

Electronic supplementary material for manuscript:

Anion-cation recognition pattern, thermal stability and DFT-calculations in the crystal structure of $\text{H}_2\text{dap}[\text{Cd}(\text{HEDTA})(\text{H}_2\text{O})]$ salt ($\text{H}_2\text{dap} = \text{H}_2(\text{N}_3,\text{N}_7)$ -2,6-diaminopurinium cation)

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Cartesian coordinates:

Figure 7a:

N	4.38350000	3.55960000	7.75160000
N	5.31030000	5.13160000	9.16020000
H	5.09080000	5.68470000	8.54360000
H	5.32180000	5.40930000	10.02230000
N	5.09180000	2.98910000	9.95480000
H	5.40260000	3.29760000	10.71020000
N	3.32300000	2.04850000	6.38230000
H	3.16900000	2.68730000	5.80190000
H	3.13930000	1.25430000	6.16110000
N	3.61220000	0.06710000	8.77740000
H	3.08150000	-0.44010000	8.19120000
N	4.59840000	0.72550000	10.68730000
C	4.90980000	3.87700000	8.94200000
C	4.63260000	1.72530000	9.76790000
C	4.05530000	1.35750000	8.57590000
C	3.92200000	2.31330000	7.53980000
C	3.96130000	-0.25300000	10.03680000
H	3.77210000	-1.09830000	10.42860000
Cd	7.30890000	2.56320000	13.66160000
O	5.91700000	0.81680000	13.27030000
H	5.67530000	0.73370000	12.53460000
H	5.25320000	0.68590000	13.72670000
O	8.89910000	1.27580000	14.70870000
O	10.99020000	0.53800000	14.52590000
O	8.08440000	1.86610000	11.52780000
O	9.03510000	2.69390000	9.69200000
O	6.31920000	2.51910000	15.89150000
O	6.39590000	3.54260000	17.88690000
H	6.16900000	2.83740000	18.21350000
O	6.05160000	3.93540000	12.30850000

O	5.00960000	5.87940000	12.02740000
N	9.44680000	3.55690000	13.15640000
N	7.21900000	4.82430000	14.62290000
C	9.62930000	4.75790000	13.99700000
H	9.89770000	4.47890000	14.90870000
H	10.35990000	5.31000000	13.62050000
C	10.49530000	2.54860000	13.40480000
H	10.79930000	2.19690000	12.53120000
H	11.26710000	3.00210000	13.82620000
C	10.10020000	1.36890000	14.28080000
C	9.38840000	3.87510000	11.71790000
H	8.83660000	4.68580000	11.58200000
H	10.30120000	4.06680000	11.38640000
C	8.79170000	2.71840000	10.92200000
C	8.36480000	5.59710000	14.08450000
H	8.13440000	5.93430000	13.18210000
H	8.53260000	6.37890000	14.66750000
C	7.26860000	4.73130000	16.08410000
H	8.21380000	4.73530000	16.37730000
H	6.82510000	5.52510000	16.47510000
C	6.59270000	3.47940000	16.60120000
C	5.95160000	5.42760000	14.17350000
H	5.21380000	5.10620000	14.75020000
H	6.00580000	6.41160000	14.26790000
C	5.64650000	5.07590000	12.71810000
Cd	3.77300000	-1.25740000	3.19960000
O	5.16490000	0.48890000	3.59090000
H	5.40650000	0.57200000	4.32660000
H	5.82860000	0.61980000	3.13450000
O	2.18280000	0.02990000	2.15250000
O	0.09160000	0.76770000	2.33530000
O	2.99750000	-0.56030000	5.33340000
O	2.04680000	-1.38810000	7.16920000
O	4.76270000	-1.21340000	0.96970000
O	4.68590000	-2.23690000	-1.02570000
H	4.91280000	-1.53160000	-1.35230000
O	5.03020000	-2.62970000	4.55270000
O	6.07220000	-4.57370000	4.83380000
N	1.63500000	-2.25120000	3.70470000
N	3.86280000	-3.51850000	2.23830000
C	1.45260000	-3.45210000	2.86420000
H	1.18420000	-3.17310000	1.95250000
H	0.72200000	-4.00430000	3.24070000
C	0.58660000	-1.24290000	3.45640000
H	0.28250000	-0.89110000	4.33000000
H	-0.18520000	-1.69640000	3.03500000
C	0.98170000	-0.06310000	2.58040000
C	1.69350000	-2.56930000	5.14330000
H	2.24520000	-3.38010000	5.27920000
H	0.78070000	-2.76110000	5.47480000
C	2.29020000	-1.41270000	5.93920000
C	2.71700000	-4.29140000	2.77670000
H	2.94740000	-4.62860000	3.67910000
H	2.54920000	-5.07320000	2.19360000
C	3.81320000	-3.42550000	0.77710000
H	2.86800000	-3.42960000	0.48390000
H	4.25670000	-4.21940000	0.38610000
C	4.48910000	-2.17360000	0.26000000
C	5.13020000	-4.12180000	2.68770000
H	5.86800000	-3.80040000	2.11100000
H	5.07600000	-5.10590000	2.59330000
C	5.43530000	-3.77020000	4.14310000
N	6.69830000	-2.25390000	9.10960000
N	5.77150000	-3.82590000	7.70100000
H	5.99100000	-4.37890000	8.31760000
H	5.76000000	-4.10360000	6.83890000
N	5.99010000	-1.68330000	6.90630000
H	5.67930000	-1.99190000	6.15100000

N	7.75880000	-0.74270000	10.47890000
H	7.91280000	-1.38160000	11.05930000
H	7.94260000	0.05150000	10.70010000
N	7.46970000	1.23860000	8.08380000
H	8.00040000	1.74580000	8.67000000
N	6.48340000	0.58020000	6.17390000
C	6.17200000	-2.57130000	7.91920000
C	6.44920000	-0.41950000	7.09330000
C	7.02650000	-0.05180000	8.28530000
C	7.15980000	-1.00760000	9.32140000
C	7.12060000	1.55870000	6.82440000
H	7.30980000	2.40410000	6.43250000

Figure 7b

N	4.38350000	3.55960000	7.75160000
N	5.31030000	5.13160000	9.16020000
H	5.09080000	5.68470000	8.54360000
H	5.32180000	5.40930000	10.02230000
N	5.09180000	2.98910000	9.95480000
H	5.40260000	3.29760000	10.71020000
N	3.32300000	2.04850000	6.38230000
H	3.16900000	2.68730000	5.80190000
H	3.13930000	1.25430000	6.16110000
N	3.61220000	0.06710000	8.77740000
H	3.08150000	-0.44010000	8.19120000
N	4.59840000	0.72550000	10.68730000
C	4.90980000	3.87700000	8.94200000
C	4.63260000	1.72530000	9.76790000
C	4.05530000	1.35750000	8.57590000
C	3.92200000	2.31330000	7.53980000
C	3.96130000	-0.25300000	10.03680000
H	3.77210000	-1.09830000	10.42860000
Cd	7.30890000	2.56320000	13.66160000
O	5.91700000	0.81680000	13.27030000
H	5.67530000	0.73370000	12.53460000
H	5.25320000	0.68590000	13.72670000
O	8.89910000	1.27580000	14.70870000
O	10.99020000	0.53800000	14.52590000
O	8.08440000	1.86610000	11.52780000
O	9.03510000	2.69390000	9.69200000
O	6.31920000	2.51910000	15.89150000
O	6.39590000	3.54260000	17.88690000
H	6.16900000	2.83740000	18.21350000
O	6.05160000	3.93540000	12.30850000
O	5.00960000	5.87940000	12.02740000
N	9.44680000	3.55690000	13.15640000
N	7.21900000	4.82430000	14.62290000
C	9.62930000	4.75790000	13.99700000
H	9.89770000	4.47890000	14.90870000
H	10.35990000	5.31000000	13.62050000
C	10.49530000	2.54860000	13.40480000
H	10.79930000	2.19690000	12.53120000
H	11.26710000	3.00210000	13.82620000
C	10.10020000	1.36890000	14.28080000
C	9.38840000	3.87510000	11.71790000
H	8.83660000	4.68580000	11.58200000
H	10.30120000	4.06680000	11.38640000
C	8.79170000	2.71840000	10.92200000
C	8.36480000	5.59710000	14.08450000
H	8.13440000	5.93430000	13.18210000
H	8.53260000	6.37890000	14.66750000
C	7.26860000	4.73130000	16.08410000
H	8.21380000	4.73530000	16.37730000
H	6.82510000	5.52510000	16.47510000
C	6.59270000	3.47940000	16.60120000
C	5.95160000	5.42760000	14.17350000
H	5.21380000	5.10620000	14.75020000
H	6.00580000	6.41160000	14.26790000

C	5.64650000	5.07590000	12.71810000
Figure 7c			
N	4.38350000	3.55960000	7.75160000
N	5.31030000	5.13160000	9.16020000
H	5.09080000	5.68470000	8.54360000
H	5.32180000	5.40930000	10.02230000
N	5.09180000	2.98910000	9.95480000
H	5.40260000	3.29760000	10.71020000
N	3.32300000	2.04850000	6.38230000
H	3.16900000	2.68730000	5.80190000
H	3.13930000	1.25430000	6.16110000
N	3.61220000	0.06710000	8.77740000
H	3.08150000	-0.44010000	8.19120000
N	4.59840000	0.72550000	10.68730000
C	4.90980000	3.87700000	8.94200000
C	4.63260000	1.72530000	9.76790000
C	4.05530000	1.35750000	8.57590000
C	3.92200000	2.31330000	7.53980000
C	3.96130000	-0.25300000	10.03680000
H	3.77210000	-1.09830000	10.42860000
Cd	3.77300000	-1.25740000	3.19960000
O	5.16490000	0.48890000	3.59090000
H	5.40650000	0.57200000	4.32660000
H	5.82860000	0.61980000	3.13450000
O	2.18280000	0.02990000	2.15250000
O	0.09160000	0.76770000	2.33530000
O	2.99750000	-0.56030000	5.33340000
O	2.04680000	-1.38810000	7.16920000
O	4.76270000	-1.21340000	0.96970000
O	4.68590000	-2.23690000	-1.02570000
H	4.91280000	-1.53160000	-1.35230000
O	5.03020000	-2.62970000	4.55270000
O	6.07220000	-4.57370000	4.83380000
N	1.63500000	-2.25120000	3.70470000
N	3.86280000	-3.51850000	2.23830000
C	1.45260000	-3.45210000	2.86420000
H	1.18420000	-3.17310000	1.95250000
H	0.72200000	-4.00430000	3.24070000
C	0.58660000	-1.24290000	3.45640000
H	0.28250000	-0.89110000	4.33000000
H	-0.18520000	-1.69640000	3.03500000
C	0.98170000	-0.06310000	2.58040000
C	1.69350000	-2.56930000	5.14330000
H	2.24520000	-3.38010000	5.27920000
H	0.78070000	-2.76110000	5.47480000
C	2.29020000	-1.41270000	5.93920000
C	2.71700000	-4.29140000	2.77670000
H	2.94740000	-4.62860000	3.67910000
H	2.54920000	-5.07320000	2.19360000
C	3.81320000	-3.42550000	0.77710000
H	2.86800000	-3.42960000	0.48390000
H	4.25670000	-4.21940000	0.38610000
C	4.48910000	-2.17360000	0.26000000
C	5.13020000	-4.12180000	2.68770000
H	5.86800000	-3.80040000	2.11100000
H	5.07600000	-5.10590000	2.59330000
C	5.43530000	-3.77020000	4.14310000
Figure 7d			
N	-2.98427444	1.13608100	0.23055801
N	-3.38862569	1.87435715	2.37665787
H	-4.00344452	2.34192443	2.00561330
H	-3.50197596	1.58732777	3.22826329
N	-1.87578911	0.16920009	2.10609819
H	-1.82243550	0.15370821	2.97748297
N	-2.71031019	0.32088754	-1.90098349

H	-3.34112774	0.85960856	-2.18469898
H	-2.26830519	-0.11436021	-2.47423713
N	-0.82158371	-1.78228823	-0.57604931
H	-0.85862022	-2.10755467	-1.45659165
N	-0.46315191	-1.75276197	1.64306174
C	-2.75125873	1.04550178	1.54672126
C	-1.26777492	-0.71994625	1.27982691
C	-1.49779669	-0.68969020	-0.07501282
C	-2.39313673	0.26760857	-0.61052286
C	-0.22962611	-2.36904186	0.48023170
H	0.30610789	-3.15094878	0.40643050
N	2.98427444	-1.13608100	-0.23055801
N	3.38862569	-1.87435715	-2.37665787
H	4.00344452	-2.34192443	-2.00561330
H	3.50197596	-1.58732777	-3.22826329
N	1.87578911	-0.16920009	-2.10609819
H	1.82243550	-0.15370821	-2.97748297
N	2.71031019	-0.32088754	1.90098349
H	3.34112774	-0.85960856	2.18469898
H	2.26830519	0.11436021	2.47423713
N	0.82158371	1.78228823	0.57604931
H	0.85862022	2.10755467	1.45659165
N	0.46315191	1.75276197	-1.64306174
C	2.75125873	-1.04550178	-1.54672126
C	1.26777492	0.71994625	-1.27982691
C	1.49779669	0.68969020	0.07501282
C	2.39313673	-0.26760857	0.61052286
C	0.22962611	2.36904186	-0.48023170
H	-0.30610789	3.15094878	-0.40643050