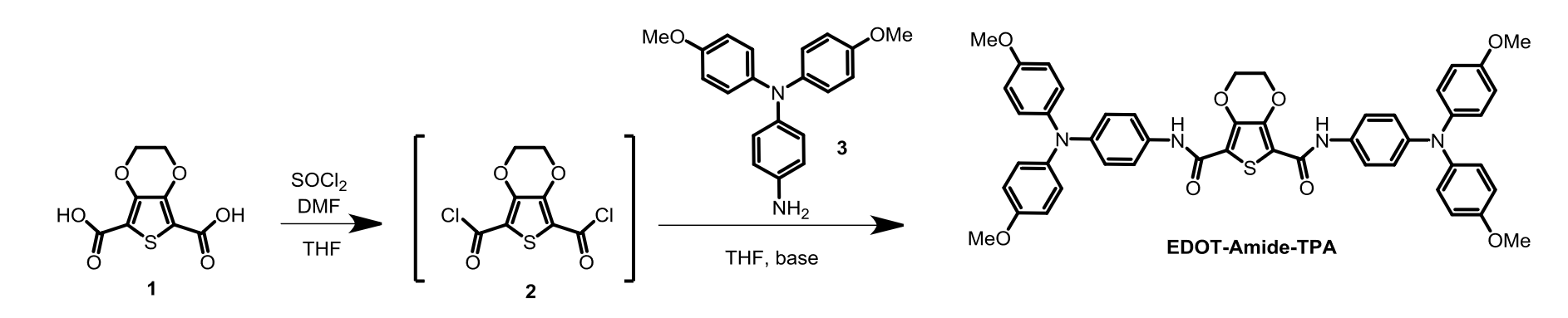
# Supplementary Information

## Behind the Scenes: Insights into the Structural Properties of Amide-Based Hole-Transporting Materials for Lead-Free Perovskite Solar Cells

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**Synthesis of (EDOT-Amide-TPA) (*N5,N7-bis(4-(bis(4-methoxyphenyl)amino)phenyl)-2,3-dihydrothieno[3,4-b][1,4]dioxine-5,7-dicarboxamide*)**



Reaction scheme 1: Synthesis of EDOT-Amide-TPA.1

**Single crystal** **synthesis**

Single crystals of EDOT-Amide-TPA were prepared by dissolving EDOT-Amide-TPA (1.0 mg) in 1 mL Dimethyl Sulfoxide upon heating to 80 °C. After cooling, the solution was filled into a crystallization tube with a diameter of 5 mm. After two weeks, orange colored, block-shaped single crystals were obtained and measured using X-ray single crystal analysis.

**Solar Cell preparation**

FTO-layered glass substrates were etched upon treatment with zinc powder and 3 m HCl and cleaned using Hellmanex (2 % in deionized water) followed by acetone and ethanol and drying under an air stream.

For the electron transport layer, a combination of a compact and a mesoporous TiO2 layer was prepared from a sol-gel precursor solution. The compact layer was created by spin-coating the solution onto the freshly prepared substrates for 45 s at 2000 rpm. The substrates were calcinated at 500 °C for 30 min at air afterwards. For the sol-gel solution a 2 m solution of HCl in dry 2-propanol was added dropwise to a vigorously stirring 0.43 mm solution of Ti-isopropoxide (99.999 %) in dry 2-propanol. As for the mesoporous TiO2 layer, 100 µL of a nanoparticle paste diluted in absolute ethanol (1:3 weight ratio) was spin-coated onto the compact TiO2 layer at 2500 rpm for 40 seconds followed by a calcination step at 500 °C for 30 minutes.

BiBr3 (224.4 mg, 0.5 mmol, 1.0 eq.) was weighed in stoichiometrically, dissolved in 1 mL DMSO at 85 °C and added to CsBr (212.8 mg, 1.0 mmol, 2.0 eq.) and AgBr (93.9 mg, 0.5 mmol, 1.0 eq.) while heating to 135 °C. After completely dissolving the precursors, both the solution and the substrates were preheated at 85 °C before spin-coating. 80 µL of the precursor solution was spin-coated dynamically at 2500 rpm for 45 seconds onto the mesoporous TiO2 substrate. After a post annealing step at 285 °C for 5 minutes under ambient conditions, the HTM was spin-coated on top.

Devices using Spiro-OMeTAD as HTM were spin-coated under inert conditions at 2000 rpm for 45 seconds. The solution was prepared dissolving 75 mg 2,2’,7,7’-tetrakis-(*N*,*N*-di-4-methoxyphenylamino)-9,9’-spirobifluorene (Borun New Material Technology Ltd., >99.9 % purity) in 1 mL Chlorobenzene. The solution was filtered before adding 4-*tert*-butylpyridine (10 µL, 6.82 ⋅ 10−5 mmol) and a 170 mg/mL bis(trifluoro-methane)sulfonamide lithium salt solution (30 µL, 1.78 ⋅ 10−2 mmol) in acetonitrile.

Devices using EDOT-amide-TPA as HTM were spin-coated under inert conditions at 2000 rpm for 45 seconds. The solution was prepared dissolving 20 mg EDOT-amide-TPA in a 1 mL mixture of Chlorobenzene and Chloroform (2:1) before adding 4-*tert*-butylpyridine (10 µL /mL) and a 170 mg/mL bis(trifluoro-methane)sulfonamide lithium salt solution (Li-TFSI, 20 µL/mL) in acetonitrile. To completely dissolve the HTM, the solution was then heated to 85 °C.

As a final step, 40 nm gold electrodes were thermally deposited under a high vacuum on top of the device.

**SEM images**

SEM data were taken with a FEI Helios NanoLab G3 UC field emission scanning electron microscope equipped with an additional concentric backscattered electron detector.

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| Figure S 1: a) SEM cross-section image of a solar cell comprising EDOT-Amide-TPA as HTM. b) SEM cross-section image of a solar cell comprising Spiro-OMeTAD as HTM without gold electrode. |

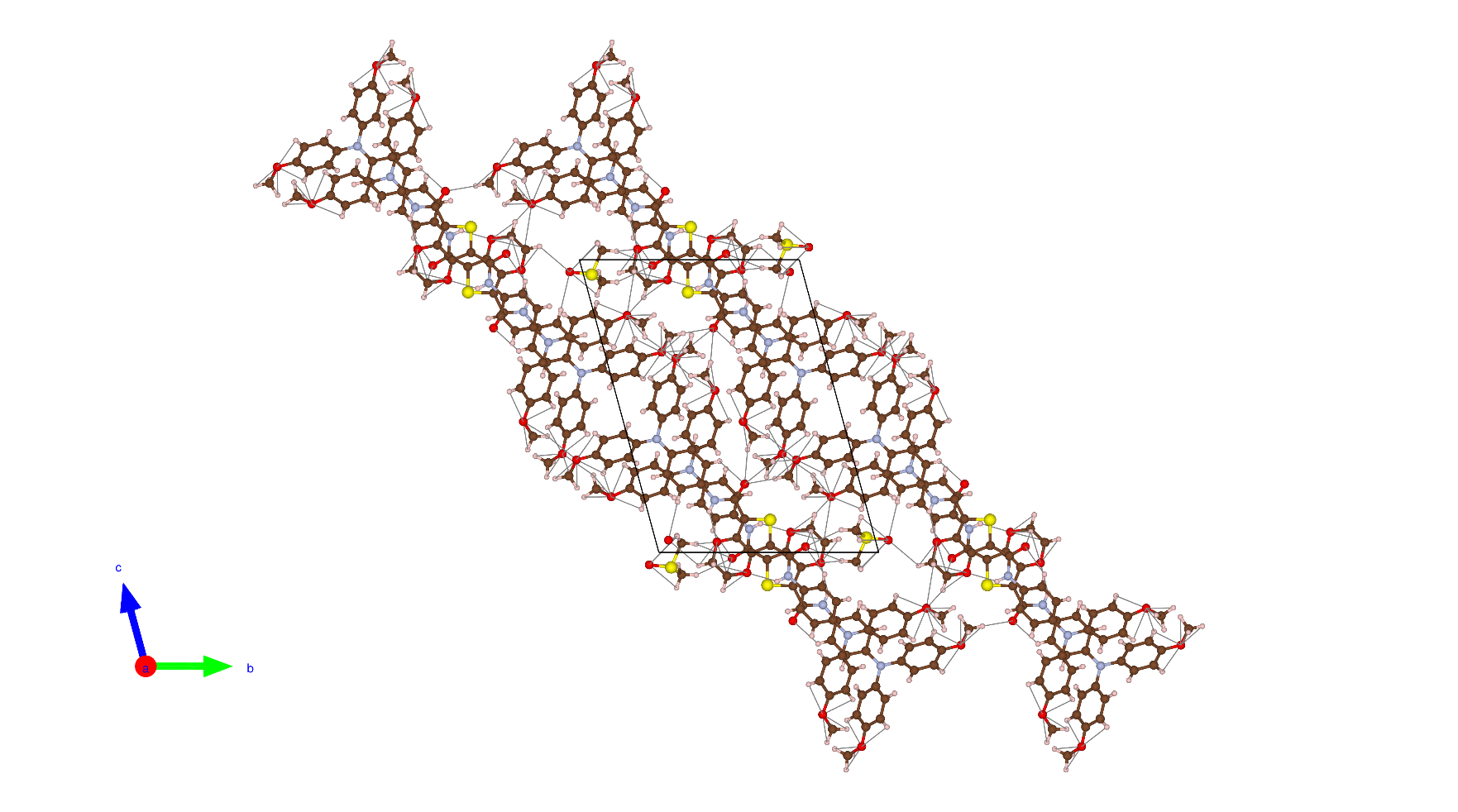
**Hydrogen bonds of EDOT-Amide TPA**

Figure S2: Crystal structure of EDOT-Amide-TPA along the a-axis with inter- and intramolecular hydrogen bonding displayed as grey connections.

**Ein Bild, das Pfeil enthält.

Automatisch generierte Beschreibung**

Figure S3: Crystal structure of EDOT-Amide-TPA along the b-axis with inter- and intramolecular hydrogen bonding displayed as grey connections.

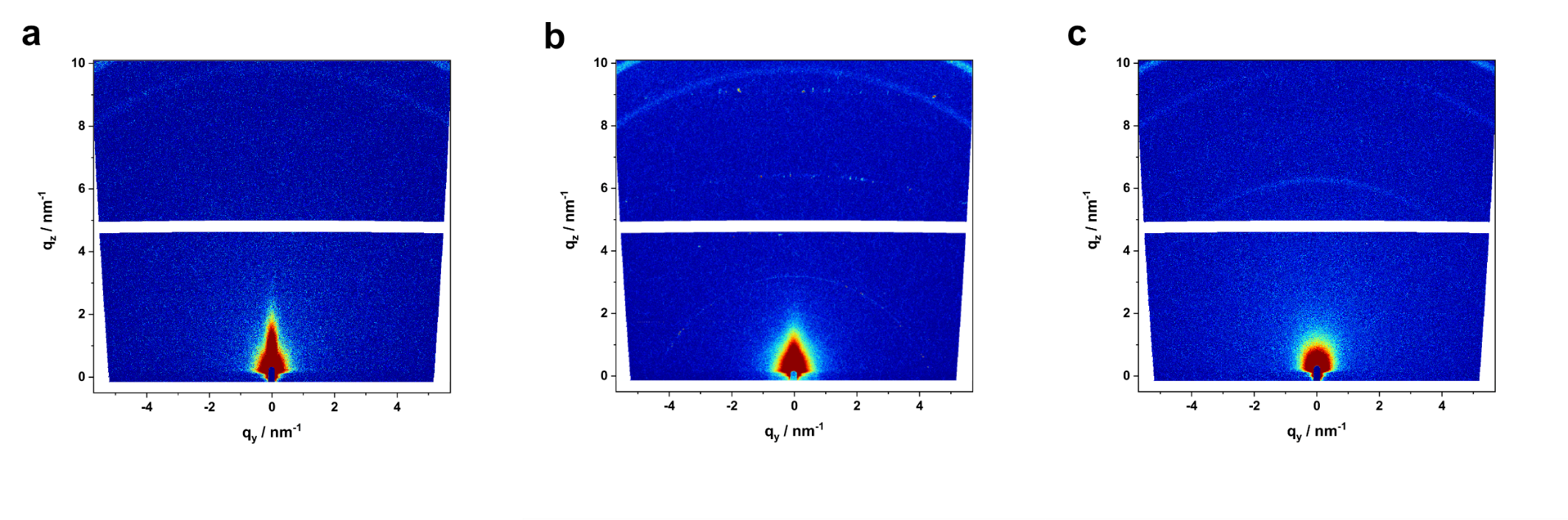
**Crystal structure of Spiro-OMeTAD**

Figure S 4: **Ein Bild, das Pfeil enthält.

Automatisch generierte Beschreibung**Crystal structure of Spiro-OMeTAD. a) Single Spiro-OMeTAD molecule viewed along a-axis, b) packing of two Spiro-OMeTAD molecules viewed along a-axis.²

**Grazing incidence wide angle X-ray scattering (GIWAXS)**

2D Grazing-incidence wide angle X-ray scattering (GIWAXS) measurements were carried out on an Anton-Paar SAXSpoint 2.0 with a Primux 100 microfocus source with Cu-Kα1 radiation (λ = 1.5406 Å) and a Dectris Eiger R 1M 2D Detector.

Figure S5: GIWAXS images of samples with the following architecture: FTO/c-TiO2, mp-TiO2/ Cs2AgBiBr6/HTM. a) Comprising Spiro-OMeTAD as HTM, and b) comprising EDOT-Amide-TPA as HTM.

The weak reflections in panel b) at qz = 3.2 nm–1 and qz = 6.3 nm–1 can be attributed to EDOT-Amide-TPA, indicating the formation of a crystalline layer of EDOT-Amide-TPA on top of the perovskite layer, while no such indication was found for the sample containing Spiro-OMeTAD as HTM.

**Photoluminescence**

Steady State Photoluminescence was measured using a 405nm diode laser with a power of 69 mW/cm². The samples were mounted in an integrating sphere and the PL was detected by a PMT.

For PLQY the obtained data from direct and indirect illumination of the sample, and the detected signal from the excitation source (all measured in an integrating sphere) was evaluated according to Mellow et. al.3

The TRPL measurements were carried out using a 375 nm pulsed diode laser with an intensity of approximately 8.3 nJ/cm² with a time interval between the pulses of 10 µs (repetition rate 100 kHz). The samples were placed in the sample holder and measured in reflection geometry. PL, PLQY and TRPL measurements were all performed with an FLS 980 Spectrometer (Edinburgh Instruments).

Fluence dependent steady state PL was measured using a 412 nm LED (Solis-415C, Thorlabs) with varying driving current. The samples were measured in transmission geometry and a silicon diode was placed behind the sample in order to monitor the integrated photoluminescence.

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| Figure S6: Steady state PL measurements of pure Spiro-OMeTAD (red), EDOT-Amide-TPA (blue) and Cs2AgBiBr6 (black). Each spin-coated on quartz-glass substrates. It is clearly shown that PL from EDOT and Cs2AgBiBr6 are very well distinguishable, whereas Spiro-OMeTAD and Cs2AgBiBr6 have overlapping PL Spectra. Therefore, results obtained by measuring layer stacks of EDOT and Cs2AgBiBr6 can be treated as reliable, whereas data measured on Spiro and Cs2AgBiBr6 will be treated carefully and should not be overinterpreted. |

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| Figure S7: Slopes of fluence dependent steady state photoluminescence measurements of Spiro-OMeTAD (red), EDOT-Amide-TPA (blue) and Cs2AgBiBr6 (black) in the sample geometry glass/Cs2AgBiBr6/HTM. The slopes of approximately 1.5 indicate an SRH dominated regime from 1mW/cm² up to 10 mW/cm² for EDOT layer stacks as well as the pure double perovskite. At higher fluences (10‑80 mW/cm²) excitonic recombination with a slope of around 1.0 is dominating followed by Auger recombination at intensities higher than 1sun. For the Spiro-OMeTAD layer stack however only Excitonic/free carrier and Auger recombination could be found as the dominating recombination mechanisms. |
|  |
| Figure S8: Slopes of fluence dependent steady state photoluminescence measurements of glass/Spiro-OMeTAD (triangle) and glass/Cs2AgBiBr6/Spiro-OMeTAD (red squares). |

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Figure S9: Full range of the time-resolved photoluminescence measurement in the time range between – 0.2 µs and 2.0 µs with the excitation baseline visible. The measurement was aborted after 1.8 µs. Baseline was measured with lower repetition rate to avoid a signal pile-up, resulting in fewer data points in that time range.

**Crystal Structure analysis**

|  |  |
| --- | --- |
| Crystal Data | |
|  |  |
| Formula | C50H48N4O9S2 |
| FW [g mol−1] | 913.04 |
| Crystal system | triclinic |
| Space Group | *P−*1 |
| Color / Habit | orange block |
| Size [mm] | 0.194 x 0.179 x 0.157 |
| *a* [Å] | 7.7358(0) |
| *b* [Å] | 14.801(30) |
| *c* [Å] | 20.429(10) |
| α [°] | 104.624 |
| *β* [°] | 95.034 |
| *γ* [°] | 94.905 |
| *V* [Å3] | 2240.5 |
| *Z* | 2 |
| *ρ*calc. [g cm−3] | 1.3533 |
| *μ* [mm−1] | 0.182 |
| *F*(000) | 960 |
| λMoKα [Å] | 0.71073 |
| *T* [K] | 129 |
| θ Min–Max [°] | 4.1, 26.4 |
| Dataset | −9: 9; −18: 18; −25: 25 |
| Reflections collected | 17423 |
| Independent refl. | 9151 |
| *R*int | 0.060 |
| Observed reflections | 5166 |
| Parameters | 600 |
| *R*1 (obs)a | 0.0627 |
| w*R*2 (all data)b | 0.1162 |
| GooFc | 0.99 |
| Resd. Dens. [e Å−3] | −0.40, 0.41 |
| Absorption correction | multi-scan |

a) *R*1 = Σ||F0|− |Fc||/ Σ|F0|; b) *wR*2 = [Σ[*w*(F02−Fc2)2]/Σ[*w*(F0)2]]1/2; *w* = [σc2(F02)+(xP)2+y*P*]−1 and *P*=(F02+2Fc2)/3; c) GooF = {Σ[*w*(Fo2−Fc2)2]/(n−p)}1/2 (n = number of reflections; p = total number of parameters).

**Bond lengths (Å)**

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Number | Atom1 | Atom2 | Length | Number | Atom1 | Atom2 | Length |
| 1 | S1 | C1 | 1.730(3) | 120 | O5 | C23 | 1.368(4) |
| 2 | S1 | C2 | 1.722(3) | 121 | O5 | C27 | 1.423(3) |
| 3 | O1 | C3 | 1.372(4) | 122 | O6 | C28 | 1.236(3) |
| 4 | O1 | C6 | 1.450(3) | 123 | O7 | C38 | 1.380(3) |
| 5 | O2 | C4 | 1.365(3) | 124 | O7 | C47 | 1.433(5) |
| 6 | O2 | C5 | 1.444(4) | 125 | O8 | C44 | 1.361(3) |
| 7 | O3 | C7 | 1.223(3) | 126 | O8 | C48 | 1.430(4) |
| 8 | O4 | C17 | 1.364(4) | 127 | N1 | C7 | 1.352(4) |
| 9 | O4 | C26 | 1.427(3) | 128 | N1 | C8 | 1.413(5) |
| 10 | O5 | C23 | 1.368(4) | 129 | N1 | H1 | 0.85(3) |
| 11 | O5 | C27 | 1.423(3) | 130 | N2 | C11 | 1.415(5) |
| 12 | O6 | C28 | 1.236(3) | 131 | N2 | C14 | 1.430(4) |
| 13 | O7 | C38 | 1.380(3) | 132 | N2 | C20 | 1.424(4) |
| 14 | O7 | C47 | 1.433(5) | 133 | N3 | C28 | 1.345(4) |
| 15 | O8 | C44 | 1.361(3) | 134 | N3 | C29 | 1.420(5) |
| 16 | O8 | C48 | 1.430(4) | 135 | N3 | H3 | 0.84(3) |
| 17 | N1 | C7 | 1.352(4) | 136 | N4 | C32 | 1.425(5) |
| 18 | N1 | C8 | 1.413(5) | 137 | N4 | C35 | 1.418(4) |
| 19 | N1 | H1 | 0.85(3) | 138 | N4 | C41 | 1.419(4) |
| 20 | N2 | C11 | 1.415(5) | 139 | C1 | C4 | 1.369(4) |
| 21 | N2 | C14 | 1.430(4) | 140 | C1 | C7 | 1.470(5) |
| 22 | N2 | C20 | 1.424(4) | 141 | C2 | C3 | 1.362(4) |
| 23 | N3 | C28 | 1.345(4) | 142 | C2 | C28 | 1.476(5) |
| 24 | N3 | C29 | 1.420(5) | 143 | C3 | C4 | 1.419(5) |
| 25 | N3 | H3 | 0.84(3) | 144 | C5 | H5A | 0.99 |
| 26 | N4 | C32 | 1.425(5) | 145 | C5 | H5B | 0.99 |
| 27 | N4 | C35 | 1.418(4) | 146 | C5 | C6 | 1.505(5) |
| 28 | N4 | C41 | 1.419(4) | 147 | C6 | H6A | 0.99 |
| 29 | C1 | C4 | 1.369(4) | 148 | C6 | H6B | 0.99 |
| 30 | C1 | C7 | 1.470(5) | 149 | C8 | C9 | 1.380(4) |
| 31 | C2 | C3 | 1.362(4) | 150 | C8 | C13 | 1.390(4) |
| 32 | C2 | C28 | 1.476(5) | 151 | C9 | H9 | 0.949 |
| 33 | C3 | C4 | 1.419(5) | 152 | C9 | C10 | 1.379(5) |
| 34 | C5 | H5A | 0.99 | 153 | C10 | H10 | 0.95 |
| 35 | C5 | H5B | 0.99 | 154 | C10 | C11 | 1.399(4) |
| 36 | C5 | C6 | 1.505(5) | 155 | C11 | C12 | 1.397(4) |
| 37 | C6 | H6A | 0.99 | 156 | C12 | H12 | 0.95 |
| 38 | C6 | H6B | 0.99 | 157 | C12 | C13 | 1.382(5) |
| 39 | C8 | C9 | 1.380(4) | 158 | C13 | H13 | 0.95 |
| 40 | C8 | C13 | 1.390(4) | 159 | C14 | C15 | 1.393(4) |
| 41 | C9 | H9 | 0.949 | 160 | C14 | C19 | 1.384(5) |
| 42 | C9 | C10 | 1.379(5) | 161 | C15 | H15 | 0.95 |
| 43 | C10 | H10 | 0.95 | 162 | C15 | C16 | 1.386(4) |
| 44 | C10 | C11 | 1.399(4) | 163 | C16 | H16 | 0.95 |
| 45 | C11 | C12 | 1.397(4) | 164 | C16 | C17 | 1.386(5) |
| 46 | C12 | H12 | 0.95 | 165 | C17 | C18 | 1.399(4) |
| 47 | C12 | C13 | 1.382(5) | 166 | C18 | H18 | 0.95 |
| 48 | C13 | H13 | 0.95 | 167 | C18 | C19 | 1.376(4) |
| 49 | C14 | C15 | 1.393(4) | 168 | C19 | H19 | 0.95 |
| 50 | C14 | C19 | 1.384(5) | 169 | C20 | C21 | 1.393(5) |
| 51 | C15 | H15 | 0.95 | 170 | C20 | C25 | 1.384(4) |
| 52 | C15 | C16 | 1.386(4) | 171 | C21 | H21 | 0.95 |
| 53 | C16 | H16 | 0.95 | 172 | C21 | C22 | 1.375(4) |
| 54 | C16 | C17 | 1.386(5) | 173 | C22 | H22 | 0.95 |
| 55 | C17 | C18 | 1.399(4) | 174 | C22 | C23 | 1.396(4) |
| 56 | C18 | H18 | 0.95 | 175 | C23 | C24 | 1.383(5) |
| 57 | C18 | C19 | 1.376(4) | 176 | C24 | H24 | 0.95 |
| 58 | C19 | H19 | 0.95 | 177 | C24 | C25 | 1.387(4) |
| 59 | C20 | C21 | 1.393(5) | 178 | C25 | H25 | 0.95 |
| 60 | C20 | C25 | 1.384(4) | 179 | C26 | H26A | 0.98 |
| 61 | C21 | H21 | 0.95 | 180 | C26 | H26B | 0.98 |
| 62 | C21 | C22 | 1.375(4) | 181 | C26 | H26C | 0.98 |
| 63 | C22 | H22 | 0.95 | 182 | C27 | H27A | 0.98 |
| 64 | C22 | C23 | 1.396(4) | 183 | C27 | H27B | 0.98 |
| 65 | C23 | C24 | 1.383(5) | 184 | C27 | H27C | 0.98 |
| 66 | C24 | H24 | 0.95 | 185 | C29 | C30 | 1.384(4) |
| 67 | C24 | C25 | 1.387(4) | 186 | C29 | C34 | 1.384(4) |
| 68 | C25 | H25 | 0.95 | 187 | C30 | H30 | 0.95 |
| 69 | C26 | H26A | 0.98 | 188 | C30 | C31 | 1.381(5) |
| 70 | C26 | H26B | 0.98 | 189 | C31 | H31 | 0.95 |
| 71 | C26 | H26C | 0.98 | 190 | C31 | C32 | 1.385(4) |
| 72 | C27 | H27A | 0.98 | 191 | C32 | C33 | 1.400(4) |
| 73 | C27 | H27B | 0.98 | 192 | C33 | H33 | 0.95 |
| 74 | C27 | H27C | 0.98 | 193 | C33 | C34 | 1.376(5) |
| 75 | C29 | C30 | 1.384(4) | 194 | C34 | H34 | 0.95 |
| 76 | C29 | C34 | 1.384(4) | 195 | C35 | C36 | 1.392(5) |
| 77 | C30 | H30 | 0.95 | 196 | C35 | C40 | 1.387(4) |
| 78 | C30 | C31 | 1.381(5) | 197 | C36 | H36 | 0.95 |
| 79 | C31 | H31 | 0.95 | 198 | C36 | C37 | 1.397(4) |
| 80 | C31 | C32 | 1.385(4) | 199 | C37 | H37 | 0.95 |
| 81 | C32 | C33 | 1.400(4) | 200 | C37 | C38 | 1.370(4) |
| 82 | C33 | H33 | 0.95 | 201 | C38 | C39 | 1.394(5) |
| 83 | C33 | C34 | 1.376(5) | 202 | C39 | H39 | 0.95 |
| 84 | C34 | H34 | 0.95 | 203 | C39 | C40 | 1.385(4) |
| 85 | C35 | C36 | 1.392(5) | 204 | C40 | H40 | 0.951 |
| 86 | C35 | C40 | 1.387(4) | 205 | C41 | C42 | 1.394(4) |
| 87 | C36 | H36 | 0.95 | 206 | C41 | C46 | 1.391(5) |
| 88 | C36 | C37 | 1.397(4) | 207 | C42 | H42 | 0.95 |
| 89 | C37 | H37 | 0.95 | 208 | C42 | C43 | 1.370(4) |
| 90 | C37 | C38 | 1.370(4) | 209 | C43 | H43 | 0.95 |
| 91 | C38 | C39 | 1.394(5) | 210 | C43 | C44 | 1.396(5) |
| 92 | C39 | H39 | 0.95 | 211 | C44 | C45 | 1.386(4) |
| 93 | C39 | C40 | 1.385(4) | 212 | C45 | H45 | 0.95 |
| 94 | C40 | H40 | 0.951 | 213 | C45 | C46 | 1.385(4) |
| 95 | C41 | C42 | 1.394(4) | 214 | C46 | H46 | 0.95 |
| 96 | C41 | C46 | 1.391(5) | 215 | C47 | H47A | 0.979 |
| 97 | C42 | H42 | 0.95 | 216 | C47 | H47B | 0.981 |
| 98 | C42 | C43 | 1.370(4) | 217 | C47 | H47C | 0.98 |
| 99 | C43 | H43 | 0.95 | 218 | C48 | H48A | 0.98 |
| 100 | C43 | C44 | 1.396(5) | 219 | C48 | H48B | 0.98 |
| 101 | C44 | C45 | 1.386(4) | 220 | C48 | H48C | 0.98 |
| 102 | C45 | H45 | 0.95 | 221 | S2 | O9 | 1.498(3) |
| 103 | C45 | C46 | 1.385(4) | 222 | S2 | C49 | 1.764(3) |
| 104 | C46 | H46 | 0.95 | 223 | S2 | C50 | 1.773(4) |
| 105 | C47 | H47A | 0.979 | 224 | C49 | H49A | 0.98 |
| 106 | C47 | H47B | 0.981 | 225 | C49 | H49B | 0.979 |
| 107 | C47 | H47C | 0.98 | 226 | C49 | H49C | 0.98 |
| 108 | C48 | H48A | 0.98 | 227 | C50 | H50A | 0.98 |
| 109 | C48 | H48B | 0.98 | 228 | C50 | H50B | 0.98 |
| 110 | C48 | H48C | 0.98 | 229 | C50 | H50C | 0.98 |
| 111 | S1 | C1 | 1.730(3) | 230 | S2 | O9 | 1.498(3) |
| 112 | S1 | C2 | 1.722(3) | 231 | S2 | C49 | 1.764(3) |
| 113 | O1 | C3 | 1.372(4) | 232 | S2 | C50 | 1.773(4) |
| 114 | O1 | C6 | 1.450(3) | 233 | C49 | H49A | 0.98 |
| 115 | O2 | C4 | 1.365(3) | 234 | C49 | H49B | 0.979 |
| 116 | O2 | C5 | 1.444(4) | 235 | C49 | H49C | 0.98 |
| 117 | O3 | C7 | 1.223(3) | 236 | C50 | H50A | 0.98 |
| 118 | O4 | C17 | 1.364(4) | 237 | C50 | H50B | 0.98 |
| 119 | O4 | C26 | 1.427(3) | 238 | C50 | H50C | 0.98 |

**Bond angles**

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Number | Atom1 | Atom2 | Atom3 | Angle | Number | Atom1 | Atom2 | Atom3 | Angle |
| 1 | C1 | S1 | C2 | 92.5(2) | 99 | C20 | C25 | H25 | 119.7 |
| 2 | C3 | O1 | C6 | 111.9(2) | 100 | C24 | C25 | H25 | 119.6 |
| 3 | C4 | O2 | C5 | 111.9(2) | 101 | O4 | C26 | H26A | 109.5 |
| 4 | C17 | O4 | C26 | 117.2(2) | 102 | O4 | C26 | H26B | 109.5 |
| 5 | C23 | O5 | C27 | 117.0(2) | 103 | O4 | C26 | H26C | 109.5 |
| 6 | C38 | O7 | C47 | 116.6(3) | 104 | H26A | C26 | H26B | 109.5 |
| 7 | C44 | O8 | C48 | 116.5(2) | 105 | H26A | C26 | H26C | 109.5 |
| 8 | C7 | N1 | C8 | 128.0(3) | 106 | H26B | C26 | H26C | 109.4 |
| 9 | C7 | N1 | H1 | 117(2) | 107 | O5 | C27 | H27A | 109.5 |
| 10 | C8 | N1 | H1 | 114(2) | 108 | O5 | C27 | H27B | 109.4 |
| 11 | C11 | N2 | C14 | 121.7(2) | 109 | O5 | C27 | H27C | 109.5 |
| 12 | C11 | N2 | C20 | 121.9(2) | 110 | H27A | C27 | H27B | 109.5 |
| 13 | C14 | N2 | C20 | 116.4(2) | 111 | H27A | C27 | H27C | 109.5 |
| 14 | C28 | N3 | C29 | 128.4(3) | 112 | H27B | C27 | H27C | 109.5 |
| 15 | C28 | N3 | H3 | 119(2) | 113 | O6 | C28 | N3 | 124.3(3) |
| 16 | C29 | N3 | H3 | 112(2) | 114 | O6 | C28 | C2 | 121.3(3) |
| 17 | C32 | N4 | C35 | 119.1(2) | 115 | N3 | C28 | C2 | 114.4(3) |
| 18 | C32 | N4 | C41 | 119.5(2) | 116 | N3 | C29 | C30 | 123.4(3) |
| 19 | C35 | N4 | C41 | 121.4(2) | 117 | N3 | C29 | C34 | 117.7(3) |
| 20 | S1 | C1 | C4 | 110.3(2) | 118 | C30 | C29 | C34 | 118.8(3) |
| 21 | S1 | C1 | C7 | 118.6(2) | 119 | C29 | C30 | H30 | 119.9 |
| 22 | C4 | C1 | C7 | 131.0(3) | 120 | C29 | C30 | C31 | 120.2(3) |
| 23 | S1 | C2 | C3 | 110.8(2) | 121 | H30 | C30 | C31 | 119.9 |
| 24 | S1 | C2 | C28 | 118.8(2) | 122 | C30 | C31 | H31 | 119.3 |
| 25 | C3 | C2 | C28 | 130.3(3) | 123 | C30 | C31 | C32 | 121.3(3) |
| 26 | O1 | C3 | C2 | 124.6(3) | 124 | H31 | C31 | C32 | 119.3 |
| 27 | O1 | C3 | C4 | 122.2(3) | 125 | N4 | C32 | C31 | 121.2(3) |
| 28 | C2 | C3 | C4 | 113.2(3) | 126 | N4 | C32 | C33 | 120.5(3) |
| 29 | O2 | C4 | C1 | 124.1(3) | 127 | C31 | C32 | C33 | 118.3(3) |
| 30 | O2 | C4 | C3 | 122.9(3) | 128 | C32 | C33 | H33 | 120 |
| 31 | C1 | C4 | C3 | 113.1(3) | 129 | C32 | C33 | C34 | 120.1(3) |
| 32 | O2 | C5 | H5A | 109.6 | 130 | H33 | C33 | C34 | 119.9 |
| 33 | O2 | C5 | H5B | 109.7 | 131 | C29 | C34 | C33 | 121.3(3) |
| 34 | O2 | C5 | C6 | 110.0(2) | 132 | C29 | C34 | H34 | 119.3 |
| 35 | H5A | C5 | H5B | 108.2 | 133 | C33 | C34 | H34 | 119.4 |
| 36 | H5A | C5 | C6 | 109.6 | 134 | N4 | C35 | C36 | 121.4(3) |
| 37 | H5B | C5 | C6 | 109.7 | 135 | N4 | C35 | C40 | 120.5(3) |
| 38 | O1 | C6 | C5 | 109.7(2) | 136 | C36 | C35 | C40 | 118.1(3) |
| 39 | O1 | C6 | H6A | 109.7 | 137 | C35 | C36 | H36 | 119.5 |
| 40 | O1 | C6 | H6B | 109.7 | 138 | C35 | C36 | C37 | 121.1(3) |
| 41 | C5 | C6 | H6A | 109.8 | 139 | H36 | C36 | C37 | 119.5 |
| 42 | C5 | C6 | H6B | 109.8 | 140 | C36 | C37 | H37 | 120.2 |
| 43 | H6A | C6 | H6B | 108.2 | 141 | C36 | C37 | C38 | 119.7(3) |
| 44 | O3 | C7 | N1 | 125.2(3) | 142 | H37 | C37 | C38 | 120.1 |
| 45 | O3 | C7 | C1 | 120.6(3) | 143 | O7 | C38 | C37 | 124.6(3) |
| 46 | N1 | C7 | C1 | 114.2(3) | 144 | O7 | C38 | C39 | 115.4(3) |
| 47 | N1 | C8 | C9 | 124.3(3) | 145 | C37 | C38 | C39 | 120.0(3) |
| 48 | N1 | C8 | C13 | 117.1(3) | 146 | C38 | C39 | H39 | 120.1 |
| 49 | C9 | C8 | C13 | 118.5(3) | 147 | C38 | C39 | C40 | 119.8(3) |
| 50 | C8 | C9 | H9 | 119.7 | 148 | H39 | C39 | C40 | 120.1 |
| 51 | C8 | C9 | C10 | 120.7(3) | 149 | C35 | C40 | C39 | 121.1(3) |
| 52 | H9 | C9 | C10 | 119.6 | 150 | C35 | C40 | H40 | 119.4 |
| 53 | C9 | C10 | H10 | 119.2 | 151 | C39 | C40 | H40 | 119.5 |
| 54 | C9 | C10 | C11 | 121.6(3) | 152 | N4 | C41 | C42 | 121.0(3) |
| 55 | H10 | C10 | C11 | 119.2 | 153 | N4 | C41 | C46 | 121.3(3) |
| 56 | N2 | C11 | C10 | 122.3(3) | 154 | C42 | C41 | C46 | 117.7(3) |
| 57 | N2 | C11 | C12 | 120.5(3) | 155 | C41 | C42 | H42 | 119.5 |
| 58 | C10 | C11 | C12 | 117.2(3) | 156 | C41 | C42 | C43 | 121.1(3) |
| 59 | C11 | C12 | H12 | 119.5 | 157 | H42 | C42 | C43 | 119.4 |
| 60 | C11 | C12 | C13 | 120.9(3) | 158 | C42 | C43 | H43 | 119.5 |
| 61 | H12 | C12 | C13 | 119.6 | 159 | C42 | C43 | C44 | 121.0(3) |
| 62 | C8 | C13 | C12 | 121.0(3) | 160 | H43 | C43 | C44 | 119.5 |
| 63 | C8 | C13 | H13 | 119.4 | 161 | O8 | C44 | C43 | 117.0(3) |
| 64 | C12 | C13 | H13 | 119.5 | 162 | O8 | C44 | C45 | 124.6(3) |
| 65 | N2 | C14 | C15 | 121.1(3) | 163 | C43 | C44 | C45 | 118.4(3) |
| 66 | N2 | C14 | C19 | 120.1(3) | 164 | C44 | C45 | H45 | 119.9 |
| 67 | C15 | C14 | C19 | 118.8(3) | 165 | C44 | C45 | C46 | 120.3(3) |
| 68 | C14 | C15 | H15 | 119.7 | 166 | H45 | C45 | C46 | 119.8 |
| 69 | C14 | C15 | C16 | 120.7(3) | 167 | C41 | C46 | C45 | 121.4(3) |
| 70 | H15 | C15 | C16 | 119.7 | 168 | C41 | C46 | H46 | 119.3 |
| 71 | C15 | C16 | H16 | 120 | 169 | C45 | C46 | H46 | 119.3 |
| 72 | C15 | C16 | C17 | 120.0(3) | 170 | O7 | C47 | H47A | 109.5 |
| 73 | H16 | C16 | C17 | 120 | 171 | O7 | C47 | H47B | 109.4 |
| 74 | O4 | C17 | C16 | 124.8(3) | 172 | O7 | C47 | H47C | 109.5 |
| 75 | O4 | C17 | C18 | 115.7(3) | 173 | H47A | C47 | H47B | 109.5 |
| 76 | C16 | C17 | C18 | 119.4(3) | 174 | H47A | C47 | H47C | 109.5 |
| 77 | C17 | C18 | H18 | 120 | 175 | H47B | C47 | H47C | 109.4 |
| 78 | C17 | C18 | C19 | 120.0(3) | 176 | O8 | C48 | H48A | 109.5 |
| 79 | H18 | C18 | C19 | 120 | 177 | O8 | C48 | H48B | 109.5 |
| 80 | C14 | C19 | C18 | 121.0(3) | 178 | O8 | C48 | H48C | 109.5 |
| 81 | C14 | C19 | H19 | 119.5 | 179 | H48A | C48 | H48B | 109.4 |
| 82 | C18 | C19 | H19 | 119.5 | 180 | H48A | C48 | H48C | 109.5 |
| 83 | N2 | C20 | C21 | 120.2(3) | 181 | H48B | C48 | H48C | 109.5 |
| 84 | N2 | C20 | C25 | 121.1(3) | 182 | O9 | S2 | C49 | 106.4(1) |
| 85 | C21 | C20 | C25 | 118.7(3) | 183 | O9 | S2 | C50 | 106.6(2) |
| 86 | C20 | C21 | H21 | 119.7 | 184 | C49 | S2 | C50 | 96.6(2) |
| 87 | C20 | C21 | C22 | 120.6(3) | 185 | S2 | C49 | H49A | 109.4 |
| 88 | H21 | C21 | C22 | 119.7 | 186 | S2 | C49 | H49B | 109.5 |
| 89 | C21 | C22 | H22 | 119.8 | 187 | S2 | C49 | H49C | 109.4 |
| 90 | C21 | C22 | C23 | 120.4(3) | 188 | H49A | C49 | H49B | 109.5 |
| 91 | H22 | C22 | C23 | 119.8 | 189 | H49A | C49 | H49C | 109.4 |
| 92 | O5 | C23 | C22 | 115.9(3) | 190 | H49B | C49 | H49C | 109.5 |
| 93 | O5 | C23 | C24 | 125.1(3) | 191 | S2 | C50 | H50A | 109.5 |
| 94 | C22 | C23 | C24 | 119.0(3) | 192 | S2 | C50 | H50B | 109.5 |
| 95 | C23 | C24 | H24 | 119.9 | 193 | S2 | C50 | H50C | 109.5 |
| 96 | C23 | C24 | C25 | 120.3(3) | 194 | H50A | C50 | H50B | 109.5 |
| 97 | H24 | C24 | C25 | 119.8 | 195 | H50A | C50 | H50C | 109.5 |
| 98 | C20 | C25 | C24 | 120.7(3) | 196 | H50B | C50 | H50C | 109.4 |

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