Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

I. Experimental section

For the synthesis of $\mathbf{L_{As,P}}$ ligand, the procedure was adapted from literature[1] and performed under inert atmosphere with distilled solvent. The synthesis of the tetrametallic metallacycle compound **A** was performed under air in a simple flask. The metallacycle derivative **B** was synthetized as previously published by our group.[2] Commercially available reagents ($[Cu(CH_3CN)_4].PF_6$ and dppm) and solvents were used as received without further purification.

^1H and $^{31}P\{^1H\}$ NMR spectra were recorded in CD_2Cl_2 on Bruker AV400 spectrometers. ^1H NMR chemical shifts were reported in parts per million (ppm) relative to Me_4Si as external standard. $^{31}P\{^1H\}$ NMR downfield chemical shifts were expressed in ppm, relative to 85% H_3PO_4 respectively.

FT-IR measurements have been performed on a Perkin Elmer Frontier spectrometer using UATR (Universal Attenuated Total Reflectance) accessory. Spectra have been recorded between 650 cm^{-1} and 4000 cm^{-1}, on pure solid samples.

UV-vis solid-state diffuse reflectance measurements were recorded on a Perkin-Elmer Lambda 650 spectrometer using a 60 mm integrating sphere. Reflectance spectra were recorded in relation to an external white reference (Spectralon®), between 800 nm and 200 nm with a spectral resolution of 1 nm on pure polycrystalline samples. The UV-vis spectra were transformed to apparent absorbance through $\log(\text{reflectance}^{-1})$.

Steady-state excitation and emission spectra measurements were recorded on a *Horiba Jobin-Yvon* (*HJY*) Fluorolog-3 (FL3-2iHR550) fluorescence spectrofluorometer equipped with an IR R928P PMT / *HJY* FL-1073 detector. Low temperature measurements were allowed by using an OptistatCF (*Oxford Inst.*) in the range of 77 K to 300 K. Excited-state lifetimes in the range of 80 K to 300 K were measured with a delta diode system allowing to measure excited-state lifetimes longer than 10 µs. Solid samples were placed in a quartz sample holder inside the cryostat and maintained at the desired temperature until equilibrium was reached before recording the spectrum.

The experimental data were then fitted according to the following equation:[3]

$$\tau(obs) = \frac{1+\frac{1}{3}\exp\left(-\frac{\Delta E_{ST}}{k_B T}\right)}{\frac{1}{\tau(T_1)}+\frac{1}{3\tau(S_1)}\exp\left(-\frac{\Delta E_{ST}}{k_B T}\right)} \qquad \text{Eq S1}$$

where $\tau(obs)$, $\tau(S_1)$, $\tau(T_1)$, k_B, T and ΔE_{ST} represent the observed lifetime, singlet state decay lifetime, triplet state decay lifetime, Boltzmann constant, temperature and singlet-triplet energy difference, respectively.

Powder X-ray diffraction diagrams have been collected using a Panalytical X'Pert Pro diffractometer with an X'celerator detector. The typical recording conditions were 45 kV, 40 mA for Cu Kα (λ = 1.542Å), the diagrams were recorded in theta/theta mode in 60 min between 4° and 40° with a step size of 0.0084° and a scan time of 50 s.

Thermal analyses have been performed using a Perkin Elmer Pyris Diamond TGA/TDA, between 25°C and 270°C in aluminum crucibles and between 25°C and 950°C in platinum crucibles under N2 atmosphere (5°C/min), and starting with a mass of sample ranging in between 5-40mg.

I.1. Synthesis

Synthesis of ligand $L_{As,P}$:

Synthesis of Ph_2AsCl was slightly adapted based on a previously reported procedure.[1] To a dry nitrogen filled Schlenk flask of chloride diphenylarsyl (7.34 mmol, 1.94 g) was added trimethylsilane diphenylphosphinemethane (7.34 mmol, 2.0 g) and the mixture was heated to 115 °C for 2.5 hours. When cooling down to room temperature, a white solid precipitate was formed. The volatile residues were removed *in vacuo* and the solid residue was washed with dry hexane and then stored at ambient atmosphere (2.88 g, yield: 92%).

^{1}H NMR (400 MHz, CD_2Cl_2, ppm): δ = 7.44 (*m*, H_{Ar}, 8H), 7.30 (*m*, H_{Ar}, 12H), 2.72 (*d*, –CH_2–, *J* = 2.3 Hz, H)

$^{31}P\{^1H\}$ NMR (161.98 MHz, CD_2Cl_2, ppm): δ = -21.56 (*s*, $P_{P,As}$)

IR (cm^{-1}): 3064, 2909, 1954 1880, 1812, 1759, 1656, 1579, 1479, 1431, 1377, 1305, 1269, 1181, 1155, 1120, 1074, 1024, 999, 969, 907, 844, 761, 733, 716, 690.

Synthesis of derivative A:

$[Cu(CH_3CN)_4]PF_6$ (55.9 mg, 0.15 mmol) and Ph_2P-CH_2-$AsPh_2$ (64.3 mg, 0.15 mmol) were dissolved in 15 ml dichloromethane and the solution was left undisturbed for 30 minutes. A methanol solution (3 ml) of KCN (4.9 mg, 0.075 mmol) was added to the crude solution. The colorless solution was stirred for 1 h. The solution was filtered over cotton and was left upon n-pentane vapor diffusion to obtain the product after crystallization (yields = 89 %).

^{1}H NMR (400 MHz, CD_2Cl_2, ppm): δ = 7.32–7.06 (*m*, H_{Ar}, 80H), 2.89 (*s*, –CH_2–, 8H)

$^{31}P\{^1H\}$ NMR (161.98 MHz, CD_2Cl_2, ppm): δ = - 9.45 (*s*, $P_{P,As}$), - 144.4 (*sept*, ^{1}J(P-F) = 711.0 Hz, PF_6^-)

IR (cm^{-1}): 3665, 3592, 3057, 2118 (υ(C≡N)), 1979, 1899, 1815, 1627, 1576, 1484, 1436, 1365, 1335, 1308, 1270, 1189, 1159, 1096, 1079, 1025, 999, 916, 833 (u = PF_6^-), 731, 691.

Positive ion ESI-MS (CH_2Cl_2, RT): m/z (%) = 429.05 $[C_{25}H_{23}AsP]^+$; 490.97 $[C_{25}H_{22}AsPCu]^+$; 919.01 $[C_{50}H_{44}As_2P_2Cu]^+$; 1009.93 overlap, major part $[C_{50}H_{44}As_2P_2Cu_2(CN)]^+$, minor part $[C_{100}H_{88}As_4P_4Cu_4(CN)_2]^{2+}$, 2162.81 $\{[C_{100}H_{88}As_4P_4Cu_4(CN)_2]^{2+}[PF_6]^-\}^+$

Negative ion ESI-MS (CH_2Cl_2, RT): m/z (%) = 144.97 $[PF_6]^-$.

Preparation of derivative A_g:

The ground sample phase $\mathbf{A_g}$ was obtained applying a manual grinding on **A** polycrystalline powder using a pestle in an agate mortar. As this grinding was conducted under UV-vis lamp light excitation (λ_{ex} = 365 nm), a greenish light emission was immediately observed at the place the grinding was applied.

^{1}H NMR (400 MHz, CD_2Cl_2, ppm): δ = 7.33–7.07 (*m*, H_{Ar}, 80H), 2.90 (*s*, $–CH_2–$, 8H)

$^{31}P\{^{1}H\}$ NMR (161.98 MHz, CD_2Cl_2, ppm): δ = - 9.59 (*s*, $P_{P,As}$), - 144.4 (*sept*, ^{1}J(P-F) = 711.0 Hz, PF_6^-)

IR (cm^{-1}): 2135 (υ(C≡N))

Characterizations of derivative A' obtained from thermal treatment of the derivative A:

^{1}H NMR (400 MHz, CD_2Cl_2, ppm): δ = 7.37–7.11 (*m*, H_{Ar}, 80H), 2.93 (*s*, $–CH_2–$, 8H)

$^{31}P\{^{1}H\}$ NMR (161.98 MHz, CD_2Cl_2, ppm): δ = - 9.69 (*s*, $P_{P,As}$), - 144.4 (*sept*, ^{1}J(P-F) = 711.0 Hz, PF_6^-)

IR (cm^{-1}): 2129 (υ(C≡N))

Characterizations of derivative A' obtained from thermal treatment of the derivative $\mathbf{A_g}$:

^{1}H NMR (400 MHz, CD_2Cl_2, ppm): δ = 7.32–7.07 (*m*, H_{Ar}, 80H), 2.89 (*s*, $–CH_2–$, 8H)

$^{31}P\{^{1}H\}$ NMR (161.98 MHz, CD_2Cl_2, ppm): δ = - 9.65 (*s*, $P_{P,As}$), - 144.4 (*sept*, ^{1}J(P-F) = 711.0 Hz, PF_6^-)

IR (cm^{-1}): 2129 (υ(C≡N))

Characterizations of derivative $\mathbf{B_g}$:

^{1}H NMR (400 MHz, CD_2Cl_2, ppm): δ = 7.69–6.81 (*m*, H_{Ar}, 80H), 3.06 (*s*, $–CH_2–$, 8H)

$^{31}P\{^{1}H\}$ NMR (161.98 MHz, CD_2Cl_2, ppm): δ = - 8.84 (*s*, $P_{P,As}$), - 10.94 (*s*, $P_{P,As}$), - 144.4 (*sept*, ^{1}J(P-F) = 711.0 Hz, PF_6^-)

IR (cm^{-1}): 2121 (υ(C≡N))

Characterizations of derivative B' obtained from thermal treatment of the derivative B:

^{1}H NMR (400 MHz, CD_2Cl_2, ppm): δ = 7.74–6.84 (*m*, H_{Ar}, 80H), 3.09 (*s*, $–CH_2–$, 8H)

$^{31}P\{^{1}H\}$ NMR (161.98 MHz, CD_2Cl_2, ppm): δ = - 8.87 (*s*, $P_{P,As}$), - 10.98 (*s*, $P_{P,As}$), - 144.4 (*sept*, ^{1}J(P-F) = 711.0 Hz, PF_6^-)

IR (cm^{-1}): 2126 (υ(C≡N))

Characterizations of derivative B' obtained from thermal treatment of the derivative $\mathbf{B_g}$:

^{1}H NMR (400 MHz, CD_2Cl_2, ppm): δ = 7.69–6.81 (*m*, H_{Ar}, 80H), 3.06 (*s*, $–CH_2–$, 8H)

$^{31}P\{^{1}H\}$ NMR (161.98 MHz, CD_2Cl_2, ppm): δ = - 8.84 (*s*, $P_{P,As}$), - 10.94 (*s*, $P_{P,As}$), - 144.4 (*sept*, ^{1}J(P-F) = 711.0 Hz, PF_6^-)

IR (cm^{-1}): 2126 (υ(C≡N))

I.2. NMR spectroscopy:

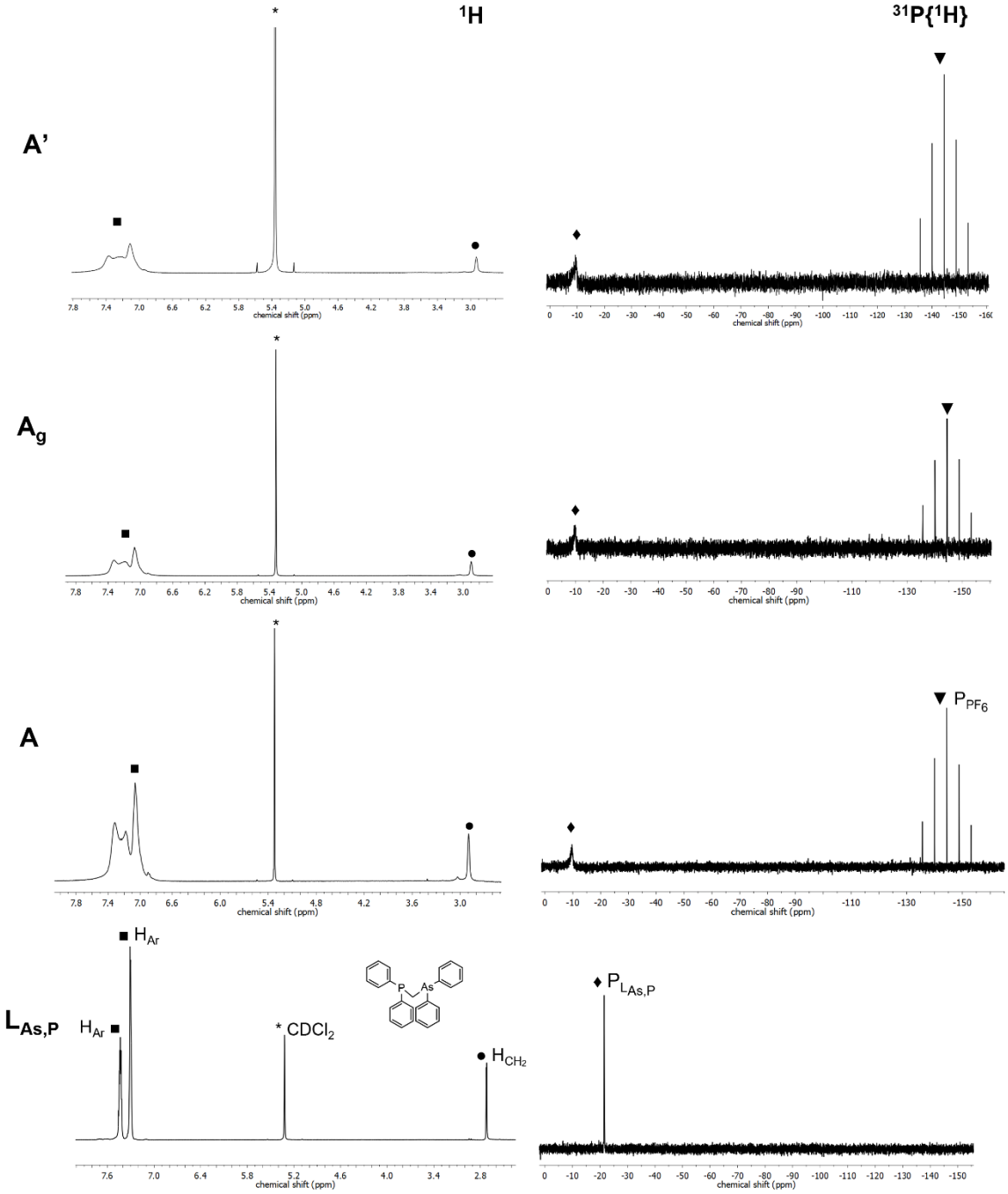

Fig. S1. ^{1}H NMR (left) and ^{31}P{^{1}H} NMR (right) spectra of **$L_{As,P}$** ligand and **A**, **A_g** and **A'** phases in CD_2Cl_2 at 400 MHz and 300 K

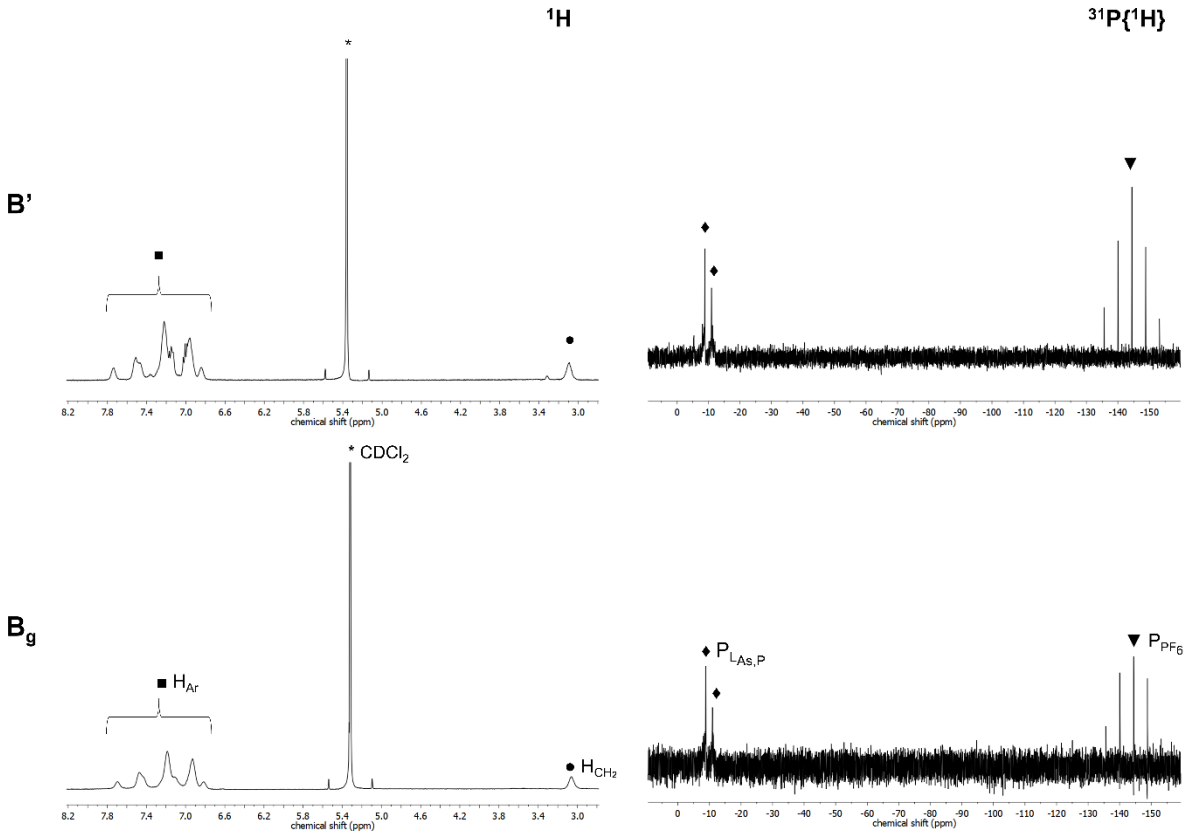

Fig. S2. ^{1}H NMR (left) and ^{31}P{^{1}H} NMR (right) spectra of **B$_g$** and **B'** phases in CD_2Cl_2 at 400 MHz and 300 K

I.3. Infrared spectroscopy:

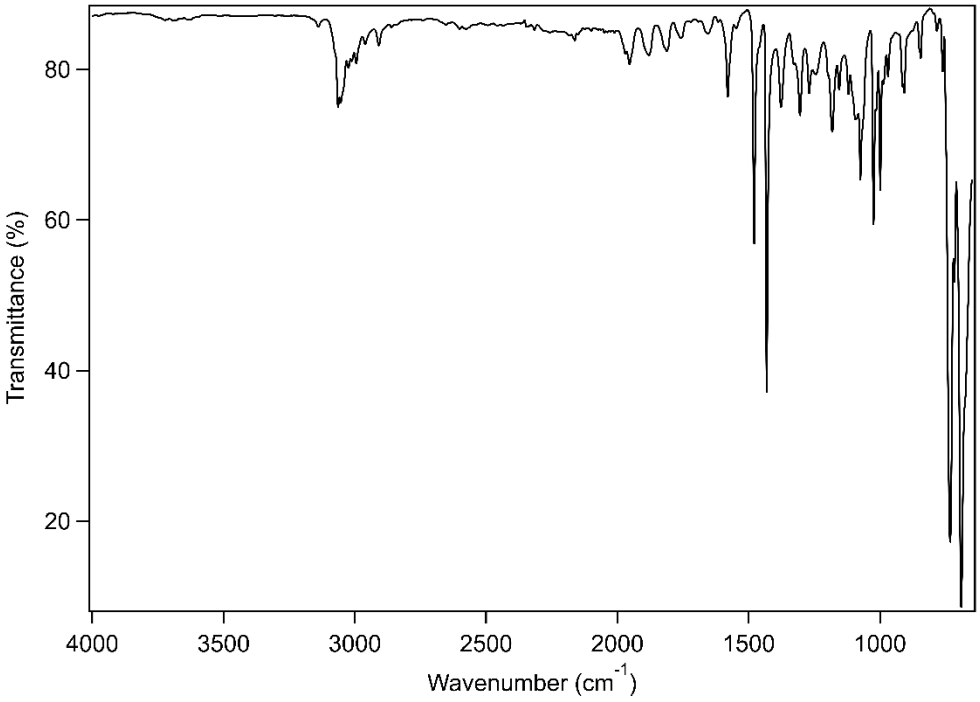

Fig. S3. Infrared spectrum of $\mathbf{L_{As,P}}$ ligand

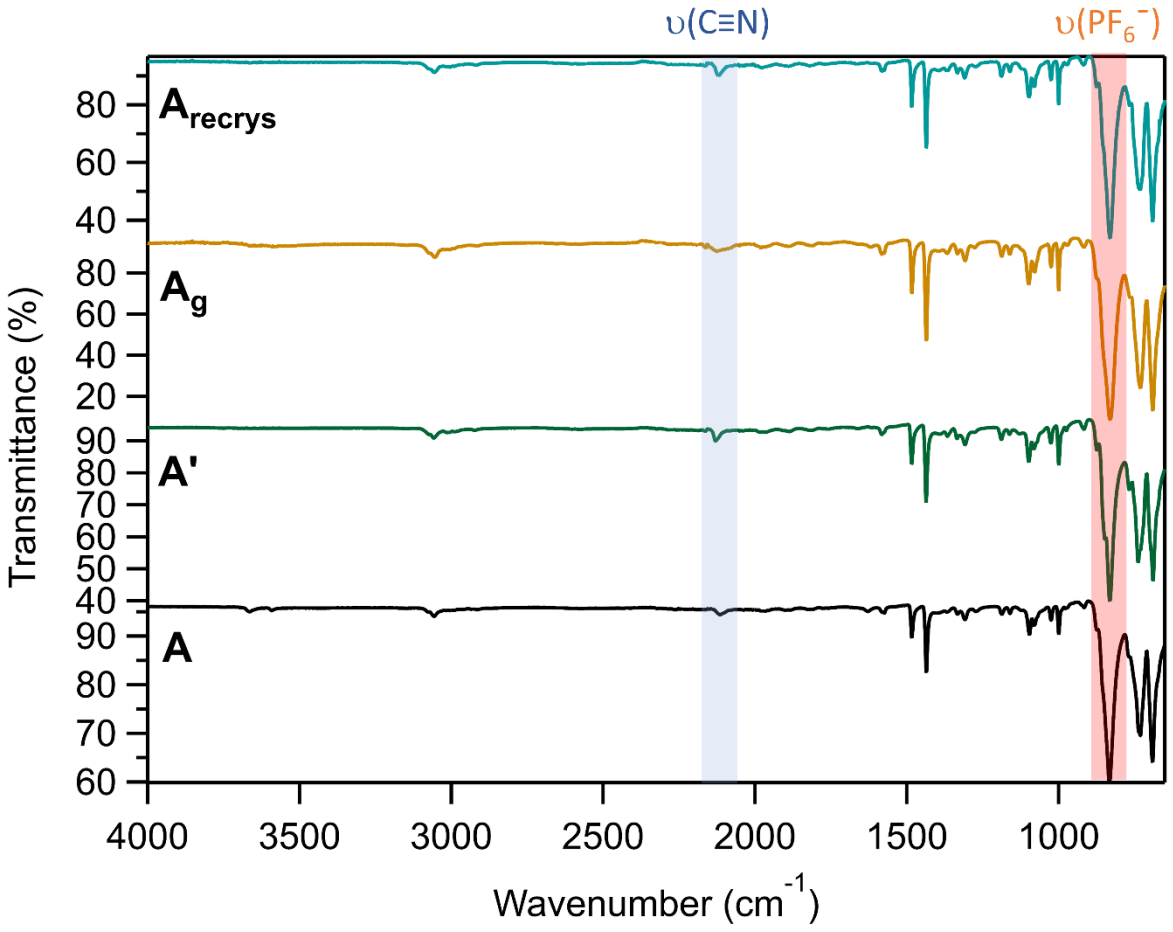

Fig. S4. Infrared spectra of derivatives **A** (black), **A'** (green), $\mathbf{A_g}$ (brown) and $\mathbf{A_{recrys}}$ (light blue).

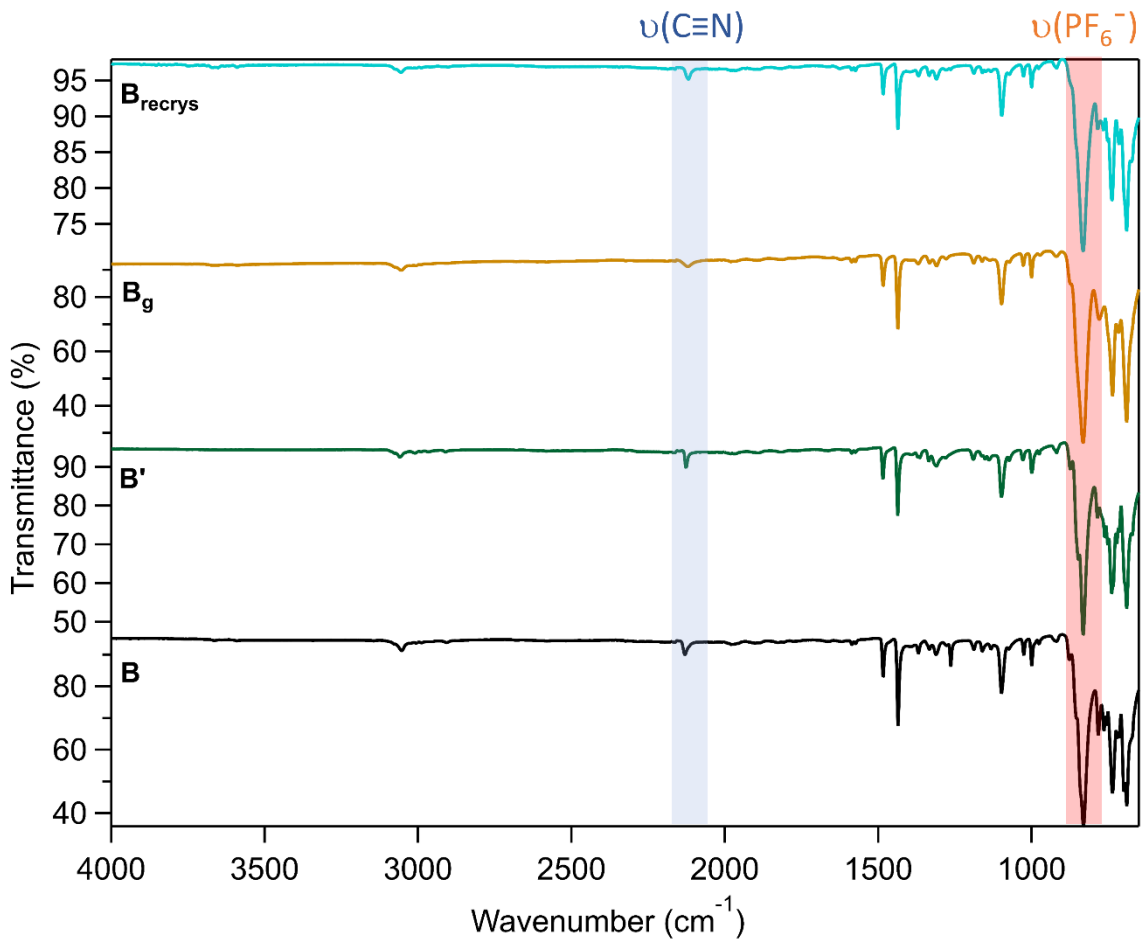

Fig. S5. Infrared spectra of derivatives **B**[2] (black), **B'** (green), $\mathbf{B_g}$ (brown) and $\mathbf{B_{recrys}}$ (light blue).

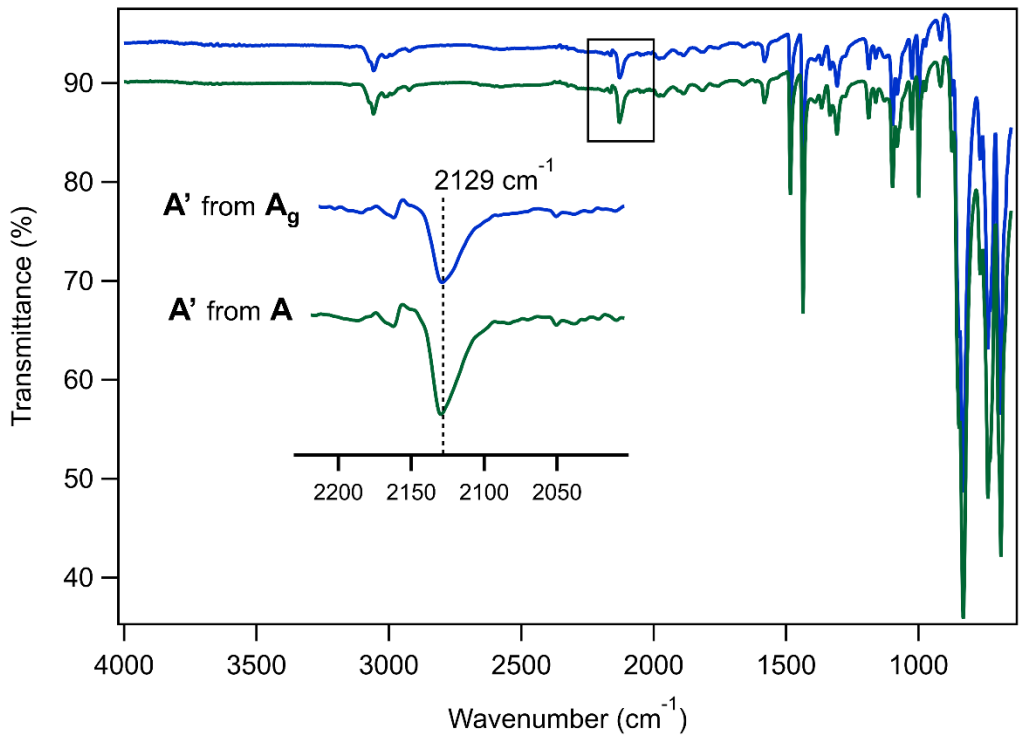

Fig. S6. Infrared spectra of derivative **A'** generated by thermal treatment of compound **A** (green curve) or of compound $\mathbf{A_g}$ (blue curve)

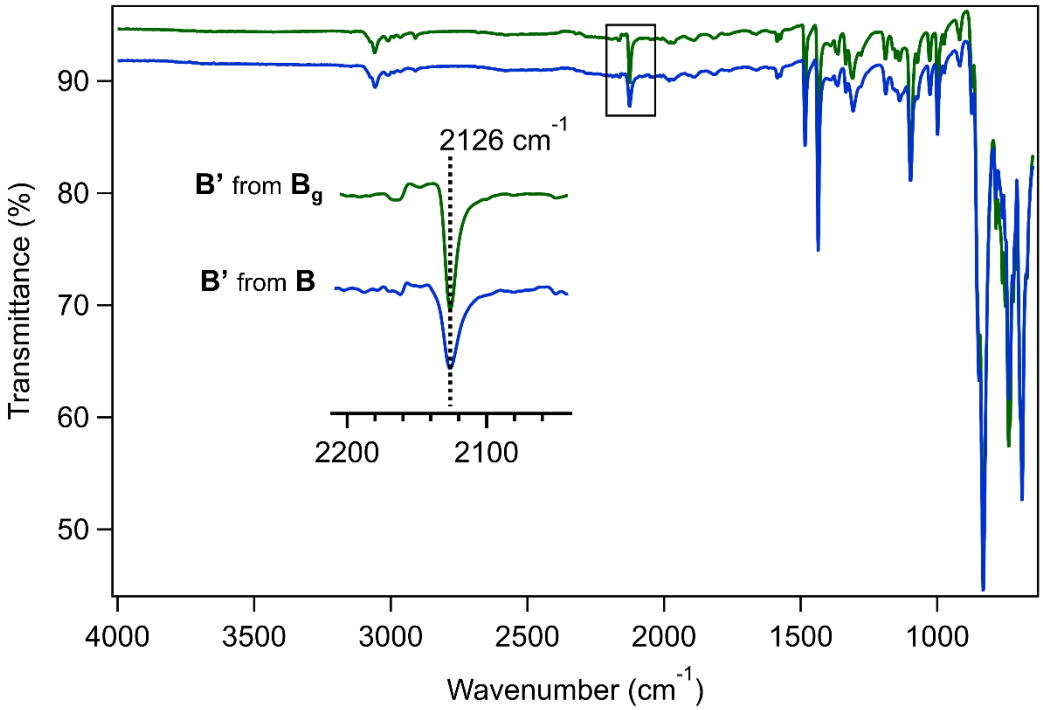

Fig. S7. Infrared spectra of derivative **B'** generated by thermal treatment of compound **B** (green curve) or of compound $\mathbf{B_g}$ (blue curve)

I.4. Powder X-Ray Diffraction diagrams:

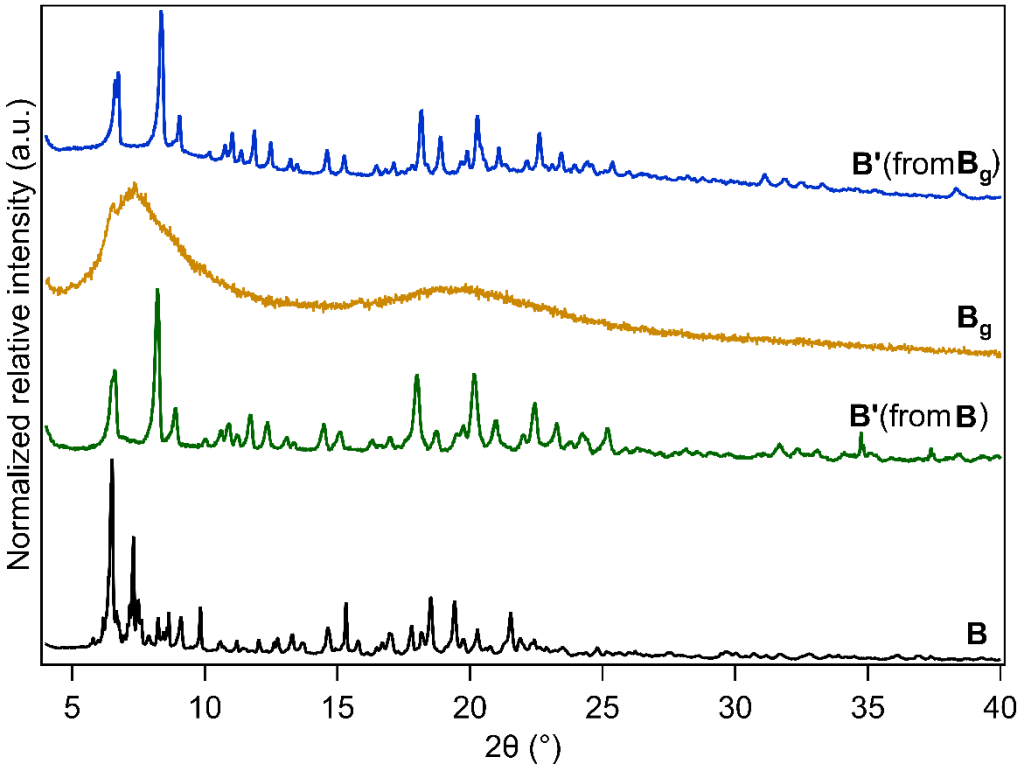

Fig. S8. Powder X-ray diffraction patterns of derivatives **B**[2] (black), **B'** (green, generated from a thermal treatment of compound **B**), $\mathbf{B_g}$, and **B'** (blue, generated from a thermal treatment of compound $\mathbf{B_g}$)

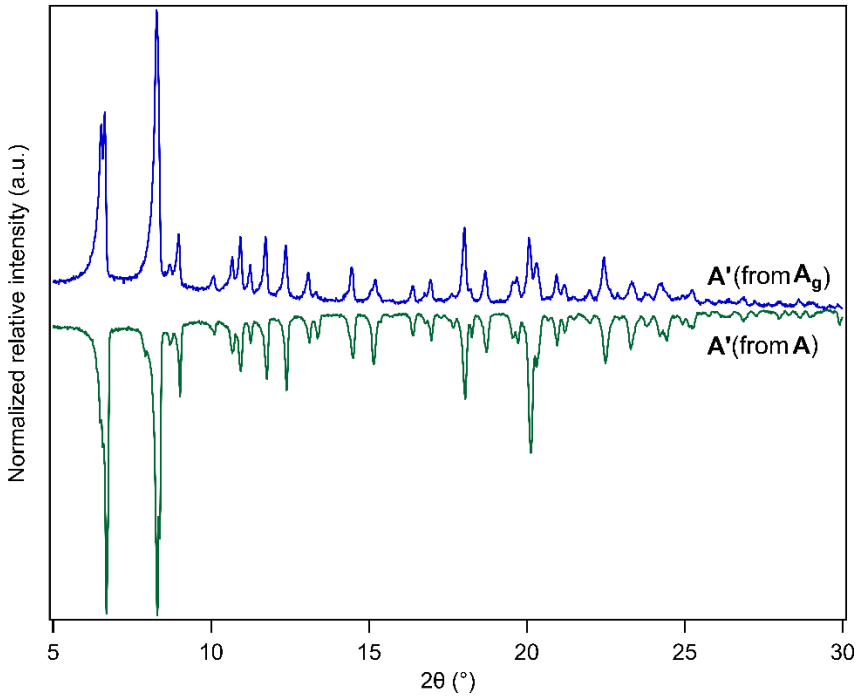

Fig. S9. Powder X-ray diffraction patterns of derivatives **A'** generated by a thermal treatment of compound **A** (green) or compound $\mathbf{A_g}$ (blue)

II. X-ray Crystallographic study

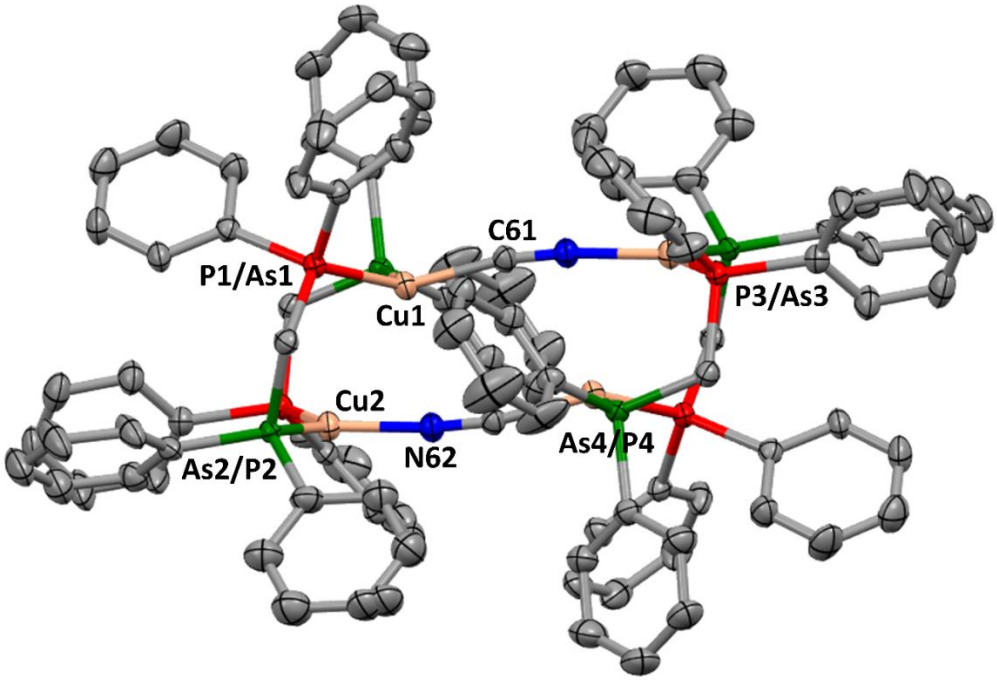

Fig. S10. ORTEP of derivative **A**

Table S1. Bond Lengths for derivative **A** at 150 K.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cu1	N61	1.946(6)	C21	C22	1.3900
Cu1	C61	1.946(6)	C22	C23	1.3900
Cu1	P1	2.2827(12)	C23	C24	1.3900
Cu1	As1	2.2827(12)	C24	C25	1.3900
Cu1	As4[1]	2.2962(12)	C20B	C21B	1.406(15)
Cu1	Cu2[1]	2.9575(12)	C20B	C25B	1.430(14)
Cu2	C62	1.919(6)	C21B	C22B	1.389(16)
Cu2	N62	1.919(6)	C22B	C23B	1.390(17)
Cu2	P3	2.2726(13)	C23B	C24B	1.369(17)
Cu2	As3	2.2726(13)	C24B	C25B	1.393(15)
Cu2	As2[1]	2.2944(12)	C31	C32	1.383(10)
P1	C7	1.873(6)	C31	C36	1.387(10)
P1	C13	1.889(6)	C32	C33	1.381(12)
P1	C1	1.900(6)	C33	C34	1.376(15)
As2	C14	1.881(7)	C34	C35	1.381(14)
As2	C20	1.882(5)	C35	C36	1.391(12)
As2	C13	1.929(6)	C37	C42	1.364(10)
P3	C31	1.862(7)	C37	C38	1.386(10)
P3	C37	1.886(7)	C38	C39	1.399(10)
P3	C43	1.906(6)	C39	C40	1.333(13)
As4	C44	1.876(7)	C40	C41	1.349(13)

As4	C50	1.900(6)	C41	C42	1.398(11)
As4	C43	1.904(6)	C44	C49	1.375(10)
As1	C7	1.873(6)	C44	C45	1.386(10)
As1	C13	1.889(6)	C45	C46	1.390(13)
As1	C1	1.900(6)	C46	C47	1.363(14)
P2	C14	1.881(7)	C47	C48	1.363(11)
P2	C20B	1.882(5)	C48	C49	1.386(10)
P2	C13	1.929(6)	C50	C51	1.380(10)
As3	C31	1.862(7)	C50	C55	1.388(10)
As3	C37	1.886(7)	C51	C52	1.372(11)
As3	C43	1.906(6)	C52	C53	1.385(13)
P4	C44	1.876(7)	C53	C54	1.363(13)
P4	C50	1.900(6)	C54	C55	1.385(11)
P4	C43	1.904(6)	C61	N62	1.155(8)
C1	C6	1.372(10)	N61	C62	1.155(8)
C1	C2	1.400(9)	P11	F1	1.571(6)
C2	C3	1.375(10)	P11	F5	1.578(7)
C3	C4	1.387(13)	P11	F2	1.579(7)
C4	C5	1.388(13)	P11	F6	1.586(6)
C5	C6	1.400(10)	P11	F3	1.606(5)
C7	C12	1.392(9)	P11	F4	1.610(5)
C7	C8	1.397(9)	C81	Cl1	1.729(13)
C8	C9	1.389(11)	C81	Cl2	1.757(13)
C9	C10	1.380(12)	C81B	Cl1B	1.733(16)
C10	C11	1.387(12)	C81B	Cl2B	1.785(16)
C11	C12	1.385(10)	C82	Cl3	1.658(13)
C14	C15	1.383(10)	C82	Cl4	1.805(14)
C14	C19	1.389(10)	C82B	Cl4B	1.651(17)
C15	C16	1.397(11)	C82B	Cl3B	1.696(14)
C16	C17	1.379(14)	C83	Cl5	1.728(14)
C17	C18	1.375(13)	C83	Cl6	1.791(14)
C18	C19	1.389(11)	C83B	Cl5B	1.725(17)
C20	C21	1.3900	C83B	Cl6B	1.778(17)
C20	C25	1.3900			

[1]1-X,1-Y,1-Z

Table S2. Bond Angles for derivative **A** 150 K

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C61	Cu1	P1	120.75(18)	C19	C14	As2	117.7(5)
N61	Cu1	As1	120.75(18)	C14	C15	C16	119.8(8)
N61	Cu1	As4[1]	110.41(17)	C17	C16	C15	120.5(8)
C61	Cu1	As4[1]	110.41(17)	C18	C17	C16	119.6(8)

P1	Cu1	As4[1]	118.91(5)	C17	C18	C19	120.4(8)
As1	Cu1	As4[1]	118.91(5)	C18	C19	C14	120.2(7)
C61	Cu1	Cu2[1]	133.73(18)	C21	C20	C25	120.0
P1	Cu1	Cu2[1]	82.14(4)	C21	C20	As2	119.7(4)
As4[1]	Cu1	Cu2[1]	85.81(4)	C25	C20	As2	120.2(4)
N62	Cu2	P3	121.24(19)	C22	C21	C20	120.0
C62	Cu2	As3	121.24(19)	C21	C22	C23	120.0
N62	Cu2	As2[1]	109.61(19)	C24	C23	C22	120.0
P3	Cu2	As2[1]	128.66(5)	C23	C24	C25	120.0
N62	Cu2	Cu1[1]	61.66(19)	C24	C25	C20	120.0
P3	Cu2	Cu1[1]	97.97(4)	C21B	C20B	C25B	113.9(10)
As2[1]	Cu2	Cu1[1]	99.87(4)	C21B	C20B	P2	126.8(8)
C7	P1	C13	105.2(3)	C25B	C20B	P2	117.4(7)
C7	P1	C1	101.2(3)	C22B	C21B	C20B	121.5(15)
C13	P1	C1	100.9(3)	C21B	C22B	C23B	121.6(17)
C7	P1	Cu1	115.56(19)	C24B	C23B	C22B	118.7(17)
C13	P1	Cu1	119.03(19)	C23B	C24B	C25B	119.4(16)
C1	P1	Cu1	112.6(2)	C24B	C25B	C20B	123.1(14)
C14	As2	C20	101.3(3)	C32	C31	C36	118.4(7)
C14	As2	C13	104.9(3)	C32	C31	As3	122.1(5)
C20	As2	C13	101.3(3)	C36	C31	As3	119.5(6)
C14	As2	Cu2[1]	123.1(2)	C32	C31	P3	122.1(5)
C20	As2	Cu2[1]	114.9(2)	C36	C31	P3	119.5(6)
C13	As2	Cu2[1]	108.89(18)	C33	C32	C31	121.2(8)
C31	P3	C37	103.4(3)	C34	C33	C32	119.9(9)
C31	P3	C43	102.3(3)	C33	C34	C35	120.1(8)
C37	P3	C43	100.8(3)	C34	C35	C36	119.6(8)
C31	P3	Cu2	117.8(2)	C31	C36	C35	120.8(8)
C37	P3	Cu2	120.3(2)	C42	C37	C38	118.3(7)
C43	P3	Cu2	109.6(2)	C42	C37	P3	122.2(5)
C44	As4	C50	103.2(3)	C38	C37	P3	119.4(5)
C44	As4	C43	103.9(3)	C42	C37	As3	122.2(5)
C50	As4	C43	101.7(3)	C38	C37	As3	119.4(5)
C44	As4	Cu1[1]	121.0(2)	C37	C38	C39	119.9(7)
C50	As4	Cu1[1]	109.9(2)	C40	C39	C38	120.4(8)
C43	As4	Cu1[1]	114.9(2)	C39	C40	C41	120.9(7)
C7	As1	C13	105.2(3)	C40	C41	C42	119.9(9)
C7	As1	C1	101.2(3)	C37	C42	C41	120.6(8)
C13	As1	C1	100.9(3)	As4	C43	P3	110.9(3)
C7	As1	Cu1	115.56(19)	P4	C43	As3	110.9(3)
C13	As1	Cu1	119.03(19)	C49	C44	C45	118.8(7)
C1	As1	Cu1	112.6(2)	C49	C44	As4	118.7(5)
C14	P2	C20B	101.3(3)	C45	C44	As4	122.5(6)

C14	P2	C13	104.9(3)	C49	C44	P4	118.7(5)
C20B	P2	C13	101.3(3)	C45	C44	P4	122.5(6)
C14	P2	Cu2[1]	123.1(2)	C44	C45	C46	119.5(8)
C13	P2	Cu2[1]	108.89(18)	C47	C46	C45	121.2(9)
C31	As3	C37	103.4(3)	C48	C47	C46	119.3(8)
C31	As3	C43	102.3(3)	C47	C48	C49	120.5(7)
C37	As3	C43	100.8(3)	C44	C49	C48	120.7(7)
C31	As3	Cu2	117.8(2)	C51	C50	C55	118.8(7)
C37	As3	Cu2	120.3(2)	C51	C50	P4	117.2(5)
C43	As3	Cu2	109.6(2)	C55	C50	P4	124.0(5)
C44	P4	C50	103.2(3)	C51	C50	As4	117.2(5)
C44	P4	C43	103.9(3)	C55	C50	As4	124.0(5)
C50	P4	C43	101.7(3)	C52	C51	C50	121.1(7)
C44	P4	Cu1[1]	121.0(2)	C51	C52	C53	120.1(8)
C50	P4	Cu1[1]	109.9(2)	C54	C53	C52	119.1(7)
C43	P4	Cu1[1]	114.9(2)	C53	C54	C55	121.4(8)
C6	C1	C2	120.7(6)	C54	C55	C50	119.5(8)
C6	C1	P1	121.3(5)	N62	C61	Cu1	170.6(6)
C2	C1	P1	118.0(5)	C61	N62	Cu2	173.6(6)
C6	C1	As1	121.3(5)	C62	N61	Cu1	170.6(6)
C2	C1	As1	118.0(5)	N61	C62	Cu2	173.6(6)
C3	C2	C1	119.7(7)	F1	P11	F5	89.4(5)
C2	C3	C4	120.6(7)	F1	P11	F2	92.0(5)
C3	C4	C5	119.3(7)	F5	P11	F2	178.6(5)
C4	C5	C6	120.8(8)	F1	P11	F6	177.8(4)
C1	C6	C5	118.9(7)	F5	P11	F6	89.3(4)
C12	C7	C8	119.1(6)	F2	P11	F6	89.3(4)
C12	C7	P1	124.5(5)	F1	P11	F3	92.1(3)
C8	C7	P1	116.3(5)	F5	P11	F3	89.4(3)
C12	C7	As1	124.5(5)	F2	P11	F3	90.8(4)
C8	C7	As1	116.3(5)	F6	P11	F3	89.7(3)
C9	C8	C7	120.4(7)	F1	P11	F4	88.6(3)
C10	C9	C8	119.9(7)	F5	P11	F4	90.7(3)
C9	C10	C11	120.1(7)	F2	P11	F4	89.1(3)
C12	C11	C10	120.3(7)	F6	P11	F4	89.6(3)
C11	C12	C7	120.1(7)	F3	P11	F4	179.3(3)
As1	C13	P2	112.2(3)	Cl1	C81	Cl2	111.7(10)
P1	C13	As2	112.2(3)	Cl1B	C81B	Cl2B	105.1(10)
C15	C14	C19	119.5(7)	Cl3	C82	Cl4	101.3(8)
C15	C14	P2	122.8(6)	Cl4B	C82B	Cl3B	114.7(8)
C19	C14	P2	117.7(5)	Cl5	C83	Cl6	112.5(8)
C15	C14	As2	122.8(6)	Cl5B	C83B	Cl6B	109.5(11)

[1]1-X,1-Y,1-Z

Table S3. Torsion Angles for derivative **A** at 150K.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
C6	C1	C2	C3	1.3(10)	C20B	C21B	C22B	C23B	9(4)
P1	C1	C2	C3	-177.9(5)	C21B	C22B	C23B	C24B	-7(4)
As1	C1	C2	C3	-177.9(5)	C22B	C23B	C24B	C25B	8(4)
C1	C2	C3	C4	0.6(11)	C23B	C24B	C25B	C20B	-12(3)
C2	C3	C4	C5	-1.0(12)	C21B	C20B	C25B	C24B	13(2)
C3	C4	C5	C6	-0.5(13)	P2	C20B	C25B	C24B	178.8(16)
C2	C1	C6	C5	-2.7(11)	C37	As3	C31	C32	-58.4(7)
P1	C1	C6	C5	176.5(6)	C43	As3	C31	C32	46.0(7)
As1	C1	C6	C5	176.5(6)	Cu2	As3	C31	C32	166.1(6)
C4	C5	C6	C1	2.3(13)	C37	As3	C31	C36	122.9(6)
C13	P1	C7	C12	-2.2(6)	C43	As3	C31	C36	-132.6(6)
C1	P1	C7	C12	-106.9(6)	Cu2	As3	C31	C36	-12.5(6)
Cu1	P1	C7	C12	131.2(5)	C37	P3	C31	C32	-58.4(7)
C13	P1	C7	C8	177.3(5)	C43	P3	C31	C32	46.0(7)
C1	P1	C7	C8	72.6(6)	Cu2	P3	C31	C32	166.1(6)
Cu1	P1	C7	C8	-49.2(6)	C37	P3	C31	C36	122.9(6)
C13	As1	C7	C12	-2.2(6)	C43	P3	C31	C36	-132.6(6)
C1	As1	C7	C12	-106.9(6)	Cu2	P3	C31	C36	-12.5(6)
Cu1	As1	C7	C12	131.2(5)	C36	C31	C32	C33	2.4(12)
C13	As1	C7	C8	177.3(5)	As3	C31	C32	C33	-176.3(7)
C1	As1	C7	C8	72.6(6)	P3	C31	C32	C33	-176.3(7)
Cu1	As1	C7	C8	-49.2(6)	C31	C32	C33	C34	-2.0(15)
C12	C7	C8	C9	-0.1(11)	C32	C33	C34	C35	0.5(15)
P1	C7	C8	C9	-179.7(7)	C33	C34	C35	C36	0.6(13)
As1	C7	C8	C9	-179.7(7)	C32	C31	C36	C35	-1.3(11)
C7	C8	C9	C10	-0.7(14)	As3	C31	C36	C35	177.4(6)
C8	C9	C10	C11	0.6(14)	P3	C31	C36	C35	177.4(6)
C9	C10	C11	C12	0.2(14)	C34	C35	C36	C31	-0.2(12)
C10	C11	C12	C7	-1.0(12)	C31	P3	C37	C42	-23.2(8)
C8	C7	C12	C11	1.0(10)	C43	P3	C37	C42	-128.8(8)
P1	C7	C12	C11	-179.5(6)	Cu2	P3	C37	C42	110.8(7)
As1	C7	C12	C11	-179.5(6)	C31	P3	C37	C38	161.4(6)
C7	As1	C13	P2	82.9(3)	C43	P3	C37	C38	55.8(6)
C1	As1	C13	P2	-172.3(3)	Cu2	P3	C37	C38	-64.6(6)
Cu1	As1	C13	P2	-48.6(4)	C31	As3	C37	C42	-23.2(8)
C7	P1	C13	As2	82.9(3)	C43	As3	C37	C42	-128.8(8)
C1	P1	C13	As2	-172.3(3)	Cu2	As3	C37	C42	110.8(7)
Cu1	P1	C13	As2	-48.6(4)	C31	As3	C37	C38	161.4(6)
C20B	P2	C14	C15	69.2(7)	C43	As3	C37	C38	55.8(6)
C13	P2	C14	C15	-35.8(7)	Cu2	As3	C37	C38	-64.6(6)

Cu2[1]	P2	C14	C15	-160.8(6)	C42	C37	C38	C39	-1.1(12)
C20B	P2	C14	C19	-113.7(6)	P3	C37	C38	C39	174.5(6)
C13	P2	C14	C19	141.3(5)	As3	C37	C38	C39	174.5(6)
Cu2[1]	P2	C14	C19	16.3(6)	C37	C38	C39	C40	1.5(12)
C20	As2	C14	C15	69.2(7)	C38	C39	C40	C41	-1.9(14)
C13	As2	C14	C15	-35.8(7)	C39	C40	C41	C42	1.8(18)
Cu2[1]	As2	C14	C15	-160.8(6)	C38	C37	C42	C41	1.1(15)
C20	As2	C14	C19	-113.7(6)	P3	C37	C42	C41	-174.5(9)
C13	As2	C14	C19	141.3(5)	As3	C37	C42	C41	-174.5(9)
Cu2[1]	As2	C14	C19	16.3(6)	C40	C41	C42	C37	-1.4(18)
C19	C14	C15	C16	-2.2(12)	C50	As4	C44	C49	-155.0(6)
P2	C14	C15	C16	174.8(7)	C43	As4	C44	C49	99.2(6)
As2	C14	C15	C16	174.8(7)	Cu1[1]	As4	C44	C49	-31.7(7)
C14	C15	C16	C17	0.9(15)	C50	As4	C44	C45	25.1(9)
C15	C16	C17	C18	1.1(16)	C43	As4	C44	C45	-80.7(9)
C16	C17	C18	C19	-1.8(15)	Cu1[1]	As4	C44	C45	148.4(8)
C17	C18	C19	C14	0.5(13)	C50	P4	C44	C49	-155.0(6)
C15	C14	C19	C18	1.6(11)	C43	P4	C44	C49	99.2(6)
P2	C14	C19	C18	-175.6(6)	Cu1[1]	P4	C44	C49	-31.7(7)
As2	C14	C19	C18	-175.6(6)	C50	P4	C44	C45	25.1(9)
C14	As2	C20	C21	14.7(5)	C43	P4	C44	C45	-80.7(9)
C13	As2	C20	C21	122.6(5)	Cu1[1]	P4	C44	C45	148.4(8)
Cu2[1]	As2	C20	C21	-120.2(4)	C49	C44	C45	C46	-0.2(17)
C14	As2	C20	C25	-168.3(5)	As4	C44	C45	C46	179.6(11)
C13	As2	C20	C25	-60.4(5)	P4	C44	C45	C46	179.6(11)
Cu2[1]	As2	C20	C25	56.8(5)	C44	C45	C46	C47	-1(2)
C25	C20	C21	C22	0.0	C45	C46	C47	C48	2(2)
As2	C20	C21	C22	177.0(5)	C46	C47	C48	C49	-0.4(16)
C20	C21	C22	C23	0.0	C45	C44	C49	C48	1.5(12)
C21	C22	C23	C24	0.0	As4	C44	C49	C48	-178.3(6)
C22	C23	C24	C25	0.0	P4	C44	C49	C48	-178.3(6)
C23	C24	C25	C20	0.0	C47	C48	C49	C44	-1.2(13)
C21	C20	C25	C24	0.0	C55	C50	C51	C52	0.0(12)
As2	C20	C25	C24	-177.0(5)	P4	C50	C51	C52	177.1(7)
C14	P2	C20B	C21B	-77.8(13)	As4	C50	C51	C52	177.1(7)
C13	P2	C20B	C21B	30.1(13)	C50	C51	C52	C53	0.6(14)
Cu2[1]	P2	C20B	C21B	147.2(12)	C51	C52	C53	C54	-0.6(15)
C14	P2	C20B	C25B	118.6(10)	C52	C53	C54	C55	-0.1(15)
C13	P2	C20B	C25B	-133.6(10)	C53	C54	C55	C50	0.8(14)
Cu2[1]	P2	C20B	C25B	-16.4(10)	C51	C50	C55	C54	-0.7(12)
C25B	C20B	C21B	C22B	-11(3)	P4	C50	C55	C54	-177.6(6)
P2	C20B	C21B	C22B	-175.6(16)	As4	C50	C55	C54	-177.6(6)

[1]1-X,1-Y,1-Z

III. SEM pictures

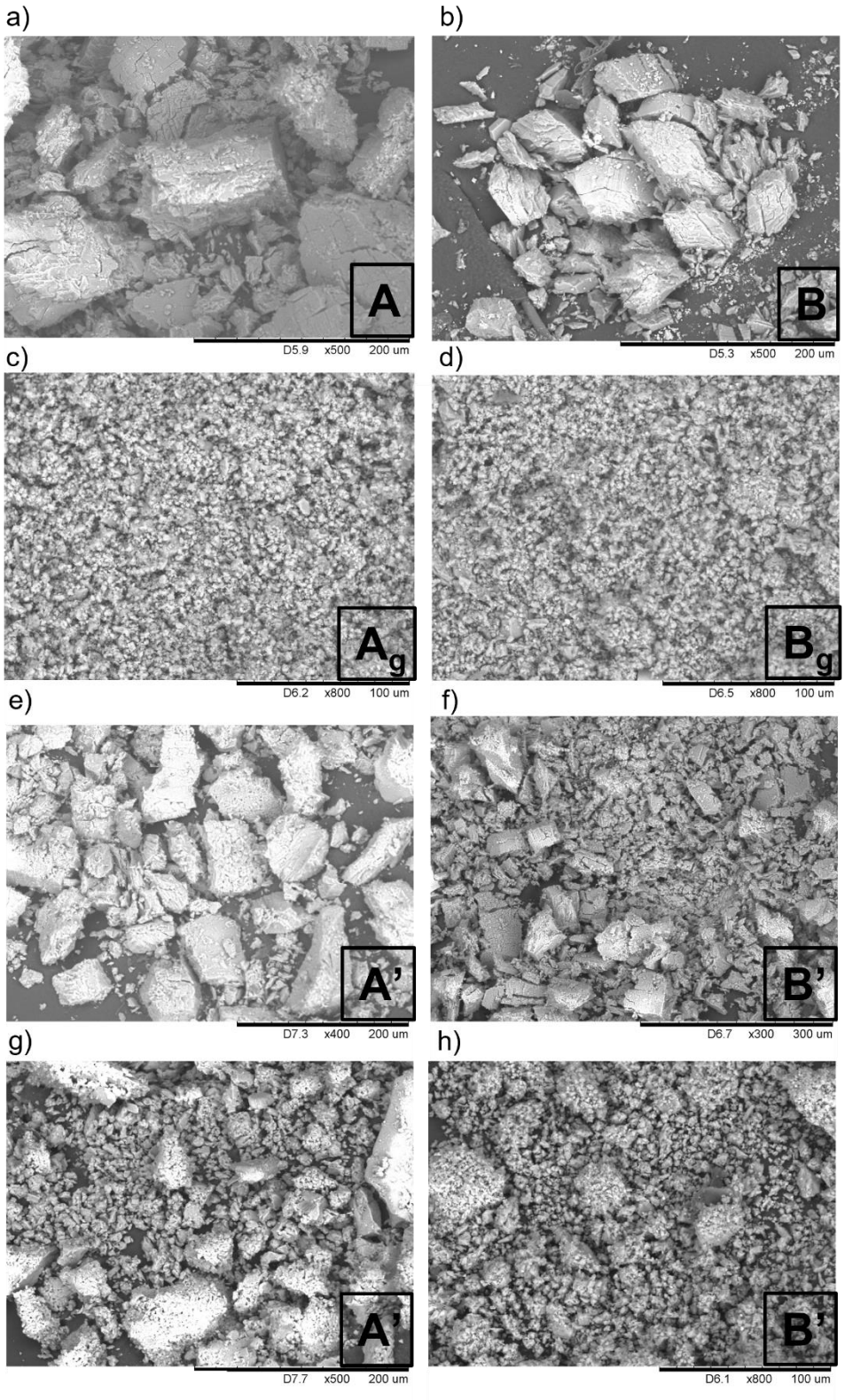

Fig. S11. SEM pictures of derivatives **A** (a), $\mathbf{A_g}$ (c), **A'** generated from **A** (e) and **A'** generated from $\mathbf{A_g}$ (g) and **B** (b), $\mathbf{B_g}$ (d), **B'** generated from B (f) and **B'** generated from $\mathbf{B_g}$ (h) taken at magnification ranging in between 250 and 800.

IV. Photophysical study

IV.1. Sample pictures

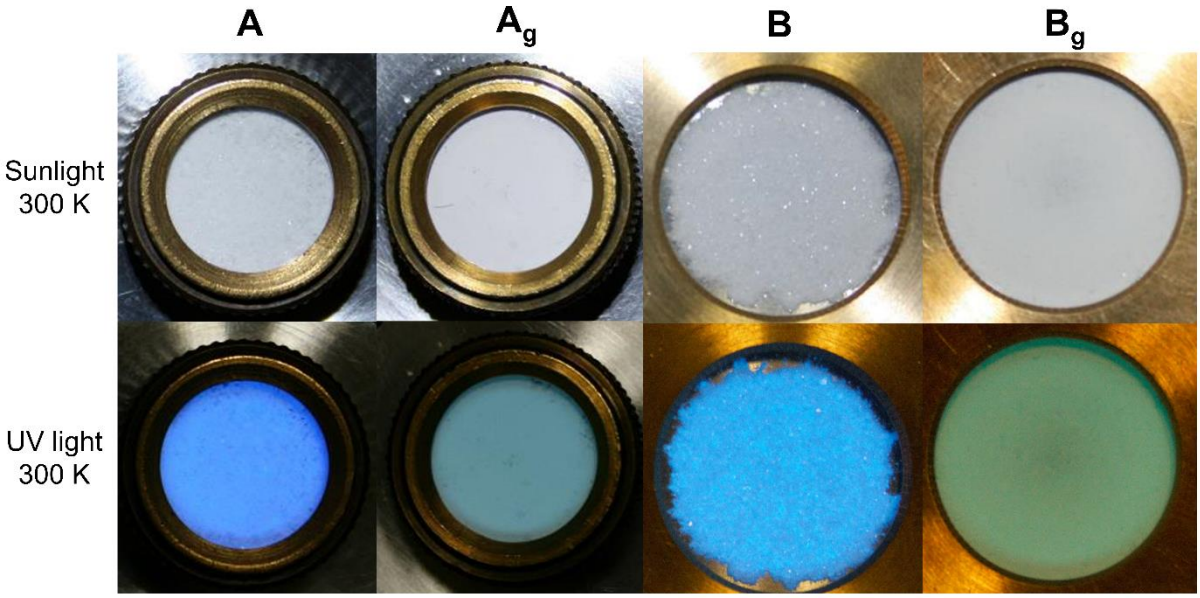

Fig. S12. Pictures of compound **A**, $\mathbf{A_g}$, **B** and $\mathbf{B_g}$ under sunlight and UV light (λ_{ex} = 365 nm) at 300 K

IV.2. Absorbance:

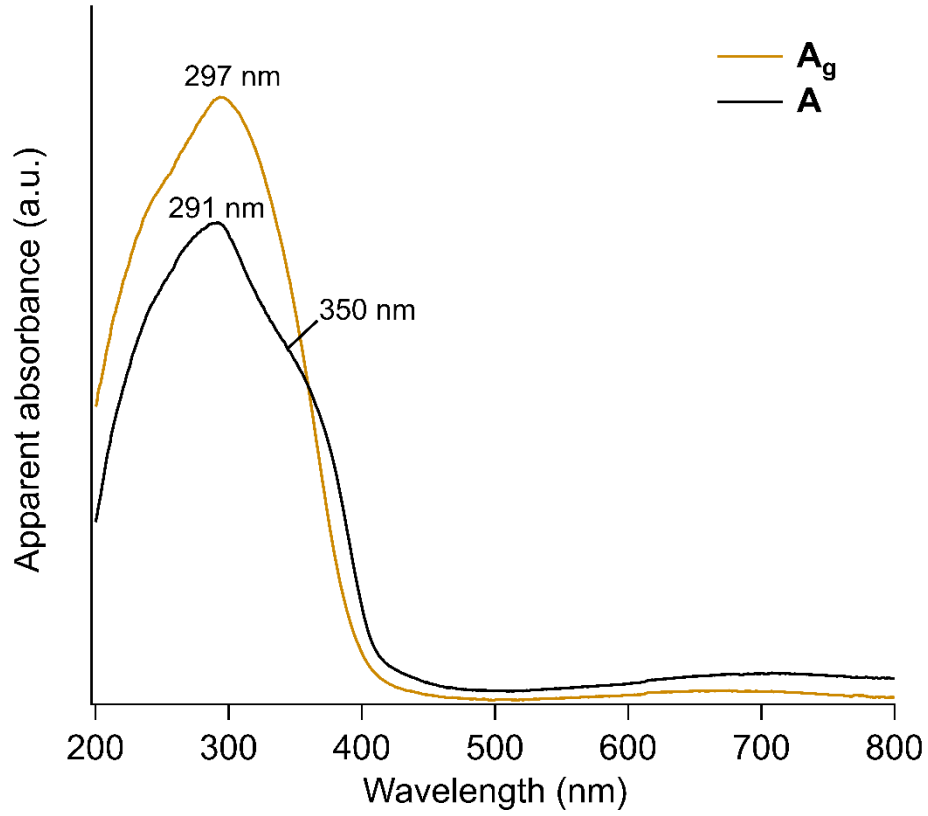

Fig. S13. Solid-state UV-Vis apparent absorbance spectra of derivatives **A** and $\mathbf{A_g}$ at 300 K.

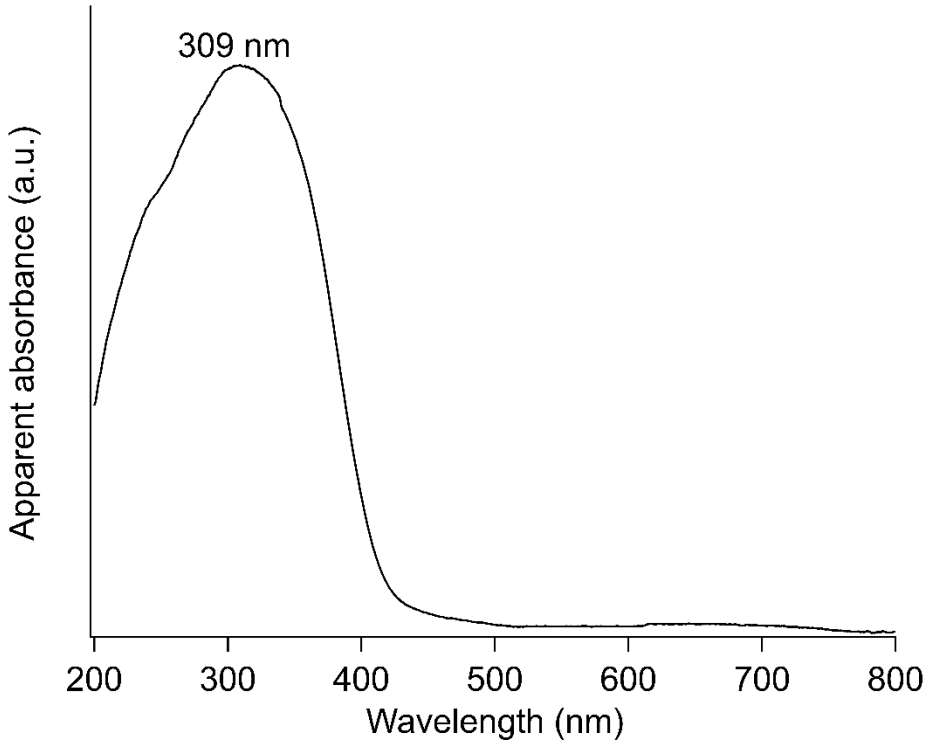

Fig. S14. Solid-state UV-Vis apparent absorbance spectra of derivative $\mathbf{B_g}$ at 300 K.

IV.3. Excitation spectra:

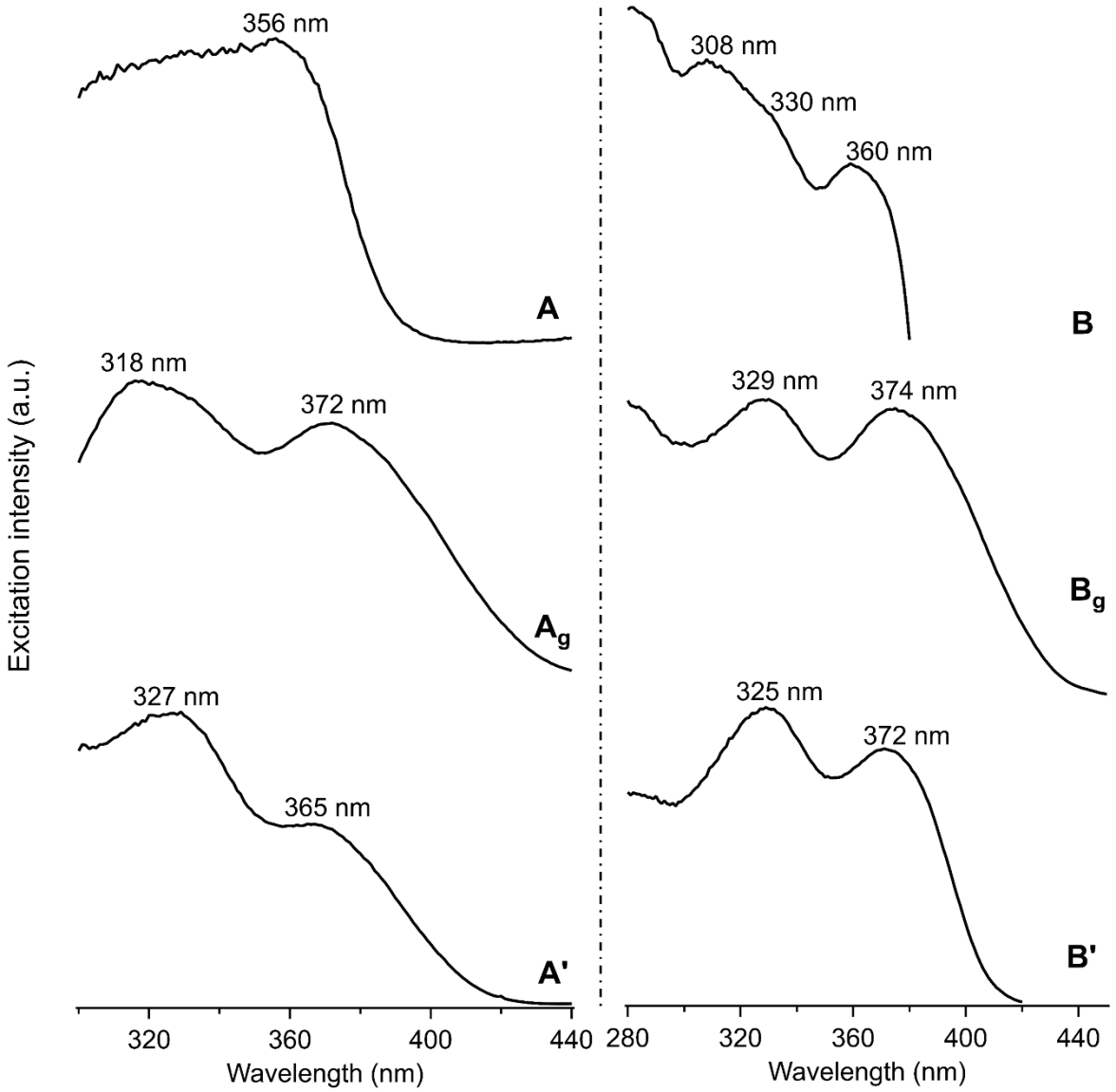

Fig. S15. Excitation spectra of derivatives **A, A_g** and **A'** at room temperature (left) and excitation spectra of derivatives **B^2** (80K)**, B_g** (300K) and **B'** (300K) (right) measured at the maximum of emission for each compound.

IV.4. Emission spectra:

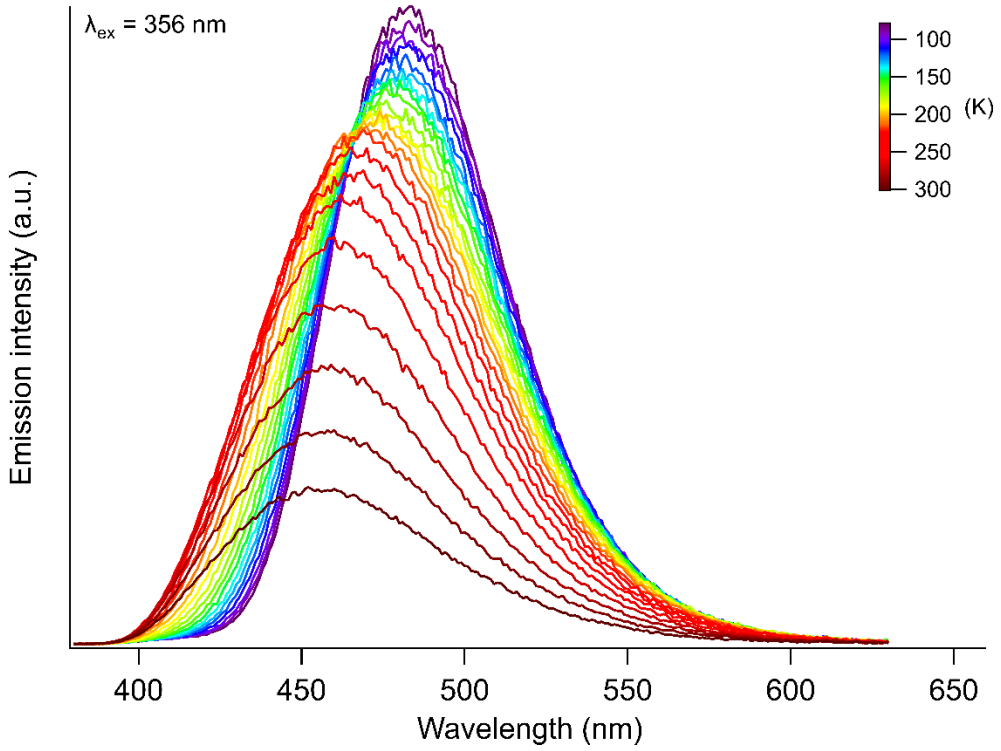

Fig. S16. Temperature dependent emission spectra of derivative **A** upon excitation at 356 nm (80–300 K).

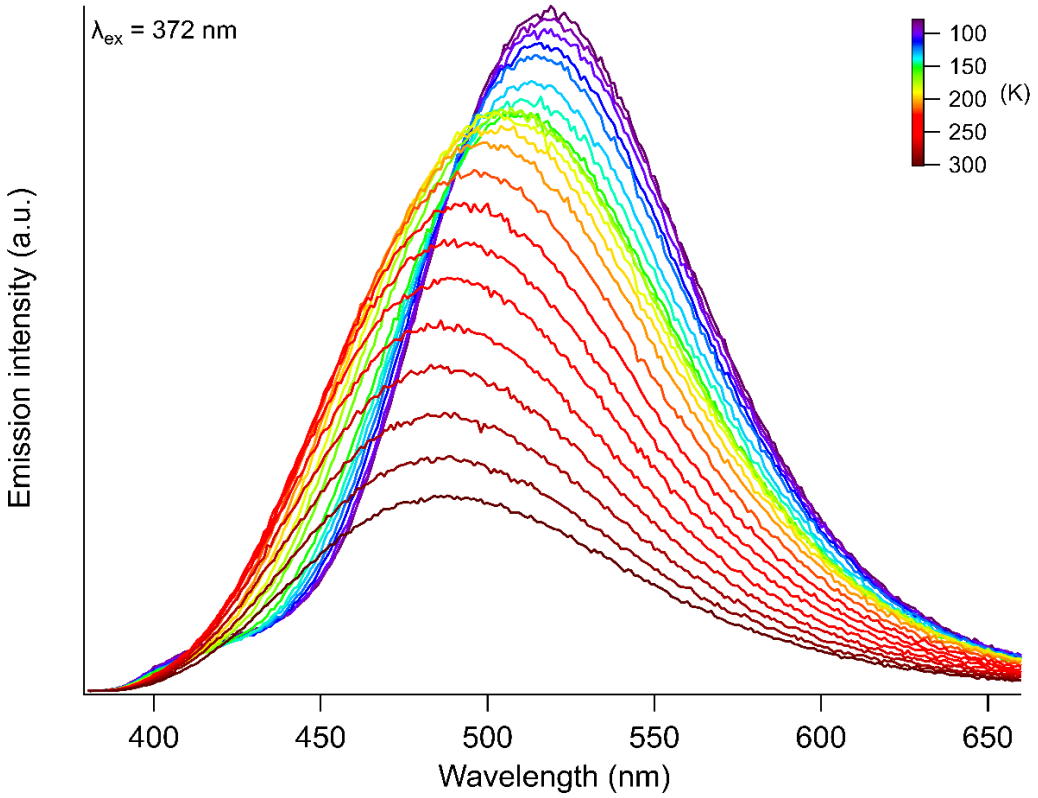

Fig. S17. Temperature dependent emission spectra of derivative $\mathbf{A_g}$ upon excitation at 372 nm (80–300 K).

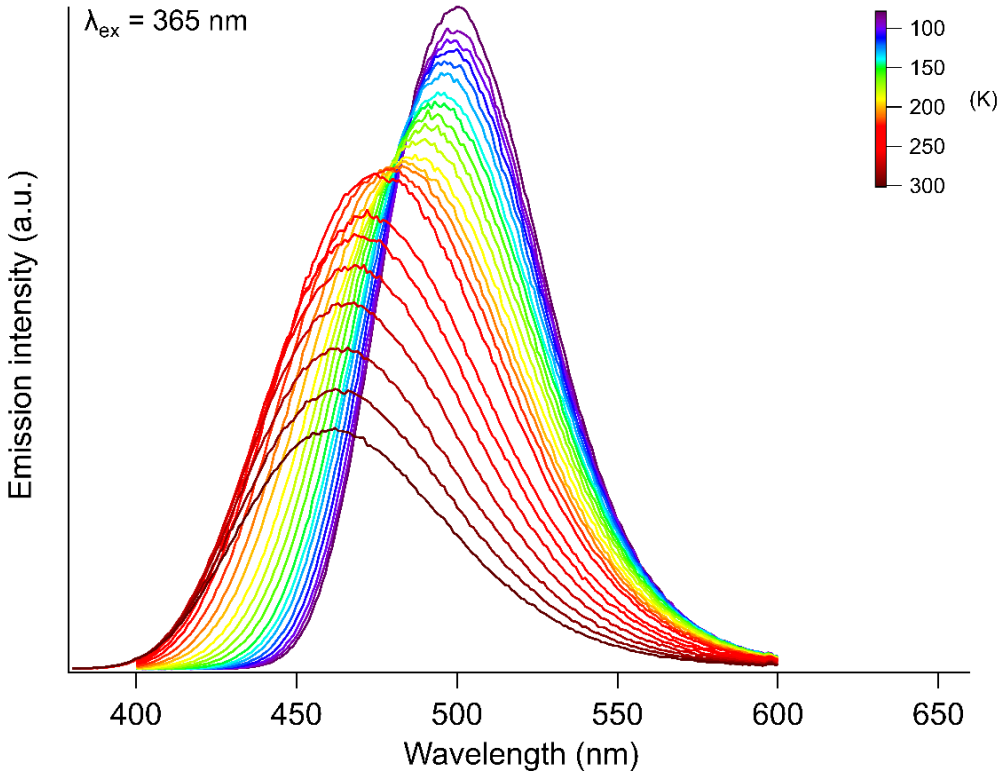

Fig. S18. Temperature dependent emission spectra of derivative **A'** upon excitation at 365 nm (80–300 K).

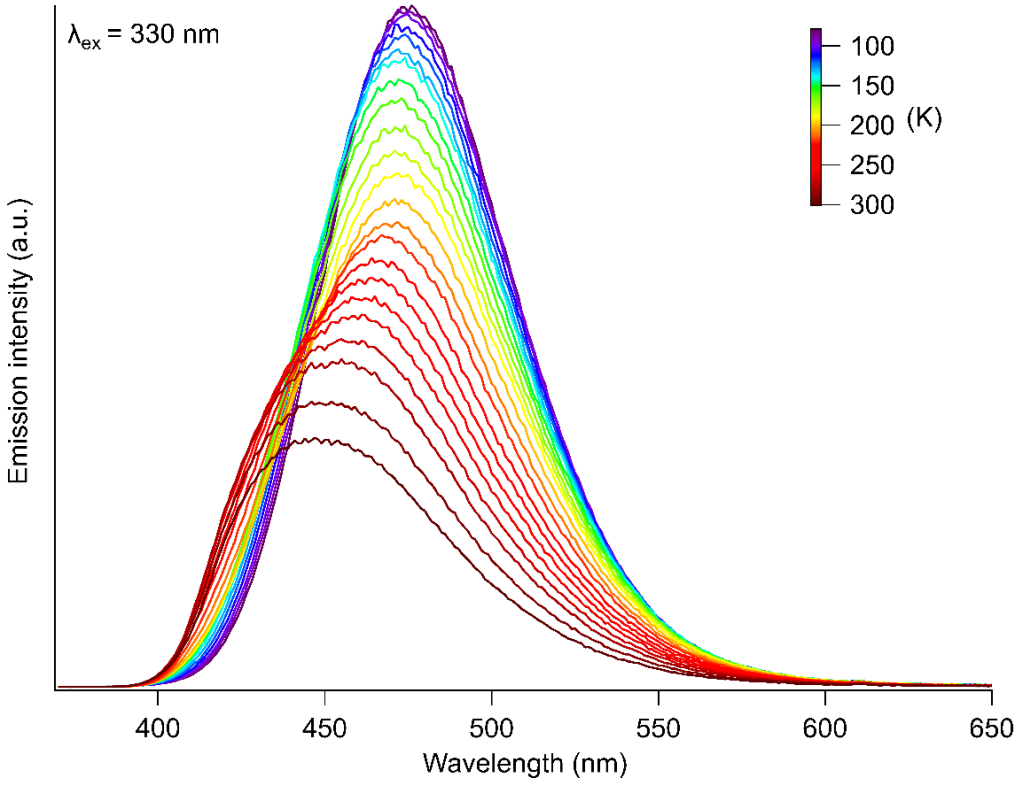

Fig. S19. Temperature dependent emission spectra of derivative **B**[2] upon excitation at 330 nm (80–300 K).

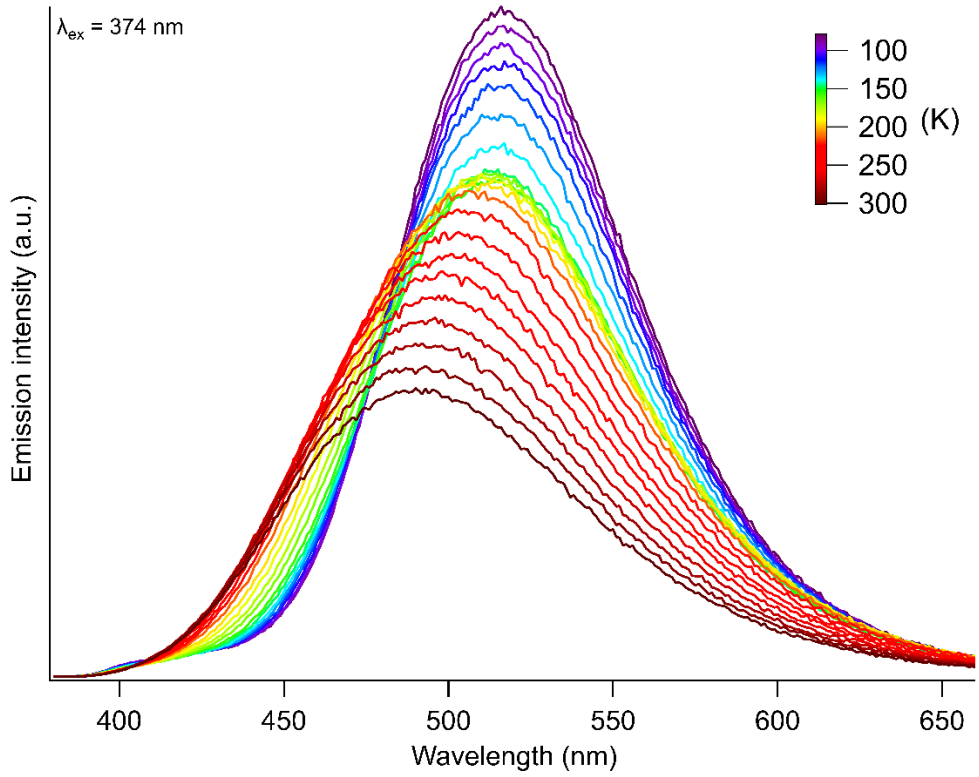

Fig. S20. Temperature dependent emission spectra of derivative $\mathbf{B_g}$ upon excitation at 374 nm (80–300 K).

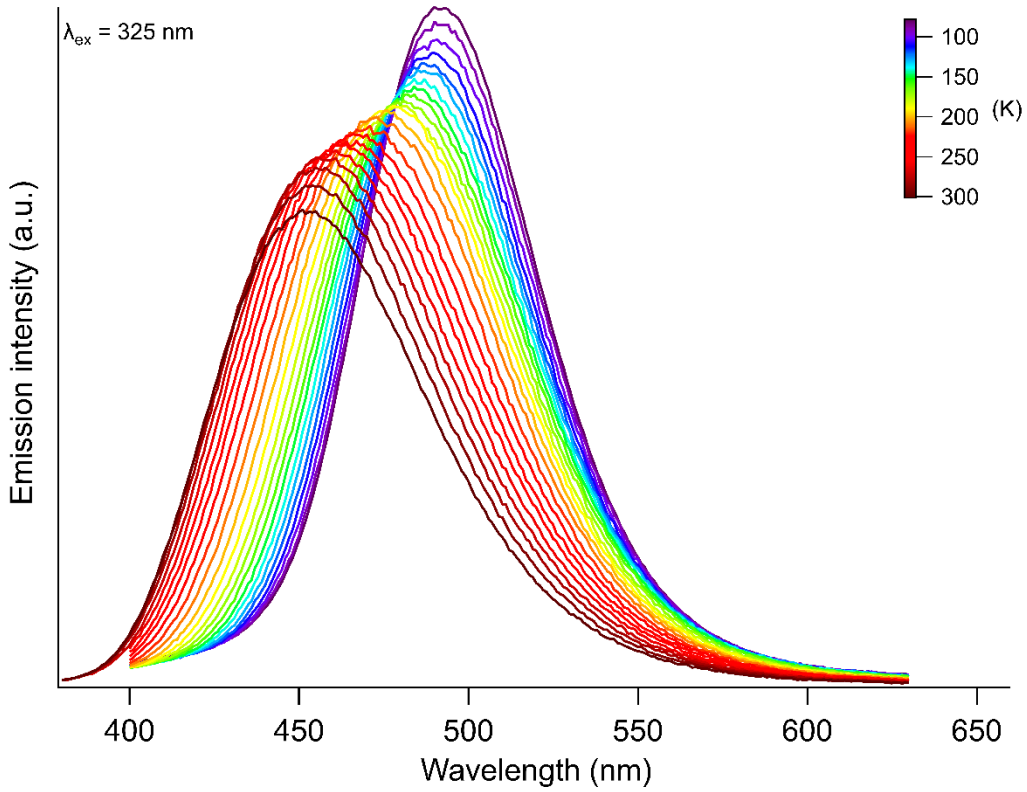

Fig. S21. Temperature dependent emission spectra of derivative **B'** upon excitation at 325 nm (80–300 K).

IV.5. Decay time:

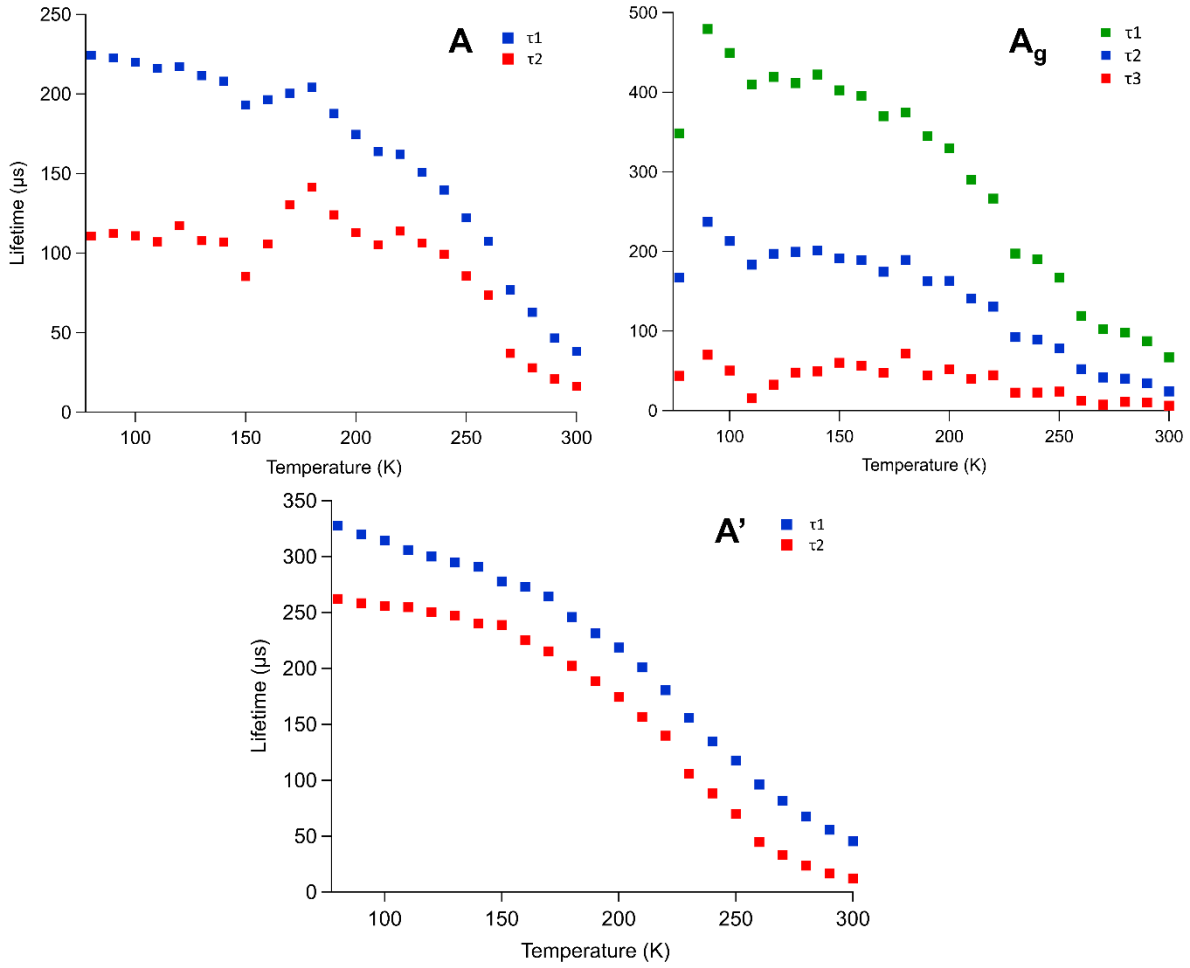

Fig. S22. Temperature dependent decay times of derivative **A** (biexponential), $\mathbf{A_g}$ (triexponential) and **A'** (biexponential) upon excitation at 375 nm (80–300 K)

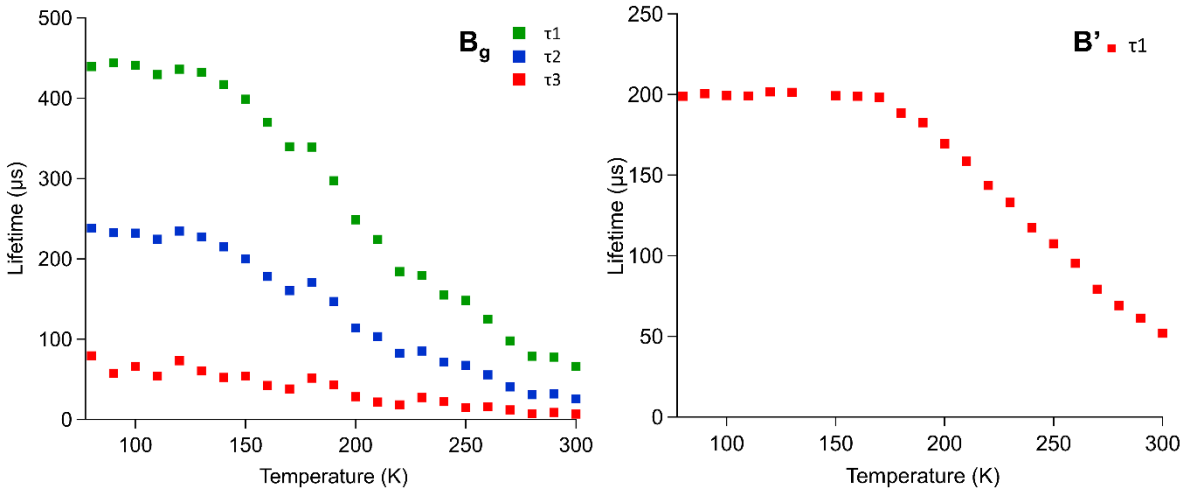

Fig. S23. Temperature dependent decay times of derivative $\mathbf{B_g}$ (triexponential) and **B'** (mono-exponential) upon excitation at 375 nm (80–300 K)

IV.6. CIE coordinates:

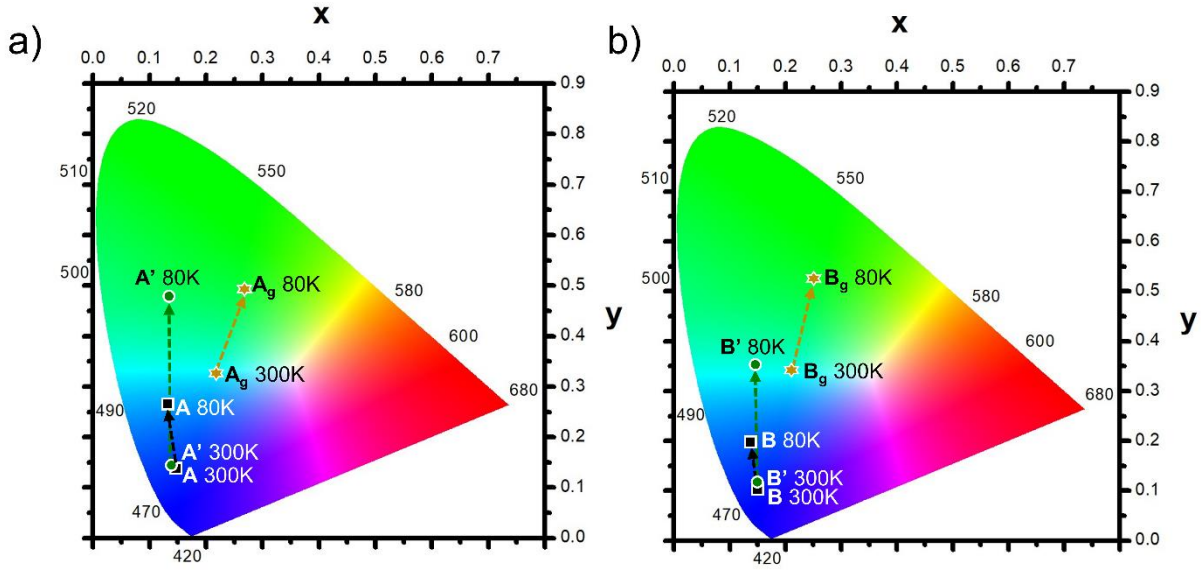

Fig. S24. CIE coordinates at 80 K and 300 K: a) **A** (λ_{ex} = 356 nm), $\mathbf{A_g}$ (λ_{ex} = 372 nm) and **A'** (λ_{ex} = 365 nm); b) $\mathbf{B}^2$ (λ_{ex} = 330 nm), $\mathbf{B_g}$ (λ_{ex} = 374 nm) and **B'** (λ_{ex} = 325 nm).

V. Thermogravimetric analyses:

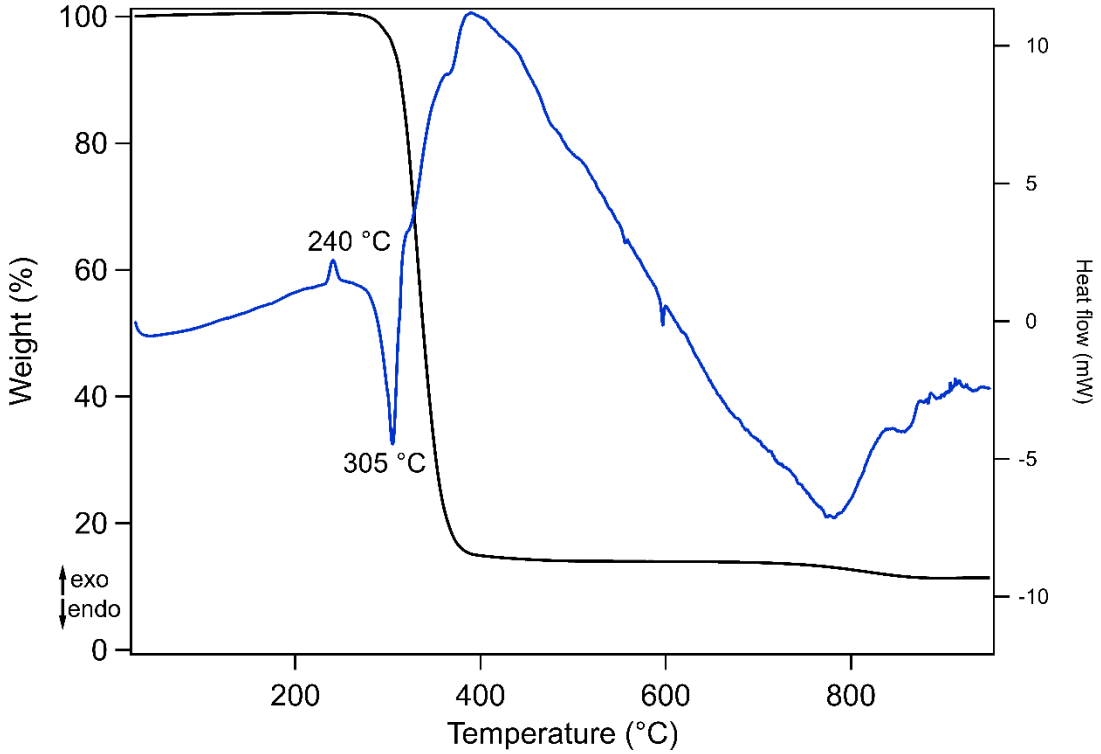

Fig. S25. TGA-TDA analysis curves of derivative **A** showing the weight loss (black curve, left axis) and the heat flow (blue curve, right axis) from 25 to 950 °C

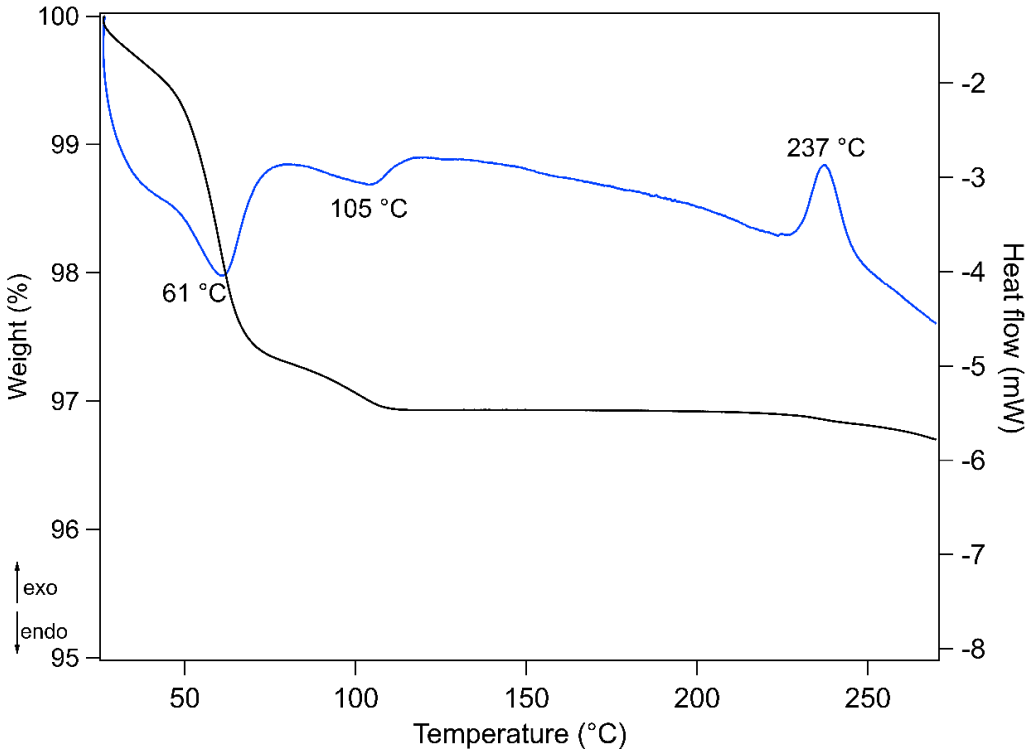

Fig. S26. TGA-TDA analysis curves of derivative **A** showing the weight loss (black curve, left axis) and the heat flow (blue curve, right axis) from 25 to 270 °C

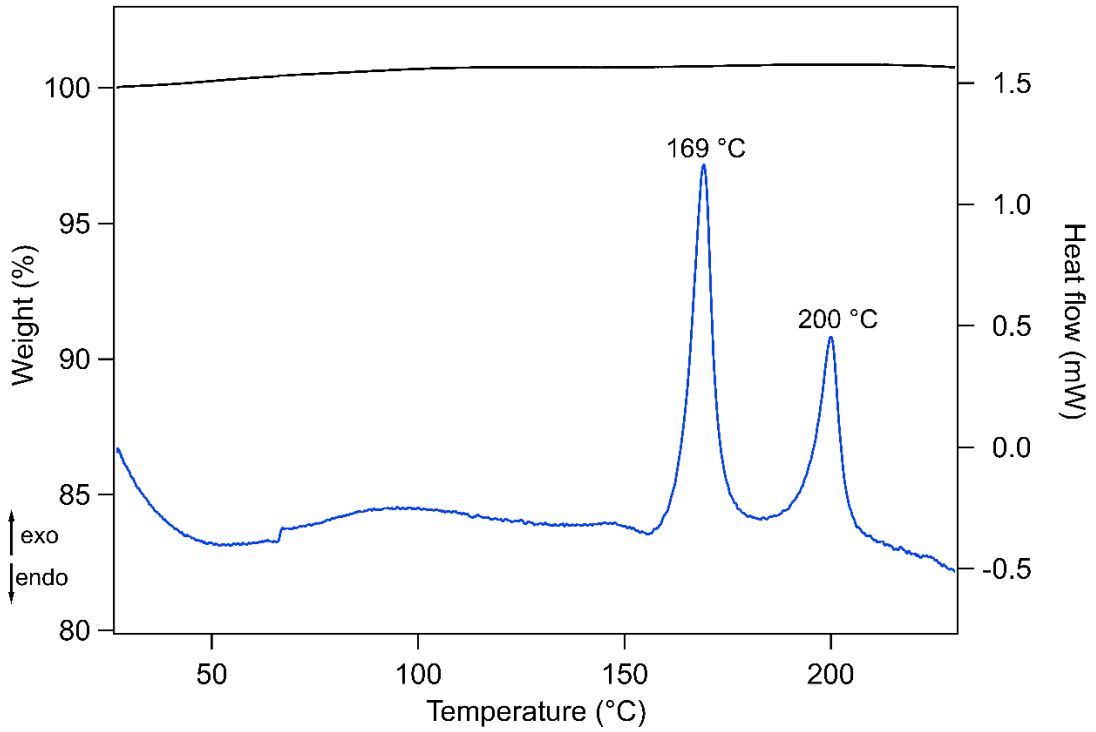

Fig. S27. TGA-TDA analysis curves of derivative $\mathbf{A_g}$ showing the weight loss (black curve, left axis) and the heat flow (blue curve, right axis) from 25 to 230 °C

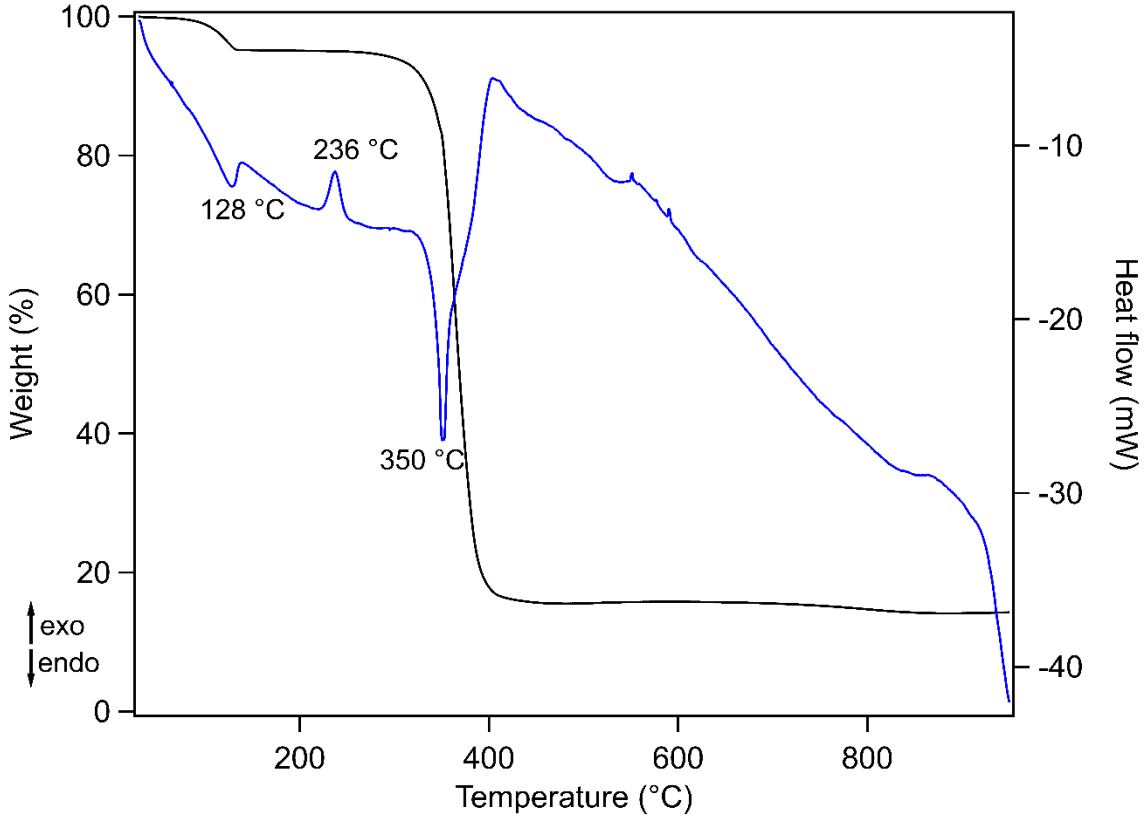

Fig. S28. TGA-TDA analysis curves of derivative **B** showing the weight loss (black curve, left axis) and the heat flow (blue curve, right axis) from 25 to 950 °C

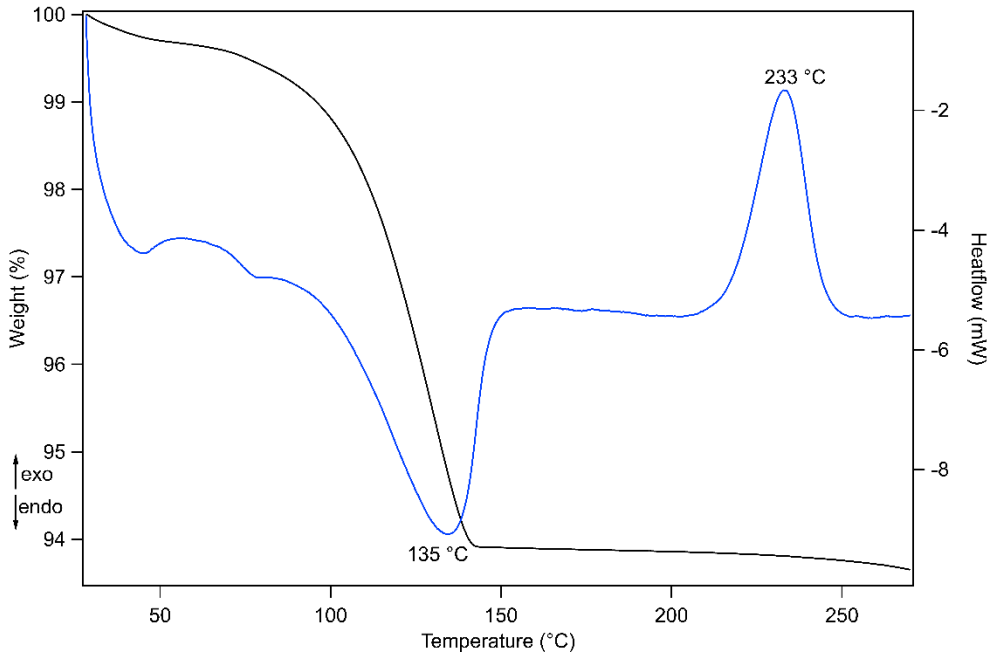

Fig. S29. TGA-TDA analysis curves of derivative **B** showing the weight loss (black curve, left axis) and the heat flow (blue curve, right axis) from 25 to 270 °C

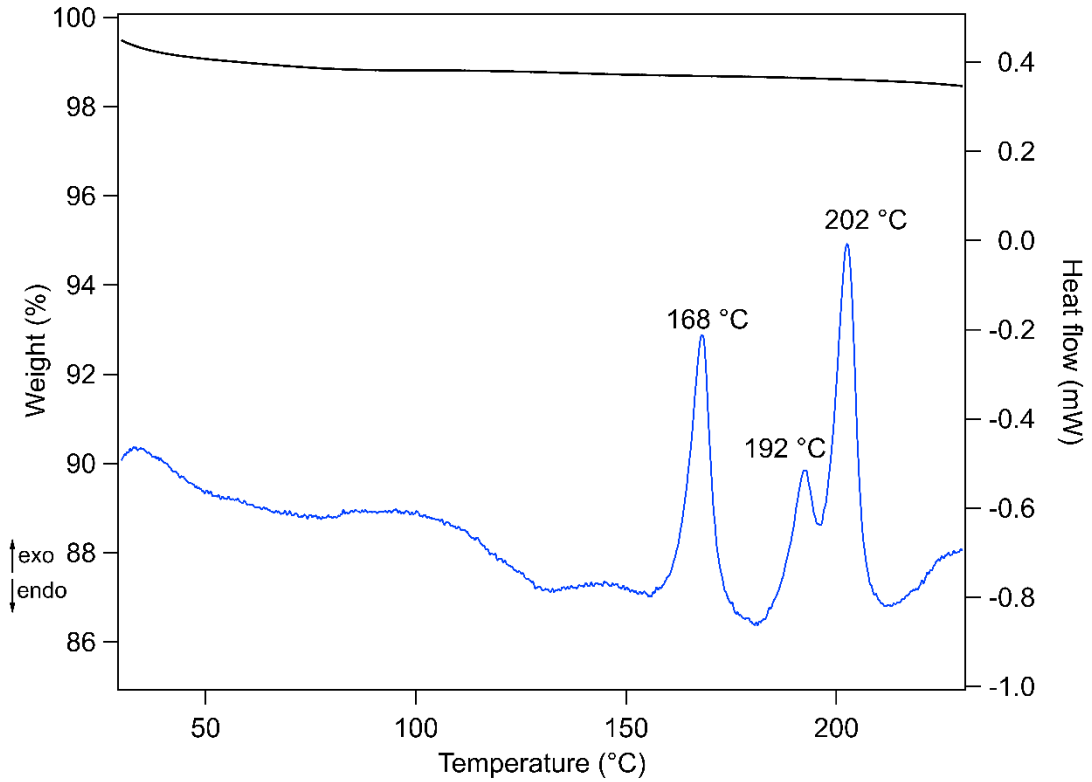

Fig. S30. TGA-TDA analysis curves of derivative $\mathbf{B_g}$ showing the weight loss (black curve, left axis) and the heat flow (blue curve, right axis) from 25 to 230 °C

VI. Computational details

DFT calculations were carried out with the ORCA 5.0 program.[4,5] The different structures and states (S_0, S_1, T_1) of **A** and **B** were optimized using PBE0[6,7] functional and SVP[8,9] atomic basis set. D3BJ dispersion correction was used. Analytic DFT for S_0 and TD-DFT for S_1, T_1 gradients were employed. Harmonic vibrational frequency calculations were not realisable because of the size of the systems (2192 and 2136 basis functions for **A** and **B** respectively). Tighter criteria of energy convergence were applied to ensure high quality of calculations (10^{-6} a.u.). For the ground state systems, two geometry optimizations were performed starting from the X-Ray structural arrangements: 1) full geometry optimizations ($\mathbf{A}_{\text{opt-full}}(S_0)$ and $\mathbf{B}_{\text{opt-full}}(S_0)$) and 2) partially constrained geometry optimizations in which the copper positions were fixed in order to indirectly simulate the crystal packing ($\mathbf{A}_{\text{opt-const}}(S_0)$ and $\mathbf{B}_{\text{opt-const}}(S_0)$). The positioning of C *versus* N in the cyano ligands, and the positioning of the P and As in the $\mathbf{L}_{\text{As,P}}$ picnogen ligands has been studied and the most stable arrangement shown in Fig. 2 was kept for the rest of the computational study. The S_1 and T_1 geometry optimizations were performed starting from the fully optimized and partially constrained optimized geometries ($\mathbf{A}_{\text{opt-full}}(S_1)$, $\mathbf{B}_{\text{opt-full}}(S_1)$, $\mathbf{A}_{\text{opt-full}}(T_1)$, $\mathbf{B}_{\text{opt-full}}(T_1)$). The cartesian coordinates are given in Table S4. The iso-surface representations were done using the GaussView program.[10] DFT 2-component spin-orbit coupling calculations were performed with the ORCA 5.0 package on the previously optimized S_0, S_1 and T_1 structures. For these calculations the same hybrid functional PBE0 was used, with an all-electron triple-zeta Slater basis set with two additional polarization functions (Def2-TZVP) and ZORA approximation.[11] In order to be more accurate, SARC/J auxiliary basis set were also employed. Calculations relying on the Tamm-Dancoff approximation (TDA) of the full TD-DFT equations were used to evaluate the lifetime of the excited states and the oscillator strengths.[12–14] Calculated emission energies include spin-orbit coupling (SOC). Note that SOC was not included in the geometry optimizations. The direct fluorescence and phosphorescence radiative rate constants, k_r^f and k_r^{ph} respectively, were calculated employing the following equations which do not take into account rovibrational aspects:

$$k_r^f = \frac{2\pi\nu^2 e^2}{\varepsilon_0 mc^3} \cdot f_{S_1 \to S_0} \; ; \; k_r^{ph} = \frac{2\pi E^2 e^2}{\varepsilon_0 h^2 mc^3} \cdot f_{T_1 \to S_0} \qquad \text{Equation S2}$$

Table S4. Cartesian coordinates of all full or partial optimized structures.

$\mathbf{A}_{\text{opt-full}}(S_0)$

Cu	1.828606	2.578258	0.000000
Cu	6.844014	2.437637	0.051653
As	0.589657	3.164037	-1.948997
P	-0.521886	0.303866	-2.483121
P	0.957817	3.220217	2.004198
As	-1.186147	0.997810	1.632969
C	1.467196	4.542344	-2.990420
C	2.672552	5.072016	-2.521307
H	3.109192	4.698893	-1.592572
C	3.322990	6.070110	-3.247447
H	4.257840	6.493034	-2.871298
C	2.779948	6.528261	-4.446245
H	3.289431	7.308962	-5.015925
C	1.575267	6.000027	-4.915263
H	1.142892	6.367550	-5.848666
C	0.913340	5.015757	-4.185371
H	-0.043467	4.628995	-4.547221
C	-1.120988	4.000066	-1.597650
C	-1.130040	5.035327	-0.652913
H	-0.200671	5.353381	-0.171869
C	-2.321478	5.678699	-0.328538
H	-2.314856	6.487017	0.406320
C	-3.514272	5.294789	-0.945399
H	-4.448557	5.800900	-0.692144
C	-3.506830	4.273484	-1.892977
H	-4.433528	3.969830	-2.385132
C	-2.313920	3.625946	-2.220910
H	-2.337941	2.825308	-2.961183
C	0.173509	1.814129	-3.299340
H	-0.484877	2.203210	-4.089606
H	1.134549	1.545223	-3.761793
C	-2.268784	0.254534	-2.975372
C	-2.660690	0.340246	-4.319752
H	-1.908301	0.385709	-5.112486
C	-4.012574	0.356090	-4.648803
H	-4.317400	0.422382	-5.695586
C	-4.979526	0.280958	-3.642520
H	-6.039476	0.292478	-3.906731
C	-4.594665	0.184114	-2.307205
H	-5.344663	0.123218	-1.515560
C	-3.240760	0.170725	-1.974209
H	-2.936327	0.111859	-0.927265
C	0.279010	-1.067458	-3.382118
C	-0.455814	-2.165633	-3.843185
H	-1.540812	-2.193199	-3.719769
C	0.195546	-3.224581	-4.475039
H	-0.386225	-4.074795	-4.838220
C	1.577339	-3.194777	-4.653433
H	2.082202	-4.021319	-5.158403
C	2.314779	-2.107052	-4.184912
H	3.398179	-2.073988	-4.316381
C	1.672421	-1.055737	-3.538384
H	2.271859	-0.224830	-3.158986
C	1.044768	5.032913	2.177072
C	2.135024	5.683229	1.581192
H	2.903974	5.097482	1.070839
C	2.243723	7.070301	1.642441
H	3.097888	7.567566	1.177873
C	1.262676	7.820246	2.289936
H	1.343739	8.908746	2.330893
C	0.173912	7.180194	2.882420
H	-0.595673	7.766088	3.390247
C	0.062830	5.791837	2.827024
H	-0.802180	5.306551	3.285070
C	1.746392	2.542522	3.505159
C	1.624814	3.169632	4.751439
H	1.085628	4.116729	4.839134
C	2.201559	2.595674	5.881529
H	2.113525	3.094445	6.849254
C	2.886871	1.384936	5.777736
H	3.328052	0.930248	6.667802
C	3.005975	0.753016	4.541095
H	3.528719	-0.201729	4.456646
C	2.451825	1.337045	3.402941
H	2.562467	0.846882	2.433838
C	-0.820668	2.826989	2.222661
H	-1.176810	2.980472	3.251602
H	-1.386305	3.484264	1.543473
C	-0.650706	-0.055689	3.155921
C	-0.967053	0.324079	4.464874
H	-1.578949	1.209713	4.654779
C	-0.503743	-0.430811	5.538698
H	-0.744807	-0.127822	6.559961
C	0.262068	-1.574646	5.309471
H	0.621417	-2.167492	6.153645
C	0.567380	-1.961919	4.007159
H	1.167854	-2.855109	3.829804
C	0.120134	-1.199264	2.929719
H	0.386849	-1.486061	1.908446
C	-3.116091	1.002092	1.703431
C	-3.805440	1.987044	0.986289
H	-3.265646	2.754091	0.423734
C	-5.197839	1.987888	0.970512
H	-5.731076	2.764385	0.417080
C	-5.905705	0.998841	1.654984
H	-6.998006	1.000648	1.643443
C	-5.218596	0.008637	2.355928
H	-5.771095	-0.766588	2.891654
C	-3.823793	0.007710	2.384143
H	-3.290177	-0.764509	2.944160
N	3.779858	2.944335	-0.056723
C	4.938390	2.796763	-0.047597
Cu	5.073534	0.390290	0.190391
Cu	0.092185	0.504332	-0.296720
P	6.253636	-0.147244	2.060551
As	7.390929	2.736974	2.356337
As	5.975725	-0.225806	-1.921360
P	8.220248	1.878265	-1.673391
C	5.435830	-1.477164	3.010694
C	4.420887	-2.209615	2.385674
H	4.092668	-1.933188	1.381241
C	3.830173	-3.287272	3.043845
H	3.055703	-3.870150	2.539578
C	4.229444	-3.621145	4.335997
H	3.765458	-4.464094	4.853424
C	5.233627	-2.885004	4.968079
H	5.553919	-3.151064	5.977918
C	5.845018	-1.825064	4.304609
H	6.651060	-1.276622	4.798474
C	7.877565	-0.912217	1.705293
C	7.891088	-1.944599	0.754907
H	6.965033	-2.243771	0.254895
C	9.073769	-2.614079	0.456732
H	9.064533	-3.421252	-0.279463
C	10.260469	-2.258693	1.103193
H	11.188698	-2.786229	0.872143
C	10.252998	-1.236821	2.049583
H	11.174413	-0.950997	2.561692
C	9.066757	-0.567241	2.354302
H	9.091566	0.225419	3.102690
C	6.587242	1.185354	3.270016
H	7.213396	0.863725	4.114804
H	5.609792	1.500535	3.666836
C	9.176559	2.802465	3.074813
C	9.416611	2.782258	4.454869
H	8.582651	2.776941	5.162751
C	10.725389	2.783875	4.930077
H	10.914115	2.768357	6.005861
C	11.794936	2.813901	4.032100
H	12.820334	2.818026	4.408803
C	11.556622	2.846578	2.659697
H	12.388925	2.874547	1.953530
C	10.247507	2.839939	2.178126
H	10.063309	2.849891	1.101298
C	6.505751	4.200399	3.260509
C	7.244967	5.310081	3.683406
H	8.331232	5.327448	3.565201

C	6.597229	6.395476	4.271832
H	7.180583	7.256540	4.605853
C	5.213892	6.377751	4.439852
H	4.708130	7.226102	4.906302
C	4.475651	5.275190	4.011568
H	3.392127	5.256307	4.137051
C	5.114197	4.191504	3.412746
H	4.511314	3.346561	3.067949
C	5.872171	-2.132683	-2.224195
C	4.696526	-2.771550	-1.809290
H	3.880453	-2.189080	-1.371737
C	4.558682	-4.149470	-1.962361
H	3.635241	-4.640115	-1.646525
C	5.596960	-4.898436	-2.515389
H	5.491711	-5.979631	-2.629202
C	6.772440	-4.267067	-2.920887
H	7.586432	-4.852586	-3.354593
C	6.912442	-2.886599	-2.777316
H	7.841208	-2.407898	-3.096562
C	5.189608	0.519203	-3.524264
C	5.566691	0.067273	-4.793043
H	6.290169	-0.746283	-4.898546
C	5.014215	0.648517	-5.931623
H	5.309233	0.293290	-6.921515
C	4.091055	1.687224	-5.806934
H	3.668872	2.151139	-6.701221
C	3.712937	2.138505	-4.544478
H	3.010315	2.968845	-4.447749
C	4.252049	1.549205	-3.400407
H	3.953639	1.900490	-2.409696
C	7.880106	0.135658	-2.156572
H	8.237027	-0.068706	-3.176724
H	8.389919	-0.533090	-1.446938
C	7.906192	2.796527	-3.213160
C	8.677027	2.562661	-4.360926
H	9.527977	1.876756	-4.321464
C	8.367522	3.212126	-5.550963
H	8.970776	3.029706	-6.443037
C	7.287021	4.095243	-5.604060
H	7.043280	4.600317	-6.541460
C	6.521242	4.333307	-4.465959
H	5.669205	5.014678	-4.509549
C	6.831538	3.688349	-3.269681
H	6.224127	3.858794	-2.376705
C	10.027328	1.932665	-1.446320
C	10.691782	0.875085	-0.813765
H	10.152008	-0.020772	-0.500666
C	12.057941	0.958680	-0.557567
H	12.565857	0.122486	-0.071871
C	12.770502	2.102291	-0.916238
H	13.843650	2.164059	-0.721581
C	12.109108	3.167443	-1.527366
H	12.661273	4.066775	-1.809077
C	10.743311	3.086666	-1.791433
H	10.235828	3.922332	-2.279772
N	3.131382	-0.006730	0.083973
C	1.983037	0.159751	-0.044233

$A_{opt\text{-}full}(S_1)$

Cu	1.828606	2.578258	0.000000
Cu	6.822476	2.384796	0.159867
As	0.526988	3.665519	-1.670099
P	-0.401109	0.715201	-2.378857
P	0.878057	3.625353	1.788834
As	-0.994236	1.157640	1.580568
C	1.580262	4.998189	-2.590819
C	2.855113	5.301984	-2.104434
H	3.240206	4.790191	-1.219499
C	3.639436	6.251226	-2.759291
H	4.633434	6.491392	-2.374254
C	3.154135	6.891698	-3.898148
H	3.766820	7.637858	-4.409475
C	1.880829	6.587729	-4.384256
H	1.499016	7.093934	-5.273738
C	1.089762	5.644810	-3.732274
H	0.088314	5.423703	-4.110760
C	-1.131959	4.561702	-1.311833
C	-1.116206	5.934319	-1.031528
H	-0.176536	6.492230	-1.053239
C	-2.306683	6.592975	-0.733075
H	-2.291893	7.665410	-0.526387
C	-3.511702	5.889666	-0.705280
H	-4.444127	6.412690	-0.481267
C	-3.525678	4.520667	-0.972892
H	-4.464705	3.962781	-0.961013
C	-2.339376	3.851500	-1.269804
H	-2.372880	2.781155	-1.480931
C	0.124572	2.364212	-3.070596
H	-0.574734	2.784635	-3.808529
H	1.088938	2.189285	-3.571669
C	-2.199906	0.660100	-2.660385
C	-2.823547	1.209421	-3.789692
H	-2.231347	1.672248	-4.583258
C	-4.209814	1.169506	-3.912312
H	-4.689483	1.599787	-4.794276
C	-4.985131	0.581352	-2.911031
H	-6.072953	0.557782	-3.008451
C	-4.372252	0.022284	-1.791394
H	-4.970670	-0.435282	-1.000977
C	-2.984975	0.060887	-1.668580
H	-2.501620	-0.365677	-0.786524
C	0.343066	-0.432238	-3.588095
C	-0.378329	-1.045638	-4.617425
H	-1.451016	-0.869380	-4.721560
C	0.273170	-1.895783	-5.510690
H	-0.295422	-2.375387	-6.310673
C	1.640606	-2.133834	-5.384979
H	2.145934	-2.798336	-6.089465
C	2.360983	-1.533586	-4.351526
H	3.429762	-1.726105	-4.237893
C	1.713471	-0.696909	-3.448314
H	2.273992	-0.252382	-2.622365
C	0.932610	5.426162	1.808771
C	2.161632	6.031649	1.496463
H	3.033204	5.411139	1.269823
C	2.268354	7.416940	1.480330
H	3.226772	7.883414	1.242831
C	1.152051	8.207520	1.766820
H	1.236495	9.296395	1.751356
C	-0.069095	7.609481	2.074379
H	-0.939880	8.227676	2.303515
C	-0.185609	6.220880	2.092677
H	-1.148459	5.764613	2.329628
C	1.785466	3.057982	3.254038
C	1.735445	3.808807	4.436883
H	1.210328	4.767391	4.459399
C	2.356566	3.328597	5.586515
H	2.318529	3.914057	6.507618
C	3.021181	2.102482	5.561543
H	3.497927	1.724021	6.468574
C	3.074405	1.356570	4.384369
H	3.578357	0.387591	4.364636
C	2.466845	1.834174	3.225972
H	2.519162	1.245670	2.307869
C	-0.849458	3.092894	1.961748
H	-1.250140	3.347967	2.954365
H	-1.426320	3.618034	1.184126
C	-0.417492	0.383824	3.258384
C	-0.833246	0.898259	4.490607
H	-1.508936	1.756520	4.538191
C	-0.397408	0.307666	5.673344
H	-0.719517	0.714000	6.634748
C	0.438361	-0.809350	5.629011
H	0.773924	-1.275960	6.558012
C	0.839456	-1.332667	4.402305
H	1.497361	-2.202424	4.368237
C	0.417476	-0.735317	3.215174
H	0.752790	-1.126401	2.249940
C	-2.917841	0.939587	1.722920
C	-3.827948	1.985223	1.554131
H	-3.484348	3.006962	1.384061
C	-5.199613	1.732807	1.602674
H	-5.906342	2.556535	1.476261

C	-5.667436	0.438886	1.820916
H	-6.741413	0.244695	1.864723
C	-4.759811	-0.607850	1.993259
H	-5.120939	-1.622629	2.175671
C	-3.390329	-0.360302	1.941621
H	-2.685544	-1.185104	2.085383
N	3.747943	2.860670	0.222968
C	4.906507	2.679471	0.199918
Cu	5.168403	0.272345	0.361680
Cu	0.342769	0.529423	-0.255289
P	6.356977	-0.110752	2.252830
As	7.536713	2.783968	2.409208
As	6.036465	-0.249519	-1.793033
P	8.236653	1.875411	-1.553844
C	5.563071	-1.368559	3.317791
C	4.485872	-2.098386	2.802379
H	4.090055	-1.857330	1.812395
C	3.919840	-3.128088	3.554082
H	3.095583	-3.711065	3.136117
C	4.405932	-3.415789	4.827538
H	3.961133	-4.222128	5.415391
C	5.471545	-2.679828	5.350298
H	5.859707	-2.909413	6.345249
C	6.056921	-1.668298	4.594856
H	6.915291	-1.126093	5.000019
C	7.984140	-0.873836	1.913418
C	8.007150	-1.880659	0.935590
H	7.086465	-2.155313	0.410631
C	9.189924	-2.552666	0.642272
H	9.189846	-3.342746	-0.112500
C	10.367642	-2.220040	1.316682
H	11.296530	-2.747376	1.087555
C	10.351448	-1.221092	2.287366
H	11.266716	-0.954793	2.820520
C	9.163937	-0.553653	2.591555
H	9.179364	0.218473	3.361655
C	6.680387	1.301320	3.379817
H	7.262526	1.022318	4.269869
H	5.694424	1.657951	3.715103
C	9.317598	2.807576	3.148015
C	9.521173	2.753930	4.533564
H	8.669398	2.733969	5.219408
C	10.815321	2.742585	5.046021
H	10.973257	2.699795	6.126045
C	11.909398	2.795817	4.179359
H	12.924224	2.790284	4.583682
C	11.707771	2.864959	2.802936
H	12.559341	2.912974	2.121556
C	10.412397	2.868528	2.283478
H	10.260454	2.908801	1.202953
C	6.736748	4.334198	3.251971
C	7.546202	5.395504	3.671180
H	8.633906	5.320673	3.599210
C	6.968871	6.552273	4.193151
H	7.608645	7.373786	4.523558
C	5.583370	6.655941	4.298482
H	5.131654	7.559851	4.713607
C	4.774940	5.601511	3.875310
H	3.689593	5.676974	3.956891
C	5.344131	4.445358	3.344421
H	4.690321	3.637302	3.004807
C	5.911992	-2.122886	-2.250456
C	4.751837	-2.793432	-1.840797
H	3.976276	-2.258123	-1.284155
C	4.587605	-4.144458	-2.139624
H	3.677878	-4.661495	-1.826608
C	5.583691	-4.835052	-2.829797
H	5.456202	-5.895433	-3.058300
C	6.746546	-4.173814	-3.223189
H	7.529511	-4.715035	-3.759583
C	6.912943	-2.819083	-2.936330
H	7.830096	-2.315696	-3.251528
C	5.241491	0.628101	-3.327049
C	5.637339	0.305435	-4.628900
H	6.372497	-0.485218	-4.804142
C	5.089263	0.984074	-5.714141
H	5.400413	0.727709	-6.729244
C	4.150888	1.994779	-5.503550
H	3.732904	2.536690	-6.354808
C	3.754226	2.317168	-4.208517
H	3.045549	3.131747	-4.042556
C	4.287725	1.627626	-3.119963
H	3.975340	1.877408	-2.104827
C	7.932022	0.134830	-2.062711
H	8.274902	-0.042310	-3.092460
H	8.470146	-0.535299	-1.376172
C	7.963975	2.821967	-3.084379
C	8.776506	2.627598	-4.210284
H	9.627920	1.942901	-4.162412
C	8.510009	3.316736	-5.388557
H	9.147466	3.166329	-6.262721
C	7.429883	4.199140	-5.452477
H	7.221066	4.736160	-6.380475
C	6.620214	4.395453	-4.336708
H	5.767673	5.075720	-4.388428
C	6.888593	3.711966	-3.151955
H	6.248459	3.851827	-2.276320
C	10.036628	1.950372	-1.274382
C	10.706083	0.885908	-0.658523
H	10.175769	-0.026111	-0.377674
C	12.066743	0.981999	-0.377853
H	12.578049	0.140677	0.095202
C	12.768678	2.144039	-0.694552
H	13.837948	2.214587	-0.482118
C	12.101381	3.217217	-1.285130
H	12.644667	4.131934	-1.532212
C	10.741475	3.124015	-1.574199
H	10.230408	3.965784	-2.048053
N	3.280248	-0.230720	0.260683
C	2.131402	-0.017420	0.099306

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Cu	1.828605	2.578258	0.000000
Cu	6.835819	2.270689	0.103828
As	0.557901	3.599946	-1.710749
P	-0.346648	0.615957	-2.379746
P	0.825212	3.576373	1.749622
As	-1.006537	1.074853	1.567756
C	1.592400	4.919663	-2.671738
C	2.873229	5.235821	-2.208986
H	3.272059	4.743515	-1.318541
C	3.644884	6.174913	-2.893004
H	4.642593	6.427195	-2.525598
C	3.141411	6.792181	-4.036916
H	3.744083	7.531053	-4.570338
C	1.862398	6.475474	-4.499059
H	1.466040	6.964426	-5.391901
C	1.083495	5.543035	-3.817804
H	0.077147	5.312155	-4.177350
C	-1.119020	4.473235	-1.381277
C	-1.121068	5.843889	-1.089709
H	-0.186326	6.410686	-1.088181
C	-2.322969	6.489223	-0.808901
H	-2.322174	7.559832	-0.592944
C	-3.521966	5.774722	-0.809573
H	-4.463233	6.287557	-0.599116
C	-3.518300	4.407981	-1.087718
H	-4.452202	3.841314	-1.098217
C	-2.320189	3.752176	-1.367296
H	-2.340006	2.683205	-1.586015
C	0.193181	2.253021	-3.081532
H	-0.483642	2.658948	-3.848405
H	1.171778	2.071885	-3.551905
C	-2.139281	0.547433	-2.698144
C	-2.741450	1.081622	-3.846342
H	-2.135509	1.551247	-4.625397
C	-4.122532	1.014732	-4.007833
H	-4.585368	1.433251	-4.904313
C	-4.914159	0.412873	-3.027572
H	-5.997903	0.366372	-3.156350
C	-4.322449	-0.130940	-1.889371
H	-4.933549	-0.599937	-1.115607
C	-2.940273	-0.063711	-1.726699

H	-2.476435	-0.478168	-0.828934
C	0.405357	-0.554878	-3.562932
C	-0.317475	-1.205028	-4.568580
H	-1.391287	-1.037542	-4.673411
C	0.333452	-2.080086	-5.437775
H	-0.237024	-2.587228	-6.219099
C	1.702498	-2.307271	-5.311957
H	2.208134	-2.991067	-5.997396
C	2.424483	-1.670409	-4.302150
H	3.494651	-1.853767	-4.188899
C	1.777438	-0.808872	-3.422256
H	2.340420	-0.336247	-2.614311
C	0.835653	5.379780	1.820945
C	2.050045	6.021478	1.522456
H	2.936945	5.427428	1.283458
C	2.124481	7.408880	1.533010
H	3.072557	7.902143	1.308012
C	0.988541	8.167905	1.828545
H	1.047251	9.258650	1.833364
C	-0.219284	7.534899	2.117933
H	-1.106096	8.127715	2.353096
C	-0.302103	6.143463	2.112391
H	-1.255492	5.661443	2.336262
C	1.735226	2.996212	3.210607
C	1.663997	3.723348	4.407194
H	1.126020	4.674449	4.443046
C	2.279512	3.228878	5.553988
H	2.222047	3.794766	6.486332
C	2.962913	2.013352	5.512703
H	3.434366	1.623334	6.417638
C	3.040037	1.292522	4.321598
H	3.557187	0.330509	4.288445
C	2.433996	1.782666	3.167751
H	2.497778	1.210161	2.240342
C	-0.894997	3.012953	1.920500
H	-1.299242	3.274953	2.910060
H	-1.481141	3.519731	1.137527
C	-0.464246	0.311874	3.262201
C	-0.920239	0.818402	4.483221
H	-1.604360	1.670789	4.513099
C	-0.514970	0.226536	5.676373
H	-0.868995	0.626307	6.629276
C	0.331149	-0.883368	5.653413
H	0.642548	-1.350181	6.590656
C	0.773290	-1.398726	4.437488
H	1.439618	-2.262944	4.419399
C	0.381350	-0.800094	3.240726
H	0.748342	-1.186504	2.285496
C	-2.930469	0.826091	1.664795
C	-3.853874	1.848826	1.438064
H	-3.523735	2.872903	1.255665
C	-5.221331	1.570685	1.443884
H	-5.938331	2.377302	1.273249
C	-5.672464	0.273198	1.675320
H	-6.743417	0.058858	1.685479
C	-4.751904	-0.751198	1.903776
H	-5.099926	-1.768693	2.096194
C	-3.386462	-0.477607	1.896215
H	-2.672457	-1.285208	2.084931
N	3.766372	2.794707	0.166089
C	4.913966	2.557238	0.138319
Cu	5.189826	0.163615	0.305666
Cu	0.381676	0.461555	-0.241174
P	6.386446	-0.223464	2.195661
As	7.543092	2.684139	2.352010
As	6.056714	-0.357784	-1.850500
P	8.250360	1.776430	-1.614747
C	5.609984	-1.482432	3.272239
C	4.485877	-2.172539	2.805165
H	4.051327	-1.911634	1.837150
C	3.924578	-3.190868	3.576093
H	3.061686	-3.742642	3.195214
C	4.466383	-3.509468	4.819254
H	4.026391	-4.307899	5.421292
C	5.582733	-2.816159	5.292128
H	6.015512	-3.071616	6.261955
C	6.160030	-1.814362	4.518160
H	7.056118	-1.304944	4.882606
C	8.017590	-0.973382	1.848843
C	8.043928	-1.979922	0.870687
H	7.122952	-2.262220	0.350365
C	9.230879	-2.641443	0.570611
H	9.233630	-3.430890	-0.184793
C	10.409318	-2.299076	1.239030
H	11.341485	-2.818169	1.004574
C	10.389655	-1.300943	2.210478
H	11.305285	-1.026994	2.739106
C	9.198209	-0.643539	2.520877
H	9.211260	0.129093	3.290489
C	6.702863	1.191544	3.321747
H	7.288111	0.915098	4.210624
H	5.714333	1.538903	3.660054
C	9.327134	2.718688	3.082198
C	9.538998	2.658425	4.466206
H	8.691251	2.628959	5.156755
C	10.836163	2.652007	4.971157
H	11.000516	2.604379	6.050009
C	11.925015	2.717041	4.098554
H	12.942139	2.715940	4.497024
C	11.715004	2.793108	2.723820
H	12.562291	2.850811	2.037868
C	10.416726	2.791691	2.211914
H	10.258373	2.836915	1.132512
C	6.730808	4.224174	3.201138
C	7.530017	5.285204	3.640143
H	8.618631	5.219094	3.574742
C	6.940644	6.430845	4.173088
H	7.572122	7.252423	4.518823
C	5.553835	6.523347	4.270243
H	5.093317	7.418581	4.694417
C	4.755439	5.469059	3.827440
H	3.668931	5.534835	3.902915
C	5.336771	4.324378	3.284889
H	4.691137	3.516417	2.930033
C	5.946447	-2.234145	-2.298630
C	4.810905	-2.922572	-1.851462
H	4.043534	-2.398366	-1.273781
C	4.658933	-4.276871	-2.142467
H	3.767873	-4.807605	-1.799872
C	5.643160	-4.952755	-2.863116
H	5.525270	-6.015468	-3.086203
C	6.782160	-4.273670	-3.294600
H	7.556111	-4.803223	-3.854990
C	6.936097	-2.916117	-3.014764
H	7.835033	-2.399213	-3.359018
C	5.261364	0.515105	-3.387176
C	5.649071	0.180645	-4.688482
H	6.377206	-0.616723	-4.861683
C	5.101536	0.855784	-5.776194
H	5.406139	0.589692	-6.790780
C	4.172429	1.875602	-5.568646
H	3.755942	2.415665	-6.421757
C	3.784036	2.209944	-4.274216
H	3.084156	3.032727	-4.110990
C	4.315808	1.523118	-3.183119
H	4.006991	1.782653	-2.169261
C	7.951256	0.034505	-2.121794
H	8.292574	-0.141805	-3.152224
H	8.492502	-0.633896	-1.435980
C	7.974604	2.720416	-3.146497
C	8.787404	2.523565	-4.271863
H	9.637844	1.837784	-4.222646
C	8.522519	3.211310	-5.451221
H	9.159806	3.058437	-6.324997
C	7.444135	4.095801	-5.516609
H	7.236265	4.631867	-6.445406
C	6.635187	4.295678	-4.401106
H	5.783861	4.977376	-4.454437
C	6.901566	3.613014	-3.215305
H	6.262102	3.756696	-2.339944
C	10.050572	1.861790	-1.339536
C	10.731030	0.798802	-0.733545
H	10.209570	-0.119905	-0.457913
C	12.091882	0.904796	-0.456845

H	12.612337	0.064682	0.008149
C	12.782678	2.075218	-0.767127
H	13.851867	2.153689	-0.557199
C	12.104314	3.146757	-1.347858
H	12.638728	4.068139	-1.589752
C	10.744442	3.043679	-1.633192
H	10.224638	3.884445	-2.099285
N	3.301994	-0.362463	0.239624
C	2.145351	-0.203512	0.103071

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Cu	11.990382	8.902615	6.655630
Cu	10.070242	6.335702	10.471699
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N	10.998956	6.101861	6.026897
As	7.751998	6.059256	10.748363
C	10.830582	7.499812	9.150713
C	10.199889	11.787711	6.835464
C	10.132918	11.392592	8.176116
H	10.561438	10.435765	8.482224
C	9.515884	12.216995	9.117102
H	9.479664	11.910002	10.165206
C	8.956459	13.430447	8.722615
H	8.475096	14.077295	9.459748
C	9.022222	13.828883	7.385401
H	8.593902	14.785441	7.077825
C	9.649124	13.016290	6.445807
H	9.724442	13.349840	5.407039
C	12.299298	11.818374	4.915607
C	13.355772	12.195652	5.759159
H	13.392966	11.833865	6.790489
C	14.359709	13.040507	5.296885
H	15.172913	13.326847	5.967652
C	14.320866	13.520818	3.985239
H	15.106430	14.188118	3.623266
C	13.271288	13.155454	3.145617
H	13.228135	13.527521	2.119533
C	12.261506	12.309294	3.607326
H	11.451593	12.045327	2.926774
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H	9.458827	11.423418	3.870377
H	8.915211	9.996970	4.785200
C	10.512859	10.359477	1.339223
C	9.473429	11.228448	0.982224
H	8.548564	11.258268	1.565421
C	9.609279	12.050472	-0.133435
H	8.798776	12.727336	-0.412997
C	10.776946	12.003246	-0.898316
H	10.878954	12.646936	-1.775016
C	11.807249	11.132877	-0.549150
H	12.720984	11.088191	-1.144848
C	11.679029	10.310998	0.570643
H	12.495222	9.640936	0.849899
C	8.762111	8.228579	2.577322
C	8.235073	8.082062	1.290932
H	8.709170	8.574759	0.438772
C	7.090207	7.309689	1.093725
H	6.679351	7.201856	0.087309
C	6.468937	6.686293	2.174230
H	5.567844	6.089268	2.017410
C	7.000722	6.823151	3.456426
H	6.523519	6.334800	4.307940
C	8.151624	7.580701	3.657517
H	8.566497	7.658983	4.665273
C	6.675747	7.658827	10.690483
C	5.290509	7.606685	10.885018
H	4.798982	6.655883	11.109492
C	4.536097	8.774195	10.810294
H	3.455712	8.734598	10.966428
C	5.160505	9.993196	10.541163
H	4.565968	10.907904	10.485375
C	6.538688	10.045831	10.346449
H	7.026091	10.997672	10.124865
C	7.299384	8.880000	10.424164
H	8.380414	8.917099	10.261421
C	6.997096	5.092498	12.241813
C	6.912869	3.697156	12.221773
H	7.208114	3.125791	11.339356
C	6.459531	3.009646	13.345964
H	6.391057	1.919769	13.318727
C	6.097133	3.708436	14.496731
H	5.736140	3.168426	15.375019
C	6.193763	5.099980	14.523958
H	5.910715	5.651972	15.423054
C	6.643679	5.793009	13.401193
H	6.706954	6.884185	13.428463
C	7.073483	5.026321	9.234591
H	7.316889	3.970529	9.427708
H	5.981501	5.143845	9.173332
C	7.128516	7.075642	7.234597
C	5.747845	7.140530	7.005909
H	5.141228	6.231221	7.038186
C	5.139793	8.359973	6.726328
H	4.063257	8.402840	6.547633
C	5.905282	9.525927	6.681428
H	5.425596	10.485495	6.476179
C	7.277984	9.467459	6.906544
H	7.872537	10.383339	6.899635
C	7.894279	8.244497	7.172146
H	8.971219	8.201715	7.347116
C	7.313359	4.284429	6.464518
C	8.067250	4.106543	5.295302
H	8.977483	4.692229	5.140421
C	7.656459	3.193766	4.327082
H	8.246262	3.069235	3.416346
C	6.499227	2.440661	4.521962
H	6.180912	1.719769	3.765620
C	5.749949	2.605158	5.686795
H	4.843749	2.015470	5.843074
C	6.153008	3.523152	6.654922
H	5.559235	3.632283	7.564830
H	17.872690	11.951583	8.223628
H	16.961233	10.367379	6.561995
C	11.442604	6.772201	5.181454
P	7.932578	5.497170	7.681707
N	11.296468	8.159072	8.309156
C	16.400927	10.561790	7.479654
As	10.387870	9.229312	2.893908
Cu	10.227442	5.404966	7.668951
Cu	12.147582	7.971880	3.852883
As	11.157166	3.594400	8.852736
P	11.770707	5.177173	11.497111
P	14.372303	8.233303	3.418780
As	14.339066	8.699219	6.483393
C	12.136782	2.414248	7.672443
C	12.153316	2.714226	6.306839
H	11.637881	3.604380	5.936614
C	12.838664	1.882957	5.420939
H	12.837235	2.110078	4.352134
C	13.519329	0.764589	5.898626
H	14.057846	0.114439	5.205261
C	13.504823	0.465464	7.262537
H	14.030211	-0.417103	7.634419
C	12.806493	1.281853	8.148914
H	12.777471	1.023994	9.211276
C	9.885090	2.358849	9.627098
C	8.852547	1.917913	8.787685
H	8.786263	2.275928	7.755559
C	7.911273	1.004831	9.256296
H	7.114748	0.660886	8.592325
C	7.994826	0.524287	10.565284
H	7.260438	-0.197649	10.929789
C	9.020282	0.960930	11.401100
H	9.092475	0.590522	12.426128
C	9.965579	1.877081	10.935758
H	10.755784	2.204885	11.612687
C	12.427091	3.926833	10.294189
H	12.722775	2.997103	10.801703
H	13.322255	4.343921	9.810227
C	11.503175	4.233051	13.026081
C	12.510339	3.430141	13.582986
H	13.506577	3.402739	13.132315
C	12.246295	2.673890	14.720555

H	13.031339	2.049721	15.153219
C	10.980656	2.717112	15.311755
H	10.778152	2.121064	16.204590
C	9.981830	3.522555	14.769897
H	8.991149	3.562936	15.226937
C	10.242975	4.280408	13.628728
H	9.456530	4.900582	13.195266
C	13.230066	6.225057	11.824669
C	13.571278	6.607711	13.126886
H	12.995111	6.237776	13.978121
C	14.661276	7.450029	13.344008
H	14.925281	7.736055	14.364640
C	15.418139	7.912773	12.269124
H	16.279646	8.561118	12.443917
C	15.073480	7.544573	10.968625
H	15.658612	7.902859	10.119097
C	13.975531	6.719617	10.745107
H	13.712622	6.464151	9.716372
C	15.349531	6.694960	3.438523
C	16.700548	6.700693	3.064997
H	17.161201	7.616923	2.685158
C	17.455162	5.536350	3.163460
H	18.506361	5.542593	2.866698
C	16.868534	4.362591	3.639769
H	17.464243	3.450431	3.719967
C	15.526134	4.352288	4.010107
H	15.067931	3.438127	4.392847
C	14.763768	5.514369	3.904067
H	13.712383	5.511744	4.202477
C	14.894961	9.068075	1.885933
C	15.169898	10.438699	1.840580
H	15.146901	11.045734	2.746840
C	15.467075	11.054077	0.625463
H	15.685581	12.124157	0.603047
C	15.489830	10.309510	-0.551947
H	15.731834	10.792093	-1.501624
C	15.207974	8.942849	-0.513871
H	15.226114	8.353220	-1.433130
C	14.908952	8.324075	0.696728
H	14.696412	7.251604	0.718206
C	15.133271	9.215861	4.773854
H	14.856811	10.274248	4.650807
H	16.229187	9.120052	4.757982
C	15.188943	7.009493	6.892025
C	16.580698	6.873244	6.877102
H	17.220667	7.727768	6.642425
C	17.165041	5.643838	7.168890
H	18.252323	5.541809	7.153084
C	16.362003	4.546080	7.478647
H	16.820326	3.580005	7.701667
C	14.975744	4.677762	7.492164
H	14.349816	3.808722	7.703153
C	14.384964	5.908320	7.202245
H	13.296282	6.006167	7.196621
C	15.176285	9.930450	7.718397
C	14.469288	10.210849	8.894357
H	13.507710	9.725024	9.086385
C	14.989176	11.106185	9.827295
H	14.434729	11.315450	10.744822
C	16.211143	11.732889	9.586654
H	16.616308	12.439757	10.314160
C	16.915514	11.460424	8.413617

A$_{\text{opt-const}}$(S_1) starting from **A**$_{\text{opt-const}}$(S_0)

Cu	1.828606	2.578258	0.000000
Cu	6.715735	2.459354	0.010866
As	0.573123	3.017675	-1.955463
P	-0.444770	0.112736	-2.374044
P	0.971202	3.036994	2.060735
As	-1.102903	0.781244	1.673595
C	1.346622	4.417975	-3.049534
C	2.429291	5.135713	-2.532517
H	2.857615	4.859311	-1.565122
C	2.962236	6.201990	-3.257971
H	3.792826	6.777282	-2.841537
C	2.434050	6.535982	-4.503499
H	2.852104	7.371437	-5.069976
C	1.360474	5.810962	-5.024627
H	0.939906	6.078294	-5.996745
C	0.808572	4.760680	-4.295282
H	-0.055253	4.223858	-4.696776
C	-1.180372	3.763425	-1.610272
C	-1.241765	4.728388	-0.595160
H	-0.336257	5.011929	-0.048205
C	-2.450625	5.347882	-0.287403
H	-2.485489	6.107620	0.497112
C	-3.609508	5.001240	-0.985792
H	-4.557868	5.487536	-0.745888
C	-3.551554	4.041730	-1.994592
H	-4.453478	3.766238	-2.545606
C	-2.339447	3.426279	-2.312472
H	-2.319895	2.680757	-3.108592
C	0.266653	1.578599	-3.244436
H	-0.339609	1.895672	-4.105062
H	1.267811	1.308323	-3.613117
C	-2.187970	0.073047	-2.883819
C	-2.553537	0.191034	-4.233644
H	-1.786146	0.271539	-5.008927
C	-3.897007	0.192658	-4.593957
H	-4.178923	0.286350	-5.645079
C	-4.883890	0.065357	-3.612463
H	-5.938127	0.065212	-3.898805
C	-4.524910	-0.070694	-2.273993
H	-5.289567	-0.174849	-1.501969
C	-3.178408	-0.065044	-1.909305
H	-2.898842	-0.154587	-0.858725
C	0.296946	-1.338916	-3.198541
C	-0.503740	-2.417872	-3.593998
H	-1.589397	-2.362554	-3.489338
C	0.078408	-3.565162	-4.130338
H	-0.557127	-4.397327	-4.441288
C	1.461458	-3.646679	-4.274649
H	1.916483	-4.543589	-4.701083
C	2.263060	-2.577522	-3.875083
H	3.347031	-2.634598	-3.985201
C	1.689815	-1.431738	-3.329867
H	2.339908	-0.614257	-3.006735
C	1.069783	4.811606	2.466256
C	2.220795	5.498207	2.051416
H	3.000443	4.968357	1.496603
C	2.367868	6.852502	2.339850
H	3.271089	7.377821	2.021824
C	1.363345	7.536694	3.024083
H	1.476873	8.600737	3.243139
C	0.209610	6.863075	3.422975
H	-0.580556	7.397910	3.954924
C	0.061627	5.504259	3.148608
H	-0.848312	4.991917	3.469098
C	1.798695	2.187673	3.452534
C	1.438040	2.441805	4.781781
H	0.679281	3.194850	5.012589
C	2.051088	1.745413	5.818558
H	1.766041	1.948299	6.853121
C	3.024515	0.785615	5.536284
H	3.495706	0.231840	6.351369
C	3.388911	0.531153	4.217263
H	4.130053	-0.239855	3.993590
C	2.785568	1.236719	3.177236
H	3.068071	1.042806	2.141952
C	-0.793153	2.607955	2.300968
H	-1.138400	2.705104	3.340637
H	-1.383467	3.275859	1.655679
C	-0.726476	-0.251657	3.258549
C	-1.486098	-0.101690	4.424732
H	-2.349475	0.569291	4.440266
C	-1.148530	-0.818809	5.569232
H	-1.744233	-0.704556	6.477684
C	-0.051134	-1.681129	5.555304
H	0.212628	-2.239953	6.456063
C	0.707370	-1.829064	4.396422
H	1.574560	-2.493062	4.388479
C	0.368723	-1.118642	3.245786
H	0.970532	-1.222530	2.338136

C	-3.033574	0.767946	1.570564
C	-3.699691	1.852063	0.988310
H	-3.150015	2.724173	0.625983
C	-5.084903	1.824084	0.845798
H	-5.596233	2.678540	0.396817
C	-5.811109	0.710954	1.268822
H	-6.898170	0.692998	1.162389
C	-5.146664	-0.380862	1.826816
H	-5.710735	-1.256694	2.155419
C	-3.760311	-0.356206	1.977542
H	-3.249801	-1.212899	2.424968
N	3.707689	3.131325	-0.076718
C	4.875155	2.966626	-0.055393
Cu	5.265200	0.350538	0.146261
Cu	0.275124	0.377443	-0.212259
P	6.691574	-0.661090	1.624363
As	7.565808	2.341323	2.205194
As	6.160425	-0.552818	-1.851783
P	7.984739	1.943957	-1.786083
C	5.801003	-2.007924	2.468524
C	4.525758	-2.380403	2.028940
H	4.068531	-1.864162	1.181502
C	3.836453	-3.404510	2.677222
H	2.843739	-3.695494	2.325603
C	4.415039	-4.056095	3.764510
H	3.876812	-4.861102	4.270348
C	5.688242	-3.687773	4.204997
H	6.144778	-4.203166	5.052910
C	6.383160	-2.669237	3.560191
H	7.385091	-2.396555	3.901857
C	8.245411	-1.400111	1.064147
C	8.235652	-2.715106	0.573246
H	7.309783	-3.295475	0.572800
C	9.410709	-3.287996	0.096098
H	9.395569	-4.315103	-0.274232
C	10.601413	-2.558760	0.098586
H	11.523493	-3.016846	-0.266268
C	10.613829	-1.250867	0.581828
H	11.541257	-0.674346	0.600227
C	9.441815	-0.667578	1.060221
H	9.482624	0.353347	1.440972
C	7.114141	0.543497	2.934373
H	7.889908	0.149294	3.608604
H	6.190994	0.693890	3.515258
C	9.453674	2.450420	2.602707
C	10.011688	1.967705	3.793482
H	9.377219	1.536582	4.572748
C	11.387370	2.041951	3.998033
H	11.819652	1.667073	4.928595
C	12.211881	2.596776	3.017348
H	13.290557	2.651370	3.181066
C	11.659967	3.083247	1.833936
H	12.298182	3.517435	1.061630
C	10.282926	3.010505	1.626376
H	9.853951	3.378216	0.691349
C	6.725456	3.432875	3.564216
C	7.443729	4.093760	4.564197
H	8.532145	4.015835	4.610311
C	6.765636	4.866690	5.507109
H	7.329639	5.383620	6.286912
C	5.377492	4.980701	5.455276
H	4.851356	5.584713	6.197936
C	4.661494	4.333379	4.448200
H	3.575308	4.428365	4.393948
C	5.333527	3.570476	3.496988
H	4.769484	3.089324	2.694533
C	6.240411	-2.448399	-2.129750
C	5.110696	-3.184879	-1.748163
H	4.235841	-2.674726	-1.334108
C	5.101393	-4.567893	-1.902897
H	4.218173	-5.140732	-1.611901
C	6.219415	-5.218376	-2.429267
H	6.212899	-6.304195	-2.547714
C	7.345006	-4.485265	-2.804846
H	8.216894	-4.995497	-3.220629
C	7.362345	-3.099559	-2.652421
H	8.252943	-2.537334	-2.940506
C	5.113428	0.094977	-3.335458
C	5.127985	-0.605191	-4.547061
H	5.674803	-1.547413	-4.637618
C	4.441038	-0.092971	-5.645840
H	4.449098	-0.638910	-6.591713
C	3.752633	1.114611	-5.537912
H	3.227187	1.520972	-6.405119
C	3.738146	1.808042	-4.327696
H	3.217531	2.764914	-4.245000
C	4.404809	1.294807	-3.217142
H	4.381165	1.839336	-2.271552
C	7.953904	0.128037	-2.138658
H	8.310364	-0.122742	-3.148935
H	8.585393	-0.376715	-1.391145
C	7.343271	2.710104	-3.316201
C	7.729497	2.264895	-4.586366
H	8.428034	1.431171	-4.695864
C	7.237066	2.892204	-5.726200
H	7.536290	2.536259	-6.714540
C	6.373931	3.982650	-5.605560
H	5.993763	4.478358	-6.501725
C	6.000982	4.440088	-4.344552
H	5.318940	5.286381	-4.248967
C	6.477769	3.802313	-3.200799
H	6.163828	4.137074	-2.207718
C	9.769050	2.339660	-1.874123
C	10.784246	1.380981	-1.809828
H	10.547683	0.317969	-1.747839
C	12.123025	1.773728	-1.827352
H	12.908919	1.016049	-1.782513
C	12.458210	3.122583	-1.911981
H	13.507119	3.426666	-1.932961
C	11.448480	4.084764	-1.980699
H	11.704114	5.143947	-2.057019
C	10.112607	3.696956	-1.959897
H	9.327353	4.456338	-2.019695
N	3.365111	0.048894	-0.133788
C	2.200369	0.188871	-0.147463

$A_{opt\text{-}const}(T_1)$ starting from $A_{opt\text{-}const}(S_0)$

Cu	1.828606	2.578258	0.000000
Cu	6.682082	2.443473	0.096318
As	0.535603	3.065430	-1.921703
P	-0.492421	0.170453	-2.360365
P	0.998472	3.067256	2.078967
As	-1.076380	0.800322	1.716248
C	1.287615	4.486264	-3.003670
C	2.400377	5.175235	-2.511932
H	2.860996	4.869710	-1.568756
C	2.921419	6.251315	-3.231609
H	3.776713	6.803670	-2.834513
C	2.348534	6.625854	-4.445362
H	2.756826	7.469291	-5.007008
C	1.242461	5.931741	-4.939939
H	0.786802	6.231329	-5.886446
C	0.704650	4.870074	-4.216751
H	-0.183242	4.356755	-4.595958
C	-1.206992	3.811223	-1.524657
C	-1.239821	4.771664	-0.504056
H	-0.319611	5.054447	0.017665
C	-2.439720	5.388027	-0.157847
H	-2.451824	6.143138	0.631817
C	-3.618095	5.044444	-0.824408
H	-4.559540	5.528339	-0.554411
C	-3.588282	4.090992	-1.840106
H	-4.505258	3.818322	-2.367132
C	-2.385530	3.477392	-2.195358
H	-2.388976	2.735641	-2.995036
C	0.193263	1.650989	-3.228382
H	-0.436230	1.983092	-4.066358
H	1.183720	1.385542	-3.628428
C	-2.249963	0.133518	-2.816970
C	-2.662241	0.282418	-4.150159
H	-1.922668	0.384267	-4.949551
C	-4.017570	0.289325	-4.463407
H	-4.335867	0.407374	-5.501605

C	-4.969804	0.136855	-3.451748
H	-6.033297	0.141286	-3.701538
C	-4.564628	-0.029549	-2.129907
H	-5.301981	-0.152596	-1.334344
C	-3.206357	-0.029325	-1.812426
H	-2.890395	-0.141622	-0.774285
C	0.237046	-1.263685	-3.224647
C	-0.567442	-2.317867	-3.674215
H	-1.653816	-2.257694	-3.580969
C	0.012888	-3.447176	-4.249699
H	-0.625041	-4.260269	-4.603295
C	1.396989	-3.535049	-4.378224
H	1.850006	-4.417737	-4.835349
C	2.202640	-2.491286	-3.922787
H	3.287674	-2.553641	-4.019217
C	1.631201	-1.363759	-3.339283
H	2.282879	-0.565627	-2.973099
C	1.072920	4.852119	2.445688
C	2.209069	5.550009	2.009486
H	2.995699	5.022097	1.463481
C	2.333159	6.913093	2.266003
H	3.224870	7.447015	1.930290
C	1.320832	7.594728	2.941010
H	1.416577	8.665228	3.135574
C	0.182106	6.909447	3.362534
H	-0.613949	7.441447	3.888506
C	0.056813	5.542502	3.118892
H	-0.842290	5.021726	3.455745
C	1.847339	2.268456	3.488017
C	1.569354	2.636867	4.810411
H	0.871049	3.452368	5.019112
C	2.191452	1.977540	5.866024
H	1.974330	2.272504	6.894945
C	3.087724	0.938421	5.610766
H	3.564861	0.414245	6.441812
C	3.368614	0.569215	4.298211
H	4.048118	-0.262392	4.095348
C	2.760365	1.240015	3.238241
H	2.981986	0.955942	2.209446
C	-0.758225	2.622049	2.351724
H	-1.079155	2.713143	3.399758
H	-1.367967	3.288131	1.722611
C	-0.642566	-0.252702	3.272833
C	-1.313578	-0.066091	4.487104
H	-2.137761	0.649055	4.559786
C	-0.938942	-0.801987	5.607686
H	-1.464480	-0.656915	6.554173
C	0.105692	-1.723511	5.520762
H	0.398843	-2.297999	6.402340
C	0.774201	-1.910733	4.313438
H	1.600317	-2.621822	4.249225
C	0.400298	-1.178181	3.187759
H	0.935230	-1.310977	2.242737
C	-3.009487	0.781895	1.681505
C	-3.693132	1.853882	1.096830
H	-3.153799	2.714454	0.693229
C	-5.082620	1.827899	1.006387
H	-5.607971	2.672832	0.555480
C	-5.795806	0.728295	1.484064
H	-6.886065	0.711547	1.417989
C	-5.114576	-0.351137	2.045655
H	-5.668850	-1.215948	2.417320
C	-3.723434	-0.328016	2.145086
H	-3.198896	-1.173775	2.596988
N	3.698207	3.182605	-0.059646
C	4.866826	3.063841	-0.005674
Cu	5.242450	0.295115	0.276980
Cu	0.255188	0.417819	-0.209210
P	6.669300	-0.704209	1.743839
As	7.524796	2.312231	2.297876
As	6.138464	-0.547780	-1.726468
P	7.967970	1.949910	-1.700053
C	5.806566	-2.062656	2.596111
C	4.548263	-2.470841	2.138858
H	4.086415	-1.963381	1.287938
C	3.886879	-3.524479	2.768486
H	2.911227	-3.849086	2.398998
C	4.473993	-4.166234	3.857193
H	3.957900	-4.994896	4.347697
C	5.727881	-3.758728	4.317928
H	6.190834	-4.266496	5.167000
C	6.396982	-2.713057	3.689391
H	7.386635	-2.412533	4.043410
C	8.233104	-1.418398	1.176356
C	8.232938	-2.725790	0.664873
H	7.311483	-3.313107	0.655563
C	9.411233	-3.281924	0.176564
H	9.403159	-4.302865	-0.210757
C	10.596419	-2.543506	0.187847
H	11.521087	-2.988359	-0.186879
C	10.599502	-1.243503	0.691616
H	11.522044	-0.659323	0.716384
C	9.423672	-0.677276	1.181488
H	9.457785	0.338110	1.576934
C	7.073246	0.522686	3.040835
H	7.844242	0.138791	3.726490
H	6.143287	0.673841	3.610737
C	9.412510	2.436205	2.697830
C	9.978718	1.953183	3.884573
H	9.352090	1.502874	4.659299
C	11.352631	2.051256	4.091376
H	11.791041	1.675554	5.018687
C	12.167420	2.631636	3.117435
H	13.244624	2.705484	3.283055
C	11.607523	3.118464	1.938004
H	12.238005	3.571746	1.170354
C	10.232540	3.020497	1.727779
H	9.799031	3.387775	0.794712
C	6.692887	3.441772	3.631295
C	7.416883	4.090964	4.635089
H	8.499187	3.965604	4.708752
C	6.754721	4.916579	5.543702
H	7.324092	5.423811	6.325887
C	5.376142	5.098349	5.451374
H	4.862113	5.747239	6.164035
C	4.655153	4.462419	4.440866
H	3.577805	4.613012	4.353506
C	5.310831	3.642154	3.526535
H	4.742826	3.168076	2.722669
C	6.224674	-2.437378	-2.078766
C	5.076554	-3.182822	-1.777800
H	4.186615	-2.686060	-1.379430
C	5.065222	-4.557335	-1.995925
H	4.166349	-5.135497	-1.770303
C	6.200581	-5.192790	-2.503284
H	6.192336	-6.272015	-2.671871
C	7.345323	-4.452106	-2.796127
H	8.231426	-4.949523	-3.197353
C	7.363552	-3.074339	-2.581643
H	8.268665	-2.507614	-2.808950
C	5.093894	0.125867	-3.202950
C	5.139078	-0.544705	-4.430791
H	5.693506	-1.481342	-4.532122
C	4.473722	-0.010905	-5.532651
H	4.506958	-0.534575	-6.490584
C	3.775057	1.189622	-5.412793
H	3.267365	1.613822	-6.282158
C	3.729709	1.853273	-4.186965
H	3.204014	2.806559	-4.093757
C	4.376751	1.318827	-3.074595
H	4.333142	1.843969	-2.119743
C	7.931853	0.132372	-2.031092
H	8.275551	-0.133488	-3.042221
H	8.572325	-0.363167	-1.284989
C	7.344925	2.720046	-3.235945
C	7.747287	2.279826	-4.502713
H	8.440420	1.440774	-4.605885
C	7.279529	2.919933	-5.645963
H	7.592151	2.568619	-6.631778
C	6.424366	4.017386	-5.532153
H	6.064183	4.522945	-6.431035
C	6.033916	4.468834	-4.274347
H	5.357867	5.320830	-4.183686
C	6.486598	3.818798	-3.127621

H	6.159010	4.151120	-2.138783
C	9.753277	2.345341	-1.777438
C	10.769161	1.388144	-1.703515
H	10.533015	0.324901	-1.643323
C	12.107635	1.782318	-1.710583
H	12.893884	1.025439	-1.659557
C	12.442419	3.131318	-1.793516
H	13.491136	3.436390	-1.806773
C	11.432178	4.092286	-1.871003
H	11.687110	5.151730	-1.946393
C	10.096716	3.702976	-1.861235
H	9.311810	4.462015	-1.929614
N	3.337573	0.027019	-0.042775
C	2.182615	0.217791	-0.109452

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Cu	3.307092	0.093718	-1.230975
C	1.373228	0.073370	-1.494421
N	0.213016	0.064639	-1.625895
Cu	-1.723151	0.056875	-1.152502
Cu	-3.339257	-0.232984	0.973987
C	-1.406887	-0.218223	1.237144
N	-0.245197	-0.208728	1.355140
Cu	1.690344	-0.204312	0.883045
P	4.448693	-1.876117	-1.085207
P	3.948211	2.284217	-1.208224
P	-3.058714	-1.666297	-1.852535
P	-2.450432	2.217979	-1.382597
P	-3.987306	-2.426656	0.941569
P	-4.483265	1.734853	0.812316
P	2.419837	-2.363088	1.109774
P	3.021471	1.526720	1.584791
C	4.158349	-2.622874	0.571511
C	-3.362599	-3.057590	-0.688299
C	-4.190494	2.474193	-0.847580
C	3.321263	2.918489	0.419158
H	4.785351	-2.054705	1.277146
H	4.468900	-3.677986	0.597539
C	-4.710264	-1.146139	-2.441794
C	-5.899733	-1.817845	-2.145166
C	-7.111178	-1.365466	-2.670759
C	-7.143539	-0.250694	-3.505177
C	-5.956037	0.414341	-3.819850
C	-4.748340	-0.029345	-3.290205
C	-2.383352	-2.468859	-3.349917
C	-2.928634	-3.652483	-3.864612
C	-2.412491	-4.209278	-5.031052
C	-1.367973	-3.575009	-5.707188
C	-0.836805	-2.387714	-5.208980
C	-1.332990	-1.840614	-4.026701
C	-5.738485	-2.903304	1.012421
C	-6.682186	-1.903788	1.263606
C	-8.041849	-2.212164	1.284907
C	-8.460064	-3.520788	1.054538
C	-7.520013	-4.526645	0.812662
C	-6.162254	-4.222812	0.795748
C	-3.168365	-3.510610	2.160861
C	-3.885971	-3.994833	3.262284
C	-3.245247	-4.758558	4.236024
C	-1.886864	-5.046492	4.119774
C	-1.166540	-4.558169	3.030422
C	-1.796781	-3.782906	2.060790
C	-2.461913	2.692321	-3.144080
C	-1.388547	2.248449	-3.930256
C	-1.342946	2.546843	-5.289723
C	-2.372536	3.278209	-5.880814
C	-3.445929	3.717867	-5.106520
C	-3.491926	3.429108	-3.743411
C	-1.533350	3.557302	-0.544310
C	-0.781592	3.251927	0.597402
C	-0.139203	4.268922	1.302472
C	-0.215117	5.586447	0.853406
C	-0.943409	5.892003	-0.296594
C	-1.607417	4.882946	-0.989888
C	-3.830659	2.962009	1.986704
C	-3.106040	2.503183	3.091809
C	-2.574036	3.409475	4.006639
C	-2.744807	4.777607	3.811682
C	-3.463869	5.242257	2.709538
C	-4.013031	4.339123	1.805325
C	-6.298730	1.841927	0.952074
C	-6.919782	2.424216	2.062145
C	-8.311266	2.434631	2.156159
C	-9.088440	1.869871	1.146470
C	-8.471231	1.280332	0.042207
C	-7.083265	1.257354	-0.052305
C	4.675550	1.008770	2.168685
C	5.862924	1.683605	1.870703
C	7.077019	1.230536	2.389535
C	7.114050	0.112451	3.219318
C	5.928757	-0.555860	3.535297
C	4.718498	-0.111859	3.011789
C	2.346071	2.329132	3.081994
C	2.894363	3.510328	3.599190
C	2.375861	4.068760	4.763759
C	1.325791	3.438769	5.435315
C	0.791494	2.253943	4.934623
C	1.290622	1.704773	3.754465
C	5.696574	2.770200	-1.284063
C	6.646187	1.774919	-1.529813
C	8.003669	2.092287	-1.557454
C	8.413604	3.405634	-1.339153
C	7.467462	4.407077	-1.102752
C	6.111846	4.094241	-1.079331
C	3.125301	3.354997	-2.436488
C	3.840796	3.819926	-3.547736
C	3.199685	4.571553	-4.530466
C	1.842989	4.867223	-4.413207
C	1.125091	4.398782	-3.313715
C	1.755497	3.634826	-2.335129
C	2.432088	-2.842044	2.870050
C	1.360331	-2.398397	3.658367
C	1.314335	-2.701993	5.016639
C	2.342273	-3.438259	5.604494
C	3.414318	-3.877554	4.828132
C	3.460571	-3.583592	3.466126
C	1.499157	-3.699049	0.269387
C	0.743637	-3.389680	-0.868787
C	0.100550	-4.404276	-1.576635
C	0.179455	-5.723659	-1.133548
C	0.911641	-6.033361	0.012797
C	1.576274	-5.026561	0.708723
C	3.790954	-3.095784	-2.264260
C	3.067325	-2.629094	-3.366821
C	2.532406	-3.529319	-4.285860
C	2.698776	-4.898874	-4.097703
C	3.416422	-5.371274	-2.998066
C	3.968969	-4.474336	-2.089717
C	6.263543	-1.981759	-1.230818
C	6.882019	-2.560904	-2.343942
C	8.273194	-2.567944	-2.442744
C	9.052560	-2.003041	-1.434841
C	8.437866	-1.416890	-0.327355
C	7.050184	-1.397256	-0.228028
H	-5.906416	-2.695584	-1.499388
H	-8.032822	-1.896304	-2.422406
H	-8.092422	0.097241	-3.919578
H	-5.967616	1.280283	-4.485711
H	-3.822005	0.489098	-3.553645
H	-3.768025	-4.141619	-3.363670
H	-2.838403	-5.134137	-5.426461
H	-0.977602	-4.006081	-6.632056
H	-0.033030	-1.877382	-5.744620
H	-0.900553	-0.923331	-3.622252
H	-2.378627	-3.522917	-0.519454
H	-4.025425	-3.831119	-1.104388
H	-6.349339	-0.876452	1.425098
H	-8.770279	-1.421779	1.478149
H	-9.524736	-3.765280	1.068681
H	-7.850341	-5.553969	0.643528
H	-5.430271	-5.016957	0.622422
H	-4.953707	-3.785084	3.357680
H	-3.816883	-5.137673	5.086127

H	-1.387997	-5.652913	4.879037
H	-0.102126	-4.775935	2.931559
H	-1.201449	-3.393770	1.230361
H	-4.252925	4.293327	-5.565858
H	-2.340758	3.505599	-6.948721
H	-0.497303	2.204830	-5.890369
H	-0.580888	1.672805	-3.470616
H	-0.703797	2.220093	0.942039
H	0.418796	4.025888	2.208748
H	0.293849	6.381094	1.403887
H	-0.998155	6.922937	-0.653410
H	-2.181154	5.129550	-1.887486
H	-4.504256	3.528272	-0.878308
H	-4.814391	1.901514	-1.552274
H	-2.946642	1.429642	3.227911
H	-2.014682	3.046225	4.869860
H	-2.317522	5.488337	4.522649
H	-3.601263	6.314766	2.556625
H	-4.588750	4.715858	0.956597
H	-6.317910	2.878530	2.852635
H	-8.790086	2.895830	3.022791
H	-10.178127	1.890064	1.219783
H	-9.072646	0.831746	-0.751893
H	-6.619127	0.769806	-0.913482
H	-4.342392	3.779509	-3.154666
H	5.866092	2.563645	1.227935
H	7.996881	1.763930	2.140049
H	8.065066	-0.236088	3.628289
H	5.943838	-1.424536	4.197526
H	3.793914	-0.633301	3.275532
H	3.738066	3.995736	3.101858
H	2.804000	4.991700	5.161249
H	0.932947	3.871720	6.358253
H	-0.016958	1.747202	5.466660
H	0.856326	0.789233	3.347988
H	2.336387	3.381367	0.249998
H	3.982333	3.694004	0.834351
H	6.319654	0.744275	-1.682879
H	8.736942	1.305310	-1.746556
H	9.476548	3.657193	-1.358220
H	7.791377	5.437930	-0.942947
H	5.374765	4.884853	-0.911470
H	4.907384	3.604544	-3.643667
H	3.769577	4.935274	-5.388433
H	1.343558	5.464421	-5.179372
H	0.062154	4.622963	-3.213886
H	1.161311	3.260587	-1.497125
H	4.220278	-4.456368	5.285051
H	2.310257	-3.669854	6.671482
H	0.470128	-2.359638	5.619092
H	0.554137	-1.818794	3.201224
H	0.664461	-2.356693	-1.209502
H	-0.460837	-4.157910	-2.479875
H	-0.329152	-6.516749	-1.686528
H	0.968599	-7.065773	0.364954
H	2.152895	-5.276525	1.603521
H	2.911098	-1.554405	-3.497707
H	1.974190	-3.160181	-5.147206
H	2.268928	-5.604712	-4.811961
H	3.550324	-6.444983	-2.850705
H	4.543337	-4.857087	-1.242803
H	6.278391	-3.014730	-3.133379
H	8.750104	-3.026597	-3.311782
H	10.142007	-2.020382	-1.512120
H	9.040959	-0.968347	0.465499
H	6.587711	-0.912294	0.635594
H	4.309915	-3.933883	2.875697

$B_{opt\text{-}full}(S_1)$

Cu	3.307092	0.093718	-1.230975
C	1.370609	0.188427	-1.373083
N	0.202146	0.236220	-1.451549
Cu	-1.681345	-0.059510	-1.039470
Cu	-3.049426	-0.353946	1.093138
C	-1.181143	-0.255954	1.490450
N	-0.009547	-0.194881	1.617091
Cu	1.849699	-0.160836	0.991661
P	4.500935	-1.846837	-1.139249
P	4.053380	2.251170	-1.313389
P	-3.120324	-1.481981	-2.125945
P	-2.584697	1.938998	-1.672549
P	-3.861601	-2.429995	0.715535
P	-4.230333	1.560613	0.843947
P	2.573177	-2.332903	1.128377
P	3.175632	1.613173	1.531188
C	4.283088	-2.614578	0.518675
C	-3.394565	-2.926919	-1.021686
C	-4.237145	2.115534	-0.927597
C	3.425277	2.947857	0.282856
H	4.952206	-2.067456	1.201348
H	4.575892	-3.675094	0.514255
C	-4.730462	-0.966655	-2.777133
C	-5.820651	-0.769759	-1.913616
C	-7.054508	-0.372429	-2.423155
C	-7.210946	-0.148808	-3.791332
C	-6.123884	-0.318726	-4.649482
C	-4.888668	-0.722827	-4.150200
C	-2.241369	-2.156737	-3.570705
C	-2.613293	-3.379382	-4.149061
C	-1.955555	-3.838175	-5.286638
C	-0.935493	-3.076859	-5.861177
C	-0.565271	-1.861011	-5.290182
C	-1.209491	-1.403921	-4.142022
C	-5.661882	-2.695752	0.804529
C	-6.398830	-1.790286	1.576275
C	-7.783981	-1.906418	1.671569
C	-8.442402	-2.931480	0.994829
C	-7.713880	-3.845527	0.231437
C	-6.329660	-3.730594	0.136520
C	-3.131755	-3.781935	1.702629
C	-3.911967	-4.748656	2.346610
C	-3.303790	-5.723536	3.136727
C	-1.919849	-5.736098	3.293784
C	-1.139450	-4.768232	2.660105
C	-1.738848	-3.791141	1.871897
C	-2.726381	2.245689	-3.440429
C	-1.529737	2.245048	-4.180386
C	-1.562411	2.437650	-5.555087
C	-2.785655	2.617232	-6.208089
C	-3.973587	2.606410	-5.479556
C	-3.950894	2.418615	-4.098649
C	-1.547814	3.271020	-1.004369
C	-0.757230	3.042772	0.129219
C	-0.071275	4.102778	0.716559
C	-0.153672	5.382028	0.167094
C	-0.927009	5.607339	-0.971595
C	-1.628984	4.556993	-1.557266
C	-3.502374	2.970588	1.750803
C	-2.618308	2.703215	2.800546
C	-2.081660	3.752166	3.545275
C	-2.413426	5.069009	3.237627
C	-3.293860	5.340735	2.188926
C	-3.845414	4.295774	1.455083
C	-6.001785	1.703114	1.286805
C	-6.316826	1.621081	2.651308
C	-7.641228	1.677289	3.073362
C	-8.669595	1.809922	2.137719
C	-8.363308	1.893333	0.782115
C	-7.035258	1.843973	0.356390
C	4.844031	1.107263	2.083029
C	6.023558	1.796263	1.786789
C	7.246036	1.340369	2.282570
C	7.298546	0.207007	3.091037
C	6.120925	-0.473966	3.408794
C	4.902706	-0.028786	2.904825
C	2.551196	2.502813	3.003262
C	3.144454	3.691173	3.451482
C	2.691463	4.301836	4.616992
C	1.661591	3.717759	5.357596
C	1.078446	2.530080	4.921914
C	1.510149	1.927429	3.740345
C	5.805003	2.726534	-1.393664
C	6.752213	1.742698	-1.684900

C	8.107877	2.067856	-1.733569
C	8.518363	3.375659	-1.487756
C	7.573568	4.366828	-1.206317
C	6.220431	4.047120	-1.165814
C	3.278211	3.275980	-2.613919
C	4.037628	3.666998	-3.725317
C	3.444815	4.368310	-4.772981
C	2.090340	4.690495	-4.721492
C	1.328632	4.297081	-3.622006
C	1.910886	3.581126	-2.577801
C	2.616808	-2.899914	2.860274
C	1.532372	-2.537315	3.673770
C	1.496715	-2.933273	5.008215
C	2.547323	-3.674951	5.548532
C	3.634145	-4.025571	4.748966
C	3.669827	-3.643634	3.408312
C	1.617581	-3.621865	0.251534
C	0.850829	-3.260495	-0.861926
C	0.189579	-4.237539	-1.604128
C	0.263029	-5.575318	-1.219550
C	1.009853	-5.938646	-0.098989
C	1.691769	-4.967701	0.629965
C	3.859223	-3.065887	-2.327878
C	3.103680	-2.598147	-3.408543
C	2.586485	-3.493418	-4.342001
C	2.800039	-4.860975	-4.188213
C	3.546222	-5.334598	-3.108227
C	4.082828	-4.441108	-2.186797
C	6.314284	-1.895894	-1.335337
C	6.911036	-2.388089	-2.501218
C	8.298197	-2.355335	-2.641825
C	9.095866	-1.838134	-1.622487
C	8.502708	-1.337619	-0.462576
C	7.118652	-1.355884	-0.321548
H	-5.722393	-0.938266	-0.840715
H	-7.898499	-0.252859	-1.740156
H	-8.182304	0.151332	-4.190651
H	-6.238473	-0.143919	-5.721544
H	-4.048000	-0.858668	-4.833331
H	-3.425858	-3.971516	-3.722022
H	-2.249017	-4.789284	-5.736380
H	-0.432448	-3.435469	-6.762373
H	0.228423	-1.259207	-5.738823
H	-0.914706	-0.456221	-3.687111
H	-2.403013	-3.403198	-0.934906
H	-4.087028	-3.658358	-1.465849
H	-5.880639	-0.976888	2.089213
H	-8.344852	-1.185072	2.269135
H	-9.528796	-3.023395	1.063188
H	-8.228893	-4.653472	-0.292995
H	-5.774478	-4.460690	-0.457763
H	-4.998514	-4.739732	2.240393
H	-3.920270	-6.473943	3.636739
H	-1.446979	-6.497570	3.918125
H	-0.056218	-4.762744	2.791825
H	-1.119373	-3.023782	1.399653
H	-4.929692	2.749678	-5.987604
H	-2.810624	2.767184	-7.289668
H	-0.628387	2.449910	-6.121422
H	-0.572650	2.097856	-3.671324
H	-0.681053	2.044770	0.562793
H	0.516599	3.924413	1.619927
H	0.385099	6.211002	0.631599
H	-0.989397	6.608291	-1.404014
H	-2.243529	4.737601	-2.443147
H	-4.616962	3.141042	-1.059332
H	-4.893664	1.416810	-1.470765
H	-2.339463	1.668274	3.017758
H	-1.387874	3.539575	4.359898
H	-1.987391	5.890379	3.818498
H	-3.560981	6.372524	1.950119
H	-4.554479	4.521782	0.654587
H	-5.516462	1.521400	3.390742
H	-7.872987	1.623006	4.139426
H	-9.709424	1.857061	2.468874
H	-9.162437	2.009154	0.046089
H	-6.822447	1.920548	-0.710668
H	-4.890584	2.414190	-3.543621
H	6.011342	2.690775	1.164005
H	8.160532	1.883398	2.034074
H	8.256079	-0.142990	3.483417
H	6.148497	-1.354623	4.054857
H	3.983196	-0.561369	3.166924
H	3.978657	4.137464	2.903707
H	3.156570	5.228064	4.961809
H	1.322323	4.188387	6.283360
H	0.283028	2.061860	5.506834
H	1.035981	1.008876	3.385074
H	2.419881	3.357012	0.097404
H	4.054680	3.771647	0.651380
H	6.428863	0.715285	-1.859842
H	8.839792	1.289564	-1.959088
H	9.579902	3.631412	-1.521659
H	7.896194	5.394728	-1.026122
H	5.484730	4.831618	-0.966235
H	5.103306	3.432127	-3.770572
H	4.050972	4.673163	-5.628967
H	1.628409	5.253263	-5.535880
H	0.268838	4.551348	-3.570892
H	1.285598	3.267438	-1.738124
H	4.458929	-4.605611	5.169264
H	2.521688	-3.977315	6.597806
H	0.644803	-2.653767	5.632029
H	0.717233	-1.938094	3.258450
H	0.786295	-2.214473	-1.160634
H	-0.376517	-3.948384	-2.492473
H	-0.260293	-6.340677	-1.797304
H	1.063243	-6.985439	0.208194
H	2.277133	-5.258708	1.506532
H	2.908849	-1.526015	-3.508795
H	2.002946	-3.122385	-5.185614
H	2.384614	-5.564520	-4.913355
H	3.715233	-6.406606	-2.986385
H	4.679692	-4.823873	-1.355591
H	6.293450	-2.806840	-3.299201
H	8.757946	-2.746790	-3.552024
H	10.182653	-1.825508	-1.731884
H	9.119050	-0.922178	0.337939
H	6.673215	-0.930671	0.581761
H	4.527425	-3.931152	2.796190

$B_{opt\text{-}full}(T_1)$

Cu	3.307092	0.093718	-1.230975
C	1.577119	0.435156	-1.984806
N	0.412262	0.464696	-2.108323
Cu	-1.454263	0.358965	-1.448844
Cu	-2.920885	-0.013211	0.682652
C	-0.957856	-0.006244	0.770947
N	0.174604	-0.058791	1.062835
Cu	2.111972	-0.113107	1.084276
P	4.919199	-1.520397	-0.945830
P	4.089448	2.245217	-1.185576
P	-2.724507	-1.428227	-2.130321
P	-2.273220	2.498198	-1.611648
P	-3.547630	-2.209063	0.708230
P	-4.192437	1.877147	0.637099
P	2.950671	-2.187563	1.281250
P	3.353663	1.636350	1.752494
C	4.695958	-2.312371	0.695534
C	-2.926180	-2.812543	-0.929058
C	-3.995036	2.693723	-0.999457
C	3.612761	2.931312	0.455830
H	5.301500	-1.732142	1.410520
H	5.088022	-3.340262	0.676089
C	-4.408659	-0.972980	-2.674965
C	-5.563962	-1.702579	-2.379139
C	-6.803491	-1.280818	-2.862800
C	-6.898056	-0.138403	-3.654504
C	-5.745464	0.585919	-3.968051
C	-4.509964	0.172678	-3.479191
C	-2.055593	-2.274636	-3.609564
C	-2.655557	-3.434889	-4.118164
C	-2.130821	-4.056018	-5.247367

C	-1.016462	-3.512545	-5.890201
C	-0.429313	-2.349260	-5.398700
C	-0.940616	-1.732421	-4.256942
C	-5.284497	-2.738802	0.786356
C	-6.256330	-1.792058	1.117141
C	-7.602874	-2.153913	1.158383
C	-7.979947	-3.461988	0.865286
C	-7.010684	-4.416827	0.544303
C	-5.666468	-4.060470	0.511167
C	-2.713631	-3.283913	1.926274
C	-3.431241	-3.786489	3.019846
C	-2.786432	-4.547071	3.993222
C	-1.424090	-4.817415	3.881870
C	-0.704848	-4.311732	2.799954
C	-1.338195	-3.534751	1.833507
C	-2.359144	3.082600	-3.337181
C	-1.333702	2.669671	-4.200647
C	-1.345907	3.056183	-5.538552
C	-2.386548	3.843123	-6.031309
C	-3.415335	4.247466	-5.181147
C	-3.403402	3.870875	-3.838965
C	-1.374357	3.808869	-0.704614
C	-0.604611	3.450520	0.409692
C	0.018253	4.434807	1.176620
C	-0.100570	5.777206	0.819519
C	-0.850241	6.138069	-0.300424
C	-1.490978	5.159232	-1.056839
C	-3.593351	3.083866	1.858841
C	-2.867145	2.600508	2.952719
C	-2.385371	3.481518	3.917890
C	-2.600389	4.850625	3.781535
C	-3.317103	5.339589	2.688566
C	-3.822382	4.459879	1.736649
C	-6.007023	1.864919	0.825967
C	-6.626552	2.331283	1.990483
C	-8.012611	2.250389	2.122801
C	-8.786259	1.710421	1.096796
C	-8.169789	1.235769	-0.061896
C	-6.786526	1.302296	-0.194721
C	5.020916	1.208503	2.370801
C	6.183966	1.934670	2.099506
C	7.401857	1.553497	2.663684
C	7.468425	0.446371	3.507279
C	6.309528	-0.278669	3.792124
C	5.094411	0.100775	3.229117
C	2.670012	2.623327	3.136141
C	3.224713	3.836991	3.562595
C	2.682191	4.507277	4.655360
C	1.599871	3.957902	5.346031
C	1.055422	2.743402	4.934864
C	1.578694	2.082542	3.824626
C	5.869169	2.478908	-1.434253
C	6.556784	1.567161	-2.241264
C	7.904605	1.764642	-2.533393
C	8.572654	2.871627	-2.016370
C	7.887168	3.796999	-1.226234
C	6.538217	3.609130	-0.942281
C	3.307942	3.336460	-2.404551
C	4.036535	3.777555	-3.519803
C	3.425332	4.584161	-4.475994
C	2.089880	4.955884	-4.329086
C	1.361769	4.514755	-3.223058
C	1.959057	3.698982	-2.269047
C	3.044567	-2.876741	2.972898
C	1.986114	-2.545864	3.831849
C	1.974018	-3.004642	5.145842
C	3.031276	-3.779005	5.624419
C	4.095341	-4.099453	4.782436
C	4.102599	-3.654914	3.460498
C	2.052075	-3.456724	0.319239
C	1.276962	-3.040995	-0.772014
C	0.627240	-3.981843	-1.568712
C	0.716643	-5.339178	-1.259035
C	1.464915	-5.756499	-0.158595
C	2.138683	-4.820493	0.623720
C	4.308117	-2.724087	-2.166557
C	3.687799	-2.233858	-3.324221
C	3.167916	-3.113778	-4.270186
C	3.262297	-4.487974	-4.066737
C	3.885834	-4.983309	-2.920162
C	4.407878	-4.108338	-1.973629
C	6.730049	-1.465454	-1.095170
C	7.387645	-2.006072	-2.206847
C	8.774767	-1.909188	-2.305849
C	9.508316	-1.271923	-1.304860
C	8.851901	-0.722753	-0.202742
C	7.468227	-0.812567	-0.097689
H	-5.519521	-2.601591	-1.764286
H	-7.698242	-1.856315	-2.615532
H	-7.869000	0.186097	-4.035621
H	-5.806246	1.475955	-4.598779
H	-3.610469	0.739952	-3.736394
H	-3.548018	-3.851349	-3.643279
H	-2.601785	-4.960484	-5.638881
H	-0.615474	-3.994540	-6.784886
H	0.430176	-1.909995	-5.910182
H	-0.469088	-0.830964	-3.860013
H	-1.907657	-3.202914	-0.775283
H	-3.536235	-3.638355	-1.324806
H	-5.958712	-0.763436	1.327906
H	-8.353866	-1.403905	1.414682
H	-9.034248	-3.746773	0.893602
H	-7.307158	-5.445537	0.327426
H	-4.910970	-4.816993	0.280162
H	-4.502557	-3.593135	3.108803
H	-3.358216	-4.938761	4.837476
H	-0.920477	-5.423985	4.638000
H	0.361457	-4.519365	2.704308
H	-0.744053	-3.129286	1.011285
H	-4.233607	4.861137	-5.564768
H	-2.400618	4.137721	-7.083058
H	-0.541215	2.732254	-6.202392
H	-0.525844	2.039741	-3.818649
H	-0.498436	2.400251	0.685325
H	0.592867	4.147332	2.060139
H	0.390588	6.547205	1.418957
H	-0.940517	7.189033	-0.584371
H	-2.080951	5.449224	-1.930761
H	-4.332602	3.740368	-0.971005
H	-4.637471	2.137680	-1.700618
H	-2.670727	1.527713	3.042231
H	-1.831649	3.097990	4.775499
H	-2.210114	5.542411	4.531368
H	-3.488488	6.412709	2.580813
H	-4.397785	4.854539	0.896128
H	-6.027962	2.766946	2.793872
H	-8.490607	2.621355	3.032168
H	-9.872519	1.659522	1.200098
H	-8.767030	0.802993	-0.867706
H	-6.320952	0.896682	-1.096793
H	-4.220065	4.193081	-3.189294
H	6.160765	2.800757	1.439281
H	8.302719	2.128806	2.438564
H	8.422245	0.150599	3.949775
H	6.348054	-1.142939	4.459287
H	4.188409	-0.465927	3.463501
H	4.095068	4.259637	3.053827
H	3.116487	5.454214	4.983711
H	1.189596	4.476324	6.215700
H	0.223588	2.300300	5.486481
H	1.144055	1.138618	3.483100
H	2.615896	3.380746	0.317713
H	4.288956	3.746847	0.756626
H	6.033301	0.699587	-2.647115
H	8.432622	1.040629	-3.156752
H	9.631528	3.023659	-2.237556
H	8.404214	4.678529	-0.840581
H	6.006948	4.362810	-0.355593
H	5.086813	3.503207	-3.636430
H	4.001835	4.930696	-5.336462
H	1.612638	5.592559	-5.077552
H	0.316629	4.801718	-3.101169
H	1.357879	3.346536	-1.428041
H	4.925127	-4.704155	5.155383

H	3.029058	-4.129920	6.658749
H	1.138381	-2.749895	5.801487
H	1.166522	-1.923306	3.460438
H	1.183034	-1.975416	-0.995037
H	0.050127	-3.650358	-2.435049
H	0.199193	-6.075158	-1.878749
H	1.527479	-6.818080	0.091158
H	2.726705	-5.153965	1.483224
H	3.602582	-1.153767	-3.482378
H	2.682660	-2.722516	-5.165904
H	2.848756	-5.179523	-4.804149
H	3.962679	-6.060769	-2.760288
H	4.888457	-4.514665	-1.081776
H	6.818182	-2.515883	-2.987919
H	9.286604	-2.345771	-3.166532
H	10.595759	-1.205649	-1.383368
H	9.419621	-0.217856	0.581986
H	6.969100	-0.361245	0.763058
H	4.943369	-3.921001	2.816454

$B_{opt\text{-}const}(S_0)$

Cu	4.961468	3.040740	10.944080
Cu	3.375500	1.095489	9.558387
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P	2.397799	0.688497	11.575421
P	5.249411	4.658361	9.345235
P	2.878935	2.968484	8.369648
N	3.876329	-0.569407	8.655326
C	4.457695	-1.483619	8.223911
C	3.159919	4.669274	13.579521
C	2.073231	5.332630	12.994034
H	1.539552	4.897993	12.146028
C	1.667260	6.573750	13.475319
H	0.812956	7.075488	13.015258
C	2.350693	7.174016	14.532835
H	2.028855	8.146084	14.913405
C	3.446598	6.528503	15.103918
H	3.987688	6.994377	15.930511
C	3.851799	5.280587	14.632298
H	4.704516	4.777627	15.094739
C	4.572824	2.240279	14.249352
C	5.894610	1.814483	14.088345
H	6.411543	2.000279	13.142613
C	6.541007	1.135149	15.119478
H	7.569941	0.797389	14.986064
C	5.868447	0.871041	16.309502
H	6.373397	0.333162	17.115049
C	4.548834	1.294766	16.476795
H	4.022195	1.092241	17.411926
C	3.904051	1.980860	15.453279
H	2.876708	2.325425	15.599745
C	2.168961	2.163453	12.647116
H	1.479545	2.825445	12.100052
H	1.726115	1.917967	13.624299
C	3.126879	-0.557980	12.692845
C	4.487031	-0.867236	12.572072
H	5.086603	-0.401825	11.787707
C	5.079527	-1.764019	13.461163
H	6.147928	-1.976309	13.382089
C	4.313939	-2.377230	14.450761
H	4.780076	-3.082846	15.142220
C	2.953436	-2.087780	14.561461
H	2.350078	-2.571786	15.332618
C	2.362626	-1.176197	13.690769
H	1.296262	-0.952756	13.783387
C	0.696816	0.108924	11.262691
C	-0.408270	0.473410	12.042632
H	-0.287418	1.127562	12.908894
C	-1.680979	0.009594	11.713165
H	-2.538284	0.296734	12.326226
C	-1.860348	-0.819392	10.605989
H	-2.859750	-1.178065	10.349740
C	-0.764290	-1.185565	9.825347
H	-0.899847	-1.835862	8.958376
C	0.508081	-0.720018	10.146880
H	1.366243	-1.007574	9.532758
C	4.810533	6.402230	9.607373
C	4.850482	7.338816	8.563418
H	5.188344	7.040646	7.566686
C	4.475561	8.657666	8.798409
H	4.507124	9.385915	7.984876
C	4.069192	9.052588	10.076172
H	3.779996	10.090360	10.257392
C	4.042484	8.129112	11.118209
H	3.730501	8.431190	12.119889
C	4.411413	6.804443	10.884206
H	4.375744	6.074221	11.694641
C	6.946349	4.731651	8.671022
C	7.443027	3.690714	7.875215
H	6.819701	2.833275	7.611159
C	8.752068	3.734677	7.403035
H	9.116467	2.929334	6.763436
C	9.588954	4.795494	7.746465
H	10.615584	4.825332	7.374593
C	9.109847	5.817252	8.564043
H	9.759398	6.651167	8.839407
C	7.794478	5.789763	9.023435
H	7.424405	6.605428	9.648766
C	4.234668	4.115534	7.890806
H	3.865364	4.976065	7.312734
H	4.886904	3.531275	7.223475
C	1.591866	4.007979	9.145805
C	0.494101	3.331756	9.700028
H	0.448275	2.239285	9.664530
C	-0.551370	4.041523	10.282823
H	-1.401646	3.500799	10.705044
C	-0.512673	5.437662	10.320016
H	-1.333307	5.995790	10.776527
C	0.570416	6.114884	9.764572
H	0.608891	7.206216	9.785490
C	1.618021	5.405582	9.174977
H	2.451930	5.962572	8.747331
C	2.104589	2.537877	6.768899
C	1.849648	1.192456	6.482578
H	2.148231	0.420336	7.194975
C	1.223157	0.839151	5.287773
H	1.006793	-0.211705	5.080925
C	0.866970	1.822333	4.367549
H	0.376469	1.545745	3.431358
C	1.123406	3.166454	4.647594
H	0.833865	3.939277	3.932089
C	1.727915	3.525288	5.848511
H	1.890650	4.582961	6.072918
Cu	5.411007	-3.040740	7.596095
Cu	6.996975	-1.095489	8.981788
P	6.632813	-3.108702	5.674462
P	7.981879	-0.704231	6.966225
P	5.108811	-4.645236	9.204735
P	7.484214	-2.967524	10.178373
N	6.496592	0.570318	9.882863
C	5.915235	1.484961	10.313444
C	7.213278	-4.694779	4.981770
C	8.303124	-5.353054	5.566841
H	8.845391	-4.908556	6.404130
C	8.702012	-6.601624	5.098764
H	9.558944	-7.099285	5.558346
C	8.008775	-7.214023	4.054779
H	8.325367	-8.191730	3.684393
C	6.909696	-6.573353	3.484214
H	6.360711	-7.048647	2.668258
C	6.511168	-5.318665	3.943018
H	5.655454	-4.820177	3.481276
C	5.819421	-2.263878	4.282374
C	4.513376	-1.792171	4.443254
H	3.997032	-1.943172	5.395426
C	3.882308	-1.112252	3.402938
H	2.866256	-0.737343	3.536706
C	4.554236	-0.895355	2.203144
H	4.061326	-0.357891	1.389899
C	5.857842	-1.366165	2.035599
H	6.383491	-1.201220	1.092546
C	6.487850	-2.051070	3.068956
H	7.502697	-2.431465	2.923092

C	8.210506	-2.182602	5.898941
H	8.898545	-2.843266	6.449247
H	8.654602	-1.940090	4.921516
C	7.256254	0.542832	5.847607
C	5.904480	0.878376	5.988762
H	5.310463	0.429818	6.787127
C	5.313494	1.777972	5.101521
H	4.250530	2.010491	5.196183
C	6.072749	2.366317	4.092366
H	5.607827	3.073451	3.401654
C	7.425586	2.050310	3.960927
H	8.023974	2.515043	3.174214
C	8.014673	1.137088	4.830858
H	9.075196	0.893664	4.722636
C	9.683588	-0.126974	7.280267
C	10.789600	-0.494698	6.503284
H	10.669754	-1.151411	5.638809
C	12.062130	-0.030744	6.833381
H	12.920181	-0.320398	6.222554
C	12.240416	0.801647	7.938101
H	13.239625	1.160639	8.194614
C	11.143445	1.170876	8.716084
H	11.278289	1.823528	9.581391
C	9.871373	0.704938	8.394088
H	9.012377	0.994318	9.006296
C	5.529011	-6.395719	8.954631
C	5.454076	-7.328170	10.000167
H	5.102279	-7.021242	10.989388
C	5.810891	-8.653818	9.775436
H	5.751820	-9.379223	10.589974
C	6.233700	-9.059173	8.506301
H	6.508125	-10.102295	8.332990
C	6.295541	-8.139248	7.462563
H	6.620391	-8.449550	6.467499
C	5.944780	-6.807866	7.686257
H	6.007207	-6.080659	6.874767
C	3.404030	-4.701727	9.859887
C	2.917148	-3.696055	10.704656
H	3.554806	-2.873036	11.035227
C	1.595988	-3.730585	11.143657
H	1.238335	-2.952856	11.820002
C	0.738939	-4.745083	10.720942
H	-0.296750	-4.766408	11.067385
C	1.210279	-5.732223	9.857277
H	0.545987	-6.531319	9.520618
C	2.536129	-5.714772	9.429823
H	2.899615	-6.504341	8.767845
C	6.121345	-4.104753	10.660730
H	6.484630	-4.966374	11.240970
H	5.473624	-3.513997	11.326552
C	8.765274	-4.018835	9.408100
C	9.868814	-3.352206	8.853750
H	9.921268	-2.259837	8.883822
C	10.912087	-4.071460	8.278648
H	11.767209	-3.538323	7.856547
C	10.865191	-5.467541	8.249269
H	11.684260	-6.033120	7.799152
C	9.775904	-6.135180	8.804150
H	9.730880	-7.226350	8.788855
C	8.730536	-5.416378	9.386133
H	7.891695	-5.966038	9.813778
C	8.262897	-2.536026	11.776683
C	8.534178	-1.191941	12.053970
H	8.243851	-0.420911	11.336949
C	9.166647	-0.838501	13.245563
H	9.396548	0.210897	13.444938
C	9.511603	-1.819841	14.172003
H	10.006538	-1.543092	15.105805
C	9.238336	-3.162538	13.901185
H	9.519064	-3.934073	14.621582
C	8.628527	-3.521884	12.703104
H	8.452830	-4.578940	12.485752

B(S_1) starting from **B**$_{opt\text{-}const}$(S_0)

Cu	4.961468	3.040740	10.944080
Cu	3.349165	1.494952	9.687345
P	3.727511	3.572595	12.794375
P	2.338873	1.126876	11.667227
P	5.159592	4.805407	9.479511
P	2.697261	3.258511	8.465136
N	4.141335	-0.092437	8.927384
C	4.864118	-0.953698	8.594914
C	3.205848	5.198156	13.407568
C	2.279630	5.931679	12.651887
H	1.870148	5.525859	11.723679
C	1.882302	7.194414	13.075511
H	1.157074	7.757200	12.483828
C	2.410334	7.738482	14.247437
H	2.094021	8.729145	14.581684
C	3.339200	7.014938	14.994877
H	3.747874	7.435695	15.916456
C	3.742059	5.747386	14.578095
H	4.464449	5.180424	15.170345
C	4.710768	2.783250	14.106584
C	6.105505	2.780673	13.966429
H	6.563170	3.244308	13.086426
C	6.906651	2.171524	14.928761
H	7.991993	2.173975	14.811926
C	6.320847	1.552595	16.030298
H	6.946960	1.065937	16.781429
C	4.932629	1.552001	16.175552
H	4.472409	1.067232	17.039053
C	4.128535	2.166669	15.221249
H	3.044870	2.156370	15.351748
C	2.144715	2.646646	12.698333
H	1.434529	3.300050	12.166382
H	1.742345	2.452469	13.703728
C	3.223183	-0.027523	12.773890
C	4.593935	-0.228729	12.568454
H	5.089454	0.245636	11.717883
C	5.321840	-1.035658	13.441652
H	6.396160	-1.163872	13.291130
C	4.677889	-1.674038	14.501184
H	5.247455	-2.313051	15.179959
C	3.307095	-1.499611	14.693274
H	2.799799	-2.008677	15.515971
C	2.581889	-0.672308	13.838867
H	1.508361	-0.536017	13.996780
C	0.636825	0.465919	11.578465
C	-0.410755	0.840605	12.429888
H	-0.245869	1.556298	13.238234
C	-1.685274	0.302873	12.251024
H	-2.497904	0.601516	12.917292
C	-1.921922	-0.616322	11.229630
H	-2.921518	-1.035077	11.093500
C	-0.882879	-0.994423	10.378582
H	-1.063079	-1.714064	9.576904
C	0.386244	-0.447305	10.543613
H	1.198769	-0.726316	9.865474
C	4.810361	6.436152	10.177252
C	4.259140	7.481408	9.425240
H	3.962358	7.327939	8.385535
C	4.124377	8.747348	9.988185
H	3.695458	9.559558	9.397313
C	4.558011	8.983555	11.293195
H	4.455268	9.979797	11.728941
C	5.131884	7.953979	12.036661
H	5.475925	8.135658	13.056169
C	5.248264	6.681919	11.485632
H	5.688682	5.870460	12.070391
C	6.825659	4.943484	8.781165
C	7.308042	3.934665	7.932723
H	6.699395	3.061647	7.687624
C	8.586923	4.032179	7.398890
H	8.947929	3.249562	6.731122
C	9.404179	5.116838	7.721587
H	10.410920	5.183769	7.303190
C	8.934635	6.112782	8.575990
H	9.567295	6.967105	8.826000
C	7.650329	6.031297	9.106912
H	7.286496	6.824458	9.762097
C	4.058748	4.447488	8.052486
H	3.732388	5.371493	7.549860

H	4.686830	3.902033	7.329149
C	1.370835	4.277437	9.206494
C	0.337065	3.577501	9.845201
H	0.376410	2.485799	9.899349
C	-0.741049	4.258772	10.403362
H	-1.536306	3.696131	10.897892
C	-0.804147	5.650971	10.324085
H	-1.648999	6.187503	10.761522
C	0.209075	6.353185	9.673909
H	0.161113	7.441895	9.597575
C	1.289640	5.670297	9.115731
H	2.068950	6.242589	8.614461
C	2.023721	2.884889	6.802567
C	1.672365	1.555475	6.545531
H	1.866726	0.794651	7.307688
C	1.080744	1.211417	5.331162
H	0.779646	0.177665	5.148682
C	0.863741	2.184963	4.358548
H	0.401130	1.915175	3.406383
C	1.225088	3.510977	4.605336
H	1.046965	4.276803	3.847064
C	1.791198	3.863242	5.827347
H	2.037565	4.910794	6.018699
Cu	5.670358	-2.598653	7.882059
Cu	7.102215	-0.727240	8.995553
P	6.679960	-2.718559	5.841115
P	8.115054	-0.313085	6.973682
P	5.346109	-4.229393	9.448247
P	7.767848	-2.539299	10.242660
N	7.009195	1.015796	9.926474
C	6.413538	1.929299	10.357273
C	7.191161	-4.293104	5.073444
C	8.261132	-5.002589	5.636554
H	8.798167	-4.611339	6.504172
C	8.642427	-6.230907	5.106246
H	9.482944	-6.770001	5.549194
C	7.948873	-6.772267	4.022968
H	8.249665	-7.735843	3.605389
C	6.870861	-6.079911	3.473819
H	6.324092	-6.500239	2.626812
C	6.491365	-4.842451	3.993460
H	5.653328	-4.300084	3.549393
C	5.679942	-1.878805	4.574937
C	4.308172	-1.741629	4.812605
H	3.878910	-2.122453	5.744357
C	3.494386	-1.111873	3.873896
H	2.423503	-1.020556	4.057958
C	4.049714	-0.589475	2.708567
H	3.413521	-0.082861	1.979273
C	5.418889	-0.715378	2.470021
H	5.855962	-0.308042	1.555840
C	6.229895	-1.368465	3.392654
H	7.296529	-1.478032	3.183693
C	8.272176	-1.797979	5.901076
H	8.996243	-2.462989	6.397868
H	8.642564	-1.570722	4.890390
C	7.304341	0.895738	5.862650
C	5.930618	1.127307	6.009188
H	5.376894	0.637099	6.811225
C	5.264017	1.974272	5.124136
H	4.187158	2.125188	5.229291
C	5.969202	2.615911	4.107183
H	5.446945	3.282189	3.416645
C	7.341147	2.403704	3.968068
H	7.896580	2.909273	3.174823
C	8.006250	1.541743	4.837229
H	9.081010	1.377947	4.719589
C	9.830338	0.280277	7.151358
C	10.867167	-0.059380	6.271986
H	10.678250	-0.702201	5.409283
C	12.159018	0.414945	6.494739
H	12.962290	0.144748	5.805489
C	12.425694	1.231515	7.593444
H	13.439792	1.598855	7.766311
C	11.399083	1.569192	8.474941
H	11.605660	2.201237	9.341547
C	10.108479	1.090515	8.262206
H	9.307138	1.339420	8.963525
C	5.788836	-5.969198	9.163711
C	5.860813	-6.894745	10.215769
H	5.617585	-6.589225	11.237493
C	6.229112	-8.211500	9.959594
H	6.286654	-8.930446	10.779967
C	6.515171	-8.616450	8.652573
H	6.800327	-9.652415	8.455136
C	6.427654	-7.705120	7.603280
H	6.645630	-8.015101	6.579271
C	6.067039	-6.382015	7.858808
H	6.014395	-5.661078	7.041067
C	3.680611	-4.326063	10.191246
C	3.183638	-3.263578	10.957913
H	3.793619	-2.379642	11.158443
C	1.892426	-3.321578	11.475410
H	1.524986	-2.498512	12.089225
C	1.073704	-4.418043	11.208326
H	0.060402	-4.455926	11.614648
C	1.553475	-5.463718	10.422522
H	0.918765	-6.326189	10.206844
C	2.851581	-5.421843	9.917354
H	3.222227	-6.253672	9.314423
C	6.432493	-3.664636	10.838844
H	6.817303	-4.504231	11.437447
H	5.818041	-3.041005	11.507641
C	9.004360	-3.604866	9.420504
C	10.056782	-2.940680	8.771692
H	10.092265	-1.847237	8.769350
C	11.067324	-3.661891	8.143302
H	11.882929	-3.129552	7.648223
C	11.037005	-5.058630	8.151621
H	11.828755	-5.626316	7.657502
C	9.998892	-5.724258	8.799528
H	9.968095	-6.815968	8.814606
C	8.987845	-5.002912	9.436788
H	8.188760	-5.550469	9.936748
C	8.625348	-2.094614	11.798434
C	8.819446	-0.746145	12.115101
H	8.450765	0.028122	11.438851
C	9.474193	-0.395974	13.296313
H	9.633393	0.658620	13.532446
C	9.930462	-1.383876	14.165439
H	10.444912	-1.108136	15.088931
C	9.743690	-2.731301	13.849055
H	10.112919	-3.508415	14.521998
C	9.101367	-3.086408	12.667059
H	8.987456	-4.144183	12.414162

B(T_1) starting from $\mathbf{B}_{\text{opt-const}}(S_0)$

Cu	4.961468	3.040740	10.944080
Cu	3.318003	1.433832	9.687427
P	3.666719	3.536668	12.771829
P	2.283598	1.067180	11.648920
P	5.175178	4.758091	9.439481
P	2.696047	3.201787	8.446911
N	4.114184	-0.154800	8.913222
C	4.830723	-1.010374	8.559264
C	3.120343	5.126814	13.460958
C	2.129588	5.849234	12.781222
H	1.678884	5.456092	11.867061
C	1.718425	7.087462	13.261880
H	0.941633	7.640571	12.729280
C	2.297333	7.619086	14.414818
H	1.969549	8.589382	14.794618
C	3.293188	6.908447	15.085191
H	3.743007	7.318987	15.992103
C	3.709280	5.665328	14.611463
H	4.482331	5.107380	15.145719
C	4.661937	2.704051	14.047836
C	6.055832	2.699471	13.897996
H	6.514047	3.203321	13.040601
C	6.860860	2.046710	14.828196
H	7.944939	2.046942	14.702327
C	6.280258	1.391262	15.910935
H	6.909509	0.872480	16.637573

C	4.893361	1.396706	16.069218
H	4.436909	0.884542	16.918781
C	4.085708	2.050896	15.145100
H	3.003227	2.041789	15.284311
C	2.093111	2.597465	12.663692
H	1.379440	3.239083	12.122145
H	1.689038	2.417286	13.671036
C	3.159116	-0.101439	12.750237
C	4.533218	-0.296647	12.555466
H	5.039318	0.205994	11.727623
C	5.251225	-1.129392	13.411605
H	6.327651	-1.251458	13.270242
C	4.595497	-1.800644	14.443809
H	5.157354	-2.460494	15.108912
C	3.223240	-1.631083	14.625814
H	2.706413	-2.164646	15.426713
C	2.507344	-0.777646	13.788519
H	1.432087	-0.646763	13.938375
C	0.572613	0.425517	11.565898
C	-0.465668	0.803853	12.427069
H	-0.287644	1.509961	13.240889
C	-1.747279	0.282031	12.252589
H	-2.551754	0.583770	12.927168
C	-2.001369	-0.625266	11.224861
H	-3.006354	-1.031889	11.092087
C	-0.972543	-1.006771	10.363302
H	-1.166333	-1.716264	9.555795
C	0.303825	-0.475483	10.524935
H	1.107462	-0.759196	9.838638
C	4.782647	6.422456	10.039859
C	4.368226	7.442795	9.171718
H	4.225441	7.247962	8.105935
C	4.166067	8.730506	9.658470
H	3.843084	9.522055	8.978555
C	4.394282	9.014165	11.006524
H	4.236000	10.027041	11.383667
C	4.836449	8.011597	11.865928
H	5.022587	8.228271	12.919379
C	5.027031	6.718247	11.384890
H	5.373860	5.932261	12.058396
C	6.837998	4.905725	8.731081
C	7.322402	3.921678	7.855735
H	6.712380	3.059564	7.577393
C	8.606349	4.028899	7.334348
H	8.967890	3.265605	6.644273
C	9.426620	5.098697	7.695796
H	10.436385	5.174366	7.285972
C	8.955362	6.069319	8.578311
H	9.590829	6.911547	8.860664
C	7.666314	5.977830	9.096488
H	7.301390	6.750926	9.775506
C	4.080971	4.351277	8.014838
H	3.766472	5.262192	7.481961
H	4.703182	3.773315	7.312309
C	1.393391	4.248440	9.190752
C	0.321224	3.567215	9.786765
H	0.320679	2.473574	9.814097
C	-0.746565	4.270635	10.336842
H	-1.573306	3.723566	10.795947
C	-0.759528	5.666310	10.294805
H	-1.597484	6.219677	10.724544
C	0.296314	6.349936	9.695139
H	0.292103	7.441515	9.654042
C	1.367334	5.645381	9.144494
H	2.183034	6.204967	8.688231
C	1.994203	2.833636	6.795287
C	1.682746	1.499159	6.513782
H	1.916328	0.726636	7.252195
C	1.079626	1.163319	5.302535
H	0.811484	0.124325	5.100599
C	0.808377	2.151156	4.358619
H	0.335968	1.887593	3.409568
C	1.126546	3.483290	4.631093
H	0.904378	4.260199	3.896175
C	1.705261	3.826035	5.849634
H	1.915534	4.876886	6.065261
Cu	5.667169	-2.641061	7.846673
Cu	7.083626	-0.745896	8.957665
P	6.671874	-2.764013	5.805974
P	8.084480	-0.340879	6.928517
P	5.336871	-4.266364	9.416379
P	7.731786	-2.548955	10.225995
N	6.964993	1.012619	9.864296
C	6.388916	1.935512	10.299402
C	7.200012	-4.338088	5.049519
C	8.270181	-5.035996	5.626722
H	8.794394	-4.636636	6.498628
C	8.667504	-6.262980	5.105352
H	9.508010	-6.793081	5.559064
C	7.989698	-6.814432	4.017163
H	8.302938	-7.777059	3.606634
C	6.911765	-6.133488	3.453924
H	6.377521	-6.561943	2.603026
C	6.516271	-4.897242	3.964492
H	5.678407	-4.363651	3.509600
C	5.655294	-1.944819	4.540086
C	4.280126	-1.842793	4.777056
H	3.859407	-2.237429	5.706995
C	3.450950	-1.233299	3.838549
H	2.377408	-1.172408	4.020827
C	3.993634	-0.695066	2.674350
H	3.345224	-0.204500	1.944899
C	5.365789	-0.785154	2.436988
H	5.792925	-0.365168	1.523870
C	6.192830	-1.418736	3.359105
H	7.262019	-1.500056	3.150706
C	8.253486	-1.826648	5.859077
H	8.985038	-2.483930	6.355171
H	8.619893	-1.597367	4.847393
C	7.260980	0.855398	5.814406
C	5.885243	1.074857	5.962079
H	5.338176	0.586997	6.770216
C	5.208567	1.906538	5.070199
H	4.130714	2.048894	5.176479
C	5.905362	2.544159	4.044904
H	5.374977	3.198004	3.348750
C	7.279142	2.344842	3.905325
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C	7.954747	1.498689	4.781931
H	9.030823	1.343971	4.663738
C	9.797241	0.260796	7.104664
C	10.836482	-0.083744	6.229953
H	10.649806	-0.729501	5.369023
C	12.128427	0.389065	6.455224
H	12.933339	0.115157	5.769370
C	12.393120	1.208659	7.552125
H	13.407370	1.574452	7.727271
C	11.363957	1.552380	8.428188
H	11.568332	2.188465	9.292295
C	10.073092	1.075902	8.212427
H	9.269653	1.331904	8.908506
C	5.799185	-6.004578	9.155694
C	5.861112	-6.919136	10.217849
H	5.596066	-6.606332	11.231916
C	6.247980	-8.234243	9.981254
H	6.298161	-8.944692	10.809450
C	6.562257	-8.648520	8.683682
H	6.862217	-9.683102	8.501634
C	6.483768	-7.748419	7.624018
H	6.723226	-8.065952	6.607135
C	6.104685	-6.426890	7.860025
H	6.058937	-5.714563	7.034433
C	3.659310	-4.369102	10.129284
C	3.141745	-3.310367	10.887273
H	3.743537	-2.424862	11.104612
C	1.839448	-3.374579	11.375529
H	1.455438	-2.554826	11.983532
C	1.030989	-4.473314	11.087804
H	0.009080	-4.515817	11.471472
C	1.532301	-5.515921	10.311333
H	0.906053	-6.380543	10.080240
C	2.841038	-5.467937	9.835365
H	3.228709	-6.297451	9.239915
C	6.397412	-3.677970	10.816478

H	6.780839	-4.508409	11.428449
H	5.768505	-3.053045	11.470405
C	8.979408	-3.610561	9.415306
C	10.023314	-2.942636	8.756751
H	10.046714	-1.849031	8.740744
C	11.041269	-3.659988	8.135960
H	11.850174	-3.124471	7.633381
C	11.026530	-5.056710	8.161334
H	11.823803	-5.621505	7.672840
C	9.997034	-5.725984	8.819262
H	9.978777	-6.817683	8.847886
C	8.979193	-5.008355	9.449749
H	8.187733	-5.558619	9.958808
C	8.578066	-2.089786	11.783232
C	8.795123	-0.738794	12.072767
H	8.442338	0.027720	11.379607
C	9.454859	-0.376038	13.247273
H	9.637000	0.679851	13.459679
C	9.889564	-1.353527	14.138879
H	10.407937	-1.067854	15.057122
C	9.676742	-2.703559	13.851439
H	10.028891	-3.472926	14.542172
C	9.032291	-3.071591	12.674583
H	8.900528	-4.132275	12.443747

Table S5. Copper-phosphorous and copper-arsenic distances of the ground state DFT optimized and partially-optimized geometries of **A** and **B** (in Å). The distances extracted from the X-ray diffraction structures at 100 K ($\mathbf{A}_{\text{exp (100 K)}}$, $\mathbf{B}_{\text{exp (100 K)}}$) are given for sake of comparison in italics.

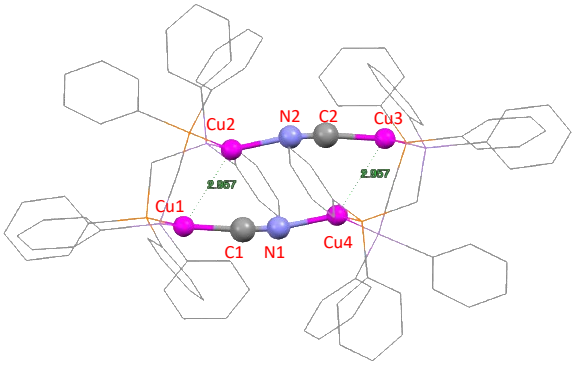
	$\mathbf{A}_{\text{opt-full}}$	$\mathbf{A}_{\text{opt-const}}$	$\mathbf{A}_{\text{exp (100 K)}}$	$\mathbf{B}_{\text{opt-full}}$	$\mathbf{B}_{\text{opt-const}}$	$\mathbf{B}_{\text{exp (100 K)}}$
Cu1-Cu2	2.710	*2.957 const*	*2.957*	2.678	*2.867 const*	*2.867*
Cu3-Cu4	2.721	*2.957 const*	*2.957*	2.687	*2.867 const*	*2.867*
Cu-P	2.278	2.280	*2.283*	2.281	2.279	*2.243*
	2.277	2.299	*2.314*	2.283	2.293	*2.264*
	2.276	2.297	*2.296*	2.290	2.278	*2.259*
	2.280	2.282	*2.273*	2.292	2.273	*2.257*
				2.288	2.278	*2.243*
				2.282	2.292	*2.264*
				2.290	2.277	*2.259*
				2.294	2.275	*2.257*
Cu-As	2.383	2.364	*2.296*			
	2.388	2.351	*2.490*			
	2.378	2.366	*2.490*			
	2.367	2.355	*2.240*			

Table S6. Selected distances and angles of the TD-DFT optimized S_1 and T_1 of derivatives **A** and **B** compared to their starting geometries *i.e.* the fully DFT-optimized and constrained ground state (S_0) (distances in Å, angles in degrees).

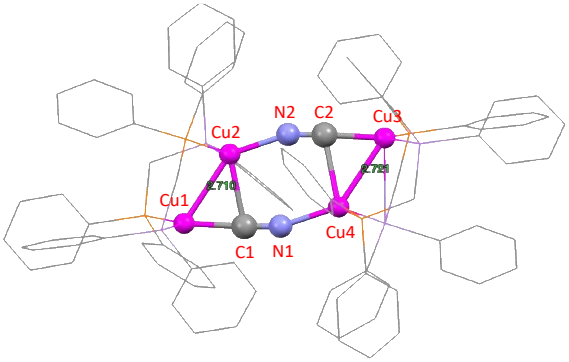
	Starting geometry $\mathbf{A}_{\text{opt-full}}$			Starting geometry $\mathbf{A}_{\text{opt-const}}$		
	S_0	S_1	T_1	S_0	S_1	T_1
Cu1-Cu2	2.710	2.691	2.681	2.957	2.563	2.592
Cu3-Cu4	2.721	2.544	2.575	2.957	2.702	2.681
Cu1-C1	1.942	1.939	1.943	1.918	1.910	1.921
Cu2-N2	1.985	1.957	1.961	1.943	1.944	1.950
Cu3-C2	1.938	1.904	1.916	1.924	1.936	1.940
Cu4-N1	1.986	1.953	1.957	1.941	1.960	1.966
C1-N1	1.168	1.173	1.172	1.166	1.179	1.176
C2-N2	1.167	1.179	1.175	1.167	1.173	1.172
Cu1-P1	2.280	2.279	2.280	2.279	2.290	2.277
Cu1-As1	2.367	2.393	2.393	2.365	2.368	2.351
Cu2-P2	2.277	2.266	2.270	2.294	2.259	2.264
Cu2-As2	2.382	2.381	2.382	2.370	2.356	2.361
Cu3-P3	2.277	2.258	2.264	2.290	2.278	2.291
Cu3-As3	2.387	2.356	2.361	2.368	2.365	2.367
Cu4-P4	2.276	2.280	2.250	2.259	2.294	2.291
Cu4-As4	2.378	2.380	2.363	2.356	2.370	2.372
N1-N2	3.025	3.127	3.192	3.087	3.102	3.176
C1-C2	3.961	3.871	3.910	4.082	3.857	3.914
Cu2-C1	2.422	2.427	2.415	2.648	2.653	2.808
Cu4-C2	2.424	2.615	2.802	2.636	2.423	2.389
Cu4-Cu3-C2	59.9	70.4	75.6	61.1	60.3	59.7

Cu1-Cu2-N2	141.9	142.3	143.1	134.9	132.3	130.2
C1-Cu1-Cu2	60.1	60.7	60.5	61.5	71.0	75.3
N1-Cu4-Cu3	139.8	134.6	130.9	135.1	141.1	143.5
Cu3-Cu4-Cu1-N1	162.2	-161.3	-168.9	160.5	167.0	167.0
Cu3-Cu4-Cu1-C1	157.9	-160.9	-161.6	159.5	167.0	168.8
Cu1-Cu2-Cu3-N2	-177.8	-177.5	-177.0	175.7	148.9	148.7
Cu1-Cu2-Cu3-C2	-175.9	-175.1	-175.5	174.0	151.2	141.8
Cu2-Cu3-Cu4-Cu1	6.3	6.6	6.2	0.0	4.7	5.4
Cu3-Cu4-Cu1-Cu2	-11.8	-12.3	-11.6	0.0	9.0	10.1
Cu4-Cu1-Cu2-Cu3	6.4	6.4	6.3	0.0	4.9	5.2
Cu1-Cu2-Cu3-Cu4	-11.9	-12.3	-11.9	0.0	9.0	9.8

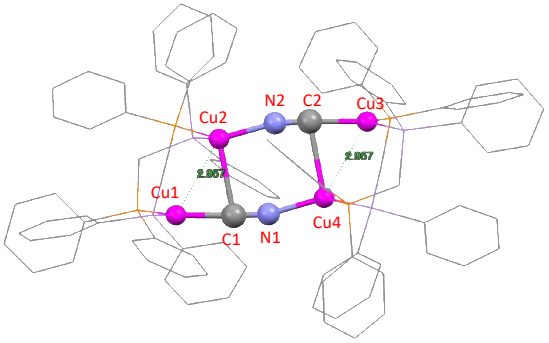
	Starting geometry $\mathbf{B}_{\text{opt-full}}$			Starting geometry $\mathbf{B}_{\text{opt-const}}$		
	S_0	S_1	T_1	S_0	S_1	T_1
Cu1-Cu2	2.678	2.670	2.614	2.867	2.563	2.620
Cu3-Cu4	2.687	2.551	2.614	2.867	2.606	2.614
Cu1-C1	1.952	1.944	1.918	1.931	1.920	1.917
Cu2-N2	1.992	1.962	1.938	1.959	1.930	1.938
Cu3-C2	1.950	1.912	1.965	1.931	1.966	1.966
Cu4-N1	1.993	1.950	1.982	1.959	1.978	1.982
C1-N1	1.168	1.172	1.172	1.166	1.172	1.172
C2-N2	1.168	1.180	1.171	1.166	1.172	1.171
Cu1-P11	2.283	2.284	2.290	2.278	2.253	2.248
Cu1-P12	2.281	2.280	2.299	2.273	2.245	2.247
Cu2-P21	2.294	2.293	2.247	2.293	2.302	2.293
Cu2-P22	2.290	2.279	2.246	2.279	2.287	2.294
Cu3-P31	2.282	2.263	2.279	2.275	2.298	2.294
Cu3-P32	2.288	2.261	2.284	2.277	2.299	2.298
Cu4-P41	2.292	2.283	2.296	2.292	2.284	2.283
Cu4-P42	2.290	2.280	2.296	2.278	2.280	2.278
N1-N2	3.028	3.106	3.223	3.110	3.233	3.224
C1-C2	3.908	3.861	3.770	3.912	3.717	3.760
Cu2-C1	2.415	2.438	3.163	2.678	3.167	3.171
Cu4-C2	2.426	2.586	2.304	2.678	2.285	2.303
Cu4-Cu3-C2	60.7	69.1	58.4	64.4	58.0	58.3
Cu1-Cu2-N2	140.7	141.7	116.4	131.1	115.5	115.9
C1-Cu1-Cu2	60.5	61.4	87.1	64.4	88.7	87.3
N1-Cu4-Cu3	140.7	135.4	143.8	131.1	143.9	143.6
Cu3-Cu4-Cu1-N1	171.6	151.9	175.9	172.0	178.6	176.3
Cu3-Cu4-Cu1-C1	171.3	151.4	171.7	162.9	175.9	172.7
Cu1-Cu2-Cu3-N2	171.2	171.0	167.7	171.6	165.6	167.7
Cu1-Cu2-Cu3-C2	171.4	171.7	28.5	162.1	18.8	25.6
Cu2-Cu3-Cu4-Cu1	0.1	0.7	2.8	0.0	3.5	3.3
Cu3-Cu4-Cu1-Cu2	0.3	1.4	5.1	0.0	6.7	6.2
Cu4-Cu1-Cu2-Cu3	0.1	0.7	2.4	0.0	3.2	3.0
Cu1-Cu2-Cu3-Cu4	0.3	1.4	4.7	0.0	6.2	5.7



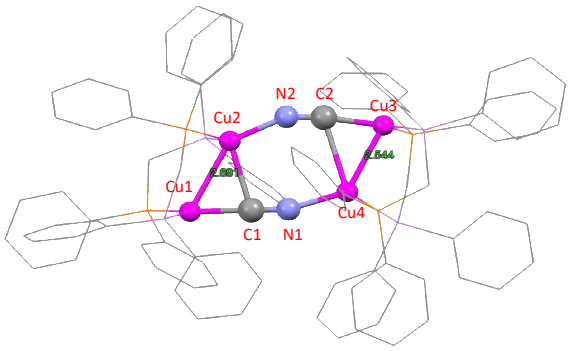
$\mathbf{A}_{exp}$ (100 K)



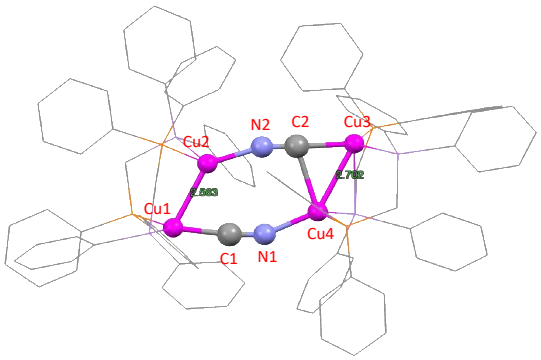
$\mathbf{A}_{opt\text{-}full}$



$\mathbf{A}_{opt\text{-}const}$



TD-DFT optimized S_1 of $\mathbf{A}_{opt\text{-}full}$



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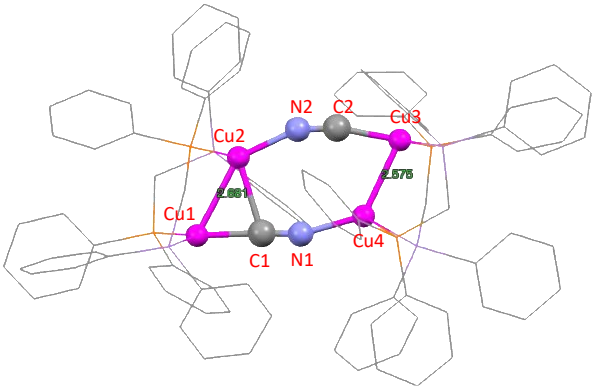

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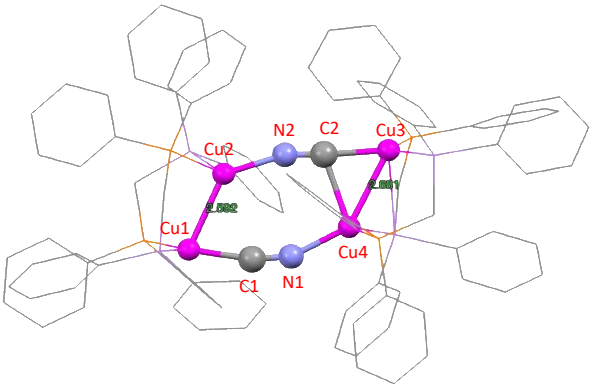

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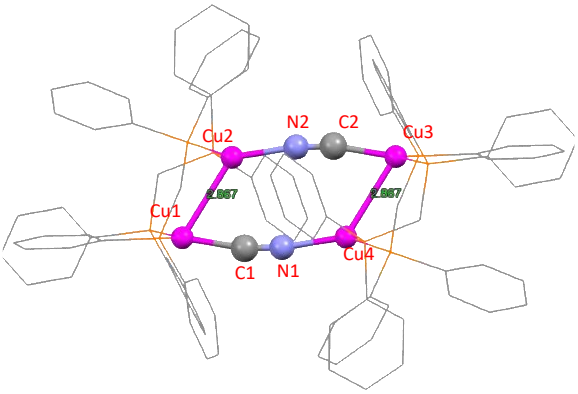
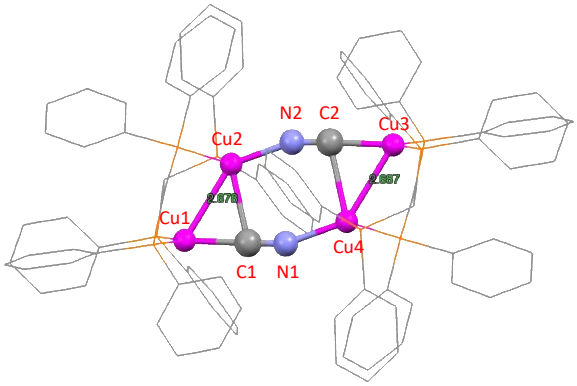


B$_{exp}$ (100 K)



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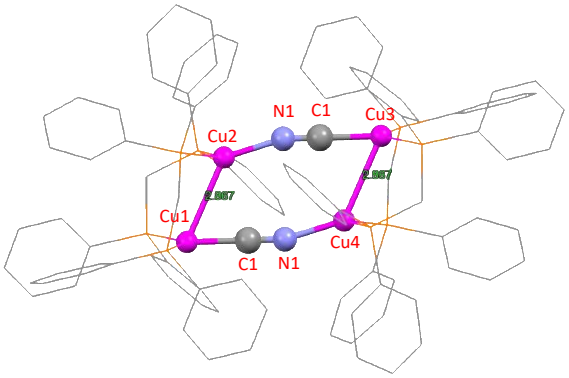

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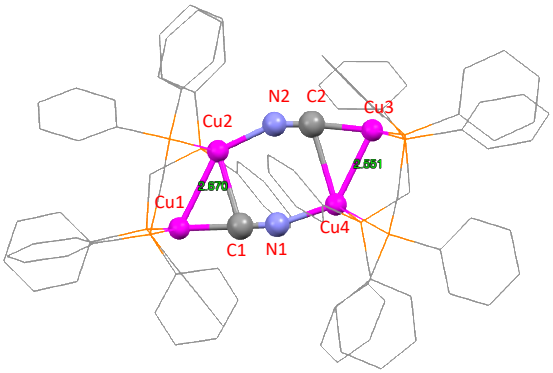

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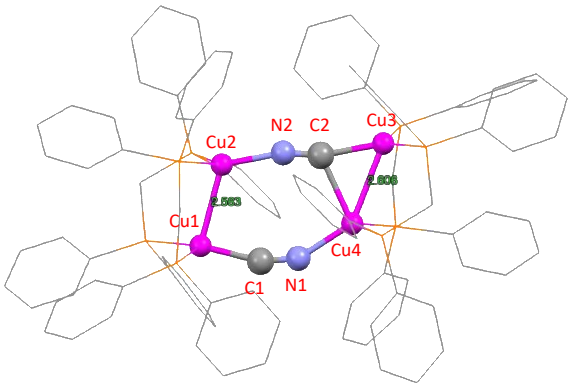
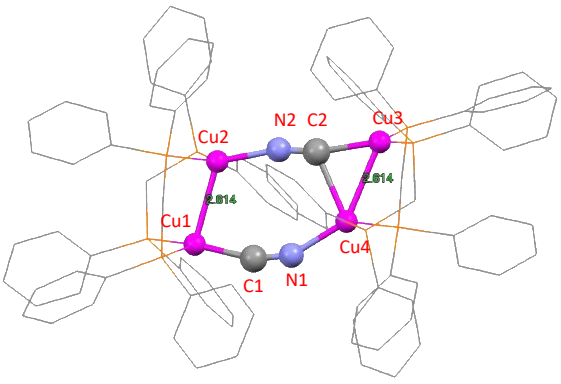
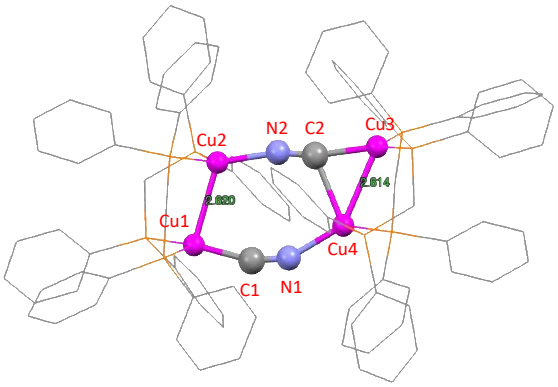


TD-DFT optimized S_1 of **B**$_{opt\text{-}const}$



TD-DFT optimized T_1 of **B**$_{opt\text{-}full}$



TD-DFT optimized T_1 of **B**$_{opt\text{-}const}$

Fig. S31. Representations of the experimental and optimized geometries of ground state, and the lowest singlet and triplet excited states of **A** and **B**.

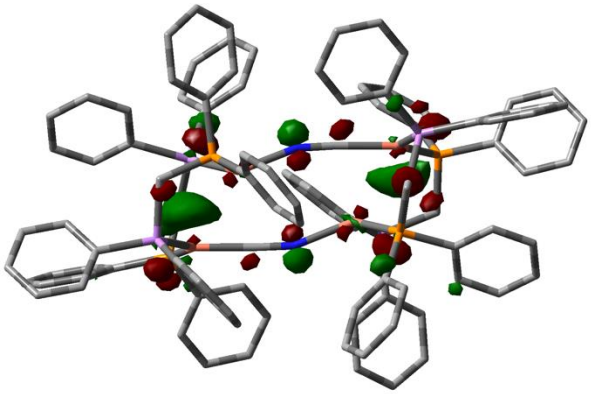
Table S7. Main characteristics of the first Franck Condon (FC) electronic excitations of $\mathbf{A}_{\text{opt-full}}$, $\mathbf{A}_{\text{opt-const}}$, $\mathbf{B}_{\text{opt-full}}$ and $\mathbf{B}_{\text{opt-const}}$. Only molecular orbitals (MOs) transition contributions of more than 10 % are given.

$\mathbf{A}_{\text{opt-full}}$	Energy (eV)	Wavelength (nm)	Oscillator strength	Nature of the excitation
T_1-FC	3.527	351	0.000	68 % HOMO to LUMO
T_2-FC	3.604	344	0.000	84 % HOMO-1 to LUMO
T_3-FC	3.656	339	0.000	45 % HOMO-2 to LUMO 26 % HOMO to LUMO+1
S_1-FC	3.746	331	0.009	77 % HOMO to LUMO
S_2-FC	3.772	328	0.003	81 % HOMO-1 to LUMO
S_3-FC	3.905	317	0.001	56 % HOMO-2 to LUMO 26 % HOMO to LUMO+1

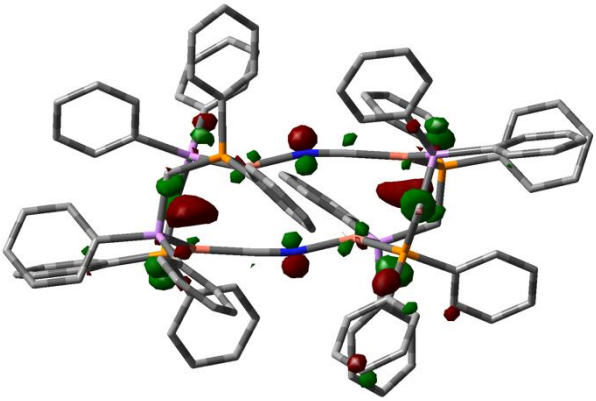
$\mathbf{A}_{\text{opt-const}}$	Energy (eV)	Wavelength (nm)	Oscillator strength	Nature of the excitation
T_1-FC	3.554	349	0.000	70 % HOMO to LUMO 13 % HOMO-1 to LUMO
T_2-FC	3.556	347	0.000	63 % HOMO-1 to LUMO 10 % HOMO to LUMO
T_3-FC	3.707	334	0.000	45 % HOMO-2 to LUMO 11 % HOMO-1 to LUMO+1 12 % HOMO to LUMO+1
S_1-FC	3.710	334	0.000	77 % HOMO to LUMO 11 % HOMO-1 to LUMO
S_2-FC	3.746	331	0.002	76 % HOMO-1 to LUMO 10 % HOMO to LUMO
S_3-FC	3.935	315	0.000	56 % HOMO-2 to LUMO 11 % HOMO-1 to LUMO+1 12 % HOMO to LUMO+1

$\mathbf{B}_{\text{opt-full}}$	Energy (eV)	Wavelength (nm)	Oscillator strength	Nature of the excitation
T_1-FC	3.527	351	0.000	69 % HOMO to LUMO
T_2-FC	3.635	341	0.000	29 % HOMO-1 to LUMO 27 % HOMO-2 to LUMO 13 % HOMO to LUMO+1
T_3-FC	3.641	340	0.000	52 % HOMO-1 to LUMO 18 % HOMO-2 to LUMO 13 % HOMO to LUMO+1
S_1-FC	3.770	329	0.017	83 % HOMO to LUMO
S_2-FC	3.807	325	0.000	88 % HOMO-1 to LUMO
S_3-FC	3.909	317	0.000	55 % HOMO-2 to LUMO 22 % HOMO to LUMO+1

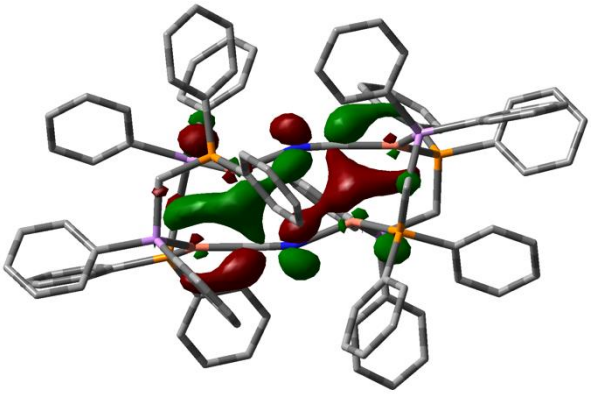
$B_{opt\text{-}const}$	E_{abs} (eV)	Wavelength (nm)	Oscillator strength	Nature of the excitation
T_1-FC	3.513	353	0.000	73 % HOMO to LUMO
T_2-FC	3.564	347	0.000	75 % HOMO-1 to LUMO
T_3-FC	3.654	339	0.000	59 % HOMO-2 to LUMO 16 % HOMO to LUMO+1
S_1-FC	3.708	334	0.006	85 % HOMO to LUMO
S_2-FC	3.743	331	0.000	85 % HOMO-1 to LUMO
S_3-FC	3.876	319	0.000	64 % HOMO-2 to LUMO 18 % HOMO to LUMO+1



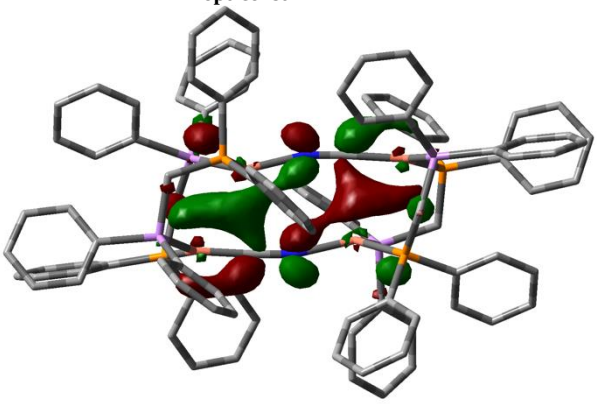
A$_{\text{opt-full}}$ LUMO+1



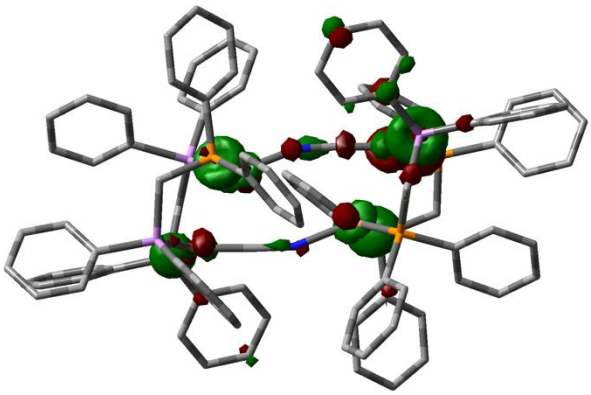
A$_{\text{opt-const}}$ LUMO+1



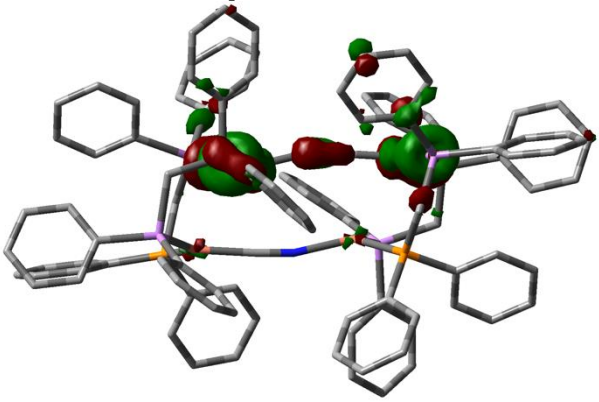
A$_{\text{opt-full}}$ LUMO



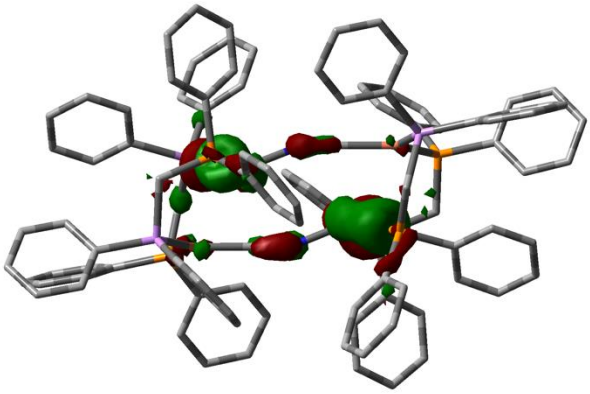
A$_{\text{opt-const}}$ LUMO



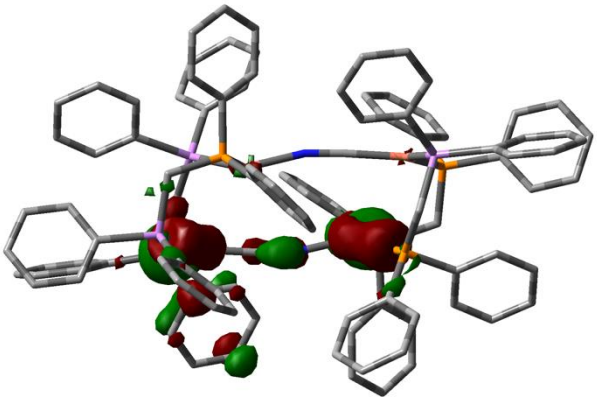
A$_{\text{opt-full}}$ HOMO



A$_{\text{opt-const}}$ HOMO



A$_{\text{opt-full}}$ HOMO-1



A$_{\text{opt-const}}$ HOMO-1

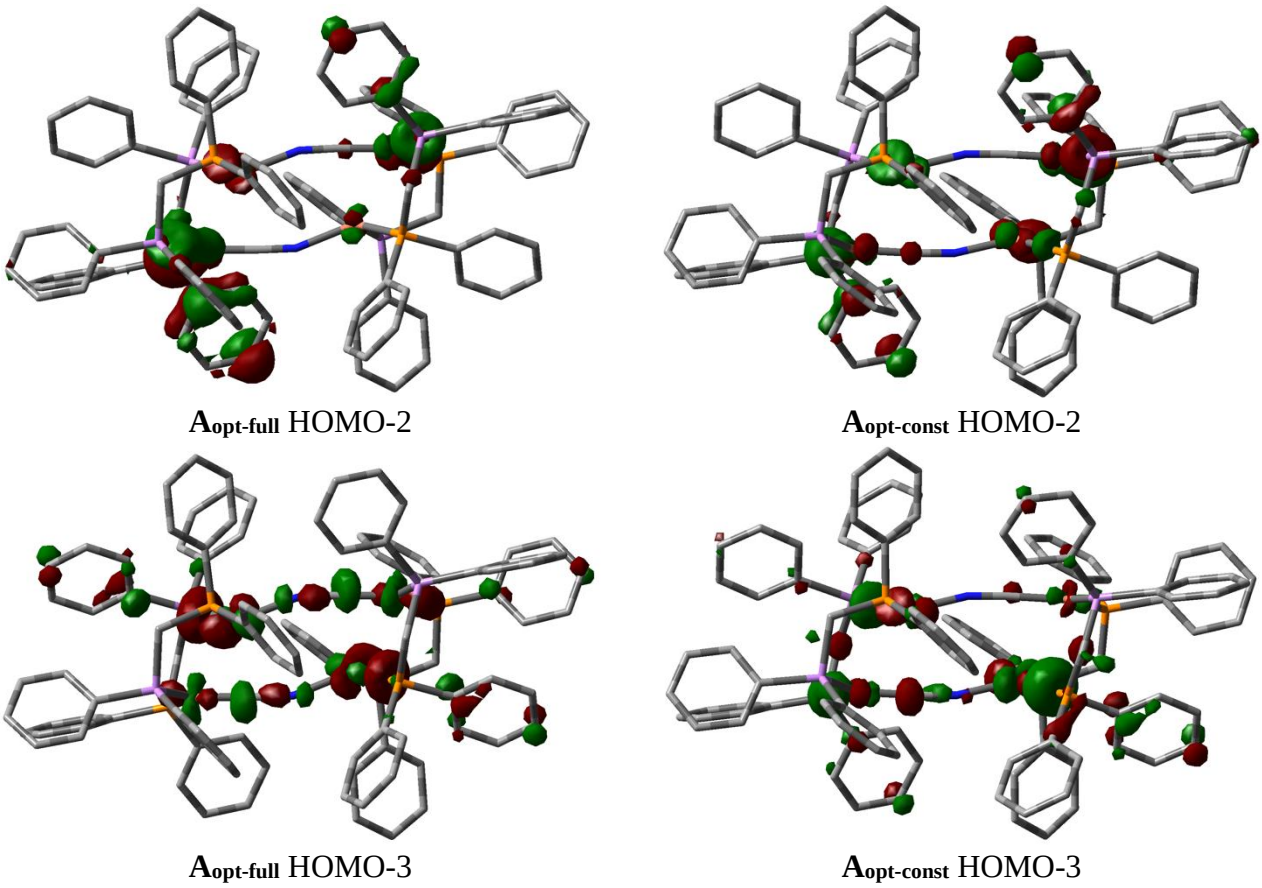
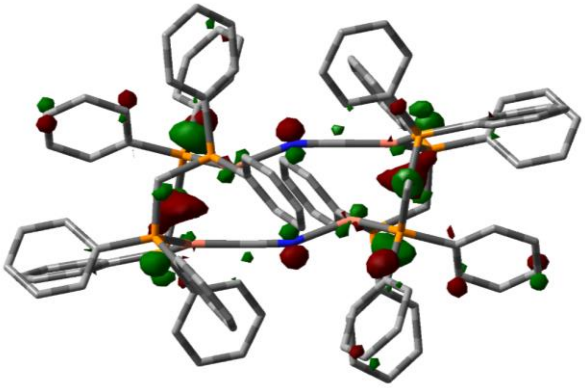
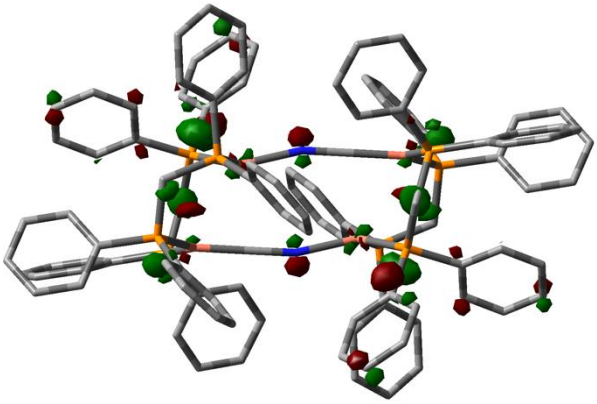


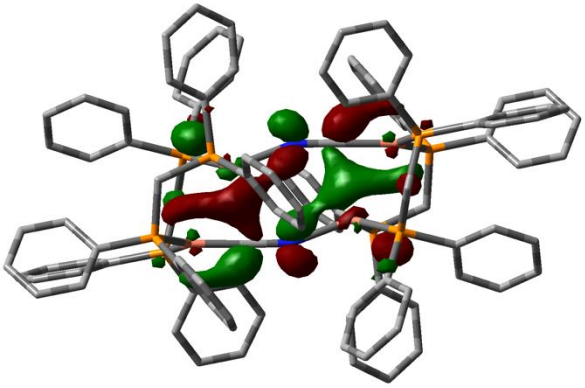
Fig. S32. Iso-contour plots of the frontier MOs involved in the description of the first FC electronic excitations of $\mathbf{A}_{\text{opt-full}}$ and $\mathbf{A}_{\text{opt-const}}$(± 0.035 [e/bohr^3]$^{1/2}$).



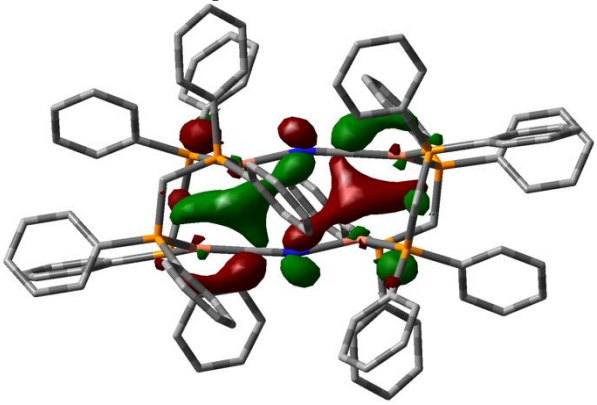
B$_{\text{opt-full}}$ LUMO+1



B$_{\text{opt-const}}$ LUMO+1



B$_{\text{opt-full}}$ LUMO



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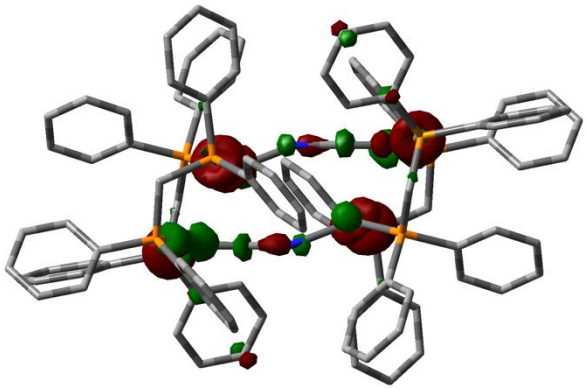
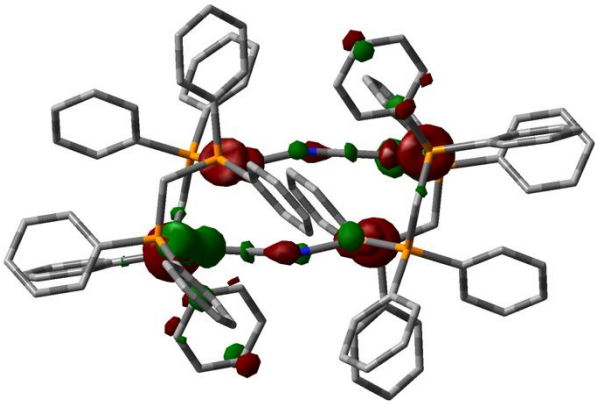
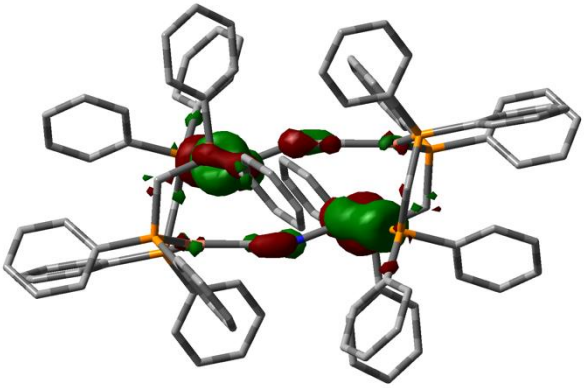


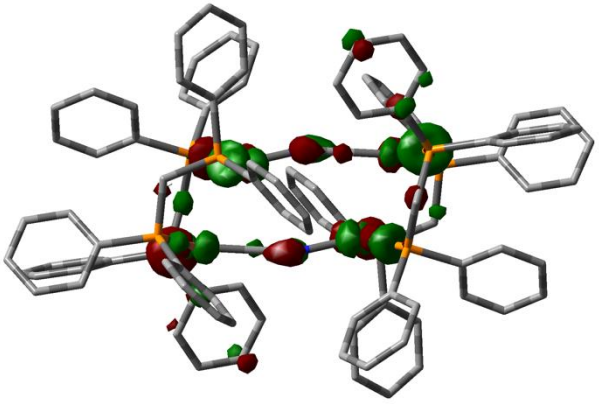
B$_{\text{opt-full}}$ HOMO



B$_{\text{opt-const}}$ HOMO



B$_{\text{opt-full}}$ HOMO-1



B$_{\text{opt-const}}$ HOMO-1

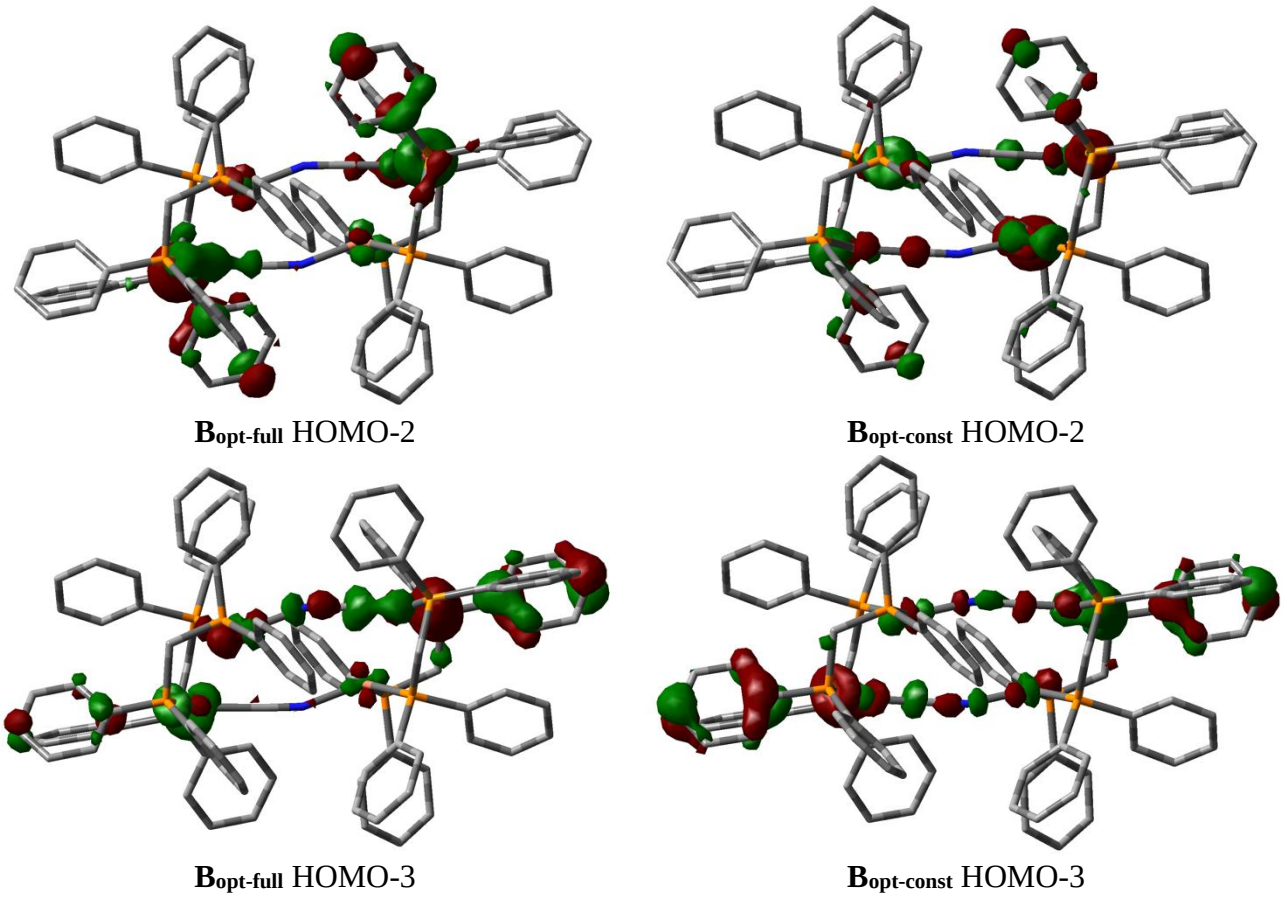
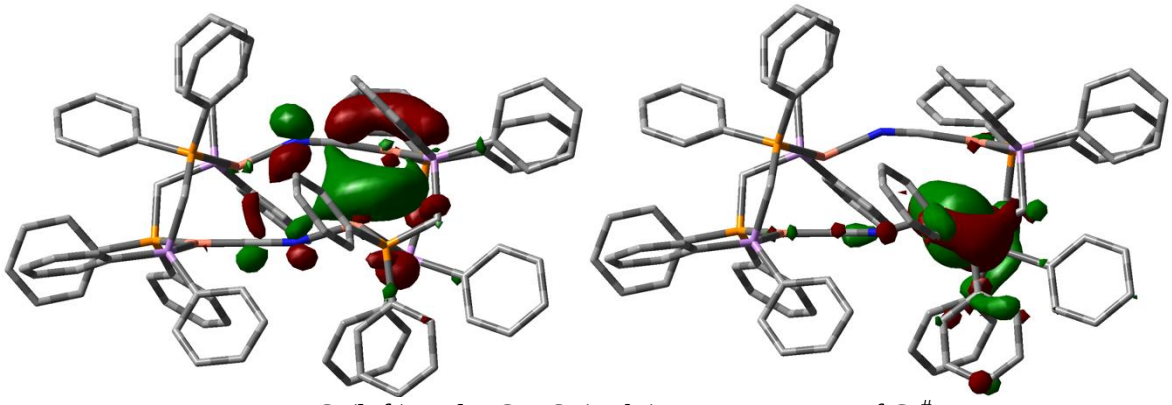


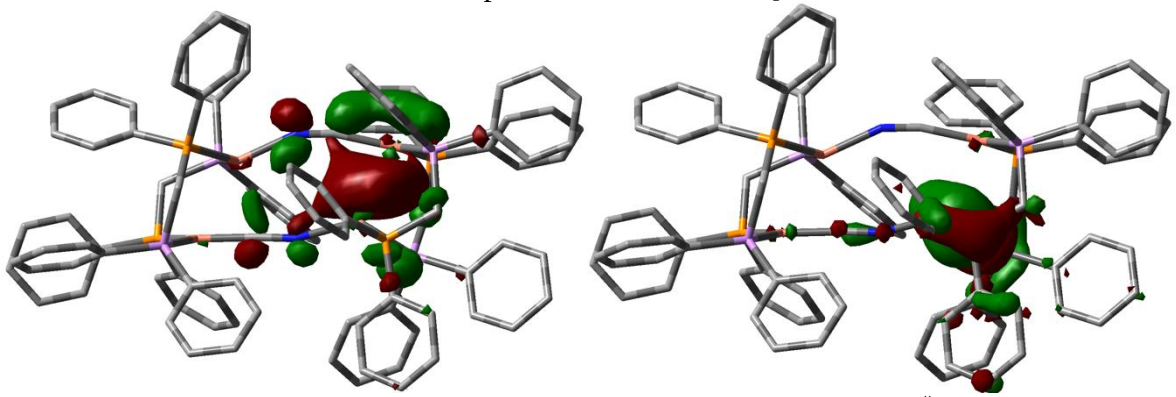
Fig. S33. Iso-contour plots of the frontier MOs involved in the description of the first FC electronic excitations of $\mathbf{B}_{\text{opt-full}}$ and $\mathbf{B}_{\text{opt-const}}$ (± 0.035 $[e/bohr^3]^{1/2}$).

Table S8. Calculated relative energies (ground state S_0 energy as reference) of the different excited states of **$A_{opt\text{-}full}$**, **$A_{opt\text{-}const}$**, **$B_{opt\text{-}full}$** and **$B_{opt\text{-}const}$** - $S_0^{\#}$ corresponds to the energy on the potential energy surface of S_0 at the geometry of S_1 or T_1; Spin orbit couplings (SOC) between states; reorganization energies ($\Delta\lambda$); computed emission energies (λ_{em}); radiative rate constants k_r^f and k_r^{ph} (Eq S1); T_1 simulated lifetimes at 80 K considering only spontaneous emission. Calculated emission wavelengths and emission energies of the different S_1 (λ_{fluo} and E_{fluo}) and T_1 (λ_{ph} and E_{ph}).

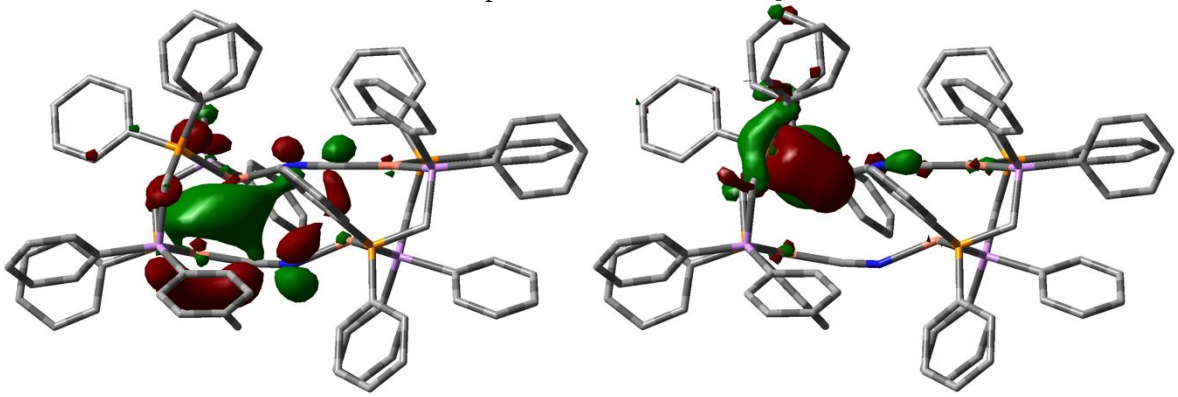
	$A_{opt\text{-}full}$	**$A_{opt\text{-}const}$**	**$B_{opt\text{-}full}$**	**$B_{opt\text{-}const}$**
E_{rel} S_0 (eV)	0.000	0.000	0.000	0.000
E_{rel} S_1 (eV)	3.042	3.102	3.061	3.105
E_{rel} $S_0^{\#}$ at S_1 geometry (eV)	0.642	0.639	0.657	0.695
E_{rel} T_1 (eV)	2.791	2.871	2.881	2.875
E_{rel} $S_0^{\#}$ at T_1 geometry (eV)	0.651	0.680	0.680	0.684
$\Delta E_{adiabatic}(S_1\text{-}T_1)$ (eV)	0.251	0.231	0.179	0.230
$\Delta E_{adiabatic}(S_1\text{-}T_1)$ (cm^{-1})	2025	1863	1445	1852
SOC S_1-FC/T_1-FC (cm^{-1})	10	6	8	9
SOC $T_1/S_0^{\#}$ (cm^{-1})	5	6	4	4
$\Delta\lambda$ S_1	0.555	0.567	0.539	0.484
$\Delta\lambda$ T_1	0.555	0.631	0.430	0.521
k_r^f (s^{-1})	$9.5\cdot10^5$	$8.5\cdot10^5$	$1.5\cdot10^6$	$8.0\cdot10^5$
k_r^{ph} (s^{-1})	$7.3\cdot10^2$	$2.5\cdot10^2$	$8.5\cdot10^2$	$8.9\cdot10^2$
T_1 lifetime (ms)	1.4	4.0	1.2	1.1
E_{fluo} (eV)	2.400	2.464	2.404	2.410
λ_{fluo} (nm)	517	504	516	514
E_{ph} (eV)	2.140	2.191	2.201	2.191
λ_{ph} (nm)	579	566	563	566



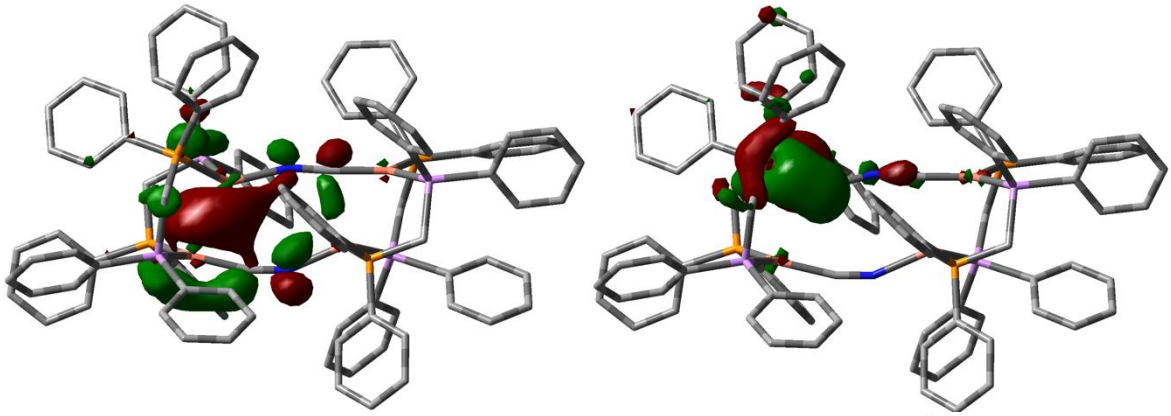
LUMO (left) and HOMO (right) representation of $S_0^{\#}$
TD-DFT optimized S_1 state of $\mathbf{A_{opt\text{-}full}}$



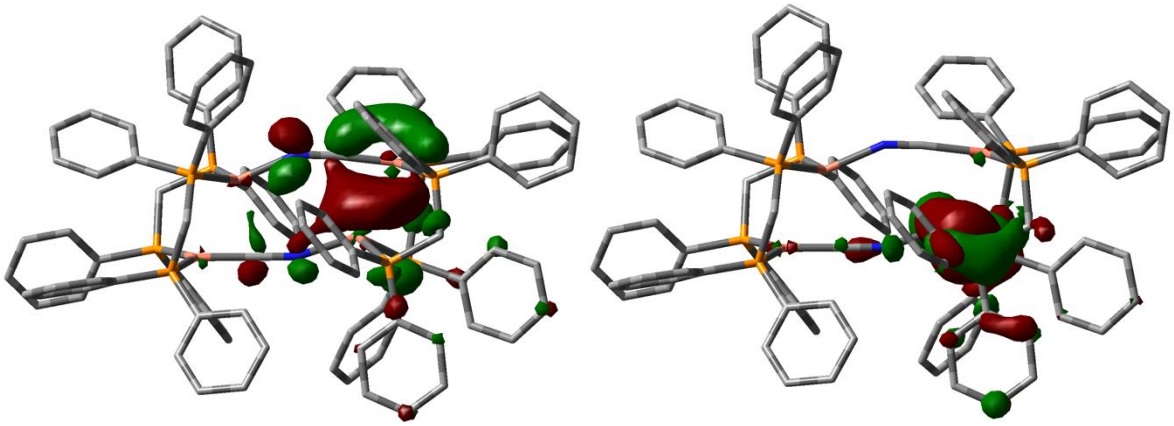
LUMO (left) and HOMO (right) representation of $S_0^{\#}$
TD-DFT optimized T_1 state of $\mathbf{A_{opt\text{-}full}}$



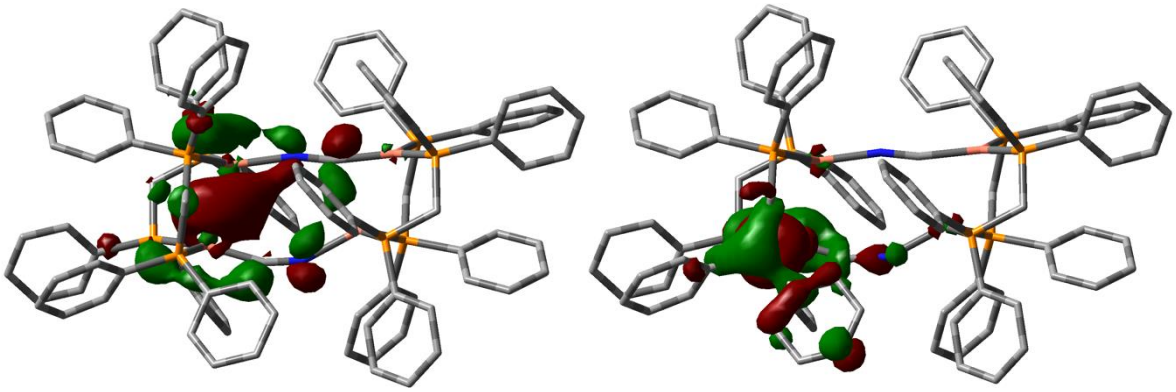
LUMO (left) and HOMO (right) representation of $S_0^{\#}$
TD-DFT optimized S_1 state of $\mathbf{A_{opt\text{-}const}}$



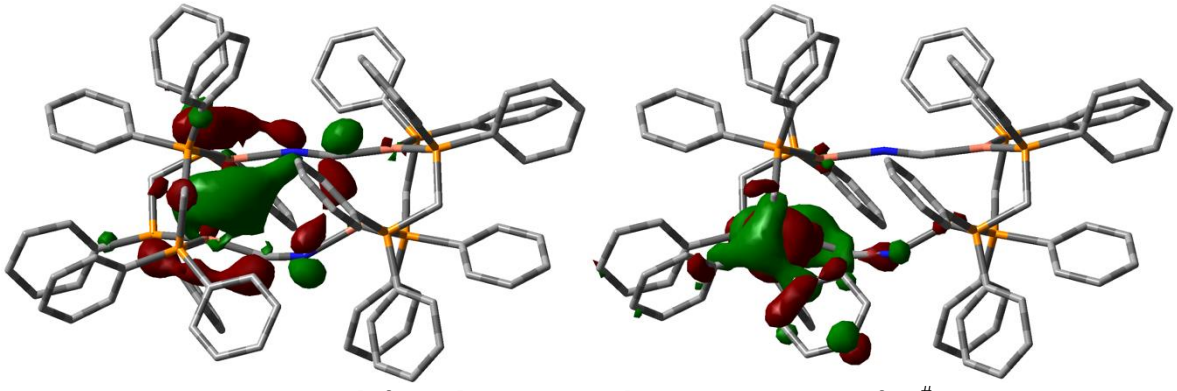
LUMO (left) and HOMO (right) representation of $S_0^{\#}$
TD-DFT optimized T_1 state of $\mathbf{A}_{\mathbf{opt\text{-}const}}$



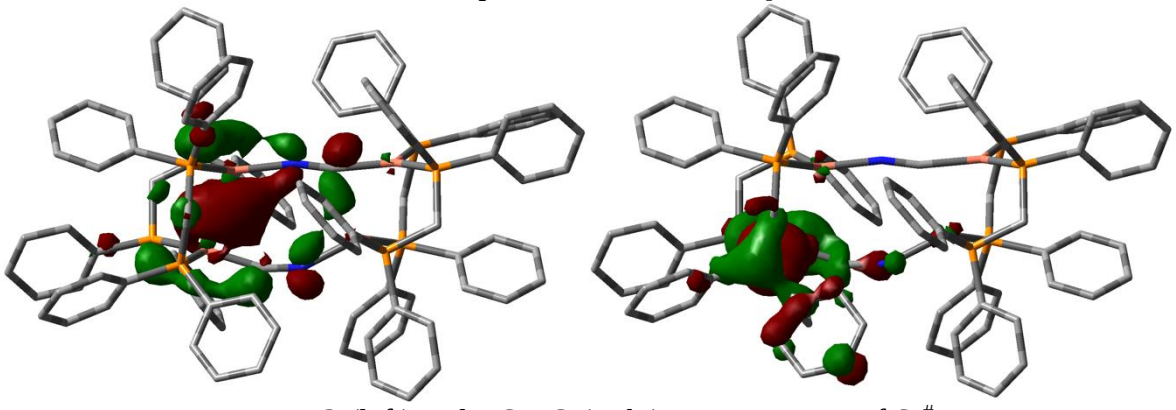
LUMO (left) and HOMO (right) representation of $S_0^{\#}$
TD-DFT optimized S_1 state of $\mathbf{B}_{\mathbf{opt\text{-}full}}$



LUMO (left) and HOMO (right) representation of $S_0^{\#}$
TD-DFT optimized T_1 state of $\mathbf{B}_{\mathbf{opt\text{-}full}}$



LUMO (left) and HOMO (right) representation of $S_0^{\#}$
TD-DFT optimized S_1 state of $\mathbf{B}_{\mathbf{opt\text{-}const}}$



LUMO (left) and HOMO (right) representation of $S_0^{\#}$
TD-DFT optimized T_1 state of $\mathbf{B}_{\mathbf{opt\text{-}const}}$

Fig. S34. Iso-contour plots of the HOMO and LUMO at the geometries S_1 and T_1 of $\mathbf{A}_{\mathbf{opt\text{-}full}}$, $\mathbf{A}_{\mathbf{opt\text{-}const}}$, $\mathbf{B}_{\mathbf{opt\text{-}full}}$ and $\mathbf{B}_{\mathbf{opt\text{-}const}}$ on the potential energy surfaces of the ground state ($S_0^{\#}$) (± 0.035 [e/bohr^3]$^{1/2}$). In all cases, the emission is mainly described by the LUMO to HOMO transition.

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