Electronic Supplementary Information for CrystEngComm

Supplementary Data
for

Oxo-anion binding by protonated (dimethylphenyl)(pyridyl)ureas

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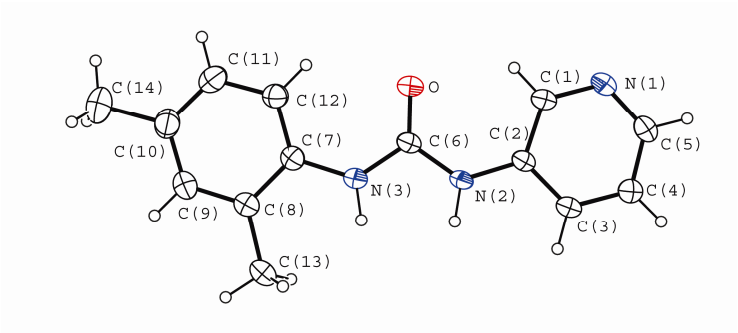


Figure S1. Molecular structure of ligand **1**.

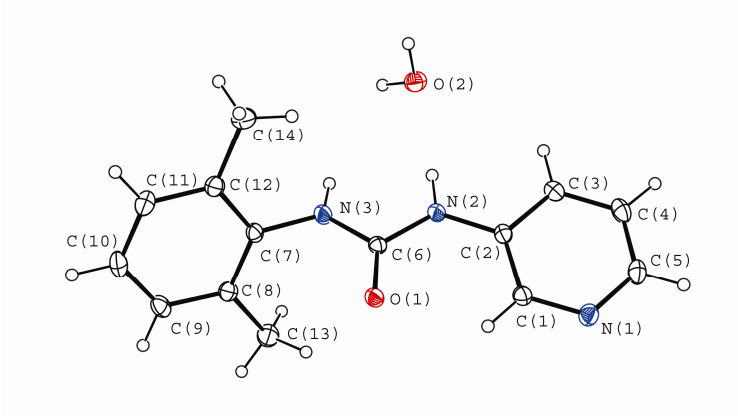


Figure S2. Molecular structure of ligand **2**·H_2O.

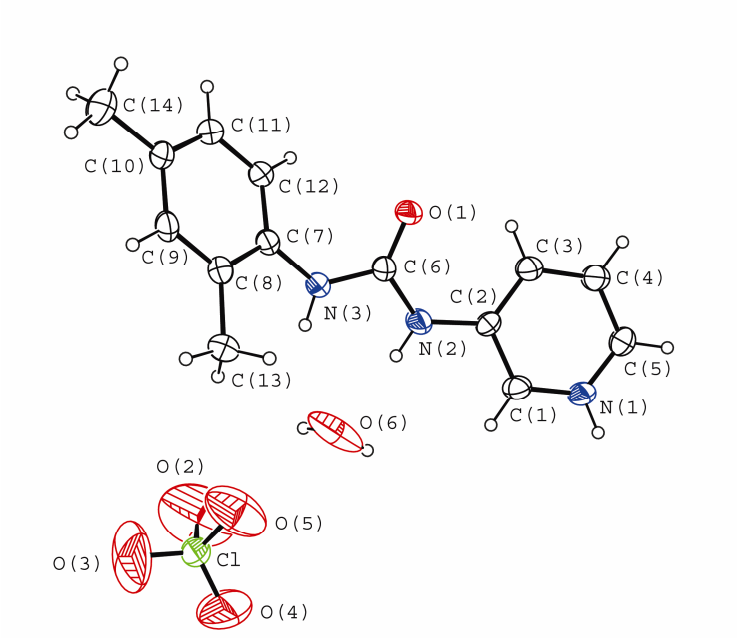


Figure S3. Molecular structure of complex **3**.

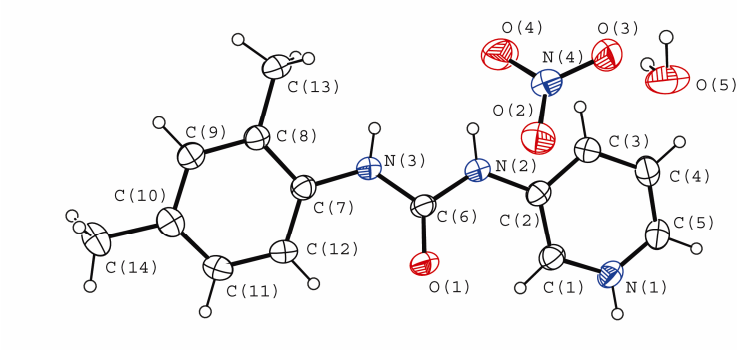


Figure S4. Molecular structure of complex **4**.

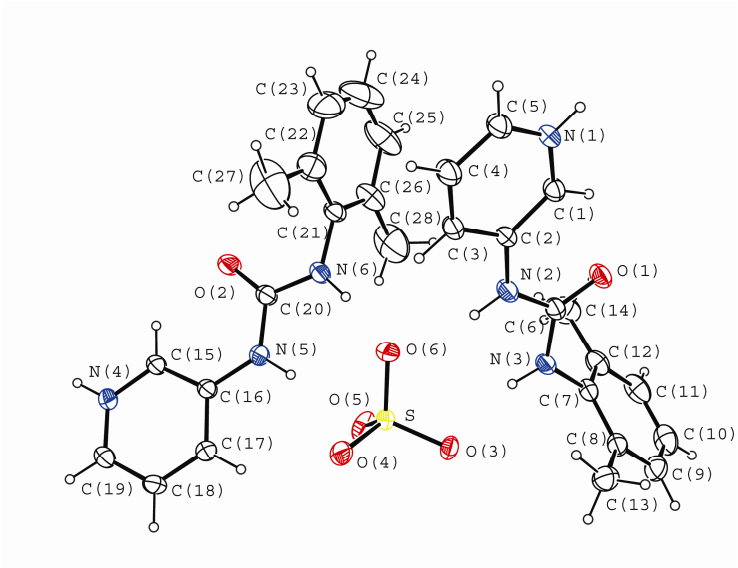


Figure S5. Molecular structure of complex **5**.

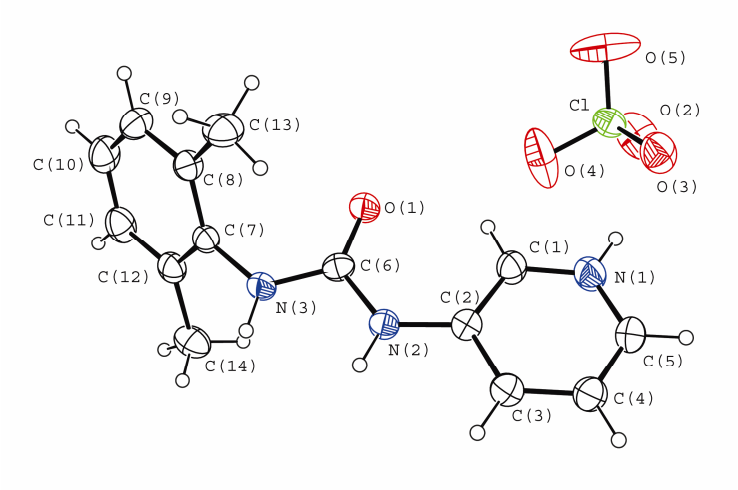


Figure S6. Molecular structure of complex **6**.

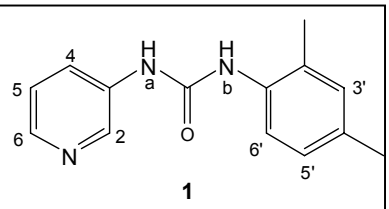
Table S1. The intramolecular C-H···O hydrogen bond parameters in **3-6**.

		D-H (Å)	H···A (Å)	D···A (Å)	∠D-H···A (°)
3	C3-H3B···O1	0.93	2.34	2.875(5)	115.9
	C12-H12A···O1	0.93	2.60	2.993(5)	105.8
4	C1-H1A···O1	0.93	2.24	2.830(4)	120.9
	C12-H12A···O1	0.93	2.34	2.899(4)	118.6
5	C1-H1A···O1	0.93	2.19	2.796(4)	122.3
	C14-H14A···O1	0.96	2.68	3.135(5)	109.2
	C15-H15A···O2	0.93	2.14	2.770(4)	124.0
	C27-H27C···O2	0.96	2.78	3.426(6)	125.7
6	C1-H1A···O1	0.93	2.17	2.784(4)	122.9
	C13-H13A···O1	0.96	2.63	3.095(4)	110.1

NMR spectroscopy

Table S2. NMR data of compound (**1**H)$ClO_4 \cdot H_2O$ (**3**) at different concentrations (DMSO-d_6)

	L (0M)	5M	10M	50M	100M	150M
NHa	9.142	9.414	9.493	9.677	9.701	9.771
H2	8.600	8.840	8.902	9.067	9.087	9.138
H4	7.959	8.139	8.177	8.271	8.292	8.318
H5	7.312	7.576	7.675	7.857	7.895	7.936
H6	8.176	8.315	8.355	8.455	8.475	8.497
NHb	7.998	8.139	8.177	8.271	8.292	8.318
H3’	6.995	7.021	7.024	7.038	7.039	7.040
H5’	6.956	6.983	6.976	6.989	6.989	6.993
H6’	7.626	7.555	7.556	7.523	7.522	7.513



1

Numbering of the protons.

Table S3. NMR data of compound (**1**H)$NO_3 \cdot H_2O$ (**4**) at different concentrations (DMSO-d_6)

	L (0M)	5 M	10 M	50 M	100 M	150 M
NHa	9.142	9.622	9.769	9.856	9.899	9.930
H2	8.600	8.920	9.110	9.142	9.151	9.155
H4	7.959	8.251	8.297	8.331	8.341	8.342
H5	7.312	7.752	7.907	7.946	7.957	7.962
H6	8.176	8.392	8.486	8.510	8.518	8.522
NHb	7.998	8.282	8.322	8.366	8.385	8.397
H3’	6.995	7.038	7.038	7.033	7.027	7.020
H5’	6.956	6.990	6.990	6.987	6.984	6.979
H6’	7.626	7.520	7.514	7.508	7.507	7.506