SUPPORTING INFORMATION

Photoredox Hetero-Bimetallic Dual Catalysis Using Engineered Covalent Organic Frameworks

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Materials and general methods.

All reagents and solvents were purchased from commercial sources and used without further purification.

Light irradiation was carried out using a 15W blue LED photoreactor thermostated at 25 °C. A spectro-radiometer equipment Stellarnet model Blue-Wave UV-NB50 was employed to measure the emission of the Blue LED used (range 300-600 Å, integration time CR2-AP + 200 ms, intensity 21.7217 W/m²).

Nuclear Magnetic Resonance (NMR) spectra were acquired on a Bruker AV-300 spectrometer, running at 300 MHz for ¹H. Chemical shifts (δ) are reported in ppm relative to residual solvent signals (CDCl₃: 7.26 ppm for ¹H-NMR. ¹³C solid state Nuclear Magnetic Resonance were acquired on a Bruker AV-400 spectrometer coupled to a multinuclear probe (¹⁵N-³¹P) CPMAS with triple channel (BL4 X/Y/²H) for a 4 mm rotor at room temperature, using 1k scans and 12 kHz of turning speed. The ¹H excitation pulse used is π/2 * 2.75 μs and the contact pulse is 3 ms.

Elemental Chemical Analyses were obtained by Servicio Interdepartamental de Apoyo a la Investigación in UAM, in an elemental analyzer LECO CHNS-932 model number 601-800-500.

IR spectra were recorded in a Perkin-Elmer 283 equipped with ATR MiRacle Single Reflection Horizontal.

Powder X-ray diffraction was obtained in a X’Pert PRO diffractometer θ/2θ geometry from Panalytical equipped with a Johansson monochromator for λ Kα, a X’Celerator fast detector in an alumina holder. The θ/2θ swept was performed from 1 to 45 ° with an angular increase of 0.0167 °/100 s. Simulated model structures of PXRD were carried out using Materials Studio 8.0 Program. Manual editing from a similar reported structure was performed and adjusted by using the forcite module.

Scanning Electron Microscopy (SEM) images were carried out on a Hitachi S-3000N electron microscope with a coupled ESED detector and an analyzer from energy dispersive X-ray from Oxford Instruments, INCAx-sight model. The images were obtained in vacuum after being metallized in a Sputter Quórum Q150T-S with gold coating. Transmission Electron Microscopy (TEM) images were collected on a Tecnai G2 F20 microscope (FEI) at 200 KV.

Diffuse reflectance was measured in a UV/Vis spectrometer by UNICAM. Emission intensities were recorded using a JASCO Spectrofluorometer FP-8600 controlled by Spectra Manager Version 2.10.01. The fluorescence emission of the materials was measured irradiating a suspension of 1 mg of the sample dispersed in 2 mL of MeOH at 390 nm. A 10x10 mm precision cell made of quartz was used for all emission measurements.

Electrochemistry: Voltammetry experiments were performed under argon atmosphere at room temperature, using 0.1 M tetrabutylammonium hexafluorophosphate solution in CH₃CN as electrolyte. Measurements were carried out by using an Ivium CompaqStat potentiostat interfaced with a computer. A standard three-electrode electrochemical cell was used. Potentials were referred to an Ag/AgCl, Et₄NBr 0.4 M reference electrode in ethylene glycol, and measured potentials were calibrated using an internal Fc/Fc+ standard. The working electrode consists of a Pt electrode coated with Teflon. A carbon paste was fabricated by mixing 30 mg of high purity carbon (>99.9%) with 3 mg of the material and 1 drop of mineral oil (Nujol). This carbon paste was deposited in the surface of the working electrode to perform the experiments.
As control experiment, a blank carbon paste containing only high purity carbon and Nujol was obtained and measured under the same conditions.

**Thermogravimetric analyses (TGA)** were performed on a TGA Q500 Thermobalance from TA instruments, heating the sample from 25 °C to 900 °C at 10 °C/min under air atmosphere.

**X Ray Photoelectron Spectroscopy (XPS)** were performed with a Phoibos 150 analyzer (SPECS GmbH) in ultra-high vacuum conditions (base pressure $4 \times 10^{-10}$ mbar) with a monochromatic aluminum $K_{\alpha}$ x-ray source (1486.74 eV) at 300 W. The energy resolution as measured by the FWHM of the Ag 3d$_{5/2}$ peak for a sputtered silver foil was 0.62 eV. The binding energy was corrected by using the C 1s line at 284.5 eV as the reference. A flood gun was used during acquisition to compensate the surface charging of the samples.

Qualitative and quantitative **Total X-Ray Fluorescence** analyses (TXRF) were performed with a benchtop S2 PicoFox TXRF spectrometer from Bruker Nano (Germany) $^{1,2}$. TXRF system was equipped with a Mo X-ray source working at 50 kV and 600 µA, a multilayer monochromator with 80% of reflectivity at 17.5 keV (Mo $K_{\alpha}$), a XFlash SDD detector with an effective area of 30 mm$^2$ and an energy resolution better than 150 eV for 5.9 keV (Mn $K_{\alpha}$). For deconvolution and integration commercial Spectra v. 7.5.3 software package from Bruker was used. Previously to the measurements, sample acid digestions were performed in a high pressure and temperature microwave. Acid digestion technology was used by mean of an UltraWAVE digestion system from Millestone (Italy) with a single reaction chamber able of operates up to 199 bar pressure and 270 °C.

**Volumetric N$_2$ sorption isotherms** were collected at 77 K (N$_2$) using an ASAP 2460 HD (Micromeritics). Temperature was controlled by using a liquid nitrogen bath.
Synthesis of building blocks and metal complexes.

**Synthesis of 1**: 3,8-dibromo-1,10-phenanthroline (1 g, 2.96 mmol), (4-formylphenyl)boronic acid (930 mg, 6.20 mmol) and K$_2$CO$_3$ (1.625 g, 8.87 mmol) were introduced into a 100 mL Schlenk equipped with a stir bar. Three vacuum-Ar cycles were performed. Then, 20 mL of purged THF and 4 mL of distilled water were added under Ar atmosphere. Finally, Pd(PPh$_3$)$_4$ (512 mg, 0.443 mmol) was added under Ar atmosphere. The reaction was heated at 70 °C during 48 hours in presence of Ar. A white solid was precipitated. Then, the reaction was cool down and filtered. The white solid was washed with water and acetone. Finally, it was recrystallized in a mixture of hot CHCl$_3$-acetone, in order to afford white crystals of **1**, that were isolated by filtration and dried under vacuum. 1118 mg obtained (97 % of yield).

\[\text{O} \quad \begin{array}{c}
\text{Br} \\
\text{Br}
\end{array} \quad \begin{array}{c}
\text{O} \\
\text{H-O}
\end{array} \quad \text{Pd(PPh$_3$)$_4$ (15 mol%)} \\
\text{K$_2$CO$_3$ (3 equiv.)} \\
\text{THF:H$_2$O (5:1)} \\
48h, 70 ^\circ C
\]

$^1$H-NMR (300 MHz, CDCl$_3$) $\delta$ **1**H NMR (300 MHz, CDCl$_3$) $\delta$ 10.14 (s, 2H), 9.50 (d, $J = 2.3$ Hz, 2H), 8.51 (d, $J = 2.3$ Hz, 2H), 8.09 (d, $J = 8.3$ Hz, 4H), 7.98 (d, $J = 8.3$ Hz, 4H), 7.96 (s, 2H) ppm.

**Elemental analysis**: calculated for C$_{26}$H$_{16}$N$_2$O$_2$: C: 80.40%; H: 4.15%; N: 7.21%. Found: C: 80.53%; H: 4.45%; N: 7.11%.

**Synthesis of the Ir precursor.**

**Step 1 – Synthesis of 2-(2,4-difluorophenyl)-5-(trifluoromethyl)pyridine (L1)**

Potassium (2,4-difluorophenyl)trifluoroborate (1.1 g, 5 mmol), 2-bromo-5-(trifluoromethyl)pyridine (753 mg, 3.33 mmol), K$_2$CO$_3$ (2.3 g, 16.7 mmol) and Pd(PPh$_3$)$_4$ (390 mg, 0.33 mmol) were placed into a 100 mL Schlenk equipped with a stir bar. Three vacuum-Ar cycles were performed. Then, 12 mL of degassed THF and 6 mL of degassed distilled water were added. The reaction was stirred at 80 °C under Ar atmosphere for 24 hours. After cooling to room temperature, it was extracted with 3x20 mL of dichloromethane. The organic layers were combined and dried with Na$_2$SO$_4$, filtrated and evaporated under reduced pressure. After purification by silica gel chromatography (cyclohexane-AcOEt 20:1), L1 was isolated as a white solid (847 mg, 97 %).
$^1$H NMR (300 MHz, CDCl$_3$): $\delta = 8.96$ (s, 1H), 8.12-8.07 (m, 1H), 7.98 (dd, $J = 8.5$, 2.0 Hz, 1H), 7.90 (d, $J = 8.5$ Hz, 1H), 7.06-7.02 (m, 1H), 6.97-6.92 (m, 1H).

**Step 2 – Synthesis of dimer [(dF(CF$_3$)ppy)$_2$-Ir-µ-Cl]$_2$**

L1 (840 mg, 3.24 mmol) and IrCl$_3$ (440 mg, 1.47 mmol) were placed into a 100 mL Schlenk equipped with a stir bar. Three vacuum-Ar cycles were performed. Then, 18 mL of degassed 2-ethoxyethanol and 6 mL of degassed distilled water were added. The reaction was stirred at 120 ºC under Ar atmosphere for 24 hours. After cooling to room temperature, the yellow solid formed was filtrated and gently washed with deionized water and cyclohexane, and finally dried under vacuum. 1.639 g obtained, 75 % yield.

$^1$H NMR (300 MHz, CDCl$_3$): 9.50 (d, $J = 1.0$ Hz, 4H), 8.45 (dd, $J = 9.0$, 3.0 Hz, 4H), 8.04 (dd, $J = 9.0$, 2.0 Hz, 4H), 6.39-6.47 (m, 4H), 5.06 (dd, $J = 9.0$, 2.0 Hz) ppm.

**Synthesis of [NiCl$_2$(phen)] complex**

A 50 mL Schlenk flask was charged with a stir bar, NiCl$_2$ (77.7 mg, 0.6 mmol), and 1,10-phenanthroline (108.1 mg, 0.6 mmol). Three vacuum/Ar cycles were performed. Then, 5 mL of degassed EtOH were added. The pink reaction mixture was stirred at room temperature overnight. A green solid appeared, indicating the completion of the reaction. The solvent was evaporated under reduced pressure, and the crude was suspended in 10 mL of THF. The green solid was isolated by filtration and dried overnight under vacuum.

Elemental Analysis: calculated for C$_{12}$H$_8$Cl$_2$N$_2$Ni: C, 46.52; H, 2.60; N, 9.04. Found: C, 46.89; H, 2.61; N, 9.04.
Figure S1: Left, Cyclic voltammetry of [NiCl₂(phen)] (black line) compared with [Ir(dF(CF₃)ppy)₂(bpy)]PF₆ (red line) measured in DMF (0.1 M TBAPF₆) at 100 mV/s using glassy carbon electrode as WE, Ag/AgCl as RE and Pt bar as CE. Right, emission spectra of [Ir(dF(CF₃)ppy)₂(bpy)]PF₆.
## Synthesis and characterization of COFs

**Table S1**: Screening of reaction conditions for the synthesis of Phen-COF.

| Entry | Solvent                          | Catalyst   | T (°C) | Time (h) | Result                                      |
|-------|----------------------------------|------------|--------|----------|---------------------------------------------|
| 1     | Dioxane                          | AcOH 6M    | 120    | 72       | Amorphous                                   |
| 2     | Mesitylene                       | AcOH 6M    | 145    | 72       | Amorphous                                   |
| 3     | NMP                              | AcOH 6M    | 120    | 72       | No material                                  |
| 4     | o-DCB                            | AcOH 6M    | 120    | 72       | No material                                  |
| 5     | TCB, tBuOH (1:1)                 | AcOH 6M    | 80     | 72       | Amorphous                                   |
| 6     | NMP, o-DCB (1:1)                 | AcOH 3M    | 100    | 96       | Amorphous                                   |
| 7     | DMA                              | AcOH 9M    | 140    | 72       | Amorphous                                   |
| 8     | ACN, DMF (1:1)                   | AcOH 6M    | 100    | 72       | Amorphous                                   |
| 9     | DMA, DMSO (1:1)                  | AcOH 9M    | 150    | 96       | Amorphous                                   |
| 10    | Dioxane, Mesitylene (1:1)        | AcOH 6M    | 120    | 72       | Amorphous, one diffraction peak with low intensity |
| 11    | Dioxane, Mesitylene (1:2)        | AcOH 6M    | 120    | 72       | Amorphous, one diffraction peak with low intensity |
| 12    | Dioxane, Mesitylene (2:1)        | AcOH 6M    | 120    | 72       | Amorphous, one diffraction peak with low intensity |
| 13    | Dioxane, Mesitylene (1:4)        | AcOH 6M    | 120    | 72       | Amorphous, one diffraction peak with low intensity |
| 14    | Dioxane, Mesitylene (4:1)        | AcOH 6M    | 120    | 72       | Amorphous                                   |
| 15    | Dioxane, Mesitylene (1:9)        | AcOH 6M    | 120    | 72       | Moderated Crystallinity                      |
| 16    | Dioxane, Mesitylene (9:1)        | AcOH 6M    | 120    | 72       | Amorphous                                   |
| 17    | Dioxane, Mesitylene (1:9)        | AcOH 3M    | 120    | 72       | Amorphous                                   |
| 18    | Dioxane, Mesitylene (1:9)        | AcOH 9M    | 120    | 72       | Amorphous                                   |
| 19    | Dioxane, Mesitylene (1:9)        | CF$_2$SO$_3$H | 120    | 72       | Black Powder                                |
| 20    | Dioxane, Mesitylene (1:9)        | Sc(OTf)$_3$ | 120    | 72       | Amorphous                                   |
| 21    | Dioxane, Mesitylene (1:9)        | AcOH 6M    | 120    | 144      | Moderated Crystallinity                      |
**Synthesis of Phen-COF:** A 45 mL solvothermal reactor was charged with 1 (100 mg, 0.257 mmol) and TAPB (60 mg, 0.170 mmol). 5.4 mL of mesitylene and 0.6 mL of anhydrous dioxane were added. Finally, 0.6 mL of aqueous acetic acid 6 M were added. The reactor was sealed and heated at 120 °C for 3 days, yielding a yellow-brown solid which was isolated by filtration and washed with DMF, MeOH and THF. The resulting powder was immersed in anhydrous THF for 24 h, filtered and dried first at room temperature under vacuum for 12 h, and then at 100 °C for 2 h to afford a yellow-brown powder, Phen-COF. 140 mg obtained.

![Synthesis of Phen-COF](image)

**Figure S2:** Fourier-Transformed Infrared Spectra of Phen-COF.
**Figure S3:** PXRD pattern of Phen-COF.

**Figure S4:** $^{13}$C-NMR-CP-MAS spectra of 1 (orange line) and Phen-COF (black line) (for the assignment of a, b and c signals, see the drawing of the molecule).

**Figure S5:** FE-SEM image of Phen-COF.
**Figure S6**: Adsorption-desorption N\textsubscript{2} isotherm at 77 K of Phen-COF and Brunauer-Emmett-Teller surface area plot of Phen-COF ($S_{\text{BET}} = 482 \text{ m}^2/\text{g}$).

**Figure S7**: Pore size distribution of Phen-COF.

**Figure S8**: Diffuse Reflectance Spectrum and Kubelka-Munk plot of Phen-COF.
**Figure S9:** Emission Spectrum of Phen-COF.

**Figure S10:** Cyclic voltammetries of Phen-COF and comparison with cyclic voltammetry of 1,10-phenanthroline (bottom, right).
Figure S11: Thermogravimetric analysis of Phen-COF. The dotted line corresponds to the first derivative of Weight %.

Synthesis of Ir,Ni@Phen-COF: in a 100 mL round bottom-flask, 140 mg of Phen-COF were suspended on 50 mL of dry acetonitrile and 1 mL of aqueous acetic acid 6 M during 30 minutes with an ultrasound bath. Then, [(dF(CF₃)ppy)₂-Ir-µ-Cl]₂ (33 mg, 0.022 mmol) and NiCl₂-glyme (19.6 mg, 0.089 mmol) were added. The mixture was stirred at 70 °C for 16 hours, yielding a yellow powder that was isolated by filtration and washed with hot DMF, acetonitrile and THF. The resulting powder was washed with acetone using Soxhlet extraction, then filtered and dried first at room temperature under vacuum for 12 h, and then at 100 °C for 2 h to afford an orange powder, Ir,Ni@Phen-COF. 151 mg obtained.
Figure S12: Fourier-Transformed Infrared Spectra of Ir,Ni@Phen-COF.

Figure S13: PXRD pattern of Ir,Ni@Phen-COF.

Figure S14: $^{13}$C-NMR-CP-MAS spectra of Ir,Ni@Phen-COF.
Figure S15: FE-SEM image of Ir,Ni@Phen-COF.
Figure S16: SEM-EDX images of Ir,Ni@Phen-COF (Ir-green, Ni-red, F and Cl-white).

Figure S17: Quantitative TXRF spectra of Ir,Ni@Phen-COF (4.0 % of Ir and 2.8 % of Ni).

Figure S18: Adsorption-desorption N₂ isotherm at 77 K of Ir,Ni@Phen-COF and Brunauer-Emmett-Teller surface area plot of Ir,Ni@Phen-COF ($S_{BET} = 432 \text{ m}^2/\text{g}$).
Figure S19: Pore size distribution of Ir,Ni@Phen-COF.

Figure S20: Diffuse Reflectance Spectrum and Kubelka-Munk plot of Ir,Ni@Phen-COF.

Figure S21: Emission Spectrum of Ir,Ni@Phen-COF.
Figure S22: Cyclic voltammetries of Ir,Ni@Phen-COF.

Figure S23: Thermogravimetric analysis of Ir,Ni@Phen-COF.
**Figure S24**: Overview of X-Ray Photoelectron Spectrum of Ir,Ni@Phen-COF.

**Figure S25**: XPS spectra of Ir,Ni@Phen-COF.
Synthesis of Ni@Phen-COF: in a 100 mL round bottom-flask, 140 mg of Phen-COF were suspended on 50 mL of dry acetonitrile and 1 mL of aqueous acetic acid 6 M during 30 minutes with an ultrasound bath. Then, NiCl₂-glyme (19.6 mg, 0.089 mmol) was added. The mixture was stirred at 70 °C for 16 hours, yielding a yellow powder that was isolated by filtration and washed with hot DMF, acetonitrile and THF. The resulting powder was washed with acetone using Soxhlet extraction, then filtered and dried first at room temperature under vacuum for 12 h, and then at 100 °C for 2 h to afford an orange powder, Ni@Phen-COF. 145 mg obtained.
**Figure S27:** Fourier-Transformed Infrared Spectra of Ni@Phen-COF.

**Figure S28:** PXRD pattern of Ni@Phen-COF.

**Figure S29:** $^{13}$C-NMR-CP-MAS spectra of Ni@Phen-COF.
Figure S30: FE-SEM image of Ni@Phen-COF.

Figure S31: SEM-EDX images of Ni@Phen-COF (Ni-green, Cl-pink).
Synthesis of Ir@Phen-COF: in a 100 mL round bottom-flask, 140 mg of Phen-COF were suspended on 50 mL of dry acetonitrile and 1 mL of aqueous acetic acid 6 M during 30 minutes with an ultrasound bath. Then, [(dF(CF$_3$)ppy)$_2$-Ir-µ-Cl]$_2$ (33 mg, 0.022 mmol) was added. The mixture was stirred at 70 °C for 16 hours, yielding a yellow powder that was isolated by filtration and washed with hot DMF, acetonitrile and THF. The resulting powder was washed with acetone using Soxhlet extraction, then filtered and dried first at room temperature under vacuum for 12 h, and then at 100 °C for 2 h to afford an orange powder, Ir@Phen-COF. 143 mg obtained.
Figure S33: Fourier-Transformed Infrared Spectra of Ir@Phen-COF.

Figure S34: PXRD pattern of Ir@Phen-COF.

Figure S35: $^{13}$C-NMR-CP-MAS spectra of Ir@Phen-COF.
**Figure S36:** FE-SEM image of Ir@Phen-COF.

**Figure S37:** SEM-EDX images of Ir@Phen-COF (Ir-blue, F-purple).
Figure S38: Quantitative TXRF spectra of Ir@Phen-COF (3.9 % of Ir).
**Figure S39:** Comparison of FTIR, PXRD, $^{13}$C-NMR-CP-MAS and SEM of pristine and functionalized Phen-COFs.
Synthesis of PF-Crystalline Laminar COF

A 45 mL solvothermal reactor was charged with TAPB (100.0 mg, 0.285 mmol), BTCA (46.0 mg, 0.285 mmol), 8.9 mL of a mixture of anhydrous dioxane : mesitylene (1:9) and 0.9 mL of 6 M acetic acid in water. The reactor was heated at 120 °C for 72 h, yielding a brown solid which was isolated by filtration and washed with DMSO, methanol and THF. The resulting powder was immersed in anhydrous THF for 24 h and dried first at room temperature under vacuum for 12 h, and then at 100 °C for 2 h to afford a brown powder. Its characterization agreed well with previous works.6,7

Then, an analogous post-functionalization protocol than the used for the synthesis of Ir,Ni@Phen-COF was followed. In a 100 mL round bottom-flask, 140 mg of Crystalline Laminar COF were suspended on 50 mL of dry acetonitrile and 1 mL of aqueous acetic acid 6 M during 30 minutes with an ultrasound bath. Then, [(dF(CF3)ppy)2-Ir-µ-Cl]2 (33 mg, 0.022 mmol) and NiCl2·glyme (19.6 mg, 0.089 mmol) were added. The mixture was stirred at 70 °C for 16 hours, yielding a yellow powder that was isolated by filtration and washed with hot DMF, acetonitrile and THF. The resulting powder was washed with acetone using Soxhlet extraction, then filtered and dried first at room temperature under vacuum for 12 h, and then at 100 °C for 2 h to afford an orange powder, PF-Crystalline Laminar COF. 138 mg obtained. In order to determine the quantity of Ir and Ni incorporated into the material, quantitative TXRF analyses were performed. Very low quantities of both Ir and Ni can be observed.

Figure S40: Quantitative TXRF analyses for PF-Crystalline Laminar COF.
General procedure for the light-mediated cross-coupling between potassium benzyltrifluoroborate and aryl bromides

An oven-dried 10 mL vial equipped with a magnetic stir bar was charged with catalyst (1.2 mg), corresponding potassium trifluoroborate salt 2 (0.15 mmol) and the corresponding aryl bromide 3 (0.075 mmol). Then, 950 µL of dry acetone and 50 µL of dry MeOH were added. Finally, 2,6-lutidine (30.5 µL, 0.26 mmol) was added. The vial was closed with a rubber septum and the reaction mixture was degassed by three cycles vacuum / Ar of “freeze-pump-thaw”. Then the vial was placed on a blue light LED photoreactor (450 nm) with an Ar balloon and the reaction mixture was stirred at 25 °C. The reaction was monitored by TLC and 1H-NMR. The yield was determined by 1H-NMR using nitromethane as internal standard.

Table S2: Screening of the reaction.

| Entry | Catalyst (mg) | Solvent       | Additive (equiv.) | NMR Yield (%) |
|-------|---------------|---------------|-------------------|---------------|
| 1     | Ir,Ni@Phen-COF (1.2 mg) | Acetone-MeOH 95:5 | 2,6-lutidine (3.5) | 51            |
| 2     | Ir,Ni@Phen-COF (1.2 mg) | THF           | 2,6-lutidine (3.5) | 6             |
| 3     | Ir,Ni@Phen-COF (1.2 mg) | Acetonitrile   | 2,6-lutidine (3.5) | 30            |
| 4     | Ir,Ni@Phen-COF (1.2 mg) | DCM           | 2,6-lutidine (3.5) | 0             |
| 5     | Ir,Ni@Phen-COF (1.2 mg) | DMF           | 2,6-lutidine (3.5) | 35            |
| 6     | Ir,Ni@Phen-COF (1.2 mg) | Toluene       | 2,6-lutidine (3.5) | 0             |
| 7     | Ir,Ni@Phen-COF (1.2 mg) | Acetone       | 2,6-lutidine (3.5) | 40            |
| 8     | Ir,Ni@Phen-COF (1.2 mg) | MeOH          | 2,6-lutidine (3.5) | 23            |
| 9     | Ir,Ni@Phen-COF (1.2 mg) | EtOH          | 2,6-lutidine (3.5) | 21            |
| 10    | Ir,Ni@Phen-COF (1.2 mg) | Acetone-MeOH 95:5 | -               | 3             |
| 11    | Ir,Ni@Phen-COF (1.2 mg) | Acetone-MeOH 95:5 | 2,6-lutidine (3.5) | 90 ±         |
| 12    | Ir,Ni@Phen-COF (1.2 mg) | Acetone-MeOH 95:5 | DIPEA (3.5)     | 76            |
| 13    | Ir,Ni@Phen-COF (1.2 mg) | Acetone-MeOH 95:5 | Cs₂CO₃ (3.5)    | 23            |
| 14    | Ir,Ni@Phen-COF (1.2 mg) | Acetone-MeOH 95:5 | K₂CO₃ (3.5)     | 12            |
| 15    | Ir,Ni@Phen-COF (1.2 mg) | Acetone-MeOH 95:5 | Na₃PO₄ (3.5)    | 10            |
| 16    | Ir,Ni@Phen-COF (1.2 mg) | Acetone-MeOH 95:5 | 2,6-lutidine (1) | 54            |
| 17    | Ir,Ni@Phen-COF (1.2 mg) | Acetone-MeOH 95:5 | 2,6-lutidine (2) | 79            |
| 18    | Ir,Ni@Phen-COF (1.2 mg) | Acetone-MeOH 95:5 | 2,6-lutidine (5) | 70            |
| 19    | Ir,Ni@Phen-COF (1.2 mg) | Acetone-MeOH 95:5 | 2,6-lutidine (7) | 43            |
| 20    | Ir,Ni@Phen-COF (0.6 mg) | Acetone-MeOH 95:5 | 2,6-lutidine (3.5) | 64          |
| 21    | Ir,Ni@Phen-COF (2.4 mg) | Acetone-MeOH 95:5 | 2,6-lutidine (3.5) | 40          |
This result was obtained when the reaction was sealed using a typical rubber septum instead of a PTFE-rubber septum. The reproducibility and the yields were significantly increased.

This material was obtained after the functionalization of the Phen-COF synthesized following the procedure presented in entry 14 of Table S1.

Variation of catalytic activity of the material depending on metal loading and Ir/Ni ratio

For the study of the influence of metal loading in the catalytic activity under the optimal conditions, a series of 6 different Ir,Ni@Phen-COF were obtained varying the amount of metal precursors on the post-functionalization stage. The results obtained appear in the following table:

**Table S3:** Study of the influence of metal loading on the catalytic activity.

| Catalyst                      | % Ir | % Ni | Molar Ratio Ni/Ir | NMR yield | TON (Ir/Ni) |
|-------------------------------|------|------|-------------------|-----------|-------------|
| Ir,Ni@Phen-COF                | 4.0  | 2.8  | 2:1               | 90        | 270/117     |
| Ir,Ni@Phen-COF                | 7.0  | 4.2  | 2:1               | 87        | 149/76      |
| Ir,Ni@Phen-COF                | 2.0  | 1.4  | 2:1               | 25        | 150/65      |
| Ir,Ni@Phen-COF                | 2.2  | 2.8  | 4:1               | 42        | 229/55      |
| Ir,Ni@Phen-COF                | 9.0  | 2.8  | 1:1               | 46        | 61/60       |

Substrate Scope

1-benzyl-4-methylbenzene (4a)
**Diphenylmethane (4b)**

\[ \text{H-NMR (300 MHz, CDCl}_3 \text{)} \delta 7.32-7.19 \text{ (m, 10H), 4.00 (s, 2H) ppm.} \]

**1-benzyl-4-(tert-butyl)benzene (4c)**

\[ \text{H-NMR (300 MHz, CDCl}_3 \text{)} \delta 7.31-7.28 \text{ (m, 4H), 7.22-7.18} \text{ (m, 3H), 7.13-7.10 \text{ (m, 2H), 3.95 (s, 2H), 1.29 (s, 9H) ppm.} \]

**1-benzyl-4-methoxybenzene (4d)**

\[ \text{H-NMR (300 MHz, CDCl}_3 \text{)} \delta 7.35-7.09 \text{ (m, 8H), 6.84-6.81 (m, 2H), 3.93 (s, 2H), 3.77 (s, 3H).} \]

**4-benzylbenzonitrile (4e)**

\[ \text{H-NMR (300 MHz, CDCl}_3 \text{)} \delta 7.58 \text{ (d, J = 8.3 Hz, 2H), 7.29 (m, 5H), 7.17 (d, J = 8.3 Hz, 2H), 4.04 (s, 2H) ppm.} \]

**4-benzylbenzaldehyde (4f)**

\[ \text{H-NMR (300 MHz, CDCl}_3 \text{)} \delta 9.98 \text{ (s, 1H), 7.81 (d, J = 8.0 Hz, 2H), 7.36 (d, J = 8.0 Hz, 2H), 7.31 (dd, J = 7.5, 7.0 Hz, 2H), 7.24 (t, J = 7.0 Hz, 1H), 7.19 (d, J = 7.5 Hz, 2H), 4.06 (s, 2H) ppm.} \]

**1-benzyl-3,5-bis(trifluoromethyl)benzene (4g)**

\[ \text{H-NMR (300 MHz, CDCl}_3 \text{)} \delta 7.72 \text{ (s, 1H), 7.63 (s, 2H), 7.35-7.31 (m, 2H), 7.28-7.24 (m, 1H), 7.18-7.16 (m, 2H), 4.09 (s, 2H) ppm.} \]

**1-benzyl-4-vinylbenzene (4h)**

\[ \text{H-NMR (300 MHz, CDCl}_3 \text{)} \delta 7.33 \text{ (d, J = 7.8 Hz, 2H), 7.28 (d, J = 7.8 Hz, 2H), 7.19-7.14 (m, 5H), 6.69 (dd, J = 17.4, 10.8 Hz, 1H), 5.70 (d, J = 17.4 Hz, 1H), 5.19 (d, J = 10.8 Hz, 1H), 3.97 (s, 2H) ppm.} \]
Recyclability experiment

An oven-dried 10 mL vial equipped with a magnetic stir bar was charged with catalyst (5 mg), corresponding potassium trifluoroborate salt 2a (0.15 mmol) and the corresponding aryl bromide 3b (0.075 mmol). Then, 950 µL of dry acetone and 50 µL of dry MeOH were added. Finally, 2,6-lutidine (30.5 µL, 0.26 mmol) was added. The vial was closed with a rubber septum and the reaction mixture was degassed by three cycles vacuum / Ar of “freeze-pump-thaw”. Then the vial was placed on a blue light LED photoreactor (450 nm) with an Ar balloon and the reaction mixture was stirred at 25 °C. After 26 h of reaction, an aliquot is analyzed by NMR to determine the yield using nitromethane as internal standard. Then, the reaction crude is centrifuged and washed with acetone 3 times. The catalyst is recovered as a yellow powder and was dried under vacuum during 2 hours before the next catalytic run. When the reaction was catalyzed by Ir,Ni@Phen-COF, 7 catalytic runs were performed, producing 0.92 mmol of diphenylmethane 4b.

Figure S41: Recyclability of Ir,Ni@Phen-COF.
Figure S42: Comparison of FTIR spectra before and after catalysis.

Figure S43: Comparison of PXRD patterns before and after catalysis.

Figure S44: Comparison of TEM images before (left) and after catalysis (right).
Leaching experiments

Once the first catalytic run was completed, the reaction was filtered in order to remove the catalyst. The supernatant was transferred to an oven-dried 10 mL vial equipped with a magnetic stir bar. The vial was closed with a PTFE / rubber septum and the reaction mixture was degassed by three cycles vacuum / oxygen of “freeze-pump-thaw”. Then the vial was placed on a blue light LED photoreactor (450 nm) and the reaction mixture was stirred at 25 °C. The reaction was monitored by 1H-NMR, observing that it did not advance further for the next 16 h. In addition, ICP-AES measurements confirmed that no detectable Ir and Ni quantities were observed in the supernatant.

Procedure for the light-mediated cross-coupling between potassium tert-butoxymethyltrifluoroborate and aryl bromides.

An oven-dried 10 mL vial equipped with a magnetic stir bar was charged with catalyst (1.2 mg), corresponding potassium (tert-butoxymethyl)trifluoroborate 5 (0.15 mmol) and the corresponding aryl bromide 3e (0.075 mmol). Then, 950 µL of dry acetone and 50 µL of dry MeOH were added. Finally, 2,6-lutidine (30.5 µL, 0.26 mmol) was added. The vial was closed with a rubber septum and the reaction mixture was degassed by three cycles vacuum / Ar of “freeze-pump-thaw”. Then the vial was placed on a blue light LED photoreactor (450 nm) with an Ar balloon and the reaction mixture was stirred at 25 °C. The reaction was monitored by TLC and 1H-NMR. The yield was determined by 1H-NMR using nitromethane as internal standard.

| Entry | Catalyst | Yield (%) |
|-------|----------|-----------|
| 1     | Ir,Ni@Phen-COF (1.2 mg) | 76        |
| 2     | Ni@Phen-COF (1.2 mg)    | 0         |
| 3     | Ir@Phen-COF (1.2 mg)    | 0         |
| 4     | Ni@Phen-COF (0.6 mg) and Ir@Phen-COF (0.6 mg) | 0         |
| 5     | [Ir(df(CF3)ppy)2(bpy)]PF6 (0.3 mol%) [NiCl2(phen)] (0.7 mol%) | 12        |
| 6     | Ir,Ni@Phen-COF (1.2 mg) (Dark conditions) | 0         |
| 7     | -                     | 0         |

4-(tert-butoxymethyl)benzonitrile (6) 14

1H-NMR (300 MHz, CDCl3) δ 7.62 (d, J = 8.1 Hz 2H), 7.46 (d, J = 8.0 Hz, 2H), 4.5 (s, 2H), 1.31 (s, 9H) ppm.
Procedure for the light-mediated cross-coupling between organic silicates and aryl bromides.

An oven-dried 10 mL vial equipped with a magnetic stir bar was charged with catalyst (2.5 mg), radical precursor 7 (102 mg, 0.225 mmol) and the corresponding aryl bromide 3e (27.3 mg, 0.15 mmol). Then, 3 μL of dry DMF were added. The vial was closed with a rubber septum and the reaction mixture was degassed by three cycles vacuum / Ar of “freeze-pump-thaw”. Then the vial was placed on a blue light LED photoreactor (450 nm) with an Ar balloon and the reaction mixture was stirred at 25 °C. The reaction was monitored by TLC and 1H-NMR. When total conversion was observed, the crude was filtered through membrane filter and extracted with 3 x 15 mL of diethyl ether and aqueous saturated solution of NaHCO₃. The organic phases were dried over Na₂SO₄, filtered, and evaporated under reduced pressure. The yield was determined by 1H-NMR using nitromethane as internal standard.

| Entry | Catalyst | Conversion (%) |
|-------|----------|----------------|
| 1     | Ir,Ni@Phen-COF (2.5 mg) | 92 |
| 2     | Ni@Phen-COF (2.5 mg) | 0 |
| 3     | Ir@Phen-COF (2.5 mg) | 0 |
| 4     | Ni@Phen-COF (1.2 mg) and Ir@Phen-COF (1.2 mg) | 0 |
| 5     | [Ir(dF(CF₃)ppy)₂(bpy)]PF₆ (0.3 mol%) | 26 |
|       | [NiCl₂(phen)] (0.7 mol%) | 26 |
| 6     | Ir,Ni@Phen-COF (2.5 mg) (Dark conditions) | 0 |
| 7     | - | 0 |

4-phenethylbenzonitrile (8)⁠¹⁵

$^1$H-NMR (300 MHz, CDCl₃) δ 7.54 (d, J = 7.8 Hz, 2H), 7.18-7.29 (m, 5H), 7.12 (d, J = 7.8 Hz, 2H), 2.90-2.99 (m, 4H) ppm.
Procedure for the light-mediated decarboxylative arylation of α-amino acids with aryl bromides.

An oven-dried 10 mL vial equipped with a magnetic stir bar was charged with catalyst (2.5 mg), Cs$_2$CO$_3$ (73 mg, 0.225 mmol) radical precursor 9 (48.4 mg, 0.225 mmol) and the corresponding aryl bromide 3e (27.3 mg, 0.15 mmol). Then, 4 μL of dry DMF were added. The vial was closed with a rubber septum and the reaction mixture was degassed by three cycles vacuum / Ar of “freeze-pump-thaw”. Then the vial was placed on a blue light LED photoreactor (450 nm) with an Ar balloon and the reaction mixture was stirred at 25 °C. The reaction was monitored by TLC and $^1$H-NMR. When total conversion was observed, the crude was filtered through membrane filter and extracted with 3 x 15 mL of diethyl ether and aqueous saturated solution of NaHCO$_3$. The organic phases were dried over Na$_2$SO$_4$, filtered, and evaporated under reduced pressure. The yield was determined by $^1$H-NMR using nitromethane as internal standard.

| Entry | Catalyst | Conversion (%) |
|-------|----------|----------------|
| 1     | Ir,Ni@Phen-COF (1.2 mg) | 86 |
| 2     | Ni@Phen-COF (1.2 mg) | 0 |
| 3     | Ir@Phen-COF (1.2 mg) | 0 |
| 4     | Ni@Phen-COF (0.6 mg) and Ir@Phen-COF (0.6 mg) | 0 |
| 5     | [Ir(dF(CF$_3$)ppy)$_2$(bpy)]PF$_6$ (0.3 mol%) [NiCl$_2$(phen)] (0.7 mol%) | 58 |
| 6     | Ir,Ni@Phen-COF (1.2 mg) (Dark conditions) | 0 |
| 7     | - | 0 |

**tert-butyl 2-(4-cyanophenyl)pyrrolidine-1-carboxylate (10)**

Product 10 gives two sets of NMR signals, due to the presence of rotamers on the tertiary amide moiety.

$^1$H-NMR (300 MHz, CDCl$_3$) δ 7.60 (d, $J = 8.0$ Hz, 2H), 7.28 (d, $J = 8.0$ Hz, 2H), 4.95-4.80 (m, 1H), 3.70-3.61 (m, 2H), 2.40-2.36 (m, 1H), 1.89-1.86 (m, 2H), 1.78-1.75 (m, 1H), 1.44 (s, 3H), 1.18 (s, 6H).
Benchmarking of catalytic results.

Table S4: Comparison of the catalytic outputs (TONs) reached using Ir,Ni@Phen-COF, homogeneous analogues and reported data in literature.

| Entry | Reaction | Catalyst | TON \(^{[a]}\) | REF |
|-------|----------|----------|----------------|-----|
| 1     | 2+3a     | Ir,Ni@Phen-COF | 129 (424) \(^{[b]}\) | This work |
| 2     | 2+3a     | [Ir\((\text{dF(CF}_3\text{ppy})_2(\text{bpy}))\text{PF}_6, [NiCl}_2(\text{phen})\)] | 33 | This work |
| 3     | 2+3a     | [Ir\((\text{dF(CF}_3\text{ppy})_2(\text{bpy}))\text{PF}_6, Ni(COD)$_2$/dtbpy | 30 | 3 |
| 4     | 5+3e     | Ir,Ni@Phen-COF | 109 | This work |
| 5     | 5+3e     | [Ir\((\text{dF(CF}_3\text{ppy})_2(\text{bpy}))\text{PF}_6, [NiCl}_2(\text{phen})\)] | 17 | This work |
| 6     | 5+3e     | [Ir\((\text{dF(CF}_3\text{ppy})_2(\text{bpy}))\text{PF}_6, NiCl}_2\text{glyme/dtbpy} | 30 | 17 |
| 7     | 7+3e     | Ir,Ni@Phen-COF | 131 | This work |
| 8     | 7+3e     | [Ir\((\text{dF(CF}_3\text{ppy})_2(\text{bpy}))\text{PF}_6, [NiCl}_2(\text{phen})\)] | 37 | This work |
| 9     | 7+3e     | [Ir\((\text{dF(CF}_3\text{ppy})_2(\text{bpy}))\text{PF}_6, Ni(COD)$_2$/dtbpy | 28 | 18 |
| 10    | 9+3e     | Ir,Ni@Phen-COF | 123 | This work |
| 11    | 9+3e     | [Ir\((\text{dF(CF}_3\text{ppy})_2(\text{bpy}))\text{PF}_6, [NiCl}_2(\text{phen})\)] | 82 | This work |
| 12    | 9+3e     | [Ir\((\text{dF(CF}_3\text{ppy})_2(\text{bpy}))\text{PF}_6, NiCl}_2\text{glyme/dtbpy} | 9.3 | 19 |

\(^{[a]}\) Calculated based on Ni catalyst loading. \(^{[b]}\) After 8 catalytic runs.
**PXRD Simulation**

**Table S5.** Atomistic coordinates for simulated PXRD pattern of Phen-COF.

| Atom | x/a | y/b     | z/c     | Symmetry operation |
|------|-----|---------|---------|--------------------|
| C1   | 0   | 0.1734  | -0.1048 | x, y, z            |
| C2   | 0   | 0.1805  | -0.083  | x, y, z            |
| C3   | 0   | 0.2162  | 0.0613  | x, y, z            |
| C4   | 0   | 0.2647  | 0.2067  | x, y, z            |
| C5   | 0   | 0.3189  | 0.3325  | x, y, z            |
| C6   | 0   | 0.3263  | 0.354   | x, y, z            |
| C7   | 0   | 0.2026  | 0.0201  | x, y, z            |
| C8   | 0   | 0.1938  | -0.0414 | x, y, z            |
| C9   | 0   | 0.1803  | -0.1252 | x, y, z            |
| C10  | 0   | 0.1735  | -0.0625 | x, y, z            |
| C11  | 0   | 0.2026  | 0.061   | x, y, z            |
| C12  | 0   | 0.258   | 0.2274  | x, y, z            |
| C13  | 0   | 0.3052  | 0.3327  | x, y, z            |
| C14  | 0   | 0.2008  | -0.0617 | x, y, z            |
| C15  | 0   | 0.2162  | 0.0202  | x, y, z            |
| C16  | 0   | 0.223   | 0.0406  | x, y, z            |
| C17  | 0   | 0.1941  | -0.0823 | x, y, z            |
| C18  | 0   | 0.2982  | 0.3125  | x, y, z            |
| C19  | 0   | 0.2648  | 0.2478  | x, y, z            |
| C20  | 0   | 0.2784  | 0.2069  | x, y, z            |
| C21  | 0   | 0.3254  | 0.3117  | x, y, z            |
| C22  | 0   | 0.1801  | -0.0419 | x, y, z            |
| C23  | 0   | 0.1958  | 0.0405  | x, y, z            |
| C24  | 0   | 0.3048  | 0.2917  | x, y, z            |
| C25  | 0   | 0.2784  | 0.2478  | x, y, z            |
| C26  | 0   | 0.3184  | 0.2915  | x, y, z            |
| C27  | 0   | 0.2852  | 0.2273  | x, y, z            |
| C28  | 0   | 0.347   | 0.3741  | x, y, z            |
| C29  | 0   | 0.3614  | 0.3738  | x, y, z            |
| C30  | 0   | 0.4515  | 0.3571  | x, y, z            |
| C31  | 0   | 0.4241  | 0.3563  | x, y, z            |
| C32  | 0   | 0.3889  | 0.3733  | x, y, z            |
| C33  | 0   | 0.3399  | 0.3539  | x, y, z            |
| C34  | 0   | 0.3686  | 0.3941  | x, y, z            |
| C35  | 0   | 0.4444  | 0.3773  | x, y, z            |
| C36  | 0   | 0.3819  | 0.3529  | x, y, z            |
| C37  | 0   | 0.4312  | 0.3361  | x, y, z            |
| C38  | 0   | 0.3683  | 0.3532  | x, y, z            |
| C39  | 0   | 0.4448  | 0.3365  | x, y, z            |
| C40  | 0   | 0.3822  | 0.3938  | x, y, z            |
| Symbol | Index | X   | Y   | Z   | Coordinates |
|--------|-------|-----|-----|-----|-------------|
| C41    | 0     | 0.4308 | 0.3769 |   | x, y, z     |
| C42    | 0     | 0.1598 | -0.1054 |   | x, y, z     |
| N43    | 0     | 0.2009 | -0.0205 |   | x, y, z     |
| C44    | 0     | 0.1951 | -0.001  |   | x, y, z     |
| N45    | 0     | 0.2979 | 0.2707  |   | x, y, z     |
| C46    | 0     | 0.2853 | 0.2695  |   | x, y, z     |
| N47    | 0     | 0.4029 | 0.3736  |   | x, y, z     |
| C48    | 0     | 0.4098 | 0.3553  |   | x, y, z     |
| C49    | 0     | 0.2574 | 0.1852  |   | x, y, z     |
| C50    | 0     | 0.264  | 0.1643  |   | x, y, z     |
| N51    | 0     | 0.2572 | 0.1446  |   | x, y, z     |
| C52    | 0     | 0.2439 | 0.1442  |   | x, y, z     |
| C53    | 0     | 0.2369 | 0.1648  |   | x, y, z     |
| C54    | 0     | 0.2437 | 0.1851  |   | x, y, z     |
| C55    | 0     | 0.2233 | 0.1647  |   | x, y, z     |
| C56    | 0     | 0.2165 | 0.1443  |   | x, y, z     |
| C57    | 0     | 0.2233 | 0.1239  |   | x, y, z     |
| C58    | 0     | 0.2371 | 0.1237  |   | x, y, z     |
| N59    | 0     | 0.2435 | 0.1036  |   | x, y, z     |
| C60    | 0     | 0.2371 | 0.0836  |   | x, y, z     |
| C61    | 0     | 0.2234 | 0.083   |   | x, y, z     |
| C62    | 0     | 0.2166 | 0.1035  |   | x, y, z     |
| C63    | 0     | 0.466  | 0.3575  |   | x, y, z     |
| C64    | 0     | 0.4731 | 0.3374  |   | x, y, z     |
| N65    | 0     | 0.4864 | 0.3377  |   | x, y, z     |
| C66    | 0     | 0.4932 | 0.3575  |   | x, y, z     |
| C67    | 0     | 0.4864 | 0.3782  |   | x, y, z     |
| C68    | 0     | 0.4728 | 0.378   |   | x, y, z     |
| C69    | 0     | 0.4932 | 0.3986  |   | x, y, z     |
| C49    | 0     | 0.7426 | 0.1852  |   | -x, 1-y, z  |
| C50    | 0     | 0.736  | 0.1643  |   | -x, 1-y, z  |
| N51    | 0     | 0.7428 | 0.1446  |   | -x, 1-y, z  |
| C52    | 0     | 0.7561 | 0.1442  |   | -x, 1-y, z  |
| C53    | 0     | 0.7631 | 0.1648  |   | -x, 1-y, z  |
| C54    | 0     | 0.7563 | 0.1851  |   | -x, 1-y, z  |
| C55    | 0     | 0.7767 | 0.1647  |   | -x, 1-y, z  |
| C56    | 0     | 0.7835 | 0.1443  |   | -x, 1-y, z  |
| C57    | 0     | 0.7767 | 0.1239  |   | -x, 1-y, z  |
| C58    | 0     | 0.7629 | 0.1237  |   | -x, 1-y, z  |
| N59    | 0     | 0.7565 | 0.1036  |   | -x, 1-y, z  |
| C60    | 0     | 0.763  | 0.0836  |   | -x, 1-y, z  |
| C61    | 0     | 0.7766 | 0.083   |   | -x, 1-y, z  |
| C62    | 0     | 0.7834 | 0.1035  |   | -x, 1-y, z  |
| C3     | 0     | 0.7838 | 0.0613  |   | -x, 1-y, z  |
| C7     | 0     | 0.7974 | 0.0201  |   | -x, 1-y, z  |
|   |   |   |   |
|---|---|---|---|
| C11 | 0 | 0.7974 | 0.061 | -x, 1-y, z |
| C15 | 0 | 0.7838 | 0.0202 | -x, 1-y, z |
| C23 | 0 | 0.8042 | 0.0405 | -x, 1-y, z |
| C4  | 0 | 0.7353 | 0.2067 | -x, 1-y, z |
| C12 | 0 | 0.742  | 0.2274 | -x, 1-y, z |
| C20 | 0 | 0.7216 | 0.2069 | -x, 1-y, z |
| N43 | 0 | 0.7991 | -0.0205 | -x, 1-y, z |
| C44 | 0 | 0.8049 | -0.001  | -x, 1-y, z |
| C16 | 0 | 0.777  | 0.0406  | -x, 1-y, z |
| C5  | 0 | 0.6811 | 0.3325  | -x, 1-y, z |
| C6  | 0 | 0.6737 | 0.354   | -x, 1-y, z |
| C13 | 0 | 0.6948 | 0.3327  | -x, 1-y, z |
| C21 | 0 | 0.6746 | 0.3117  | -x, 1-y, z |
| C24 | 0 | 0.6952 | 0.2917  | -x, 1-y, z |
| C25 | 0 | 0.7216 | 0.2478  | -x, 1-y, z |
| C26 | 0 | 0.6816 | 0.2915  | -x, 1-y, z |
| C27 | 0 | 0.7148 | 0.2273  | -x, 1-y, z |
| N45 | 0 | 0.7021 | 0.2707  | -x, 1-y, z |
| C46 | 0 | 0.7147 | 0.2695  | -x, 1-y, z |
| C19 | 0 | 0.7352 | 0.2478  | -x, 1-y, z |
| C1  | 0 | 0.8266 | -0.1048 | -x, 1-y, z |
| C2  | 0 | 0.8195 | -0.083  | -x, 1-y, z |
| C8  | 0 | 0.8062 | -0.0414 | -x, 1-y, z |
| C9  | 0 | 0.8197 | -0.1252 | -x, 1-y, z |
| C10 | 0 | 0.8265 | -0.0625 | -x, 1-y, z |
| C14 | 0 | 0.7992 | -0.0617 | -x, 1-y, z |
| C22 | 0 | 0.8198 | -0.0419 | -x, 1-y, z |
| C28 | 0 | 0.653  | 0.3741  | -x, 1-y, z |
| C29 | 0 | 0.6385 | 0.3738  | -x, 1-y, z |
| C32 | 0 | 0.6111 | 0.3733  | -x, 1-y, z |
| C33 | 0 | 0.6601 | 0.3539  | -x, 1-y, z |
| C34 | 0 | 0.6314 | 0.3941  | -x, 1-y, z |
| C36 | 0 | 0.6181 | 0.3529  | -x, 1-y, z |
| C38 | 0 | 0.6318 | 0.3532  | -x, 1-y, z |
| C40 | 0 | 0.6178 | 0.3938  | -x, 1-y, z |
| C18 | 0 | 0.7018 | 0.3125  | -x, 1-y, z |
| C17 | 0 | 0.8059 | -0.0823 | -x, 1-y, z |
| C42 | 0 | 0.8402 | -0.1054 | -x, 1-y, z |
| N47 | 0 | 0.5971 | 0.3736  | -x, 1-y, z |
| C48 | 0 | 0.5901 | 0.3553  | -x, 1-y, z |
| C30 | 0 | 0.5485 | 0.3571  | -x, 1-y, z |
| C31 | 0 | 0.5759 | 0.3563  | -x, 1-y, z |
| C35 | 0 | 0.5556 | 0.3773  | -x, 1-y, z |
| C37 | 0 | 0.5688 | 0.3361  | -x, 1-y, z |
| C39 | 0 | 0.5552 | 0.3365  | -x, 1-y, z |
| C41 | 0  | 0.5692 | 0.3769 | -x, 1-y, z |
|-----|----|--------|--------|------------|
| C63 | 0  | 0.534  | 0.3575 | -x, 1-y, z |
| C64 | 0  | 0.5269 | 0.3374 | -x, 1-y, z |
| N65 | 0  | 0.5136 | 0.3377 | -x, 1-y, z |
| C66 | 0  | 0.5068 | 0.3575 | -x, 1-y, z |
| C67 | 0  | 0.5136 | 0.3782 | -x, 1-y, z |
| C68 | 0  | 0.5272 | 0.378  | -x, 1-y, z |
| C69 | 0  | 0.5068 | 0.3986 | -x, 1-y, z |
| C6  | 0  | 0.8263 | -0.146 | x, 1/2+y, -1/2+z |
| C6  | 0  | 0.1737 | -0.146 | x, 1/2+y, -1/2+z |
| C9  | 0  | 0.6803 | 0.3748 | x, 1/2+y, 1/2+z |
| C9  | 0  | 0.3197 | 0.3748 | -x, 1/2-y, 1/2+z |
| C28 | 0  | 0.847  | -0.1259| x, 1/2+y, -1/2+z |
| C28 | 0  | 0.153  | -0.1259| -x, 1/2-y, -1/2+z |
| C42 | 0  | 0.6598 | 0.3946 | x, 1/2+y, 1/2+z |
| C42 | 0  | 0.3402 | 0.3946 | -x, 1/2-y, 1/2+z |
| C1  | 0  | -0.3266| 0.3952 | x, -1/2+y, 1/2+z |
| C2  | 0  | -0.3195| 0.417  | x, -1/2+y, 1/2+z |
| C3  | 0  | -0.2838| 0.5613 | x, -1/2+y, 1/2+z |
| C4  | 0  | -0.2353| 0.7067 | x, -1/2+y, 1/2+z |
| C5  | 0  | -0.1811| 0.8325 | x, -1/2+y, 1/2+z |
| C6  | 0  | -0.1737| 0.854  | x, -1/2+y, 1/2+z |
| C7  | 0  | -0.2974| 0.5201 | x, -1/2+y, 1/2+z |
| C8  | 0  | -0.3062| 0.4586 | x, -1/2+y, 1/2+z |
| C9  | 0  | -0.3197| 0.3748 | x, -1/2+y, 1/2+z |
| C10 | 0  | -0.3265| 0.4375 | x, -1/2+y, 1/2+z |
| C11 | 0  | -0.2974| 0.561  | x, -1/2+y, 1/2+z |
| C12 | 0  | -0.242 | 0.7274 | x, -1/2+y, 1/2+z |
| C13 | 0  | -0.1948| 0.8327 | x, -1/2+y, 1/2+z |
| C14 | 0  | -0.2992| 0.4383 | x, -1/2+y, 1/2+z |
| C15 | 0  | -0.2838| 0.5202 | x, -1/2+y, 1/2+z |
| C16 | 0  | -0.277 | 0.5406 | x, -1/2+y, 1/2+z |
| C17 | 0  | -0.3059| 0.4177 | x, -1/2+y, 1/2+z |
| C18 | 0  | -0.2018| 0.8125 | x, -1/2+y, 1/2+z |
| C19 | 0  | -0.2352| 0.7478 | x, -1/2+y, 1/2+z |
| C20 | 0  | -0.2216| 0.7069 | x, -1/2+y, 1/2+z |
| C21 | 0  | -0.1746| 0.8117 | x, -1/2+y, 1/2+z |
| C22 | 0  | -0.3199| 0.4581 | x, -1/2+y, 1/2+z |
| C23 | 0  | -0.3042| 0.5405 | x, -1/2+y, 1/2+z |
| C24 | 0  | -0.1952| 0.7917 | x, -1/2+y, 1/2+z |
| C25 | 0  | -0.2216| 0.7478 | x, -1/2+y, 1/2+z |
| C26 | 0  | -0.1816| 0.7915 | x, -1/2+y, 1/2+z |
| C27 | 0  | -0.2148| 0.7273 | x, -1/2+y, 1/2+z |
| C28 | 0  | -0.153 | 0.8741 | x, -1/2+y, 1/2+z |
| C29 | 0  | -0.1386| 0.8738 | x, -1/2+y, 1/2+z |
| C30  | 0  | -0.0485 | 0.8571 | x, -1/2+y, 1/2+z |
|------|----|---------|--------|-----------------|
| C31  | 0  | -0.0759 | 0.8563 | x, -1/2+y, 1/2+z |
| C32  | 0  | -0.1111 | 0.8733 | x, -1/2+y, 1/2+z |
| C33  | 0  | -0.1601 | 0.8539 | x, -1/2+y, 1/2+z |
| C34  | 0  | -0.1314 | 0.8941 | x, -1/2+y, 1/2+z |
| C35  | 0  | -0.0556 | 0.8773 | x, -1/2+y, 1/2+z |
| C36  | 0  | -0.1181 | 0.8529 | x, -1/2+y, 1/2+z |
| C37  | 0  | -0.0688 | 0.8361 | x, -1/2+y, 1/2+z |
| C38  | 0  | -0.1317 | 0.8532 | x, -1/2+y, 1/2+z |
| C39  | 0  | -0.0552 | 0.8365 | x, -1/2+y, 1/2+z |
| C40  | 0  | -0.1178 | 0.8938 | x, -1/2+y, 1/2+z |
| C41  | 0  | -0.0692 | 0.8769 | x, -1/2+y, 1/2+z |
| C42  | 0  | -0.3402 | 0.3946 | x, -1/2+y, 1/2+z |
| N43  | 0  | -0.2991 | 0.4795 | x, -1/2+y, 1/2+z |
| C44  | 0  | -0.3049 | 0.499  | x, -1/2+y, 1/2+z |
| N45  | 0  | -0.2021 | 0.7707 | x, -1/2+y, 1/2+z |
| C46  | 0  | -0.2147 | 0.7695 | x, -1/2+y, 1/2+z |
| N47  | 0  | -0.0971 | 0.8736 | x, -1/2+y, 1/2+z |
| C48  | 0  | -0.0902 | 0.8553 | x, -1/2+y, 1/2+z |
| C49  | 0  | -0.2426 | 0.6852 | x, -1/2+y, 1/2+z |
| C50  | 0  | -0.236  | 0.6643 | x, -1/2+y, 1/2+z |
| N51  | 0  | -0.2428 | 0.6446 | x, -1/2+y, 1/2+z |
| C52  | 0  | -0.2561 | 0.6442 | x, -1/2+y, 1/2+z |
| C53  | 0  | -0.2631 | 0.6648 | x, -1/2+y, 1/2+z |
| C54  | 0  | -0.2563 | 0.6851 | x, -1/2+y, 1/2+z |
| C55  | 0  | -0.2767 | 0.6647 | x, -1/2+y, 1/2+z |
| C56  | 0  | -0.2835 | 0.6443 | x, -1/2+y, 1/2+z |
| C57  | 0  | -0.2767 | 0.6239 | x, -1/2+y, 1/2+z |
| C58  | 0  | -0.2629 | 0.6237 | x, -1/2+y, 1/2+z |
| N59  | 0  | -0.2565 | 0.6036 | x, -1/2+y, 1/2+z |
| C60  | 0  | -0.263  | 0.5836 | x, -1/2+y, 1/2+z |
| C61  | 0  | -0.2766 | 0.583  | x, -1/2+y, 1/2+z |
| C62  | 0  | -0.2834 | 0.6035 | x, -1/2+y, 1/2+z |
| C63  | 0  | -0.034  | 0.8575 | x, -1/2+y, 1/2+z |
| C64  | 0  | -0.0269 | 0.8374 | x, -1/2+y, 1/2+z |
| N65  | 0  | -0.0136 | 0.8377 | x, -1/2+y, 1/2+z |
| C66  | 0  | -0.0068 | 0.8575 | x, -1/2+y, 1/2+z |
| C67  | 0  | -0.0136 | 0.8782 | x, -1/2+y, 1/2+z |
| C68  | 0  | -0.0272 | 0.878  | x, -1/2+y, 1/2+z |
| C69  | 0  | -0.0068 | 0.8986 | x, -1/2+y, 1/2+z |
| C49  | 0  | 0.2426  | 0.6852 | -x, 1/2-y, 1/2+z |
| C50  | 0  | 0.236   | 0.6643 | -x, 1/2-y, 1/2+z |
| N51  | 0  | 0.2428  | 0.6446 | -x, 1/2-y, 1/2+z |
| C52  | 0  | 0.2561  | 0.6442 | -x, 1/2-y, 1/2+z |
| C53  | 0  | 0.2631  | 0.6648 | -x, 1/2-y, 1/2+z |
| #  | x   | y   | z   | Coordinates                  |
|----|-----|-----|-----|------------------------------|
| C54| 0   | 0.2563 | 0.6851 | -x, 1/2-y, 1/2+z |
| C55| 0   | 0.2767 | 0.6647 | -x, 1/2-y, 1/2+z |
| C56| 0   | 0.2835 | 0.6443 | -x, 1/2-y, 1/2+z |
| C57| 0   | 0.2767 | 0.6239 | -x, 1/2-y, 1/2+z |
| C58| 0   | 0.2629 | 0.6237 | -x, 1/2-y, 1/2+z |
| N59| 0   | 0.2565 | 0.6036 | -x, 1/2-y, 1/2+z |
| C60| 0   | 0.263  | 0.5836 | -x, 1/2-y, 1/2+z |
| C61| 0   | 0.2766 | 0.583  | -x, 1/2-y, 1/2+z |
| C62| 0   | 0.2834 | 0.6035 | -x, 1/2-y, 1/2+z |
| C3 | 0   | 0.2838 | 0.5613 | -x, 1/2-y, 1/2+z |
| C7 | 0   | 0.2974 | 0.5201 | -x, 1/2-y, 1/2+z |
| C11| 0   | 0.2974 | 0.561  | -x, 1/2-y, 1/2+z |
| C15| 0   | 0.2838 | 0.5202 | -x, 1/2-y, 1/2+z |
| C23| 0   | 0.3042 | 0.5405 | -x, 1/2-y, 1/2+z |
| C4 | 0   | 0.2353 | 0.7067 | -x, 1/2-y, 1/2+z |
| C12| 0   | 0.242  | 0.7274 | -x, 1/2-y, 1/2+z |
| C20| 0   | 0.2216 | 0.7069 | -x, 1/2-y, 1/2+z |
| N43| 0   | 0.2991 | 0.4795 | -x, 1/2-y, 1/2+z |
| C44| 0   | 0.3049 | 0.499  | -x, 1/2-y, 1/2+z |
| C16| 0   | 0.277  | 0.5406 | -x, 1/2-y, 1/2+z |
| C5 | 0   | 0.1811 | 0.8325 | -x, 1/2-y, 1/2+z |
| C6 | 0   | 0.1737 | 0.854  | -x, 1/2-y, 1/2+z |
| C13| 0   | 0.1948 | 0.8327 | -x, 1/2-y, 1/2+z |
| C21| 0   | 0.1746 | 0.8117 | -x, 1/2-y, 1/2+z |
| C24| 0   | 0.1952 | 0.7917 | -x, 1/2-y, 1/2+z |
| C25| 0   | 0.2216 | 0.7478 | -x, 1/2-y, 1/2+z |
| C26| 0   | 0.1816 | 0.7915 | -x, 1/2-y, 1/2+z |
| C27| 0   | 0.2148 | 0.7273 | -x, 1/2-y, 1/2+z |
| N45| 0   | 0.2021 | 0.7707 | -x, 1/2-y, 1/2+z |
| C46| 0   | 0.2147 | 0.7695 | -x, 1/2-y, 1/2+z |
| C19| 0   | 0.2352 | 0.7478 | -x, 1/2-y, 1/2+z |
| C1 | 0   | 0.3266 | 0.3952 | -x, 1/2-y, 1/2+z |
| C2 | 0   | 0.3195 | 0.417  | -x, 1/2-y, 1/2+z |
| C8 | 0   | 0.3062 | 0.4586 | -x, 1/2-y, 1/2+z |
| C10| 0   | 0.3265 | 0.4375 | -x, 1/2-y, 1/2+z |
| C14| 0   | 0.2992 | 0.4383 | -x, 1/2-y, 1/2+z |
| C22| 0   | 0.3198 | 0.4581 | -x, 1/2-y, 1/2+z |
| C28| 0   | 0.153  | 0.8741 | -x, 1/2-y, 1/2+z |
| C29| 0   | 0.1385 | 0.8738 | -x, 1/2-y, 1/2+z |
| C32| 0   | 0.1111 | 0.8733 | -x, 1/2-y, 1/2+z |
| C33| 0   | 0.1601 | 0.8539 | -x, 1/2-y, 1/2+z |
| C34| 0   | 0.1314 | 0.8941 | -x, 1/2-y, 1/2+z |
| C36| 0   | 0.1181 | 0.8529 | -x, 1/2-y, 1/2+z |
| C38| 0   | 0.1318 | 0.8532 | -x, 1/2-y, 1/2+z |
| C40| 0   | 0.1178 | 0.8938 | -x, 1/2-y, 1/2+z |
| Symbol | x  | y  | z   | Coordinates          |
|--------|----|----|-----|----------------------|
| C18    | 0  | 0.2018 | 0.8125 | -x, 1/2-y, 1/2+z     |
| C17    | 0  | 0.3059 | 0.4177 | -x, 1/2-y, 1/2+z     |
| N47    | 0  | 0.0971 | 0.8736 | -x, 1/2-y, 1/2+z     |
| C48    | 0  | 0.0901 | 0.8553 | -x, 1/2-y, 1/2+z     |
| C30    | 0  | 0.0485 | 0.8571 | -x, 1/2-y, 1/2+z     |
| C31    | 0  | 0.0759 | 0.8563 | -x, 1/2-y, 1/2+z     |
| C35    | 0  | 0.0556 | 0.8773 | -x, 1/2-y, 1/2+z     |
| C37    | 0  | 0.0688 | 0.8361 | -x, 1/2-y, 1/2+z     |
| C39    | 0  | 0.0552 | 0.8365 | -x, 1/2-y, 1/2+z     |
| C41    | 0  | 0.0692 | 0.8769 | -x, 1/2-y, 1/2+z     |
| C63    | 0  | 0.034  | 0.8575 | -x, 1/2-y, 1/2+z     |
| C64    | 0  | 0.0269 | 0.8374 | -x, 1/2-y, 1/2+z     |
| N65    | 0  | 0.0136 | 0.8377 | -x, 1/2-y, 1/2+z     |
| C66    | 0  | 0.0068 | 0.8575 | -x, 1/2-y, 1/2+z     |
| C67    | 0  | 0.0136 | 0.8782 | -x, 1/2-y, 1/2+z     |
| C68    | 0  | 0.0272 | 0.878  | -x, 1/2-y, 1/2+z     |
| C69    | 0  | 0.0068 | 0.8986 | -x, 1/2-y, 1/2+z     |
| C6    | 0  | -0.3263 | 0.354  | -x, -y, z            |
| C9     | 0  | 0.1803 | 0.8748 | x, y, 1+z            |
| C9     | 0  | -0.1803 | 0.8748 | -x, -y, 1+z          |
| C28    | 0  | -0.347 | 0.3741 | -x, -y, z            |
| C42    | 0  | 0.1598 | 0.8946 | x, y, 1+z            |
| C42    | 0  | -0.1598 | 0.8946 | -x, -y, 1+z          |
| C1     | 0  | 0.6734 | 0.3952 | x, 1/2+y, 1/2+z      |
| C2     | 0  | 0.6805 | 0.417  | x, 1/2+y, 1/2+z      |
| C3     | 0  | 0.7162 | 0.5613 | x, 1/2+y, 1/2+z      |
| C4     | 0  | 0.7647 | 0.7067 | x, 1/2+y, 1/2+z      |
| C5     | 0  | 0.8189 | 0.8325 | x, 1/2+y, 1/2+z      |
| C6     | 0  | 0.8263 | 0.854  | x, 1/2+y, 1/2+z      |
| C7     | 0  | 0.7026 | 0.5201 | x, 1/2+y, 1/2+z      |
| C8     | 0  | 0.6938 | 0.4586 | x, 1/2+y, 1/2+z      |
| C10    | 0  | 0.6735 | 0.4375 | x, 1/2+y, 1/2+z      |
| C11    | 0  | 0.7026 | 0.561  | x, 1/2+y, 1/2+z      |
| C12    | 0  | 0.758  | 0.7274 | x, 1/2+y, 1/2+z      |
| C13    | 0  | 0.8052 | 0.8327 | x, 1/2+y, 1/2+z      |
| C14    | 0  | 0.7008 | 0.4383 | x, 1/2+y, 1/2+z      |
| C15    | 0  | 0.7162 | 0.5202 | x, 1/2+y, 1/2+z      |
| C16    | 0  | 0.723  | 0.5406 | x, 1/2+y, 1/2+z      |
| C17    | 0  | 0.6941 | 0.4177 | x, 1/2+y, 1/2+z      |
| C18    | 0  | 0.7982 | 0.8125 | x, 1/2+y, 1/2+z      |
| C19    | 0  | 0.7648 | 0.7478 | x, 1/2+y, 1/2+z      |
| C20    | 0  | 0.7784 | 0.7069 | x, 1/2+y, 1/2+z      |
| C21    | 0  | 0.8254 | 0.8117 | x, 1/2+y, 1/2+z      |
| C22    | 0  | 0.6802 | 0.4581 | x, 1/2+y, 1/2+z      |
| C23    | 0  | 0.6958 | 0.5405 | x, 1/2+y, 1/2+z      |
| C24 | 0  | 0.8048 | 0.7917 | x, 1/2+y, 1/2+z |
|-----|----|--------|--------|-----------------|
| C25 | 0  | 0.7784 | 0.7478 | x, 1/2+y, 1/2+z |
| C26 | 0  | 0.8184 | 0.7915 | x, 1/2+y, 1/2+z |
| C27 | 0  | 0.7852 | 0.7273 | x, 1/2+y, 1/2+z |
| C28 | 0  | 0.8470 | 0.8741 | x, 1/2+y, 1/2+z |
| C29 | 0  | 0.8615 | 0.8738 | x, 1/2+y, 1/2+z |
| C30 | 0  | 0.9515 | 0.8571 | x, 1/2+y, 1/2+z |
| C31 | 0  | 0.9241 | 0.8563 | x, 1/2+y, 1/2+z |
| C32 | 0  | 0.8889 | 0.8733 | x, 1/2+y, 1/2+z |
| C33 | 0  | 0.8399 | 0.8539 | x, 1/2+y, 1/2+z |
| C34 | 0  | 0.8686 | 0.8941 | x, 1/2+y, 1/2+z |
| C35 | 0  | 0.9444 | 0.8773 | x, 1/2+y, 1/2+z |
| C36 | 0  | 0.8819 | 0.8529 | x, 1/2+y, 1/2+z |
| C37 | 0  | 0.9312 | 0.8361 | x, 1/2+y, 1/2+z |
| C38 | 0  | 0.8682 | 0.8532 | x, 1/2+y, 1/2+z |
| C39 | 0  | 0.9448 | 0.8365 | x, 1/2+y, 1/2+z |
| C40 | 0  | 0.8822 | 0.8938 | x, 1/2+y, 1/2+z |
| C41 | 0  | 0.9308 | 0.8769 | x, 1/2+y, 1/2+z |
| N43 | 0  | 0.7009 | 0.4795 | x, 1/2+y, 1/2+z |
| C44 | 0  | 0.6951 | 0.4990 | x, 1/2+y, 1/2+z |
| N45 | 0  | 0.7979 | 0.7707 | x, 1/2+y, 1/2+z |
| C46 | 0  | 0.7853 | 0.7695 | x, 1/2+y, 1/2+z |
| N47 | 0  | 0.9029 | 0.8736 | x, 1/2+y, 1/2+z |
| C48 | 0  | 0.9099 | 0.8553 | x, 1/2+y, 1/2+z |
| C49 | 0  | 0.7574 | 0.6852 | x, 1/2+y, 1/2+z |
| C50 | 0  | 0.7640 | 0.6643 | x, 1/2+y, 1/2+z |
| N51 | 0  | 0.7572 | 0.6446 | x, 1/2+y, 1/2+z |
| C52 | 0  | 0.7439 | 0.6442 | x, 1/2+y, 1/2+z |
| C53 | 0  | 0.7369 | 0.6648 | x, 1/2+y, 1/2+z |
| C54 | 0  | 0.7437 | 0.6851 | x, 1/2+y, 1/2+z |
| C55 | 0  | 0.7233 | 0.6647 | x, 1/2+y, 1/2+z |
| C56 | 0  | 0.7165 | 0.6443 | x, 1/2+y, 1/2+z |
| C57 | 0  | 0.7233 | 0.6239 | x, 1/2+y, 1/2+z |
| C58 | 0  | 0.7371 | 0.6237 | x, 1/2+y, 1/2+z |
| N59 | 0  | 0.7435 | 0.6036 | x, 1/2+y, 1/2+z |
| C60 | 0  | 0.737  | 0.5836 | x, 1/2+y, 1/2+z |
| C61 | 0  | 0.7234 | 0.583  | x, 1/2+y, 1/2+z |
| C62 | 0  | 0.7166 | 0.6035 | x, 1/2+y, 1/2+z |
| C63 | 0  | 0.966  | 0.8575 | x, 1/2+y, 1/2+z |
| C64 | 0  | 0.9731 | 0.8374 | x, 1/2+y, 1/2+z |
| N65 | 0  | 0.9864 | 0.8377 | x, 1/2+y, 1/2+z |
| C66 | 0  | 0.9932 | 0.8575 | x, 1/2+y, 1/2+z |
| C67 | 0  | 0.9864 | 0.8782 | x, 1/2+y, 1/2+z |
| C68 | 0  | 0.9728 | 0.878  | x, 1/2+y, 1/2+z |
| C69 | 0  | 0.9932 | 0.8986 | x, 1/2+y, 1/2+z |
| C49 | 0  | 1.2426 | 0.6852 | -x, 1.5-y, 1/2+z |
|-----|----|--------|--------|------------------|
| C50 | 0  | 1.2361 | 0.6643 | -x, 1.5-y, 1/2+z |
| N51 | 0  | 1.2428 | 0.6446 | -x, 1.5-y, 1/2+z |
| C52 | 0  | 1.2561 | 0.6442 | -x, 1.5-y, 1/2+z |
| C53 | 0  | 1.2631 | 0.6648 | -x, 1.5-y, 1/2+z |
| C54 | 0  | 1.2563 | 0.6851 | -x, 1.5-y, 1/2+z |
| C55 | 0  | 1.2767 | 0.6647 | -x, 1.5-y, 1/2+z |
| C56 | 0  | 1.2835 | 0.6443 | -x, 1.5-y, 1/2+z |
| C57 | 0  | 1.2767 | 0.6239 | -x, 1.5-y, 1/2+z |
| C58 | 0  | 1.2629 | 0.6237 | -x, 1.5-y, 1/2+z |
| N59 | 0  | 1.2565 | 0.6036 | -x, 1.5-y, 1/2+z |
| C60 | 0  | 1.263  | 0.5836 | -x, 1.5-y, 1/2+z |
| C61 | 0  | 1.2766 | 0.583  | -x, 1.5-y, 1/2+z |
| C62 | 0  | 1.2834 | 0.6035 | -x, 1.5-y, 1/2+z |
| C3  | 0  | 1.2838 | 0.5613 | -x, 1.5-y, 1/2+z |
| C7  | 0  | 1.2974 | 0.5201 | -x, 1.5-y, 1/2+z |
| C11 | 0  | 1.2974 | 0.561  | -x, 1.5-y, 1/2+z |
| C15 | 0  | 1.2838 | 0.5202 | -x, 1.5-y, 1/2+z |
| C23 | 0  | 1.3042 | 0.5405 | -x, 1.5-y, 1/2+z |
| C4  | 0  | 1.2353 | 0.7067 | -x, 1.5-y, 1/2+z |
| C12 | 0  | 1.242  | 0.7274 | -x, 1.5-y, 1/2+z |
| C20 | 0  | 1.2216 | 0.7069 | -x, 1.5-y, 1/2+z |
| N43 | 0  | 1.2991 | 0.4795 | -x, 1.5-y, 1/2+z |
| C44 | 0  | 1.3049 | 0.499  | -x, 1.5-y, 1/2+z |
| C16 | 0  | 1.277  | 0.5406 | -x, 1.5-y, 1/2+z |
| C5  | 0  | 1.1811 | 0.8325 | -x, 1.5-y, 1/2+z |
| C6  | 0  | 1.1738 | 0.854  | -x, 1.5-y, 1/2+z |
| C13 | 0  | 1.1948 | 0.8327 | -x, 1.5-y, 1/2+z |
| C21 | 0  | 1.1745 | 0.8117 | -x, 1.5-y, 1/2+z |
| C24 | 0  | 1.1952 | 0.7917 | -x, 1.5-y, 1/2+z |
| C25 | 0  | 1.2216 | 0.7478 | -x, 1.5-y, 1/2+z |
| C26 | 0  | 1.1816 | 0.7915 | -x, 1.5-y, 1/2+z |
| C27 | 0  | 1.2148 | 0.7273 | -x, 1.5-y, 1/2+z |
| N45 | 0  | 1.2021 | 0.7707 | -x, 1.5-y, 1/2+z |
| C46 | 0  | 1.2147 | 0.7695 | -x, 1.5-y, 1/2+z |
| C19 | 0  | 1.2352 | 0.7478 | -x, 1.5-y, 1/2+z |
| C1  | 0  | 1.3266 | 0.3952 | -x, 1.5-y, 1/2+z |
| C2  | 0  | 1.3195 | 0.417  | -x, 1.5-y, 1/2+z |
| C8  | 0  | 1.3062 | 0.4586 | -x, 1.5-y, 1/2+z |
| C9  | 0  | 1.3197 | 0.3748 | -x, 1.5-y, 1/2+z |
| C10 | 0  | 1.3264 | 0.4375 | -x, 1.5-y, 1/2+z |
| C14 | 0  | 1.2992 | 0.4383 | -x, 1.5-y, 1/2+z |
| C22 | 0  | 1.3198 | 0.4581 | -x, 1.5-y, 1/2+z |
| C28 | 0  | 1.153  | 0.8741 | -x, 1.5-y, 1/2+z |
| C29 | 0  | 1.1385 | 0.8738 | -x, 1.5-y, 1/2+z |
|   |   |   |   |   |
|---|---|---|---|---|
| C32 | 0 | 1.1111 | 0.8733 | -x, 1.5-y, 1/2+z |
| C33 | 0 | 1.1601 | 0.8539 | -x, 1.5-y, 1/2+z |
| C34 | 0 | 1.1314 | 0.8941 | -x, 1.5-y, 1/2+z |
| C36 | 0 | 1.1181 | 0.8529 | -x, 1.5-y, 1/2+z |
| C38 | 0 | 1.1318 | 0.8532 | -x, 1.5-y, 1/2+z |
| C40 | 0 | 1.1178 | 0.8938 | -x, 1.5-y, 1/2+z |
| C18 | 0 | 1.2018 | 0.8125 | -x, 1.5-y, 1/2+z |
| C17 | 0 | 1.3059 | 0.4177 | -x, 1.5-y, 1/2+z |
| C42 | 0 | 1.3402 | 0.3946 | -x, 1.5-y, 1/2+z |
| N47 | 0 | 1.0971 | 0.8736 | -x, 1.5-y, 1/2+z |
| C48 | 0 | 1.0901 | 0.8553 | -x, 1.5-y, 1/2+z |
| C30 | 0 | 1.0485 | 0.8571 | -x, 1.5-y, 1/2+z |
| C31 | 0 | 1.0759 | 0.8563 | -x, 1.5-y, 1/2+z |
| C35 | 0 | 1.0556 | 0.8773 | -x, 1.5-y, 1/2+z |
| C37 | 0 | 1.0688 | 0.8361 | -x, 1.5-y, 1/2+z |
| C39 | 0 | 1.0552 | 0.8365 | -x, 1.5-y, 1/2+z |
| C41 | 0 | 1.0692 | 0.8769 | -x, 1.5-y, 1/2+z |
| C63 | 0 | 1.034 | 0.8575 | -x, 1.5-y, 1/2+z |
| C64 | 0 | 1.0269 | 0.8374 | -x, 1.5-y, 1/2+z |
| N65 | 0 | 1.0136 | 0.8377 | -x, 1.5-y, 1/2+z |
| C66 | 0 | 1.0068 | 0.8575 | -x, 1.5-y, 1/2+z |
| C67 | 0 | 1.0136 | 0.8782 | -x, 1.5-y, 1/2+z |
| C68 | 0 | 1.0272 | 0.878 | -x, 1.5-y, 1/2+z |
| C69 | 0 | 1.0068 | 0.8986 | -x, 1.5-y, 1/2+z |
| C6 | 0 | 1.3262 | 0.354 | x, 1+y, z |
| C9 | 0 | 1.1803 | 0.8748 | x, 1+y, 1+z |
| C9 | 0 | 0.8197 | 0.8748 | -x, 1-y, 1+z |
| C28 | 0 | 1.347 | 0.3741 | x, 1+y, z |
| C42 | 0 | 1.1598 | 0.8946 | x, 1+y, 1+z |
| C42 | 0 | 0.8402 | 0.8946 | -x, 1-y, 1+z |
| C1 | 1 | 0.1734 | -0.1048 | 1+x, y, z |
| C2 | 1 | 0.1805 | -0.083 | 1+x, y, z |
| C3 | 1 | 0.2162 | 0.0613 | 1+x, y, z |
| C4 | 1 | 0.2647 | 0.2067 | 1+x, y, z |
| C5 | 1 | 0.3189 | 0.3325 | 1+x, y, z |
| C6 | 1 | 0.3263 | 0.354 | 1+x, y, z |
| C7 | 1 | 0.2026 | 0.0201 | 1+x, y, z |
| C8 | 1 | 0.1938 | -0.0414 | 1+x, y, z |
| C9 | 1 | 0.1803 | -0.1252 | 1+x, y, z |
| C10 | 1 | 0.1735 | -0.0625 | 1+x, y, z |
| C11 | 1 | 0.2026 | 0.061 | 1+x, y, z |
| C12 | 1 | 0.258 | 0.2274 | 1+x, y, z |
| C13 | 1 | 0.3052 | 0.3327 | 1+x, y, z |
| C14 | 1 | 0.2008 | -0.0617 | 1+x, y, z |
| C15 | 1 | 0.2162 | 0.0202 | 1+x, y, z |
| C16 | 1 | 0.223 | 0.0406 | 1+x, y, z |
| C17 | 1 | 0.1941 | -0.0823 | 1+x, y, z |
| C18 | 1 | 0.2982 | 0.3125 | 1+x, y, z |
| C19 | 1 | 0.2648 | 0.2478 | 1+x, y, z |
| C20 | 1 | 0.2784 | 0.2069 | 1+x, y, z |
| C21 | 1 | 0.3254 | 0.3117 | 1+x, y, z |
| C22 | 1 | 0.1801 | -0.0419 | 1+x, y, z |
| C23 | 1 | 0.1958 | 0.0405 | 1+x, y, z |
| C24 | 1 | 0.2982 | 0.3125 | 1+x, y, z |
| C25 | 1 | 0.2784 | 0.2478 | 1+x, y, z |
| C26 | 1 | 0.3184 | 0.2915 | 1+x, y, z |
| C27 | 1 | 0.2852 | 0.2273 | 1+x, y, z |
| C28 | 1 | 0.347 | 0.3741 | 1+x, y, z |
| C29 | 1 | 0.3614 | 0.3738 | 1+x, y, z |
| C30 | 1 | 0.4515 | 0.3571 | 1+x, y, z |
| C31 | 1 | 0.4241 | 0.3563 | 1+x, y, z |
| C32 | 1 | 0.3889 | 0.3733 | 1+x, y, z |
| C33 | 1 | 0.3399 | 0.3539 | 1+x, y, z |
| C34 | 1 | 0.3686 | 0.3941 | 1+x, y, z |
| C35 | 1 | 0.4444 | 0.3773 | 1+x, y, z |
| C36 | 1 | 0.3819 | 0.3529 | 1+x, y, z |
| C37 | 1 | 0.4312 | 0.3361 | 1+x, y, z |
| C38 | 1 | 0.3683 | 0.3532 | 1+x, y, z |
| C39 | 1 | 0.4448 | 0.3365 | 1+x, y, z |
| C40 | 1 | 0.3822 | 0.3938 | 1+x, y, z |
| C41 | 1 | 0.4308 | 0.3769 | 1+x, y, z |
| C42 | 1 | 0.1598 | -0.1054 | 1+x, y, z |
| N43 | 1 | 0.2009 | -0.0205 | 1+x, y, z |
| C44 | 1 | 0.1951 | -0.001 | 1+x, y, z |
| N45 | 1 | 0.2979 | 0.2707 | 1+x, y, z |
| C46 | 1 | 0.2853 | 0.2695 | 1+x, y, z |
| N47 | 1 | 0.4029 | 0.3736 | 1+x, y, z |
| C48 | 1 | 0.4098 | 0.3553 | 1+x, y, z |
| C49 | 1 | 0.2574 | 0.1852 | 1+x, y, z |
| C50 | 1 | 0.264 | 0.1643 | 1+x, y, z |
| N51 | 1 | 0.2572 | 0.1446 | 1+x, y, z |
| C52 | 1 | 0.2439 | 0.1442 | 1+x, y, z |
| C53 | 1 | 0.2369 | 0.1648 | 1+x, y, z |
| C54 | 1 | 0.2437 | 0.1851 | 1+x, y, z |
| C55 | 1 | 0.2233 | 0.1647 | 1+x, y, z |
| C56 | 1 | 0.2165 | 0.1443 | 1+x, y, z |
| C57 | 1 | 0.2233 | 0.1239 | 1+x, y, z |
| C58 | 1 | 0.2371 | 0.1237 | 1+x, y, z |
| N59 | 1 | 0.2435 | 0.1036 | 1+x, y, z |
| C60 | 1 | 0.2371 | 0.0836 | 1+x, y, z |
|   |   |   |   |
|---|---|---|---|
| C61 | 1 | 0.2234 | 0.083 | 1+x, y, z |
| C62 | 1 | 0.2166 | 0.1035 | 1+x, y, z |
| C63 | 1 | 0.4660 | 0.3575 | 1+x, y, z |
| C64 | 1 | 0.4731 | 0.3374 | 1+x, y, z |
| N65 | 1 | 0.4864 | 0.3377 | 1+x, y, z |
| C66 | 1 | 0.4932 | 0.3575 | 1+x, y, z |
| C67 | 1 | 0.4864 | 0.3782 | 1+x, y, z |
| C68 | 1 | 0.4728 | 0.3780 | 1+x, y, z |
| C69 | 1 | 0.4932 | 0.3986 | 1+x, y, z |
| C70 | 1 | 0.7363 | 0.1643 | 1-x, 1-y, z |
| N51 | 1 | 0.7426 | 0.1852 | 1-x, 1-y, z |
| C52 | 1 | 0.7561 | 0.1442 | 1-x, 1-y, z |
| C53 | 1 | 0.7631 | 0.1648 | 1-x, 1-y, z |
| C54 | 1 | 0.7563 | 0.1851 | 1-x, 1-y, z |
| C55 | 1 | 0.7767 | 0.1647 | 1-x, 1-y, z |
| C56 | 1 | 0.7835 | 0.1443 | 1-x, 1-y, z |
| C57 | 1 | 0.7767 | 0.1239 | 1-x, 1-y, z |
| C58 | 1 | 0.7629 | 0.1237 | 1-x, 1-y, z |
| N59 | 1 | 0.7565 | 0.1036 | 1-x, 1-y, z |
| C60 | 1 | 0.7630 | 0.0836 | 1-x, 1-y, z |
| C61 | 1 | 0.7766 | 0.0830 | 1-x, 1-y, z |
| C62 | 1 | 0.7834 | 0.1035 | 1-x, 1-y, z |
| C3  | 1 | 0.7838 | 0.0613 | 1-x, 1-y, z |
| C7  | 1 | 0.7974 | 0.0201 | 1-x, 1-y, z |
| C11 | 1 | 0.7974 | 0.0610 | 1-x, 1-y, z |
| C15 | 1 | 0.7838 | 0.0202 | 1-x, 1-y, z |
| C23 | 1 | 0.8042 | 0.0405 | 1-x, 1-y, z |
| C4  | 1 | 0.7353 | 0.2067 | 1-x, 1-y, z |
| C12 | 1 | 0.7420 | 0.2274 | 1-x, 1-y, z |
| C20 | 1 | 0.7216 | 0.2069 | 1-x, 1-y, z |
| N43 | 1 | 0.7991 | -0.0205 | 1-x, 1-y, z |
| C44 | 1 | 0.8049 | -0.0000 | 1-x, 1-y, z |
| C16 | 1 | 0.7772 | 0.0406 | 1-x, 1-y, z |
| C5  | 1 | 0.6811 | 0.3325 | 1-x, 1-y, z |
| C6  | 1 | 0.6737 | 0.3540 | 1-x, 1-y, z |
| C13 | 1 | 0.6948 | 0.3327 | 1-x, 1-y, z |
| C21 | 1 | 0.6746 | 0.3117 | 1-x, 1-y, z |
| C24 | 1 | 0.6952 | 0.2917 | 1-x, 1-y, z |
| C25 | 1 | 0.7216 | 0.2478 | 1-x, 1-y, z |
| C26 | 1 | 0.6816 | 0.2915 | 1-x, 1-y, z |
| C27 | 1 | 0.7148 | 0.2273 | 1-x, 1-y, z |
| N45 | 1 | 0.7021 | 0.2707 | 1-x, 1-y, z |
| C46 | 1 | 0.7147 | 0.2695 | 1-x, 1-y, z |
| C19 | 1 | 0.7352 | 0.2478 | 1-x, 1-y, z |
| C1  | 1  | 0.8266 | -0.1048 | 1-x, 1-y, z  |
| C2  | 1  | 0.8195 | -0.0483 | 1-x, 1-y, z  |
| C8  | 1  | 0.8062 | -0.0414 | 1-x, 1-y, z  |
| C9  | 1  | 0.8197 | -0.1252 | 1-x, 1-y, z  |
| C10 | 1  | 0.8265 | -0.0625 | 1-x, 1-y, z  |
| C14 | 1  | 0.7992 | -0.0617 | 1-x, 1-y, z  |
| C22 | 1  | 0.8198 | -0.0419 | 1-x, 1-y, z  |
| C28 | 1  | 0.6385 | 0.3738  | 1-x, 1-y, z  |
| C32 | 1  | 0.6111 | 0.3733  | 1-x, 1-y, z  |
| C33 | 1  | 0.6601 | 0.3539  | 1-x, 1-y, z  |
| C34 | 1  | 0.6314 | 0.3941  | 1-x, 1-y, z  |
| C36 | 1  | 0.6181 | 0.3529  | 1-x, 1-y, z  |
| C38 | 1  | 0.6318 | 0.3532  | 1-x, 1-y, z  |
| C40 | 1  | 0.6178 | 0.3938  | 1-x, 1-y, z  |
| C18 | 1  | 0.7018 | 0.3125  | 1-x, 1-y, z  |
| C17 | 1  | 0.8059 | -0.0823 | 1-x, 1-y, z  |
| C42 | 1  | 0.8402 | -0.1054 | 1-x, 1-y, z  |
| N47 | 1  | 0.5971 | 0.3736  | 1-x, 1-y, z  |
| C48 | 1  | 0.5901 | 0.3553  | 1-x, 1-y, z  |
| C30 | 1  | 0.5485 | 0.3571  | 1-x, 1-y, z  |
| C31 | 1  | 0.5759 | 0.3563  | 1-x, 1-y, z  |
| C35 | 1  | 0.5556 | 0.3773  | 1-x, 1-y, z  |
| C37 | 1  | 0.5688 | 0.3361  | 1-x, 1-y, z  |
| C39 | 1  | 0.5552 | 0.3365  | 1-x, 1-y, z  |
| C41 | 1  | 0.5692 | 0.3769  | 1-x, 1-y, z  |
| C63 | 1  | 0.534  | 0.3575  | 1-x, 1-y, z  |
| C64 | 1  | 0.5269 | 0.3374  | 1-x, 1-y, z  |
| N65 | 1  | 0.5136 | 0.3377  | 1-x, 1-y, z  |
| C66 | 1  | 0.5068 | 0.3575  | 1-x, 1-y, z  |
| C67 | 1  | 0.5136 | 0.3782  | 1-x, 1-y, z  |
| C68 | 1  | 0.5272 | 0.378   | 1-x, 1-y, z  |
| C69 | 1  | 0.5068 | 0.3986  | 1-x, 1-y, z  |
| C6  | 1  | 0.8263 | -0.146  | 1+x, 1/2+y, -1/2+z |
| C6  | 1  | 0.1737 | -0.146  | 1-x, 1/2-y, -1/2+z |
| C9  | 1  | 0.6803 | 0.3748  | 1+x, 1/2+y, 1/2+z |
| C9  | 1  | 0.3197 | 0.3748  | 1-x, 1/2-y, 1/2+z |
| C28 | 1  | 0.847  | -0.1259 | 1+x, 1/2+y, -1/2+z |
| C28 | 1  | 0.153  | -0.1259 | 1-x, 1/2-y, -1/2+z |
| C42 | 1  | 0.6598 | 0.3946  | 1+x, 1/2+y, 1/2+z |
| C42 | 1  | 0.3402 | 0.3946  | 1-x, 1/2-y, 1/2+z |
| C1  | 1  | -0.3266| 0.3952  | 1+x, -1/2+y, 1/2+z |
| C2  | 1  | -0.3195| 0.417   | 1+x, -1/2+y, 1/2+z |
| C3  | 1  | -0.2838| 0.5613  | 1+x, -1/2+y, 1/2+z |
| C4  | 1  | -0.2353| 0.7067  | 1+x, -1/2+y, 1/2+z |
|   |   |   |   |
|---|---|---|---|
| C5 | 1 | -0.1811 | 0.8325 | $1+x, -1/2+y, 1/2+z$ |
| C6 | 1 | -0.1737 | 0.854 | $1+x, -1/2+y, 1/2+z$ |
| C7 | 1 | -0.2974 | 0.5201 | $1+x, -1/2+y, 1/2+z$ |
| C8 | 1 | -0.3062 | 0.4586 | $1+x, -1/2+y, 1/2+z$ |
| C9 | 1 | -0.3197 | 0.3748 | $1+x, -1/2+y, 1/2+z$ |
| C10 | 1 | -0.3265 | 0.4375 | $1+x, -1/2+y, 1/2+z$ |
| C11 | 1 | -0.2974 | 0.561 | $1+x, -1/2+y, 1/2+z$ |
| C12 | 1 | -0.242 | 0.7274 | $1+x, -1/2+y, 1/2+z$ |
| C13 | 1 | -0.3062 | 0.4586 | $1+x, -1/2+y, 1/2+z$ |
| C14 | 1 | -0.2992 | 0.4383 | $1+x, -1/2+y, 1/2+z$ |
| C15 | 1 | -0.2838 | 0.5202 | $1+x, -1/2+y, 1/2+z$ |
| C16 | 1 | -0.277 | 0.5406 | $1+x, -1/2+y, 1/2+z$ |
| C17 | 1 | -0.3059 | 0.4177 | $1+x, -1/2+y, 1/2+z$ |
| C18 | 1 | -0.2018 | 0.8125 | $1+x, -1/2+y, 1/2+z$ |
| C19 | 1 | -0.2352 | 0.7478 | $1+x, -1/2+y, 1/2+z$ |
| C20 | 1 | -0.2216 | 0.7069 | $1+x, -1/2+y, 1/2+z$ |
| C21 | 1 | -0.1746 | 0.8117 | $1+x, -1/2+y, 1/2+z$ |
| C22 | 1 | -0.3199 | 0.4581 | $1+x, -1/2+y, 1/2+z$ |
| C23 | 1 | -0.3042 | 0.5405 | $1+x, -1/2+y, 1/2+z$ |
| C24 | 1 | -0.1952 | 0.7917 | $1+x, -1/2+y, 1/2+z$ |
| C25 | 1 | -0.2216 | 0.7478 | $1+x, -1/2+y, 1/2+z$ |
| C26 | 1 | -0.1816 | 0.7915 | $1+x, -1/2+y, 1/2+z$ |
| C27 | 1 | -0.2148 | 0.7273 | $1+x, -1/2+y, 1/2+z$ |
| C28 | 1 | -0.153 | 0.8741 | $1+x, -1/2+y, 1/2+z$ |
| C29 | 1 | -0.1386 | 0.8738 | $1+x, -1/2+y, 1/2+z$ |
| C30 | 1 | -0.0485 | 0.8571 | $1+x, -1/2+y, 1/2+z$ |
| C31 | 1 | -0.0759 | 0.8563 | $1+x, -1/2+y, 1/2+z$ |
| C32 | 1 | -0.1111 | 0.8733 | $1+x, -1/2+y, 1/2+z$ |
| C33 | 1 | -0.1601 | 0.8539 | $1+x, -1/2+y, 1/2+z$ |
| C34 | 1 | -0.1314 | 0.8941 | $1+x, -1/2+y, 1/2+z$ |
| C35 | 1 | -0.0556 | 0.8773 | $1+x, -1/2+y, 1/2+z$ |
| C36 | 1 | -0.1181 | 0.8529 | $1+x, -1/2+y, 1/2+z$ |
| C37 | 1 | -0.0688 | 0.8361 | $1+x, -1/2+y, 1/2+z$ |
| C38 | 1 | -0.1317 | 0.8532 | $1+x, -1/2+y, 1/2+z$ |
| C39 | 1 | -0.0552 | 0.8365 | $1+x, -1/2+y, 1/2+z$ |
| C40 | 1 | -0.1178 | 0.8938 | $1+x, -1/2+y, 1/2+z$ |
| C41 | 1 | -0.0692 | 0.8769 | $1+x, -1/2+y, 1/2+z$ |
| C42 | 1 | -0.3402 | 0.3946 | $1+x, -1/2+y, 1/2+z$ |
| N43 | 1 | -0.2991 | 0.4795 | $1+x, -1/2+y, 1/2+z$ |
| C44 | 1 | -0.3049 | 0.499 | $1+x, -1/2+y, 1/2+z$ |
| N44 | 1 | -0.2021 | 0.7707 | $1+x, -1/2+y, 1/2+z$ |
| C46 | 1 | -0.2147 | 0.7695 | $1+x, -1/2+y, 1/2+z$ |
| N47 | 1 | -0.0971 | 0.8736 | $1+x, -1/2+y, 1/2+z$ |
| C48 | 1 | -0.0902 | 0.8553 | $1+x, -1/2+y, 1/2+z$ |
| C49 | 1 | -0.2426 | 0.6852 | $1+x, -1/2+y, 1/2+z$ |
|   |   |   |   |   |
|---|---|---|---|---|
| C50 | 1 | -0.236 | 0.6643 | \(1+x, -1/2+y, 1/2+z\) |
| N51 | 1 | -0.2428 | 0.6446 | \(1+x, -1/2+y, 1/2+z\) |
| C52 | 1 | -0.2561 | 0.6442 | \(1+x, -1/2+y, 1/2+z\) |
| C53 | 1 | -0.2631 | 0.6648 | \(1+x, -1/2+y, 1/2+z\) |
| C54 | 1 | -0.2563 | 0.6851 | \(1+x, -1/2+y, 1/2+z\) |
| C55 | 1 | -0.2767 | 0.6647 | \(1+x, -1/2+y, 1/2+z\) |
| C56 | 1 | -0.2835 | 0.6443 | \(1+x, -1/2+y, 1/2+z\) |
| C57 | 1 | -0.2767 | 0.6239 | \(1+x, -1/2+y, 1/2+z\) |
| C58 | 1 | -0.2629 | 0.6237 | \(1+x, -1/2+y, 1/2+z\) |
| N59 | 1 | -0.2565 | 0.6036 | \(1+x, -1/2+y, 1/2+z\) |
| C60 | 1 | -0.263 | 0.5836 | \(1+x, -1/2+y, 1/2+z\) |
| C61 | 1 | -0.2766 | 0.583 | \(1+x, -1/2+y, 1/2+z\) |
| C62 | 1 | -0.2834 | 0.6035 | \(1+x, -1/2+y, 1/2+z\) |
| C63 | 1 | -0.034 | 0.8575 | \(1+x, -1/2+y, 1/2+z\) |
| C64 | 1 | -0.0269 | 0.8374 | \(1+x, -1/2+y, 1/2+z\) |
| N65 | 1 | -0.0136 | 0.8377 | \(1+x, -1/2+y, 1/2+z\) |
| C66 | 1 | -0.0068 | 0.8575 | \(1+x, -1/2+y, 1/2+z\) |
| C67 | 1 | -0.0136 | 0.8782 | \(1+x, -1/2+y, 1/2+z\) |
| C68 | 1 | -0.0272 | 0.878 | \(1+x, -1/2+y, 1/2+z\) |
| C69 | 1 | -0.0068 | 0.8986 | \(1+x, -1/2+y, 1/2+z\) |
| C49 | 1 | 0.2426 | 0.6852 | \(1-x, 1/2-y, 1/2+z\) |
| C50 | 1 | 0.236 | 0.6643 | \(1-x, 1/2-y, 1/2+z\) |
| N51 | 1 | 0.2428 | 0.6446 | \(1-x, 1/2-y, 1/2+z\) |
| C52 | 1 | 0.2561 | 0.6442 | \(1-x, 1/2-y, 1/2+z\) |
| C53 | 1 | 0.2631 | 0.6648 | \(1-x, 1/2-y, 1/2+z\) |
| C54 | 1 | 0.2563 | 0.6851 | \(1-x, 1/2-y, 1/2+z\) |
| C55 | 1 | 0.2767 | 0.6647 | \(1-x, 1/2-y, 1/2+z\) |
| C56 | 1 | 0.2835 | 0.6443 | \(1-x, 1/2-y, 1/2+z\) |
| C57 | 1 | 0.2767 | 0.6239 | \(1-x, 1/2-y, 1/2+z\) |
| C58 | 1 | 0.2629 | 0.6237 | \(1-x, 1/2-y, 1/2+z\) |
| N59 | 1 | 0.2565 | 0.6036 | \(1-x, 1/2-y, 1/2+z\) |
| C60 | 1 | 0.263 | 0.5836 | \(1-x, 1/2-y, 1/2+z\) |
| C61 | 1 | 0.2766 | 0.583 | \(1-x, 1/2-y, 1/2+z\) |
| C62 | 1 | 0.2834 | 0.6035 | \(1-x, 1/2-y, 1/2+z\) |
| C3 | 1 | 0.2838 | 0.5613 | \(1-x, 1/2-y, 1/2+z\) |
| C7 | 1 | 0.2974 | 0.5201 | \(1-x, 1/2-y, 1/2+z\) |
| C11 | 1 | 0.2974 | 0.561 | \(1-x, 1/2-y, 1/2+z\) |
| C15 | 1 | 0.2838 | 0.5202 | \(1-x, 1/2-y, 1/2+z\) |
| C23 | 1 | 0.3042 | 0.5405 | \(1-x, 1/2-y, 1/2+z\) |
| C4 | 1 | 0.2353 | 0.7067 | \(1-x, 1/2-y, 1/2+z\) |
| C12 | 1 | 0.242 | 0.7274 | \(1-x, 1/2-y, 1/2+z\) |
| C20 | 1 | 0.2216 | 0.7069 | \(1-x, 1/2-y, 1/2+z\) |
| N43 | 1 | 0.2991 | 0.4795 | \(1-x, 1/2-y, 1/2+z\) |
| C44 | 1 | 0.3049 | 0.499 | \(1-x, 1/2-y, 1/2+z\) |
| C16 | 1 | 0.277 | 0.5406 | \(1-x, 1/2-y, 1/2+z\) |
| C5 | 1  | 0.1811 | 0.8325 | 1-x, 1/2-y, 1/2+z |
|----|----|--------|--------|--------------------|
| C6 | 1  | 0.1737 | 0.854  | 1-x, 1/2-y, 1/2+z |
| C13| 1  | 0.1948 | 0.8327 | 1-x, 1/2-y, 1/2+z |
| C21| 1  | 0.1746 | 0.8117 | 1-x, 1/2-y, 1/2+z |
| C24| 1  | 0.1952 | 0.7917 | 1-x, 1/2-y, 1/2+z |
| C25| 1  | 0.2216 | 0.7478 | 1-x, 1/2-y, 1/2+z |
| C26| 1  | 0.1816 | 0.7915 | 1-x, 1/2-y, 1/2+z |
| C27| 1  | 0.2148 | 0.7273 | 1-x, 1/2-y, 1/2+z |
| C19| 1  | 0.2352 | 0.7478 | 1-x, 1/2-y, 1/2+z |
| C22| 1  | 0.3198 | 0.4581 | 1-x, 1/2-y, 1/2+z |
| C28| 1  | 0.153  | 0.8741 | 1-x, 1/2-y, 1/2+z |
| C29| 1  | 0.1385 | 0.8738 | 1-x, 1/2-y, 1/2+z |
| C32| 1  | 0.1111 | 0.8733 | 1-x, 1/2-y, 1/2+z |
| C33| 1  | 0.1601 | 0.8539 | 1-x, 1/2-y, 1/2+z |
| C34| 1  | 0.1314 | 0.8941 | 1-x, 1/2-y, 1/2+z |
| C36| 1  | 0.1181 | 0.8529 | 1-x, 1/2-y, 1/2+z |
| C38| 1  | 0.1318 | 0.8532 | 1-x, 1/2-y, 1/2+z |
| C40| 1  | 0.1178 | 0.8938 | 1-x, 1/2-y, 1/2+z |
| C18| 1  | 0.2018 | 0.8125 | 1-x, 1/2-y, 1/2+z |
| C17| 1  | 0.3059 | 0.4177 | 1-x, 1/2-y, 1/2+z |
| N47| 1  | 0.0971 | 0.8736 | 1-x, 1/2-y, 1/2+z |
| C48| 1  | 0.0901 | 0.8553 | 1-x, 1/2-y, 1/2+z |
| C30| 1  | 0.0485 | 0.8571 | 1-x, 1/2-y, 1/2+z |
| C31| 1  | 0.0759 | 0.8563 | 1-x, 1/2-y, 1/2+z |
| C35| 1  | 0.0556 | 0.8773 | 1-x, 1/2-y, 1/2+z |
| C37| 1  | 0.0688 | 0.8361 | 1-x, 1/2-y, 1/2+z |
| C39| 1  | 0.0552 | 0.8365 | 1-x, 1/2-y, 1/2+z |
| C41| 1  | 0.0692 | 0.8769 | 1-x, 1/2-y, 1/2+z |
| C63| 1  | 0.034  | 0.8575 | 1-x, 1/2-y, 1/2+z |
| C64| 1  | 0.0269 | 0.8374 | 1-x, 1/2-y, 1/2+z |
| N65| 1  | 0.0136 | 0.8377 | 1-x, 1/2-y, 1/2+z |
| C66| 1  | 0.0068 | 0.8575 | 1-x, 1/2-y, 1/2+z |
| C67| 1  | 0.0136 | 0.8782 | 1-x, 1/2-y, 1/2+z |
| C68| 1  | 0.0272 | 0.878  | 1-x, 1/2-y, 1/2+z |
| C69| 1  | 0.0068 | 0.8986 | 1-x, 1/2-y, 1/2+z |
| C6 | 1  | -0.3263| 0.354  | 1-x, -y, z        |
| C9 | 1  | 0.1803 | 0.8748 | 1+x, y, 1+z       |
| C9 | 1  | -0.1803| 0.8748 | 1-x, -y, 1+z     |
| C28 | 1  | -0.347 | 0.3741 | 1-x, -y, z |
|-----|----|--------|--------|------------|
| C42 | 1  | 0.1598 | 0.8946 | 1+x, y, 1+z |
| C42 | 1  | -0.1598 | 0.8946 | 1-x, -y, 1+z |
| C1  | 1  | 0.6734 | 0.3952 | 1+x, 1/2+y, 1/2+z |
| C2  | 1  | 0.6805 | 0.417  | 1+x, 1/2+y, 1/2+z |
| C3  | 1  | 0.7162 | 0.5613 | 1+x, 1/2+y, 1/2+z |
| C4  | 1  | 0.7647 | 0.7067 | 1+x, 1/2+y, 1/2+z |
| C5  | 1  | 0.8189 | 0.8325 | 1+x, 1/2+y, 1/2+z |
| C6  | 1  | 0.8263 | 0.854  | 1+x, 1/2+y, 1/2+z |
| C7  | 1  | 0.7026 | 0.5201 | 1+x, 1/2+y, 1/2+z |
| C8  | 1  | 0.6938 | 0.4586 | 1+x, 1/2+y, 1/2+z |
| C10 | 1  | 0.6735 | 0.4375 | 1+x, 1/2+y, 1/2+z |
| C11 | 1  | 0.7026 | 0.561  | 1+x, 1/2+y, 1/2+z |
| C12 | 1  | 0.758  | 0.7274 | 1+x, 1/2+y, 1/2+z |
| C13 | 1  | 0.8052 | 0.8327 | 1+x, 1/2+y, 1/2+z |
| C14 | 1  | 0.7008 | 0.4383 | 1+x, 1/2+y, 1/2+z |
| C15 | 1  | 0.7162 | 0.5202 | 1+x, 1/2+y, 1/2+z |
| C16 | 1  | 0.723  | 0.5406 | 1+x, 1/2+y, 1/2+z |
| C17 | 1  | 0.6941 | 0.4177 | 1+x, 1/2+y, 1/2+z |
| C18 | 1  | 0.7982 | 0.8125 | 1+x, 1/2+y, 1/2+z |
| C19 | 1  | 0.7648 | 0.7478 | 1+x, 1/2+y, 1/2+z |
| C20 | 1  | 0.7784 | 0.7069 | 1+x, 1/2+y, 1/2+z |
| C21 | 1  | 0.8254 | 0.8117 | 1+x, 1/2+y, 1/2+z |
| C22 | 1  | 0.6802 | 0.4581 | 1+x, 1/2+y, 1/2+z |
| C23 | 1  | 0.6958 | 0.5405 | 1+x, 1/2+y, 1/2+z |
| C24 | 1  | 0.8048 | 0.7917 | 1+x, 1/2+y, 1/2+z |
| C25 | 1  | 0.7784 | 0.7478 | 1+x, 1/2+y, 1/2+z |
| C26 | 1  | 0.8184 | 0.7915 | 1+x, 1/2+y, 1/2+z |
| C27 | 1  | 0.7852 | 0.7273 | 1+x, 1/2+y, 1/2+z |
| C28 | 1  | 0.847  | 0.8741 | 1+x, 1/2+y, 1/2+z |
| C29 | 1  | 0.8615 | 0.8738 | 1+x, 1/2+y, 1/2+z |
| C30 | 1  | 0.9515 | 0.8571 | 1+x, 1/2+y, 1/2+z |
| C31 | 1  | 0.9241 | 0.8563 | 1+x, 1/2+y, 1/2+z |
| C32 | 1  | 0.8889 | 0.8733 | 1+x, 1/2+y, 1/2+z |
| C33 | 1  | 0.8399 | 0.8539 | 1+x, 1/2+y, 1/2+z |
| C34 | 1  | 0.8686 | 0.8941 | 1+x, 1/2+y, 1/2+z |
| C35 | 1  | 0.9444 | 0.8773 | 1+x, 1/2+y, 1/2+z |
| C36 | 1  | 0.8819 | 0.8529 | 1+x, 1/2+y, 1/2+z |
| C37 | 1  | 0.9312 | 0.8361 | 1+x, 1/2+y, 1/2+z |
| C38 | 1  | 0.8682 | 0.8532 | 1+x, 1/2+y, 1/2+z |
| C39 | 1  | 0.9448 | 0.8365 | 1+x, 1/2+y, 1/2+z |
| C40 | 1  | 0.8822 | 0.8938 | 1+x, 1/2+y, 1/2+z |
| C41 | 1  | 0.9308 | 0.8769 | 1+x, 1/2+y, 1/2+z |
| N43 | 1  | 0.7009 | 0.4795 | 1+x, 1/2+y, 1/2+z |
| C44 | 1  | 0.6951 | 0.499  | 1+x, 1/2+y, 1/2+z |
|   |   |   |   |
|---|---|---|---|
| N45 | 1 | 0.7979 | 0.7707 | 1+x, 1/2+y, 1/2+z |
| C46 | 1 | 0.7853 | 0.7695 | 1+x, 1/2+y, 1/2+z |
| N47 | 1 | 0.9029 | 0.8736 | 1+x, 1/2+y, 1/2+z |
| C48 | 1 | 0.9099 | 0.8553 | 1+x, 1/2+y, 1/2+z |
| C49 | 1 | 0.7574 | 0.6852 | 1+x, 1/2+y, 1/2+z |
| C50 | 1 | 0.764 | 0.6643 | 1+x, 1/2+y, 1/2+z |
| N51 | 1 | 0.7572 | 0.6446 | 1+x, 1/2+y, 1/2+z |
| C52 | 1 | 0.7439 | 0.6442 | 1+x, 1/2+y, 1/2+z |
| C53 | 1 | 0.7369 | 0.6648 | 1+x, 1/2+y, 1/2+z |
| C54 | 1 | 0.7437 | 0.6851 | 1+x, 1/2+y, 1/2+z |
| C55 | 1 | 0.7233 | 0.6647 | 1+x, 1/2+y, 1/2+z |
| C56 | 1 | 0.7165 | 0.6443 | 1+x, 1/2+y, 1/2+z |
| C57 | 1 | 0.7233 | 0.6239 | 1+x, 1/2+y, 1/2+z |
| C58 | 1 | 0.7371 | 0.6237 | 1+x, 1/2+y, 1/2+z |
| N59 | 1 | 0.7435 | 0.6036 | 1+x, 1/2+y, 1/2+z |
| C60 | 1 | 0.737 | 0.5836 | 1+x, 1/2+y, 1/2+z |
| C61 | 1 | 0.7234 | 0.583 | 1+x, 1/2+y, 1/2+z |
| C62 | 1 | 0.7166 | 0.6035 | 1+x, 1/2+y, 1/2+z |
| C63 | 1 | 0.966 | 0.8575 | 1+x, 1/2+y, 1/2+z |
| C64 | 1 | 0.9731 | 0.8374 | 1+x, 1/2+y, 1/2+z |
| N65 | 1 | 0.9864 | 0.8377 | 1+x, 1/2+y, 1/2+z |
| C66 | 1 | 0.9932 | 0.8575 | 1+x, 1/2+y, 1/2+z |
| C67 | 1 | 0.9864 | 0.8782 | 1+x, 1/2+y, 1/2+z |
| C68 | 1 | 0.9728 | 0.878 | 1+x, 1/2+y, 1/2+z |
| C69 | 1 | 0.9932 | 0.8986 | 1+x, 1/2+y, 1/2+z |
| C49 | 1 | 1.2426 | 0.6852 | 1-x, 1.5-y, 1/2+z |
| C50 | 1 | 1.2361 | 0.6643 | 1-x, 1.5-y, 1/2+z |
| N51 | 1 | 1.2428 | 0.6446 | 1-x, 1.5-y, 1/2+z |
| C52 | 1 | 1.2561 | 0.6442 | 1-x, 1.5-y, 1/2+z |
| C53 | 1 | 1.2631 | 0.6648 | 1-x, 1.5-y, 1/2+z |
| C54 | 1 | 1.2563 | 0.6851 | 1-x, 1.5-y, 1/2+z |
| C55 | 1 | 1.2767 | 0.6647 | 1-x, 1.5-y, 1/2+z |
| C56 | 1 | 1.2835 | 0.6443 | 1-x, 1.5-y, 1/2+z |
| C57 | 1 | 1.2767 | 0.6239 | 1-x, 1.5-y, 1/2+z |
| C58 | 1 | 1.2629 | 0.6239 | 1-x, 1.5-y, 1/2+z |
| N59 | 1 | 1.2565 | 0.6036 | 1-x, 1.5-y, 1/2+z |
| C60 | 1 | 1.263 | 0.5836 | 1-x, 1.5-y, 1/2+z |
| C61 | 1 | 1.2766 | 0.583 | 1-x, 1.5-y, 1/2+z |
| C62 | 1 | 1.2834 | 0.6035 | 1-x, 1.5-y, 1/2+z |
| C3 | 1 | 1.2838 | 0.5613 | 1-x, 1.5-y, 1/2+z |
| C7 | 1 | 1.2974 | 0.5201 | 1-x, 1.5-y, 1/2+z |
| C11 | 1 | 1.2974 | 0.561 | 1-x, 1.5-y, 1/2+z |
| C15 | 1 | 1.2838 | 0.5202 | 1-x, 1.5-y, 1/2+z |
| C23 | 1 | 1.3042 | 0.5405 | 1-x, 1.5-y, 1/2+z |
| C4 | 1 | 1.2353 | 0.7067 | 1-x, 1.5-y, 1/2+z |
| Atoms | Z | V | C | Formula |
|-------|---|---|---|---------|
| C12   | 1 | 1.242 | 0.7274 | 1-x, 1.5-y, 1/2+z |
| C20   | 1 | 1.2216 | 0.7069 | 1-x, 1.5-y, 1/2+z |
| N43   | 1 | 1.2991 | 0.4795 | 1-x, 1.5-y, 1/2+z |
| C44   | 1 | 1.2021 | 0.7707 | 1-x, 1.5-y, 1/2+z |
| C18   | 1 | 1.2018 | 0.8125 | 1-x, 1.5-y, 1/2+z |
| C6    | 1 | 1.178 | 0.3748 | 1-x, 1.5-y, 1/2+z |
| C21   | 1 | 1.1952 | 0.7917 | 1-x, 1.5-y, 1/2+z |
| C4   | 1 | 1.153 | 0.8741 | 1-x, 1.5-y, 1/2+z |
| C32   | 1 | 1.1601 | 0.8539 | 1-x, 1.5-y, 1/2+z |
| C10   | 1 | 1.3264 | 0.4375 | 1-x, 1.5-y, 1/2+z |
| N47   | 1 | 1.0971 | 0.8736 | 1-x, 1.5-y, 1/2+z |
| C40   | 1 | 1.1314 | 0.8941 | 1-x, 1.5-y, 1/2+z |
| C17   | 1 | 1.3059 | 0.4177 | 1-x, 1.5-y, 1/2+z |
| C48   | 1 | 1.0556 | 0.8773 | 1-x, 1.5-y, 1/2+z |
| C30   | 1 | 1.0485 | 0.8571 | 1-x, 1.5-y, 1/2+z |
| C31   | 1 | 1.0759 | 0.8563 | 1-x, 1.5-y, 1/2+z |
| C35   | 1 | 1.0688 | 0.8361 | 1-x, 1.5-y, 1/2+z |
| C39   | 1 | 1.0552 | 0.8365 | 1-x, 1.5-y, 1/2+z |
| C41   | 1 | 1.0692 | 0.8769 | 1-x, 1.5-y, 1/2+z |
| C64   | 1 | 1.0269 | 0.8374 | 1-x, 1.5-y, 1/2+z |
| N65   | 1 | 1.0136 | 0.8377 | 1-x, 1.5-y, 1/2+z |
|   |   |   |   |
|---|---|---|---|
| C66 | 1 | 1.0068 | 0.8575 | 1-x, 1.5-y, 1/2+z |
| C67 | 1 | 1.0136 | 0.8782 | 1-x, 1.5-y, 1/2+z |
| C68 | 1 | 1.0272 | 0.878 | 1-x, 1.5-y, 1/2+z |
| C69 | 1 | 1.0068 | 0.8986 | 1-x, 1.5-y, 1/2+z |
| C6  | 1 | 1.3262 | 0.354 | 1+x, 1+y, z |
| C9  | 1 | 1.1803 | 0.8748 | 1+x, 1+y, 1+z |
| C9  | 1 | 0.8197 | 0.8748 | 1-x, 1-y, 1+z |
| C28 | 1 | 1.347 | 0.3741 | 1+x, 1+y, z |
| C42 | 1 | 1.1598 | 0.8946 | 1+x, 1+y, 1+z |
| C42 | 1 | 0.8402 | 0.8946 | 1-x, 1-y, 1+z |
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