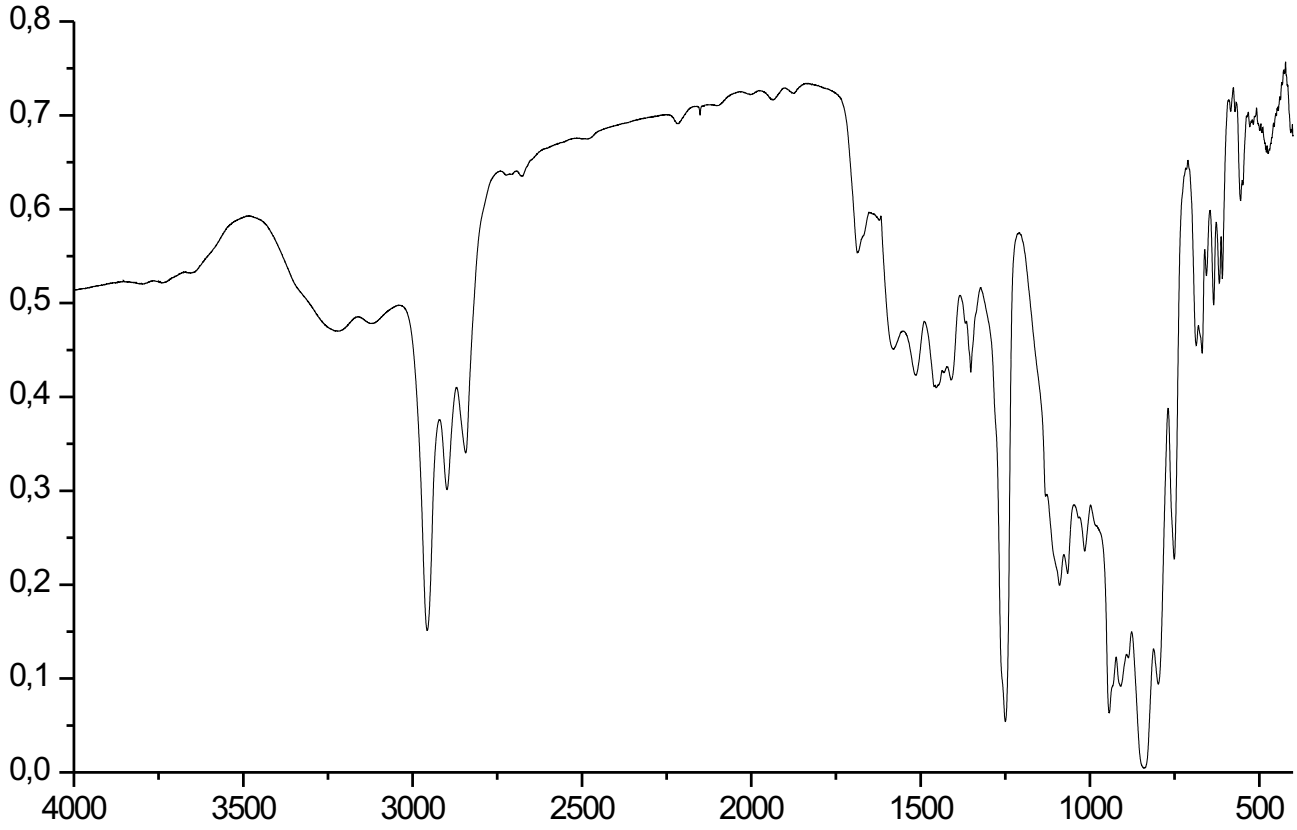

Supp. Mat. Figure S1. MIR spectra of **1**.

Supp. Mat.

Table S1. Charge contributions of model **I**.[a]

Orbital	Label	Energy [Hartree]	Charge decompositon [%][b]			
			V-d	N	N_{AD}[c]	N_{AM}[d]
d_{z^2}	169	-0.04625	61	1	11	0
$d_{x^2-y^2}\_p_y$	168	-0.05598	62	10	8	1
d_{yz}	167	-0.07935	70	2	11	0
N_{AM}	166	-0.19597	5	8	11	36
$N_{AD}\_p_z$	165	-0.19989	2	10	36	13
$N_{AM}\_p_z$	164	-0.21017	3	5	16	37
$N_{AD}\_d_{yz}\_p_y$	163	-0.21708	8	5	33	20
N_{AD}	162	-0.22056	2	5	48	8
$N_{AD}\_d_{x^2-y^2}\_p_{yz}$	161	-0.22363	12	7	45	1
$p_y\_d_{xy}$	160	-0.25720	24	40	13	1
$N_{AD}\_p_z$	159	-0.26146	7	26	33	1
$p_z\_d_{yz}$	158	-0.26514	30	38	11	0
$p_x\_d_\sigma$	150	-0.29833	11	13	5	1
$p_{xy}\_d_{xy}$	147	-0.30156	13	17	7	1
$p_{xy}\_d_{xy}$	143	-0.30722	9	9	10	2
$p_x\_d_\sigma$	142	-0.30790	17	18	11	4
$p_{xy}\_d_{xy}$	141	-0.31046	21	22	15	3
$p_{xy}\_d_{xy}$	140	-0.31859	24	29	5	9
$p_y\_d_{x^2-y^2}$	138	-0.32492	9	9	12	20
$d_{xz}\_p_z$	137	-0.32495	18	9	17	12

[a] Only selected orbitals are listed. [b] The charge decomposition gives the sum of all contributions of the corresponding atoms. [c] N_{AD} are the nitrogen atoms of the amido groups. [d] N_{AM} are the nitrogen atoms of the amino groups.