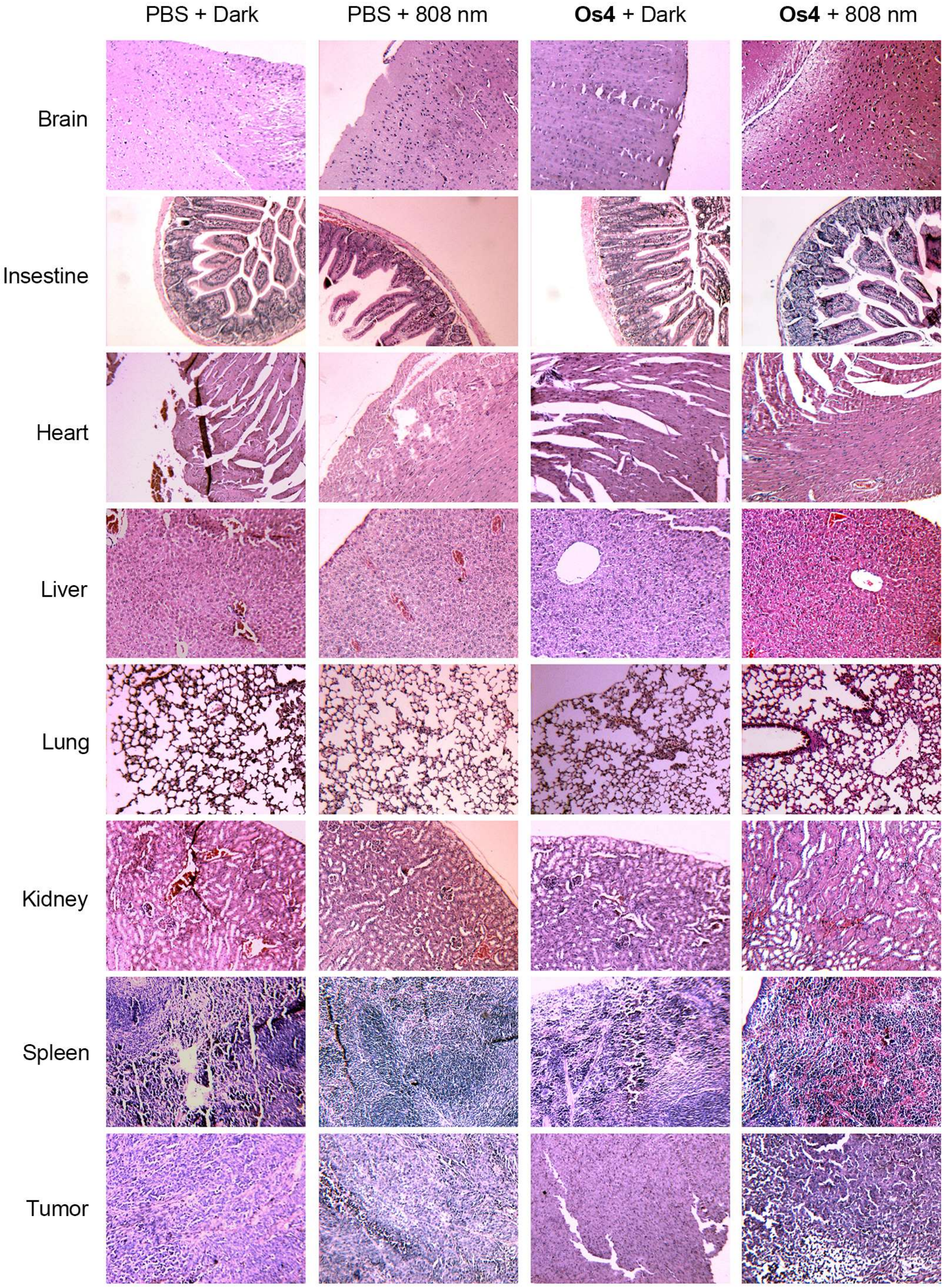


Fig. S24. H&E staining of organ slices from different groups.

5. Supplementary Tables

Table S1. Photophysical and Electrochemical Data for Os(II) complexes

DOC	λ_{abs}/nm[a] (ε/×10^4 M^{-1} cm^{-1})	λ_{em}/nm[b]	E_{ox}/V[c]	E_{red}/V[d]	ΔE/V[e]
Os1	287 (9.75), 397 (2.76), 420 (4.22), 478 (2.87), 631 (0.79)	714, 808	+0.59	-0.43, -1.08, -1.83	1.02
Os2	289 (13.69), 399 (3.13), 422 (4.25), 487 (3.24), 659 (0.81)	732, 794	+0.51	-0.42, -1.06, -1.87	0.93
Os3	264 (8.15), 398 (2.33), 421 (3.49), 479 (2.40), 627 (0.60)	708, 811	+0.58	-0.44, -1.04, -1.83	1.02
Os4	279 (15.56), 400 (2.65), 444 (3.75), 495 (3.02), 660 (0.74)	712, 804	+0.57	-0.56, -1.13, -1.81	1.13

[a] Maximum absorption wavelength in aqueous solution.

[b] Maximum emission wavelength in aqueous solution.

[c] Oxidation potential of Os(III)/Os(II) couple.

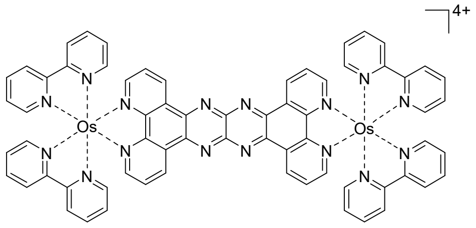
[d] Ligand-centered reduction potential of Os(II) complex.

[e] Potential difference obtained by $\Delta E = E_{ox} - E_{red(first)}$.

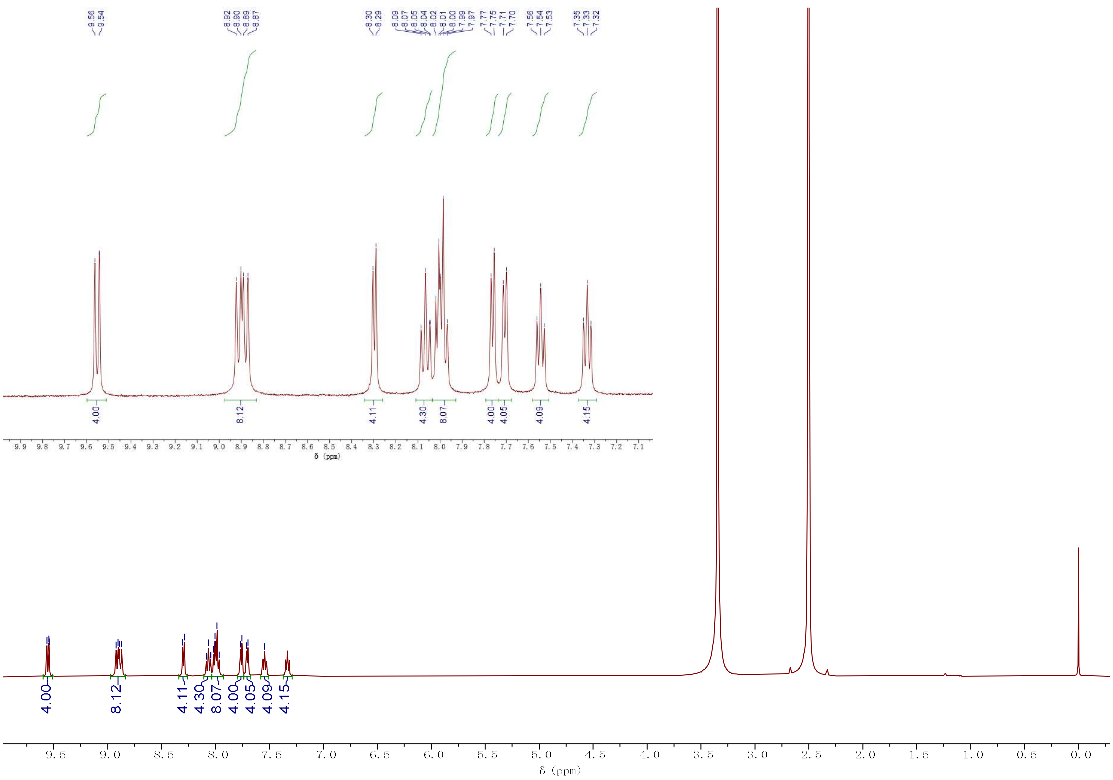
Table S2. Experimental and Computational Absorption Spectral Data of Os(II) complexes, together with the Calculated Excitation Energies (ΔE), Oscillator Strengths (f > 0.01), by MN15/Lanl2DZ (D3-BJ) method in Aqueous Solution (CPCM).

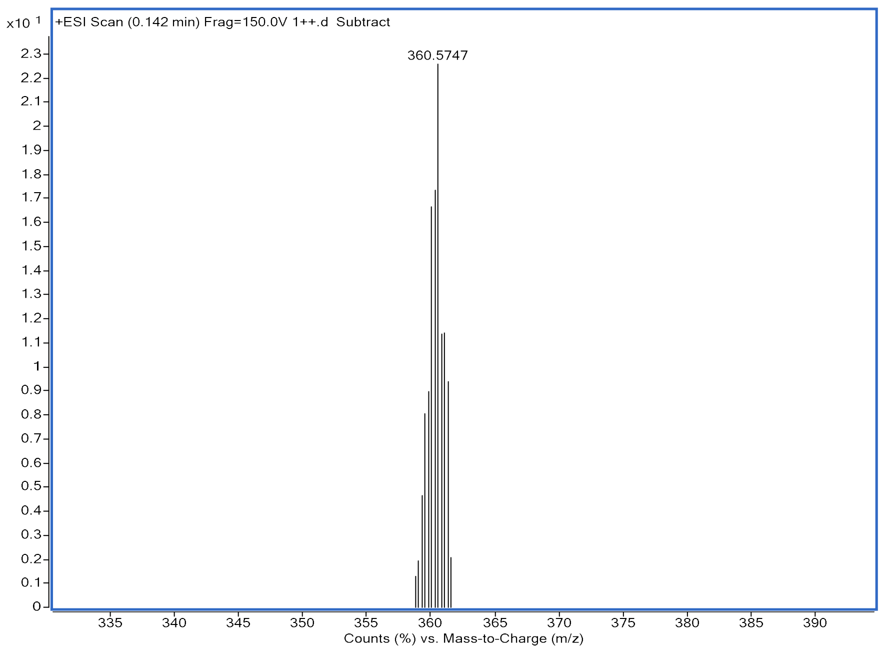
DOC	λ_{exp}/nm (ε/×10^4 M^{-1} cm^{-1})	λ_{cal}/nm	f	ΔE/eV	Excited State	Character
Os1	631(0.79)	568.03	0.266	2.18	S3	MLCT/IL(pppp)
	478(2.87)	444.26	0.016	2.79	S16	MLCT
		444.23	0.028	2.79	S17	MLCT
		443.07	0.236	2.80	S18	MLCT/LLCT
		424.59	0.012	2.92	S21	MLCT
	420(4.22)	418.65	0.529	2.96	S22	MLCT
		415.93	0.162	2.98	S24	MLCT
		415.79	0.228	2.98	S25	MLCT
Os2	659(0.81)	595.77	0.251	2.08	S3	MLCT/IL(pppp)
	487(3.24)	478.88	0.010	2.59	S14	MLCT
		450.11	0.326	2.75	S16	MLCT
		448.38	0.029	2.77	S18	MLCT
		448.31	0.047	2.77	S19	MLCT
		435.95	0.099	2.84	S20	MLCT
		427.27	0.402	2.90	S22	MLCT
	422(4.25)	421.82	0.204	2.94	S24	MLCT
		421.68	0.289	2.94	S25	MLCT
		404.05	0.172	3.07	S26	MLCT
Os3	627(0.60)	569.98	0.277	2.18	S3	MLCT/IL(pppp)
	479(2.40)	439.87	0.313	2.82	S16	MLCT
		439.17	0.028	2.82	S17	MLCT
		439.11	0.042	2.82	S18	MLCT
		423.69	0.017	2.93	S20	MLCT
	421(3.49)	417.05	0.392	2.97	S22	MLCT
		413.15	0.119	3.00	S24	MLCT
		413.40	0.180	3.00	S25	MLCT
		403.11	0.128	3.08	S26	MLCT
		396.15	0.217	3.13	S28	MLCT/LLCT
Os4	660(0.74)	586.39	0.289	2.11	S3	MLCT/IL(pppp)
		513.58	0.012	2.41	S7	MLCT
	495(3.02)	490.37	0.017	2.53	S11	MLCT
		474.94	0.041	2.61	S14	MLCT/LLCT
		474.39	0.015	2.61	S15	MLCT/LLCT
		455.49	0.069	2.72	S16	MLCT
		455.44	0.058	2.72	S17	MLCT
		452.80	0.428	2.74	S18	MLCT
	444(3.75)	431.18	0.196	2.88	S20	MLCT
		430.08	0.161	2.88	S22	MLCT
		429.55	0.269	2.89	S23	MLCT
		429.37	0.388	2.89	S24	MLCT
		415.45	0.263	2.98	S26	MLCT
		408.01	0.192	3.04	S28	MLCT
		407.92	0.156	3.04	S29	MLCT
		405.68	0.371	3.06	S30	MLCT/LLCT

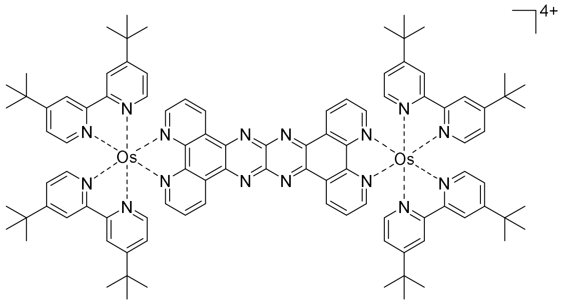
6. ^{1}H NMR, Mass, and FT-IR Spectra of DOCs Os1–4



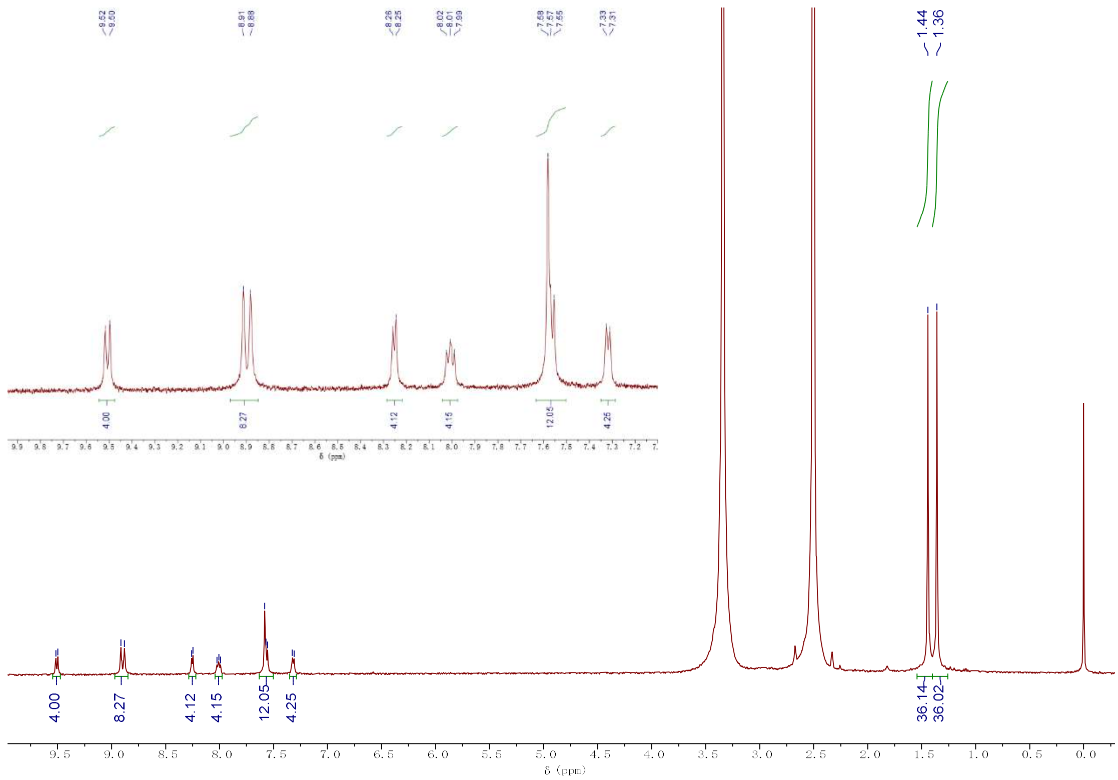
Os1

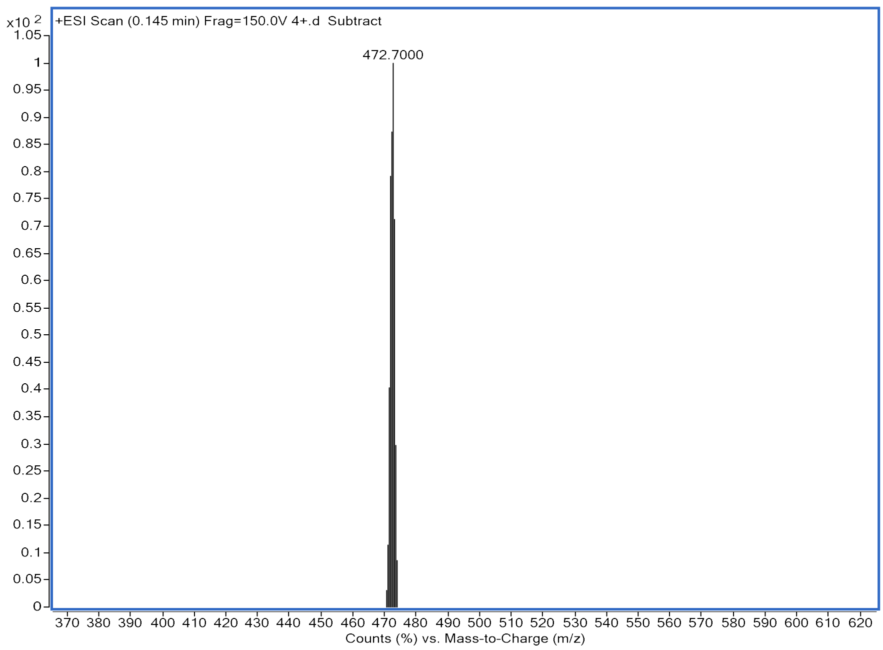


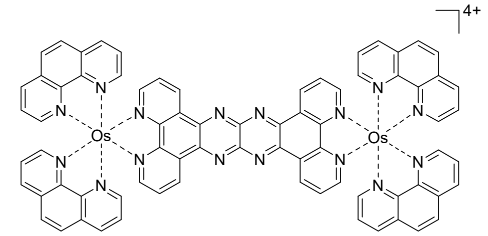




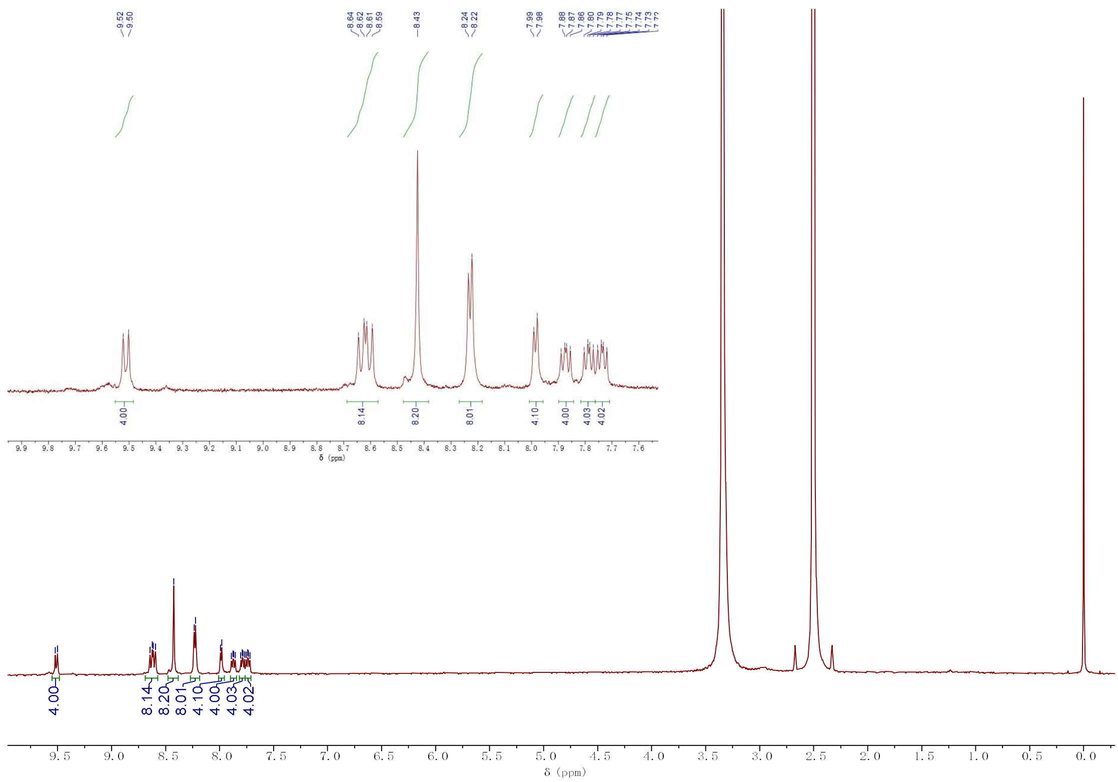
Os2

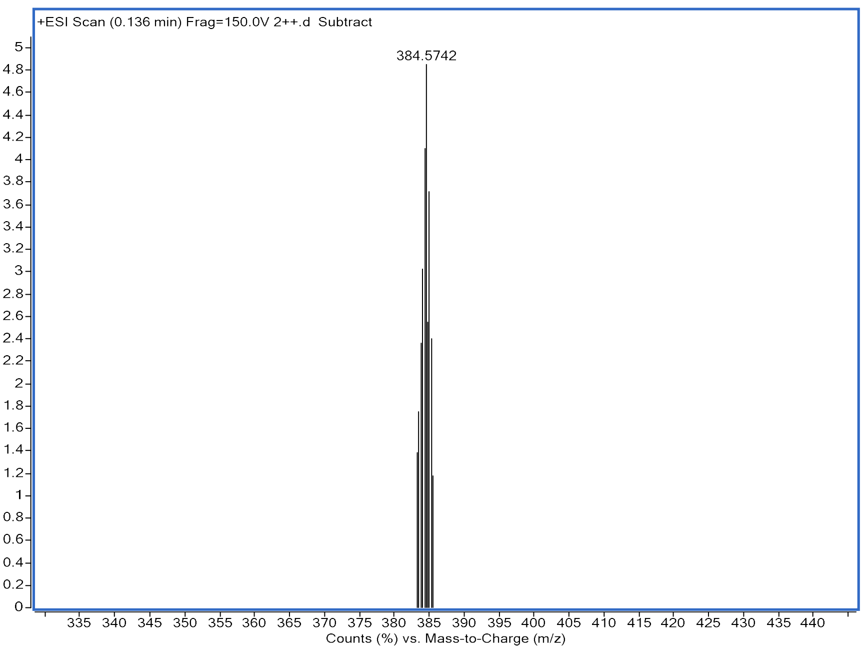


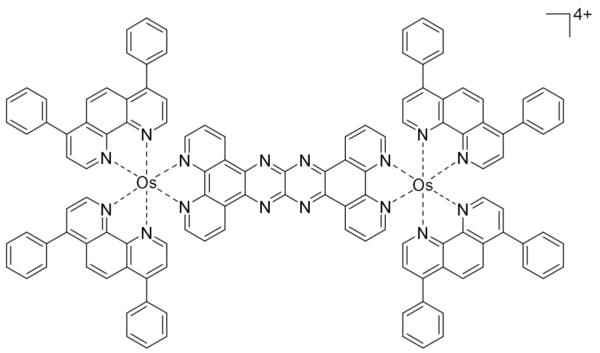

+ESI Scan (0.145 min) Frag=150.0V 4+.d Subtract
472.7000
Counts (%) vs. Mass-to-Charge (m/z)



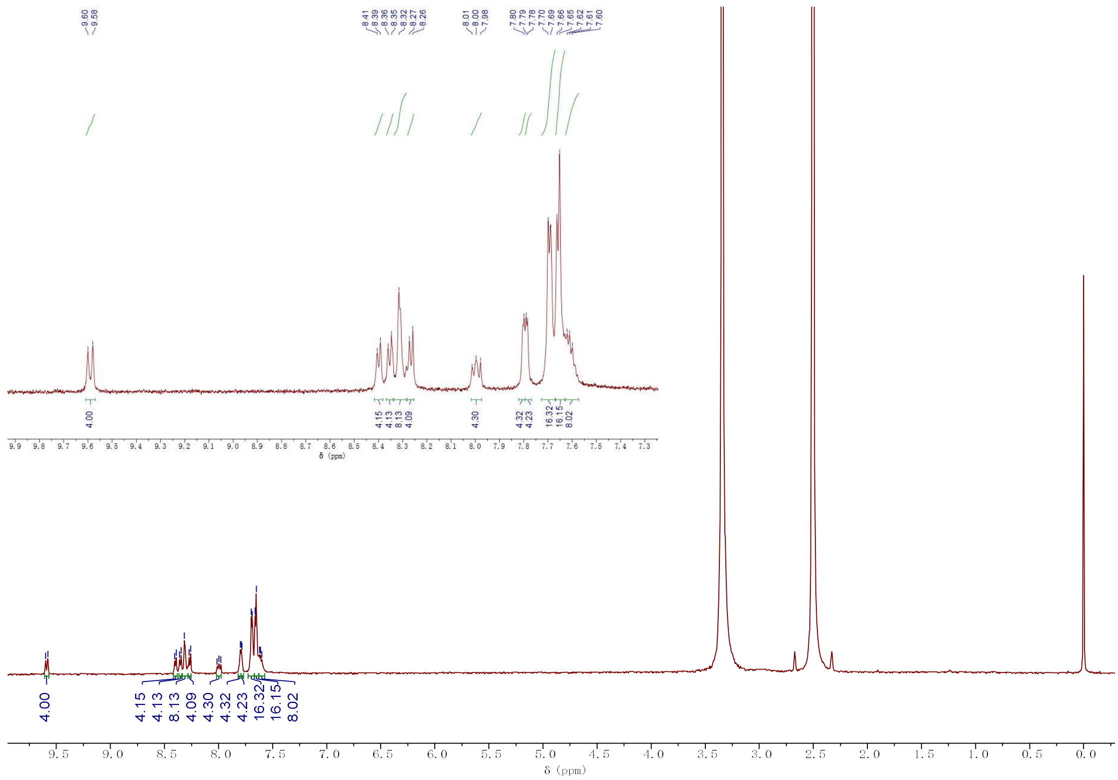
Os3

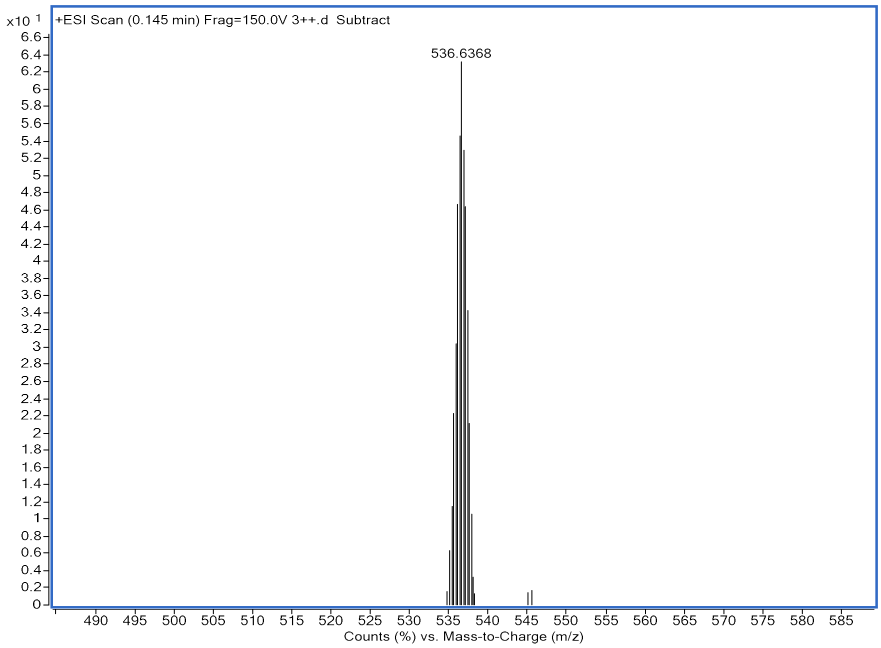


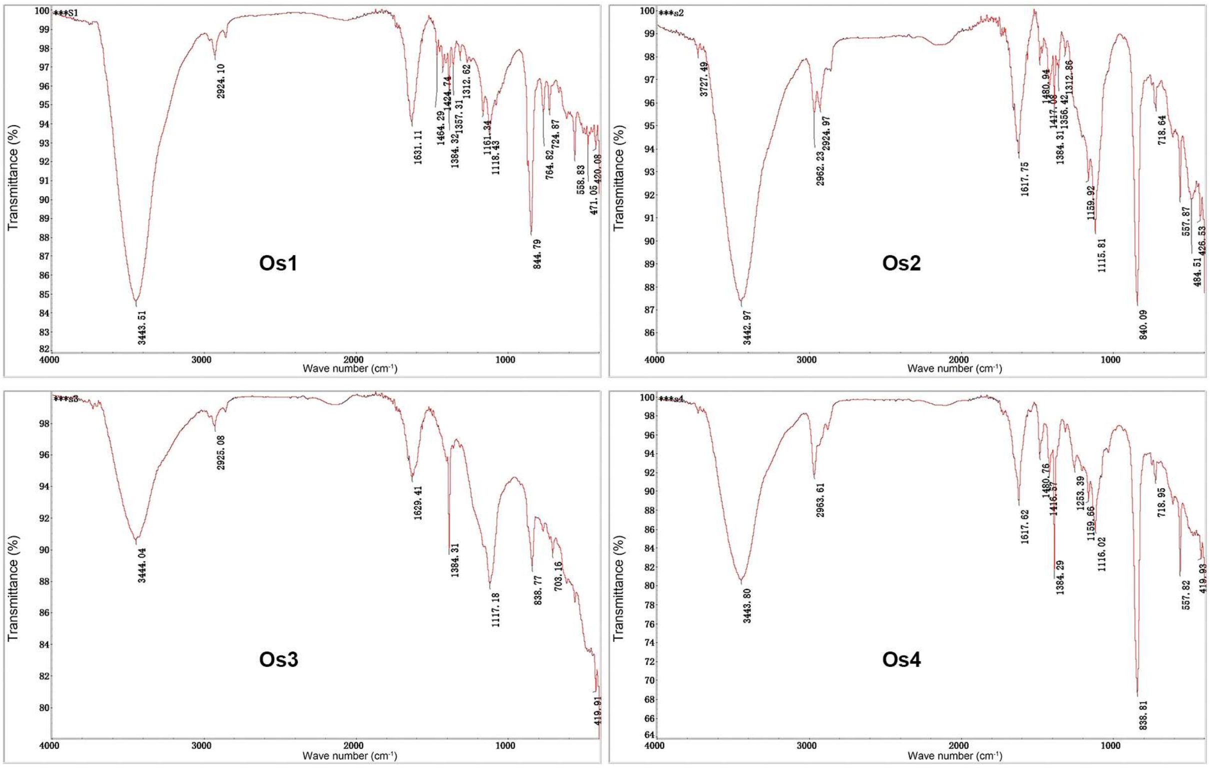

+ESI Scan (0.136 min) Frag=150.0V 2++.d Subtract
384.5742
Counts (%) vs. Mass-to-Charge (m/z)



Os4




+ESI Scan (0.145 min) Frag=150.0V 3++.d Subtract
536.6368
Counts (%) vs. Mass-to-Charge (m/z)


Os1
Os2
Os3
Os4
Transmittance (%)
Wave number (cm-1)

7. Cartesian coordinates of DFT/TDDFT (MN15/Lanl2dz, GD3BJ, CPCM for water, Gaussian 16) optimized Os1–4 for the ground state (S0), first excited singlet state (S1) and first excited triplet state (T1).

Os1	S0			S1			T1		
Symbol	X	Y	Z	X	Y	Z	X	Y	Z
Os	7.609402	0	0	7.616889	-0.000009	-0.000005	-7.62334	0	0
Os	-7.6094	0	0	-7.61906	0.000003	0.000006	7.623336	0	0
N	1.172821	0.006504	1.417174	1.178266	0.026611	1.425996	-1.17019	0.018332	1.425448
N	1.172821	-0.0065	-1.41717	1.178264	-0.026848	-1.425994	-1.17019	-0.01833	-1.42545
N	6.018728	-0.0023	1.314472	6.044149	0.012987	1.3353	-6.03371	0.077471	1.323485
N	6.018728	0.002298	-1.31447	6.044146	-0.013118	-1.335304	-6.03371	-0.07747	-1.32349
N	7.714404	2.036723	0.301883	7.668892	2.03023	0.3596	-7.69765	-2.00159	0.491997
N	9.098107	0.132	1.416241	9.147572	0.128984	1.382223	-9.1359	-0.02223	1.400101
N	7.714404	-2.03672	-0.30188	7.669047	-2.030241	-0.359622	-7.69765	2.001586	-0.492
N	9.098107	-0.132	-1.41624	9.147586	-0.128877	-1.38223	-9.1359	0.022229	-1.4001
N	-7.7144	-2.03672	0.301883	-7.71554	-2.032033	0.324242	7.697645	2.001586	0.491997
N	-9.09811	-0.132	1.416241	-9.10431	-0.121731	1.418579	9.135902	0.022229	1.400101
N	-7.7144	2.036723	-0.30188	-7.7154	2.032045	-0.324232	7.697645	-2.00159	-0.492
N	-9.09811	0.132	-1.41624	-9.10431	0.121835	-1.418565	9.135902	-0.02223	-1.4001
N	-1.17282	-0.0065	1.417174	-1.16452	0.0133	1.417303	1.170188	-0.01833	1.425448
N	-1.17282	0.006504	-1.41717	-1.16452	-0.013523	-1.417298	1.170188	0.018332	-1.42545
N	-6.01873	-0.0023	-1.31447	-6.02907	-0.018983	-1.319487	6.03371	0.077471	-1.32349
N	-6.01873	0.002298	1.314472	-6.02907	0.018895	1.319497	6.03371	-0.07747	1.323485
C	2.316008	-0.00638	-0.72816	2.330505	-0.016682	-0.724827	-2.33157	-0.01596	-0.7132
C	2.316008	0.00638	0.728163	2.330506	0.016453	0.724829	-2.33157	0.015956	0.713195
C	3.586483	0.014914	1.457234	3.595572	0.034107	1.438918	-3.59269	0.04897	1.438244
C	4.781397	0.004906	0.722457	4.809777	0.00854	0.70825	-4.79994	0.033866	0.71634
C	4.781397	-0.00491	-0.72246	4.809776	-0.008711	-0.708252	-4.79994	-0.03387	-0.71634
C	3.586483	-0.01491	-1.45723	3.59557	-0.034318	-1.438918	-3.59269	-0.04897	-1.43824
C	3.663441	0.029128	2.864311	3.681828	0.077057	2.846568	-3.67451	0.101276	2.851101
C	4.926991	0.03267	3.466363	4.936112	0.09996	3.467875	-4.92943	0.133141	3.460849
C	6.084822	0.016287	2.669234	6.10432	0.072105	2.679691	-6.09857	0.11764	2.67122
C	6.084822	-0.01629	-2.66923	6.104318	-0.072251	-2.679694	-6.09857	-0.11764	-2.67122
C	4.926991	-0.03267	-3.46636	4.93611	-0.100155	-3.467877	-4.92943	-0.13314	-3.46085
C	3.663441	-0.02913	-2.86431	3.681827	-0.07728	-2.846568	-3.67451	-0.10128	-2.8511
C	7.952753	4.767652	0.881906	7.835866	4.73536	1.012796	-7.89123	-4.66174	1.327721
C	7.011471	4.31463	-0.06022	6.86552	4.281289	0.103789	-6.92999	-4.28027	0.375214
C	6.918326	2.945798	-0.3242	6.803219	2.917679	-0.195742	-6.85693	-2.94114	-0.01701
C	8.634808	2.47004	1.224016	8.613569	2.460097	1.258337	-8.63385	-2.36177	1.429552
C	8.770645	3.831761	1.528763	8.714617	3.812633	1.600294	-8.74832	-3.68899	1.861671
C	9.432245	1.395813	1.836768	9.455077	1.390865	1.823161	-9.46089	-1.24877	1.924198

C	9.776149	-0.93788	1.913759	9.869083	-0.937725	1.812169	-9.84081	1.07921	1.772605
C	10.80252	-0.79058	2.850286	10.91882	-0.78838	2.722975	-10.8883	1.002055	2.694177
C	10.45462	1.602176	2.773662	10.5011	1.599293	2.729188	-10.5051	-1.38447	2.847577
C	11.14917	0.499992	3.289525	11.23879	0.498146	3.188327	-11.2266	-0.2484	3.240679
C	7.952753	-4.76765	-0.88191	7.836222	-4.735352	-1.012841	-7.89123	4.661735	-1.32772
C	7.011471	-4.31463	0.060217	6.865835	-4.281359	-0.10384	-6.92999	4.280272	-0.37521
C	6.918326	-2.9458	0.324203	6.803431	-2.917757	0.195701	-6.85693	2.941136	0.01701
C	8.634808	-2.47004	-1.22402	8.613763	-2.460031	-1.258354	-8.63385	2.361774	-1.42955
C	8.770645	-3.83176	-1.52876	8.714912	-3.812557	-1.600324	-8.74832	3.688989	-1.86167
C	9.432245	-1.39581	-1.83677	9.455195	-1.390734	-1.823166	-9.46089	1.248766	-1.9242
C	9.776149	0.937882	-1.91376	9.869016	0.937889	-1.81217	-9.84081	-1.07921	-1.77261
C	10.80252	0.790578	-2.85029	10.91877	0.788627	-2.722964	-10.8883	-1.00206	-2.69418
C	10.45462	-1.60218	-2.77366	10.50125	-1.59908	-2.729179	-10.5051	1.384472	-2.84758
C	11.14917	-0.49999	-3.28953	11.23885	-0.497875	-3.188311	-11.2266	0.248395	-3.24068
C	-7.95275	-4.76765	0.881906	-7.93316	-4.756865	0.943348	7.891226	4.661735	1.327721
C	-7.01147	-4.31463	-0.06022	-6.99863	-4.310237	-0.008805	6.929991	4.280272	0.375214
C	-6.91833	-2.9458	-0.3242	-6.91537	-2.944646	-0.291912	6.856932	2.941136	-0.01701
C	-8.63481	-2.47004	1.224016	-8.62922	-2.459138	1.256226	8.633848	2.361774	1.429552
C	-8.77065	-3.83176	1.528763	-8.75448	-3.817561	1.580607	8.74832	3.688989	1.861671
C	-9.43225	-1.39581	1.836768	-9.43125	-1.381688	1.856585	9.460891	1.248766	1.924198
C	-9.77615	0.937882	1.913759	-9.78797	0.950976	1.902801	9.840805	-1.07921	1.772605
C	-10.8025	0.790578	2.850286	-10.8123	0.810693	2.842423	10.88829	-1.00206	2.694177
C	-10.4546	-1.60218	2.773662	-10.4518	-1.580992	2.79729	10.50513	1.384472	2.847577
C	-11.1492	-0.49999	3.289525	-11.1517	-0.475942	3.299378	11.22662	0.248395	3.240679
C	-7.95275	4.767652	-0.88191	-7.93284	4.756889	-0.943348	7.891226	-4.66174	-1.32772
C	-7.01147	4.31463	0.060217	-6.99833	4.3102	0.008807	6.929991	-4.28027	-0.37521
C	-6.91833	2.945798	0.324203	-6.91517	2.944604	0.291919	6.856932	-2.94114	0.01701
C	-8.63481	2.47004	-1.22402	-8.62906	2.459211	-1.256217	8.633848	-2.36177	-1.42955
C	-8.77065	3.831761	-1.52876	-8.75422	3.81764	-1.580604	8.74832	-3.68899	-1.86167
C	-9.43225	1.395813	-1.83677	-9.43116	1.381813	-1.85657	9.460891	-1.24877	-1.9242
C	-9.77615	-0.93788	-1.91376	-9.78803	-0.950827	-1.902782	9.840805	1.07921	-1.77261
C	-10.8025	-0.79058	-2.85029	-10.8124	-0.810476	-2.842399	10.88829	1.002055	-2.69418
C	-10.4546	1.602176	-2.77366	-10.4517	1.581185	-2.797268	10.50513	-1.38447	-2.84758
C	-11.1492	0.499992	-3.28953	-11.1516	0.476181	-3.299353	11.22662	-0.2484	-3.24068
C	0	0	0.719647	-5.7E-05	0.010172	0.728773	0	0	0.733534
C	0	0	-0.71965	-5.8E-05	-0.010407	-0.728769	0	0	-0.73353
C	-2.31601	0.00638	-0.72816	-2.3267	-0.004208	-0.714214	2.331569	0.015956	-0.7132
C	-2.31601	-0.00638	0.728163	-2.3267	0.004005	0.714219	2.331569	-0.01596	0.713195
C	-3.58648	0.014914	-1.45723	-3.58865	-0.006474	-1.445133	3.592686	0.04897	-1.43824
C	-4.7814	0.004906	-0.72246	-4.79234	-0.004972	-0.719051	4.799937	0.033866	-0.71634
C	-4.7814	-0.00491	0.722457	-4.79233	0.004842	0.719059	4.799937	-0.03387	0.71634
C	-3.58648	-0.01491	1.457234	-3.58865	0.0063	1.44514	3.592686	-0.04897	1.438244

C	-3.66344	0.029128	-2.86431	-3.66687	-0.013283	-2.85664	3.674506	0.101276	-2.8511
C	-4.92699	0.03267	-3.46636	-4.92527	-0.017422	-3.462964	4.929431	0.133141	-3.46085
C	-6.08482	0.016287	-2.66923	-6.09101	-0.020158	-2.67038	6.098565	0.11764	-2.67122
C	-3.66344	-0.02913	2.864311	-3.66687	0.013103	2.856647	3.674506	-0.10128	2.851101
C	-4.92699	-0.03267	3.466363	-4.92527	0.017278	3.462972	4.929431	-0.13314	3.460849
C	-6.08482	-0.01629	2.669234	-6.091	0.020061	2.670389	6.098565	-0.11764	2.67122
H	2.751718	0.036643	3.451358	2.765154	0.09586	3.427144	-2.75822	0.11531	3.4312
H	5.031873	0.044763	4.544588	5.028444	0.136762	4.546134	-5.02694	0.172048	4.539208
H	7.074646	0.006821	3.111377	7.089419	0.081358	3.133986	-7.08451	0.151108	3.121281
H	7.074646	-0.00682	-3.11138	7.089417	-0.081474	-3.13399	-7.08451	-0.15111	-3.12128
H	5.031873	-0.04476	-4.54459	5.028441	-0.136969	-4.546135	-5.02694	-0.17205	-4.53921
H	2.751718	-0.03664	-3.45136	2.765151	-0.096113	-3.427143	-2.75822	-0.11531	-3.4312
H	6.359939	5.004663	-0.58355	6.16658	4.963596	-0.364228	-6.247	-5.00128	-0.05782
H	6.212213	2.557545	-1.04905	6.072014	2.524237	-0.891715	-6.13493	-2.60596	-0.75232
H	9.500499	4.158613	2.260365	9.457695	4.14625	2.314398	-9.48822	-3.9629	2.604409
H	9.475817	-1.9149	1.553197	9.587775	-1.911601	1.428494	-9.5452	2.023338	1.329778
H	11.31507	-1.66996	3.222492	11.46872	-1.6615	3.052283	-11.4233	1.902647	2.971016
H	10.70792	2.605951	3.094945	10.74274	2.598445	3.071101	-10.7567	-2.35742	3.252916
H	6.359939	-5.00466	0.583548	6.166939	-4.963721	0.364163	-6.247	5.001279	0.057823
H	6.212213	-2.55755	1.049049	6.072189	-2.524373	0.891668	-6.13493	2.605956	0.752318
H	9.500499	-4.15861	-2.26037	9.458019	-4.146113	-2.314426	-9.48822	3.9629	-2.60441
H	9.475817	1.914895	-1.5532	9.587628	1.911743	-1.428499	-9.5452	-2.02334	-1.32978
H	11.31507	1.669957	-3.22249	11.46861	1.66179	-3.052268	-11.4233	-1.90265	-2.97102
H	10.70792	-2.60595	-3.09495	10.74297	-2.598214	-3.071085	-10.7567	2.357424	-3.25292
H	-6.35994	-5.00466	-0.58355	-6.34423	-5.003055	-0.524955	6.247003	5.001279	-0.05782
H	-6.21221	-2.55755	-1.04905	-6.21403	-2.560794	-1.023795	6.134929	2.605956	-0.75232
H	-9.5005	-4.15861	2.260365	-9.47848	-4.138892	2.320513	9.488222	3.9629	2.604409
H	-9.47582	1.914895	1.553197	-9.49298	1.924366	1.527976	9.545199	-2.02334	1.329778
H	-11.3151	1.669957	3.222492	-11.3294	1.692131	3.203536	11.42327	-1.90265	2.971016
H	-10.7079	-2.60595	3.094945	-10.6999	-2.5819	3.131519	10.75667	2.357424	3.252916
H	-6.35994	5.004663	0.583548	-6.34389	5.002975	0.524954	6.247003	-5.00128	0.057823
H	-6.21221	2.557545	1.049049	-6.21386	2.560706	1.023803	6.134929	-2.60596	0.752318
H	-9.5005	4.158613	-2.26037	-9.4782	4.13902	-2.320513	9.488222	-3.9629	-2.60441
H	-9.47582	-1.9149	-1.5532	-9.49311	-1.924236	-1.527958	9.545199	2.023338	-1.32978
H	-11.3151	-1.66996	-3.22249	-11.3295	-1.691881	-3.203509	11.42327	1.902647	-2.97102
H	-10.7079	2.605951	-3.09495	-10.6997	2.582109	-3.131496	10.75667	-2.35742	-3.25292
H	-2.75172	0.036643	-3.45136	-2.75211	-0.015519	-3.439062	2.758224	0.11531	-3.4312
H	-5.03187	0.044763	-4.54459	-5.02587	-0.021546	-4.541964	5.02694	0.172048	-4.53921
H	-7.07465	0.006821	-3.11138	-7.07844	-0.034384	-3.118248	7.084508	0.151108	-3.12128
H	-2.75172	-0.03664	3.451358	-2.75211	0.015307	3.439067	2.758224	-0.11531	3.4312
H	-5.03187	-0.04476	4.544588	-5.02587	0.021398	4.541972	5.02694	-0.17205	4.539208
H	-7.07465	-0.00682	3.111377	-7.07843	0.034321	3.118259	7.084508	-0.15111	3.121281

H	-8.04623	-5.82453	1.10639	-8.01833	-5.811169	1.182857	7.968712	5.694016	1.65069
H	8.046225	5.824525	1.10639	7.903774	5.787651	1.265258	-7.96871	-5.69402	1.65069
H	-8.04623	5.824525	-1.10639	-8.01793	5.811198	-1.182862	7.968712	-5.69402	-1.65069
H	8.046225	-5.82453	-1.10639	7.904208	-5.787637	-1.265312	-7.96871	5.694016	-1.65069
H	-11.9422	-0.64298	4.015295	-11.9433	-0.613486	4.027827	12.03694	0.337136	3.955837
H	11.94222	0.64298	4.015295	12.05049	0.642547	3.892549	-12.0369	-0.33714	3.955837
H	-11.9422	0.64298	-4.0153	-11.9432	0.613777	-4.027796	12.03694	-0.33714	-3.95584
H	11.94222	-0.64298	-4.0153	12.05058	-0.642212	-3.892521	-12.0369	0.337136	-3.95584

Os2	S0			S1			T1		
Symbol	X	Y	Z	X	Y	Z	X	Y	Z
Os	-7.6083	0	0	-7.61943	0	0	-7.6239	0	0
Os	7.608301	0	0	7.619431	0	0	7.623896	0	0
N	7.72278	2.036564	0.294512	7.702023	2.004675	0.464588	7.707032	2.002644	0.479192
N	9.096985	0.142826	1.414429	9.132937	0.045751	1.396479	9.135298	0.035528	1.397486
N	7.72278	-2.03656	-0.29451	7.702023	-2.00468	-0.46459	7.707032	-2.00264	-0.47919
N	9.096985	-0.14283	-1.41443	9.132937	-0.04575	-1.39648	9.135298	-0.03553	-1.39749
N	1.172854	0.008201	1.41709	1.171179	-0.01438	1.42235	1.170272	-0.01571	1.425452
N	1.172854	-0.0082	-1.41709	1.171179	0.014378	-1.42235	1.170272	0.015712	-1.42545
N	6.01972	0.004439	1.31288	6.036064	-0.06656	1.324781	6.03434	-0.06822	1.323153
N	6.01972	-0.00444	-1.31288	6.036064	0.06656	-1.32478	6.03434	0.068217	-1.32315
N	-1.17285	-0.0082	1.41709	-1.17118	0.014378	1.42235	-1.17027	0.015712	1.425452
N	-1.17285	0.008201	-1.41709	-1.17118	-0.01438	-1.42235	-1.17027	-0.01571	-1.42545
N	-6.01972	0.004439	-1.31288	-6.03606	-0.06656	-1.32478	-6.03434	-0.06822	-1.32315
N	-6.01972	-0.00444	1.31288	-6.03606	0.06656	1.324781	-6.03434	0.068217	1.323153
N	-7.72278	2.036564	-0.29451	-7.70202	2.004675	-0.46459	-7.70703	2.002644	-0.47919
N	-9.09699	0.142826	-1.41443	-9.13294	0.045751	-1.39648	-9.1353	0.035528	-1.39749
N	-7.72278	-2.03656	0.294512	-7.70202	-2.00468	0.464588	-7.70703	-2.00264	0.479192
N	-9.09699	-0.14283	1.414429	-9.13294	-0.04575	1.396479	-9.1353	-0.03553	1.397486
C	7.979776	4.799328	0.864606	7.926518	4.709751	1.254834	7.928482	4.700618	1.292956
C	7.03594	4.316531	-0.07261	6.951822	4.286157	0.32119	6.958422	4.285228	0.350761
C	6.932272	2.952666	-0.33071	6.862237	2.946475	-0.04553	6.870444	2.948851	-0.02789
C	8.644198	2.47764	1.207642	8.647063	2.384724	1.381718	8.647648	2.374365	1.404034
C	8.785973	3.841657	1.501428	8.77426	3.720416	1.783107	8.773266	3.706674	1.81723
C	9.43967	1.403728	1.827408	9.471719	1.275872	1.895171	9.471312	1.261367	1.909481
C	9.777848	-0.91989	1.926239	9.840204	-1.04592	1.795608	9.843518	-1.05955	1.786904
C	10.80107	-0.76229	2.85694	10.88706	-0.94881	2.708012	10.88784	-0.97022	2.702596
C	10.46418	1.613078	2.761868	10.52048	1.424381	2.811802	10.51765	1.401567	2.829871
C	11.17332	0.528044	3.302618	11.25576	0.307115	3.244237	11.25345	0.28079	3.252637
C	8.081192	6.297994	1.143934	8.015705	6.182456	1.649071	8.016399	6.170103	1.699289
C	12.29831	0.688972	4.323807	12.40812	0.401717	4.242165	12.40306	0.366727	4.254329
C	7.979776	-4.79933	-0.86461	7.926518	-4.70975	-1.25483	7.928482	-4.70062	-1.29296
C	7.03594	-4.31653	0.07261	6.951822	-4.28616	-0.32119	6.958422	-4.28523	-0.35076
C	6.932272	-2.95267	0.330708	6.862237	-2.94648	0.045526	6.870444	-2.94885	0.027894
C	8.644198	-2.47764	-1.20764	8.647063	-2.38472	-1.38172	8.647648	-2.37437	-1.40403
C	8.785973	-3.84166	-1.50143	8.77426	-3.72042	-1.78311	8.773266	-3.70667	-1.81723
C	9.43967	-1.40373	-1.82741	9.471719	-1.27587	-1.89517	9.471312	-1.26137	-1.90948
C	9.777848	0.919892	-1.92624	9.840204	1.045919	-1.79561	9.843518	1.059552	-1.7869
C	10.80107	0.762292	-2.85694	10.88706	0.948809	-2.70801	10.88784	0.970218	-2.7026
C	10.46418	-1.61308	-2.76187	10.52048	-1.42438	-2.8118	10.51765	-1.40157	-2.82987
C	11.17332	-0.52804	-3.30262	11.25576	-0.30712	-3.24424	11.25345	-0.28079	-3.25264

C	8.081192	-6.29799	-1.14393	8.015705	-6.18246	-1.64907	8.016399	-6.1701	-1.69929
C	12.29831	-0.68897	-4.32381	12.40812	-0.40172	-4.24217	12.40306	-0.36673	-4.25433
C	2.316315	-0.00803	-0.72831	2.329597	0.013081	-0.71809	2.331973	0.013706	-0.71323
C	2.316315	0.008031	0.728306	2.329597	-0.01308	0.718089	2.331973	-0.01371	0.713231
C	3.586687	0.019963	1.457589	3.592395	-0.0411	1.44049	3.593125	-0.0423	1.438789
C	4.781371	0.008012	0.722123	4.800956	-0.02903	0.71396	4.800251	-0.02961	0.716561
C	4.781371	-0.00801	-0.72212	4.800956	0.029026	-0.71396	4.800251	0.029605	-0.71656
C	3.586687	-0.01996	-1.45759	3.592395	0.041103	-1.44049	3.593125	0.042303	-1.43879
C	3.66422	0.040359	2.864387	3.67508	-0.0841	2.851209	3.675318	-0.08713	2.851842
C	4.928676	0.048498	3.465369	4.930792	-0.1089	3.463195	4.930733	-0.11339	3.461162
C	6.086053	0.030153	2.667992	6.098697	-0.09597	2.671971	6.099587	-0.10016	2.671071
C	6.086053	-0.03015	-2.66799	6.098697	0.095974	-2.67197	6.099587	0.10016	-2.67107
C	4.928676	-0.0485	-3.46537	4.930792	0.108896	-3.4632	4.930733	0.11339	-3.46116
C	3.66422	-0.04036	-2.86439	3.67508	0.084095	-2.85121	3.675318	0.087129	-2.85184
C	0	0	0.719591	0	0	0.72979	0	0	0.733551
C	0	0	-0.71959	0	0	-0.72979	0	0	-0.73355
C	-2.31632	0.008031	-0.72831	-2.3296	-0.01308	-0.71809	-2.33197	-0.01371	-0.71323
C	-2.31632	-0.00803	0.728306	-2.3296	0.013081	0.718089	-2.33197	0.013706	0.713231
C	-3.58669	0.019963	-1.45759	-3.5924	-0.0411	-1.44049	-3.59313	-0.0423	-1.43879
C	-4.78137	0.008012	-0.72212	-4.80096	-0.02903	-0.71396	-4.80025	-0.02961	-0.71656
C	-4.78137	-0.00801	0.722123	-4.80096	0.029026	0.71396	-4.80025	0.029605	0.716561
C	-3.58669	-0.01996	1.457589	-3.5924	0.041103	1.44049	-3.59313	0.042303	1.438789
C	-3.66422	0.040359	-2.86439	-3.67508	-0.0841	-2.85121	-3.67532	-0.08713	-2.85184
C	-4.92868	0.048498	-3.46537	-4.93079	-0.1089	-3.4632	-4.93073	-0.11339	-3.46116
C	-6.08605	0.030153	-2.66799	-6.0987	-0.09597	-2.67197	-6.09959	-0.10016	-2.67107
C	-3.66422	-0.04036	2.864387	-3.67508	0.084095	2.851209	-3.67532	0.087129	2.851842
C	-4.92868	-0.0485	3.465369	-4.93079	0.108896	3.463195	-4.93073	0.11339	3.461162
C	-6.08605	-0.03015	2.667992	-6.0987	0.095974	2.671971	-6.09959	0.10016	2.671071
C	-7.97978	4.799328	-0.86461	-7.92652	4.709751	-1.25483	-7.92848	4.700618	-1.29296
C	-7.03594	4.316531	0.07261	-6.95182	4.286157	-0.32119	-6.95842	4.285228	-0.35076
C	-6.93227	2.952666	0.330708	-6.86224	2.946475	0.045526	-6.87044	2.948851	0.027894
C	-8.6442	2.47764	-1.20764	-8.64706	2.384724	-1.38172	-8.64765	2.374365	-1.40403
C	-8.78597	3.841657	-1.50143	-8.77426	3.720416	-1.78311	-8.77327	3.706674	-1.81723
C	-9.43967	1.403728	-1.82741	-9.47172	1.275872	-1.89517	-9.47131	1.261367	-1.90948
C	-9.77785	-0.91989	-1.92624	-9.8402	-1.04592	-1.79561	-9.84352	-1.05955	-1.7869
C	-10.8011	-0.76229	-2.85694	-10.8871	-0.94881	-2.70801	-10.8878	-0.97022	-2.7026
C	-10.4642	1.613078	-2.76187	-10.5205	1.424381	-2.8118	-10.5177	1.401567	-2.82987
C	-11.1733	0.528044	-3.30262	-11.2558	0.307115	-3.24424	-11.2535	0.28079	-3.25264
C	-8.08119	6.297994	-1.14393	-8.01571	6.182456	-1.64907	-8.0164	6.170103	-1.69929
C	-12.2983	0.688972	-4.32381	-12.4081	0.401717	-4.24217	-12.4031	0.366727	-4.25433
C	-7.97978	-4.79933	0.864606	-7.92652	-4.70975	1.254834	-7.92848	-4.70062	1.292956
C	-7.03594	-4.31653	-0.07261	-6.95182	-4.28616	0.32119	-6.95842	-4.28523	0.350761

C	-6.93227	-2.95267	-0.33071	-6.86224	-2.94648	-0.04553	-6.87044	-2.94885	-0.02789
C	-8.6442	-2.47764	1.207642	-8.64706	-2.38472	1.381718	-8.64765	-2.37437	1.404034
C	-8.78597	-3.84166	1.501428	-8.77426	-3.72042	1.783107	-8.77327	-3.70667	1.81723
C	-9.43967	-1.40373	1.827408	-9.47172	-1.27587	1.895171	-9.47131	-1.26137	1.909481
C	-9.77785	0.919892	1.926239	-9.8402	1.045919	1.795608	-9.84352	1.059552	1.786904
C	-10.8011	0.762292	2.85694	-10.8871	0.948809	2.708012	-10.8878	0.970218	2.702596
C	-10.4642	-1.61308	2.761868	-10.5205	-1.42438	2.811802	-10.5177	-1.40157	2.829871
C	-11.1733	-0.52804	3.302618	-11.2558	-0.30712	3.244237	-11.2535	-0.28079	3.252637
C	-8.08119	-6.29799	1.143934	-8.01571	-6.18246	1.649071	-8.0164	-6.1701	1.699289
C	-12.2983	-0.68897	4.323807	-12.4081	-0.40172	4.242165	-12.4031	-0.36673	4.254329
C	8.414425	7.034498	-0.17416	8.284059	7.024544	0.379817	8.291248	7.022071	0.438024
C	6.719171	6.799766	1.677659	6.667971	6.613953	2.27307	6.665867	6.597334	2.320164
C	9.168025	6.624618	2.180504	9.138691	6.447195	2.664418	9.134716	6.426202	2.721952
C	12.56154	2.162512	4.672937	12.65768	1.844346	4.709644	12.65055	1.805028	4.736018
C	11.91248	-0.06643	5.616793	12.07384	-0.4698	5.475311	12.06581	-0.51664	5.478267
C	13.59459	0.077595	3.74337	13.6948	-0.13371	3.571584	13.69188	-0.16163	3.582178
C	12.56154	-2.16251	-4.67294	12.65768	-1.84435	-4.70964	12.65055	-1.80503	-4.73602
C	11.91248	0.066431	-5.61679	12.07384	0.469801	-5.47531	12.06581	0.516644	-5.47827
C	13.59459	-0.0776	-3.74337	13.6948	0.133711	-3.57158	13.69188	0.161626	-3.58218
C	8.414425	-7.0345	0.174157	8.284059	-7.02454	-0.37982	8.291248	-7.02207	-0.43802
C	6.719171	-6.79977	-1.67766	6.667971	-6.61395	-2.27307	6.665867	-6.59733	-2.32016
C	9.168025	-6.62462	-2.1805	9.138691	-6.4472	-2.66442	9.134716	-6.4262	-2.72195
C	-6.71917	6.799766	-1.67766	-6.66797	6.613953	-2.27307	-6.66587	6.597334	-2.32016
C	-8.41443	7.034498	0.174157	-8.28406	7.024544	-0.37982	-8.29125	7.022071	-0.43802
C	-9.16803	6.624618	-2.1805	-9.13869	6.447195	-2.66442	-9.13472	6.426202	-2.72195
C	-11.9125	0.066431	5.616793	-12.0738	0.469801	5.475311	-12.0658	0.516644	5.478267
C	-13.5946	-0.0776	3.74337	-13.6948	0.133711	3.571584	-13.6919	0.161626	3.582178
C	-12.5615	-2.16251	4.672937	-12.6577	-1.84435	4.709644	-12.6505	-1.80503	4.736018
C	-6.71917	-6.79977	1.677659	-6.66797	-6.61395	2.27307	-6.66587	-6.59733	2.320164
C	-9.16803	-6.62462	2.180504	-9.13869	-6.4472	2.664418	-9.13472	-6.4262	2.721952
C	-8.41443	-7.0345	-0.17416	-8.28406	-7.02454	0.379817	-8.29125	-7.02207	0.438024
C	-12.5615	2.162512	-4.67294	-12.6577	1.844346	-4.70964	-12.6505	1.805028	-4.73602
C	-13.5946	0.077595	-3.74337	-13.6948	-0.13371	-3.57158	-13.6919	-0.16163	-3.58218
C	-11.9125	-0.06643	-5.61679	-12.0738	-0.4698	-5.47531	-12.0658	-0.51664	-5.47827
H	6.378242	4.995655	-0.60581	6.258698	4.992158	-0.12449	6.267807	4.99517	-0.09249
H	6.219399	2.567998	-1.05104	6.125543	2.605988	-0.76374	6.137751	2.614972	-0.75336
H	9.525846	4.151345	2.230129	9.531949	3.985979	2.510508	9.527785	3.965952	2.550194
H	9.478536	-1.90148	1.577033	9.542514	-2.00036	1.376814	9.548435	-2.01011	1.357583
H	11.30387	-1.64981	3.228177	11.41045	-1.85557	2.993457	11.41195	-1.87909	2.97978
H	10.70647	2.625654	3.062355	10.76336	2.412339	3.184166	10.75853	2.385959	3.212812
H	6.378242	-4.99566	0.605812	6.258698	-4.99216	0.124485	6.267807	-4.99517	0.092491
H	6.219399	-2.568	1.051041	6.125543	-2.60599	0.763743	6.137751	-2.61497	0.75336

H	9.525846	-4.15135	-2.23013	9.531949	-3.98598	-2.51051	9.527785	-3.96595	-2.55019
H	9.478536	1.901484	-1.57703	9.542514	2.000362	-1.37681	9.548435	2.010111	-1.35758
H	11.30387	1.649808	-3.22818	11.41045	1.855568	-2.99346	11.41195	1.879093	-2.97978
H	10.70647	-2.62565	-3.06236	10.76336	-2.41234	-3.18417	10.75853	-2.38596	-3.21281
H	2.753015	0.049477	3.452196	2.759364	-0.09629	3.432657	2.759376	-0.09966	3.432494
H	5.03406	0.065984	4.543547	5.027857	-0.14029	4.54175	5.028521	-0.14603	4.53977
H	7.076597	0.025067	3.108791	7.085577	-0.12256	3.121106	7.08632	-0.12857	3.119924
H	7.076597	-0.02507	-3.10879	7.085577	0.122559	-3.12111	7.08632	0.128568	-3.11992
H	5.03406	-0.06598	-4.54355	5.027857	0.140287	-4.54175	5.028521	0.146031	-4.53977
H	2.753015	-0.04948	-3.4522	2.759364	0.096292	-3.43266	2.759376	0.099664	-3.43249
H	-2.75302	0.049477	-3.4522	-2.75936	-0.09629	-3.43266	-2.75938	-0.09966	-3.43249
H	-5.03406	0.065984	-4.54355	-5.02786	-0.14029	-4.54175	-5.02852	-0.14603	-4.53977
H	-7.0766	0.025067	-3.10879	-7.08558	-0.12256	-3.12111	-7.08632	-0.12857	-3.11992
H	-2.75302	-0.04948	3.452196	-2.75936	0.096292	3.432657	-2.75938	0.099664	3.432494
H	-5.03406	-0.06598	4.543547	-5.02786	0.140287	4.54175	-5.02852	0.146031	4.53977
H	-7.0766	-0.02507	3.108791	-7.08558	0.122559	3.121106	-7.08632	0.128568	3.119924
H	-6.37824	4.995655	0.605812	-6.2587	4.992158	0.124485	-6.26781	4.99517	0.092491
H	-6.2194	2.567998	1.051041	-6.12554	2.605988	0.763743	-6.13775	2.614972	0.75336
H	-9.52585	4.151345	-2.23013	-9.53195	3.985979	-2.51051	-9.52779	3.965952	-2.55019
H	-9.47854	-1.90148	-1.57703	-9.54251	-2.00036	-1.37681	-9.54844	-2.01011	-1.35758
H	-11.3039	-1.64981	-3.22818	-11.4104	-1.85557	-2.99346	-11.412	-1.87909	-2.97978
H	-10.7065	2.625654	-3.06236	-10.7634	2.412339	-3.18417	-10.7585	2.385959	-3.21281
H	-6.37824	-4.99566	-0.60581	-6.2587	-4.99216	-0.12449	-6.26781	-4.99517	-0.09249
H	-6.2194	-2.568	-1.05104	-6.12554	-2.60599	-0.76374	-6.13775	-2.61497	-0.75336
H	-9.52585	-4.15135	2.230129	-9.53195	-3.98598	2.510508	-9.52779	-3.96595	2.550194
H	-9.47854	1.901484	1.577033	-9.54251	2.000362	1.376814	-9.54844	2.010111	1.357583
H	-11.3039	1.649808	3.228177	-11.4104	1.855568	2.993457	-11.412	1.879093	2.97978
H	-10.7065	-2.62565	3.062355	-10.7634	-2.41234	3.184166	-10.7585	-2.38596	3.212812
H	7.642799	6.871581	-0.93751	7.48506	6.907721	-0.36349	7.495874	6.91154	-0.31013
H	8.475243	8.113604	0.018829	8.33572	8.08593	0.655301	8.34193	8.081204	0.722204
H	9.378444	6.699806	-0.57858	9.236284	6.740906	-0.08657	9.245658	6.741769	-0.0259
H	6.777822	7.880309	1.863234	6.718062	7.677172	2.541636	6.715231	7.658356	2.597391
H	5.91069	6.624312	0.956294	5.834038	6.481616	1.572011	5.835294	6.471096	1.614006
H	6.45796	6.299886	2.619405	6.452641	6.036544	3.181333	6.445784	6.012886	3.222759
H	8.96165	6.149573	3.149153	8.978603	5.896703	3.601323	8.969993	5.868495	3.65377
H	10.16354	6.31065	1.838504	10.12405	6.178482	2.260241	10.12179	6.160117	2.320221
H	9.195319	7.709895	2.339507	9.156285	7.517412	2.904936	9.15178	7.494489	2.970917
H	12.8653	2.741139	3.79004	12.92952	2.502117	3.873031	12.92427	2.470794	3.906369
H	11.67858	2.638698	5.120446	11.77996	2.264493	5.219133	11.77133	2.219932	5.247191
H	13.37715	2.215755	5.404939	13.49166	1.848356	5.422439	13.48265	1.802695	5.450996
H	11.74928	-1.13552	5.42954	11.92543	-1.52236	5.202241	11.91884	-1.56668	5.194883
H	12.72526	0.028293	6.348844	12.90667	-0.42056	6.188796	12.89667	-0.47359	6.194422

H	10.99823	0.351497	6.057785	11.16615	-0.11022	5.97683	11.15654	-0.16234	5.980679
H	14.40293	0.174709	4.47997	14.52402	-0.083	4.289122	14.51901	-0.11716	4.302519
H	13.47399	-0.98881	3.513444	13.58498	-1.17916	3.256184	13.58373	-1.20409	3.256562
H	13.8975	0.597951	2.825538	13.95977	0.467856	2.692582	13.95892	0.448461	2.709708
H	12.8653	-2.74114	-3.79004	12.92952	-2.50212	-3.87303	12.92427	-2.47079	-3.90637
H	11.67858	-2.6387	-5.12045	11.77996	-2.26449	-5.21913	11.77133	-2.21993	-5.24719
H	13.37715	-2.21576	-5.40494	13.49166	-1.84836	-5.42244	13.48265	-1.8027	-5.451
H	11.74928	1.135516	-5.42954	11.92543	1.522361	-5.20224	11.91884	1.566675	-5.19488
H	12.72526	-0.02829	-6.34884	12.90667	0.420562	-6.1888	12.89667	0.473586	-6.19442
H	10.99823	-0.3515	-6.05779	11.16615	0.110217	-5.97683	11.15654	0.162337	-5.98068
H	14.40293	-0.17471	-4.47997	14.52402	0.083001	-4.28912	14.51901	0.117157	-4.30252
H	13.47399	0.988809	-3.51344	13.58498	1.179156	-3.25618	13.58373	1.204091	-3.25656
H	13.8975	-0.59795	-2.82554	13.95977	-0.46786	-2.69258	13.95892	-0.44846	-2.70971
H	7.642799	-6.87158	0.937507	7.48506	-6.90772	0.363487	7.495874	-6.91154	0.310132
H	8.475243	-8.1136	-0.01883	8.33572	-8.08593	-0.6553	8.34193	-8.0812	-0.7222
H	9.378444	-6.69981	0.578578	9.236284	-6.74091	0.086567	9.245658	-6.74177	0.025895
H	6.777822	-7.88031	-1.86323	6.718062	-7.67717	-2.54164	6.715231	-7.65836	-2.59739
H	5.91069	-6.62431	-0.95629	5.834038	-6.48162	-1.57201	5.835294	-6.4711	-1.61401
H	6.45796	-6.29989	-2.61941	6.452641	-6.03654	-3.18133	6.445784	-6.01289	-3.22276
H	8.96165	-6.14957	-3.14915	8.978603	-5.8967	-3.60132	8.969993	-5.8685	-3.65377
H	10.16354	-6.31065	-1.8385	10.12405	-6.17848	-2.26024	10.12179	-6.16012	-2.32022
H	9.195319	-7.7099	-2.33951	9.156285	-7.51741	-2.90494	9.15178	-7.49449	-2.97092
H	-6.77782	7.880309	-1.86323	-6.71806	7.677172	-2.54164	-6.71523	7.658356	-2.59739
H	-5.91069	6.624312	-0.95629	-5.83404	6.481616	-1.57201	-5.83529	6.471096	-1.61401
H	-6.45796	6.299886	-2.61941	-6.45264	6.036544	-3.18133	-6.44578	6.012886	-3.22276
H	-7.6428	6.871581	0.937507	-7.48506	6.907721	0.363487	-7.49587	6.91154	0.310132
H	-8.47524	8.113604	-0.01883	-8.33572	8.08593	-0.6553	-8.34193	8.081204	-0.7222
H	-9.37844	6.699806	0.578578	-9.23628	6.740906	0.086567	-9.24566	6.741769	0.025895
H	-8.96165	6.149573	-3.14915	-8.9786	5.896703	-3.60132	-8.96999	5.868495	-3.65377
H	-10.1635	6.31065	-1.8385	-10.1241	6.178482	-2.26024	-10.1218	6.160117	-2.32022
H	-9.19532	7.709895	-2.33951	-9.15629	7.517412	-2.90494	-9.15178	7.494489	-2.97092
H	-11.7493	1.135516	5.42954	-11.9254	1.522361	5.202241	-11.9188	1.566675	5.194883
H	-12.7253	-0.02829	6.348844	-12.9067	0.420562	6.188796	-12.8967	0.473586	6.194422
H	-10.9982	-0.3515	6.057785	-11.1662	0.110217	5.97683	-11.1565	0.162337	5.980679
H	-14.4029	-0.17471	4.47997	-14.524	0.083001	4.289122	-14.519	0.117157	4.302519
H	-13.474	0.988809	3.513444	-13.585	1.179156	3.256184	-13.5837	1.204091	3.256562
H	-13.8975	-0.59795	2.825538	-13.9598	-0.46786	2.692582	-13.9589	-0.44846	2.709708
H	-12.8653	-2.74114	3.79004	-12.9295	-2.50212	3.873031	-12.9243	-2.47079	3.906369
H	-11.6786	-2.6387	5.120446	-11.78	-2.26449	5.219133	-11.7713	-2.21993	5.247191
H	-13.3772	-2.21576	5.404939	-13.4917	-1.84836	5.422439	-13.4827	-1.8027	5.450996
H	-6.77782	-7.88031	1.863234	-6.71806	-7.67717	2.541636	-6.71523	-7.65836	2.597391
H	-5.91069	-6.62431	0.956294	-5.83404	-6.48162	1.572011	-5.83529	-6.4711	1.614006

H	-6.45796	-6.29989	2.619405	-6.45264	-6.03654	3.181333	-6.44578	-6.01289	3.222759
H	-8.96165	-6.14957	3.149153	-8.9786	-5.8967	3.601323	-8.96999	-5.8685	3.65377
H	-10.1635	-6.31065	1.838504	-10.1241	-6.17848	2.260241	-10.1218	-6.16012	2.320221
H	-9.19532	-7.7099	2.339507	-9.15629	-7.51741	2.904936	-9.15178	-7.49449	2.970917
H	-7.6428	-6.87158	-0.93751	-7.48506	-6.90772	-0.36349	-7.49587	-6.91154	-0.31013
H	-8.47524	-8.1136	0.018829	-8.33572	-8.08593	0.655301	-8.34193	-8.0812	0.722204
H	-9.37844	-6.69981	-0.57858	-9.23628	-6.74091	-0.08657	-9.24566	-6.74177	-0.0259
H	-12.8653	2.741139	-3.79004	-12.9295	2.502117	-3.87303	-12.9243	2.470794	-3.90637
H	-11.6786	2.638698	-5.12045	-11.78	2.264493	-5.21913	-11.7713	2.219932	-5.24719
H	-13.3772	2.215755	-5.40494	-13.4917	1.848356	-5.42244	-13.4827	1.802695	-5.451
H	-14.4029	0.174709	-4.47997	-14.524	-0.083	-4.28912	-14.519	-0.11716	-4.30252
H	-13.474	-0.98881	-3.51344	-13.585	-1.17916	-3.25618	-13.5837	-1.20409	-3.25656
H	-13.8975	0.597951	-2.82554	-13.9598	0.467856	-2.69258	-13.9589	0.448461	-2.70971
H	-11.7493	-1.13552	-5.42954	-11.9254	-1.52236	-5.20224	-11.9188	-1.56668	-5.19488
H	-12.7253	0.028293	-6.34884	-12.9067	-0.42056	-6.1888	-12.8967	-0.47359	-6.19442
H	-10.9982	0.351497	-6.05779	-11.1662	-0.11022	-5.97683	-11.1565	-0.16234	-5.98068

Os3	S0			S1			T1		
Symbol	X	Y	Z	X	Y	Z	X	Y	Z
Os	7.606776	0	0	7.614808	0	0	7.619539	0	0
Os	-7.60678	0	0	-7.61481	0	0	-7.61954	0	0
N	7.715131	2.044906	0.278666	7.692936	2.025767	0.395295	7.698638	2.022947	0.417107
N	9.100883	0.10254	1.424019	9.134569	0.04173	1.406596	9.136025	0.025409	1.407921
N	7.715131	-2.04491	-0.27867	7.692936	-2.02577	-0.3953	7.698638	-2.02295	-0.41711
N	9.100883	-0.10254	-1.42402	9.134569	-0.04173	-1.4066	9.136025	-0.02541	-1.40792
N	1.17285	-0.00231	1.417165	1.171178	-0.01532	1.42226	1.170235	-0.01814	1.425486
N	1.17285	0.002312	-1.41717	1.171178	0.015324	-1.42226	1.170235	0.018135	-1.42549
N	6.018893	-0.02821	1.31396	6.035937	-0.06834	1.325049	6.034008	-0.07386	1.323412
N	6.018893	0.028206	-1.31396	6.035937	0.068338	-1.32505	6.034008	0.073862	-1.32341
N	-1.17285	0.002312	1.417165	-1.17118	0.015324	1.42226	-1.17024	0.018135	1.425486
N	-1.17285	-0.00231	-1.41717	-1.17118	-0.01532	-1.42226	-1.17024	-0.01814	-1.42549
N	-6.01889	-0.02821	-1.31396	-6.03594	-0.06834	-1.32505	-6.03401	-0.07386	-1.32341
N	-6.01889	0.028206	1.31396	-6.03594	0.068338	1.325049	-6.03401	0.073862	1.323412
N	-7.71513	2.044906	-0.27867	-7.69294	2.025767	-0.3953	-7.69864	2.022947	-0.41711
N	-9.10088	0.10254	-1.42402	-9.13457	0.04173	-1.4066	-9.13603	0.025409	-1.40792
N	-7.71513	-2.04491	0.278666	-7.69294	-2.02577	0.395295	-7.69864	-2.02295	0.417107
N	-9.10088	-0.10254	1.424019	-9.13457	-0.04173	1.406596	-9.13603	-0.02541	1.407921
C	8.097847	4.77057	0.909159	8.04217	4.711135	1.172742	8.046352	4.698063	1.228757
C	7.137387	4.369161	-0.01741	7.057328	4.345785	0.257223	7.065527	4.344738	0.304226
C	6.967268	2.997448	-0.31418	6.901302	2.9906	-0.11311	6.910411	2.994419	-0.08372
C	8.660723	2.435013	1.203951	8.65825	2.376765	1.315718	8.660014	2.361642	1.346013
C	8.893684	3.783373	1.549639	8.876475	3.706207	1.733098	8.877674	3.685844	1.780281
C	9.416018	1.387444	1.813983	9.440056	1.309554	1.853131	9.439829	1.287681	1.872046
C	9.792973	-0.9199	1.965867	9.852617	-0.99903	1.869572	9.853623	-1.02162	1.859041
C	10.81283	-0.70441	2.921057	10.89283	-0.81929	2.810512	10.89059	-0.85374	2.805142
C	10.41682	1.683325	2.764008	10.46033	1.569754	2.791886	10.45759	1.535575	2.816691
C	11.12904	0.590714	3.32698	11.19967	0.457102	3.276706	11.19571	0.416724	3.288966
C	8.097847	-4.77057	-0.90916	8.04217	-4.71114	-1.17274	8.046352	-4.69806	-1.22876
C	7.137387	-4.36916	0.017406	7.057328	-4.34579	-0.25722	7.065527	-4.34474	-0.30423
C	6.967268	-2.99745	0.314179	6.901302	-2.9906	0.113109	6.910411	-2.99442	0.083718
C	8.660723	-2.43501	-1.20395	8.65825	-2.37677	-1.31572	8.660014	-2.36164	-1.34601
C	8.893684	-3.78337	-1.54964	8.876475	-3.70621	-1.7331	8.877674	-3.68584	-1.78028
C	9.416018	-1.38744	-1.81398	9.440056	-1.30955	-1.85313	9.439829	-1.28768	-1.87205
C	9.792973	0.919897	-1.96587	9.852617	0.99903	-1.86957	9.853623	1.021623	-1.85904
C	10.81283	0.704408	-2.92106	10.89283	0.819291	-2.81051	10.89059	0.853741	-2.80514
C	10.41682	-1.68333	-2.76401	10.46033	-1.56975	-2.79189	10.45759	-1.53558	-2.81669
C	11.12904	-0.59071	-3.32698	11.19967	-0.4571	-3.27671	11.19571	-0.41672	-3.28897
C	2.316102	0.002248	-0.72821	2.329268	0.013945	-0.7182	2.331744	0.0158	-0.71315
C	2.316102	-0.00225	0.728211	2.329268	-0.01395	0.718203	2.331744	-0.0158	0.713152

C	3.586583	-0.00956	1.457311	3.592179	-0.0433	1.440363	3.592919	-0.04789	1.43831
C	4.78143	-0.00909	0.722419	4.800678	-0.03049	0.713701	4.80004	-0.03298	0.716343
C	4.78143	0.00909	-0.72242	4.800678	0.030493	-0.7137	4.80004	0.032982	-0.71634
C	3.586583	0.009559	-1.45731	3.592179	0.043304	-1.44036	3.592919	0.04789	-1.43831
C	3.663603	-0.02091	2.864396	3.67478	-0.08809	2.850846	3.674886	-0.09819	2.851226
C	4.927258	-0.03066	3.46619	4.930438	-0.1142	3.463205	4.929938	-0.128	3.460865
C	6.084989	-0.03403	2.668842	6.098297	-0.10031	2.672389	6.09898	-0.11214	2.671218
C	6.084989	0.034026	-2.66884	6.098297	0.100314	-2.67239	6.09898	0.11214	-2.67122
C	4.927258	0.030664	-3.46619	4.930438	0.114203	-3.46321	4.929938	0.128002	-3.46087
C	3.663603	0.020913	-2.8644	3.67478	0.088088	-2.85085	3.674886	0.09819	-2.85123
C	0	0	0.719629	0	0	0.729665	0	0	0.733592
C	0	0	-0.71963	0	0	-0.72967	0	0	-0.73359
C	-2.3161	-0.00225	-0.72821	-2.32927	-0.01395	-0.7182	-2.33174	-0.0158	-0.71315
C	-2.3161	0.002248	0.728211	-2.32927	0.013945	0.718203	-2.33174	0.0158	0.713152
C	-3.58658	-0.00956	-1.45731	-3.59218	-0.0433	-1.44036	-3.59292	-0.04789	-1.43831
C	-4.78143	-0.00909	-0.72242	-4.80068	-0.03049	-0.7137	-4.80004	-0.03298	-0.71634
C	-4.78143	0.00909	0.722419	-4.80068	0.030493	0.713701	-4.80004	0.032982	0.716343
C	-3.58658	0.009559	1.457311	-3.59218	0.043304	1.440363	-3.59292	0.04789	1.43831
C	-3.6636	-0.02091	-2.8644	-3.67478	-0.08809	-2.85085	-3.67489	-0.09819	-2.85123
C	-4.92726	-0.03066	-3.46619	-4.93044	-0.1142	-3.46321	-4.92994	-0.128	-3.46087
C	-6.08499	-0.03403	-2.66884	-6.0983	-0.10031	-2.67239	-6.09898	-0.11214	-2.67122
C	-3.6636	0.020913	2.864396	-3.67478	0.088088	2.850846	-3.67489	0.09819	2.851226
C	-4.92726	0.030664	3.46619	-4.93044	0.114203	3.463205	-4.92994	0.128002	3.460865
C	-6.08499	0.034026	2.668842	-6.0983	0.100314	2.672389	-6.09898	0.11214	2.671218
C	-8.09785	4.77057	-0.90916	-8.04217	4.711135	-1.17274	-8.04635	4.698063	-1.22876
C	-7.13739	4.369161	0.017406	-7.05733	4.345785	-0.25722	-7.06553	4.344738	-0.30423
C	-6.96727	2.997448	0.314179	-6.9013	2.9906	0.113109	-6.91041	2.994419	0.083718
C	-8.66072	2.435013	-1.20395	-8.65825	2.376765	-1.31572	-8.66001	2.361642	-1.34601
C	-8.89368	3.783373	-1.54964	-8.87648	3.706207	-1.7331	-8.87767	3.685844	-1.78028
C	-9.41602	1.387444	-1.81398	-9.44006	1.309554	-1.85313	-9.43983	1.287681	-1.87205
C	-9.79297	-0.9199	-1.96587	-9.85262	-0.99903	-1.86957	-9.85362	-1.02162	-1.85904
C	-10.8128	-0.70441	-2.92106	-10.8928	-0.81929	-2.81051	-10.8906	-0.85374	-2.80514
C	-10.4168	1.683325	-2.76401	-10.4603	1.569754	-2.79189	-10.4576	1.535575	-2.81669
C	-11.129	0.590714	-3.32698	-11.1997	0.457102	-3.27671	-11.1957	0.416724	-3.28897
C	-8.09785	-4.77057	0.909159	-8.04217	-4.71114	1.172742	-8.04635	-4.69806	1.228757
C	-7.13739	-4.36916	-0.01741	-7.05733	-4.34579	0.257223	-7.06553	-4.34474	0.304226
C	-6.96727	-2.99745	-0.31418	-6.9013	-2.9906	-0.11311	-6.91041	-2.99442	-0.08372
C	-8.66072	-2.43501	1.203951	-8.65825	-2.37677	1.315718	-8.66001	-2.36164	1.346013
C	-8.89368	-3.78337	1.549639	-8.87648	-3.70621	1.733098	-8.87767	-3.68584	1.780281
C	-9.41602	-1.38744	1.813983	-9.44006	-1.30955	1.853131	-9.43983	-1.28768	1.872046
C	-9.79297	0.919897	1.965867	-9.85262	0.99903	1.869572	-9.85362	1.021623	1.859041
C	-10.8128	0.704408	2.921057	-10.8928	0.819291	2.810512	-10.8906	0.853741	2.805142

C	-10.4168	-1.68333	2.764008	-10.4603	-1.56975	2.791886	-10.4576	-1.53558	2.816691
C	-11.129	-0.59071	3.32698	-11.1997	-0.4571	3.276706	-11.1957	-0.41672	3.288966
C	-9.91997	-4.07524	2.525166	-9.92302	-3.96206	2.696428	-9.92134	-3.92911	2.749938
C	-10.6523	-3.06822	3.105544	-10.6857	-2.93713	3.201842	-10.6821	-2.89754	3.244607
C	-10.6523	3.068218	-3.10554	-10.6857	2.937125	-3.20184	-10.6821	2.897542	-3.24461
C	-9.91997	4.075243	-2.52517	-9.92302	3.96206	-2.69643	-9.92134	3.929107	-2.74994
C	9.919973	-4.07524	-2.52517	9.923017	-3.96206	-2.69643	9.921335	-3.92911	-2.74994
C	10.65225	-3.06822	-3.10554	10.68569	-2.93713	-3.20184	10.68214	-2.89754	-3.24461
C	10.65225	3.068218	3.105544	10.68569	2.937125	3.201842	10.68214	2.897542	3.244607
C	9.919973	4.075243	2.525166	9.923017	3.96206	2.696428	9.921335	3.929107	2.749938
H	6.511142	5.093508	-0.52498	6.401199	5.085798	-0.18511	6.411932	5.090588	-0.13199
H	6.231542	2.668821	-1.03986	6.146226	2.688682	-0.83019	6.158816	2.702147	-0.80852
H	9.528518	-1.92148	1.645143	9.593698	-1.98582	1.501842	9.596507	-2.00355	1.477359
H	11.33581	-1.56234	3.327191	11.43763	-1.68906	3.157703	11.43481	-1.72774	3.142424
H	6.511142	-5.09351	0.524975	6.401199	-5.0858	0.185113	6.411932	-5.09059	0.131991
H	6.231542	-2.66882	1.039855	6.146226	-2.68868	0.830185	6.158816	-2.70215	0.808516
H	9.528518	1.921483	-1.64514	9.593698	1.985817	-1.50184	9.596507	2.003554	-1.47736
H	11.33581	1.562338	-3.32719	11.43763	1.689058	-3.1577	11.43481	1.727741	-3.14242
H	2.751948	-0.02228	3.451598	2.758983	-0.10058	3.432171	2.758671	-0.1121	3.431434
H	5.0323	-0.03816	4.544444	5.027392	-0.14717	4.541656	5.027638	-0.16518	4.53927
H	7.074883	-0.05093	3.110595	7.084687	-0.12731	3.122304	7.085105	-0.14266	3.120966
H	7.074883	0.050934	-3.1106	7.084687	0.12731	-3.1223	7.085105	0.142655	-3.12097
H	5.0323	0.038164	-4.54444	5.027392	0.147173	-4.54166	5.027638	0.165179	-4.53927
H	2.751948	0.02228	-3.4516	2.758983	0.100584	-3.43217	2.758671	0.112103	-3.43143
H	-2.75195	-0.02228	-3.4516	-2.75898	-0.10058	-3.43217	-2.75867	-0.1121	-3.43143
H	-5.0323	-0.03816	-4.54444	-5.02739	-0.14717	-4.54166	-5.02764	-0.16518	-4.53927
H	-7.07488	-0.05093	-3.1106	-7.08469	-0.12731	-3.1223	-7.08511	-0.14266	-3.12097
H	-2.75195	0.02228	3.451598	-2.75898	0.100584	3.432171	-2.75867	0.112103	3.431434
H	-5.0323	0.038164	4.544444	-5.02739	0.147173	4.541656	-5.02764	0.165179	4.53927
H	-7.07488	0.050934	3.110595	-7.08469	0.12731	3.122304	-7.08511	0.142655	3.120966
H	-6.51114	5.093508	0.524975	-6.4012	5.085798	0.185113	-6.41193	5.090588	0.131991
H	-6.23154	2.668821	1.039855	-6.14623	2.688682	0.830185	-6.15882	2.702147	0.808516
H	-9.52852	-1.92148	-1.64514	-9.5937	-1.98582	-1.50184	-9.59651	-2.00355	-1.47736
H	-11.3358	-1.56234	-3.32719	-11.4376	-1.68906	-3.1577	-11.4348	-1.72774	-3.14242
H	-6.51114	-5.09351	-0.52498	-6.4012	-5.0858	-0.18511	-6.41193	-5.09059	-0.13199
H	-6.23154	-2.66882	-1.03986	-6.14623	-2.68868	-0.83019	-6.15882	-2.70215	-0.80852
H	-9.52852	1.921483	1.645143	-9.5937	1.985817	1.501842	-9.59651	2.003554	1.477359
H	-11.3358	1.562338	3.327191	-11.4376	1.689058	3.157703	-11.4348	1.727741	3.142424
H	-8.24177	-5.82087	1.144094	-8.17425	-5.74913	1.462735	-8.17774	-5.73232	1.532047
H	-11.9071	-0.77091	4.062661	-11.9931	-0.60845	4.00229	-11.9871	-0.55874	4.018651
H	-10.1008	-5.11356	2.788855	-10.0943	-4.98695	3.0126	-10.0923	-4.94992	3.079177
H	-11.4236	-3.29519	3.836099	-11.4724	-3.13673	3.923682	-11.4669	-3.08769	3.971069

H	-8.24177	5.820866	-1.14409	-8.17425	5.749134	-1.46274	-8.17774	5.732321	-1.53205
H	-11.9071	0.770913	-4.06266	-11.9931	0.608448	-4.00229	-11.9871	0.558736	-4.01865
H	-11.4236	3.295193	-3.8361	-11.4724	3.136731	-3.92368	-11.4669	3.087688	-3.97107
H	-10.1008	5.113555	-2.78886	-10.0943	4.986945	-3.0126	-10.0923	4.949916	-3.07918
H	8.241773	-5.82087	-1.14409	8.174249	-5.74913	-1.46274	8.177736	-5.73232	-1.53205
H	11.90708	-0.77091	-4.06266	11.99307	-0.60845	-4.00229	11.98708	-0.55874	-4.01865
H	10.10078	-5.11356	-2.78886	10.09426	-4.98695	-3.0126	10.09232	-4.94992	-3.07918
H	11.42359	-3.29519	-3.8361	11.47236	-3.13673	-3.92368	11.46687	-3.08769	-3.97107
H	8.241773	5.820866	1.144094	8.174249	5.749134	1.462735	8.177736	5.732321	1.532047
H	11.90708	0.770913	4.062661	11.99307	0.608448	4.00229	11.98708	0.558736	4.018651
H	11.42359	3.295193	3.836099	11.47236	3.136731	3.923682	11.46687	3.087688	3.971069
H	10.10078	5.113555	2.788855	10.09426	4.986945	3.0126	10.09232	4.949916	3.079177

Os4	S0			S1			T1		
Symbol	X	Y	Z	X	Y	Z	X	Y	Z
Os	-7.60791	0	0	-7.61716	0	0	-7.62235	0	0
Os	7.607908	0	0	7.617156	0	0	7.622348	0	0
N	7.716529	2.02948	0.34956	7.692109	2.027273	0.366482	7.698189	2.030368	0.361572
N	9.091376	0.07201	1.427597	9.127669	0.082614	1.402371	9.125208	0.08411	1.405981
N	7.716529	-2.02948	-0.34956	7.692109	-2.02727	-0.36648	7.698189	-2.03037	-0.36157
N	9.091376	-0.07201	-1.4276	9.127669	-0.08261	-1.40237	9.125208	-0.08411	-1.40598
N	1.172818	-0.01166	1.417117	1.171233	-0.00448	1.422374	1.170312	0.000001	1.425553
N	1.172818	0.01166	-1.41712	1.171233	0.004476	-1.42237	1.170312	-1E-06	-1.42555
N	6.018671	-0.05785	1.313807	6.035859	-0.03582	1.326761	6.033992	-0.0233	1.325919
N	6.018671	0.057849	-1.31381	6.035859	0.035824	-1.32676	6.033992	0.023295	-1.32592
N	-1.17282	0.01166	1.417117	-1.17123	0.004476	1.422374	-1.17031	-1E-06	1.425553
N	-1.17282	-0.01166	-1.41712	-1.17123	-0.00448	-1.42237	-1.17031	0.000001	-1.42555
N	-6.01867	-0.05785	-1.31381	-6.03586	-0.03582	-1.32676	-6.03399	-0.0233	-1.32592
N	-6.01867	0.057849	1.313807	-6.03586	0.035824	1.326761	-6.03399	0.023295	1.325919
N	-7.71653	2.02948	-0.34956	-7.69211	2.027273	-0.36648	-7.69819	2.030368	-0.36157
N	-9.09138	0.07201	-1.4276	-9.12767	0.082614	-1.40237	-9.12521	0.08411	-1.40598
N	-7.71653	-2.02948	0.34956	-7.69211	-2.02727	0.366482	-7.69819	-2.03037	0.361572
N	-9.09138	-0.07201	1.427597	-9.12767	-0.08261	1.402371	-9.12521	-0.08411	1.405981
C	8.026093	4.756806	1.103145	7.965577	4.747996	1.138675	7.965005	4.750088	1.138647
C	7.125202	4.351277	0.110335	7.033089	4.331965	0.179682	7.04425	4.33569	0.167764
C	6.991908	2.996928	-0.2477	6.915003	2.978866	-0.18675	6.929686	2.982924	-0.20138
C	8.625491	2.402606	1.317984	8.625156	2.407558	1.308735	8.620554	2.408893	1.314696
C	8.834847	3.743098	1.712654	8.819376	3.747429	1.709626	8.811318	3.748405	1.718769
C	9.384374	1.335431	1.898033	9.413433	1.349796	1.865576	9.404314	1.350692	1.876333
C	9.806474	-0.96553	1.907013	9.873653	-0.94642	1.848398	9.870733	-0.94543	1.854212
C	10.79651	-0.7916	2.891687	10.88806	-0.76102	2.805615	10.87586	-0.76116	2.820399
C	10.37429	1.591853	2.873181	10.4274	1.61814	2.811003	10.40978	1.617481	2.831047
C	11.08953	0.474335	3.414362	11.17327	0.507325	3.326958	11.15328	0.506114	3.349732
C	8.026093	-4.75681	-1.10315	7.965577	-4.748	-1.13868	7.965005	-4.75009	-1.13865
C	7.125202	-4.35128	-0.11034	7.033089	-4.33197	-0.17968	7.04425	-4.33569	-0.16776
C	6.991908	-2.99693	0.247695	6.915003	-2.97887	0.186748	6.929686	-2.98292	0.201384
C	8.625491	-2.40261	-1.31798	8.625156	-2.40756	-1.30874	8.620554	-2.40889	-1.3147
C	8.834847	-3.7431	-1.71265	8.819376	-3.74743	-1.70963	8.811318	-3.74841	-1.71877
C	9.384374	-1.33543	-1.89803	9.413433	-1.3498	-1.86558	9.404314	-1.35069	-1.87633
C	9.806474	0.965529	-1.90701	9.873653	0.946422	-1.8484	9.870733	0.945425	-1.85421
C	10.79651	0.791599	-2.89169	10.88806	0.761022	-2.80562	10.87586	0.761159	-2.8204
C	10.37429	-1.59185	-2.87318	10.4274	-1.61814	-2.811	10.40978	-1.61748	-2.83105
C	11.08953	-0.47434	-3.41436	11.17327	-0.50733	-3.32696	11.15328	-0.50611	-3.34973
C	2.316038	0.011325	-0.72808	2.329531	0.004057	-0.71814	2.33192	-4.8E-05	-0.7133
C	2.316038	-0.01133	0.72808	2.329531	-0.00406	0.718138	2.33192	0.000048	0.7133

C	3.586532	-0.0359	1.456698	3.592449	-0.01505	1.44078	3.593184	-0.0036	1.439121
C	4.781627	-0.02399	0.722137	4.801059	-0.01461	0.714455	4.800515	-0.00808	0.717234
C	4.781627	0.023992	-0.72214	4.801059	0.014613	-0.71446	4.800515	0.008076	-0.71723
C	3.586532	0.035898	-1.4567	3.592449	0.015051	-1.44078	3.593184	0.0036	-1.43912
C	3.662743	-0.07587	2.863276	3.674581	-0.02787	2.85216	3.674645	-0.00433	2.852959
C	4.925996	-0.10234	3.465305	4.929902	-0.03502	3.465239	4.929424	-0.00494	3.463751
C	6.083931	-0.09226	2.66845	6.098007	-0.03551	2.674436	6.098598	-0.01153	2.674204
C	6.083931	0.092255	-2.66845	6.098007	0.03551	-2.67444	6.098598	0.011527	-2.6742
C	4.925996	0.102338	-3.46531	4.929902	0.035024	-3.46524	4.929424	0.004937	-3.46375
C	3.662743	0.075871	-2.86328	3.674581	0.027872	-2.85216	3.674645	0.004331	-2.85296
C	0	0	0.719631	0	0	0.729805	0	0	0.733563
C	0	0	-0.71963	0	0	-0.72981	0	0	-0.73356
C	-2.31604	-0.01133	-0.72808	-2.32953	-0.00406	-0.71814	-2.33192	0.000048	-0.7133
C	-2.31604	0.011325	0.72808	-2.32953	0.004057	0.718138	-2.33192	-4.8E-05	0.7133
C	-3.58653	-0.0359	-1.4567	-3.59245	-0.01505	-1.44078	-3.59318	-0.0036	-1.43912
C	-4.78163	-0.02399	-0.72214	-4.80106	-0.01461	-0.71446	-4.80052	-0.00808	-0.71723
C	-4.78163	0.023992	0.722137	-4.80106	0.014613	0.714455	-4.80052	0.008076	0.717234
C	-3.58653	0.035898	1.456698	-3.59245	0.015051	1.44078	-3.59318	0.0036	1.439121
C	-3.66274	-0.07587	-2.86328	-3.67458	-0.02787	-2.85216	-3.67465	-0.00433	-2.85296
C	-4.926	-0.10234	-3.46531	-4.9299	-0.03502	-3.46524	-4.92942	-0.00494	-3.46375
C	-6.08393	-0.09226	-2.66845	-6.09801	-0.03551	-2.67444	-6.0986	-0.01153	-2.6742
C	-3.66274	0.075871	2.863276	-3.67458	0.027872	2.85216	-3.67465	0.004331	2.852959
C	-4.926	0.102338	3.465305	-4.9299	0.035024	3.465239	-4.92942	0.004937	3.463751
C	-6.08393	0.092255	2.66845	-6.09801	0.03551	2.674436	-6.0986	0.011527	2.674204
C	-8.02609	4.756806	-1.10315	-7.96558	4.747996	-1.13868	-7.96501	4.750088	-1.13865
C	-7.1252	4.351277	-0.11034	-7.03309	4.331965	-0.17968	-7.04425	4.33569	-0.16776
C	-6.99191	2.996928	0.247695	-6.915	2.978866	0.186748	-6.92969	2.982924	0.201384
C	-8.62549	2.402606	-1.31798	-8.62516	2.407558	-1.30874	-8.62055	2.408893	-1.3147
C	-8.83485	3.743098	-1.71265	-8.81938	3.747429	-1.70963	-8.81132	3.748405	-1.71877
C	-9.38437	1.335431	-1.89803	-9.41343	1.349796	-1.86558	-9.40431	1.350692	-1.87633
C	-9.80647	-0.96553	-1.90701	-9.87365	-0.94642	-1.8484	-9.87073	-0.94543	-1.85421
C	-10.7965	-0.7916	-2.89169	-10.8881	-0.76102	-2.80562	-10.8759	-0.76116	-2.8204
C	-10.3743	1.591853	-2.87318	-10.4274	1.61814	-2.811	-10.4098	1.617481	-2.83105
C	-11.0895	0.474335	-3.41436	-11.1733	0.507325	-3.32696	-11.1533	0.506114	-3.34973
C	-8.02609	-4.75681	1.103145	-7.96558	-4.748	1.138675	-7.96501	-4.75009	1.138647
C	-7.1252	-4.35128	0.110335	-7.03309	-4.33197	0.179682	-7.04425	-4.33569	0.167764
C	-6.99191	-2.99693	-0.2477	-6.915	-2.97887	-0.18675	-6.92969	-2.98292	-0.20138
C	-8.62549	-2.40261	1.317984	-8.62516	-2.40756	1.308735	-8.62055	-2.40889	1.314696
C	-8.83485	-3.7431	1.712654	-8.81938	-3.74743	1.709626	-8.81132	-3.74841	1.718769
C	-9.38437	-1.33543	1.898033	-9.41343	-1.3498	1.865576	-9.40431	-1.35069	1.876333
C	-9.80647	0.965529	1.907013	-9.87365	0.946422	1.848398	-9.87073	0.945425	1.854212
C	-10.7965	0.791599	2.891687	-10.8881	0.761022	2.805615	-10.8759	0.761159	2.820399

C	-10.3743	-1.59185	2.873181	-10.4274	-1.61814	2.811003	-10.4098	-1.61748	2.831047
C	-11.0895	-0.47434	3.414362	-11.1733	-0.50733	3.326958	-11.1533	-0.50611	3.349732
C	-9.90056	-3.99668	2.655158	-9.91035	-4.01529	2.617889	-9.89295	-4.01475	2.638418
C	-10.6341	-2.97419	3.204798	-10.6778	-3.00256	3.13897	-10.6558	-3.00125	3.164744
C	-10.6341	2.974191	-3.2048	-10.6778	3.002557	-3.13897	-10.6558	3.001251	-3.16474
C	-9.90056	3.996684	-2.65516	-9.91035	4.015291	-2.61789	-9.89295	4.014747	-2.63842
C	9.900555	-3.99668	-2.65516	9.910346	-4.01529	-2.61789	9.89295	-4.01475	-2.63842
C	10.63414	-2.97419	-3.2048	10.67777	-3.00256	-3.13897	10.65584	-3.00125	-3.16474
C	10.63414	2.974191	3.204798	10.67777	3.002557	3.13897	10.65584	3.001251	3.164744
C	9.900555	3.996684	2.655158	9.910346	4.015291	2.617889	9.89295	4.014747	2.638418
C	8.097774	6.18893	1.490332	8.021048	6.177385	1.535005	8.017488	6.179155	1.536674
C	8.07673	6.576835	2.84809	8.047304	6.554281	2.895859	8.028016	6.554935	2.898017
C	8.124637	7.185639	0.491062	7.983071	7.180728	0.542617	7.993215	7.183293	0.544704
C	8.092838	7.936043	3.198751	8.045621	7.91095	3.255779	8.024466	7.911337	3.258986
C	8.149593	8.54476	0.842159	7.992092	8.537266	0.903141	8.000217	8.53955	0.906405
C	8.134664	8.924015	2.197339	8.023582	8.906195	2.260937	8.016174	8.907386	2.264756
C	12.09899	0.606857	4.495869	12.20688	0.650987	4.382704	12.17659	0.647583	4.415269
C	11.82783	1.364525	5.656357	11.95405	1.405705	5.549274	11.91286	1.400037	5.581013
C	13.32654	-0.08312	4.396799	13.43911	-0.02553	4.253194	13.40997	-0.02894	4.296022
C	12.77152	1.438232	6.693008	12.92131	1.48962	6.562903	12.87048	1.481612	6.603866
C	14.27376	-0.00227	5.429826	14.41004	0.067338	5.262606	14.37131	0.061843	5.314637
C	13.99922	0.759322	6.58102	14.15388	0.825461	6.420355	14.10429	0.817613	6.471506
C	12.09899	-0.60686	-4.49587	12.20688	-0.65099	-4.3827	12.17659	-0.64758	-4.41527
C	11.82783	-1.36453	-5.65636	11.95405	-1.40571	-5.54927	11.91286	-1.40004	-5.58101
C	13.32654	0.083118	-4.3968	13.43911	0.025527	-4.25319	13.40997	0.028939	-4.29602
C	12.77152	-1.43823	-6.69301	12.92131	-1.48962	-6.5629	12.87048	-1.48161	-6.60387
C	14.27376	0.00227	-5.42983	14.41004	-0.06734	-5.26261	14.37131	-0.06184	-5.31464
C	13.99922	-0.75932	-6.58102	14.15388	-0.82546	-6.42036	14.10429	-0.81761	-6.47151
C	8.097774	-6.18893	-1.49033	8.021048	-6.17739	-1.53501	8.017488	-6.17916	-1.53667
C	8.07673	-6.57684	-2.84809	8.047304	-6.55428	-2.89586	8.028016	-6.55494	-2.89802
C	8.124637	-7.18564	-0.49106	7.983071	-7.18073	-0.54262	7.993215	-7.18329	-0.5447
C	8.092838	-7.93604	-3.19875	8.045621	-7.91095	-3.25578	8.024466	-7.91134	-3.25899
C	8.149593	-8.54476	-0.84216	7.992092	-8.53727	-0.90314	8.000217	-8.53955	-0.90641
C	8.134664	-8.92402	-2.19734	8.023582	-8.9062	-2.26094	8.016174	-8.90739	-2.26476
C	-8.09777	6.18893	-1.49033	-8.02105	6.177385	-1.53501	-8.01749	6.179155	-1.53667
C	-8.07673	6.576835	-2.84809	-8.0473	6.554281	-2.89586	-8.02802	6.554935	-2.89802
C	-8.12464	7.185639	-0.49106	-7.98307	7.180728	-0.54262	-7.99322	7.183293	-0.5447
C	-8.09284	7.936043	-3.19875	-8.04562	7.91095	-3.25578	-8.02447	7.911337	-3.25899
C	-8.14959	8.54476	-0.84216	-7.99209	8.537266	-0.90314	-8.00022	8.53955	-0.90641
C	-8.13466	8.924015	-2.19734	-8.02358	8.906195	-2.26094	-8.01617	8.907386	-2.26476
C	-12.099	0.606857	-4.49587	-12.2069	0.650987	-4.3827	-12.1766	0.647583	-4.41527
C	-11.8278	1.364525	-5.65636	-11.954	1.405705	-5.54927	-11.9129	1.400037	-5.58101

C	-13.3265	-0.08312	-4.3968	-13.4391	-0.02553	-4.25319	-13.41	-0.02894	-4.29602
C	-12.7715	1.438232	-6.69301	-12.9213	1.48962	-6.5629	-12.8705	1.481612	-6.60387
C	-14.2738	-0.00227	-5.42983	-14.41	0.067338	-5.26261	-14.3713	0.061843	-5.31464
C	-13.9992	0.759322	-6.58102	-14.1539	0.825461	-6.42036	-14.1043	0.817613	-6.47151
C	-12.099	-0.60686	4.495869	-12.2069	-0.65099	4.382704	-12.1766	-0.64758	4.415269
C	-11.8278	-1.36453	5.656357	-11.954	-1.40571	5.549274	-11.9129	-1.40004	5.581013
C	-13.3265	0.083118	4.396799	-13.4391	0.025527	4.253194	-13.41	0.028939	4.296022
C	-12.7715	-1.43823	6.693008	-12.9213	-1.48962	6.562903	-12.8705	-1.48161	6.603866
C	-14.2738	0.00227	5.429826	-14.41	-0.06734	5.262606	-14.3713	-0.06184	5.314637
C	-13.9992	-0.75932	6.58102	-14.1539	-0.82546	6.420355	-14.1043	-0.81761	6.471506
C	-8.09777	-6.18893	1.490332	-8.02105	-6.17739	1.535005	-8.01749	-6.17916	1.536674
C	-8.07673	-6.57684	2.84809	-8.0473	-6.55428	2.895859	-8.02802	-6.55494	2.898017
C	-8.12464	-7.18564	0.491062	-7.98307	-7.18073	0.542617	-7.99322	-7.18329	0.544704
C	-8.09284	-7.93604	3.198751	-8.04562	-7.91095	3.255779	-8.02447	-7.91134	3.258986
C	-8.14959	-8.54476	0.842159	-7.99209	-8.53727	0.903141	-8.00022	-8.53955	0.906405
C	-8.13466	-8.92402	2.197339	-8.02358	-8.9062	2.260937	-8.01617	-8.90739	2.264756
H	6.488264	5.081069	-0.37859	6.359851	5.051482	-0.27397	6.37729	5.05609	-0.29367
H	6.289974	2.687938	-1.01412	6.188108	2.661012	-0.9256	6.211747	2.6663	-0.94964
H	9.570242	-1.95055	1.520436	9.642432	-1.93312	1.462798	9.645492	-1.93107	1.462535
H	11.31045	-1.66944	3.269313	11.4262	-1.63181	3.164563	11.41305	-1.63201	3.180535
H	6.488264	-5.08107	0.378589	6.359851	-5.05148	0.273967	6.37729	-5.05609	0.293674
H	6.289974	-2.68794	1.014115	6.188108	-2.66101	0.925597	6.211747	-2.6663	0.949638
H	9.570242	1.950553	-1.52044	9.642432	1.933118	-1.4628	9.645492	1.931069	-1.46254
H	11.31045	1.669437	-3.26931	11.4262	1.631806	-3.16456	11.41305	1.632011	-3.18054
H	2.750728	-0.08665	3.449803	2.758476	-0.03026	3.433099	2.758226	-0.00248	3.432968
H	5.030578	-0.13303	4.543201	5.026756	-0.04256	4.544203	5.02678	-0.00261	4.542839
H	7.073422	-0.12216	3.110557	7.084353	-0.0498	3.125098	7.084664	-0.02186	3.125039
H	7.073422	0.122164	-3.11056	7.084353	0.049801	-3.1251	7.084664	0.021855	-3.12504
H	5.030578	0.133029	-4.5432	5.026756	0.042564	-4.5442	5.02678	0.002611	-4.54284
H	2.750728	0.086649	-3.4498	2.758476	0.030259	-3.4331	2.758226	0.002481	-3.43297
H	-2.75073	-0.08665	-3.4498	-2.75848	-0.03026	-3.4331	-2.75823	-0.00248	-3.43297
H	-5.03058	-0.13303	-4.5432	-5.02676	-0.04256	-4.5442	-5.02678	-0.00261	-4.54284
H	-7.07342	-0.12216	-3.11056	-7.08435	-0.0498	-3.1251	-7.08466	-0.02186	-3.12504
H	-2.75073	0.086649	3.449803	-2.75848	0.030259	3.433099	-2.75823	0.002481	3.432968
H	-5.03058	0.133029	4.543201	-5.02676	0.042564	4.544203	-5.02678	0.002611	4.542839
H	-7.07342	0.122164	3.110557	-7.08435	0.049801	3.125098	-7.08466	0.021855	3.125039
H	-6.48826	5.081069	0.378589	-6.35985	5.051482	0.273967	-6.37729	5.05609	0.293674
H	-6.28997	2.687938	1.014115	-6.18811	2.661012	0.925597	-6.21175	2.6663	0.949638
H	-9.57024	-1.95055	-1.52044	-9.64243	-1.93312	-1.4628	-9.64549	-1.93107	-1.46254
H	-11.3104	-1.66944	-3.26931	-11.4262	-1.63181	-3.16456	-11.4131	-1.63201	-3.18054
H	-6.48826	-5.08107	-0.37859	-6.35985	-5.05148	-0.27397	-6.37729	-5.05609	-0.29367
H	-6.28997	-2.68794	-1.01412	-6.18811	-2.66101	-0.9256	-6.21175	-2.6663	-0.94964

H	-9.57024	1.950553	1.520436	-9.64243	1.933118	1.462798	-9.64549	1.931069	1.462535
H	-11.3104	1.669437	3.269313	-11.4262	1.631806	3.164563	-11.4131	1.632011	3.180535
H	-10.1458	-5.02482	2.900226	-10.1463	-5.04617	2.859781	-10.1263	-5.04521	2.88447
H	-11.4531	-3.2035	3.878539	-11.5146	-3.24202	3.786487	-11.4866	-3.23986	3.820338
H	-11.4531	3.2035	-3.87854	-11.5146	3.242023	-3.78649	-11.4866	3.239863	-3.82034
H	-10.1458	5.024824	-2.90023	-10.1463	5.046173	-2.85978	-10.1263	5.045214	-2.88447
H	10.1458	-5.02482	-2.90023	10.14626	-5.04617	-2.85978	10.12634	-5.04521	-2.88447
H	11.45312	-3.2035	-3.87854	11.51459	-3.24202	-3.78649	11.48657	-3.23986	-3.82034
H	11.45312	3.2035	3.878539	11.51459	3.242023	3.786487	11.48657	3.239863	3.820338
H	10.1458	5.024824	2.900226	10.14626	5.046173	2.859781	10.12634	5.045214	2.88447
H	8.014365	5.819992	3.62701	8.03366	5.791283	3.67101	8.003717	5.791342	3.672337
H	8.147149	6.896187	-0.55754	7.969395	6.89929	-0.50823	7.991709	6.902733	-0.50647
H	8.067104	8.222577	4.246222	8.055409	8.189767	4.305498	8.022259	8.189307	4.308976
H	8.182187	9.302753	0.064732	7.97569	9.301252	0.131234	7.994379	9.304154	0.134954
H	8.151289	9.975725	2.469437	8.026893	9.956048	2.540414	8.018072	9.957016	2.545083
H	10.86925	1.867555	5.763233	10.99243	1.896988	5.680001	10.95002	1.890924	5.703908
H	13.54679	-0.66387	3.503488	13.64471	-0.60374	3.354827	13.62423	-0.60512	3.398391
H	12.548	2.016577	7.584924	12.71253	2.064531	7.460478	12.65329	2.05456	7.500682
H	15.21982	-0.52805	5.337334	15.35988	-0.44673	5.147149	15.3222	-0.45199	5.207041
H	14.73074	0.819964	7.382036	14.90375	0.894675	7.20344	14.84676	0.885107	7.261756
H	10.86925	-1.86756	-5.76323	10.99243	-1.89699	-5.68	10.95002	-1.89092	-5.70391
H	13.54679	0.663874	-3.50349	13.64471	0.603737	-3.35483	13.62423	0.605121	-3.39839
H	12.548	-2.01658	-7.58492	12.71253	-2.06453	-7.46048	12.65329	-2.05456	-7.50068
H	15.21982	0.528046	-5.33733	15.35988	0.446727	-5.14715	15.3222	0.451988	-5.20704
H	14.73074	-0.81996	-7.38204	14.90375	-0.89468	-7.20344	14.84676	-0.88511	-7.26176
H	8.014365	-5.81999	-3.62701	8.03366	-5.79128	-3.67101	8.003717	-5.79134	-3.67234
H	8.147149	-6.89619	0.557536	7.969395	-6.89929	0.50823	7.991709	-6.90273	0.50647
H	8.067104	-8.22258	-4.24622	8.055409	-8.18977	-4.3055	8.022259	-8.18931	-4.30898
H	8.182187	-9.30275	-0.06473	7.97569	-9.30125	-0.13123	7.994379	-9.30415	-0.13495
H	8.151289	-9.97573	-2.46944	8.026893	-9.95605	-2.54041	8.018072	-9.95702	-2.54508
H	-8.01437	5.819992	-3.62701	-8.03366	5.791283	-3.67101	-8.00372	5.791342	-3.67234
H	-8.14715	6.896187	0.557536	-7.9694	6.89929	0.50823	-7.99171	6.902733	0.50647
H	-8.0671	8.222577	-4.24622	-8.05541	8.189767	-4.3055	-8.02226	8.189307	-4.30898
H	-8.18219	9.302753	-0.06473	-7.97569	9.301252	-0.13123	-7.99438	9.304154	-0.13495
H	-8.15129	9.975725	-2.46944	-8.02689	9.956048	-2.54041	-8.01807	9.957016	-2.54508
H	-10.8693	1.867555	-5.76323	-10.9924	1.896988	-5.68	-10.95	1.890924	-5.70391
H	-13.5468	-0.66387	-3.50349	-13.6447	-0.60374	-3.35483	-13.6242	-0.60512	-3.39839
H	-12.548	2.016577	-7.58492	-12.7125	2.064531	-7.46048	-12.6533	2.05456	-7.50068
H	-15.2198	-0.52805	-5.33733	-15.3599	-0.44673	-5.14715	-15.3222	-0.45199	-5.20704
H	-14.7307	0.819964	-7.38204	-14.9037	0.894675	-7.20344	-14.8468	0.885107	-7.26176
H	-10.8693	-1.86756	5.763233	-10.9924	-1.89699	5.680001	-10.95	-1.89092	5.703908
H	-13.5468	0.663874	3.503488	-13.6447	0.603737	3.354827	-13.6242	0.605121	3.398391

H	-12.548	-2.01658	7.584924	-12.7125	-2.06453	7.460478	-12.6533	-2.05456	7.500682
H	-15.2198	0.528046	5.337334	-15.3599	0.446727	5.147149	-15.3222	0.451988	5.207041
H	-14.7307	-0.81996	7.382036	-14.9037	-0.89468	7.20344	-14.8468	-0.88511	7.261756
H	-8.01437	-5.81999	3.62701	-8.03366	-5.79128	3.67101	-8.00372	-5.79134	3.672337
H	-8.14715	-6.89619	-0.55754	-7.9694	-6.89929	-0.50823	-7.99171	-6.90273	-0.50647
H	-8.0671	-8.22258	4.246222	-8.05541	-8.18977	4.305498	-8.02226	-8.18931	4.308976
H	-8.18219	-9.30275	0.064732	-7.97569	-9.30125	0.131234	-7.99438	-9.30415	0.134954
H	-8.15129	-9.97573	2.469437	-8.02689	-9.95605	2.540414	-8.01807	-9.95702	2.545083

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