# An investigation on the second-order nonlinear optical response of cationic bipyridine or phenanthroline iridium(III) complexes bearing cyclometallated 2-phenylpyridines with a triphenylamine substituent.

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# Supporting Information

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## Structure of ligands L1-L3

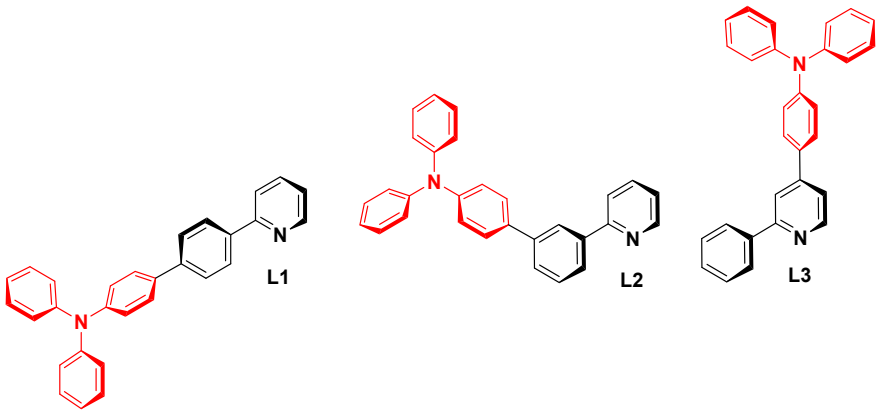



**Chart S1.** Ligands **L1-L3** used in this study

## X-ray Crystallography

Single crystals of sufficient quality of **3a** were grown from $CH_2Cl_2$/Hexane via vapor diffusion. X-ray diffraction data for **3a** were collected at 173 K by using a Rigaku FR-X Ultrahigh Brilliance Microfocus RA generator/confocal optics with XtaLAB P200 diffractometer [Mo Kα radiation (λ = 0.71075 Å)]. Intensity data were collected using ω steps accumulating area detector images spanning at least a hemisphere of reciprocal space. All data were corrected for Lorentz polarisation effects. A multiscan absorption correction was applied by using CrystalClear.[1] Structures were solved by dual-space methods (SHELXT)[2] and refined by full-matrix least-squares against $F^2$ (SHELXL-2016).[3] Non-hydrogen atoms

were refined anisotropically, and hydrogen atoms were refined using a riding model. All calculations were performed using the CrystalStructure[4] interface. Selected bond lengths, angles, and inter-planar angles are presented in Table S1, and selected crystallographic data are presented in Table S2. CCDC 1817920 contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures.

**Table S1**. Selected crystallographic parameters for complex **3a**

| | **Bond Length / Å** | | | **Bond Angle / °** | | **Inter-planar angle[a] / °** |
|---|---|---|---|---|---|---|
| | Ir-$C_{C^N}$ | Ir-$N_{C^N}$ | Ir-$N_{N^N}$ | $N_{N^N}$-Ir-$N_{N^N}$ | $C_{C^N}$-Ir-$N_{C^N}$ | |
| **3a** | 1.992(13)<br>1.994(13) | 2.027(10)<br>2.041(10) | 2.129(9)<br>2.131(10) | 75.9(4) | 79.9(4)<br>81.3(4) | 16.5(6)<br>41.4(3) |

[a] Angle between the ring-plane of the pyridine of the C^N ligand and that of the (non-coordinating) phenyl bound to that pyridine.

Table **S2.** Crystallographic data for complex **3a**

| | **3a** |
|---|---|
| Formula | $C_{77.25}H_{68.5}Cl_{2.5}F_6IrN_6P$ |
| Formula weight | 1506.75 |
| Crystal colour, habit | orange needle |
| Crystal dimensions ($mm^3$) | 0.13× 0.03× 0.01 |
| Space group | $P\bar{1}$ (No. 2) |
| a (Å) | 12.508(5) |
| b (Å) | 17.601(8) |
| c (Å) | 18.137(8) |
| $\alpha$ (°) | 111.009(8) |
| $\beta$ (°) | 102.642(9) |
| $\gamma$ (°) | 90.125(7) |
| Volume ($Å^3$) | 3623(3) |
| Z | 2 |
| $\rho_{calcd}$ (g $cm^{-3}$) | 1.381 |
| Temperature (K) | 173 |
| μ ($mm^{-1}$) | 2.023 |
| $\theta$ range | 1.834 – 25.242 |
| Reflections collected | 43499 |
| Independent reflections ($R_{int}$) | 13028 (0.1828) |
| Data/restraints/parameters | 13028/9/866 |
| $R_1$ [$I$>2σ($I$)] | 0.0869 |
| $wR_2$ (all data) | 0.2173 |
| Residual electron peak, hole | 1.61, -1.20 |

**Photophysical data**

Samples for all complexes were prepared in HPLC grade $CHCl_3$ with varying concentrations in the order of micromolar. Absorption spectra were recorded at room temperature using either a Shimadzu UV-1800 double beam spectrophotometer or a Biotek Instruments XS

spectrometer. Molar absorptivity determination was verified by linear least-squares fit of values obtained from at least four independent solutions at varying concentrations ranging from $3.93 \times 10^{-5}$ to $5.88 \times 10^{-6}$ M. The sample solutions for the emission spectra of **1a**, **2a** and **3a** were prepared in HPLC grade MeCN and degassed via three freeze−pump−thaw cycles using an in-house designed quartz cuvette. Steady-state and time-resolved emission spectra were recorded at room temperature using a Gilden photonics Fluorimeter. For steady-state measurements at room temperature, the complexes were excited at 420 nm. The excited-state lifetimes of the complex were obtained by time correlated single photon counting (TCSPC) at an excitation wavelength of 378 nm using an Edinburgh Instruments FLS980 fluorimeter using a pulsed diode laser, and PL emission was detected at the corresponding steady-state emission maximum for the complex. The room temperature PL decays were fitted with a multi exponential decay function. Emission quantum yields were determined using the optically dilute method.[5] A stock solution with absorbance of ca. 0.2 was prepared, and then four dilutions were prepared with dilution factors between 2 and 20 to obtain solutions with absorbances of ca. 0.100, 0.071, 0.052, and 0.026, respectively. The Beer−Lambert law was found to be linear at the concentrations of the solutions. For each sample, linearity between absorption and emission intensity was verified through linear regression analysis, and additional measurements were acquired until the Pearson regression factor ($R^2$) for the linear fit of the data set surpassed 0.9. Individual relative quantum yield values were calculated for each solution, and the values reported represent the slope value. The $\Phi_s = \Phi_r(A_r/A_s)(I_s/I_r)(n_s/n_r)^2$ equation was used to calculate the relative quantum yield of each of the samples, where $\Phi_r$ is the absolute quantum yield of the reference, $n$ is the refractive index of the solvent, $A$ is the absorbance at the excitation wavelength, and $I$ is the integrated area under the corrected emission curve. The subscripts $s$ and $r$ in the equation refer to the sample and

reference, respectively. A solution of $[Ru(bpy)_3](PF_6)_2$ in iaerated MeCN at 298 K ($\Phi_{PL}$ = 1.8%) was used as a reference.[6]

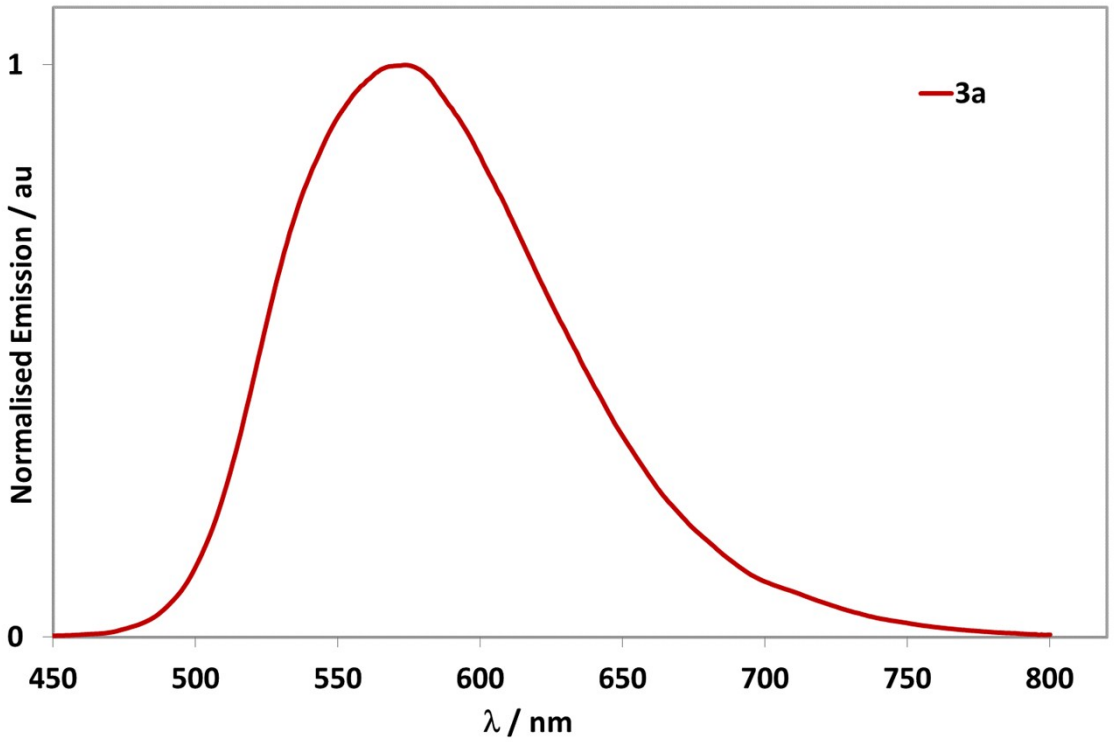



Figure **S1**. Normalised emission spectrum of **3a** in deaerated MeCN at 298 K.

Table **S3**. Photophysical properties of **3a** in deaerated MeCN at 298 K.

| | $\lambda_{em}$[a] / nm | $\Phi_{PL}$[b] / % | $\tau_{PL}$[c] / ns |
|---|---|---|---|
| | | | 77 (28%) |
| **3a** | 573 | 7 | 671 (42%) |
| | | | 5107 (30%) |

[a] $\lambda_{exc}$ = 420 nm; [b] $[Ru(bpy)_3](PF_6)_2$ in MeCN as reference ($\Phi_{PL}$ = 1.8% in aerated MeCN at 298 K);[6] [c] $\lambda_{exc}$ = 378 nm.

**Cyclovoltammetry**

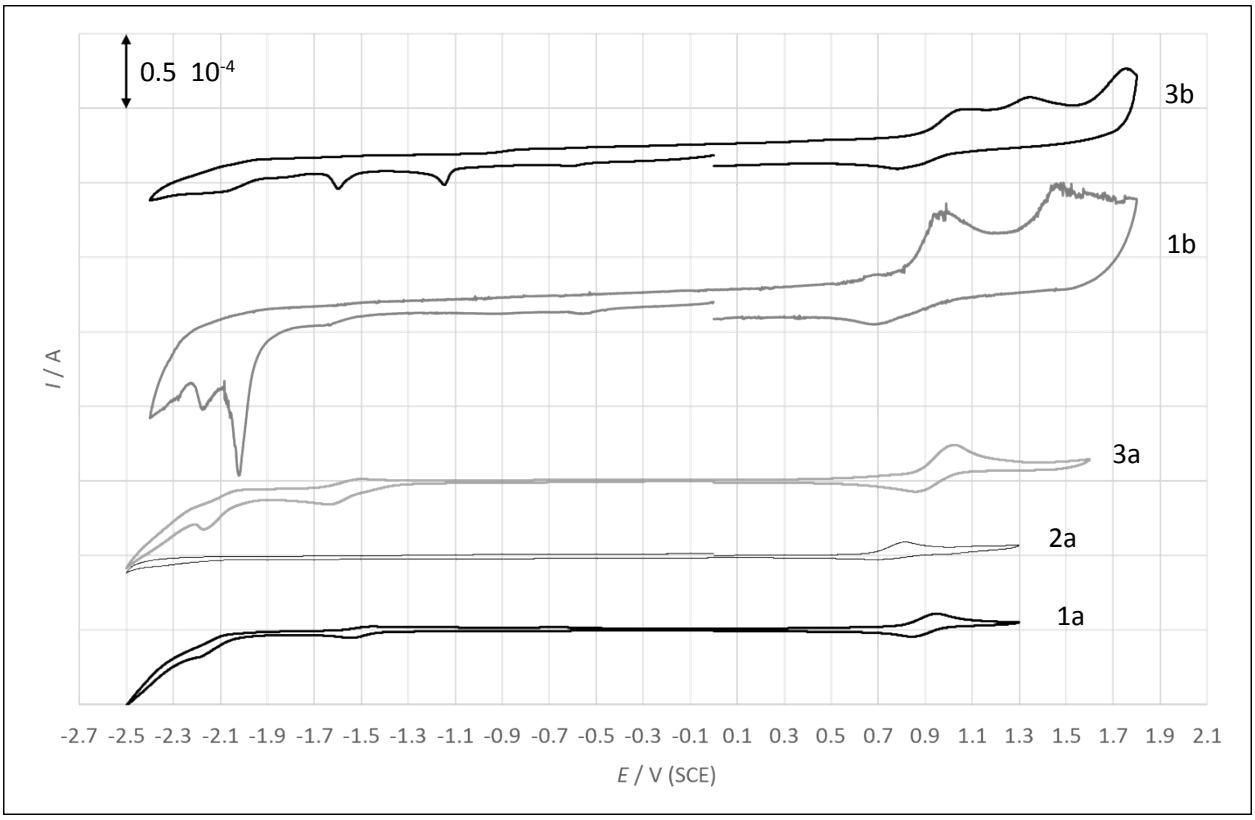



**Figure S2** Cyclic voltammograms of complexes 1a, 2a, 3a, 1b and 3b (0.001 M), scanned on GC at 100 mV $s^{-1}$ in acetonitrile with 0.1 M TBAP as supporting electrolyte.

The complexes were characterised by cyclic voltammetry (CV), at 0.1 V $s^{-1}$ potential scan rate in 1 mM solutions of acetonitrile (ACN), deaerated by $N_2$ purging before each experiment. 0.1 M tetrabutylammonium perchlorate (TBAP) was used as the supporting electrolyte. The experiments were carried out using an Autolab PGSTAT 12 potentiostat (EcoChemie, The Netherlands), run by a PC with NOVA 2.1.2 software. The working electrode was a 0.071 $cm^2$ glassy carbon (GC) disk embedded in Teflon® (Amel, Italy), polished with a diamond powder of 1 μm in diameter (Aldrich) on a wet Struers DP–Nap cloth, before each scan. The counter electrode was a platinum wire, while the reference electrode was an aqueous saturated calomel (SCE).

**Theoretical data**

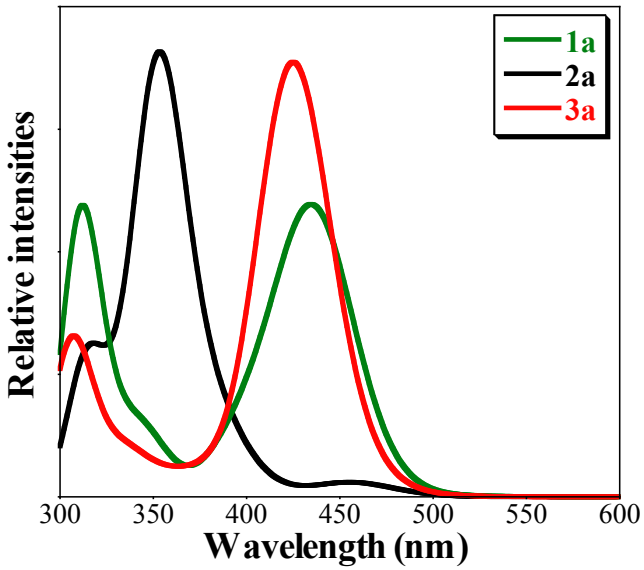


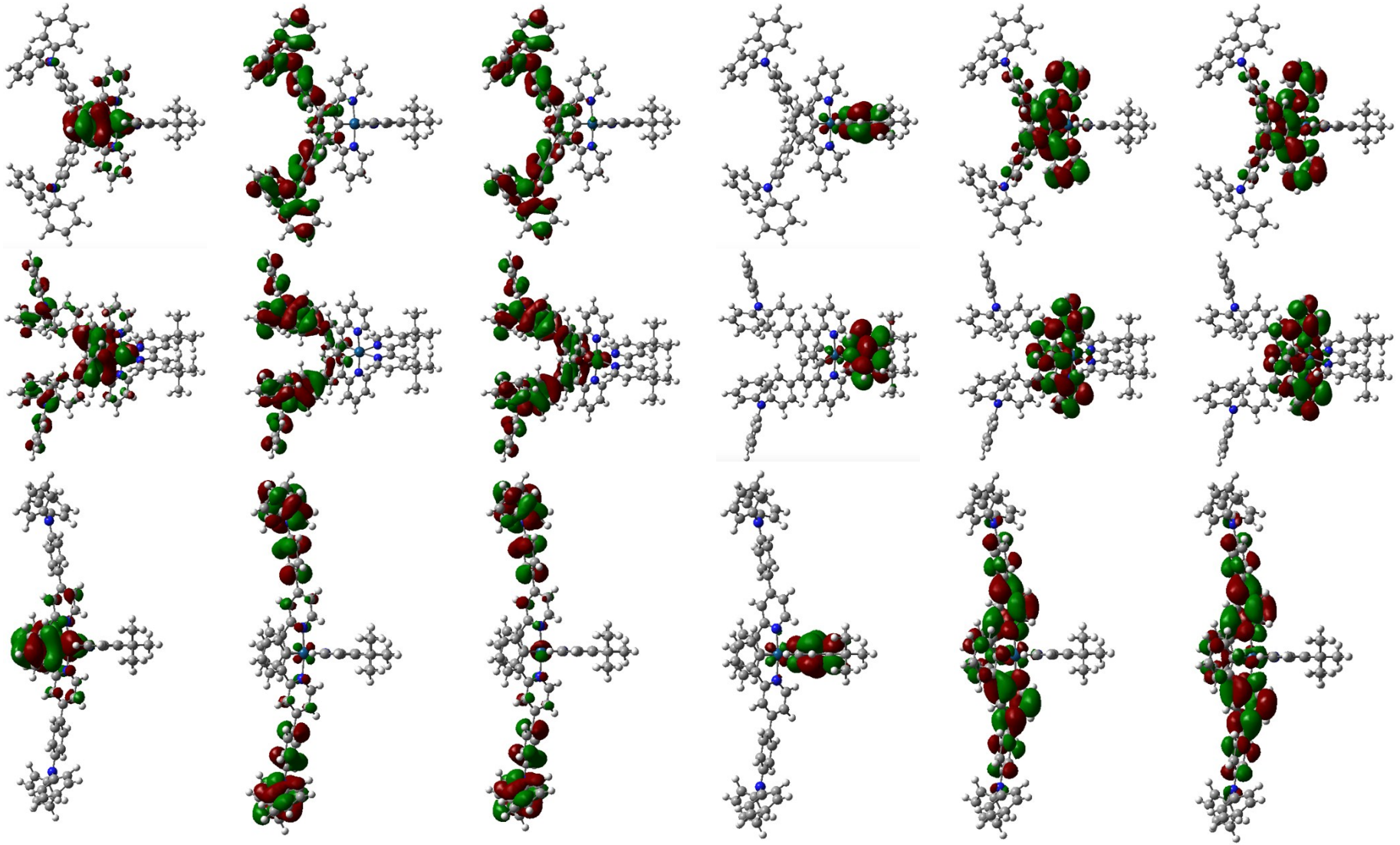

Figure **S3**. TD-DFT simulated spectra for **1a**, **2a** and **3a.** Broadening Gaussian HWHM used: 0.15 eV.

Table **S4**. TD-DFT data for the different complexes: first three significantly (dipole-)allowed excited-states.

| Compound | λ/nm | f | Dominant MO composition |
|---|---|---|---|
| **1a** | 440 | 0.86 | H to L+1 (0.63) |
| | 433 | 0.35 | H-1 to L+1 (0.61) |
| | 411 | 0.25 | H-1 to L+2 (0.49); H-2 to L+1 (0.48) |
| **1b** | 449 | 0.39 | H to L+2 (0.49); H to L+3 (0.37) |
| | 445 | 0.57 | H to L+3 (0.51); H to L+2 (0.34) |
| | 440 | 0.28 | H-1 to L+3 (0.59); H to L+4 (0.21) |
| **2a** | 458 | 0.06 | H to L+1 (0.61) |
| | 386 | 0.35 | H-4 to L (0.60); H-2 to L (0.30) |
| | 366 | 0.31 | H to L+5 (0.57); H-2 to L+1 (0.21) |
| **2b** | 472 | 0.14 | H-5 to L+2 (0.56); H-3 to L (0.21) |
| | 361 | 0.21 | H-2 to L+2 (0.33); H-16 to L (0.31) |
| | 360 | 0.15 | H-18 to L (0.63) |
| **3a** | 428 | 1.52 | H to L+1 (0.44); H-2 to L+1 (0.42); H-1 to L+2 (0.32) |
| | 416 | 0.46 | H-2 to L (0.54); H to L+1 (0.29); H-1 to L+2 (0.29) |
| | 388 | 0.08 | H-3 to L+1 (0.62); H-5 to L (0.22) |
| **3b** | 433 | 0.12 | H to L+3 (0.45); H-1 to L+4 (0.37); H-2 to L+3 (0.21) |
| | 430 | 1.80 | H to L+6 (0.56); H to L+7 (0.21) |
| | 356 | 0.08 | H-1 to L+3 (0.59); H to L+4 (0.21) |

Table **S5**. TD-DFT composition of the two lowest (vertical) triplet excited-states of **1a**, **2a** and **3a**.

| Compound | λ/nm | Dominant MO composition |
|---|---|---|
| **1a** | 534 | H to L+1 (0.44); H-1 to L+2 (-0.29) |
| | 531 | H-1 to L+1 (0.39); H to L+2 (-0.34) |
| **2a** | 568 | H to L (0.63); H-2 to L (0.30) |
| | 512 | H to L+1 (0.47); H-2 to L+2 (0.34) |
| **3a** | 511 | H-2 to L (0.62) |
| | 509 | H-1 to L+1 (0.41); H to L+2 (-0.41) |



H-2 H-1 H L L+1 L+2

Figure **S4**. Frontier orbitals of **1a** (top) **2a** (middle) and **3a** (bottom).

**DFT Cartesian coordinates (Å).**

**1a**

| | | | |
|---|---|---|---|
| 77 | 0.000000 | 0.000000 | 1.711661 |
| 7 | 0.799392 | 1.058599 | 3.434913 |
| 6 | 1.576299 | 2.152270 | 3.363879 |
| 6 | 0.432448 | 0.602033 | 4.654630 |
| 6 | 2.025046 | 2.828282 | 4.489403 |
| 1 | 1.844624 | 2.484362 | 2.359213 |
| 6 | 0.851762 | 1.241610 | 5.825304 |
| 6 | 1.666586 | 2.377311 | 5.771086 |
| 1 | 2.652836 | 3.707348 | 4.349577 |
| 7 | -0.799392 | -1.058599 | 3.434913 |
| 6 | -0.432448 | -0.602033 | 4.654630 |
| 6 | -1.576299 | -2.152270 | 3.363879 |
| 6 | -0.851762 | -1.241610 | 5.825304 |
| 6 | -2.025046 | -2.828282 | 4.489403 |
| 6 | -1.666586 | -2.377311 | 5.771086 |
| 1 | -2.652836 | -3.707348 | 4.349577 |
| 7 | -1.464032 | 1.443709 | 1.580016 |
| 6 | -2.595284 | 1.456308 | 2.310611 |
| 6 | -1.258999 | 2.401024 | 0.627537 |
| 6 | -3.589162 | 2.409065 | 2.133178 |
| 1 | -2.702694 | 0.660184 | 3.047960 |
| 6 | -2.228285 | 3.389999 | 0.407264 |
| 6 | -3.398796 | 3.395592 | 1.156247 |
| 1 | -4.488130 | 2.370911 | 2.743740 |
| 1 | -2.060430 | 4.144839 | -0.358716 |
| 6 | 0.783841 | 1.141689 | 0.264236 |
| 6 | 2.012085 | 0.968017 | -0.387182 |
| 6 | -0.000000 | 2.269366 | -0.093158 |
| 6 | 2.472076 | 1.864197 | -1.369620 |
| 1 | 2.654382 | 0.126532 | -0.111300 |
| 6 | 0.446806 | 3.175674 | -1.069281 |
| 6 | 1.668869 | 2.975811 | -1.700793 |
| 1 | -0.158800 | 4.039218 | -1.350125 |
| 1 | -1.844624 | -2.484362 | 2.359213 |
| 7 | 1.464032 | -1.443709 | 1.580016 |
| 6 | 2.595284 | -1.456308 | 2.310611 |
| 6 | 1.258999 | -2.401024 | 0.627537 |
| 6 | 3.589162 | -2.409065 | 2.133178 |
| 1 | 2.702694 | -0.660184 | 3.047960 |
| 6 | 2.228285 | -3.389999 | 0.407264 |
| 6 | -0.000000 | -2.269366 | -0.093158 |
| 6 | 3.398796 | -3.395592 | 1.156247 |
| 1 | 4.488130 | -2.370911 | 2.743740 |
| 1 | 2.060430 | -4.144839 | -0.358716 |
| 6 | -0.446806 | -3.175674 | -1.069281 |

| | | | |
|---|---|---|---|
| 6 | -2.012085 | -0.968017 | -0.387182 |
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| 1 | 0.158800 | -4.039218 | -1.350125 |
| 6 | -2.472076 | -1.864197 | -1.369620 |
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| 6 | -0.783841 | -1.141689 | 0.264236 |
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| 1 | 0.534463 | 0.849044 | 6.788743 |
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| 6 | -2.150518 | -3.119422 | 7.007945 |
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| 1 | 4.158168 | -4.156864 | 0.983046 |
| 1 | -1.989986 | -3.664757 | -2.482654 |
| 1 | 1.989986 | 3.664757 | -2.482654 |
| 6 | 3.765702 | 1.644198 | -2.043804 |
| 6 | 4.552304 | 2.723043 | -2.486277 |
| 6 | 4.262387 | 0.347359 | -2.269802 |
| 6 | 5.778517 | 2.523383 | -3.113987 |
| 1 | 4.220954 | 3.745801 | -2.298936 |
| 6 | 5.479150 | 0.134566 | -2.911479 |
| 1 | 3.663141 | -0.518821 | -1.981547 |
| 6 | 6.262129 | 1.221895 | -3.342068 |
| 1 | 6.375949 | 3.381944 | -3.421522 |
| 1 | 5.822974 | -0.883055 | -3.098401 |
| 6 | -3.765702 | -1.644198 | -2.043804 |
| 6 | -4.552304 | -2.723043 | -2.486277 |
| 6 | -4.262387 | -0.347359 | -2.269802 |
| 6 | -5.778517 | -2.523383 | -3.113987 |
| 1 | -4.220954 | -3.745801 | -2.298936 |
| 6 | -5.479150 | -0.134566 | -2.911479 |
| 1 | -3.663141 | 0.518821 | -1.981547 |
| 6 | -6.262129 | -1.221895 | -3.342068 |
| 1 | -6.375949 | -3.381944 | -3.421522 |
| 1 | -5.822974 | 0.883055 | -3.098401 |
| 7 | -7.496398 | -1.013314 | -3.987922 |
| 7 | 7.496398 | 1.013314 | -3.987922 |
| 6 | 7.932656 | 1.898429 | -5.008501 |
| 6 | 7.040355 | 2.343619 | -5.997467 |
| 6 | 9.269179 | 2.327547 | -5.044835 |
| 6 | 7.479508 | 3.212330 | -6.998853 |
| 1 | 6.003842 | 2.004333 | -5.978965 |
| 6 | 9.704416 | 3.184050 | -6.058416 |
| 1 | 9.963747 | 1.986380 | -4.276085 |
| 6 | 8.813334 | 3.635587 | -7.038948 |
| 1 | 6.776520 | 3.548170 | -7.761323 |
| 1 | 10.744654 | 3.509534 | -6.073967 |
| 1 | 9.154328 | 4.307967 | -7.825641 |
| 6 | 8.315641 | -0.090194 | -3.635747 |
| 6 | 8.519870 | -0.426553 | -2.287415 |
| 6 | 8.943029 | -0.850660 | -4.635892 |
| 6 | 9.330712 | -1.512384 | -1.949796 |

| | | | |
|---|---|---|---|
| 1 | 8.044418 | 0.169028 | -1.506948 |
| 6 | 9.764131 | -1.925953 | -4.289734 |
| 1 | 8.784012 | -0.593890 | -5.683989 |
| 6 | 9.960633 | -2.267210 | -2.946509 |
| 1 | 9.483730 | -1.759251 | -0.898988 |
| 1 | 10.244269 | -2.507380 | -5.076926 |
| 1 | 10.598917 | -3.109033 | -2.679696 |
| 6 | -8.315641 | 0.090194 | -3.635747 |
| 6 | -8.943029 | 0.850660 | -4.635892 |
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| 1 | -8.784012 | 0.593890 | -5.683989 |
| 6 | -9.330712 | 1.512384 | -1.949796 |
| 1 | -8.044418 | -0.169028 | -1.506948 |
| 6 | -9.960633 | 2.267210 | -2.946509 |
| 1 | -10.244269 | 2.507380 | -5.076926 |
| 1 | -9.483730 | 1.759251 | -0.898988 |
| 1 | -10.598917 | 3.109033 | -2.679696 |
| 6 | -7.932656 | -1.898429 | -5.008501 |
| 6 | -9.269179 | -2.327547 | -5.044835 |
| 6 | -7.040355 | -2.343619 | -5.997467 |
| 6 | -9.704416 | -3.184050 | -6.058416 |
| 1 | -9.963747 | -1.986380 | -4.276085 |
| 6 | -7.479508 | -3.212330 | -6.998853 |
| 1 | -6.003842 | -2.004333 | -5.978965 |
| 6 | -8.813334 | -3.635587 | -7.038948 |
| 1 | -10.744654 | -3.509534 | -6.073967 |
| 1 | -6.776520 | -3.548170 | -7.761323 |
| 1 | -9.154328 | -4.307967 | -7.825641 |
| 6 | -1.686174 | -2.454115 | 8.304081 |
| 1 | -0.589664 | -2.430673 | 8.384688 |
| 1 | -2.068950 | -1.427257 | 8.399120 |
| 1 | -2.064984 | -3.026467 | 9.161615 |
| 6 | 1.686174 | 2.454115 | 8.304081 |
| 1 | 0.589664 | 2.430673 | 8.384688 |
| 1 | 2.068950 | 1.427257 | 8.399120 |
| 1 | 2.064984 | 3.026467 | 9.161615 |
| 6 | -1.599374 | -4.554301 | 6.966812 |
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| 1 | -1.938597 | -5.101707 | 6.076905 |
| 1 | -0.500140 | -4.555520 | 6.970972 |
| 6 | -3.687279 | -3.158089 | 7.001629 |
| 1 | -4.087197 | -3.675601 | 6.119165 |
| 1 | -4.044327 | -3.695792 | 7.891291 |
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| 6 | 3.687279 | 3.158089 | 7.001629 |
| 1 | 4.087197 | 3.675601 | 6.119165 |
| 1 | 4.044327 | 3.695792 | 7.891291 |
| 1 | 4.108894 | 2.143209 | 7.024470 |
| 6 | 1.599374 | 4.554301 | 6.966812 |
| 1 | 1.945504 | 5.107220 | 7.851533 |

| | | | |
|---|---|---|---|
| 1 | 1.938597 | 5.101707 | 6.076905 |
| 1 | 0.500140 | 4.555520 | 6.970972 |

**1b**

| | | | |
|---|---|---|---|
| 77 | 0.032570 | 2.018928 | 0.076601 |
| 7 | -0.796652 | 3.762121 | 1.095045 |
| 6 | -1.706498 | 3.758286 | 2.068369 |
| 6 | -0.281729 | 4.953099 | 0.685737 |
| 6 | -2.168094 | 4.934284 | 2.687987 |
| 1 | -2.089852 | 2.779207 | 2.363679 |
| 6 | -0.692903 | 6.177612 | 1.248534 |
| 6 | -1.661334 | 6.153019 | 2.276360 |
| 1 | -2.914241 | 4.863131 | 3.475629 |
| 7 | 1.044954 | 3.716393 | -0.862281 |
| 6 | 0.704553 | 4.938073 | -0.364692 |
| 6 | 1.924111 | 3.643768 | -1.857134 |
| 6 | 1.279566 | 6.142229 | -0.840651 |
| 6 | 2.518008 | 4.788026 | -2.412958 |
| 6 | 2.204922 | 6.036158 | -1.907576 |
| 1 | 3.223026 | 4.679296 | -3.233646 |
| 7 | 1.335560 | 1.784229 | 1.657208 |
| 6 | 2.498360 | 2.449147 | 1.796013 |
| 6 | 0.984026 | 0.830502 | 2.569597 |
| 6 | 3.378769 | 2.205843 | 2.840950 |
| 1 | 2.728549 | 3.187240 | 1.027189 |
| 6 | 1.832827 | 0.546941 | 3.649062 |
| 6 | 3.034787 | 1.230745 | 3.786883 |
| 1 | 4.309257 | 2.764771 | 2.904032 |
| 1 | 1.546943 | -0.216345 | 4.370358 |
| 6 | -0.935934 | 0.598733 | 1.102587 |
| 6 | -2.169020 | 0.015546 | 0.786137 |
| 6 | -0.289094 | 0.179284 | 2.293639 |
| 6 | -2.762756 | -0.966719 | 1.600641 |
| 1 | -2.706572 | 0.342478 | -0.108437 |
| 6 | -0.871782 | -0.795577 | 3.120561 |
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| 6 | -1.900331 | 0.876450 | -3.546244 |
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| 6 | 1.833708 | -1.424904 | -2.778140 |

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| 6 | 0.861055 | 0.557026 | -1.011735 |
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| 1 | -3.710125 | 1.561267 | -4.494494 |
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| 6 | -4.425306 | -1.729607 | -0.121670 |
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| 6 | 8.284994 | -2.277046 | 1.261626 |
| 6 | 9.331151 | -4.297676 | 2.882456 |
| 1 | 8.429885 | -5.677836 | 1.481583 |
| 6 | 9.007038 | -1.950849 | 2.411609 |
| 1 | 7.888245 | -1.490025 | 0.618927 |
| 6 | 9.537657 | -2.956974 | 3.227806 |
| 1 | 9.734569 | -5.091838 | 3.510805 |
| 1 | 9.169921 | -0.902234 | 2.661489 |
| 1 | 10.107472 | -2.699429 | 4.120145 |
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| 6 | 0.827684 | 7.365752 | -0.220263 |
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| 1 | 2.668090 | 6.924992 | -2.323654 |

**2a**

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| 6 | -1.238354 | 2.365005 | 3.917011 |
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| 1 | -1.418490 | 2.753873 | 2.912843 |
| 6 | -0.738430 | 1.310385 | 6.376373 |
| 6 | -1.399711 | 2.541877 | 6.324380 |
| 1 | -2.159610 | 4.015866 | 4.905377 |
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| 1 | -4.103845 | -2.968532 | 3.325395 |
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| 6 | -0.000000 | 2.235608 | 0.152600 |
| 6 | -2.065404 | 1.056741 | 0.518316 |
| 6 | -0.644748 | 3.057163 | -0.772785 |
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| 6 | -2.709979 | 1.879511 | -0.417121 |
| 6 | -2.012124 | 2.898686 | -1.076973 |
| 1 | -3.762713 | 1.716062 | -0.659628 |
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| 7 | 1.943410 | 0.668850 | 2.142626 |
| 6 | 2.440962 | 1.693248 | 2.860977 |
| 6 | 2.736730 | 0.021595 | 1.240019 |
| 6 | 3.750747 | 2.132733 | 2.726104 |
| 1 | 1.750978 | 2.176225 | 3.553546 |
| 6 | 4.068516 | 0.419978 | 1.065822 |
| 6 | 2.065404 | -1.056741 | 0.518316 |
| 6 | 4.580911 | 1.478267 | 1.807385 |
| 1 | 4.103845 | 2.968532 | 3.325395 |
| 1 | 4.694090 | -0.097858 | 0.341233 |
| 6 | 2.709979 | -1.879511 | -0.417121 |
| 6 | 0.000000 | -2.235608 | 0.152600 |
| 6 | 2.012124 | -2.898686 | -1.076973 |
| 1 | 3.762713 | -1.716062 | -0.659628 |
| 6 | 0.644748 | -3.057163 | -0.772785 |
| 1 | -1.061666 | -2.405190 | 0.351150 |
| 6 | 0.691085 | -1.217918 | 0.831614 |
| 1 | 0.525895 | -0.850869 | 7.338977 |
| 1 | -0.525895 | 0.850869 | 7.338977 |
| 6 | -1.855590 | 3.298187 | 7.563135 |
| 6 | 1.855590 | -3.298187 | 7.563135 |
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| 1 | 5.691283 | -3.965694 | -5.403085 |

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| 1 | 8.867842 | -7.768083 | -5.841272 |
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| 1 | -3.736770 | 3.964264 | 8.413896 |
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| 1 | -1.531359 | 5.287137 | 6.674252 |
| 1 | -1.558923 | 5.255246 | 8.446241 |
| 1 | -0.133420 | 4.648057 | 7.571625 |
| 6 | -1.448953 | 2.593476 | 8.857884 |
| 1 | -1.905929 | 1.597020 | 8.945908 |
| 1 | -0.357252 | 2.490131 | 8.944246 |
| 1 | -1.792133 | 3.186663 | 9.716215 |
| 6 | 1.448953 | -2.593476 | 8.857884 |
| 1 | 1.905929 | -1.597020 | 8.945908 |
| 1 | 0.357252 | -2.490131 | 8.944246 |
| 1 | 1.792133 | -3.186663 | 9.716215 |
| 6 | 1.231136 | -4.702762 | 7.554441 |
| 1 | 1.531359 | -5.287137 | 6.674252 |
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| 1 | 0.081049 | -3.859369 | -1.253485 |
| 1 | -0.081049 | 3.859369 | -1.253485 |

**2b**

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| 6 | 2.942737 | 4.048469 | 0.349136 |
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| 6 | 3.844867 | 5.119527 | 0.432475 |
| 6 | 3.352541 | 6.404033 | 0.333080 |
| 1 | 4.905195 | 4.939119 | 0.589587 |
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| 6 | 0.091355 | 3.318496 | 2.908456 |

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| 6 | -1.384325 | 1.382088 | -0.212190 |
| 6 | -1.843174 | 0.725441 | -1.365637 |
| 6 | -2.116115 | 1.170733 | 0.983999 |
| 6 | -2.980159 | -0.083396 | -1.332985 |
| 1 | -1.316225 | 0.847268 | -2.315534 |
| 6 | -3.255031 | 0.353052 | 1.014761 |
| 6 | -3.711051 | -0.285846 | -0.145170 |
| 1 | -3.785732 | 0.185300 | 1.954736 |
| 1 | 3.283545 | 3.016701 | 0.450123 |
| 7 | 0.763444 | 2.439169 | -2.006492 |
| 6 | 0.322841 | 3.191367 | -3.033003 |
| 6 | 1.659939 | 1.435654 | -2.232841 |
| 6 | 0.745364 | 2.991240 | -4.339761 |
| 1 | -0.402291 | 3.967548 | -2.787398 |
| 6 | 2.122832 | 1.190456 | -3.532073 |
| 6 | 2.042696 | 0.693592 | -1.034192 |
| 6 | 1.666639 | 1.966819 | -4.591149 |
| 1 | 0.356312 | 3.622041 | -5.135323 |
| 1 | 2.834173 | 0.385368 | -3.706467 |
| 6 | 2.982666 | -0.346873 | -1.038404 |
| 6 | 1.712604 | 0.404344 | 1.331959 |
| 6 | 3.307786 | -1.024719 | 0.143193 |
| 1 | 3.453565 | -0.658435 | -1.973553 |
| 6 | 2.652480 | -0.627857 | 1.326061 |
| 1 | 1.235349 | 0.671510 | 2.278267 |
| 6 | 1.386442 | 1.099230 | 0.155812 |
| 1 | -1.877832 | 2.400357 | 5.510029 |
| 1 | 2.020214 | 1.776323 | -5.603379 |
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| 6 | -5.995088 | -0.860042 | 0.732760 |
| 6 | -5.038402 | -2.252954 | -0.974441 |
| 6 | -7.139903 | -1.652962 | 0.748386 |
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| 8 | -0.143340 | 7.180318 | 1.305647 |
| 8 | 0.518782 | 7.733638 | -0.680679 |

## References


1 In: CrystalClear-SM Expert v. 2.1; . Rigaku Americas, Rigaku Americas, The Woodlands, Texas, USA and Rigaku Corporation, Tokyo, Japan, (2015)

2 Sheldrick, G. M. *Acta Crystallogr., Sect. A*. **2015**, *71*, 3.

3 Sheldrick, G.: Crystal structure refinement with SHELXL. *Acta Crystallogr., Sect. C: Cryst. Struct. Commun*. 2015, **71**, 3.

4 In: CrystalStructure v4.2. The Woodlands, Texas, USA and Rigaku Corporation, Tokyo, Japan, (2015)

5 J. N. Demas and G. A. Crosby, *J. Phys. Chem.,* 1971, **75**, 991.

6 K. Suzuki, A. Kobayashi, S. Kaneko, K. Takehira, T. Yoshihara, H. Ishida, Y. Shiina, S. Oishi and S. Tobita, *Phys. Chem. Chem. Phys.*, 2009, **11**, 9850.