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## **Supporting Information**

## For

### Color-tunable and white circularly polarized luminescence through

## confining guests into chiral MOFs

Hong-Ru Fu,<sup>ac</sup> Ruo-Yu Zhang,<sup>ab</sup> Ting Li,<sup>a\*</sup> Chen-Ying Wei,<sup>a</sup> Shuang Liu,<sup>a</sup> Jia-Yi Xu,<sup>a</sup> Xueli Zhu,<sup>a</sup> Jiaojiao Wei,<sup>a\*</sup> Qing-Rong Ding,<sup>c\*</sup> Lu-Fang Ma<sup>a</sup>

<sup>a</sup>College of Chemistry and Chemical Engineering, Luoyang Normal University, Luoyang 471934, P. R. China.
 <sup>b</sup>College of Chemistry and Chemical Engineering, Henan Normal University, Xinxiang 453007 China.
 <sup>c</sup>State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian, 350002, China.

\* Corresponding author E-mails: liting880202@163.com, jjwei1992@163.com, qrding@fjirsm.ac.cn

HR Fu: writing—reviewing and editing, funding acquisition. RY Zhang: data curation, formal analysis. T Li: data curation, formal analysis. CY Wei: formal analysis. S Liu: formal analysis. JY Xu: formal analysis. XL. Zhu: formal analysis, funding acquisition. JJ Wei: writing, funding acquisition. QR Ding: Critical revision. LF Ma: Supervision.

#### 1. Materials and Methods.

All reagents and solvents were purchased commercially. Ethyl alcohol (EtOH) and N, Ndimethylformamide (DMF) (China National Pharmaceutical Group Co., Ltd.). 4-(1H-Pyrazol-4-Yl)Pyridine (4-HPPD) (CHEMSOON), Nile Red (NIR) (TCI), Coumarin 152 (C152) (TCI).

Powder X-ray diffraction (PXRD) was performed using a Rigaku Smart Lab diffractometer with a Cu K $\alpha$  source (1.541 Å), where diffraction data were collected at  $2\theta$  angle from 5° to 50°, using a 0.01° step size and 1° min<sup>-1</sup> step speed. Solid state diffuse reflectance spectra were recorded on a UV-2600 Shimadzu spectrophotometer using a standard sample holder. Solid state emission was measured using FLS1000 spectrofluorometer. Thermogravimetric analysis (TGA) was performed on a PerkinElmer TG-7 analyzer heated from 30 °C to 700 °C at the atmosphere with a ramp rate of 5 °C/min. The fluorescence and phosphorescence spectra were conducted on Edinburgh FLS1000 with xenon arc lamp and nanosecond flash-lamp. The intrinsic circularly polarized luminescence (CPL) spectra were measured at the scanning speed rate of 100 nm/min on JASCO CPL-300 spectrometer. The circular dichroism (CD) spectra were measured from 200-800 nm range using JASCO J-810 circular dichroism spectrometer.

# 1.1 Synthesis of $[Zn_2(M-4-PPD)_2(NO_3)_2]$ ·DMA·H<sub>2</sub>O·EtOH (DCF-20) and $[Zn_2(P-4-PPD)_2(NO_3)_2]$ ·DMA·2H<sub>2</sub>O·EtOH (LCF-20)

A mixture of  $Zn(NO_3)_2 \cdot 6H_2O$  (60 mg, 0.2 mmol), 4-HPPD (4-(1H-pyrazol-4-yl)pyridine, 15 mg, 0.1 mmol) and D-cam (D-camphoric acid, 20 mg, 0.1 mmol) in the solution of H<sub>2</sub>O (1 mL), EtOH (2 mL), and DMA (N,N-dimethylacetamide, 4 mL) was sealed in a 25 mL Teflon-lined stainless steel autoclave. The autoclave was heated at 100°C for 72 h under an autogenous presser and then cooled slowly to room temperature at a rate of 10 °C·h<sup>-1</sup>. Colorless rodlike crystals were obtained and washed with DMA and ethanol. The yield was 81% (based on 4-HPPD). Elemental analysis: Calcd for DCF-20 (C<sub>16</sub>H<sub>21.5</sub>N<sub>3.5</sub>O<sub>3.5</sub>Zn): C, 49.97; H, 5.59; N, 12.75. Found: C, 49.47; H, 6.01; N, 12.32. LCF-20 was synthesized by using L-cam.

#### 1.2 Synthesis of Guests@MOFs

The host-guest systems were prepared via an in-situ approach. Similar to the synthesis of parent crystals, a series of dyes solution were added under the different molar ratio of 4-PPD and guest. The molar ratio of 4-PPD and guest is as follows: 1.0:0.3, 1.0:0.2, 1.0:0.1, namely, 8.6, 5.7 and 2.8 mg for HBT1 were added, 8.1, 5.4 and 2.7 mg for HBT2, 7.5, 5.0 and 2.5 mg C152 as well as 9.0, 6.0 and 3.0 mg for NIR were added, while the total volume is equal to that of the host materials. After decanting the solution, the crystals were washed thoroughly with DMF and deionized water and dried in the air..

The white light was realized by introducing three dyes. The  $5 \times 10^{-3}$  mol/L DMA solution of HBT1, C152 and NIR were added in the parent solution with different concentration gradients, the total volume is equal to that of the host materials. The detail synthesis processes and final results were shown in Table S4 and Figure S30-36.

#### 1.3 X-ray Data Collection and Structure Determinations

Crystallographic data of DCF-20 and LCF-20 was collected on a Rigaku Supernova diffractometer at 290 (2) K or ambient temperature with Mo-K $\alpha$  radiation ( $\lambda = 0.71073$  Å) by  $\omega$  scan mode. The determination of the unit cell and data collection was performed with CrysAlisPro.

The structure was determined by direct methods and refined by the full-matrix least-squares method with the SHELX<sup>1</sup> and OLEX2.0<sup>2</sup> program package. All non-hydrogen atoms were located successfully from Fourier maps and were refined anisotropically. The H atoms on the ligands were placed in idealized positions and refined using a riding model. The disordered guest molecules could not be located successfully from fourier maps, and the highly disordered lattice guest molecules were removed using the SQUEEZE procedure by PLATON.<sup>3</sup> Selected crystal parameters and refinement are summarized in Table S6. The numbers of CCDC are 2364863 and 2364864. These data are provided free of charge by the Cambridge Crystallographic Data Centre.

In addition, the crystal quantity of Guests@DCF-20 and Guests@LCF-20 are good, and they are suitable to X-ray single crystal diffraction, however, only the host structure can be resolved, no lattice diffraction of guest molecules can be confirmed. This can be attributed to two factors, one the one hand, the guest molecules into the pores still own molecular vibration, further present the structure disorder, one the other hand, the integrity of guest is low resulting from the restrictions of crystallography occupancy.

Besides, although many efforts have been tried, we could not obtain the guest-loaded crystal structure. However, the guest-loaded crystals also keep the intact morphology and crystallinity, we could obtain the accurate structure of the host framework by single crystal X-ray diffraction.

#### 1.4 The loading amounts of guests

The loading amounts of guest dyes in compounds were determined by fluorescence spectra. For example, the fluorescence intensity-concentration relationship was adopted. The luminescent intensities of different concentrations of C152 in DMA solution were measured and repeated five times, and then the average values were calculated, respectively. Therefore, the relationship for the emission intensity-concentration of C152 in DMA solution could be obtained. 10 mg dye-encapsulated C152@MOFs were dissolved in 2 mL DMA solution, which was achieved by adding HCl (0.25 mL, 37%) to obtain clear solution, then the emission intensity of the mixture solution was measured under the same condition. Through combining the function of C152 pure solution and the intensity of C152 from composition, we could obtain the specific loading capacity of C152 at each concentration gradient (Figure S21-24).

#### 1.5 Theoretical simulation

The density functional theory (DFT) calculations were performed using a Dmol3 module of Material Studio 2020.<sup>4</sup> The generalized gradient approximation (GGA) method with Perdew-Burke-Ernzerhof (PBE) function was employed to describe the interactions between core and electrons. The force and energy convergence criterion were set to 0.002 Ha Å-1 and 10-5 Ha, respectively. When the optimization was completed, the ESP and mulliken charge calculations were performed.

The binding energy ( $\Delta E$ ) was calculated as

 $\Delta E(eV) = 27.212*(Etotal(Ha)-E1(Ha)-E2(Ha))$ 

where the Etotal is the energy of the optimized system; E1 is the energy of the material; Emolecule is the energy of micromolecule.

The coordinate sites were listed in Table S7 and S8.

#### 1.6 The CD and CPL measurements of MOFs

CD spectra was measured on a JASCO J-810 spectrophotometer. The samples were prepared by using the method for infrared measurement. A mixture of MOFs and KBr (crystal/KBr 1:400, weight ratio, total weight of 100 mg) was finely ground and pressed into a transparent pellet with a diameter of 13 mm. The pellet was directly used for measurement of CD. The wavelength and bandwidth of the monochromator were set to 280.0 and 1.0 nm, and the time-per-point of each sampling point was 0.5 s.

CPL spectra for all samples were recorded on a JASCO CPL-300 spectrophotometer in the solid state with scanning speed. The basic mode is used. Ex slit width, Em slit width, and accumulations of 100 nm min<sup>-1</sup>, 2000 um, 2000 um, and 2, respectively. The excitation wavelength was 280 nm and the DV values were about 0.5 V for DCF-20/LCF-20 and the corresponding wavelengths for Guests@DCF-20 and Guests@LCF-20.

#### 1.7 The preparation of WLED

For the UV-pumped white LED, the grounded WD-5 were blended with (Polymethyl Methacrylate) PMMA to form a well-distributed mixture; then, the composite was coated on the surface of a 365 nm UV LED chip and cured for 30 min at room temperature.

#### 2. Other figures and data

Table S1. The results of crystal parameter under different molar ratio of 4-PPD and D-cam.

Molar ratio	4-HPPD (mg)	D-cam (mg)	Solution	Space group
1:5	15	100	4:2:1	P41212
1:10	7.5	100	4:2:1	P41212
1:10	15	200	8:4:2	P41212
1:20	8	200	4:2:1	P41212

Solution: DMA:EtOH:H<sub>2</sub>O (mL:mL:mL)

The effect of stoichiometric ratio was preliminary investigated, it can find that the space group has no inversion and change.



**Figure S1.** (a) The emission of 4-HPPD in DMA; (b) the delayed lifetimes of DCF-20 and LCF-20.



**Figure S2.** (a) PXRD patterns of as-synthesized DCF-20 and LCF-20; (b) PXRD of WD-5 and WL-5 with white-lighting emission. All simulated patterns are calculated from the corresponding single-crystal structures. Test conditions: working voltage and current is 40 kV and 40 mA, respectively.



Figure S3. (a,b) PXRD patterns of as-synthesized HBT1@DCF-20 and HBT1@LCF-20; (c,d) PXRD of HBT2@DCF-20 and HBT2@LCF-20.



Figure S4. (a,b) PXRD patterns of as-synthesized C152@DCF-20 and C152@LCF-20; (c,d) PXRD of NIR@DCF-20 and NIR@LCF-20.



Figure S5. Thermogravimetric analysis of guests@MOFs. (a) HBT1@DCF-20/HBT1@LCF-20; (b) HBT2@DCF-20/HBT2@LCF-20; (d) C152@DCF-20/C152@LCF-20; (d) NIR@DCF-20/NIR@LCF-20.



**Figure S6.** The emission behaviors of guest emitters under different excitation wavelength. (a) HBT1; (b) HBT2; (c) C152; (d) NIR.



Figure S7. The emission behaviors including emission peaks and CIE coordinates of HBT1@LCF-20-1.



Figure S8. The emission behaviors including emission peaks and CIE coordinates of HBT1@LCF-20-2.



Figure S9. The emission behaviors including emission peaks and CIE coordinates of HBT1@LCF-20-3.



Figure S10. The emission behaviors including emission peaks and CIE coordinates of HBT2@DCF-20-1.



Figure S11. The emission behaviors including emission peaks and CIE coordinates of HBT2@DCF-20-2.



Figure S12. The emission behaviors including emission peaks and CIE coordinates of HBT2@DCF-20-3.



Figure S13. The emission behaviors including emission peaks and CIE coordinates of HBT2@LCF-20-3.



Figure S14. The emission behaviors including emission peaks and CIE coordinates of C152@LCF-20-1.



Figure S15. The emission behaviors including emission peaks and CIE coordinates of C152@LCF-20-2.







Figure S17. The emission behaviors including emission peaks and CIE coordinates of C152@DCF-20-1.



Figure S18. The emission behaviors including emission peaks and CIE coordinates of C152@DCF-20-2.



Figure S19. The emission behaviors including emission peaks and CIE coordinates of NIR@DCF-20-1.



Figure S20. The emission behaviors including emission peaks and CIE coordinates of NIR@DCF-20 and NIR@LCF-20.



**Figure S21.** (a) The emission intensity of HBT1 in DMA solution with different concentrations; (b) the relationship for the intensity-concentration of HBT1 in DMA solution could be obtained; (c) HBT1@DCF-20 (10 mg) crystal sample was decomposed in DMA (2 mL) with HCl (0.25 mL, 37%); (d) the final amounts of HBT1 in host framework.

When the data at 375 nm was adopted, the below equation can be obtained, as follows: **Equation S1:** Y = 1741309.5X + 205.24 (cyan fitting line), the concentration of HBT1 is below 1 × 10<sup>-4</sup> mol/L.



**Figure S22.** (a) The emission intensity of HBT2 in DMA solution with different concentrations; (b) the relationship for the intensity-concentration of HBT2 in DMA solution could be obtained; (c) HBT2@DCF-20 (10 mg) crystal sample was decomposed in DMA (2 mL) with HCl (0.25 mL, 37%); (d) the final amounts of HBT2 in host framework.

When the intensity at 550 nm was adopted, the below equation can be obtained, as follows: **Equation S1:** Y = 3.47714E7X + 1245.28571 (cyan fitting line), the concentration of HBT2 is below  $1 \times 10^{-4}$  mol/L.

Equation S2: Y = -7817478.39749X + 3965.42655 (orange fitting line). The concentration of HBT2 ranges from  $1 \times 10^{-4}$  to  $1 \times 10^{-3}$  mol/L.



**Figure S23.** (a) The emission intensity of C152 in DMA solution with different concentrations; (b) the relationship for the intensity-concentration of C152 in DMA solution could be obtained; (c) C152@DCF-20 (10 mg) crystal sample was decomposed in DMA (2 mL) with HCl (0.25 mL, 37%); (d) the final amounts of C152 in host framework.

When the data at 500 nm was adopted, the below equation can be obtained, as follows:

Equation S1: Y = 2.687E7X + 1756.91111 (cyan fitting line), the concentration of C152 is below  $1 \times 10^{-4}$  mol/L.

Equation S2: Y = -9492000X + 5092.2 (orange fitting line). The concentration of C152 ranges from  $1 \times 10^{-4}$  to  $1 \times 10^{-3}$  mol/L.



**Figure S24.** (a) The emission intensity of NIR in DMA solution with different concentrations; (b) the relationship for the intensity-concentration of NIR in DMA solution could be obtained; (c) NIR@DCF-20 (10 mg) crystal sample was decomposed in DMA (2 mL) with HCl (0.25 mL, 37%); (d) the final amounts of NIR in host framework.

When the data at 640 nm was adopted, the below equation can be obtained, as follows:

Equation S1: Y = 1504200X + 24.74022 (cyan fitting line), the concentration of NIR is below  $1 \times 10^{-4}$  mol/L.

Equation S2: Y = 396700X + 143.6 (orange fitting line). The concentration of NIR ranges from 1  $\times 10^{-4}$  to  $1 \times 10^{-3}$  mol/L.

	$\Phi_{\rm f}(100\%)$		$\Phi_{\rm f}(100\%)$
HBT1@DCF-20-1	24.32	HBT2@DCF-20-1	62.31
HBT1@DCF-20-2	22.31	HBT2@DCF-20-2	58.32
HBT1@DCF-20-3	21.35	HBT2@DCF-20-3	57.98
HBT1@LCF-20-1	22.31	HBT2@LCF-20-1	61.32
HBT1@LCF-20-2	20.13	HBT2@LCF-20-2	59.00
HBT1@LCF-20-3	20.01	HBT2@LCF-20-3	57.31

Table S2. The quantum yields of Guests@MOFs.

Table S3. The quantum yields of Guests@MOFs.

	$\Phi_{\rm f}(100\%)$		$\Phi_{\rm f}(100\%)$
C152@DCF-20-1	68.01	NIR@DCF-20-1	22.36
C152@DCF-20-2	68.12	NIR@DCF-20-2	23.25
C152@DCF-20-3	67.32	NIR@DCF-20-3	21.46
C152@LCF-20-1	69.22	NIR@LCF-20-1	23.25
C152@LCF-20-2	68.23	NIR@LCF-20-2	21.33
C152@LCF-20-3	68.19	NIR@LCF-20-3	29.25



**Figure S25.** (a) The solid state UV-vis absorption spectrum of DCF-20/LCF-20; (b) the solid state UV-vis absorption spectra of four guests and the emission of 4-HPPD; (c) the solid state UV-vis absorption spectra of C152@DCF-20; (d) the solid state UV-vis absorption spectra of C152@LCF-20.



**Figure S26.** The solid state UV-vis absorption spectrum of HBT1@DCF-20/HBT1@LCF-20, and HBT2@DCF-20/HBT2@LCF-20.



Figure S27. The solid state UV-vis absorption spectrum of NIR@DCF-20/NIR@LCF-20,





 Figure S28. (a) CD spectra of DCF-20/LCF-20; (b) HBT1@DCF-20/HBT1@LCF-20; (c)

 HBT1@DCF-20/HBT1@LCF-20;
 (d)
 C152@DCF-20/C152@LCF-20.



Figure S29. CPL and glum of HBT1@DCF-20 and LCF-20 under 360 nm excitation.

Table S4. A summary of reported host-guest MOFs-based CPL materials.

Entry	MOFs	Guests	Emission (nm)	g <sub>lum</sub> (×10 <sup>-3</sup> )	Ref.
1	Chiral ZIF-8	dyes	505,578	±0.3,±1.2	Angew. Chem. Int. Ed.
					2019, 58, 4978–4982
2	CD-HF	PyC-	500	3.5	J. Am. Chem. Soc.
					2022, 144, 9380–9389
3	P-/M-Et(Cd)	o/p/m-PhF	512,507,513	-8.3/8.4, -	Adv. Sci. 2023, 10
				8.3/8.7, -8.4/8.6	2207333
4	(P-(+)/M-	DSM	615	+2.1/-1.3	Chem. Sci. 2020, 11,
	(-)-TbBTC)				9154–9161
5	DCF/LCF-12	pyrene	612	- 3.7/+5.1	Adv. Funct. Mater.
					2023, 33, 2300105
6	SURchirMOF	Ln(acac) <sub>3</sub>	550	+8.5/-8.5	Nano Res. 2021, 15,
					1102–1108
7	L/D-CMOF	CBS, FS, RB,	435,535,618,585,	+11.5/-11.5,	Adv. Mater. 2020, 20,
		R6G, AR	610	+3.4/-3.4, +7.5/-	2002914
				7.5, +11/-11,	
				+3.5/-3.5	
8	DCF-1/LCF-1	C6, MCz	535, 525	none, +9.1/-13.9	ACS Mater. Lett. 2024,
					6, 2559–2568
9	DCF-20/LCF-20	HBT1, HBT2,	550,550, ,500,	+2.5/-7.5,	this work
		C152, NIR	650	+10.9/-10.9,	
				+1.2/-1.2,	
				+14.7/-16.3	



Figure 30. Linear dichroism spectra for DCF-20/LCF-20 and composites. (a) DCF-20/LCF-20; (b)HBT1@DCF-20-3/HBT1@LCF-20-3; (c) HBT2@DCF-20-3/HBT2@LCF-20-3; (d) C152@DCF-20-3/C152@LCF-20-3.



**Figure 31.** (a) Polarized emission spectra of DCF-20 crystal powder at changed angles (0–360°); (b) maximum emission intensity of DCF-20 at different polarizer rotation angles; (c) Polarized emission spectra of C152@DCF-20-3 crystal powder at changed angles (0–360°); (d) maximum emission intensity of C152@DCF-20-3 at different polarizer rotation angles; (e) Polarized emission spectra of HBT2@DCF-20-3 crystal powder at changed angles (0–360°); (f) maximum emission intensity of HBT2@DCF-20-3 at different polarizer rotation angles.

	HBT1 $(5 \times 10^3)$	C152 (5 $\times$ 10 <sup>3</sup>	NIR $(5 \times 10^3)$	White or not
	mol/L), mL	mol/L), mL	mol/L), mL	
WD-1	1.00	0.80	0.40	Yes
WD-2	0.60	0.60	0.30	Yes
WD-3	1.00	0.40	0.40	
WD-4	0.40	0.80	0.60	
WD-5	0.40	0.20	0.20	Yes
WD-6	0.40	0.30	0.15	

**Table S5.** The program for the generation of white-lighting emission.

When LCF-20 was used as host to encapsulate these guest molecules, the same processed were carried out.



Figure S32. The photographs of WD-1 to WD-6 under UV lamp and day light at ambient conditions.



Figure S33. The emission behaviors including emission peaks and CIE coordinates of WD-1.



Figure S34. The emission behaviors including emission peaks and CIE coordinates of WD-2.



Figure S35. The emission behaviors including emission peaks and CIE coordinates of WD-3.



Figure S36. The emission behaviors including emission peaks and CIE coordinates of WD-4.



Figure S37. The emission behaviors including emission peaks and CIE coordinates of WD-5.



Figure S38. The emission behaviors including emission peaks and CIE coordinates of WD-6.







Figure S40. The fluorescence quantum yields of WL-5.



Figure S41. The optimized host-guest structure of HBT1@DCF-20 and HBT2@DCF-20.



**Figure S42.** (a) CPL spectra of HBT1/C152/NIR@DCF-20 and HBT1/C152/NIR@LCF-20 ( $\lambda$  ex. of 340 nm); (b) glum of HBT1@C152@NIR@DCF-20 and HBT1@C152@NIR@LCF-20; (c) PL spectrum the white light emitting devices, the CIE coordinate diagram of the WLED.

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Identification code	DCF-20	LCF-20
Number of CCDC	2364863	2364864
Empirical formula	$C_{16}H_{21.50}N_{3.50}O_{3.50}Zn$	$C_{16}H_{22.50}N_{3.50}O_4Zn$
Formula weight	384.24	393.24
Temperature/K	290	290
Crystal system	tetragonal	tetragonal
Space group	P4 <sub>1</sub> 2 <sub>1</sub> 2	P4 <sub>3</sub> 2 <sub>1</sub> 2
a / Å	18.1052(4)	18.1042(4)
b / Å	18.1052(4)	18.1042(4)
c / Å	13.2724(3)	13.2792(4)
α / °	90	90
eta / °	90	90
γ / °	90	90
Volume/ Å <sup>3</sup>	4350.7(2)	4352.4(2)
Ζ	8	8
$ ho calcg/cm^3$	1.173	1.200
$\mu$ / mm <sup>-1</sup>	1.147	1.150
F(000)	1264	1640
Crystal size/ mm <sup>3</sup>	$0.08 \times 0.10 \times 0.13$	$0.08 \times 0.10 \times 0.13$
Radiation	Mo-K $\alpha$ ( $\lambda = 0.71073$ )	Mo-K $\alpha$ ( $\lambda = 0.71073$ )
$2\theta$ range for data collection/°	7.592 to 54.166	7.596 to 59.5556
Inday manage	-21 $\leq h \leq$ 24, -24 $\leq k \leq$ 19, -	-11 $\leq$ h $\leq$ 24, -24 $\leq$ k $\leq$ 15, -
Index ranges	$18 \le 1 \le 9$	$18 \leq l \leq 16$
Reflections collected	10487	11548
T. 1	5016 [ $R_{int} = 0.0273$ , $R_{sigma} =$	5024 [ $R_{int} = 0.0298$ , $R_{sigma} =$
Independent reflections	0.0525]	0.0482]
Goodness-of-fit on F <sup>2</sup>	1.077	1.064
Flcak	0.028(11)	0.000(11)
$R_1 \left[I > 2\sigma \left(I\right)\right]$	$R_1 = 0.0379, wR_2 = 0.0846$	$R_1 = 0.0375, wR_2 = 0.0889$
wR <sub>2</sub> (all data)	$R_1 = 0.0475, wR_2 = 0.0880$	$R_1 = 0.0458, wR_2 = 0.0925$
$R = \Sigma   F_{\rm o}  -  F_{\rm c}   / \Sigma  F_{\rm o} ,$	$wR = \{\Sigma[w( F_o 2 -  F_c ^2) -  F_c ^2\}$	$( F_o 4)]^{1/2}, \qquad w =$
1/[\s^2^(Fo^2^)+(0.0519P)^2^]	where $P = (Fo^2 + 2Fc^2)/3$ for	r DCF-20.
$W = 1/[\sqrt{s^2}(Fo^2) + (0.0470P)]$	$^{2^{1}}$ where P = (Fo <sup>2^</sup> +2Fc <sup>2</sup> )	/3 for LCF-15.

Table S6. The crystallographic parameters of DCF-20 and LCF-20

label	type_symbol	Z	у	Z	U_iso_or_equiv	adp_type	occupanc
							у
Zn1	Zn	0.41756	0.19601	0.64991	0.02363	Uani	1.00
N2	Ν	0.49019	0.18162	0.41075	0.02436	Uani	1.00
N3	Ν	0.50019	0.18054	0.53660	0.02825	Uani	1.00
N4	Ν	0.81262	0.07705	0.41263	0.03374	Uani	1.00
05	0	0.45747	0.20756	0.80908	0.08893	Uani	1.00
C6	С	0.60659	0.15183	0.44837	0.02847	Uani	1.00
C7	С	0.67956	0.12717	0.43305	0.03421	Uani	1.00
C8	С	0.55377	0.16400	0.35366	0.03101	Uani	1.00
H9	Н	0.56066	0.16002	0.25112	0.04900	Uiso	1.00
C10	С	0.57091	0.16298	0.56295	0.03154	Uani	1.00
H11	Н	0.59284	0.15677	0.65850	0.04900	Uiso	1.00
C12	С	0.74801	0.07047	0.33691	0.04589	Uani	1.00
H13	Н	0.74808	0.04568	0.27013	0.07100	Uiso	1.00
C14	С	0.68128	0.09578	0.34381	0.05184	Uani	1.00
H15	Н	0.63049	0.09008	0.28276	0.08000	Uiso	1.00
C16	С	0.81311	0.10779	0.49875	0.05198	Uani	1.00
H17	Н	0.86480	0.11205	0.55889	0.08200	Uiso	1.00
C18	С	0.74614	0.13308	0.51190	0.05169	Uani	1.00
H19	Н	0.74623	0.15698	0.58253	0.08000	Uiso	1.00
N20	Ν	0.47592	0.17244	0.87079	0.08829	Uani	1.00
O21	0	0.47256	0.13796	0.81208	0.12208	Uani	1.00
O22	0	0.49888	0.17330	0.98958	0.13402	Uani	1.00
Zn23	Zn	0.58061	0.30513	0.14273	0.02358	Uani	1.00
N24	Ν	0.51056	0.31693	0.90135	0.02440	Uani	1.00
N25	Ν	0.49883	0.31944	0.02683	0.02824	Uani	1.00
N26	Ν	0.18468	0.41780	0.89373	0.03383	Uani	1.00
O27	0	0.53896	0.29410	0.30315	0.08944	Uani	1.00
C28	С	0.38972	0.34281	0.93243	0.02860	Uani	1.00
C29	С	0.31530	0.36589	0.91131	0.03428	Uani	1.00
C30	С	0.44580	0.33148	0.84074	0.03107	Uani	1.00
H31	Н	0.44024	0.33390	0.73758	0.04900	Uiso	1.00
C32	С	0.42520	0.33458	0.04942	0.03163	Uani	1.00
H33	Н	0.40074	0.34104	0.14366	0.04900	Uiso	1.00
C34	С	0.24982	0.42389	0.81623	0.04618	Uani	1.00
H35	Н	0.25147	0.44922	0.75004	0.07100	Uiso	1.00
C36	С	0.31506	0.39757	0.82111	0.05219	Uani	1.00
H37	Н	0.36670	0.40333	0.75990	0.08000	Uiso	1.00
C38	С	0.18201	0.38634	0.97900	0.05259	Uani	1.00
H39	Н	0.13006	0.38252	0.04080	0.08200	Uiso	1.00
C40	С	0.24771	0.36009	-0.00933	0.05215	Uani	1.00
H41	Н	0.24672	0.33622	0.06273	0.08000	Uiso	1.00
N42	N	0.51944	0.32951	0.36076	0.08808	Uani	1.00
043	0	0.52008	0.36343	0.29650	0.12230	Uani	1.00
044	0	0.49835	0.32949	0.48124	0.13405	Uani	1.00
Zn45	Zn	0.09934	0.45599	0.88471	0.02357	Uani	1.00
N46	N	0.12899	0.49296	0.64558	0.02440	Uani	1.00
N47	N	0.12994	0.49785	0.77148	0.02829	Uani	1.00
N48	N	0.34185	0.15339	0.65928	0.03396	Uani	1.00
049	0	0.07361	0.47611	0.04373	0.08818	Uani	1.00

 Table S7. Atomic coordinates of optimized HBT1@DCF-20 models.

C50	С	0.18550	0.05284	0.60117	0.02857	Uani	1.00
C51	C C	0.18550	0.05264	0.67559	0.02837	Uani	1.00
C52	C C	0.25007	0.52515	0.58903	0.03108	Uani	1.00
С52 H53	н	0.10+2+	0.02756	0.38503	0.03108	Uiso	1.00
C54	n C	0.1755	0.02750	0.90633	0.03175	Uani	1.00
U54 U55	ч	0.10039	0.03388	0.00033	0.03175	Uiso	1.00
П33 С56	П	0.1/140	0.04755	0.90127	0.04900	UISO	1.00
C30	U U	0.33370	0.12034	0.56515	0.04041	Uani	1.00
П37 С59	П	0.40428	0.11941	0.51775	0.07100	UISO	1.00
U38 1150	U	0.300/3	0.08812	0.58/90	0.05247	Uani	1.00
H39	H	0.3113/	0.00221	0.52097	0.08000	UISO	1.00
	U	0.27910	0.10010	0.74550	0.05248	Uani	1.00
	H	0.27105	0.18139	0.80413	0.08200		1.00
C62	U U	0.22599	0.12264	0.75455	0.05226	Uani	1.00
H63	H	0.1//28	0.12383	0.82399	0.08000	U1SO	1.00
N64	N	0.14208	0.48657	0.10341	0.08822	Uani	1.00
065	0	0.21070	0.48438	0.04394	0.12288	Uanı	1.00
066	0	0.13923	0.49948	0.22087	0.13492	Uani	1.00
Zn67	Zn	0.90071	0.04078	0.40008	0.02351	Uani	1.00
N68	Ν	0.87371	0.00668	0.15936	0.02434	Uani	1.00
N69	Ν	0.87335	-0.00029	0.28467	0.02823	Uani	1.00
N70	Ν	0.65654	0.34806	0.15027	0.03384	Uani	1.00
O71	0	0.92695	0.01989	0.55831	0.08877	Uani	1.00
C72	С	0.81269	0.44878	0.18876	0.02852	Uani	1.00
C73	С	0.76115	0.41296	0.17133	0.03428	Uani	1.00
C74	С	0.83806	-0.02443	0.10069	0.03100	Uani	1.00
H75	Н	0.82650	0.47543	-0.00592	0.04900	Uiso	1.00
C76	С	0.83773	0.46457	0.30428	0.03165	Uani	1.00
H77	Н	0.82566	0.45244	0.39927	0.04900	Uiso	1.00
C78	С	0.64726	0.38114	0.07260	0.04608	Uani	1.00
H79	Н	0.59869	0.38239	0.00487	0.07100	Uiso	1.00
C80	С	0.70016	0.41369	0.07974	0.05220	Uani	1.00
H81	Н	0.69147	0.43983	0.01774	0.08000	Uiso	1.00
C82	С	0.71635	0.34619	0.23794	0.05229	Uani	1.00
H83	Н	0.72178	0.31983	0.29982	0.08200	Uiso	1.00
C84	С	0.76898	0.37875	0.25132	0.05193	Uani	1.00
H85	Н	0.81521	0.37729	0.32346	0.08000	Uiso	1.00
N86	Ν	0.85879	0.00984	0.62276	0.08818	Uani	1.00
087	0	0.79027	0.00928	0.56479	0.12208	Uani	1.00
O88	0	0.86219	-0.00040	0.74333	0.13454	Uani	1.00
Zn89	Zn	0.08119	0.44664	0.57286	0.02363	Uani	1.00
N90	Ν	0.00848	0.43215	0.81204	0.02439	Uani	1.00
N91	Ν	-0.00202	0.43155	0.68637	0.02825	Uani	1.00
N92	Ν	0.68736	0.32859	0.81825	0.03376	Uani	1.00
O93	Ο	0.04232	0.45841	0.41248	0.08892	Uani	1.00
C94	С	0.89130	0.40371	0.77701	0.02852	Uani	1.00
C95	С	0.81870	0.37918	0.79465	0.03423	Uani	1.00
C96	С	-0.05518	0.41509	0.87054	0.03105	Uani	1.00
H97	Н	0.93855	0.41077	0.97327	0.04900	Uiso	1.00
C98	С	0.92665	0.41478	0.66149	0.03158	Uani	1.00
H99	Н	0.90418	0.40891	0.56649	0.04900	Uiso	1.00
C100	С	0.75211	0.32230	0.89442	0.04610	Uani	1.00
H101	Н	0.75305	0.29739	0.96219	0.07100	Uiso	1.00
C102	С	0.81804	0.34780	0.88577	0.05203	Uani	1.00

11102		0.0(021	0.24212	0.04(50	0.00000	<b>T</b> 1'	1.00
H103	H	0.86921	0.34213	0.94658	0.08000	Uiso	1.00
C104	C U	0.68554	0.35948	0.73093	0.05219	Uani	1.00
H105	H	0.63362	0.36357	0.67076	0.08200	Uiso	1.00
C106	С	0.75167	0.38507	0.71627	0.05192	Uanı	1.00
H107	Н	0.75074	0.40904	0.64456	0.08000	Uiso	1.00
N108	Ν	0.02316	0.42328	0.35378	0.08838	Uani	1.00
O109	0	0.02429	0.38905	0.41618	0.12268	Uani	1.00
O110	0	0.00176	0.42389	0.23419	0.13472	Uani	1.00
Zn111	Zn	0.91930	0.05424	0.08808	0.02357	Uani	1.00
N112	Ν	0.99010	0.06741	0.32659	0.02434	Uani	1.00
N113	Ν	1.00080	0.06954	0.20067	0.02819	Uani	1.00
N114	Ν	0.31297	0.17054	0.32781	0.03365	Uani	1.00
O115	Ο	0.95991	0.04380	0.92711	0.08958	Uani	1.00
C116	С	0.10634	0.09741	0.28958	0.02849	Uani	1.00
C117	С	0.17965	0.12132	0.30619	0.03420	Uani	1.00
C118	С	1.05299	0.08457	0.38408	0.03098	Uani	1.00
H119	Н	0.05924	0.08762	0.48683	0.04900	Uiso	1.00
C120	С	0.07151	0.08727	0.17458	0.03150	Uani	1.00
H121	Н	0.09424	0.09404	0.07917	0.04900	Uiso	1.00
C122	С	0.24784	0.17700	0.40496	0.04581	Uani	1.00
H123	Н	0.24741	0.20152	0.472.77	0.07100	Uiso	1.00
C124	C	0 18101	0.15207	0 39760	0.05182	Uani	1.00
H125	н	0.12976	0.15207	0.45963	0.08000	Uiso	1.00
C126	C C	0.31405	0.14018	0.24032	0.05210	Uani	1.00
H127	н	0.31403	0.13605	0.17880	0.03210	Uiso	1.00
C128	II C	0.30000	0.11536	0.17665	0.05166	Uani	1.00
U120	с u	0.24097	0.11330	0.22030	0.03100	Uiso	1.00
N120	II N	0.24/44	0.09190	0.13447	0.08000	Uiso	1.00
N130	N	0.97007	0.07939	0.80030	0.08851	Uani	1.00
0131	0	0.9/3/0	0.11338	0.92814	0.12192	Uani	1.00
7 122	0	0.99624	0.07944	0.74549	0.13435	Uani	1.00
Zn133	Zn	0.40008	0.20723	0.33/32	0.02352	Uani	1.00
N134	N	0.37030	0.24274	0.5/630	0.02441	Uani	1.00
N135	N	0.37090	0.24879	0.45055	0.02828	Uani	1.00
N136	N	0.15616	0.40332	0.56556	0.03404	Uani	1.00
0137	0	0.42578	0.22776	0.17772	0.08862	Uanı	1.00
C138	С	0.31112	0.30162	0.53803	0.02864	Uani	1.00
C139	С	0.26007	0.33777	0.55160	0.03438	Uani	1.00
C140	С	0.33310	0.27415	0.63286	0.03110	Uani	1.00
H141	Н	0.32162	0.27644	0.73495	0.04900	Uiso	1.00
C142	С	0.33628	0.28463	0.42391	0.03180	Uani	1.00
H143	Н	0.32529	0.29627	0.32828	0.04900	Uiso	1.00
C144	С	0.14231	0.36993	0.64021	0.04649	Uani	1.00
H145	Н	0.09082	0.36877	0.70362	0.07100	Uiso	1.00
C146	С	0.19463	0.33701	0.63651	0.05262	Uani	1.00
H147	Н	0.18261	0.31072	0.69648	0.08000	Uiso	1.00
C148	С	0.22011	0.40513	0.48368	0.05284	Uani	1.00
H149	Н	0.22921	0.43180	0.42425	0.08200	Uiso	1.00
C150	С	0.27267	0.37217	0.47384	0.05247	Uani	1.00
H151	Н	0.32250	0.37345	0.40648	0.08000	Uiso	1.00
N152	Ν	0.35730	0.23764	0.11562	0.08794	Uani	1.00
O153	0	0.28863	0.23752	0.17549	0.12253	Uani	1.00
0154	0	0.36040	0.24823	-0.00476	0.13427	Uani	1.00
Zn155	Zn	0.60156	0.29141	0.83149	0.02356	Uani	1.00

N156         N         0.62897         0.25779         0.07501         0.02436         Uani         1.00           N157         N         0.62998         0.25077         0.95011         0.02232         Uani         1.00           N158         N         0.84201         0.09659         0.08219         0.03394         Uani         1.00           C160         C         0.657738         0.27017         0.67415         0.08820         Uani         1.00           C161         C         0.73734         0.16182         0.03344         0.04900         Uiani         1.00           C164         C         0.66427         0.22649         0.13594         0.03103         Uani         1.00           C164         C         0.66436         0.21460         0.92838         0.03170         Uani         1.00           H165         H         0.67634         0.20222         0.83429         0.04900         Uiso         1.00           C164         C         0.87634         0.21434         0.8000         Uiso         1.00           H167         H         0.90133         0.13016         0.22545         0.07100         Uiso         1.00           C170 <th></th> <th></th> <th></th> <th></th> <th></th> <th></th> <th></th> <th></th>								
N157         N         0.62998         0.25077         0.95011         0.02228         Uani         1.00           N158         N         0.84201         0.09659         0.08219         0.03394         Uani         1.00           0159         0         0.57738         0.27017         0.67415         0.08820         Uani         1.00           C160         C         0.67314         0.16182         0.06354         0.03430         Uani         1.00           C161         C         0.67373         0.12247         0.23844         0.04900         Uiso         1.00           C164         C         0.66436         0.21460         0.92838         0.03170         Uani         1.00           C164         C         0.66436         0.21272         0.15923         0.04616         Uani         1.00           C166         C         0.7807         0.02247         0.02230         Uani         1.00           H165         H         0.90133         0.1316         0.22453         0.07100         Uiso         1.00           C168         C         0.79200         0.16199         0.15322         Uani         1.00           C177         C	N156	Ν	0.62897	0.25779	0.07501	0.02436	Uani	1.00
N158         N         0.84201         0.09659         0.08219         0.03394         Uani         1.00           0159         O         0.57738         0.27017         0.67415         0.08820         Uani         1.00           C160         C         0.65741         0.19826         0.04343         Uani         1.00           C161         C         0.67350         0.22472         0.23844         0.04900         Uiso         1.00           C164         C         0.66436         0.21460         0.92838         0.03170         Uani         1.00           H165         H         0.67634         0.20221         0.83429         0.04900         Uiso         1.00           H167         H         0.90133         0.13016         0.22545         0.07100         Uiso         1.00           H167         H         0.90133         0.13016         0.22545         0.07100         Uiso         1.00           H167         H         0.9037         0.15922         0.05220         Uani         1.00           C168         C         0.77807         0.0957         -0.02289         0.05197         Uani         1.00           C1717         C	N157	Ν	0.62998	0.25077	0.95011	0.02828	Uani	1.00
0159         0         0.57738         0.27017         0.67415         0.08820         Uani         1.00           C160         C         0.68741         0.19826         0.04489         0.02851         Uani         1.00           C161         C         0.73734         0.16182         0.03334         0.03103         Uani         1.00           C162         C         0.66427         0.22649         0.13594         0.03103         Uani         1.00           H163         H         0.67350         0.22472         0.23844         0.04900         Uiso         1.00           H165         H         0.67634         0.22122         0.83429         0.04900         Uiso         1.00           H167         H         0.9633         0.13101         0.22454         0.07100         Uiso         1.00           H167         H         0.80868         0.18787         0.21434         0.08000         Uiso         1.00           H171         H         0.74777         0.06897         0.93599         0.08220         Uani         1.00           H173         H         0.68091         0.12690         0.61320         0.89815         Uani         1.00      <	N158	Ν	0.84201	0.09659	0.08219	0.03394	Uani	1.00
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	O159	0	0.57738	0.27017	0.67415	0.08820	Uani	1.00
C161         C         0.73734         0.16182         0.06354         0.03103         Uani         1.00           C162         C         0.66427         0.22472         0.23844         0.04900         Uiso         1.00           C164         C         0.66436         0.22472         0.23844         0.04900         Uiso         1.00           C164         C         0.66436         0.22227         0.5223         0.04616         Uani         1.00           H167         H         0.90133         0.13016         0.22545         0.07100         Uiso         1.00           H167         H         0.90133         0.13016         0.22545         0.07100         Uiso         1.00           H168         H         0.8068         0.18787         0.21434         0.8000         Uiso         1.00           C170         C         0.78087         0.93599         0.08200         Uiso         1.00           H171         H         0.64030         0.12690         0.91437         0.08000         Uiso         1.00           N174         N         0.46432         0.2236         Uani         1.00           N174         N         0.46432	C160	С	0.68741	0.19826	0.04489	0.02851	Uani	1.00
C162         C         0.66427         0.23249         0.13594         0.03103         Uani         1.00           H163         H         0.67350         0.22472         0.23844         0.04900         Uiso         1.00           H165         H         0.67634         0.2222         0.83429         0.04900         Uiso         1.00           C166         C         0.85205         0.12927         0.15923         0.04616         Uani         1.00           H167         H         0.90133         0.13016         0.22545         0.07100         Uiso         1.00           H167         H         0.90133         0.13106         0.22545         0.07100         Uiso         1.00           H171         H         0.77477         0.06897         0.91539         0.82200         Uiso         1.00           H173         H         0.66891         0.12690         0.91437         0.08000         Uiso         1.00           C172         C         0.72803         0.12780         0.68125         Uani         1.00           D175         O         0.71451         0.26050         0.67122         0.1220         Uani         1.00           D177	C161	С	0.73734	0.16182	0.06354	0.03430	Uani	1.00
H163         H         0.67350         0.22472         0.23844         0.04900         Uiso         1.00           C164         C         0.66436         0.21460         0.92838         0.03170         Uani         1.00           C166         C         0.85205         0.12927         0.15923         0.04616         Uani         1.00           H167         H         0.90133         0.13016         0.22545         0.07100         Uiso         1.00           H169         H         0.8068         0.1877         0.21434         0.08000         Uiso         1.00           H171         H         0.7477         0.06897         0.93599         0.08200         Uiso         1.00           H173         H         0.66091         0.12690         0.91437         0.08000         Uiso         1.00           N174         N         0.44632         0.23596         0.06123         0.08815         Uani         1.00           N174         N         0.44632         0.22547         0.49311         0.131418         Uani         1.00           N174         N         0.44633         0.68155         0.46823         0.02436         Uani         1.00 <t< td=""><td>C162</td><td>С</td><td>0.66427</td><td>0.22649</td><td>0.13594</td><td>0.03103</td><td>Uani</td><td>1.00</td></t<>	C162	С	0.66427	0.22649	0.13594	0.03103	Uani	1.00
C164         C         0.66436         0.21400         0.92838         0.03170         Uani         1.00           H165         H         0.67634         0.20222         0.83429         0.04900         Uiso         1.00           C166         C         0.85205         0.12927         0.15232         0.04616         Uani         1.00           H167         H         0.90133         0.13016         0.22545         0.07100         Uiso         1.00           C168         C         0.79920         0.16199         0.15322         0.05220         Uani         1.00           H171         H         0.77477         0.06897         0.93599         0.08200         Uiso         1.00           H173         H         0.64032         0.25906         0.61230         0.08815         Uani         1.00           N174         N         0.64632         0.2596         0.61230         0.08815         Uani         1.00           N174         N         0.64632         0.2596         0.61230         0.08815         Uani         1.00           N174         N         0.64632         0.25903         0.64823         0.02363         Uani         1.00      <	H163	Н	0.67350	0.22472	0.23844	0.04900	Uiso	1.00
H165         H         0.67634         0.20222         0.83429         0.04900         Uiso         1.00           C166         C         0.85205         0.12927         0.15923         0.04616         Uani         1.00           H167         H         0.90133         0.13016         0.25245         0.07100         Uiso         1.00           C168         C         0.79920         0.16199         0.15322         0.05223         Uani         1.00           H169         H         0.80868         0.18787         0.21434         0.08000         Uiso         1.00           C170         C         0.72803         0.12786         0.98498         0.05197         Uani         1.00           H171         H         0.68091         0.12690         0.61220         0.2220         Uani         1.00           N174         N         0.64632         0.26050         0.67122         0.1220         Uani         1.00           N174         N         0.4938         0.68175         0.40832         0.02363         Uani         1.00           N178         N         0.49388         0.68175         0.3374         Uani         1.00           N179	C164	С	0.66436	0.21460	0.92838	0.03170	Uani	1.00
C166         C $0.85205$ $0.12927$ $0.15923$ $0.04616$ Uani $1.00$ H167         H $0.90133$ $0.13016$ $0.22245$ $0.07100$ Uiso $1.00$ C168         C $0.79920$ $0.16199$ $0.15322$ $0.05223$ Uani $1.00$ C170         C $0.78087$ $0.09507$ $-0.00289$ $0.5220$ Uani $1.00$ H171         H $0.77477$ $0.06897$ $0.93599$ $0.08200$ Uiso $1.00$ N174         N $0.64632$ $0.25906$ $0.61230$ $0.0815$ Uani $1.00$ O175         O $0.71451$ $0.26050$ $0.67122$ $0.12220$ Uani $1.00$ O176         O $0.64328$ $0.26333$ Uani $1.00$ O177         Zn $0.41756$ $0.69630$ $0.64823$ $0.02363$ Uani $1.00$ N178         N $0.48938$ $0.68127$ $0.04038$ $0.03374$ U	H165	Н	0.67634	0.20222	0.83429	0.04900	Uiso	1.00
H167H $0.90133$ $0.13016$ $0.22545$ $0.07100$ Uiso $1.00$ C168C $0.79920$ $0.16199$ $0.15322$ $0.05223$ Uani $1.00$ H169H $0.80868$ $0.18787$ $0.21434$ $0.08000$ Uiso $1.00$ C170C $0.78087$ $0.09507$ $-0.02289$ $0.05220$ Uani $1.00$ H171H $0.77477$ $0.06897$ $0.93599$ $0.08200$ Uiso $1.00$ C172C $0.72803$ $0.12786$ $0.98498$ $0.05197$ Uani $1.00$ H173H $0.66091$ $0.12690$ $0.91437$ $0.088000$ Uiso $1.00$ N174N $0.64632$ $0.25996$ $0.61230$ $0.08815$ Uani $1.00$ O175O $0.71451$ $0.26050$ $0.67122$ $0.12220$ Uani $1.00$ N174N $0.46432$ $0.24874$ $0.49313$ $0.02835$ Uani $1.00$ N175N $0.48938$ $0.68175$ $0.40832$ $0.02436$ Uani $1.00$ N178N $0.48938$ $0.68175$ $0.02847$ Uani $1.00$ N180N $0.81244$ $0.57680$ $0.03374$ Uani $1.00$ O181O $0.45783$ $0.77768$ $0.038471$ Uani $1.00$ C182C $0.55905$ $0.65904$ $0.44669$ $0.04900$ Uiso $1.00$ C183C $0.5772$ $0.43260$ $0.03374$ Uani $1.00$	C166	С	0.85205	0.12927	0.15923	0.04616	Uani	1.00
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	H167	Н	0.90133	0.13016	0.22545	0.07100	Uiso	1.00
H169H $0.80868$ $0.18787$ $0.21434$ $0.08000$ Uiso $1.00$ C170C $0.78087$ $0.09507$ $-0.00289$ $0.05220$ Uani $1.00$ H171H $0.77477$ $0.06897$ $0.93599$ $0.08200$ Uiso $1.00$ C172C $0.72803$ $0.12786$ $0.98498$ $0.05197$ Uani $1.00$ H173H $0.68091$ $0.12690$ $0.91437$ $0.08000$ Uiso $1.00$ N174N $0.64632$ $0.25996$ $0.61230$ $0.08815$ Uani $1.00$ O175O $0.71451$ $0.26050$ $0.67122$ $0.1220$ Uani $1.00$ O176O $0.64406$ $0.24874$ $0.49311$ $0.13418$ Uani $1.00$ N178N $0.44938$ $0.68175$ $0.40832$ $0.02436$ Uani $1.00$ N178N $0.48938$ $0.68175$ $0.40832$ $0.02436$ Uani $1.00$ N180N $0.81244$ $0.57680$ $0.01498$ $0.03374$ Uani $1.00$ O181O $0.45783$ $0.70768$ $0.80720$ $0.08893$ Uani $1.00$ C182C $0.66319$ $0.24906$ $0.03421$ Uani $1.00$ C184C $0.55208$ $0.65304$ $0.24906$ $0.03421$ Uani $1.00$ C184C $0.55208$ $0.65904$ $0.24906$ $0.03421$ Uani $1.00$ H185H $0.59150$ $0.65924$ $0.44589$	C168	С	0.79920	0.16199	0.15322	0.05223	Uani	1.00
C170C $0.78087$ $0.09507$ $-0.00289$ $0.05220$ Uani $1.00$ H171H $0.77477$ $0.06897$ $0.93599$ $0.08200$ Uiso $1.00$ C172C $0.72803$ $0.12786$ $0.98498$ $0.05197$ Uani $1.00$ H173H $0.68091$ $0.12690$ $0.91437$ $0.08000$ Uiso $1.00$ N174N $0.64632$ $0.22996$ $0.61230$ $0.08815$ Uani $1.00$ O175O $0.71451$ $0.26050$ $0.67122$ $0.12220$ Uani $1.00$ Zn177Zn $0.41756$ $0.69630$ $0.64823$ $0.02363$ Uani $1.00$ N178N $0.48938$ $0.68053$ $0.53421$ $0.02825$ Uani $1.00$ N179N $0.49938$ $0.65054$ $0.08817$ Uani $1.00$ N180N $0.81244$ $0.57680$ $0.41098$ $0.03374$ Uani $1.00$ C182C $0.60435$ $0.65040$ $0.44669$ $0.02847$ Uani $1.00$ C183C $0.67749$ $0.65272$ $0.33157$ $0.3101$ Uani $1.00$ C184C $0.55208$ $0.66309$ $0.35157$ $0.03101$ Uani $1.00$ C184C $0.56923$ $0.66212$ $0.56080$ $0.3154$ Uani $1.00$ C184C $0.56923$ $0.66212$ $0.56080$ $0.3154$ Uani $1.00$ C184C $0.56876$ $0.33924$ $0.04589$	H169	Н	0.80868	0.18787	0.21434	0.08000	Uiso	1.00
H171         H         0.77477         0.06897         0.93599         0.08200         Uiso         1.00           C172         C         0.72803         0.12786         0.98498         0.05197         Uani         1.00           H173         H         0.66091         0.12690         0.91437         0.08000         Uiso         1.00           N174         N         0.64632         0.25996         0.61230         0.08815         Uani         1.00           O175         O         0.71451         0.26050         0.67122         0.12220         Uani         1.00           O176         O         0.64406         0.24874         0.49311         0.13418         Uani         1.00           N178         N         0.48938         0.68175         0.40832         0.02436         Uani         1.00           N179         N         0.49938         0.68175         0.40832         Uani         1.00           N180         N         0.81244         0.57680         0.03374         Uani         1.00           C181         O         0.45783         0.70768         0.80720         0.08893         Uani         1.00           C182         C	C170	С	0.78087	0.09507	-0.00289	0.05220	Uani	1.00
C172C $0.72803$ $0.12786$ $0.98498$ $0.05197$ Uani $1.00$ H173H $0.68091$ $0.12690$ $0.91437$ $0.08000$ Uiso $1.00$ N174N $0.64632$ $0.25996$ $0.61230$ $0.08815$ Uani $1.00$ O175O $0.71451$ $0.26050$ $0.67122$ $0.12220$ Uani $1.00$ O176O $0.64406$ $0.24874$ $0.49311$ $0.13418$ Uani $1.00$ Zn177Zn $0.41756$ $0.69630$ $0.64823$ $0.02363$ Uani $1.00$ N178N $0.48938$ $0.68175$ $0.40832$ $0.02436$ Uani $1.00$ N179N $0.49938$ $0.68053$ $0.53421$ $0.02825$ Uani $1.00$ O181O $0.45783$ $0.70768$ $0.80720$ $0.08893$ Uani $1.00$ C182C $0.60435$ $0.65040$ $0.44669$ $0.02847$ Uani $1.00$ C183C $0.67749$ $0.62572$ $0.43260$ $0.03421$ Uani $1.00$ C184C $0.55905$ $0.65094$ $0.24906$ $0.04900$ Uiso $1.00$ C185C $0.74664$ $0.56876$ $0.33924$ $0.04589$ Uani $1.00$ H187H $0.59119$ $0.65251$ $0.6300$ Uiso $1.00$ C188C $0.74664$ $0.56876$ $0.33924$ $0.04589$ Uani $1.00$ C190C $0.67856$ $0.53912$ $0.3481$	H171	Н	0.77477	0.06897	0.93599	0.08200	Uiso	1.00
H173         H         0.68091         0.12690         0.91437         0.08000         Uiso         1.00           N174         N         0.64632         0.25996         0.61230         0.08815         Uani         1.00           O175         O         0.71451         0.26050         0.67122         0.12220         Uani         1.00           O176         O         0.64406         0.24874         0.49311         0.13418         Uani         1.00           Zn177         Zn         0.41756         0.69630         0.64823         0.02363         Uani         1.00           N178         N         0.48938         0.68175         0.40832         0.02455         Uani         1.00           N179         N         0.49938         0.68053         0.53421         0.03374         Uani         1.00           O181         O         0.45783         0.70768         0.80720         0.08893         Uani         1.00           C183         C         0.66749         0.62572         0.43260         0.03421         Uani         1.00           C184         C         0.55905         0.65904         0.24906         0.04900         Uiso         1.00	C172	С	0.72803	0.12786	0.98498	0.05197	Uani	1.00
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	H173	Н	0.68091	0.12690	0.91437	0.08000	Uiso	1.00
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	N174	N	0.64632	0.25996	0.61230	0.08815	Uani	1.00
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0175	0	0 71451	0.26050	0.67122	0 12220	Uani	1.00
21177 $Zn$ $0.41756$ $0.69630$ $0.6423$ $0.02363$ $Uani$ $1.00$ $N178$ N $0.44938$ $0.68175$ $0.40832$ $0.02436$ $Uani$ $1.00$ $N179$ N $0.49938$ $0.68053$ $0.53421$ $0.02825$ $Uani$ $1.00$ $N180$ N $0.81244$ $0.57680$ $0.41098$ $0.03374$ $Uani$ $1.00$ $O181$ O $0.475783$ $0.70768$ $0.80720$ $0.08893$ $Uani$ $1.00$ $O181$ O $0.45783$ $0.70768$ $0.80720$ $0.02847$ $Uani$ $1.00$ $C182$ C $0.60435$ $0.65040$ $0.44669$ $0.03421$ $Uani$ $1.00$ $C184$ C $0.55205$ $0.65904$ $0.24906$ $0.03421$ $Uani$ $1.00$ $H185$ H $0.55905$ $0.65904$ $0.24906$ $0.04900$ $Uiso$ $1.00$ $C186$ C $0.56923$ $0.66212$ $0.56080$ $0.03154$ $Uani$ $1.00$ $H187$ H $0.59119$ $0.65591$ $0.65626$ $0.04900$ $Uiso$ $1.00$ $C188$ C $0.74664$ $0.56876$ $0.33924$ $0.04589$ $Uani$ $1.00$ $H187$ H $0.62510$ $0.59312$ $0.34818$ $0.05184$ $Uani$ $1.00$ $C190$ C $0.67856$ $0.59312$ $0.34818$ $0.05184$ $Uani$ $1.00$ $H191$ H $0.62610$ $0.58761$ $0.57655$ $0.08000$ $Uiso$ $1.00$ <td>0176</td> <td>0 0</td> <td>0.64406</td> <td>0.24874</td> <td>0.49311</td> <td>0.13418</td> <td>Uani</td> <td>1.00</td>	0176	0 0	0.64406	0.24874	0.49311	0.13418	Uani	1.00
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Zn177	Zn	0.41756	0.69630	0.64823	0.02363	Uani	1.00
N179       N       0.49938       0.68053       0.53421       0.02825       Uani       1.00         N180       N       0.81244       0.57680       0.41098       0.03374       Uani       1.00         0181       O       0.45783       0.70768       0.80720       0.08893       Uani       1.00         C182       C       0.60435       0.65040       0.44669       0.02847       Uani       1.00         C183       C       0.67749       0.62572       0.43260       0.03421       Uani       1.00         C184       C       0.55905       0.65904       0.24906       0.04900       Uiso       1.00         C186       C       0.55915       0.65021       0.63210       Uani       1.00         H187       H       0.55913       0.6526       0.04900       Uiso       1.00         H187       H       0.59119       0.65591       0.65626       0.04900       Uiso       1.00         H189       H       0.74640       0.54337       0.27478       0.07100       Uiso       1.00         H189       H       0.62610       0.58571       0.29345       0.08000       Uiso       1.00	N178	N	0.48938	0.69050	0.40832	0.02305	Uani	1.00
N170         N         0.57536         0.50535         0.50421         0.03255         0.11         1.00           N180         N         0.81244         0.57680         0.41098         0.03374         Uani         1.00           0181         O         0.45783         0.70768         0.80720         0.08893         Uani         1.00           C182         C         0.60435         0.65040         0.44669         0.02847         Uani         1.00           C183         C         0.67749         0.62572         0.43260         0.03421         Uani         1.00           C184         C         0.55905         0.65904         0.24906         0.04900         Uiso         1.00           C186         C         0.56923         0.66212         0.56080         0.03154         Uani         1.00           H187         H         0.59119         0.65526         0.04900         Uiso         1.00           C188         C         0.74664         0.56876         0.33924         0.04589         Uani         1.00           H189         H         0.74640         0.54337         0.27478         0.07100         Uiso         1.00           C190 <td>N179</td> <td>N</td> <td>0.40038</td> <td>0.68053</td> <td>0.53421</td> <td>0.02825</td> <td>Uani</td> <td>1.00</td>	N179	N	0.40038	0.68053	0.53421	0.02825	Uani	1.00
Nilo         N         0.51244         0.57050         0.41053         0.03814         Uani         1.00           O181         O         0.45783         0.70768         0.80720         0.08893         Uani         1.00           C182         C         0.60435         0.65040         0.44669         0.02847         Uani         1.00           C183         C         0.67749         0.62572         0.43260         0.03421         Uani         1.00           C184         C         0.55905         0.65904         0.24906         0.04900         Uiso         1.00           H185         H         0.55905         0.65911         0.65626         0.04900         Uiso         1.00           H187         H         0.59119         0.65521         0.65626         0.04900         Uiso         1.00           C188         C         0.74664         0.56876         0.33924         0.04589         Uani         1.00           H189         H         0.74640         0.54337         0.27478         0.07100         Uiso         1.00           C190         C         0.67856         0.59312         0.34818         0.05184         Uani         1.00	N180	N	0.81244	0.00055	0.33421	0.02823	Uani	1.00
Oracle         0.43783         0.70768         0.80720         0.00893         Oracle         1.00           C182         C         0.60435         0.65040         0.44669         0.02847         Uani         1.00           C183         C         0.67749         0.62572         0.43260         0.03421         Uani         1.00           C184         C         0.55208         0.66309         0.35157         0.03101         Uani         1.00           H185         H         0.55905         0.66212         0.56080         0.03154         Uani         1.00           C186         C         0.56923         0.66212         0.56080         0.03154         Uani         1.00           C188         C         0.74664         0.56876         0.33924         0.04589         Uani         1.00           H189         H         0.74640         0.54337         0.27478         0.07100         Uiso         1.00           C190         C         0.67856         0.59312         0.34818         0.05184         Uani         1.00           H191         H         0.62610         0.58571         0.29345         0.8000         Uiso         1.00 <td< td=""><td>0181</td><td>N</td><td>0.01244</td><td>0.37080</td><td>0.41036</td><td>0.03374</td><td>Uani</td><td>1.00</td></td<>	0181	N	0.01244	0.37080	0.41036	0.03374	Uani	1.00
C182C $0.50435$ $0.05040$ $0.43057$ $0.02847$ $0.0111$ $1.00$ C183C $0.67749$ $0.62572$ $0.43260$ $0.03421$ Uani $1.00$ C184C $0.55208$ $0.66309$ $0.35157$ $0.03101$ Uani $1.00$ H185H $0.55905$ $0.65904$ $0.24906$ $0.04900$ Uiso $1.00$ C186C $0.56923$ $0.66212$ $0.56080$ $0.03154$ Uani $1.00$ H187H $0.59119$ $0.65591$ $0.65626$ $0.04900$ Uiso $1.00$ C188C $0.74664$ $0.56876$ $0.33924$ $0.04589$ Uani $1.00$ H189H $0.74640$ $0.54337$ $0.27478$ $0.07100$ Uiso $1.00$ C190C $0.67856$ $0.59312$ $0.34818$ $0.05184$ Uani $1.00$ H191H $0.62610$ $0.58571$ $0.29345$ $0.08000$ Uiso $1.00$ C192C $0.81281$ $0.60821$ $0.49470$ $0.05198$ Uani $1.00$ H193H $0.86511$ $0.61349$ $0.55255$ $0.08200$ Uiso $1.00$ C194C $0.74536$ $0.67235$ $0.86735$ $0.08829$ Uani $1.00$ H195H $0.74536$ $0.67265$ $0.12208$ Uani $1.00$ N196N $0.47326$ $0.63826$ $0.86655$ $0.12208$ Uani $1.00$ N196N $0.47631$ $0.67263$ $0.9$	C182	C C	0.45785	0.70708	0.80720	0.03893	Uani	1.00
C183C $0.07/49$ $0.025/2$ $0.43200$ $0.03421$ Can1.00C184C $0.55208$ $0.66309$ $0.35157$ $0.03101$ Uani $1.00$ H185H $0.55905$ $0.65904$ $0.24906$ $0.04900$ Uiso $1.00$ C186C $0.56923$ $0.66212$ $0.56080$ $0.03154$ Uani $1.00$ H187H $0.59119$ $0.65591$ $0.65626$ $0.04900$ Uiso $1.00$ C188C $0.74664$ $0.56876$ $0.33924$ $0.04589$ Uani $1.00$ C189H $0.74640$ $0.54337$ $0.27478$ $0.07100$ Uiso $1.00$ C190C $0.67856$ $0.59312$ $0.34818$ $0.05184$ Uani $1.00$ H191H $0.62610$ $0.58571$ $0.29345$ $0.08000$ Uiso $1.00$ C192C $0.81281$ $0.60821$ $0.49470$ $0.5198$ Uani $1.00$ H193H $0.86511$ $0.61349$ $0.55255$ $0.08200$ Uiso $1.00$ C194C $0.74506$ $0.63303$ $0.50799$ $0.5169$ Uani $1.00$ H195H $0.74536$ $0.67255$ $0.88000$ Uiso $1.00$ N196N $0.47631$ $0.67235$ $0.86675$ $0.12208$ Uani $1.00$ N196N $0.47631$ $0.67263$ $0.98652$ $0.13402$ Uani $1.00$ N200N $0.51128$ $0.81902$ $0.91438$ <td>C182</td> <td>C C</td> <td>0.00433</td> <td>0.03040</td> <td>0.44009</td> <td>0.02847</td> <td>Uani</td> <td>1.00</td>	C182	C C	0.00433	0.03040	0.44009	0.02847	Uani	1.00
C184       C       0.53208       0.68309       0.53137       0.03101       Uani       1.00         H185       H       0.55905       0.65904       0.24906       0.04900       Uiso       1.00         C186       C       0.56923       0.66212       0.56080       0.03154       Uani       1.00         H187       H       0.59119       0.65591       0.65626       0.04900       Uiso       1.00         C188       C       0.74664       0.56876       0.33924       0.04589       Uani       1.00         H189       H       0.74640       0.54337       0.27478       0.07100       Uiso       1.00         C190       C       0.67856       0.59312       0.34818       0.05184       Uani       1.00         H191       H       0.62610       0.58571       0.29345       0.08000       Uiso       1.00         C192       C       0.81281       0.60821       0.49470       0.05198       Uani       1.00         H193       H       0.86511       0.61349       0.55255       0.08200       Uiso       1.00         N196       N       0.47631       0.67235       0.86735       0.08209       Uani </td <td>C185</td> <td>C C</td> <td>0.07749</td> <td>0.02372</td> <td>0.45200</td> <td>0.03421</td> <td>Uani</td> <td>1.00</td>	C185	C C	0.07749	0.02372	0.45200	0.03421	Uani	1.00
H183       H       0.53903       0.63904       0.24906       0.04900       0.050       1.00         C186       C       0.56923       0.66212       0.56080       0.03154       Uani       1.00         H187       H       0.59119       0.65591       0.65626       0.04900       Uiso       1.00         C188       C       0.74664       0.56876       0.33924       0.04589       Uani       1.00         H189       H       0.74640       0.54337       0.27478       0.07100       Uiso       1.00         C190       C       0.67856       0.59312       0.34818       0.05184       Uani       1.00         H191       H       0.62610       0.58571       0.29345       0.08000       Uiso       1.00         C192       C       0.81281       0.60821       0.49470       0.05198       Uani       1.00         H193       H       0.86511       0.61349       0.55255       0.08200       Uiso       1.00         C194       C       0.74506       0.63303       0.50799       0.05169       Uani       1.00         N196       N       0.47631       0.67235       0.86735       0.08829       Uani<	U104		0.55005	0.00309	0.33137	0.03101	Ulian	1.00
C186       C       0.36923       0.60212       0.36080       0.03134       Uani       1.00         H187       H       0.59119       0.65591       0.65626       0.04900       Uiso       1.00         C188       C       0.74664       0.56876       0.33924       0.04589       Uani       1.00         H189       H       0.74640       0.54337       0.27478       0.07100       Uiso       1.00         C190       C       0.67856       0.59312       0.34818       0.05184       Uani       1.00         H191       H       0.62610       0.58571       0.29345       0.08000       Uiso       1.00         C192       C       0.81281       0.60821       0.49470       0.05198       Uani       1.00         H193       H       0.86511       0.61349       0.55255       0.08200       Uiso       1.00         C194       C       0.74506       0.63303       0.50799       0.05169       Uani       1.00         H195       H       0.74536       0.6764       0.57605       0.08000       Uiso       1.00         N196       N       0.47631       0.67235       0.86735       0.12208       Uani <td>П165</td> <td>П</td> <td>0.55905</td> <td>0.03904</td> <td>0.24900</td> <td>0.04900</td> <td>UISO</td> <td>1.00</td>	П165	П	0.55905	0.03904	0.24900	0.04900	UISO	1.00
H187H0.591190.653910.650260.04900Uiso1.00C188C0.746640.568760.339240.04589Uani1.00H189H0.746400.543370.274780.07100Uiso1.00C190C0.678560.593120.348180.05184Uani1.00H191H0.626100.585710.293450.08000Uiso1.00C192C0.812810.608210.494700.05198Uani1.00C194C0.745060.633030.507990.05169Uani1.00H195H0.745360.657640.576050.08000Uiso1.00N196N0.476310.672350.867350.0829Uani1.00O197O0.473260.638260.806550.12208Uani1.00O198O0.498630.672630.986520.13402Uani1.00N200N0.511280.819020.914380.02440Uani1.00N201N0.501150.820790.040370.02824Uani1.00N202N0.187040.922230.910920.03383Uani1.00O203O0.541960.793330.313780.08944Uani1.00	C180	U	0.50925	0.00212	0.50080	0.03134	Uani	1.00
C188C $0.74664$ $0.56876$ $0.3324$ $0.04589$ Uani $1.00$ H189H $0.74640$ $0.54337$ $0.27478$ $0.07100$ Uiso $1.00$ C190C $0.67856$ $0.59312$ $0.34818$ $0.05184$ Uani $1.00$ H191H $0.62610$ $0.58571$ $0.29345$ $0.08000$ Uiso $1.00$ C192C $0.81281$ $0.60821$ $0.49470$ $0.05198$ Uani $1.00$ H193H $0.86511$ $0.61349$ $0.55255$ $0.08200$ Uiso $1.00$ C194C $0.74506$ $0.63303$ $0.50799$ $0.05169$ Uani $1.00$ H195H $0.74536$ $0.65764$ $0.57605$ $0.08000$ Uiso $1.00$ N196N $0.47631$ $0.67235$ $0.86735$ $0.08829$ Uani $1.00$ O197O $0.47326$ $0.63826$ $0.80655$ $0.12208$ Uani $1.00$ O198O $0.49863$ $0.67263$ $0.98652$ $0.13402$ Uani $1.00$ N200N $0.51128$ $0.81902$ $0.91438$ $0.02440$ Uani $1.00$ N201N $0.50115$ $0.82079$ $0.04037$ $0.02824$ Uani $1.00$ N202N $0.18704$ $0.92223$ $0.91092$ $0.03383$ Uani $1.00$ N202N $0.18704$ $0.92223$ $0.9192$ $0.03383$ Uani $1.00$ N204C $0.39500$ $0.84916$ <	H18/	H	0.59119	0.65591	0.05626	0.04900	UISO	1.00
H189H $0.74640$ $0.54337$ $0.27478$ $0.07100$ Uiso $1.00$ C190C $0.67856$ $0.59312$ $0.34818$ $0.05184$ Uani $1.00$ H191H $0.62610$ $0.58571$ $0.29345$ $0.08000$ Uiso $1.00$ C192C $0.81281$ $0.60821$ $0.49470$ $0.05198$ Uani $1.00$ H193H $0.86511$ $0.61349$ $0.55255$ $0.08200$ Uiso $1.00$ C194C $0.74506$ $0.63303$ $0.50799$ $0.05169$ Uani $1.00$ H195H $0.74536$ $0.65764$ $0.57605$ $0.08000$ Uiso $1.00$ N196N $0.47631$ $0.67235$ $0.86735$ $0.08829$ Uani $1.00$ O197O $0.47326$ $0.63826$ $0.80655$ $0.12208$ Uani $1.00$ O198O $0.49863$ $0.67263$ $0.98652$ $0.13402$ Uani $1.00$ N200N $0.51128$ $0.81902$ $0.91438$ $0.02440$ Uani $1.00$ N201N $0.50115$ $0.82079$ $0.04037$ $0.02824$ Uani $1.00$ N202N $0.18704$ $0.92223$ $0.91092$ $0.03383$ Uani $1.00$ O203O $0.54196$ $0.79333$ $0.31378$ $0.02860$ Uani $1.00$	C188	C U	0.74664	0.56876	0.33924	0.04589	Uani	1.00
C190C0.678560.593120.348180.05184Uani1.00H191H0.626100.585710.293450.08000Uiso1.00C192C0.812810.608210.494700.05198Uani1.00H193H0.865110.613490.552550.08200Uiso1.00C194C0.745060.633030.507990.05169Uani1.00H195H0.745360.657640.576050.08000Uiso1.00N196N0.476310.672350.867350.08829Uani1.00O197O0.473260.638260.806550.12208Uani1.00O198O0.498630.672630.986520.13402Uani1.00N200N0.511280.819020.914380.02440Uani1.00N201N0.501150.820790.040370.02824Uani1.00N202N0.187040.922230.910920.03383Uani1.00O203O0.541960.793330.313780.08944Uani1.00	H189	H	0.74640	0.54337	0.27478	0.07100	Uiso	1.00
H191H0.626100.585710.293450.08000Uiso1.00C192C0.812810.608210.494700.05198Uani1.00H193H0.865110.613490.552550.08200Uiso1.00C194C0.745060.633030.507990.05169Uani1.00H195H0.745360.657640.576050.08000Uiso1.00N196N0.476310.672350.867350.08829Uani1.00O197O0.473260.638260.806550.12208Uani1.00O198O0.498630.672630.986520.13402Uani1.00Zn199Zn0.582860.804510.152990.02358Uani1.00N200N0.511280.819020.914380.02440Uani1.00N201N0.501150.820790.040370.02824Uani1.00N202N0.187040.922230.910920.03383Uani1.00O203O0.541960.793330.313780.08944Uani1.00C204C0.395000.849160.951830.02860Uani1.00	C190	C	0.67856	0.59312	0.34818	0.05184	Uani	1.00
C192       C       0.81281       0.60821       0.49470       0.05198       Uani       1.00         H193       H       0.86511       0.61349       0.55255       0.08200       Uiso       1.00         C194       C       0.74506       0.63303       0.50799       0.05169       Uani       1.00         H195       H       0.74536       0.65764       0.57605       0.08000       Uiso       1.00         N196       N       0.47631       0.67235       0.86735       0.0829       Uani       1.00         O197       O       0.47326       0.63826       0.80655       0.12208       Uani       1.00         O198       O       0.49863       0.67263       0.98652       0.13402       Uani       1.00         Zn199       Zn       0.58286       0.80451       0.15299       0.02358       Uani       1.00         N200       N       0.51128       0.81902       0.91438       0.02440       Uani       1.00         N201       N       0.50115       0.82079       0.04037       0.02824       Uani       1.00         N202       N       0.18704       0.92223       0.91092       0.03383       Uani<	H191	H	0.62610	0.58571	0.29345	0.08000	Uiso	1.00
H193H $0.86511$ $0.61349$ $0.55255$ $0.08200$ Uiso $1.00$ C194C $0.74506$ $0.63303$ $0.50799$ $0.05169$ Uani $1.00$ H195H $0.74536$ $0.65764$ $0.57605$ $0.08000$ Uiso $1.00$ N196N $0.47631$ $0.67235$ $0.86735$ $0.08829$ Uani $1.00$ O197O $0.47326$ $0.63826$ $0.80655$ $0.12208$ Uani $1.00$ O198O $0.49863$ $0.67263$ $0.98652$ $0.13402$ Uani $1.00$ Zn199Zn $0.58286$ $0.80451$ $0.15299$ $0.02358$ Uani $1.00$ N200N $0.51128$ $0.81902$ $0.91438$ $0.02440$ Uani $1.00$ N201N $0.50115$ $0.82079$ $0.04037$ $0.02824$ Uani $1.00$ N202N $0.18704$ $0.92223$ $0.91092$ $0.03383$ Uani $1.00$ O203O $0.54196$ $0.79333$ $0.31378$ $0.02860$ Uani $1.00$	C192	С	0.81281	0.60821	0.49470	0.05198	Uani	1.00
C194       C       0.74506       0.63303       0.50799       0.05169       Uani       1.00         H195       H       0.74536       0.65764       0.57605       0.08000       Uiso       1.00         N196       N       0.47631       0.67235       0.86735       0.08829       Uani       1.00         O197       O       0.47326       0.63826       0.80655       0.12208       Uani       1.00         O198       O       0.49863       0.67263       0.98652       0.13402       Uani       1.00         Zn199       Zn       0.58286       0.80451       0.15299       0.02358       Uani       1.00         N200       N       0.51128       0.81902       0.91438       0.02440       Uani       1.00         N201       N       0.50115       0.82079       0.04037       0.02824       Uani       1.00         N202       N       0.18704       0.92223       0.91092       0.03383       Uani       1.00         O203       O       0.54196       0.79333       0.31378       0.08944       Uani       1.00         C204       C       0.39500       0.84916       0.95183       0.02860       Uani	H193	H	0.86511	0.61349	0.55255	0.08200	Uiso	1.00
H195H0.745360.657640.576050.08000Uiso1.00N196N0.476310.672350.867350.08829Uani1.00O197O0.473260.638260.806550.12208Uani1.00O198O0.498630.672630.986520.13402Uani1.00Zn199Zn0.582860.804510.152990.02358Uani1.00N200N0.511280.819020.914380.02440Uani1.00N201N0.501150.820790.040370.02824Uani1.00N202N0.187040.922230.910920.03383Uani1.00O203O0.541960.793330.313780.08944Uani1.00C204C0.395000.849160.951830.02860Uani1.00	C194	С	0.74506	0.63303	0.50799	0.05169	Uani	1.00
N196       N       0.47631       0.67235       0.86735       0.08829       Uani       1.00         O197       O       0.47326       0.63826       0.80655       0.12208       Uani       1.00         O198       O       0.49863       0.67263       0.98652       0.13402       Uani       1.00         Zn199       Zn       0.58286       0.80451       0.15299       0.02358       Uani       1.00         N200       N       0.51128       0.81902       0.91438       0.02440       Uani       1.00         N201       N       0.50115       0.82079       0.04037       0.02824       Uani       1.00         N202       N       0.18704       0.92223       0.91092       0.03383       Uani       1.00         O203       O       0.54196       0.79333       0.31378       0.08944       Uani       1.00         C204       C       0.39500       0.84916       0.95183       0.02860       Uani       1.00	H195	Н	0.74536	0.65764	0.57605	0.08000	Uiso	1.00
O197         O         0.47326         0.63826         0.80655         0.12208         Uani         1.00           O198         O         0.49863         0.67263         0.98652         0.13402         Uani         1.00           Zn199         Zn         0.58286         0.80451         0.15299         0.02358         Uani         1.00           N200         N         0.51128         0.81902         0.91438         0.02440         Uani         1.00           N201         N         0.50115         0.82079         0.04037         0.02824         Uani         1.00           N202         N         0.18704         0.92223         0.91092         0.03383         Uani         1.00           O203         O         0.54196         0.79333         0.31378         0.08944         Uani         1.00           C204         C         0.39500         0.84916         0.95183         0.02860         Uani         1.00	N196	N	0.47631	0.67235	0.86735	0.08829	Uani	1.00
O198         O         0.49863         0.67263         0.98652         0.13402         Uani         1.00           Zn199         Zn         0.58286         0.80451         0.15299         0.02358         Uani         1.00           N200         N         0.51128         0.81902         0.91438         0.02440         Uani         1.00           N201         N         0.50115         0.82079         0.04037         0.02824         Uani         1.00           N202         N         0.18704         0.92223         0.91092         0.03383         Uani         1.00           O203         O         0.54196         0.79333         0.31378         0.08944         Uani         1.00           C204         C         0.39500         0.84916         0.95183         0.02860         Uani         1.00	O197	0	0.47326	0.63826	0.80655	0.12208	Uani	1.00
Zn199         Zn         0.58286         0.80451         0.15299         0.02358         Uani         1.00           N200         N         0.51128         0.81902         0.91438         0.02440         Uani         1.00           N201         N         0.50115         0.82079         0.04037         0.02824         Uani         1.00           N202         N         0.18704         0.92223         0.91092         0.03383         Uani         1.00           O203         O         0.54196         0.79333         0.31378         0.08944         Uani         1.00           C204         C         0.39500         0.84916         0.95183         0.02860         Uani         1.00	O198	0	0.49863	0.67263	0.98652	0.13402	Uani	1.00
N200         N         0.51128         0.81902         0.91438         0.02440         Uani         1.00           N201         N         0.50115         0.82079         0.04037         0.02824         Uani         1.00           N202         N         0.18704         0.92223         0.91092         0.03383         Uani         1.00           O203         O         0.54196         0.79333         0.31378         0.08944         Uani         1.00           C204         C         0.39500         0.84916         0.95183         0.02860         Uani         1.00	Zn199	Zn	0.58286	0.80451	0.15299	0.02358	Uani	1.00
N201         N         0.50115         0.82079         0.04037         0.02824         Uani         1.00           N202         N         0.18704         0.92223         0.91092         0.03383         Uani         1.00           O203         O         0.54196         0.79333         0.31378         0.08944         Uani         1.00           C204         C         0.39500         0.84916         0.95183         0.02860         Uani         1.00	N200	Ν	0.51128	0.81902	0.91438	0.02440	Uani	1.00
N202         N         0.18704         0.92223         0.91092         0.03383         Uani         1.00           O203         O         0.54196         0.79333         0.31378         0.08944         Uani         1.00           C204         C         0.39500         0.84916         0.95183         0.02860         Uani         1.00	N201	Ν	0.50115	0.82079	0.04037	0.02824	Uani	1.00
O203         O         0.54196         0.79333         0.31378         0.08944         Uani         1.00           C204         C         0.39500         0.84916         0.95183         0.02860         Uani         1.00	N202	Ν	0.18704	0.92223	0.91092	0.03383	Uani	1.00
C204 C 0.39500 0.84916 0.95183 0.02860 Uani 1.00	O203	Ο	0.54196	0.79333	0.31378	0.08944	Uani	1.00
C204 C 0.55500 0.04510 0.55105 0.02000 Cam 1.00	C204	С	0.39500	0.84916	0.95183	0.02860	Uani	1.00
C205 C 0.32146 0.87325 0.93511 0.03428 Uani 1.00	C205	С	0.32146	0.87325	0.93511	0.03428	Uani	1.00
C206 C 0.44794 0.83641 0.85710 0.03107 Uani 1.00	C206	С	0.44794	0.83641	0.85710	0.03107	Uani	1.00
H207 H 0.44107 0.83962 0.75432 0.04900 Uiso 1.00	H207	Н	0.44107	0.83962	0.75432	0.04900	Uiso	1.00
C208 C 0.43040 0.83860 0.06671 0.03163 Uani 1.00	C208	С	0.43040	0.83860	0.06671	0.03163	Uani	1.00

H209         H         0.40796         0.84507         0.16215         0.04001         Uiso         1.00           11211         H         0.25210         0.93562         0.76512         0.07100         Uiso         1.00           11211         H         0.32550         0.9176         0.99980         0.05259         Uani         1.00           1213         H         0.13452         0.88766         0.04810         Uiso         1.00           1214         C         0.13452         0.88766         0.08200         Uiso         1.00           1215         H         0.13452         0.88766         0.03127         Uani         1.00           1217         H         0.52420         0.88434         0.08779         0.08800         Uani         1.00           1218         N         0.52476         0.82847         0.98797         0.13405         Uani         1.00           1221         Zn         0.08707         0.95842         0.89760         0.03356         Uani         1.00           1222         N         0.12760         0.9387         0.65632         0.02357         Uani         1.00           1222         N         0.12764								
C210         C         0.25219         0.92901         0.83400         0.04618         Uani         1.00           C212         C         0.31961         0.90424         0.84272         0.05219         Uani         1.00           C214         C         0.37085         0.91011         0.78077         0.08000         Uiso         1.00           H213         H         0.37085         0.89176         0.99980         0.05259         Uani         1.00           H215         H         0.13452         0.88737         0.06006         0.08200         Uiso         1.00           H217         H         0.25242         0.88706         0.037374         0.08000         Uiso         1.00           D218         N         0.52476         0.83867         0.37374         0.08008         Uani         1.00           C219         O         0.52623         0.83867         0.033407         0.12630         Uani         1.00           C222         N         0.12671         1.00000         0.78190         0.02829         Uani         1.00           C225         O         0.07164         0.55176         0.68425         0.023571         Uani         1.00	H209	Н	0.40796	0.84507	0.16215	0.04900	Uiso	1.00
H211         H         0.25210         0.93362         0.7612         0.07100         Uiso         1.00           C212         C         0.31965         0.9011         0.78077         0.08000         Uiso         1.00           C214         C         0.37085         0.9101         0.78077         0.08000         Uiso         1.00           C214         C         0.37085         0.89176         0.08200         Uiso         1.00           C214         C         0.25424         0.86706         0.01489         0.05215         Uani         1.00           C217         H         0.25420         0.84344         0.08779         0.08808         Uani         1.00           C219         O         0.52823         0.86300         0.31207         0.12405         Uani         1.00           C221         N         0.12670         0.98842         0.89376         0.02357         Uani         1.00           C222         N         0.12671         1.00000         0.78190         0.02357         Uani         1.00           C223         N         0.12671         1.00000         0.78190         0.02357         Uani         1.00           C223	C210	С	0.25219	0.92901	0.83400	0.04618	Uani	1.00
C212         C         0.31961         0.90424         0.84272         0.05219         Uani         1.00           H213         H         0.37085         0.91010         0.78077         0.08000         Uiso         1.00           H215         H         0.13452         0.88737         0.06096         0.08210         Uiani         1.00           H215         H         0.25420         0.88737         0.06096         0.08200         Uiao         1.00           H217         H         0.25476         0.83774         0.08800         Uani         1.00           N18         N         0.52476         0.83267         0.37374         0.08808         Uani         1.00           O219         O         0.52823         0.83600         0.31207         Uani         1.00           N222         N         0.12671         1.00000         0.73190         0.03237         Uani         1.00           N224         N         0.1271         1.00000         0.73190         0.03364         Uani         1.00           N224         N         0.12740         0.53176         0.64825         0.02837         Uani         1.00           N223         N	H211	Н	0.25210	0.95362	0.76512	0.07100	Uiso	1.00
H213         H         0.37085         0.91011         0.78077         0.08000         Uiso         1.00           C214         C         0.18659         0.89176         0.99980         0.05259         Uani         1.00           C216         C         0.25424         0.88737         0.06096         0.08200         Uiso         1.00           C216         C         0.25420         0.84344         0.08779         0.08000         Uiani         1.00           N11         0.52420         0.84344         0.08779         0.08080         Uani         1.00           N218         N         0.52476         0.82867         0.37374         0.08808         Uani         1.00           X222         O         0.52823         0.86300         0.31207         0.12306         Uani         1.00           X222         N         0.12760         0.99387         0.65652         0.02440         Uani         1.00           X223         N         0.12761         1.00000         0.03396         Uani         1.00           X224         N         0.34111         0.6557         0.08481         Uani         1.00           X225         C         0.107146 <td>C212</td> <td>С</td> <td>0.31961</td> <td>0.90424</td> <td>0.84272</td> <td>0.05219</td> <td>Uani</td> <td>1.00</td>	C212	С	0.31961	0.90424	0.84272	0.05219	Uani	1.00
C214         C         0.18659         0.89176         0.99980         0.05259         Uani         1.00           H215         H         0.13452         0.88737         0.06096         0.08200         Uiso         1.00           H217         H         0.25420         0.88706         0.03779         0.08000         Uiso         1.00           P218         N         0.52476         0.82867         0.37374         0.08000         Uiso         1.00           Q219         O         0.52823         0.86300         0.31270         0.12330         Uani         1.00           Zn21         Zn         0.09870         0.95842         0.89796         0.02357         Uani         1.00           N222         N         0.12671         1.00000         0.78190         0.02829         Uani         1.00           N224         N         0.34111         0.65372         0.0818         Uani         1.00           N225         O         0.07146         0.57970         0.08818         Uani         1.00           N226         C         0.16398         1.02544         0.58050         0.03175         Uani         1.00           N227         C	H213	Н	0.37085	0.91011	0.78077	0.08000	Uiso	1.00
H215         H         0.13452         0.88737         0.06096         0.08200         Uiso         1.00           C216         C         0.25424         0.88706         0.01489         0.05215         Uani         1.00           N18         N         0.52476         0.82867         0.37374         0.08808         Uani         1.00           0219         O         0.52823         0.86300         0.12230         Uani         1.00           Za21         Zn         0.09870         0.95842         0.89796         0.02357         Uani         1.00           X222         N         0.12670         0.99387         0.65652         0.02440         Uani         1.00           N224         N         0.12671         1.00000         0.78190         0.02827         Uani         1.00           N224         N         0.12671         1.00000         0.78190         0.03396         Uani         1.00           N224         N         0.31171         Uani         1.00         1.00         1.00           N225         C         0.16318         0.5347         0.79839         0.03175         Uani         1.00           N227         H <td< td=""><td>C214</td><td>С</td><td>0.18659</td><td>0.89176</td><td>0.99980</td><td>0.05259</td><td>Uani</td><td>1.00</td></td<>	C214	С	0.18659	0.89176	0.99980	0.05259	Uani	1.00
C216         C         0.25424         0.86706         0.01489         0.05215         Uani         1.00           H217         H         0.25420         0.84344         0.08779         0.08000         Uiso         1.00           0218         N         0.52476         0.82867         0.37374         0.08000         Uiso         1.00           0219         O         0.58233         0.86300         0.31207         0.12300         Uani         1.00           0220         O         0.50272         0.8816         0.49379         0.12305         Uani         1.00           N222         N         0.12671         1.00000         0.78190         0.02389         Uani         1.00           N223         N         0.3111         0.63572         0.68481         Uani         1.00           0224         N         0.31141         0.65552         0.62857         Uani         1.00           0225         O         0.01746         0.97902         0.03168         Uani         1.00           0226         C         0.16388         1.02541         0.59800         0.3108         Uani         1.00           1223         H         0.17348	H215	Н	0.13452	0.88737	0.06096	0.08200	Uiso	1.00
H217         H         0.25420         0.84344         0.08779         0.08000         Uiso         1.00           N218         N         0.52476         0.82867         0.37374         0.08808         Uani         1.00           0219         0         0.52823         0.86300         0.31207         0.12320         Uani         1.00           0220         0         0.50272         0.88766         0.02357         Uani         1.00           2.221         N         0.12670         0.99387         0.65652         0.02440         Uani         1.00           N2224         N         0.12671         1.00000         0.78190         0.02829         Uani         1.00           N224         N         0.31746         0.57970         0.08818         Uani         1.00           C225         O         0.18724         0.55176         0.68425         0.02857         Uani         1.00           C227         C         0.23661         0.58855         0.04930         Uani         1.00           C228         C         0.16418         0.53847         0.79839         0.03175         Uani         1.00           C234         C         0.29355	C216	С	0.25424	0.86706	0.01489	0.05215	Uani	1.00
N218         N         0.52476         0.37374         0.08808         Uani         1.00           0219         0         0.52823         0.86300         0.31207         0.12230         Uani         1.00           Zn21         Zn         0.09870         0.95842         0.89796         0.02357         Uani         1.00           N222         N         0.12760         0.99877         0.66652         0.02440         Uani         1.00           N223         N         0.12761         1.00000         0.78190         0.02829         Uani         1.00           N224         N         0.34111         0.65372         0.6579         0.08818         Uani         1.00           C226         C         0.1746         0.97912         0.03108         Uani         1.00           C227         C         0.23661         0.58855         0.67058         0.03108         Uani         1.00           C230         C         0.16418         0.5347         0.79839         0.03175         Uani         1.00           C331         H         0.39348         0.62428         0.49620         0.07100         Uiso         1.00           C3232         C	H217	Н	0.25420	0.84344	0.08779	0.08000	Uiso	1.00
O219         O         0.52823         0.86300         0.31207         0.12230         Uani         1.00           O220         O         0.50272         0.82816         0.49379         0.13405         Uani         1.00           N2212         N         0.12760         0.99387         0.65652         0.02440         Uani         1.00           N222         N         0.12671         1.00000         0.78190         0.02829         Uani         1.00           N224         N         0.34111         0.65770         0.08818         Uani         1.00           C225         O         0.07146         0.97902         0.05579         0.08818         Uani         1.00           C226         C         0.16398         1.02534         0.59800         0.03108         Uani         1.00           C228         C         0.16398         1.02534         0.59800         0.03108         Uani         1.00           L221         H         0.17348         0.5281         0.4461         Uani         1.00           L231         H         0.17348         0.5237         0.04611         Uani         1.00           L232         C         0.34744	N218	Ν	0.52476	0.82867	0.37374	0.08808	Uani	1.00
O220         O         0.50272         0.82816         0.49379         0.13405         Uani         1.00           Xn221         Xn         0.09870         0.95842         0.89766         0.02357         Uani         1.00           N222         N         0.12671         1.00000         0.78190         0.02829         Uani         1.00           N224         N         0.34111         0.65372         0.65700         0.03396         Uani         1.00           0225         C         0.1746         0.97902         0.05579         0.08818         Uani         1.00           0227         C         0.23661         0.55876         0.03433         Uani         1.00           0228         C         0.1398         1.02534         0.58855         0.04900         Uiso         1.00           0230         C         0.16418         0.5347         0.79839         0.03175         Uani         1.00           1231         H         0.17556         0.54430         0.89416         0.49000         Uiso         1.00           1233         H         0.39348         0.62428         0.49620         0.07100         Uiso         1.00           1234	O219	0	0.52823	0.86300	0.31207	0.12230	Uani	1.00
Zn211         Zn         0.09870         0.95842         0.89796         0.02357         Uani         1.00           N2223         N         0.12760         0.99387         0.65652         0.02440         Uani         1.00           N224         N         0.34111         0.65372         0.65700         0.03396         Uani         1.00           0225         O         0.07146         0.97902         0.05579         0.08818         Uani         1.00           0226         C         0.18724         0.55176         0.68425         0.02857         Uani         1.00           0227         C         0.23661         0.58855         0.67058         0.03433         Uani         1.00           0228         C         0.16398         1.02334         0.59800         0.03175         Uani         1.00           1231         H         0.17556         0.54430         0.89416         0.04900         Uiso         1.00           1233         H         0.39348         0.65247         Uani         1.00           1234         H         0.29855         0.59137         0.57186         0.52248         Uani         1.00           1235         H	O220	0	0.50272	0.82816	0.49379	0.13405	Uani	1.00
N222         N         0.12760         0.99387         0.65652         0.02440         Uani         1.00           N223         N         0.12671         1.00000         0.78190         0.02829         Uani         1.00           N224         N         0.31111         0.65370         0.03396         Uani         1.00           C225         O         0.07146         0.97902         0.05579         0.08818         Uani         1.00           C226         C         0.18724         0.55176         0.68425         0.02857         Uani         1.00           C228         C         0.16398         1.02344         0.59800         0.03108         Uani         1.00           H         0.17556         0.54430         0.89416         0.04900         Uiso         1.00           C323         C         0.34744         0.62428         0.49620         0.07100         Uiso         1.00           L233         H         0.39348         0.62428         0.49620         0.07100         Uiso         1.00           L235         H         0.29455         0.59137         0.57156         0.05248         Uani         1.00           L235         H	Zn221	Zn	0.09870	0.95842	0.89796	0.02357	Uani	1.00
N223         N         0.12671         1.00000         0.78190         0.02829         Uani         1.00           N224         N         0.34111         0.65372         0.65700         0.03396         Uani         1.00           0225         O         0.017146         0.97902         0.05579         0.08818         Uani         1.00           0226         C         0.18724         0.55176         0.68425         0.02857         Uani         1.00           0227         C         0.23661         0.58855         0.67058         0.03433         Uani         1.00           0228         C         0.16398         1.02344         0.59800         0.03175         Uani         1.00           1229         H         0.17556         0.54430         0.89416         0.04900         Uiso         1.00           1233         H         0.39348         0.62428         0.49620         0.07100         Uiso         1.00           1235         H         0.29355         0.59137         0.57186         0.05247         Uani         1.00           1237         H         0.28167         0.67511         0.82197         0.08200         Uiso         1.00	N222	Ν	0.12760	0.99387	0.65652	0.02440	Uani	1.00
N224         N         0.34111         0.65372         0.65700         0.03396         Uani         1.00           0225         O         0.07146         0.97902         0.05579         0.08818         Uani         1.00           0226         C         0.18724         0.55176         0.68425         0.02857         Uani         1.00           0227         C         0.23661         0.55855         0.6708         0.03433         Uani         1.00           0220         C         0.16398         1.02534         0.59800         0.03108         Uani         1.00           0230         C         0.16418         0.53431         0.79839         0.03175         Uani         1.00           0231         H         0.17556         0.54430         0.89416         0.04900         Uiso         1.00           0232         C         0.34744         0.62242         0.56957         0.04641         Uani         1.00           1233         H         0.29355         0.59137         0.57156         0.05247         Uani         1.00           1235         H         0.29350         0.59137         0.57126         Uanis         1.00           1234 <td>N223</td> <td>Ν</td> <td>0.12671</td> <td>1.00000</td> <td>0.78190</td> <td>0.02829</td> <td>Uani</td> <td>1.00</td>	N223	Ν	0.12671	1.00000	0.78190	0.02829	Uani	1.00
O225         O         0.07146         0.97902         0.05579         0.08818         Uani         1.00           C226         C         0.18724         0.55176         0.68425         0.02857         Uani         1.00           C227         C         0.23661         0.58855         0.67058         0.03133         Uani         1.00           C228         C         0.16398         1.02534         0.59800         0.03175         Uani         1.00           C230         C         0.16418         0.5347         0.79839         0.03175         Uani         1.00           C232         C         0.34744         0.62342         0.56957         0.04641         Uani         1.00           C234         C         0.29355         0.59137         0.57156         0.05247         Uani         1.00           C234         C         0.29365         0.59137         0.57186         0.05248         Uani         1.00           C235         C         0.224848         0.65254         0.71186         0.05248         Uani         1.00           C238         C         0.23222         0.61958         0.71192         0.05226         Uani         1.00	N224	Ν	0.34111	0.65372	0.65700	0.03396	Uani	1.00
C226         C         0.18724         0.55176         0.68425         0.02857         Uani         1.00           C227         C         0.23661         0.58855         0.67058         0.03433         Uani         1.00           C228         C         0.16398         1.02534         0.59800         0.03108         Uani         1.00           H229         H         0.17348         0.52861         0.48655         0.04900         Uiso         1.00           H231         H         0.17556         0.54430         0.89416         0.04900         Uiso         1.00           C232         C         0.34744         0.62428         0.49620         0.7100         Uiso         1.00           C234         C         0.29355         0.59137         0.57156         0.05247         Uani         1.00           H235         H         0.29863         0.56817         0.49930         0.08000         Uiso         1.00           C236         C         0.28448         0.65254         0.75192         0.63226         Uani         1.00           C238         C         0.23222         0.61958         0.76192         0.63226         Uani         1.00      <	O225	0	0.07146	0.97902	0.05579	0.08818	Uani	1.00
C227         C         0.23661         0.58855         0.67058         0.03433         Uani         1.00           C228         C         0.16398         1.02534         0.59800         0.03108         Uani         1.00           H229         H         0.17348         0.52861         0.48655         0.04900         Uiso         1.00           C230         C         0.16418         0.53347         0.79839         0.03175         Uani         1.00           C232         C         0.34744         0.62342         0.56957         0.04641         Uani         1.00           C234         C         0.29853         0.59137         0.57156         0.5247         Uani         1.00           C236         C         0.28448         0.65254         0.75186         0.05248         Uani         1.00           H237         H         0.28167         0.67651         0.82197         0.08200         Uiso         1.00           H239         H         0.18912         0.61828         0.84029         0.08000         Uiso         1.00           H237         H         0.2823         0.98943         0.05902         0.12288         Uani         1.00 <t< td=""><td>C226</td><td>С</td><td>0.18724</td><td>0.55176</td><td>0.68425</td><td>0.02857</td><td>Uani</td><td>1.00</td></t<>	C226	С	0.18724	0.55176	0.68425	0.02857	Uani	1.00
C228         C         0.16398         1.02534         0.59800         0.03108         Uani         1.00           H229         H         0.17348         0.52861         0.48655         0.04900         Uiso         1.00           C230         C         0.16418         0.53347         0.79839         0.03175         Uani         1.00           H231         H         0.17556         0.54430         0.89416         0.04900         Uiso         1.00           C232         C         0.34744         0.62342         0.49620         0.07100         Uiso         1.00           H233         H         0.39348         0.62428         0.49620         0.07100         Uiso         1.00           C234         C         0.29355         0.59137         0.57156         0.5247         Uani         1.00           C235         C         0.28448         0.65254         0.75186         0.05248         Uani         1.00           C238         C         0.23222         0.61958         0.76192         0.0526         Uani         1.00           C439         H         0.18912         0.61828         0.84029         0.8000         Uiso         1.00 <tr< td=""><td>C227</td><td>С</td><td>0.23661</td><td>0.58855</td><td>0.67058</td><td>0.03433</td><td>Uani</td><td>1.00</td></tr<>	C227	С	0.23661	0.58855	0.67058	0.03433	Uani	1.00
H229       H       0.17348       0.52861       0.48655       0.04900       Uiso       1.00         C230       C       0.16418       0.53347       0.79839       0.03175       Uani       1.00         H231       H       0.17556       0.54430       0.89416       0.04900       Uiso       1.00         C232       C       0.34744       0.62342       0.56957       0.04641       Uani       1.00         H233       H       0.39348       0.62428       0.49620       0.07100       Uiso       1.00         H235       H       0.29355       0.55817       0.49930       0.08000       Uiso       1.00         H235       H       0.29863       0.56817       0.49930       0.08200       Uiso       1.00         H237       H       0.28167       0.67651       0.82197       0.08200       Uiso       1.00         H239       H       0.18912       0.61828       0.48029       0.08000       Uiso       1.00         N240       N       0.13925       0.98950       0.11784       0.08822       Uani       1.00         N244       N       0.87470       0.33677       0.02351       Uani       1.00	C228	С	0.16398	1.02534	0.59800	0.03108	Uani	1.00
C230         C         0.16418         0.53347         0.79839         0.03175         Uani         1.00           H231         H         0.17556         0.54430         0.89416         0.04900         Uiso         1.00           C232         C         0.34744         0.62342         0.56957         0.04641         Uani         1.00           H233         H         0.39348         0.62428         0.49620         0.07100         Uiso         1.00           C234         C         0.29355         0.59137         0.57156         0.05247         Uani         1.00           C236         C         0.28448         0.65254         0.75186         0.05248         Uani         1.00           H237         H         0.28167         0.67651         0.82197         0.08200         Uiso         1.00           H239         H         0.18912         0.61828         0.84029         0.08000         Uiso         1.00           O2440         N         0.13925         0.98950         0.1784         0.0822         Uani         1.00           O242         O         0.13509         1.00057         0.23311         Uani         1.00           N244	H229	Н	0.17348	0.52861	0.48655	0.04900	Uiso	1.00
L231         H         0.17556         0.54430         0.89416         0.04641         Uiso         1.00           L233         H         0.39348         0.62428         0.49620         0.07100         Uiso         1.00           L233         H         0.39348         0.62428         0.49620         0.07100         Uiso         1.00           C234         C         0.29355         0.59137         0.57156         0.05247         Uani         1.00           H235         H         0.29863         0.56817         0.49930         0.88000         Uiso         1.00           C236         C         0.28448         0.65254         0.75186         0.05226         Uani         1.00           C238         C         0.23222         0.61828         0.84029         0.08000         Uiso         1.00           C444         N         0.13925         0.98950         0.11784         0.08822         Uani         1.00           C441         O         0.13509         1.0057         0.23712         0.13492         Uani         1.00           C442         O         0.39677         0.02381         Uani         1.00           C444         N	C230	C	0.16418	0.53347	0.79839	0.03175	Uani	1.00
Hart         Original         Original         Original         Original         Original         Original           1233         H         0.34744         0.62342         0.56957         0.04641         Uani         1.00           1233         H         0.39348         0.62428         0.49620         0.07100         Uiso         1.00           1235         H         0.29355         0.59137         0.57156         0.05247         Uani         1.00           1235         H         0.29863         0.6517         0.49930         0.08000         Uiso         1.00           1237         H         0.28167         0.67651         0.82197         0.08200         Uiso         1.00           1237         H         0.28167         0.67651         0.82197         0.08226         Uani         1.00           1239         H         0.18912         0.61828         0.84029         0.08000         Uiso         1.00           0240         N         0.13925         0.98950         0.11784         0.08822         Uani         1.00           2n243         Zn         0.90211         0.5112         0.12481         Uani         1.00           2n243	H231	н	0.17556	0 54430	0.89416	0.04900	Uiso	1.00
C224         C         0.39348         0.62428         0.49670         Uiso         1.00           C234         C         0.39348         0.62428         0.49620         0.07100         Uiso         1.00           H235         H         0.29355         0.59137         0.57156         0.05247         Uani         1.00           C236         C         0.28448         0.65254         0.75186         0.05248         Uani         1.00           C238         C         0.23222         0.61958         0.76192         0.05226         Uani         1.00           C238         C         0.23222         0.61958         0.76192         0.08000         Uiso         1.00           D240         N         0.13925         0.98950         0.11784         0.08822         Uani         1.00           D241         O         0.20823         0.98943         0.05902         0.12288         Uani         1.00           Zn243         Zn         0.90211         0.54109         0.39677         0.02351         Uani         1.00           N244         N         0.87470         0.50721         0.15512         0.02434         Uani         1.00           N245 </td <td>C232</td> <td>C C</td> <td>0 34744</td> <td>0.62342</td> <td>0.56957</td> <td>0.04641</td> <td>Uani</td> <td>1.00</td>	C232	C C	0 34744	0.62342	0.56957	0.04641	Uani	1.00
1125       1       0.5916       0.5917       0.5916       0.5917       0.5916       0.05147       Uani       1.00         1235       H       0.29355       0.59137       0.57156       0.05247       Uani       1.00         1235       H       0.29355       0.59137       0.49930       0.08000       Uiso       1.00         1237       H       0.28167       0.67651       0.82197       0.08200       Uiso       1.00         1239       H       0.13922       0.61958       0.76192       0.05226       Uani       1.00         0241       O       0.20823       0.98950       0.11784       0.08802       Uani       1.00         0242       O       0.13509       1.00057       0.23512       Uani       1.00         2743       Zn       0.90211       0.54109       0.39677       0.02351       Uani       1.00         N244       N       0.87470       0.50721       0.15512       0.02434       Uani       1.00         N245       N       0.87475       0.53346       0.08877       Uani       1.00         N246       N       0.66016       0.84657       0.19357       0.02352       Uani	H233	е н	0 39348	0.62428	0.49620	0.07100	Uiso	1.00
CL236         C         0.29863         0.5153         0.05153         0.05247         Can         1.00           1235         H         0.29863         0.56817         0.49930         0.08000         Uiso         1.00           C236         C         0.28448         0.65254         0.75186         0.05248         Uani         1.00           C238         C         0.23222         0.61958         0.76192         0.05226         Uani         1.00           H239         H         0.18912         0.61828         0.84029         0.08000         Uiso         1.00           O241         O         0.20823         0.98943         0.05902         0.12288         Uani         1.00           O242         O         0.13509         1.00057         0.23712         0.13492         Uani         1.00           N244         N         0.87470         0.50721         0.15512         0.02434         Uani         1.00           N245         N         0.87435         0.50008         0.28037         0.02852         Uani         1.00           N244         N         0.66016         0.84657         0.15937         0.0384         Uani         1.00 <t< td=""><td>C234</td><td>п С</td><td>0.29355</td><td>0.59137</td><td>0.57156</td><td>0.05247</td><td>Uani</td><td>1.00</td></t<>	C234	п С	0.29355	0.59137	0.57156	0.05247	Uani	1.00
112.57       11       0.23605       0.73505       0.75186       0.05000       0.180       1.00         C236       C       0.28448       0.65254       0.75186       0.08200       Uiso       1.00         1237       H       0.28122       0.61958       0.76192       0.05226       Uani       1.00         1239       H       0.18912       0.61828       0.84029       0.08000       Uiso       1.00         0241       O       0.20823       0.98950       0.11784       0.08822       Uani       1.00         0242       O       0.13509       1.00057       0.23712       0.13492       Uani       1.00         2n243       Zn       0.90211       0.54109       0.39677       0.02351       Uani       1.00         N244       N       0.87470       0.50721       0.15512       0.02434       Uani       1.00         N245       N       0.87435       0.50008       0.28037       0.02823       Uani       1.00         N246       N       0.66016       0.84657       0.15376       0.0384       Uani       1.00         C247       O       0.93161       0.51977       0.55346       0.08877       U	H235	н	0.27555	0.57137	0.37130	0.03247	Uiso	1.00
C230         C         0.02244         0.01244         0.01244         0.01244         0.01244         0.01244         0.01244         0.01244         0.01244         0.01244         0.01244         0.01244         0.01244         0.01244         0.01242         0.01242         0.01242         0.01243         0.01243         0.013925         0.98950         0.11784         0.08200         Uiso         1.00           0241         O         0.20823         0.98943         0.05902         0.12288         Uani         1.00           0242         O         0.13509         1.00057         0.23712         0.13492         Uani         1.00           2n243         Zn         0.90211         0.54109         0.39677         0.02323         Uani         1.00           N244         N         0.87470         0.50721         0.15512         0.02434         Uani         1.00           N245         N         0.87435         0.50008         0.28037         0.02823         Uani         1.00           N246         N         0.66016         0.84657         0.15937         0.0384         Uani         1.00           C248         C         0.81613         0.51977         0.55346         0.	C236	n C	0.29003	0.65254	0.75186	0.05248	Uani	1.00
112.57       11       0.23101       0.0311       0.03217       0.03220       0.61958       0.76192       0.05226       Uani       1.00         1239       H       0.18912       0.61958       0.76192       0.05226       Uani       1.00         0240       N       0.13925       0.98950       0.11784       0.08822       Uani       1.00         0241       O       0.20823       0.98950       0.11784       0.08822       Uani       1.00         0242       O       0.13509       1.00057       0.23712       0.13492       Uani       1.00         0242       O       0.13509       1.00057       0.23712       0.13492       Uani       1.00         N244       N       0.87470       0.50721       0.15512       0.02434       Uani       1.00         N245       N       0.87435       0.50008       0.28037       0.02823       Uani       1.00         N246       N       0.66016       0.84657       0.15937       0.03384       Uani       1.00         C248       C       0.81525       0.94744       0.19357       0.02852       Uani       1.00         C249       C       0.76475       0.91	H237	н	0.28167	0.05254	0.75100	0.03248	Uiso	1.00
C235       C       0.01322       0.011938       0.01192       0.03200       Uani       1.00         H239       H       0.18912       0.61828       0.84029       0.08000       Uiso       1.00         N240       N       0.13925       0.98950       0.11784       0.08822       Uani       1.00         O241       O       0.20823       0.98943       0.05902       0.12288       Uani       1.00         O242       O       0.13509       1.00057       0.23712       0.13492       Uani       1.00         V244       N       0.87470       0.50721       0.15512       0.02434       Uani       1.00         N244       N       0.87435       0.50008       0.28037       0.02823       Uani       1.00         N245       N       0.86016       0.84657       0.15937       0.03384       Uani       1.00         N246       N       0.66016       0.84657       0.19377       0.02852       Uani       1.00         C248       C       0.81525       0.94744       0.19357       0.02852       Uani       1.00         C250       C       0.83693       0.47674       0.09626       0.03100       Uani<	C238	II C	0.20107	0.61058	0.02177	0.05226	Uani	1.00
112.57       11       0.16912       0.01023       0.04025       0.08000       0.050       1.00         N240       N       0.13925       0.98950       0.11784       0.08822       Uani       1.00         O241       O       0.20823       0.98943       0.05902       0.12288       Uani       1.00         O242       O       0.13509       1.00057       0.23712       0.13492       Uani       1.00         Zn243       Zn       0.90211       0.54109       0.39677       0.02351       Uani       1.00         N244       N       0.87435       0.50008       0.28037       0.02823       Uani       1.00         N245       N       0.87435       0.50008       0.28037       0.02852       Uani       1.00         N246       N       0.66016       0.84657       0.15937       0.0384       Uani       1.00         C247       O       0.93161       0.51977       0.55346       0.08877       Uani       1.00         C248       C       0.76475       0.91137       0.1707       0.03428       Uani       1.00         C250       C       0.83693       0.47674       0.09626       0.03100       Ua	U230	ч	0.23222	0.61938	0.70192	0.03220	Uiso	1.00
N240       N       0.1392.5       0.98943       0.0592.2       0.411       1.00         O241       O       0.20823       0.98943       0.05902       0.12288       Uani       1.00         O242       O       0.13509       1.00057       0.23712       0.13492       Uani       1.00         Zn243       Zn       0.90211       0.54109       0.39677       0.02351       Uani       1.00         N244       N       0.87470       0.50721       0.15512       0.02423       Uani       1.00         N245       N       0.87435       0.50008       0.28037       0.02823       Uani       1.00         N246       N       0.66016       0.84657       0.15937       0.03384       Uani       1.00         O247       O       0.93161       0.51977       0.55346       0.08877       Uani       1.00         C248       C       0.81525       0.94744       0.19357       0.02852       Uani       1.00         C250       C       0.83693       0.47674       0.09626       0.03100       Uani       1.00         H251       H       0.82789       0.97399       -0.0153       0.04900       Uiso       1.00	N240	II N	0.10912	0.01020	0.04029	0.08000	UISO	1.00
0241 $0$ $0.2023$ $0.93943$ $0.03902$ $0.12288$ $0.11$ $1.00$ $0242$ $O$ $0.13509$ $1.00057$ $0.23712$ $0.13492$ $Uani$ $1.00$ $Zn243$ $Zn$ $0.90211$ $0.54109$ $0.39677$ $0.02351$ $Uani$ $1.00$ $N244$ $N$ $0.87470$ $0.50721$ $0.15512$ $0.02434$ $Uani$ $1.00$ $N245$ $N$ $0.87435$ $0.50008$ $0.28037$ $0.02823$ $Uani$ $1.00$ $N246$ $N$ $0.66016$ $0.84657$ $0.15937$ $0.03384$ $Uani$ $1.00$ $0247$ $O$ $0.93161$ $0.51977$ $0.55346$ $0.08877$ $Uani$ $1.00$ $0247$ $O$ $0.93161$ $0.51977$ $0.55346$ $0.08877$ $Uani$ $1.00$ $0247$ $O$ $0.93161$ $0.51977$ $0.55346$ $0.08877$ $Uani$ $1.00$ $0247$ $O$ $0.81525$ $0.94744$ $0.19357$ $0.02852$ $Uani$ $1.00$ $0249$ $C$ $0.76475$ $0.91137$ $0.17707$ $0.03428$ $Uani$ $1.00$ $0250$ $C$ $0.83693$ $0.47674$ $0.09626$ $0.03100$ $Uani$ $1.00$ $1251$ $H$ $0.82789$ $0.97399$ $-0.00153$ $0.04900$ $Uiso$ $1.00$ $1253$ $H$ $0.82686$ $0.95148$ $0.40385$ $0.04900$ $Uiso$ $1.00$ $1255$ $H$ $0.60165$ $0.88067$ $0.01401$ $0.07100$	N240	N O	0.13923	0.98930	0.11/04	0.08822	Uani	1.00
0.242 $0$ $0.13309$ $1.00037$ $0.23712$ $0.13492$ $0.011$ $0.0011$ $Zn243$ $Zn$ $0.90211$ $0.54109$ $0.39677$ $0.02351$ $Uani$ $1.00$ $N244$ N $0.87470$ $0.50721$ $0.15512$ $0.02434$ $Uani$ $1.00$ $N245$ N $0.87435$ $0.50008$ $0.28037$ $0.02823$ $Uani$ $1.00$ $N246$ N $0.66016$ $0.84657$ $0.15937$ $0.03384$ $Uani$ $1.00$ $0247$ O $0.93161$ $0.51977$ $0.55346$ $0.08877$ $Uani$ $1.00$ $C248$ C $0.81525$ $0.94744$ $0.19357$ $0.02852$ $Uani$ $1.00$ $C249$ C $0.76475$ $0.91137$ $0.17707$ $0.03428$ $Uani$ $1.00$ $C250$ C $0.83693$ $0.47674$ $0.09626$ $0.03100$ $Uani$ $1.00$ $H$ $0.82789$ $0.97399$ $-0.00153$ $0.04900$ $Uiso$ $1.00$ $H$ $0.82686$ $0.95148$ $0.40385$ $0.04900$ $Uiso$ $1.00$ $H253$ H $0.60165$ $0.88067$ $0.01401$ $0.07100$ $Uiso$ $1.00$ $H255$ H $0.60165$ $0.88067$ $0.01401$ $0.07100$ $Uiso$ $1.00$ $H255$ H $0.60165$ $0.88067$ $0.01401$ $0.07100$ $Uiso$ $1.00$ $H255$ H $0.60165$ $0.88067$ $0.01401$ $0.07100$ $Uiso$ $1.00$ $H25$	0241	0	0.20625	1.00057	0.03902	0.12200	Uani	1.00
2h243       2h       0.90211       0.94109       0.39677       0.02351       0ani       1.00         N244       N       0.87470       0.50721       0.15512       0.02434       Uani       1.00         N245       N       0.87435       0.50008       0.28037       0.02823       Uani       1.00         N246       N       0.66016       0.84657       0.15937       0.03384       Uani       1.00         O247       O       0.93161       0.51977       0.55346       0.08877       Uani       1.00         C248       C       0.81525       0.94744       0.19357       0.02852       Uani       1.00         C249       C       0.76475       0.91137       0.17707       0.03428       Uani       1.00         C250       C       0.83693       0.47674       0.09626       0.03100       Uani       1.00         H251       H       0.82789       0.97399       -0.00153       0.04900       Uiso       1.00         C252       C       0.83887       0.96370       0.30892       0.03165       Uani       1.00         H253       H       0.82686       0.95148       0.40385       0.04900       Uis	0242	0	0.13309	1.00057	0.23/12	0.13492	Uani	1.00
N244       N       0.8/4/0       0.30721       0.15312       0.02434       Uani       1.00         N245       N       0.87435       0.50008       0.28037       0.02823       Uani       1.00         N246       N       0.66016       0.84657       0.15937       0.03384       Uani       1.00         O247       O       0.93161       0.51977       0.55346       0.08877       Uani       1.00         C248       C       0.81525       0.94744       0.19357       0.02852       Uani       1.00         C249       C       0.76475       0.91137       0.17707       0.03428       Uani       1.00         C250       C       0.83693       0.47674       0.09626       0.03100       Uani       1.00         H251       H       0.82789       0.97399       -0.00153       0.04900       Uiso       1.00         C252       C       0.83887       0.96370       0.30892       0.03165       Uani       1.00         H253       H       0.82686       0.95148       0.40385       0.04900       Uiso       1.00         H255       H       0.60165       0.88067       0.01401       0.07100       Uiso<	Zn245	Zn	0.90211	0.54109	0.390//	0.02331	Uani	1.00
N245       N       0.87435       0.50008       0.28037       0.02825       0.ani       1.00         N246       N       0.66016       0.84657       0.15937       0.03384       Uani       1.00         O247       O       0.93161       0.51977       0.55346       0.08877       Uani       1.00         C248       C       0.81525       0.94744       0.19357       0.02852       Uani       1.00         C249       C       0.76475       0.91137       0.17707       0.03428       Uani       1.00         C250       C       0.83693       0.47674       0.09626       0.03100       Uani       1.00         H251       H       0.82789       0.97399       -0.00153       0.04900       Uiso       1.00         C252       C       0.83887       0.96370       0.30892       0.03165       Uani       1.00         H253       H       0.82686       0.95148       0.40385       0.04900       Uiso       1.00         C254       C       0.65049       0.87947       0.08111       0.04608       Uani       1.00         H255       H       0.60165       0.88067       0.01401       0.07100       Uiso	N244	N N	0.8/4/0	0.50/21	0.15512	0.02434	Uani	1.00
N246       N       0.66016       0.84657       0.15937       0.03384       Uani       1.00         O247       O       0.93161       0.51977       0.55346       0.08877       Uani       1.00         C248       C       0.81525       0.94744       0.19357       0.02852       Uani       1.00         C249       C       0.76475       0.91137       0.17707       0.03428       Uani       1.00         C250       C       0.83693       0.47674       0.09626       0.03100       Uani       1.00         H251       H       0.82789       0.97399       -0.00153       0.04900       Uiso       1.00         C252       C       0.83887       0.96370       0.30892       0.03165       Uani       1.00         H253       H       0.82686       0.95148       0.40385       0.04900       Uiso       1.00         H255       H       0.60165       0.88067       0.01401       0.07100       Uiso       1.00         H255       H       0.60165       0.88067       0.01401       0.07100       Uiso       1.00         H255       H       0.60165       0.88067       0.02402       0.08000       Uiso<	N245	N	0.8/435	0.50008	0.28037	0.02823	Uani	1.00
C247       C       0.93161       0.31977       0.53346       0.08877       Uani       1.00         C248       C       0.81525       0.94744       0.19357       0.02852       Uani       1.00         C249       C       0.76475       0.91137       0.17707       0.03428       Uani       1.00         C250       C       0.83693       0.47674       0.09626       0.03100       Uani       1.00         H251       H       0.82789       0.97399       -0.00153       0.04900       Uiso       1.00         C252       C       0.83887       0.96370       0.30892       0.03165       Uani       1.00         H253       H       0.82686       0.95148       0.40385       0.04900       Uiso       1.00         H255       H       0.60165       0.88067       0.01401       0.07100       Uiso       1.00         H255       H       0.60165       0.88067       0.01401       0.07100       Uiso       1.00         H255       H       0.69429       0.93792       0.02402       0.08000       Uiso       1.00         H257       H       0.69429       0.93792       0.02402       0.08000       Uiso<	N246	N	0.00010	0.84657	0.15937	0.03384	Uani	1.00
C248C0.815250.947440.195570.02852Uani1.00C249C0.764750.911370.177070.03428Uani1.00C250C0.836930.476740.096260.03100Uani1.00H251H0.827890.97399-0.001530.04900Uiso1.00C252C0.838870.963700.308920.03165Uani1.00H253H0.826860.951480.403850.04900Uiso1.00C254C0.650490.879470.081110.04608Uani1.00H255H0.601650.880670.014010.07100Uiso1.00C256C0.703320.911950.086590.05220Uani1.00H257H0.694290.937920.024020.08000Uiso1.00H257H0.720740.844690.245650.05229Uani1.00H259H0.726500.818450.307920.08200Uiso1.00H259H0.726500.877260.257330.05193Uani1.00H261H0.820250.875990.328640.08000Uiso1.00	0247	0	0.93161	0.519//	0.55346	0.08877	Uani	1.00
C249C0.764750.911370.177070.03428Uani1.00C250C0.836930.476740.096260.03100Uani1.00H251H0.827890.97399-0.001530.04900Uiso1.00C252C0.838870.963700.308920.03165Uani1.00H253H0.826860.951480.403850.04900Uiso1.00C254C0.650490.879470.081110.04608Uani1.00H255H0.601650.880670.014010.07100Uiso1.00C256C0.703320.911950.086590.05220Uani1.00H257H0.694290.937920.024020.08000Uiso1.00H259H0.726500.818450.307920.08200Uiso1.00H259H0.726500.877260.257330.05193Uani1.00H261H0.820250.875990.328640.08000Uiso1.00	C248	C	0.81525	0.94/44	0.19357	0.02852	Uani	1.00
C250C0.836930.476740.096260.03100Uani1.00H251H0.827890.97399-0.001530.04900Uiso1.00C252C0.838870.963700.308920.03165Uani1.00H253H0.826860.951480.403850.04900Uiso1.00C254C0.650490.879470.081110.04608Uani1.00H255H0.601650.880670.014010.07100Uiso1.00C256C0.703320.911950.086590.05220Uani1.00H257H0.694290.937920.024020.08000Uiso1.00C258C0.720740.844690.245650.05229Uani1.00H259H0.726500.818450.307920.08200Uiso1.00H261H0.820250.875990.328640.08000Uiso1.00	C249	C	0.76475	0.91137	0.17/07	0.03428	Uani	1.00
H251H0.827890.97399-0.001530.04900Uiso1.00C252C0.838870.963700.308920.03165Uani1.00H253H0.826860.951480.403850.04900Uiso1.00C254C0.650490.879470.081110.04608Uani1.00H255H0.601650.880670.014010.07100Uiso1.00C256C0.703320.911950.086590.05220Uani1.00H257H0.694290.937920.024020.08000Uiso1.00C258C0.720740.844690.245650.05229Uani1.00H259H0.726500.818450.307920.08200Uiso1.00C260C0.773500.877260.257330.05193Uani1.00H261H0.820250.875990.328640.08000Uiso1.00	C250	C	0.83693	0.47674	0.09626	0.03100	Uani	1.00
C252       C       0.83887       0.96370       0.30892       0.03165       Uani       1.00         H253       H       0.82686       0.95148       0.40385       0.04900       Uiso       1.00         C254       C       0.65049       0.87947       0.08111       0.04608       Uani       1.00         H255       H       0.60165       0.88067       0.01401       0.07100       Uiso       1.00         C256       C       0.70332       0.91195       0.08659       0.05220       Uani       1.00         H257       H       0.69429       0.93792       0.02402       0.08000       Uiso       1.00         C258       C       0.72074       0.84469       0.24565       0.05229       Uani       1.00         H259       H       0.72650       0.81845       0.30792       0.08200       Uiso       1.00         C260       C       0.77350       0.87726       0.25733       0.05193       Uani       1.00         H261       H       0.82025       0.87599       0.32864       0.08000       Uiso       1.00	H251	Н	0.82789	0.97399	-0.00153	0.04900	Uiso	1.00
H253H0.826860.951480.403850.04900Uiso1.00C254C0.650490.879470.081110.04608Uani1.00H255H0.601650.880670.014010.07100Uiso1.00C256C0.703320.911950.086590.05220Uani1.00H257H0.694290.937920.024020.08000Uiso1.00C258C0.720740.844690.245650.05229Uani1.00H259H0.726500.818450.307920.08200Uiso1.00C260C0.773500.877260.257330.05193Uani1.00H261H0.820250.875990.328640.08000Uiso1.00	C252	C	0.83887	0.96370	0.30892	0.03165	Uani	1.00
C254C0.650490.879470.081110.04608Uani1.00H255H0.601650.880670.014010.07100Uiso1.00C256C0.703320.911950.086590.05220Uani1.00H257H0.694290.937920.024020.08000Uiso1.00C258C0.720740.844690.245650.05229Uani1.00H259H0.726500.818450.307920.08200Uiso1.00C260C0.773500.877260.257330.05193Uani1.00H261H0.820250.875990.328640.08000Uiso1.00	H253	H	0.82686	0.95148	0.40385	0.04900	Uiso	1.00
H255       H       0.60165       0.88067       0.01401       0.07100       Uiso       1.00         C256       C       0.70332       0.91195       0.08659       0.05220       Uani       1.00         H257       H       0.69429       0.93792       0.02402       0.08000       Uiso       1.00         C258       C       0.72074       0.84469       0.24565       0.05229       Uani       1.00         H259       H       0.72650       0.81845       0.30792       0.08200       Uiso       1.00         C260       C       0.77350       0.87726       0.25733       0.05193       Uani       1.00         H261       H       0.82025       0.87599       0.32864       0.08000       Uiso       1.00	C254	C	0.65049	0.87947	0.08111	0.04608	Uani	1.00
C256       C       0.70332       0.91195       0.08659       0.05220       Uani       1.00         H257       H       0.69429       0.93792       0.02402       0.08000       Uiso       1.00         C258       C       0.72074       0.84469       0.24565       0.05229       Uani       1.00         H259       H       0.72650       0.81845       0.30792       0.08200       Uiso       1.00         C260       C       0.77350       0.87726       0.25733       0.05193       Uani       1.00         H261       H       0.82025       0.87599       0.32864       0.08000       Uiso       1.00	H255	Н	0.60165	0.88067	0.01401	0.07100	Uiso	1.00
H257H0.694290.937920.024020.08000Uiso1.00C258C0.720740.844690.245650.05229Uani1.00H259H0.726500.818450.307920.08200Uiso1.00C260C0.773500.877260.257330.05193Uani1.00H261H0.820250.875990.328640.08000Uiso1.00	C256	С	0.70332	0.91195	0.08659	0.05220	Uani	1.00
C258         C         0.72074         0.84469         0.24565         0.05229         Uani         1.00           H259         H         0.72650         0.81845         0.30792         0.08200         Uiso         1.00           C260         C         0.77350         0.87726         0.25733         0.05193         Uani         1.00           H261         H         0.82025         0.87599         0.32864         0.08000         Uiso         1.00	H257	Н	0.69429	0.93792	0.02402	0.08000	Uiso	1.00
H259         H         0.72650         0.81845         0.30792         0.08200         Uiso         1.00           C260         C         0.77350         0.87726         0.25733         0.05193         Uani         1.00           H261         H         0.82025         0.87599         0.32864         0.08000         Uiso         1.00	C258	С	0.72074	0.84469	0.24565	0.05229	Uani	1.00
C260         C         0.77350         0.87726         0.25733         0.05193         Uani         1.00           H261         H         0.82025         0.87599         0.32864         0.08000         Uiso         1.00	H259	Н	0.72650	0.81845	0.30792	0.08200	Uiso	1.00
H261 H 0.82025 0.87599 0.32864 0.08000 Uiso 1.00	C260	С	0.77350	0.87726	0.25733	0.05193	Uani	1.00
	H261	Н	0.82025	0.87599	0.32864	0.08000	Uiso	1.00

N262	N	0 86540	0 51245	0.62626	0.08818	Uani	1.00
0263	N O	0.79448	0.51245	0.02020	0.12208	Uani	1.00
0263	0	0.7290	0.50151	0.74563	0.12200	Uani	1.00
7n265	Zn	0.08265	0.94679	0.58577	0.02363	Uani	1.00
N266	N	0.00205	0.93219	0.82540	0.02339	Uani	1.00
N267	N	0.00770	0.93219	0.62040	0.02435	Uani	1.00
N268	N	0.68820	0.93095	0.07755	0.02325	Uani	1.00
0260	N	0.00029	0.02031	0.82044	0.03370	Uani	1.00
C270	0 C	0.04204	0.93773	0.42550	0.03852	Uani	1.00
C270	C C	0.89407	0.90230	0.70030	0.02832	Uani	1.00
C271	C C	0.62110	0.07625	0.804/5	0.03425	Uani	1.00
U272	C U	-0.03300	0.91409	0.00570	0.03103	Uani	1.00
П273 С274	П	0.93900	0.91066	0.98579	0.04900	UISO	1.00
C2/4	U	0.93003	0.91551	0.0/304	0.03138	Uani	1.00
H2/5	H	0.90854	0.90740	0.07851	0.04900		1.00
C2/6	C U	0.75291	0.82150	0.90241	0.04610	Uani	1.00
H2//	H	0.75298	0.79654	0.96995	0.07100	U1SO	1.00
C278	C	0.81951	0.84662	0.89489	0.05203	Uani	1.00
H279	н	0.87033	0.84060	0.95614	0.08000	U1SO	1.00
C280	C	0.68766	0.85949	0./3944	0.05219	∪anı	1.00
H281	Н	0.63595	0.86409	0.67916	0.08200	U1SO	1.00
C282	C	0.75455	0.88461	0.72563	0.05192	∪anı	1.00
H283	H	0.75443	0.90870	0.65426	0.08000	Uiso	1.00
N284	Ν	0.02602	0.92229	0.36659	0.08838	Uani	1.00
0285	0	0.02956	0.88808	0.42882	0.12268	Uani	1.00
0286	0	0.00450	0.92261	0.24704	0.13472	Uani	1.00
Zn287	Zn	0.92216	0.55447	0.08425	0.02357	Uani	1.00
N288	Ν	0.99113	0.56826	0.32321	0.02434	Uani	1.00
N289	Ν	1.00273	0.56957	0.19749	0.02819	Uani	1.00
N290	Ν	0.31123	0.67393	0.32145	0.03365	Uani	1.00
O291	0	0.96456	0.54385	0.92462	0.08958	Uani	1.00
C292	С	0.10637	0.59931	0.28559	0.02849	Uani	1.00
C293	С	0.17859	0.62420	0.30048	0.03420	Uani	1.00
C294	С	1.05296	0.58657	0.38032	0.03098	Uani	1.00
H295	Н	0.05848	0.59044	0.48290	0.04900	Uiso	1.00
C296	С	0.07282	0.58780	0.17113	0.03150	Uani	1.00
H297	Н	0.09569	0.59417	0.07558	0.04900	Uiso	1.00
C298	С	0.24598	0.68031	0.39849	0.04581	Uani	1.00
H299	Н	0.24572	0.70458	0.46724	0.07100	Uiso	1.00
C300	С	0.17945	0.65511	0.39145	0.05182	Uani	1.00
H301	Н	0.12840	0.66039	0.45426	0.08000	Uiso	1.00
C302	С	0.31205	0.64402	0.23257	0.05210	Uani	1.00
H303	Н	0.36372	0.64036	0.17035	0.08200	Uiso	1.00
C304	С	0.24544	0.61890	0.21930	0.05166	Uani	1.00
H305	Н	0.24607	0.59561	0.14672	0.08000	Uiso	1.00
N306	Ν	0.98080	0.57932	0.86310	0.08831	Uani	1.00
O307	0	0.97765	0.61350	0.92372	0.12192	Uani	1.00
O308	0	1.00151	0.57906	0.74246	0.13435	Uani	1.00
Zn309	Zn	0.40037	0.70921	0.33511	0.02352	Uani	1.00
N310	Ν	0.37192	0.74354	0.57646	0.02441	Uani	1.00
N311	Ν	0.37210	0.75034	0.45108	0.02828	Uani	1.00
N312	Ν	0.16005	0.90466	0.57910	0.03404	Uani	1.00
O313	Ο	0.42831	0.73044	0.17728	0.08862	Uani	1.00
C314	С	0.31505	0.80326	0.54316	0.02864	Uani	1.00

C316         C         0.246491         0.83961         0.56066         0.03138         Uani         1.00           H317         H         0.32714         0.77702         0.73830         0.04900         Uiso         1.00           H317         H         0.32714         0.77702         0.73830         0.04900         Uiso         1.00           C318         C         0.33846         0.73665         0.42373         0.03180         Uani         1.00           C320         C         0.14973         0.87185         0.65758         0.04649         Uani         1.00           H321         H         0.10304         0.81327         0.71425         0.80200         Uiso         1.00           H323         H         0.22775         0.93261         0.43033         0.05247         Uani         1.00           H327         H         0.32757         0.74205         0.17242         0.88000         Uiso         1.00           N328         N         0.3667         0.71348         0.11399         0.01245         Uani         1.00           N334         N         0.62864         0.75716         0.72326         0.13242         Uani         1.00								
C316         C         0.33707         0.77510         0.63575         0.03110         Uam         1.00           C318         C         0.33846         0.78665         0.42735         0.03180         Uani         1.00           C319         H         0.32705         0.78983         0.33266         0.04490         Uiao         1.00           H311         H         0.10022         0.87079         0.72498         0.07100         Uiso         1.00           H321         H         0.10022         0.87079         0.72498         0.07100         Uiso         1.00           H323         H         0.103944         0.81327         0.71425         0.08000         Uiso         1.00           H324         C         0.22150         0.990639         0.49244         0.08204         Uiso         1.00           H325         H         0.32187         0.87440         0.48661         0.80200         Uiso         1.00           H328         N         0.36588         0.73226         0.08574         Uani         1.00           H328         N         0.62860         0.77143         0.84460         0.8324         Uani         1.00           H332 <td>C315</td> <td>С</td> <td>0.26491</td> <td>0.83961</td> <td>0.56066</td> <td>0.03438</td> <td>Uani</td> <td>1.00</td>	C315	С	0.26491	0.83961	0.56066	0.03438	Uani	1.00
H317         H         0.32714         0.77702         0.73830         0.04900         Uiso         1.00           H319         H         0.32705         0.77893         0.33266         0.04190         Uiso         1.00           H319         H         0.32705         0.78993         0.33266         0.04490         Uiso         1.00           G120         C         0.1973         0.87185         0.65758         0.04649         Uani         1.00           G122         C         0.20269         0.83922         0.65174         0.05262         Uani         1.00           G132         H         0.10344         0.81327         0.71425         0.05200         Uiso         1.00           G132         C         0.22755         0.93261         0.43033         0.05247         Uani         1.00           G132         H         0.32787         0.74138         0.11399         0.08794         Uani         1.00           G330         O         0.63848         0.75100         0.94544         Uani         1.00           G333         N         0.62848         0.7510         0.94534         Uani         1.00           G333         N	C316	С	0.33707	0.77510	0.63575	0.03110	Uani	1.00
C318         C         0.33846         0.78665         0.42735         0.03100         Uani         1.00           C320         C         0.14973         0.87185         0.65758         0.04649         Uani         1.00           C321         H         0.10022         0.87079         0.72498         0.07100         Uiso         1.00           H321         H         0.19304         0.81327         0.71425         0.08000         Uiso         1.00           C324         C         0.22150         0.99639         0.49244         0.05244         Uani         1.00           C325         H         0.22175         0.93261         0.43015         0.08200         Uiso         1.00           C326         C         0.27445         0.87364         0.48033         0.05247         Uani         1.00           N28         N         0.36080         C.71418         0.11399         0.0874         Uani         1.00           N328         N         0.36080         0.71422         0.12253         Uani         1.00           N330         N         0.62860         0.75716         0.04317         0.04326         Uani         1.00           N333	H317	Н	0.32714	0.77702	0.73830	0.04900	Uiso	1.00
H319         H         0.32705         0.78933         0.33266         0.04940         Uias         1.00           C330         C         0.10022         0.87079         0.72498         0.07100         Uiso         1.00           C322         C         0.20269         0.83922         0.65174         0.05262         Uani         1.00           C324         C         0.22150         0.90639         0.49244         0.05284         Uani         1.00           C325         C         0.22175         0.93261         0.43015         0.08200         Uiso         1.00           H325         H         0.22175         0.93261         0.43015         0.08200         Uiso         1.00           H325         H         0.22175         0.74138         0.11399         0.08794         Uani         1.00           N328         N         0.36558         0.75236         -0.02356         Uani         1.00           N331         N         0.62484         0.7516         0.8137         0.02435         Uani         1.00           N333         N         0.62484         0.75170         0.63238         Uani         1.00           N334         N	C318	С	0.33846	0.78665	0.42735	0.03180	Uani	1.00
C320         C         0.14973         0.87185         0.65758         0.04649         Uari         1.00           H321         H         0.10022         0.87079         0.72498         0.07100         Uiso         1.00           H323         H         0.19304         0.81327         0.71425         0.80000         Uiso         1.00           H324         C         0.22175         0.93261         0.43015         0.08200         Uiso         1.00           C326         C         0.27455         0.87366         0.48033         0.05247         Uari         1.00           M328         N         0.36087         0.74138         0.11399         0.08794         Uari         1.00           M328         N         0.60042         0.75246         -0.00594         Uari         1.00           M333         N         0.62860         0.7516         0.08137         0.02456         Uari         1.00           M333         N         0.62840         0.75106         0.03828         Uari         1.00           M334         N         0.62840         0.75106         0.03828         Uari         1.00           M334         N         0.66875	H319	Н	0.32705	0.79893	0.33266	0.04900	Uiso	1.00
H321         H         0.10022         0.87079         0.72498         0.07100         Uiso         1.00           C322         C         0.20269         0.83922         0.65174         0.05262         Uani         1.00           C324         C         0.22150         0.90639         0.49244         0.05284         Uani         1.00           H325         H         0.22175         0.93261         0.43015         0.08200         Uiso         1.00           H327         H         0.32187         0.87474         0.40801         0.08000         Uiso         1.00           M328         N         0.36087         0.71435         0.11242         0.12253         Uani         1.00           M332         N         0.62860         0.75716         0.08137         0.02436         Uani         1.00           M333         N         0.62860         0.7516         0.08137         0.02436         Uani         1.00           M334         N         0.42641         0.57932         0.0726         0.03394         Uani         1.00           M333         N         0.62860         0.75176         0.03394         Uani         1.00           M334	C320	С	0.14973	0.87185	0.65758	0.04649	Uani	1.00
C322         C         0.20269         0.83922         0.65174         0.05262         Uani         1.00           H223         H         0.19304         0.81327         0.71425         0.08000         Uiso         1.00           H325         H         0.22775         0.93261         0.43015         0.08200         Uiso         1.00           H327         H         0.22175         0.93261         0.43015         0.08200         Uiso         1.00           M327         H         0.22175         0.97444         0.40861         0.08000         Uiso         1.00           M328         N         0.36087         0.74138         0.112253         Uani         1.00           Zn331         Zn         0.60042         0.79247         0.84040         0.02356         Uani         1.00           M333         N         0.62848         0.75116         0.08137         0.0236         Uani         1.00           M333         N         0.62848         0.7516         0.08324         Uani         1.00           M333         N         0.62848         0.7516         0.08324         Uani         1.00           M334         N         0.62655	H321	Н	0.10022	0.87079	0.72498	0.07100	Uiso	1.00
H         0.19304         0.81327         0.71425         0.08000         Uiso         1.00           C324         C         0.22150         0.90639         0.49244         0.05240         Uiso         1.00           C326         C         0.27445         0.87366         0.48033         0.05247         Uani         1.00           C327         H         0.32187         0.87374         0.40800         Uiso         1.00           M328         N         0.36087         0.71438         0.11399         0.08794         Uani         1.00           O330         O         0.29175         0.74205         0.17242         0.12253         Uani         1.00           N333         N         0.62860         0.75716         0.08137         0.02436         Uani         1.00           N333         N         0.62848         0.75100         0.93544         0.03340         Uani         1.00           C335         O         0.57366         0.77187         0.68328         0.0810         Uani         1.00           C336         C         0.68935         0.69851         0.49400         Uasi         1.00           C337         C         0.67646	C322	С	0.20269	0.83922	0.65174	0.05262	Uani	1.00
C324         C         0.22150         0.90639         0.49244         0.05284         Uani         1.00           H325         H         0.22775         0.93261         0.43015         0.08200         Uiso         1.00           H327         H         0.32187         0.87366         0.48033         0.05247         Uani         1.00           M328         N         0.36087         0.71138         0.01399         0.08794         Uani         1.00           O329         O         0.29175         0.74205         0.17242         0.12535         Uani         1.00           M330         O         0.36558         0.75236         -0.00594         0.13427         Uani         1.00           M331         N         0.62848         0.75100         0.95604         0.02828         Uani         1.00           M333         N         0.62848         0.75100         0.95812         0.03394         Uani         1.00           C335         O         0.7716         0.08130         Uani         1.00           C334         C         0.67646         0.72357         0.24116         0.04300         Uiso         1.00           C338         C	H323	Н	0.19304	0.81327	0.71425	0.08000	Uiso	1.00
H325         H         0.22775         0.93261         0.43015         0.08200         Uiso         1.00           C326         C         0.27445         0.87364         0.48033         0.05247         Uani         1.00           N327         H         0.32187         0.87474         0.40801         Uani         1.00           N328         N         0.36087         0.74138         0.11399         0.08794         Uani         1.00           0330         O         0.35658         0.75236         -0.00994         0.13247         Uani         1.00           X331         N         0.6042         0.79247         0.84040         0.02356         Uani         1.00           N333         N         0.62848         0.75106         0.03394         Uani         1.00           0335         O         0.57366         0.77187         0.68328         0.08820         Uani         1.00           C337         C         0.71414         0.66248         0.03944         Uani         1.00           C338         C         0.66575         0.72580         0.13908         0.3103         Uani         1.00           C340         C         0.67646	C324	С	0.22150	0.90639	0.49244	0.05284	Uani	1.00
C326         C         0.27445         0.87366         0.48033         0.05247         Uani         1.00           H327         H         0.32187         0.87474         0.40861         0.08000         Uiso         1.00           0329         O         0.29175         0.74205         0.17242         0.12253         Uani         1.00           0330         O         0.36558         0.75236         -0.00594         0.13427         Uani         1.00           X331         Zn         0.60042         0.79247         0.84040         0.02356         Uani         1.00           N333         N         0.62848         0.75100         0.95604         0.02828         Uani         1.00           0.335         O         0.5766         0.7187         0.68328         0.08340         Uani         1.00           0.335         O         0.5766         0.7187         0.68328         0.08137         Uani         1.00           0.334         PH         0.6746         0.72357         0.24116         0.04900         Uiso         1.00           0.334         C         0.66420         0.1541         0.99077         0.3170         Uani         1.00	H325	Н	0.22775	0.93261	0.43015	0.08200	Uiso	1.00
H327         H         0.32187         0.87474         0.40861         0.08000         Uiso         1.00           N328         N         0.36087         0.74138         0.11399         0.08794         Uani         1.00           0329         O         0.29175         0.74205         0.122253         Uani         1.00           0330         O         0.36558         0.75236         -0.00594         0.13427         Uani         1.00           N332         N         0.62848         0.75100         0.95604         0.02828         Uani         1.00           N333         N         0.62848         0.75100         0.95604         0.02828         Uani         1.00           C335         C         0.66955         0.72828         0.03304         Uani         1.00           C336         C         0.66955         0.72808         0.03430         Uani         1.00           C337         C         0.74114         0.66248         0.05984         0.03103         Uani         1.00           C338         C         0.66450         0.71247         0.2316         Uani         1.00           C340         C         0.66460         0.72357	C326	С	0.27445	0.87366	0.48033	0.05247	Uani	1.00
N328         N         0.36087         0.74138         0.11399         0.08794         Uani         1.00           0330         O         0.36558         0.75236         -0.00594         0.113427         Uani         1.00           2n311         Zn         0.60042         0.79247         0.84040         0.02356         Uani         1.00           N332         N         0.62860         0.75716         0.08137         0.02436         Uani         1.00           N3334         N         0.62848         0.75100         0.95604         0.02828         Uani         1.00           0335         O         0.57366         0.77187         0.68328         0.08820         Uani         1.00           0335         O         0.57366         0.77187         0.68328         0.03030         Uani         1.00           0337         C         0.74114         0.66248         0.03103         Uani         1.00           1339         H         0.67655         0.72580         0.13908         0.03103         Uani         1.00           1341         H         0.67655         0.72580         0.13908         0.03103         Uani         1.00           134	H327	Н	0.32187	0.87474	0.40861	0.08000	Uiso	1.00
O329         O         0.29175         0.74205         0.17242         0.12253         Uani         1.00           O330         O         0.36558         0.75236         -0.00594         0.13427         Uani         1.00           Xa31         Zn         0.60042         0.75716         0.8137         0.02436         Uani         1.00           N333         N         0.62840         0.75116         0.08137         0.02436         Uani         1.00           O335         O         0.57366         0.77187         0.63282         Uani         1.00           C336         C         0.66935         0.65981         0.04532         0.02851         Uani         1.00           C337         C         0.74114         0.66248         0.05984         0.03430         Uani         1.00           C338         C         0.66470         0.71541         0.93077         0.03170         Uani         1.00           H339         H         0.67646         0.72357         0.24116         0.04900         Uiso         1.00           C340         C         0.68420         0.71541         0.93077         0.03170         Uani         1.00           C344 <td>N328</td> <td>Ν</td> <td>0.36087</td> <td>0.74138</td> <td>0.11399</td> <td>0.08794</td> <td>Uani</td> <td>1.00</td>	N328	Ν	0.36087	0.74138	0.11399	0.08794	Uani	1.00
O330         O         0.36558         0.75236         -0.00594         0.13427         Uani         1.00           Xn331         Zn         0.60042         0.79247         0.84040         0.02356         Uani         1.00           N332         N         0.62848         0.75716         0.08137         0.02436         Uani         1.00           N333         N         0.62848         0.75716         0.03394         Uani         1.00           C335         O         0.57366         0.771187         0.68328         0.08820         Uani         1.00           C336         C         0.66935         0.04552         0.02851         Uani         1.00           C338         C         0.66675         0.72580         0.13908         0.03103         Uani         1.00           C340         C         0.66620         0.71571         0.24116         0.04900         Uiso         1.00           C342         C         0.85162         0.62233         0.16241         0.04616         Uani         1.00           C344         C         0.79203         0.6276         0.25507         0.07100         Uiso         1.00           C344         C	O329	0	0.29175	0.74205	0.17242	0.12253	Uani	1.00
Zn331         Zn         0.60042         0.79247         0.84040         0.02356         Uani         1.00           N332         N         0.62860         0.75716         0.08137         0.02436         Uani         1.00           N333         N         0.62848         0.75100         0.95604         0.02828         Uani         1.00           0335         O         0.57366         0.77187         0.68328         0.08820         Uani         1.00           C336         C         0.66675         0.72580         0.03103         Uani         1.00           C337         C         0.66675         0.72580         0.31030         Uani         1.00           C338         C         0.66675         0.72580         0.31030         Uani         1.00           H339         H         0.66766         0.7397         0.03170         Uani         1.00           C340         C         0.66420         0.71541         0.93077         0.03170         Uani         1.00           H341         H         0.89723         0.62776         0.23507         0.07100         Uiso         1.00           C344         C         0.79826         0.66076	O330	0	0.36558	0.75236	-0.00594	0.13427	Uani	1.00
N332         N         0.62860         0.75716         0.08137         0.02436         Uani         1.00           N333         N         0.62848         0.75100         0.95604         0.02828         Uani         1.00           0335         O         0.57366         0.77187         0.68328         0.08820         Uani         1.00           0335         O         0.57366         0.77187         0.68328         0.08820         Uani         1.00           C336         C         0.68935         0.04532         0.02851         Uani         1.00           C337         C         0.71141         0.66248         0.05984         0.03103         Uani         1.00           C338         C         0.66457         0.72580         0.13908         0.03103         Uani         1.00           C340         C         0.66420         0.71541         0.99077         0.03170         Uani         1.00           C344         C         0.85162         0.6223         0.16241         0.04616         Uani         1.00           C344         C         0.79102         0.59806         -0.01762         0.5220         Uani         1.00           C344	Zn331	Zn	0.60042	0.79247	0.84040	0.02356	Uani	1.00
N333         N         0.62848         0.75100         0.95604         0.02828         Uani         1.00           N334         N         0.84621         0.59732         0.07726         0.03394         Uani         1.00           0335         C         0.68935         0.68328         0.08820         Uani         1.00           C336         C         0.666575         0.72580         0.13908         0.03103         Uani         1.00           C338         C         0.666755         0.72580         0.13908         0.03103         Uani         1.00           C340         C         0.666420         0.71541         0.93077         0.03170         Uani         1.00           C341         H         0.67056         0.70399         0.83543         0.04900         Uiso         1.00           C342         C         0.85162         0.62823         0.16241         0.04616         Uani         1.00           C344         C         0.79826         0.6676         0.1723         0.5223         Uani         1.00           C344         C         0.79102         0.59806         -0.01762         0.5220         Uani         1.00           C346 <td>N332</td> <td>Ν</td> <td>0.62860</td> <td>0.75716</td> <td>0.08137</td> <td>0.02436</td> <td>Uani</td> <td>1.00</td>	N332	Ν	0.62860	0.75716	0.08137	0.02436	Uani	1.00
N334         N         0.84621         0.5732         0.07726         0.03394         Uani         1.00           O335         O         0.57366         0.77187         0.68328         0.08820         Uani         1.00           C336         C         0.68935         0.69881         0.04532         0.02851         Uani         1.00           C337         C         0.74114         0.66248         0.03984         0.03103         Uani         1.00           C338         C         0.66575         0.72580         0.03103         Uani         1.00           C340         C         0.66420         0.71541         0.93077         0.03170         Uani         1.00           C341         C         0.66420         0.71541         0.93077         0.03170         Uani         1.00           C342         C         0.85162         0.62823         0.16241         0.04616         Uani         1.00           C344         C         0.79826         0.66076         0.15723         0.05223         Uani         1.00           C344         C         0.79102         0.59806         0.07078         0.05197         Uani         1.00           C344	N333	Ν	0.62848	0.75100	0.95604	0.02828	Uani	1.00
O335         O         0.57366         0.77187         0.68328         0.08820         Uani         1.00           C336         C         0.68935         0.69851         0.04532         0.02851         Uani         1.00           C337         C         0.71141         0.66248         0.05984         0.03103         Uani         1.00           C338         C         0.66575         0.72580         0.13908         0.03103         Uani         1.00           C340         C         0.66420         0.71541         0.93077         0.03170         Uani         1.00           C340         C         0.66420         0.71541         0.93077         0.03170         Uani         1.00           H343         H         0.87605         0.70399         0.83543         0.04900         Uiso         1.00           C344         C         0.79826         0.66076         0.15723         0.07100         Uiso         1.00           C344         C         0.79826         0.66076         0.15723         0.08200         Uiso         1.00           C344         C         0.79826         0.66076         0.5723         Uani         1.00           C348	N334	Ν	0.84621	0.59732	0.07726	0.03394	Uani	1.00
C336         C         0.68935         0.69831         0.04532         0.02851         Uani         1.00           C337         C         0.74114         0.66248         0.05984         0.03430         Uani         1.00           C338         C         0.66575         0.72580         0.13908         0.03103         Uani         1.00           C340         C         0.66420         0.71541         0.93077         0.03170         Uani         1.00           C341         H         0.67665         0.70399         0.83543         0.04700         Uiso         1.00           C342         C         0.85162         0.62823         0.16241         0.04616         Uani         1.00           C344         C         0.79826         0.66076         0.15723         0.05223         Uani         1.00           H345         H         0.80369         0.68501         0.22587         0.08000         Uiso         1.00           C346         C         0.73822         0.63085         0.97078         0.05197         Uani         1.00           C348         C         0.71822         0.63157         0.89295         0.8000         Uiso         1.00      <	0335	0	0.57366	0.77187	0.68328	0.08820	Uani	1.00
Color         Color         Color         Color         Color         Color         Color           C337         C         0.66575         0.72580         0.13908         0.03103         Uani         1.00           H339         H         0.66764         0.72357         0.24116         0.04900         Uiso         1.00           C340         C         0.66420         0.71541         0.93977         0.03170         Uani         1.00           H341         H         0.67605         0.70399         0.83543         0.04900         Uiso         1.00           G342         C         0.85162         0.62823         0.16241         0.04010         Uiso         1.00           G344         C         0.79826         0.66076         0.15723         0.05223         Uani         1.00           H345         H         0.80369         0.68501         0.22587         0.08000         Uiso         1.00           G344         C         0.73824         0.91328         0.08200         Uiso         1.00           G348         C         0.73822         0.63157         0.89295         0.8000         Uiso         1.00           G351         O	C336	C	0.68935	0.69851	0.04532	0.02851	Uani	1.00
Construct         Construct         Construct         Construct         Construct         Construct         Construct           H339         H         0.66757         0.72580         0.13908         0.03103         Uani         1.00           C340         C         0.66420         0.71541         0.93077         0.03170         Uani         1.00           C341         H         0.67646         0.72380         0.16241         0.04616         Uani         1.00           C342         C         0.85162         0.62823         0.16241         0.04616         Uani         1.00           C344         C         0.79826         0.66076         0.15723         0.05223         Uani         1.00           H343         H         0.890369         0.68501         0.22587         0.08000         Uiso         1.00           C346         C         0.79102         0.59806         -0.01762         0.05220         Uani         1.00           H347         H         0.69072         0.63157         0.89295         0.80000         Uiso         1.00           G348         C         0.73822         0.63085         0.97078         0.05197         Uani         1.00 <td>C337</td> <td>C</td> <td>0.74114</td> <td>0.66248</td> <td>0.05984</td> <td>0.03430</td> <td>Uani</td> <td>1.00</td>	C337	C	0.74114	0.66248	0.05984	0.03430	Uani	1.00
Construct         Construct         Construct         Construct         Construct         Construct           1339         H         0.67646         0.72357         0.24116         0.04900         Uiso         1.00           C340         C         0.66420         0.71541         0.93077         0.03170         Uani         1.00           C342         C         0.85162         0.62823         0.16241         0.04616         Uani         1.00           C344         C         0.79826         0.66076         0.15723         0.05223         Uani         1.00           C344         C         0.79826         0.66076         0.15723         0.08000         Uiso         1.00           C346         C         0.79102         0.59806         -0.01762         0.59220         Uani         1.00           H347         H         0.79020         0.57384         0.91328         0.08200         Uiso         1.00           C348         C         0.73822         0.63157         0.89295         0.8000         Uiso         1.00           O351         O         0.71067         0.76180         0.67463         0.1220         Uani         1.00           C353 <td>C338</td> <td>C C</td> <td>0.66575</td> <td>0.72580</td> <td>0.13908</td> <td>0.03103</td> <td>Uani</td> <td>1.00</td>	C338	C C	0.66575	0.72580	0.13908	0.03103	Uani	1.00
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Н339	е н	0.67646	0.72357	0.24116	0.04900	Uiso	1.00
Construct         Construct         Construct         Construct         Construct         Construct           C342         C         0.67605         0.70399         0.83543         0.04900         Uiso         1.00           H341         H         0.8705         0.62823         0.16241         0.04616         Uani         1.00           H343         H         0.89723         0.62776         0.23507         0.07100         Uiso         1.00           C344         C         0.79826         0.66076         0.15723         0.05223         Uani         1.00           H345         H         0.80369         0.68501         0.22587         0.08000         Uiso         1.00           H347         H         0.79020         0.57384         0.91328         0.08200         Uiso         1.00           H349         H         0.69572         0.63157         0.89295         0.8000         Uiso         1.00           N350         N         0.64136         0.76084         0.61925         0.8815         Uani         1.00           O351         O         0.71067         0.76180         0.67463         0.1220         Uani         1.00           C353C	C340	п С	0.66420	0.72557	0.93077	0.03170	Uani	1.00
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	H341	с н	0.00420	0.70399	0.83543	0.04900	Uiso	1.00
H343         H         0.89723         0.62736         0.10241         0.00010         Uiso         1.00           H343         H         0.89723         0.62776         0.23507         0.07100         Uiso         1.00           C344         C         0.79826         0.66076         0.15723         0.05223         Uani         1.00           H345         H         0.80369         0.68501         0.22587         0.08000         Uiso         1.00           C346         C         0.79102         0.59806         -0.01762         0.05220         Uani         1.00           H347         H         0.79020         0.57384         0.91328         0.08200         Uiso         1.00           C348         C         0.73822         0.63157         0.89295         0.8000         Uiso         1.00           N350         N         0.64136         0.76084         0.61925         0.08815         Uani         1.00           O351         O         0.71067         0.76180         0.67463         0.1220         Uani         1.00           C353         C         0.55931         0.57305         1.01186         0.00000         Uiso         1.00      <	C342	n C	0.85162	0.70377	0.05545	0.04500	Uani	1.00
C344       C       0.79826       0.66076       0.15723       0.05120       Uani       1.00         H345       H       0.80369       0.68501       0.22587       0.08000       Uiso       1.00         H345       H       0.79926       0.68501       0.22587       0.08000       Uiso       1.00         H347       H       0.79020       0.57384       0.91328       0.08200       Uiso       1.00         C348       C       0.73822       0.63085       0.97078       0.05197       Uani       1.00         H349       H       0.69572       0.63157       0.89295       0.08000       Uiso       1.00         N350       N       0.64136       0.76084       0.61925       0.08815       Uani       1.00         O351       O       0.71067       0.76180       0.67463       0.12220       Uani       1.00         C353       C       0.55931       0.57305       1.01186       0.00000       Uiso       1.00         C354       C       0.47591       0.57281       1.03176       0.00000       Uiso       1.00         C355       C       0.42540       0.55631       0.93889       0.00000       Uiso </td <td>H343</td> <td>с н</td> <td>0.89723</td> <td>0.62776</td> <td>0.10241</td> <td>0.07100</td> <td>Uiso</td> <td>1.00</td>	H343	с н	0.89723	0.62776	0.10241	0.07100	Uiso	1.00
Construction         Construction         Construction         Construction         Construction           H345         H         0.80369         0.68501         0.22587         0.08000         Uiso         1.00           C346         C         0.79102         0.59806         -0.01762         0.05220         Uani         1.00           H347         H         0.79020         0.57384         0.91328         0.08200         Uiso         1.00           C348         C         0.73822         0.63085         0.97078         0.05197         Uani         1.00           H349         H         0.69572         0.63157         0.89295         0.08000         Uiso         1.00           N350         N         0.64136         0.76084         0.61925         0.08815         Uani         1.00           O351         O         0.71067         0.76180         0.67463         0.12220         Uani         1.00           C353         C         0.55931         0.57305         1.01186         0.00000         Uiso         1.00           C355         C         0.42540         0.55631         0.93889         0.00000         Uiso         1.00           C355	C344	n C	0.09725	0.62776	0.15723	0.05223	Uani	1.00
11343       11       0.30303       0.32301       0.32307       0.03000       Uiso       1.00         C346       C       0.79102       0.59806       -0.01762       0.05220       Uani       1.00         H347       H       0.79020       0.57384       0.91328       0.08200       Uiso       1.00         C348       C       0.73822       0.63085       0.97078       0.05197       Uani       1.00         H349       H       0.69572       0.63157       0.89295       0.08000       Uiso       1.00         N350       N       0.64136       0.76084       0.61925       0.08815       Uani       1.00         O351       O       0.71067       0.76180       0.67463       0.12220       Uani       1.00         C353       C       0.55931       0.57305       1.0186       0.00000       Uiso       1.00         C355       C       0.47591       0.57281       1.03176       0.0000       Uiso       1.00         C355       C       0.45987       0.54005       0.82802       0.00000       Uiso       1.00         C355       C       0.45987       0.54005       0.82802       0.00000       Uiso<	U344 U345	ч	0.79820	0.00070	0.13723	0.03223	Uiso	1.00
C346       C       0.7902       0.59806       0.01102       0.08220       Uani       1.00         H347       H       0.79020       0.57384       0.91328       0.08220       Uiso       1.00         C348       C       0.73822       0.63085       0.97078       0.05197       Uani       1.00         H349       H       0.69572       0.63157       0.89295       0.08000       Uiso       1.00         N350       N       0.64136       0.76084       0.61925       0.08815       Uani       1.00         O351       O       0.71067       0.76180       0.67463       0.12220       Uani       1.00         C353       C       0.55931       0.57305       1.0186       0.00000       Uiso       1.00         C355       C       0.47591       0.57281       1.03176       0.00000       Uiso       1.00         C355       C       0.45987       0.54005       0.82802       0.00000       Uiso       1.00         C355       C       0.45987       0.54005       0.82802       0.00000       Uiso       1.00         C357       C       0.54132       0.54080       0.80859       0.00000       Uiso <td>C346</td> <td>II C</td> <td>0.00507</td> <td>0.000001</td> <td>0.22587</td> <td>0.05220</td> <td>Uani</td> <td>1.00</td>	C346	II C	0.00507	0.000001	0.22587	0.05220	Uani	1.00
I1347I10.79200.573840.713280.082000.080.08C348C0.738220.630850.970780.05197Uani1.00H349H0.695720.631570.892950.08000Uiso1.00N350N0.641360.760840.619250.08815Uani1.00O351O0.710670.761800.674630.12220Uani1.00O352O0.636860.748630.501310.13418Uani1.00C353C0.559310.573051.011860.00000Uiso1.00C354C0.475910.572811.031760.00000Uiso1.00C355C0.425400.556310.938890.00000Uiso1.00C356C0.459870.540050.828020.00000Uiso1.00C357C0.592460.556700.899550.00000Uiso1.00C360C0.501520.514740.626480.00000Uiso1.00C361S0.409630.519690.703310.00000Uiso1.00C362C0.584700.488380.441790.00000Uiso1.00C363C0.594650.482380.309330.00000Uiso1.00C364C0.594650.482380.309330.00000Uiso1.00C364C0.594650.482380.309330.0000	U247	с u	0.79102	0.57384	-0.01702	0.03220	Uiso	1.00
C348C0.738220.630330.970780.03197Cann1.00H349H0.695720.631570.892950.08000Uiso1.00N350N0.641360.760840.619250.08815Uani1.00O351O0.710670.761800.674630.12220Uani1.00O352O0.636860.748630.501310.13418Uani1.00C353C0.559310.573051.011860.00000Uiso1.00C354C0.475910.572811.031760.00000Uiso1.00C355C0.425400.556310.938890.00000Uiso1.00C356C0.459870.540050.828020.00000Uiso1.00C357C0.541320.540800.808590.00000Uiso1.00C358C0.592460.556700.899550.00000Uiso1.00N359N0.565300.526840.694570.00000Uiso1.00C360C0.501520.514740.626480.00000Uiso1.00C361S0.409630.519690.703310.00000Uiso1.00C363C0.594650.482380.309330.00000Uiso1.00C364C0.594650.482380.309330.00000Uiso1.00C364C0.530560.487940.226520.00000	C249	II C	0.79020	0.57504	0.91526	0.08200	UISO	1.00
N350N0.693720.031370.032930.000000.0300.030N350N0.641360.760840.619250.08815Uani1.00O351O0.710670.761800.674630.12220Uani1.00O352O0.636860.748630.501310.13418Uani1.00C353C0.559310.573051.011860.00000Uiso1.00C354C0.475910.572811.031760.00000Uiso1.00C355C0.425400.556310.938890.00000Uiso1.00C356C0.459870.540050.828020.00000Uiso1.00C357C0.541320.540800.808590.00000Uiso1.00C358C0.592460.556700.899550.00000Uiso1.00C360C0.501520.514740.626480.00000Uiso1.00C361S0.409630.519690.703310.00000Uiso1.00C362C0.510560.502430.490570.00000Uiso1.00C363C0.530560.482380.309330.00000Uiso1.00C364C0.594650.482380.309330.00000Uiso1.00C364C0.530560.487940.226520.00000Uiso1.00C364C0.454870.498590.275470.000	C348	U U	0.75822	0.03083	0.97078	0.03197	Uani	1.00
N350N0.641360.760840.619230.08813Oan1.00O351O0.710670.761800.674630.12220Uani1.00O352O0.636860.748630.501310.13418Uani1.00C353C0.559310.573051.011860.00000Uiso1.00C354C0.475910.572811.031760.00000Uiso1.00C355C0.425400.556310.938890.00000Uiso1.00C356C0.459870.540050.828020.00000Uiso1.00C357C0.541320.540800.808590.00000Uiso1.00C358C0.592460.556700.899550.00000Uiso1.00N359N0.565300.526840.694570.00000Uiso1.00C360C0.511520.514740.626480.00000Uiso1.00C361S0.409630.519690.703310.00000Uiso1.00C362C0.584700.488380.441790.00000Uiso1.00C364C0.594650.482380.309330.00000Uiso1.00C364C0.530560.487940.226520.00000Uiso1.00C364C0.454870.498590.275470.00000Uiso1.00C366C0.445810.506720.406550.00000<	N250	n N	0.09372	0.03137	0.69295	0.08000	UISO	1.00
0331       0       0.71067       0.76180       0.674853       0.12220       0       0ani       1.00         0352       0       0.63686       0.74863       0.50131       0.13418       Uani       1.00         C353       C       0.55931       0.57305       1.01186       0.00000       Uiso       1.00         C354       C       0.47591       0.57281       1.03176       0.00000       Uiso       1.00         C355       C       0.42540       0.55631       0.93889       0.00000       Uiso       1.00         C356       C       0.445987       0.54005       0.82802       0.00000       Uiso       1.00         C357       C       0.54132       0.54080       0.8859       0.00000       Uiso       1.00         C358       C       0.59246       0.55670       0.89955       0.00000       Uiso       1.00         N359       N       0.56530       0.52684       0.69457       0.00000       Uiso       1.00         C360       C       0.50152       0.51474       0.62648       0.00000       Uiso       1.00         C362       C       0.51056       0.50243       0.49057       0.00000 <td>N350 0251</td> <td>N</td> <td>0.04130</td> <td>0.76084</td> <td>0.01925</td> <td>0.08815</td> <td>Uani</td> <td>1.00</td>	N350 0251	N	0.04130	0.76084	0.01925	0.08815	Uani	1.00
0352       0       0.65886       0.74883       0.50131       0.13418       0 ani       1.00         C353       C       0.55931       0.57305       1.01186       0.00000       Uiso       1.00         C354       C       0.47591       0.57281       1.03176       0.00000       Uiso       1.00         C355       C       0.42540       0.55631       0.93889       0.00000       Uiso       1.00         C356       C       0.45987       0.54005       0.82802       0.00000       Uiso       1.00         C357       C       0.54132       0.54080       0.80859       0.00000       Uiso       1.00         C358       C       0.59246       0.55670       0.89955       0.00000       Uiso       1.00         N359       N       0.56530       0.52684       0.69457       0.00000       Uiso       1.00         C360       C       0.50152       0.51474       0.62648       0.00000       Uiso       1.00         S361       S       0.40963       0.51969       0.70331       0.00000       Uiso       1.00         C362       C       0.58470       0.48838       0.44179       0.00000       Uiso<	0351	0	0./100/	0.70180	0.0/403	0.12220	Uani	1.00
C353       C       0.35931       0.37305       1.01186       0.00000       Uiso       1.00         C354       C       0.47591       0.57281       1.03176       0.00000       Uiso       1.00         C355       C       0.42540       0.55631       0.93889       0.00000       Uiso       1.00         C356       C       0.45987       0.54005       0.82802       0.00000       Uiso       1.00         C357       C       0.54132       0.54080       0.80859       0.00000       Uiso       1.00         C358       C       0.59246       0.55670       0.89955       0.00000       Uiso       1.00         N359       N       0.56530       0.52684       0.69457       0.00000       Uiso       1.00         C360       C       0.50152       0.51474       0.62648       0.00000       Uiso       1.00         S361       S       0.40963       0.51969       0.70331       0.00000       Uiso       1.00         C362       C       0.58470       0.48838       0.44179       0.00000       Uiso       1.00         C363       C       0.59465       0.48238       0.30933       0.00000       Uiso </td <td>0352</td> <td>0</td> <td>0.03080</td> <td>0.74863</td> <td>0.50131</td> <td>0.13418</td> <td>Uani</td> <td>1.00</td>	0352	0	0.03080	0.74863	0.50131	0.13418	Uani	1.00
C354C0.475910.572811.031760.00000Uiso1.00C355C0.425400.556310.938890.00000Uiso1.00C356C0.459870.540050.828020.00000Uiso1.00C357C0.541320.540800.808590.00000Uiso1.00C358C0.592460.556700.899550.00000Uiso1.00N359N0.565300.526840.694570.00000Uiso1.00C360C0.501520.514740.626480.00000Uiso1.00C361S0.409630.519690.703310.00000Uiso1.00C362C0.510560.502430.490570.00000Uiso1.00C363C0.594650.48380.441790.00000Uiso1.00C364C0.594650.482380.309330.00000Uiso1.00C365C0.454870.498590.275470.00000Uiso1.00C366C0.445810.506720.406550.00000Uiso1.00	C353	C	0.55931	0.57305	1.01186	0.00000	UISO	1.00
C355C0.425400.556310.938890.00000Uiso1.00C356C0.459870.540050.828020.00000Uiso1.00C357C0.541320.540800.808590.00000Uiso1.00C358C0.592460.556700.899550.00000Uiso1.00N359N0.565300.526840.694570.00000Uiso1.00C360C0.501520.514740.626480.00000Uiso1.00C361S0.409630.519690.703310.00000Uiso1.00C362C0.510560.502430.490570.00000Uiso1.00C363C0.584700.488380.441790.00000Uiso1.00C364C0.594650.482380.309330.00000Uiso1.00C365C0.454870.498590.275470.00000Uiso1.00C366C0.445810.506720.406550.0000Uiso1.00	C354	C	0.4/591	0.57281	1.031/6	0.00000	U1SO	1.00
C356C0.459870.540050.828020.00000Uiso1.00C357C0.541320.540800.808590.00000Uiso1.00C358C0.592460.556700.899550.00000Uiso1.00N359N0.565300.526840.694570.00000Uiso1.00C360C0.501520.514740.626480.00000Uiso1.00S361S0.409630.519690.703310.00000Uiso1.00C362C0.510560.502430.490570.00000Uiso1.00C363C0.594650.48380.441790.00000Uiso1.00C364C0.594650.482380.309330.00000Uiso1.00C365C0.454870.498590.275470.00000Uiso1.00C366C0.445810.506720.406550.0000Uiso1.00	0355	C	0.42540	0.55631	0.93889	0.00000	U1SO	1.00
C357C0.541320.540800.808590.00000Uiso1.00C358C0.592460.556700.899550.00000Uiso1.00N359N0.565300.526840.694570.00000Uiso1.00C360C0.501520.514740.626480.00000Uiso1.00S361S0.409630.519690.703310.00000Uiso1.00C362C0.510560.502430.490570.00000Uiso1.00C363C0.584700.488380.441790.00000Uiso1.00C364C0.594650.482380.309330.00000Uiso1.00C365C0.454870.498590.275470.00000Uiso1.00C366C0.445810.506720.406550.00000Uiso1.00	C356	C	0.45987	0.54005	0.82802	0.00000	U1SO	1.00
C358       C       0.59246       0.55670       0.89955       0.00000       Uiso       1.00         N359       N       0.56530       0.52684       0.69457       0.00000       Uiso       1.00         C360       C       0.50152       0.51474       0.62648       0.00000       Uiso       1.00         S361       S       0.40963       0.51969       0.70331       0.00000       Uiso       1.00         C362       C       0.51056       0.50243       0.49057       0.00000       Uiso       1.00         C363       C       0.58470       0.48838       0.44179       0.00000       Uiso       1.00         C364       C       0.59465       0.48238       0.30933       0.00000       Uiso       1.00         C365       C       0.53056       0.48794       0.22652       0.00000       Uiso       1.00         C366       C       0.45487       0.49859       0.27547       0.00000       Uiso       1.00         C367       C       0.44581       0.50672       0.40655       0.00000       Uiso       1.00	C357	C	0.54132	0.54080	0.80859	0.00000	U1SO	1.00
N359         N         0.56530         0.52684         0.69457         0.00000         Uiso         1.00           C360         C         0.50152         0.51474         0.62648         0.00000         Uiso         1.00           S361         S         0.40963         0.51969         0.70331         0.00000         Uiso         1.00           C362         C         0.51056         0.50243         0.49057         0.00000         Uiso         1.00           C363         C         0.58470         0.48838         0.44179         0.00000         Uiso         1.00           C364         C         0.59465         0.48238         0.30933         0.00000         Uiso         1.00           C365         C         0.53056         0.48794         0.22652         0.00000         Uiso         1.00           C366         C         0.45487         0.49859         0.27547         0.00000         Uiso         1.00           C367         C         0.44581         0.50672         0.40655         0.00000         Uiso         1.00	C358	C	0.59246	0.55670	0.89955	0.00000	Uiso	1.00
C360       C       0.50152       0.51474       0.62648       0.00000       Uiso       1.00         S361       S       0.40963       0.51969       0.70331       0.00000       Uiso       1.00         C362       C       0.51056       0.50243       0.49057       0.00000       Uiso       1.00         C363       C       0.58470       0.48838       0.44179       0.00000       Uiso       1.00         C364       C       0.59465       0.48238       0.30933       0.00000       Uiso       1.00         C365       C       0.53056       0.48794       0.22652       0.00000       Uiso       1.00         C366       C       0.45487       0.49859       0.27547       0.00000       Uiso       1.00         C367       C       0.44581       0.50672       0.40655       0.00000       Uiso       1.00	N359	N	0.56530	0.52684	0.69457	0.00000	Uiso	1.00
S361       S       0.40963       0.51969       0.70331       0.00000       Uiso       1.00         C362       C       0.51056       0.50243       0.49057       0.00000       Uiso       1.00         C363       C       0.58470       0.48838       0.44179       0.00000       Uiso       1.00         C364       C       0.59465       0.48238       0.30933       0.00000       Uiso       1.00         C365       C       0.53056       0.48794       0.22652       0.00000       Uiso       1.00         C366       C       0.45487       0.49859       0.27547       0.00000       Uiso       1.00         C367       C       0.44581       0.50672       0.40655       0.00000       Uiso       1.00	C360	С	0.50152	0.51474	0.62648	0.00000	Uiso	1.00
C362       C       0.51056       0.50243       0.49057       0.00000       Uiso       1.00         C363       C       0.58470       0.48838       0.44179       0.00000       Uiso       1.00         C364       C       0.59465       0.48238       0.30933       0.00000       Uiso       1.00         C365       C       0.53056       0.48794       0.22652       0.00000       Uiso       1.00         C366       C       0.45487       0.49859       0.27547       0.00000       Uiso       1.00         C367       C       0.44581       0.50672       0.40655       0.00000       Uiso       1.00	S361	S	0.40963	0.51969	0.70331	0.00000	Uiso	1.00
C363       C       0.58470       0.4838       0.44179       0.00000       Uiso       1.00         C364       C       0.59465       0.48238       0.30933       0.00000       Uiso       1.00         C365       C       0.53056       0.48794       0.22652       0.00000       Uiso       1.00         C366       C       0.45487       0.49859       0.27547       0.00000       Uiso       1.00         C367       C       0.44581       0.50672       0.40655       0.00000       Uiso       1.00	C362	С	0.51056	0.50243	0.49057	0.00000	Uiso	1.00
C364         C         0.59465         0.48238         0.30933         0.00000         Uiso         1.00           C365         C         0.53056         0.48794         0.22652         0.00000         Uiso         1.00           C366         C         0.45487         0.49859         0.27547         0.00000         Uiso         1.00           C367         C         0.44581         0.50672         0.40655         0.00000         Uiso         1.00	C363	С	0.58470	0.48838	0.44179	0.00000	Uiso	1.00
C365         C         0.53056         0.48794         0.22652         0.00000         Uiso         1.00           C366         C         0.45487         0.49859         0.27547         0.00000         Uiso         1.00           C367         C         0.44581         0.50672         0.40655         0.00000         Uiso         1.00	C364	С	0.59465	0.48238	0.30933	0.00000	Uiso	1.00
C366         C         0.45487         0.49859         0.27547         0.00000         Uiso         1.00           C367         C         0.44581         0.50672         0.40655         0.00000         Uiso         1.00	C365	С	0.53056	0.48794	0.22652	0.00000	Uiso	1.00
C367 C 0.44581 0.50672 0.40655 0.00000 Uiso 1.00	C366	С	0.45487	0.49859	0.27547	0.00000	Uiso	1.00
	C367	С	0.44581	0.50672	0.40655	0.00000	Uiso	1.00

C368	С	0.38462	0.50065	0.19043	0.00000	Uiso	1.00
O369	0	0.64696	0.47912	0.52565	0.00000	Uiso	1.00
H370	Н	0.59802	0.58629	1.08214	0.00000	Uiso	1.00
H371	Н	0.45078	0.58531	1.11891	0.00000	Uiso	1.00
H372	Н	0.36107	0.55640	0.95285	0.00000	Uiso	1.00
H373	Н	0.65628	0.55673	0.88271	0.00000	Uiso	1.00
H374	Н	0.65203	0.47305	0.27061	0.00000	Uiso	1.00
H375	Н	0.53964	0.48308	0.12455	0.00000	Uiso	1.00
H376	Н	0.38778	0.51609	0.44256	0.00000	Uiso	1.00
O377	Ο	0.37998	0.47753	0.07876	0.00000	Uiso	1.00
H378	Н	0.69429	0.46554	0.48206	0.00000	Uiso	1.00
O379	Ο	0.33030	0.52419	0.21486	0.00000	Uiso	1.00
C380	С	0.39694	0.43537	0.09396	0.00000	Uiso	1.00
H381	Н	0.42985	0.42477	0.00746	0.00000	Uiso	1.00
H382	Н	0.33951	0.41904	0.10457	0.00000	Uiso	1.00
H383	Н	0.43329	0.42760	0.17926	0.00000	Uiso	1.00

 Table S8. Atomic coordinates of optimized HBT2@DCF-20 models.

label	type_symbol	Z	у	Z	U_iso_or_equiv	adp_type	occupancy
Zn1	Zn	0.42103	0.19493	0.65114	0.02351	Uani	1.00
N2	Ν	0.49289	0.18031	0.41031	0.02423	Uani	1.00
N3	Ν	0.50211	0.17829	0.53733	0.02806	Uani	1.00
N4	Ν	0.81708	0.07835	0.40973	0.03341	Uani	1.00
O5	0	0.46051	0.20439	0.81382	0.08912	Uani	1.00
C6	С	0.60803	0.14995	0.44816	0.02829	Uani	1.00
C7	С	0.68186	0.12638	0.43194	0.03396	Uani	1.00
C8	С	0.55610	0.16276	0.35254	0.03081	Uani	1.00
H9	Н	0.56394	0.15984	0.24892	0.04900	Uiso	1.00
C10	С	0.57219	0.16042	0.56393	0.03127	Uani	1.00
H11	Н	0.59415	0.15411	0.66023	0.04900	Uiso	1.00
C12	С	0.75251	0.07014	0.33490	0.04552	Uani	1.00
H13	Н	0.75334	0.04480	0.26841	0.07100	Uiso	1.00
C14	С	0.68460	0.09440	0.34269	0.05140	Uani	1.00
H15	Н	0.63379	0.08739	0.28253	0.08000	Uiso	1.00
C16	С	0.81649	0.10970	0.49590	0.05162	Uani	1.00
H17	Н	0.86817	0.11525	0.55544	0.08200	Uiso	1.00
C18	С	0.74838	0.13398	0.50996	0.05131	Uani	1.00
H19	Н	0.74757	0.15839	0.58055	0.08000	Uiso	1.00
N20	Ν	0.47548	0.16807	0.87241	0.08782	Uani	1.00
O21	0	0.47106	0.13405	0.80839	0.12143	Uani	1.00
O22	0	0.49643	0.16729	0.99337	0.13360	Uani	1.00
Zn23	Zn	0.58240	0.30811	0.15622	0.02349	Uani	1.00
N24	Ν	0.51260	0.32316	0.91346	0.02425	Uani	1.00
N25	Ν	0.50356	0.32645	0.04036	0.02805	Uani	1.00
N26	Ν	0.18563	0.42337	0.90326	0.03343	Uani	1.00
O27	0	0.53883	0.29916	0.31714	0.08940	Uani	1.00
C28	С	0.39748	0.35407	0.94956	0.02834	Uani	1.00
C29	С	0.32250	0.37660	0.93073	0.03398	Uani	1.00
C30	С	0.44944	0.34022	0.85484	0.03082	Uani	1.00

H31       H       0.44112       0.34164       0.75115       0.04900         C32       C       0.43341       0.34470       0.06594       0.03130         H33       H       0.41083       0.35142       0.16185       0.04900	Uiso 1	.00
C32         C         0.43341         0.34470         0.06594         0.03130           H33         H         0.41083         0.35142         0.16185         0.04900	TT ' 1	
H33 H 0.41083 0.35142 0.16185 0.04900	Uani I	.00
	Uiso 1	.00
C34 C 0.24983 0.43075 0.82558 0.04560	Uani 1	.00
H35 H 0.24786 0.45489 0.75453 0.07100	Uiso 1	.00
C36 C 0.31841 0.40701 0.83576 0.05152	Uani 1	.00
H37 H 0.36880 0.41321 0.77291 0.08000	Uiso 1	.00
C38 C 0.18728 0.39329 0.99444 0.05186	Uani 1	.00
H39 H 0.13596 0.38837 0.05626 0.08200	Uiso 1	.00
C40 C 0.25610 0.36967 0.01103 0.05147	Uani 1	.00
H41 H 0.25773 0.34648 0.08601 0.08000	Uiso 1	.00
N42 N 0.52536 0.33572 0.37482 0.08772	Uani 1	.00
O43 O 0.53256 0.36965 0.31020 0.12143	Uani 1	.00
O44 O 0.50377 0.33689 0.49582 0.13357	Uani 1	.00
Zn45 Zn 0.09526 0.45816 0.88648 0.02336	Uani 1	.00
N46 N 0.12488 0.49304 0.64280 0.02425	Uani 1	.00
N47 N 0.12138 0.50024 0.76870 0.02815	Uani 1	.00
N48 N 0.34193 0.15367 0.65558 0.03388	Uani 1	.00
O49 O 0.06520 0.47876 0.04432 0.08742	Uani 1	.00
C50 C 0.18230 0.05387 0.68852 0.02841	Uani 1	.00
C51 C 0.23407 0.08978 0.67157 0.03419	Uani 1	00
C52 $C$ $0.16242$ $0.52434$ $0.58402$ $0.03089$	Uani 1	00
H53 H 0.17210 0.02727 0.49250 0.04900	Uiso 1	00
$C_{54} = C = 0.15810 = 0.03722 = 0.80528 = 0.03167 = 0.015810 = 0.03722 = 0.80528 = 0.03167 = 0.015810 = 0.03722 = 0.80528 = 0.03167 = 0.015810 = 0.03722 = 0.80528 = 0.03167 = 0.015810 = 0.03722 = 0.80528 = 0.03167 = 0.015810 = 0.00158100 = 0.00158100 = 0.00158100 = 0.00158100000000000000000000000000000000$	Uani 1	.00
H55 H 0.16971 0.04935 0.90063 0.04900	Uiso 1	.00
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Ulso I Uani I	.00
$H_{57}$ H 0.40126 0.11873 0.51145 0.07100	Uiro 1	.00
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Ulso I Uani I	.00
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Uani I Uico 1	.00
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	UISU I	.00
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Uani I	.00
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		.00
$C_{02}$ C $0.22552$ $0.12415$ $0.75151$ $0.05215$	Uani I	.00
H05 H 0.17778 0.12389 0.82226 0.08000		.00
N64 N 0.13150 0.49220 0.10504 0.08748	Uani I	.00
065 0 0.19871 0.49513 0.04308 0.12204	Uani I	.00
	Uani I	.00
Zn6/ Zn 0.90644 0.04314 0.39662 0.02334	Uani I	.00
N68 N 0.87864 0.00841 0.15390 0.02422	Uani I	.00
N69 N 0.88067 0.00126 0.28000 0.02812	Uani I	.00
N/U N 0.66456 0.34777 0.16512 0.03382	Uani 1	.00
0/1 0 0.93390 0.02245 0.55578 0.08761	∪anı l	.00
C/Z C 0.82572 0.44706 0.20006 0.02838	Uani 1	.00
C/3 C 0.7/520 0.41050 0.18305 0.03416	Uani 1	.00
C/4 C 0.84162 -0.02290 0.09552 0.03084	Uani 1	.00
H75 H 0.83920 0.47326 0.00297 0.04900	Uiso 1	.00
C76 C 0.84720 0.46454 0.31659 0.03162	Uani 1	.00
H77 H 0.83460 0.45275 0.41240 0.04900	Uiso 1	.00
C78 C 0.66650 0.37749 0.07298 0.04610	Uani 1	.00
Н79 Н 0.62362 0.37746 -0.00452 0.07100	Uiso 1	.00
C80 C 0.72403 0.40801 0.07680 0.05228	Uani 1	.00
H81 H 0.72567 0.43055 0.00017 0.08000	Uiso 1	.00
C82 C 0.71672 0.34787 0.26558 0.05217	Uani 1	.00
H83 H 0.71321 0.32423 0.33887 0.08200	Uiso 1	.00

C84 C 0.7718	0.37968	0.27801	0.05194	Uani	1.00
H85 H 0.8104	7 0.38044	0.36157	0.08000	Uiso	1.00
N86 N 0.86680	0 01091	0.61980	0.08749	Uani	1.00
0.00000000000000000000000000000000000	7 0.01033	0.56182	0.12168	Uani	1.00
O88 O 0.8710	-0.00035	0.74029	0.13407	Uani	1.00
7n89 $7n$ $0.0829'$	0.00000000000000000000000000000000000	0.57276	0.02351	Uani	1.00
N90 N 0.00252	2 0.47961	0.81226	0.02331	Uani	1.00
N01 N 0.0098	5 0.42785	0.68521	0.02424	Uani	1.00
NO2 N 0.6880	0.42703	0.000021	0.02307	Uani	1.00
0.032 0 0.0444	5 0.52002	0.01017	0.03341	Uani	1.00
$C_{0,0}^{0,0} = 0$	0.45578	0.40933	0.03912	Uani	1.00
$C_{94} C 0.8901$	0.39801	0.77340	0.02831	Uani	1.00
C95 C 0.8255	0.37330	0.76945	0.03390	Uani	1.00
107 II $0.0201$	0.41120	0.80932	0.03082	Uani	1.00
П9/ П 0.93910	0.40798	0.9/508	0.04900	UISO	1.00
	0.40922	0.05/98	0.03129	Uani	1.00
H99 H 0.9106	0.40256	0.56156	0.04900	Uiso	1.00
C100 C 0./5400	0.31/24	0.88944	0.04558	Uani	1.00
H101 H 0.75358	8 0.29202	0.95700	0.07100	Uiso	1.00
C102 C 0.8221	0.34121	0.8/814	0.05145	Uani	1.00
H103 H 0.87379	9 0.33408	0.93637	0.08000	Uiso	1.00
C104 C 0.687/9	0.35728	0./3106	0.05168	Uanı	1.00
H105 H 0.63490	6 0.36326	0.67450	0.08200	Uiso	1.00
C106 C 0.75582	2 0.38135	0.71386	0.05138	Uani	1.00
Н107 Н 0.75543	5 0.40603	0.64375	0.08000	Uiso	1.00
N108 N 0.02940	6 0.41743	0.35169	0.08784	Uani	1.00
O109 O 0.03458	8 0.38342	0.41623	0.12161	Uani	1.00
O110 O 0.00758	8 0.41662	0.23120	0.13380	Uani	1.00
Zn111 Zn 0.92093	5 0.05718	0.08290	0.02348	Uani	1.00
N112 N 0.99344	4 0.07123	0.32231	0.02423	Uani	1.00
N113 N 1.00262	2 0.07349	0.19520	0.02804	Uani	1.00
N114 N 0.3168	0.17379	0.32235	0.03338	Uani	1.00
O115 O 0.96053	5 0.04754	0.91979	0.08944	Uani	1.00
C116 C 0.10824	4 0.10199	0.28319	0.02831	Uani	1.00
C117 C 0.1817:	5 0.12580	0.29901	0.03396	Uani	1.00
C118 C 1.05640	0.08883	0.37935	0.03079	Uani	1.00
Н119 Н 0.06393	5 0.09174	0.48287	0.04900	Uiso	1.00
C120 C 0.07252	2 0.09161	0.16778	0.03126	Uani	1.00
Н121 Н 0.0942	0.09833	0.07125	0.04900	Uiso	1.00
C122 C 0.25209	9 0.18152	0.39858	0.04549	Uani	1.00
H123 H 0.2528	7 0.20640	0.46685	0.07100	Uiso	1.00
C124 C 0.18428	3 0.15726	0.39020	0.05141	Uani	1.00
Н125 Н 0.13340	0.16382	0.45168	0.08000	Uiso	1.00
C126 C 0.31638	8 0.14301	0.23412	0.05171	Uani	1.00
H127 H 0.36810	6 0.13786	0.17351	0.08200	Uiso	1.00
C128 C 0.24842	0.11879	0.21948	0.05133	Uani	1.00
Н129 Н 0.24792	2 0.09481	0.14742	0.08000	Uiso	1.00
N130 N 0.97629	9 0.08378	0.86113	0.08779	Uani	1.00
O131 O 0.97125	5 0.11785	0.92483	0.12132	Uani	1.00
O132 O 0.99828	8 0.08443	0.74028	0.13365	Uani	1.00
Zn133 Zn 0.40646	6 0.20874	0.33658	0.02335	Uani	1.00
N134 N 0.37919	9 0.24356	0.58032	0.02425	Uani	1.00
N135 N 0.38069	9 0.25054	0.45406	0.02815	Uani	1.00
N136 N 0.16184	5 0.40308	0 57156	0.02200	T.T	1.00

O137	0	0.43559	0.22979	0.17818	0.08755	Uani	1.00
C138	С	0.32285	0.30369	0.54619	0.02843	Uani	1.00
C139	С	0.27089	0.33959	0.56164	0.03420	Uani	1.00
C140	С	0.34348	0.27520	0.63966	0.03089	Uani	1.00
H141	Н	0.33098	0.27670	0.74243	0.04900	Uiso	1.00
C142	С	0.34766	0.28714	0.42991	0.03168	Uani	1.00
H143	Н	0.33671	0.29940	0.33429	0.04900	Uiso	1.00
C144	С	0.15161	0.36992	0.64982	0.04630	Uani	1.00
H145	Н	0.10058	0.36794	0.71353	0.07100	Uiso	1.00
C146	С	0.20646	0.33802	0.64797	0.05247	Uani	1.00
H147	Н	0.19670	0.31165	0.70956	0.08000	Uiso	1.00
C148	С	0.22526	0.40598	0.48969	0.05242	Uani	1.00
H149	Н	0.23131	0.43250	0.42790	0.08200	Uiso	1.00
C150	C	0.28065	0.37412	0.48233	0.05220	Uani	1.00
H151	н	0.32998	0.37608	0.41470	0.08000	Uiso	1.00
N152	N	0.36942	0.24224	0.11434	0.08000	Uani	1.00
0153	0	0.30021	0.24224	0.17107	0.12104	Uani	1.00
0153	0	0.30021	0.24231	0.17107	0.12194	Uani	1.00
0134 7n155	0 7n	0.57545	0.23490	-0.00403	0.13403	Uani	1.00
Zn155	Zn	0.396/1	0.29207	0.83990	0.02336	Uani	1.00
N156	N	0.62320	0.25881	0.08628	0.02423	Uani	1.00
N15/	N	0.62111	0.25131	0.96043	0.02814	Uani	1.00
N158	N	0.84196	0.09891	0.08017	0.03385	Uani	1.00
0159	0	0.56501	0.27127	0.68428	0.08744	Uani	1.00
C160	С	0.68127	0.19887	0.05329	0.02837	Uani	1.00
C161	С	0.73357	0.16295	0.06862	0.03416	Uani	1.00
C162	С	0.66055	0.22766	0.14589	0.03085	Uani	1.00
H163	Η	0.67407	0.22672	0.24815	0.04900	Uiso	1.00
C164	С	0.65509	0.21487	0.93719	0.03163	Uani	1.00
H165	Н	0.66601	0.20244	0.84184	0.04900	Uiso	1.00
C166	С	0.85211	0.13218	0.15731	0.04613	Uani	1.00
H167	Н	0.90285	0.13404	0.22080	0.07100	Uiso	1.00
C168	С	0.79760	0.16432	0.15473	0.05229	Uani	1.00
H169	Н	0.80729	0.19068	0.21574	0.08000	Uiso	1.00
C170	С	0.77903	0.09627	-0.00179	0.05214	Uani	1.00
H171	Н	0.77271	0.06972	0.93695	0.08200	Uiso	1.00
C172	С	0.72419	0.12840	0.98984	0.05196	Uani	1.00
H173	Н	0.67544	0.12649	0.92184	0.08000	Uiso	1.00
N174	Ν	0.63029	0.25952	0.61591	0.08748	Uani	1.00
O175	0	0.69974	0.25735	0.67027	0.12172	Uani	1.00
O176	0	0.62301	0.24913	0.49526	0.13397	Uani	1.00
Zn177	Zn	0.41834	0.69559	0.65461	0.02351	Uani	1.00
N178	Ν	0.49278	0.68122	0.41619	0.02423	Uani	1.00
N179	N	0.50101	0.67945	0.54338	0.02806	Uani	1.00
N180	N	0.81670	0 57868	0 42278	0.03341	Uani	1.00
0181	0	0 45623	0 70539	0.81790	0.08912	Uani	1.00
C182	C	0.15025	0.65018	0 45735	0.00912	Uani	1.00
C183	C	0.68081	0.62640	0.44340	0.02029	Uani	1.00
C103	C	0.00001	0.02040	0.26022	0.03370	Uani	1.00
U104	с u	0.55000	0.00300	0.30023	0.03081		1.00
П183 С197	п	0.56428	0.03933	0.20088	0.04900	U1SO	1.00
C186	C	0.57037	0.66117	0.57202	0.03127	Uanı	1.00
H187	H	0.59106	0.65472	0.66898	0.04900	Uiso	1.00
C188	C	0.75385	0.57152	0.34340	0.04552	Uani	1.00
H189	Н	0.75700	0.54745	0.27296	0.07100	Uiso	1.00

C190	С	0.68560	0.59555	0.35043	0.05140	Uani	1.00
H191	Н	0.63630	0.58933	0.28614	0.08000	Uiso	1.00
C192	С	0.81408	0.60885	0.51300	0.05162	Uani	1.00
H193	Н	0.86434	0.61357	0.57635	0.08200	Uiso	1.00
C194	С	0.74563	0.63296	0.52620	0.05131	Uani	1.00
H195	Н	0.74336	0.65650	0.59966	0.08000	Uiso	1.00
N196	Ν	0.47231	0.66909	0.87541	0.08782	Uani	1.00
O197	0	0.46581	0.63518	0.81145	0.12143	Uani	1.00
O198	0	0.49589	0.66815	0.99504	0.13360	Uani	1.00
Zn199	Zn	0.58252	0.80679	0.16064	0.02349	Uani	1.00
N200	Ν	0.51121	0.82066	0.91993	0.02425	Uani	1.00
N201	Ν	0.50133	0.82303	0.04684	0.02805	Uani	1.00
N202	Ν	0.18748	0.92339	0.91337	0.03343	Uani	1.00
0203	0	0.54244	0.79695	0.32355	0.08940	Uani	1.00
C204	C	0.39601	0.85142	0.95650	0.02834	Uani	1.00
C205	C	0.32238	0.87516	0.93891	0.03398	Uani	1.00
C205	C	0.44839	0.83811	0.86148	0.03082	Uani	1.00
U200	с ц	0.44125	0.84077	0.75777	0.03002	Lliso	1.00
C208	n C	0.43124	0.84121	0.07274	0.03130	Ulani	1.00
C208	ш	0.43124	0.04121	0.07274	0.03130	Ulian	1.00
П209	п	0.40900	0.04005	0.10878	0.04900	UISO	1.00
C210	U U	0.25201	0.95037	0.85012	0.04300	Uam	1.00
H211	H	0.25120	0.95521	0.76650	0.07100	U1SO	1.00
C212	C H	0.31972	0.90616	0.84556	0.05152	Uani	1.00
H213	H	0.37050	0.91235	0.78345	0.08000	U1so	1.00
C214	С	0.18793	0.89295	1.00334	0.05186	Uani	1.00
H215	H	0.13636	0.88828	0.06487	0.08200	U1so	1.00
C216	С	0.25580	0.86863	0.01910	0.05147	Uanı	1.00
H217	Н	0.25639	0.84503	0.09285	0.08000	Uiso	1.00
N218	Ν	0.52658	0.83310	0.38213	0.08772	Uanı	1.00
O219	0	0.53083	0.86724	0.31807	0.12143	Uani	1.00
O220	0	0.50507	0.83358	0.50321	0.13357	Uani	1.00
Zn221	Zn	0.09844	0.95894	0.89981	0.02336	Uani	1.00
N222	Ν	0.12477	0.99407	0.65558	0.02425	Uani	1.00
N223	Ν	0.12441	1.00081	0.78184	0.02815	Uani	1.00
N224	Ν	0.34020	0.65360	0.65562	0.03388	Uani	1.00
O225	0	0.07096	0.97993	0.05864	0.08742	Uani	1.00
C226	С	0.18144	0.55304	0.67735	0.02841	Uani	1.00
C227	С	0.23292	0.58923	0.66360	0.03419	Uani	1.00
C228	С	0.16051	1.02562	0.59553	0.03089	Uani	1.00
H229	Н	0.17677	0.52555	0.48180	0.04900	Uiso	1.00
C230	С	0.15403	0.53687	0.79272	0.03167	Uani	1.00
H231	Η	0.16263	0.54967	0.88794	0.04900	Uiso	1.00
C232	С	0.35169	0.62066	0.57725	0.04628	Uani	1.00
H233	Н	0.40302	0.61912	0.51410	0.07100	Uiso	1.00
C234	С	0.29745	0.58852	0.57741	0.05243	Uani	1.00
H235	Н	0.30771	0.56266	0.51435	0.08000	Uiso	1.00
C236	С	0.27661	0.65567	0.73748	0.05231	Uani	1.00
H237	Н	0.26932	0.68194	0.79982	0.08200	Uiso	1.00
C238	С	0.22239	0.62331	0.74425	0.05213	Uani	1.00
H239	Н	0.17319	0.62471	0.81238	0.08000	Uiso	1.00
N240	Ν	0.13804	0.99163	0.12101	0.08748	Uani	1.00
O241	0	0.20650	0.99202	0.06189	0.12204	Uani	1.00

Zn243	Zn	0.90595	0.54329	0.40863	0.02334	Uani	1.00
N244	Ν	0.88098	0.50763	0.16565	0.02422	Uani	1.00
N245	Ν	0.87999	0.50121	0.29216	0.02812	Uani	1.00
N246	Ν	0.66085	0.84862	0.16368	0.03382	Uani	1.00
O247	0	0.93383	0.52238	0.56734	0.08761	Uani	1.00
C248	С	0.82066	0.94865	0.18946	0.02838	Uani	1.00
C249	С	0.76848	0.91277	0.17526	0.03416	Uani	1.00
C250	С	0.84832	0.47530	0.10630	0.03084	Uani	1.00
H251	Н	0.82861	0.97578	-0.00686	0.04900	Uiso	1.00
C252	С	0.84667	0.96494	0.30496	0.03162	Uani	1.00
H253	Н	0.83583	0.95274	0.40086	0.04900	Uiso	1.00
C254	С	0.65096	0.88173	0.08517	0.04610	Uani	1.00
H255	Н	0.60080	0.88340	0.02039	0.07100	Uiso	1.00
C256	С	0.70509	0.91394	0.08787	0.05228	Uani	1.00
H257	Н	0.69565	0.94018	0.02573	0.08000	Uiso	1.00
C258	С	0.72303	0.84621	0.24723	0.05217	Uani	1.00
H259	Н	0.72906	0.81977	0.30953	0.08200	Uiso	1.00
C260	С	0.77744	0.87843	0.25576	0.05194	Uani	1.00
H261	Н	0.82555	0.87674	0.32506	0.08000	Uiso	1.00
N262	N	0.86701	0.51035	0.63138	0.08749	Uani	1.00
0263	0	0.79828	0.51036	0.57452	0.12168	Uani	1.00
0264	0	0.87207	0.49797	0.75071	0.13407	Uani	1.00
Zn265	Zn	0.08150	0.94580	0.58573	0.02351	Uani	1.00
N266	N	0.00196	0.93115	0.82778	0.02331	Uani	1.00
N267	N	0.01080	0.93113	0.82778	0.02424	Uani	1.00
N269	N	0.00074	0.92940	0.70090	0.02307	Uani	1.00
0260	N O	0.08794	0.02014	0.05556	0.03341	Uani	1.00
C270	C	0.04120	0.95507	0.42308	0.03912	Uani	1.00
C270	C C	0.89303	0.90009	0.79210	0.02851	Uani	1.00
C271	C C	0.02224	0.0/001	0.80930	0.03390	Uani	1.00
C272	U	-0.05182	0.91544	0.88072	0.03082	Uani	1.00
H2/3	н	0.94121	0.91021	0.99046	0.04900		1.00
C2/4	C	0.93063	0.91146	0.6/568	0.03129	Uani	1.00
H2/5	Н	0.90820	0.90515	0.5/981	0.04900	Uiso	1.00
C276	C	0.75257	0.82046	0.90890	0.04558	Uanı	1.00
H277	H	0.75209	0.79528	0.97657	0.07100	Uiso	1.00
C278	С	0.82001	0.84504	0.90028	0.05145	Uani	1.00
H279	Н	0.87087	0.83844	0.96097	0.08000	Uiso	1.00
C280	С	0.68803	0.85929	0.74589	0.05168	Uani	1.00
H281	Н	0.63634	0.86442	0.68587	0.08200	Uiso	1.00
C282	С	0.75559	0.88388	0.73111	0.05138	Uani	1.00
H283	Н	0.75588	0.90812	0.65953	0.08000	Uiso	1.00
N284	Ν	0.02600	0.91945	0.36546	0.08784	Uani	1.00
0285	0	0.02983	0.88538	0.42996	0.12161	Uani	1.00
0286	0	0.00522	0.91881	0.24443	0.13380	Uani	1.00
Zn287	Zn	0.92244	0.55635	0.09387	0.02348	Uani	1.00
N288	Ν	0.99340	0.57121	0.33362	0.02423	Uani	1.00
N289	Ν	1.00324	0.57296	0.20651	0.02804	Uani	1.00
N290	Ν	0.31667	0.67368	0.32907	0.03338	Uani	1.00
O291	0	0.96184	0.54676	0.93056	0.08944	Uani	1.00
C292	С	0.10884	0.60132	0.29434	0.02831	Uani	1.00
C293	С	0.18230	0.62512	0.30942	0.03396	Uani	1.00
C294	С	1.05638	0.58882	0.39053	0.03079	Uani	1.00
	TT	0.06262	0.50210	0 /0305	0.04000	Llico	1.00

C296	С	0.07343	0.59072	0.17906	0.03126	Uani	1.00
H297	Н	0.09572	0.59688	0.08248	0.04900	Uiso	1.00
C298	С	0.25125	0.68224	0.40282	0.04549	Uani	1.00
H299	Н	0.25113	0.70803	0.46758	0.07100	Uiso	1.00
C300	С	0.18374	0.65777	0.39623	0.05141	Uani	1.00
H301	Н	0.13226	0.66506	0.45553	0.08000	Uiso	1.00
C302	С	0.31731	0.64170	0.24518	0.05171	Uani	1.00
H303	Н	0.36966	0.63585	0.18655	0.08200	Uiso	1.00
C304	С	0.24969	0.61712	0.23247	0.05133	Uani	1.00
H305	Н	0.24995	0.59217	0.16378	0.08000	Uiso	1.00
N306	Ν	0.97644	0.58309	0.87162	0.08779	Uani	1.00
0307	Ο	0.97317	0.61704	0.93621	0.12132	Uani	1.00
<b>D308</b>	0	0.99586	0.58393	0.74964	0.13365	Uani	1.00
Zn309	Zn	0.40570	0.70905	0.34125	0.02335	Uani	1.00
N310	Ν	0.37649	0.74411	0.58336	0.02425	Uani	1.00
N311	Ν	0.37881	0.75116	0.45723	0.02815	Uani	1.00
N312	Ν	0.16002	0.90419	0.58008	0.03390	Uani	1.00
0313	0	0.43350	0.72958	0.18171	0.08755	Uani	1.00
C314	С	0.31953	0.80408	0.54874	0.02843	Uani	1.00
2315	C	0.26750	0.84001	0.56442	0.03420	Uani	1.00
316	C	0.34012	0.77561	0.64234	0.03089	Uani	1.00
4317	н	0.32727	0.77701	0.74501	0.04900	Uiso	1.00
7318	C C	0.34534	0.78766	0.43273	0.03168	Uani	1.00
310	н	0.33/81	0.70002	0.33702	0.03100	Uiso	1.00
7320	n C	0.15057	0.77772	0.55762	0.04500	Ulso	1.00
J221	с u	0.10072	0.8/100	0.03803	0.04030	Uiso	1.00
7277	II C	0.10073	0.80937	0.72480	0.07100	Ulso	1.00
1222		0.20409	0.03000	0.03401	0.03247	Uani	1.00
7224	П	0.19338	0.01202	0.71041	0.08000	Ulso	1.00
1225	C U	0.22100	0.90002	0.49459	0.03242	Uani	1.00
1323	H	0.22719	0.93308	0.43195	0.08200		1.00
.320	C U	0.27604	0.8/43/	0.48384	0.03220	Uani	1.00
1327	H	0.32372	0.8/604	0.41295	0.08000	Uiso	1.00
N328	N	0.36648	0./415/	0.11932	0.08/40	Uani	1.00
0329	0	0.29799	0.74197	0.17832	0.12194	Uani	1.00
5330	0	0.37092	0.75354	-0.00052	0.13405	Uani	1.00
2n331	Zn	0.59887	0.79269	0.84722	0.02336	Uani	1.00
N332	Ν	0.62592	0.75815	0.09109	0.02423	Uani	1.00
N333	Ν	0.62470	0.75093	0.96515	0.02814	Uani	1.00
N334	Ν	0.84335	0.59795	0.08985	0.03385	Uani	1.00
0335	0	0.57165	0.77178	0.68872	0.08744	Uani	1.00
2336	С	0.68397	0.69827	0.05809	0.02837	Uani	1.00
2337	С	0.73598	0.66230	0.07432	0.03416	Uani	1.00
2338	С	0.66249	0.72684	0.15089	0.03085	Uani	1.00
1339	Н	0.67481	0.72558	0.25352	0.04900	Uiso	1.00
2340	С	0.65866	0.71449	0.94171	0.03163	Uani	1.00
1341	Н	0.67001	0.70218	0.84629	0.04900	Uiso	1.00
2342	С	0.85276	0.63116	0.16749	0.04613	Uani	1.00
H343	Н	0.90253	0.63287	0.23297	0.07100	Uiso	1.00
C <b>3</b> 44	С	0.79851	0.66337	0.16331	0.05229	Uani	1.00
H345	Н	0.80739	0.68958	0.22529	0.08000	Uiso	1.00
2346	С	0.78178	0.59559	0.00510	0.05214	Uani	1.00
H347	Н	0.77625	0.56916	0.94311	0.08200	Uiso	1.00
	C	0 72782	0.62801	0 99417	0.05106	Honi	1.00

H349	Н	0.68073	0.62659	0.92313	0.08000	Uiso	1.00
N350	Ν	0.63880	0.76020	0.62513	0.08748	Uani	1.00
O351	Ο	0.70725	0.75979	0.68315	0.12172	Uani	1.00
O352	Ο	0.63460	0.74875	0.50501	0.13397	Uani	1.00
C353	С	0.53954	0.56516	0.96474	0.00000	Uiso	1.00
C354	С	0.46145	0.55432	1.00105	0.00000	Uiso	1.00
C355	С	0.41251	0.53327	0.91411	0.00000	Uiso	1.00
C356	С	0.44289	0.52355	0.79194	0.00000	Uiso	1.00
C357	С	0.51885	0.53439	0.75598	0.00000	Uiso	1.00
C358	С	0.56879	0.55520	0.84093	0.00000	Uiso	1.00
N359	Ν	0.53866	0.52359	0.63495	0.00000	Uiso	1.00
C360	С	0.47729	0.50400	0.57781	0.00000	Uiso	1.00
S361	S	0.39307	0.49862	0.67369	0.00000	Uiso	1.00
C362	С	0.48075	0.48997	0.44021	0.00000	Uiso	1.00
C363	С	0.55223	0.49131	0.36643	0.00000	Uiso	1.00
C364	С	0.55065	0.48179	0.23207	0.00000	Uiso	1.00
C365	С	0.47965	0.46757	0.17708	0.00000	Uiso	1.00
C366	С	0.41037	0.46412	0.25120	0.00000	Uiso	1.00
C367	С	0.41093	0.47556	0.38125	0.00000	Uiso	1.00
C368	С	0.33479	0.44937	0.19131	0.00000	Uiso	1.00
O369	Ο	0.62324	0.50135	0.42913	0.00000	Uiso	1.00
H370	Н	0.57702	0.58118	1.03261	0.00000	Uiso	1.00
H371	Н	0.43921	0.56203	1.09649	0.00000	Uiso	1.00
H372	Н	0.35239	0.52480	0.94126	0.00000	Uiso	1.00
H373	Н	0.62868	0.56350	0.81207	0.00000	Uiso	1.00
C374	С	0.62008	0.48881	0.14566	0.00000	Uiso	1.00
H375	Н	0.47772	0.45956	0.07534	0.00000	Uiso	1.00
H376	Н	0.35567	0.47371	0.43519	0.00000	Uiso	1.00
H377	Н	0.28457	0.46890	0.22356	0.00000	Uiso	1.00
H378	Н	0.32311	0.41750	0.22211	0.00000	Uiso	1.00
H379	Н	0.33824	0.45057	0.08398	0.00000	Uiso	1.00
H380	Н	0.67324	0.49073	0.38604	0.00000	Uiso	1.00
O381	Ο	0.61550	0.48241	0.02971	0.00000	Uiso	1.00
H382	Н	0.67553	0.50042	0.18175	0.00000	Uiso	1.00

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