

Electronic Supplementary Information

Quasi-aromatic Möbius chelates of Cadmium(II) nitrite and/or nitrate

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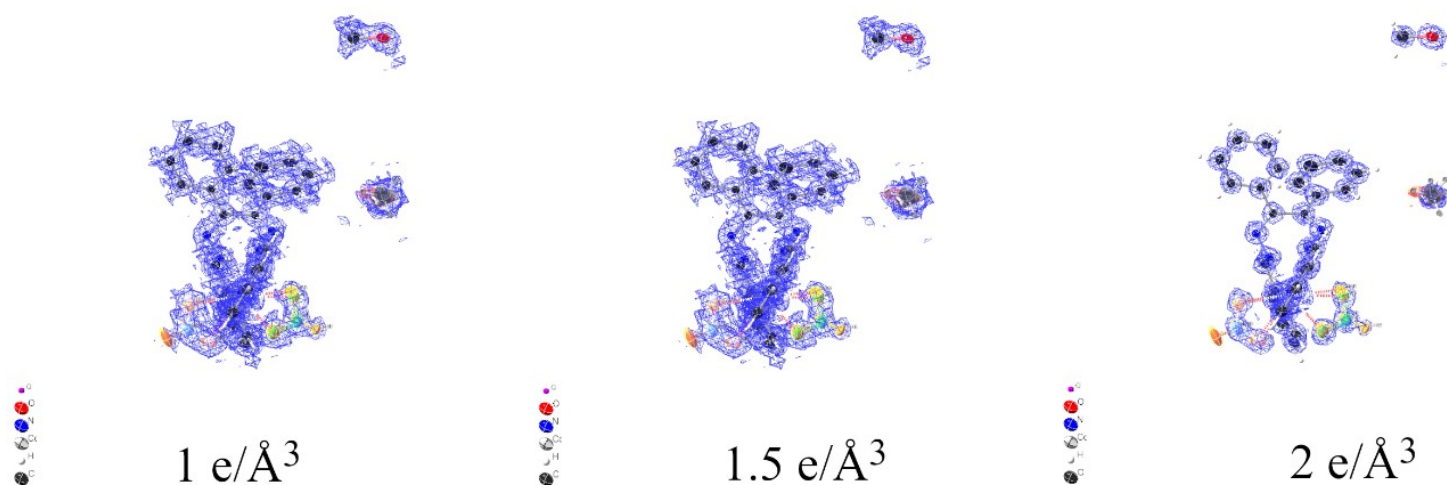


Fig. S1 F_o electron density at different levels for **1-100K** as evidence for the applied $\text{NO}_2^-/\text{NO}_3^-$ disorder. The $\text{NO}_2^-/\text{NO}_3^-$ disorder refines to 92.5/7.5 for the set on the left, to 74.6/25.4 on the right. Disorder is highlighted in different colours.

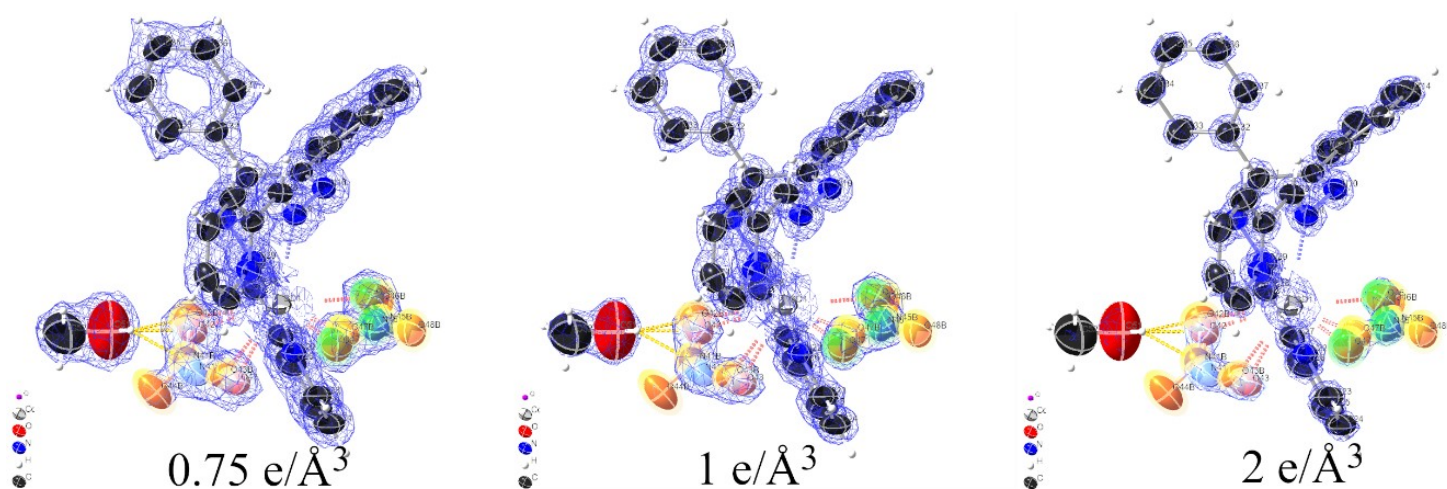


Fig.S2 F_o electron density at different levels for **1-296K** as evidence for the applied $\text{NO}_2^-/\text{NO}_3^-$ disorder. The $\text{NO}_2^-/\text{NO}_3^-$ disorder refines to 74/16 for the set on the left, to 83/17 on the right. Disorder is highlighted in different colours.

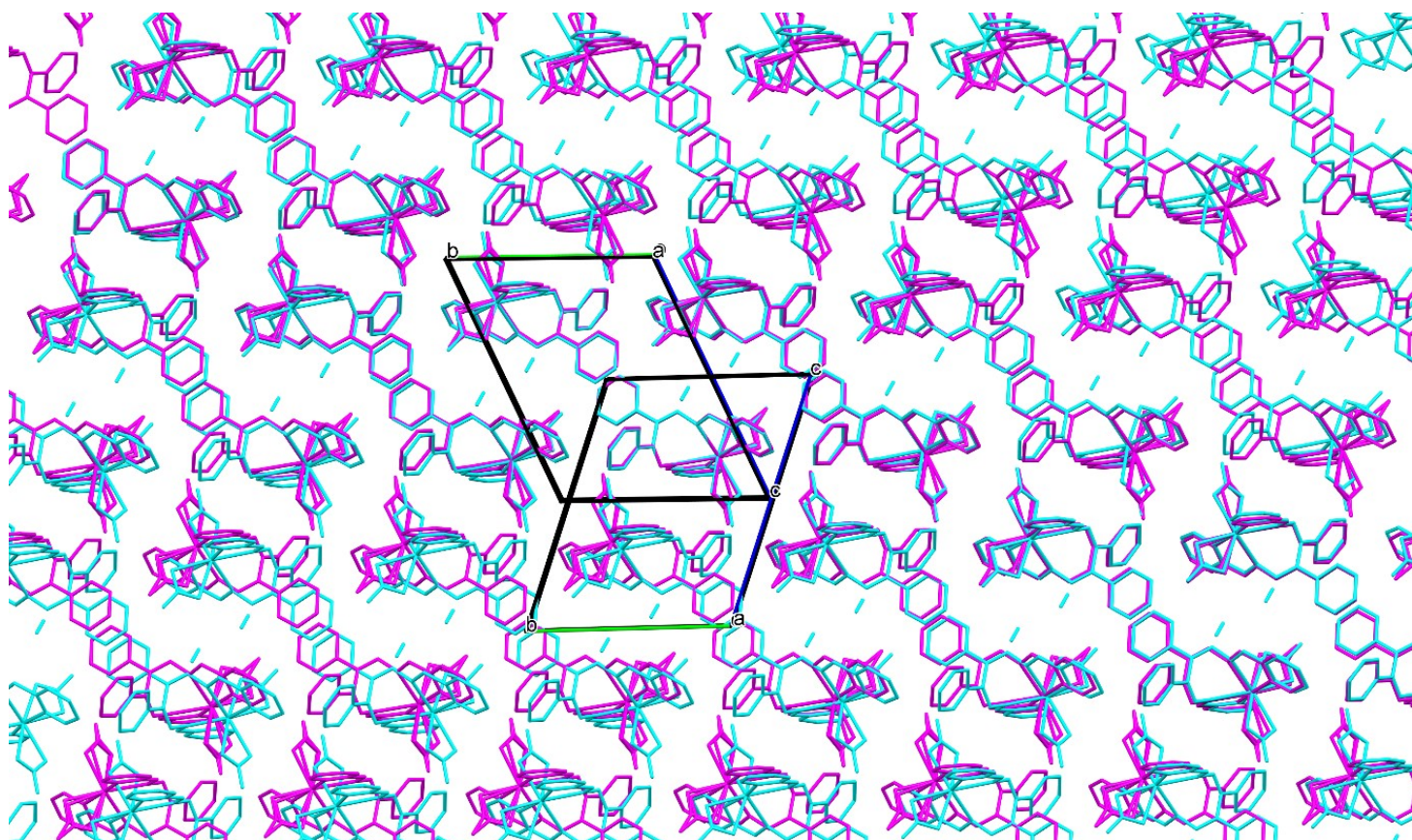


Fig. S3 Superposition of **1-296K** (magenta) and **2** (cyan) to show the packing similarities between both structures. The central complexes are superposed onto each other, and the difference between both packings becomes apparent when moving away from the central units. The upper unit cell belongs to **2**, while the bottom unit cell belongs to **1-296K**.

XYZ parameters (models from Fig. 4)Left ($\pi\cdots\pi/\text{C}-\text{H}\cdots\pi$)

H	-0.50323500	9.97109600	1.86439200
C	-0.28523700	8.50980900	3.25048400
H	-1.06721500	8.04629100	3.05526000
H	4.99237800	16.49916700	-1.02492700
C	0.56209600	8.06781300	4.24333900
C	2.98806400	14.49753400	2.47544400
C	1.59880900	11.57108500	2.18790600
H	1.15160600	11.84152700	1.41816500
C	1.21987000	10.33283700	2.87816400
H	0.35518800	7.30503300	4.73279400
C	1.72680000	8.77474100	4.50410300
H	0.38533900	14.96904000	2.08750500
O	5.03753800	8.96154800	3.90769300
C	3.63706000	15.64175100	1.79188000
C	3.95257100	16.79209900	2.51002600
H	9.03641400	10.78474500	5.62664300
C	7.05099600	10.98259200	5.23061600
H	6.87967900	10.07001900	5.17762700
C	5.13402700	14.05683200	5.09730600
H	5.23465200	14.97163500	5.23480000
C	4.01667300	15.54372600	0.46156600
H	3.79218400	14.78737800	-0.03067800
N	6.04486300	11.82862900	5.05240400
C	2.36638200	14.76474300	3.82346800
H	2.30449900	8.45926000	5.16228800
C	1.12772000	15.57841900	3.86934500
C	0.86731200	16.40496300	4.97124700
H	1.46857000	16.44453400	5.67963200
C	-0.29714500	17.16312500	4.99634700
H	-0.46631800	17.72218000	5.72007100
C	-1.21222700	17.09761600	3.95050300
H	-1.98750100	17.60972100	3.97420900

C	-0.95869700	16.26067100	2.87119100
H	-1.57540900	16.20011200	2.17814500
C	0.21216600	15.51317400	2.82099100
Cd	3.88969700	11.17115900	4.43954000
C	6.29368600	13.15085200	5.17051500
N	3.99703200	13.56191100	4.84225900
N	2.87663600	14.36862200	4.93025000
N	3.01251400	13.34380100	1.91054800
N	2.55343900	12.27093200	2.66634500
N	2.04958400	9.88847300	3.84801000
N	3.07172800	10.65724200	7.16040800
N	5.19234200	9.24309100	2.69033000
O	2.48545800	11.53578400	6.46568900
O	3.99382900	9.99420800	6.61057300
C	0.04671500	9.65822900	2.54628200
H	3.68728500	16.87209200	3.39829700
C	4.66256000	17.82097800	1.90622600
C	7.56642200	13.65112800	5.39516200
H	4.87387800	18.58749200	2.39149700
O	2.76075000	10.46982500	8.33844700
C	5.05643000	17.71065400	0.58985600
H	7.71415500	14.56829400	5.43839100
O	4.83654400	10.41066800	2.31410500
H	5.53983200	18.39701000	0.18964600
C	4.73080100	16.57276700	-0.13526300
C	8.61758000	12.75863900	5.55552500
H	9.48268900	13.06677200	5.70054900
C	8.35561000	11.40477400	5.49416900
O	5.65495400	8.44340200	1.88614500
C	4.42239300	1.67583200	5.17051500
C	5.69513000	2.17610800	5.39516200
H	5.84286200	3.09327400	5.43839100
C	6.74628700	1.28361900	5.55552500
H	7.61139700	1.59175100	5.70054900

C	6.48431700	−0.07024600	5.49416900
H	7.16512100	−0.69027500	5.62664300
C	5.17970300	−0.49242900	5.23061600
H	5.00838600	−1.40500100	5.17762700
C	3.26273400	2.58181200	5.09730600
H	3.36335900	3.49661500	5.23480000
C	0.49508900	3.28972300	3.82346800
C	1.11677100	3.02251400	2.47544400
C	−0.27248400	0.09606500	2.18790600
H	−0.71968700	0.36650700	1.41816500
C	−0.65142300	−1.14218400	2.87816400
C	−1.82457800	−1.81679100	2.54628200
H	−2.37452800	−1.50392400	1.86439200
C	−2.15653000	−2.96521200	3.25048400
H	−2.93850800	−3.42873000	3.05526000
C	−1.30919700	−3.40720700	4.24333900
H	−1.51610500	−4.16998700	4.73279400
C	−0.14449200	−2.70027900	4.50410300
H	0.43320700	−3.01576000	5.16228800
C	−0.74357200	4.10339900	3.86934500
C	−1.00398100	4.92994300	4.97124700
H	−0.40272300	4.96951300	5.67963200
C	−2.16843800	5.68810500	4.99634700
H	−2.33761100	6.24716000	5.72007100
C	−3.08352000	5.62259600	3.95050300
H	−3.85879300	6.13470100	3.97420900
C	−2.82999000	4.78565000	2.87119100
H	−3.44670200	4.72509200	2.17814500
C	−1.65912700	4.03815400	2.82099100
H	−1.48595400	3.49402000	2.08750500
C	1.76576700	4.16673000	1.79188000
C	2.08127800	5.31707900	2.51002600
H	1.81599200	5.39707200	3.39829700
C	2.79126700	6.34595800	1.90622600

H	3.00258500	7.11247200	2.39149700
C	3.18513700	6.23563400	0.58985600
H	3.66853900	6.92198900	0.18964600
C	2.85950800	5.09774600	−0.13526300
H	3.12108500	5.02414700	−1.02492700
C	2.14538000	4.06870600	0.46156600
H	1.92089100	3.31235800	−0.03067800
N	4.17357000	0.35360900	5.05240400
N	2.12573900	2.08689100	4.84225900
N	1.00534300	2.89360100	4.93025000
N	1.14122100	1.86878000	1.91054800
N	0.68214600	0.79591200	2.66634500
N	0.17829100	−1.58654700	3.84801000
N	1.20043500	−0.81777800	7.16040800
N	3.32104900	−2.23192900	2.69033000
O	0.61416500	0.06076300	6.46568900
O	2.12253600	−1.48081200	6.61057300
O	0.88945700	−1.00519500	8.33844700
O	2.96525100	−1.06435300	2.31410500
O	3.78366200	−3.03161800	1.88614500
O	3.16624500	−2.51347300	3.90769300
Cd	2.01840500	−0.30386100	4.43954000

Right (O–H···O)

C	8.17540600	3.23682600	8.77407600
C	6.90267000	2.73655000	8.54942900
H	6.75493800	1.81938400	8.50620100
C	5.85151300	3.62903900	8.38906600
H	4.98640300	3.32090600	8.24404300
C	6.11348200	4.98290400	8.45042200
H	5.43267800	5.60293300	8.31794900
C	7.41809600	5.40508600	8.71397500
H	7.58941300	6.31765900	8.76696500
C	9.33506500	2.33084600	8.84728600
H	9.23444000	1.41604300	8.70979200
C	12.10271000	1.62293500	10.12112400
C	11.48102800	1.89014400	11.46914800
C	12.87028300	4.81659300	11.75668500
H	13.31748600	4.54615100	12.52642700
C	13.24922300	6.05484100	11.06642800
C	14.42237700	6.72944900	11.39830900
H	14.97232700	6.41658200	12.08020000
C	14.75432900	7.87786900	10.69410700
H	15.53630800	8.34138700	10.88933200
C	13.90699600	8.31986500	9.70125200
H	14.11390400	9.08264400	9.21179700
C	12.74229200	7.61293700	9.44048800
H	12.16459300	7.92841800	8.78230400
C	13.34137200	0.80925900	10.07524600
C	13.60178000	−0.01728500	8.97334500
H	13.00052200	−0.05685600	8.26495900
C	14.76623700	−0.77544700	8.94824400
H	14.93541000	−1.33450200	8.22452000
C	15.68131900	−0.70993800	9.99408900
H	16.45659300	−1.22204300	9.97038300
C	15.42778900	0.12700700	11.07340000
H	16.04450100	0.18756600	11.76644600

C	14.25692600	0.87450400	11.12360100
H	14.08375300	1.41863800	11.85708600
C	10.83203200	0.74592700	12.15271200
C	10.51652100	−0.40442100	11.43456500
H	10.78180800	−0.48441400	10.54629500
C	9.80653200	−1.43330000	12.03836600
H	9.59521400	−2.19981400	11.55309400
C	9.41266200	−1.32297600	13.35473500
H	8.92926000	−2.00933200	13.75494500
C	9.73829100	−0.18508900	14.07985400
H	9.47671400	−0.11148900	14.96951900
C	10.45241900	0.84395200	13.48302600
H	10.67690800	1.60030000	13.97527000
N	8.42422900	4.55904900	8.89218700
N	10.47206000	2.82576700	9.10233200
N	11.59245600	2.01905600	9.01434200
N	11.45657800	3.04387700	12.03404300
N	11.91565300	4.11674600	11.27824600
N	12.41950800	6.49920500	10.09658200
N	11.39736400	5.73043600	6.78418300
N	9.27675000	7.14458700	11.25426200
O	11.98363400	4.85189400	7.47890300
O	10.47526300	6.39347000	7.33401800
O	11.70834200	5.91785300	5.60614400
O	9.63254800	5.97701000	11.63048700
O	8.81413800	7.94427600	12.05844600
O	9.43155500	7.42613000	10.03689900
Cd	10.57939500	5.21651900	9.50505200
C	8.69289200	6.44051700	15.14801000
H	8.82100600	6.42213000	16.09903100
H	7.99711800	5.82423500	14.90676800
H	8.44308200	7.32698200	14.87609000
O	9.86867200	6.07797800	14.51632000
H	9.77085500	6.09630700	13.72147800