

Supplementary Information for

## Acidic medium synthesis of zeolites – an avenue to control the structure-directing power of the organic template

Guangying Fu,<sup>a</sup> Eddy Dib,<sup>b</sup> Qiaolin Lang,<sup>a</sup> Haonuan Zhao,<sup>a,b</sup> Songxia Wang,<sup>a</sup> Ruiqin Ding,<sup>a</sup> Xiaobo Yang,<sup>\*a</sup> and Valentin Valtchev<sup>\*a,b</sup>

<sup>a</sup> The ZeoMat Group, Qingdao Institute of Bioenergy and Bioprocess Technology, CAS, Laoshan District, CN-266101 Qingdao, China.

<sup>b</sup> Normandie University, ENSICAEN, UNICAEN, CNRS, Laboratoire Catalyse et Spectrochimie, F-14000 Caen, France.

### Table of Contents

#### S1. Additional synthesis and characterization results

**Figure S1.1.** The XRD patterns of the crystallizing **MTN** material obtained from a hydrogel with high F<sup>-</sup> content (1SiO<sub>2</sub>: 0.5HMTA: 0.12NH<sub>4</sub>F: 0.18HF: 50H<sub>2</sub>O, pH = 5.9) after 31 days of 160°C hydrothermal treatment, Sample A1.

**Figure S1.2.** XRD of the recovered solid products in the experiment series of temperature tests: Sample C10, 1SiO<sub>2</sub>:0.5HMTA:0.056NH<sub>4</sub>F:0.083HF:50H<sub>2</sub>O, pH = 6.5, crystallizes into cristobalite at 180°C in 36 days; Sample C11, 1SiO<sub>2</sub>:0.5HMTA:0.125HF:50H<sub>2</sub>O, pH = 5.6, remains amorphous at 140°C in 39 days.

**Figure S1.3.** XRD pattern of |TMA<sup>+</sup>,F<sup>-</sup>|-dodecasil 3C-**MTN** crystallized at basic conditions as a reference material. Sample was R1 obtained at 180°C in 14 days.

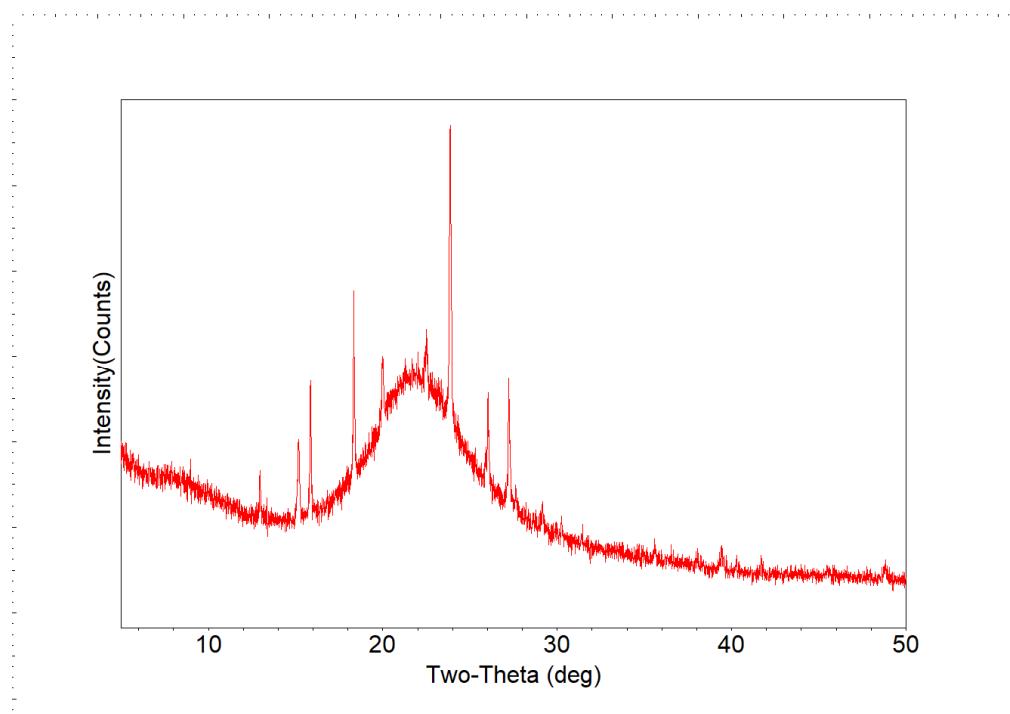
**Figure S1.4.** SEM pictures of |TMA<sup>+</sup>,F<sup>-</sup>|-dodecasil 3C-**MTN** crystallized at basic conditions as a reference material. Sample R1 was obtained at 180°C in 14 days.

#### S2. Model validation by Rietveld refinement

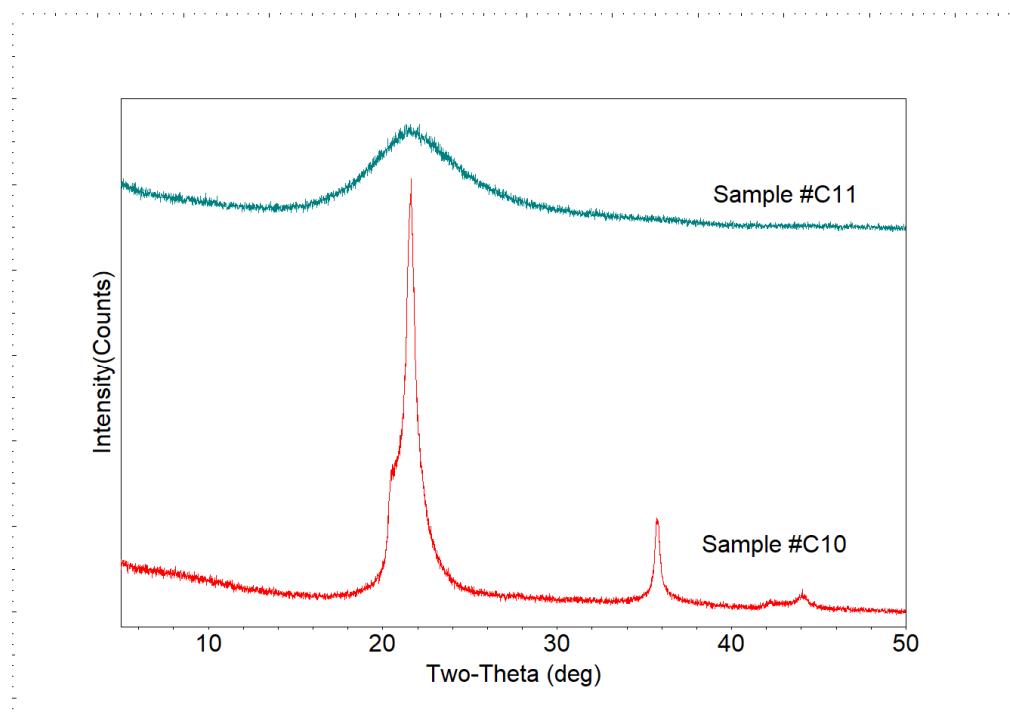
**Figure S2.1** Population of HMTA<sup>+</sup> ions at the centers of hexakaidecahedral [5<sup>12</sup>6<sup>4</sup>] cages as the results of energy minimization of 5 million Monte Carlo configurations.

**Table S2.1.** Refined atomic coordinates in the unit cell (cubic, a = 19.39662 Å).

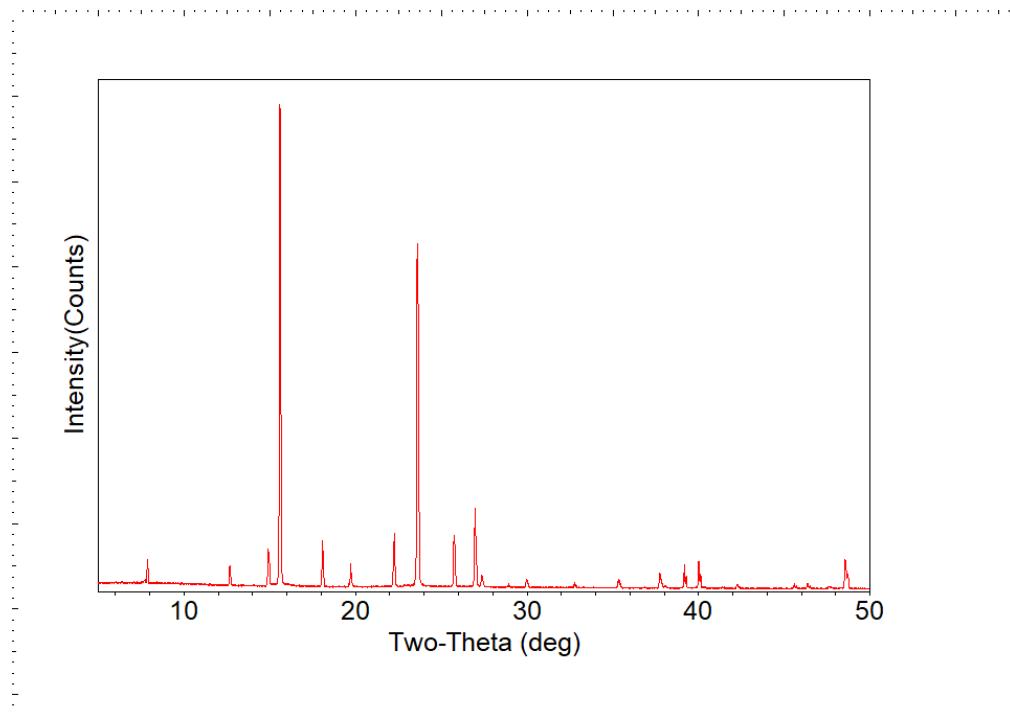
## S1. Additional synthesis and characterization results



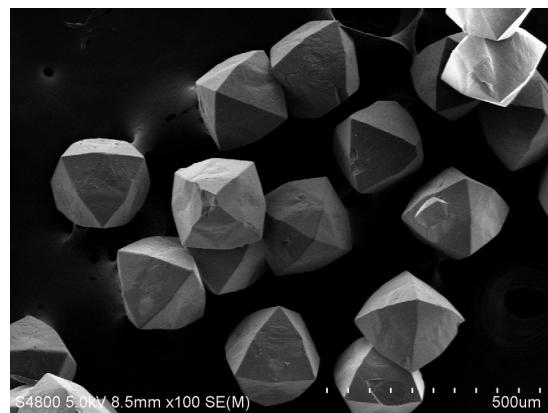
**Figure S1.1.** The XRD patterns of the crystallizing **MTN** material obtained from a hydrogel with high F<sup>-</sup> content (1SiO<sub>2</sub>: 0.5HMTA: 0.12NH<sub>4</sub>F: 0.18HF: 50H<sub>2</sub>O, pH = 5.9) after 31 days of 160°C hydrothermal treatment.



**Figure S1.2.** XRD of the recovered solid products in the experiment series of temperature tests: Sample C10, 1SiO<sub>2</sub>:0.5HMTA:0.056NH<sub>4</sub>F:0.083HF:50H<sub>2</sub>O, pH = 6.5, crystallizes into cristobalite at 180°C in 36 days; Sample C11, 1SiO<sub>2</sub>:0.5HMTA:0.125HF:50H<sub>2</sub>O, pH = 5.6, remains amorphous at 140°C in 39 days.

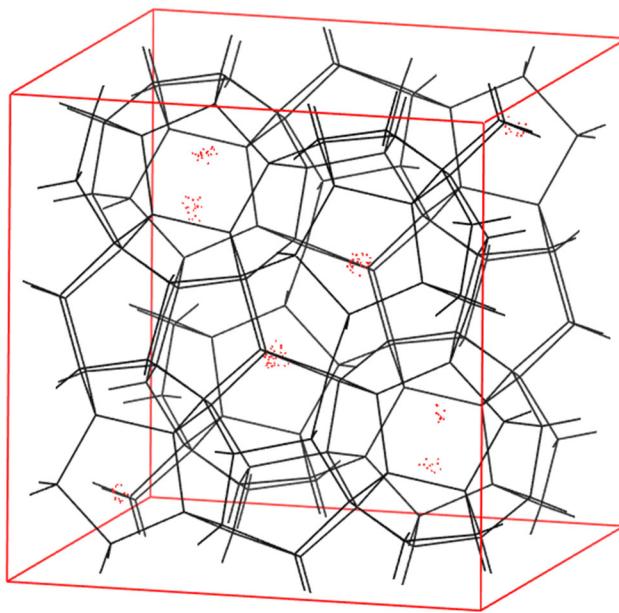


**Figure S1.3.** XRD patterns of  $|\text{TMA}^+, \text{F}^-|$ -dodecasil 3C-**MTN** crystallized at basic conditions as a reference material. Sample R1 was obtained at 180°C for 14 days.



**Figure S1.4.** SEM pictures of  $|\text{TMA}^+, \text{F}^-|$ -dodecasil 3C-**MTN** crystallized at basic conditions as a reference material. Sample R1 was obtained at 180°C in 14 days.

## S2. Model validation by Rietveld refinement



**Figure S2.1** Population of HMTA<sup>+</sup> ions at the centers of hexakaidecahedral [5<sup>12</sup>6<sup>4</sup>] cages as the results of energy minimization of 5 million Monte Carlo configurations (The corresponding 3D model in the file HMTA+population.msi).

**Table S2.1.** Refined atomic coordinates in the unit cell (cubic,  $a = 19.39662$ ).

Site Label	Atom Type	x	y	z	Multiplicity
O1	O	0.0485	0.0485	0.2952	1
Si2	Si	0.068	0.068	0.3712	1
O3	O	0.0485	0.5485	0.7952	1
Si4	Si	0.068	0.568	0.8712	1
O5	O	0.5485	0.0485	0.7952	1
Si6	Si	0.568	0.068	0.8712	1
O7	O	0.5485	0.5485	0.2952	1
Si8	Si	0.568	0.568	0.3712	1
O9	O	0.7015	0.2015	0.7952	1
Si10	Si	0.682	0.182	0.8712	1
O11	O	0.7015	0.7015	0.2952	1
Si12	Si	0.682	0.682	0.3712	1
O13	O	0.2015	0.5485	0.4548	1
Si14	Si	0.182	0.568	0.3788	1
O15	O	0.2015	0.0485	0.9548	1
Si16	Si	0.182	0.068	0.8788	1
O17	O	0.7015	0.0485	0.4548	1
Si18	Si	0.682	0.068	0.3788	1
O19	O	0.5485	0.7015	0.9548	1

Si20	Si	0.568	0.682	0.8788	1
O21	O	0.0485	0.7015	0.4548	1
Si22	Si	0.068	0.682	0.3788	1
O23	O	0.2952	0.0485	0.0485	1
Si24	Si	0.3712	0.068	0.068	1
O25	O	0.2952	0.5485	0.5485	1
Si26	Si	0.3712	0.568	0.568	1
O27	O	0.7952	0.0485	0.5485	1
Si28	Si	0.8712	0.068	0.568	1
O29	O	0.7952	0.5485	0.0485	1
Si30	Si	0.8712	0.568	0.068	1
O31	O	0.7952	0.7015	0.2015	1
Si32	Si	0.8712	0.682	0.182	1
O33	O	0.2952	0.7015	0.7015	1
Si34	Si	0.3712	0.682	0.682	1
O35	O	0.4548	0.2015	0.5485	1
Si36	Si	0.3788	0.182	0.568	1
O37	O	0.4548	0.7015	0.0485	1
Si38	Si	0.3788	0.682	0.068	1
O39	O	0.9548	0.5485	0.7015	1
Si40	Si	0.8788	0.568	0.682	1
O41	O	0.9548	0.0485	0.2015	1
Si42	Si	0.8788	0.068	0.182	1
O43	O	0.4548	0.0485	0.7015	1
Si44	Si	0.3788	0.068	0.682	1
O45	O	0.0485	0.2952	0.0485	1
Si46	Si	0.068	0.3712	0.068	1
O47	O	0.0485	0.7952	0.5485	1
Si48	Si	0.068	0.8712	0.568	1
O49	O	0.5485	0.2952	0.5485	1
Si50	Si	0.568	0.3712	0.568	1
O51	O	0.5485	0.7952	0.0485	1
Si52	Si	0.568	0.8712	0.068	1
O53	O	0.2015	0.7952	0.7015	1
Si54	Si	0.182	0.8712	0.682	1
O55	O	0.2015	0.2952	0.2015	1
Si56	Si	0.182	0.3712	0.182	1
O57	O	0.7015	0.2952	0.7015	1
Si58	Si	0.682	0.3712	0.682	1
O59	O	0.5485	0.4548	0.2015	1
Si60	Si	0.568	0.3788	0.182	1
O61	O	0.0485	0.4548	0.7015	1
Si62	Si	0.068	0.3788	0.682	1
O63	O	0.7015	0.9548	0.5485	1
Si64	Si	0.682	0.8788	0.568	1
O65	O	0.7015	0.4548	0.0485	1

Si66	Si	0.682	0.3788	0.068	1
O67	O	0.7985	0.2985	0.2048	1
Si68	Si	0.818	0.318	0.1288	1
O69	O	0.7985	0.7985	0.7048	1
Si70	Si	0.818	0.818	0.6288	1
O71	O	0.9515	0.9515	0.7048	1
Si72	Si	0.932	0.932	0.6288	1
O73	O	0.9515	0.4515	0.2048	1
Si74	Si	0.932	0.432	0.1288	1
O75	O	0.4515	0.9515	0.2048	1
Si76	Si	0.432	0.932	0.1288	1
O77	O	0.4515	0.4515	0.7048	1
Si78	Si	0.432	0.432	0.6288	1
O79	O	0.2985	0.4515	0.0452	1
Si80	Si	0.318	0.432	0.1212	1
O81	O	0.2985	0.9515	0.5452	1
Si82	Si	0.318	0.932	0.6212	1
O83	O	0.7985	0.9515	0.0452	1
Si84	Si	0.818	0.932	0.1212	1
O85	O	0.4515	0.7985	0.5452	1
Si86	Si	0.432	0.818	0.6212	1
O87	O	0.9515	0.7985	0.0452	1
Si88	Si	0.932	0.818	0.1212	1
O89	O	0.7985	0.5452	0.4515	1
Si90	Si	0.818	0.6212	0.432	1
O91	O	0.7985	0.0452	0.9515	1
Si92	Si	0.818	0.1212	0.932	1
O93	O	0.4515	0.0452	0.2985	1
Si94	Si	0.432	0.1212	0.318	1
O95	O	0.9515	0.0452	0.7985	1
Si96	Si	0.932	0.1212	0.818	1
O97	O	0.9515	0.7048	0.9515	1
Si98	Si	0.932	0.6288	0.932	1
O99	O	0.9515	0.2048	0.4515	1
Si100	Si	0.932	0.1288	0.432	1
O101	O	0.4515	0.7048	0.4515	1
Si102	Si	0.432	0.6288	0.432	1
O103	O	0.4515	0.2048	0.9515	1
Si104	Si	0.432	0.1288	0.932	1
O105	O	0.2985	0.2048	0.7985	1
Si106	Si	0.318	0.1288	0.818	1
O107	O	0.2985	0.7048	0.2985	1
Si108	Si	0.318	0.6288	0.318	1
O109	O	0.7985	0.7048	0.7985	1
Si110	Si	0.818	0.6288	0.818	1
O111	O	0.0452	0.2985	0.4515	1

Si112	Si	0.1212	0.318	0.432	1
O113	O	0.0452	0.7985	0.9515	1
Si114	Si	0.1212	0.818	0.932	1
O115	O	0.5452	0.4515	0.7985	1
Si116	Si	0.6212	0.432	0.818	1
O117	O	0.5452	0.9515	0.2985	1
Si118	Si	0.6212	0.932	0.318	1
O119	O	0.0452	0.9515	0.7985	1
Si120	Si	0.1212	0.932	0.818	1
O121	O	0.2048	0.7985	0.2985	1
Si122	Si	0.1288	0.818	0.318	1
O123	O	0.7048	0.7985	0.7985	1
Si124	Si	0.6288	0.818	0.818	1
O125	O	0.7048	0.9515	0.9515	1
Si126	Si	0.6288	0.932	0.932	1
O127	O	0.7048	0.4515	0.4515	1
Si128	Si	0.6288	0.432	0.432	1
O129	O	0.2048	0.9515	0.4515	1
Si130	Si	0.1288	0.932	0.432	1
O131	O	0.2048	0.4515	0.9515	1
Si132	Si	0.1288	0.432	0.932	1
O133	O	0.2985	0.7985	0.2048	1
Si134	Si	0.318	0.818	0.1288	1
O135	O	0.2985	0.2985	0.7048	1
Si136	Si	0.318	0.318	0.6288	1
O137	O	0.7985	0.4515	0.5452	1
Si138	Si	0.818	0.432	0.6212	1
O139	O	0.4515	0.2985	0.0452	1
Si140	Si	0.432	0.318	0.1212	1
O141	O	0.9515	0.2985	0.5452	1
Si142	Si	0.932	0.318	0.6212	1
O143	O	0.2048	0.2985	0.7985	1
Si144	Si	0.1288	0.318	0.818	1
O145	O	0.7048	0.2985	0.2985	1
Si146	Si	0.6288	0.318	0.318	1
O147	O	0.5452	0.7985	0.4515	1
Si148	Si	0.6212	0.818	0.432	1
O149	O	0.5452	0.2985	0.9515	1
Si150	Si	0.6212	0.318	0.932	1
O151	O	0.0452	0.4515	0.2985	1
Si152	Si	0.1212	0.432	0.318	1
O153	O	0.7985	0.2048	0.2985	1
Si154	Si	0.818	0.1288	0.318	1
O155	O	0.4515	0.5452	0.7985	1
Si156	Si	0.432	0.6212	0.818	1
O157	O	0.9515	0.5452	0.2985	1

Si158	Si	0.932	0.6212	0.318	1
O159	O	0.2985	0.0452	0.4515	1
Si160	Si	0.318	0.1212	0.432	1
O161	O	0.2985	0.5452	0.9515	1
Si162	Si	0.318	0.6212	0.932	1
O163	O	0.2015	0.7015	0.7952	1
Si164	Si	0.182	0.682	0.8712	1
O165	O	0.2015	0.2015	0.2952	1
Si166	Si	0.182	0.182	0.3712	1
O167	O	0.7015	0.5485	0.9548	1
Si168	Si	0.682	0.568	0.8788	1
O169	O	0.5485	0.2015	0.4548	1
Si170	Si	0.568	0.182	0.3788	1
O171	O	0.0485	0.2015	0.9548	1
Si172	Si	0.068	0.182	0.8788	1
O173	O	0.2015	0.4548	0.5485	1
Si174	Si	0.182	0.3788	0.568	1
O175	O	0.2015	0.9548	0.0485	1
Si176	Si	0.182	0.8788	0.068	1
O177	O	0.5485	0.9548	0.7015	1
Si178	Si	0.568	0.8788	0.682	1
O179	O	0.0485	0.9548	0.2015	1
Si180	Si	0.068	0.8788	0.182	1
O181	O	0.7015	0.7952	0.2015	1
Si182	Si	0.682	0.8712	0.182	1
O183	O	0.9548	0.7015	0.5485	1
Si184	Si	0.8788	0.682	0.568	1
O185	O	0.9548	0.2015	0.0485	1
Si186	Si	0.8788	0.182	0.068	1
O187	O	0.4548	0.5485	0.2015	1
Si188	Si	0.3788	0.568	0.182	1
O189	O	0.7952	0.2015	0.7015	1
Si190	Si	0.8712	0.182	0.682	1
O191	O	0.2952	0.2015	0.2015	1
Si192	Si	0.3712	0.182	0.182	1
O193	O	0.0931	0	0.4069	1
O194	O	0.0931	0.5	0.9069	1
O195	O	0.6569	0.25	0.9069	1
O196	O	0.6569	0.75	0.4069	1
O197	O	0.1569	0.75	0.9069	1
O198	O	0.1569	0.5	0.3431	1
O199	O	0.1569	0	0.8431	1
O200	O	0.6569	0.5	0.8431	1
O201	O	0.5931	0.75	0.8431	1
O202	O	0.5931	0.25	0.3431	1
O203	O	0.4069	0.0931	0	1

O204	O	0.4069	0.5931	0.5	1
O205	O	0.9069	0.6569	0.25	1
O206	O	0.9069	0.1569	0.75	1
O207	O	0.3431	0.1569	0.5	1
O208	O	0.3431	0.6569	0	1
O209	O	0.8431	0.6569	0.5	1
O210	O	0.8431	0.5931	0.75	1
O211	O	0.8431	0.0931	0.25	1
O212	O	0.3431	0.5931	0.25	1
O213	O	0	0.4069	0.0931	1
O214	O	0.5	0.4069	0.5931	1
O215	O	0.25	0.9069	0.6569	1
O216	O	0.75	0.9069	0.1569	1
O217	O	0.5	0.3431	0.1569	1
O218	O	0.5	0.8431	0.6569	1
O219	O	0	0.3431	0.6569	1
O220	O	0.75	0.8431	0.5931	1
O221	O	0.25	0.8431	0.0931	1
O222	O	0.25	0.3431	0.5931	1
O223	O	0.75	0.3431	0.0931	1
O224	O	0	0.9069	0.5931	1
O225	O	0.5	0.9069	0.0931	1
O226	O	0.25	0.4069	0.1569	1
O227	O	0.75	0.4069	0.6569	1
O228	O	0	0.8431	0.1569	1
O229	O	0.8431	0.1569	0	1
O230	O	0.4069	0.1569	0.25	1
O231	O	0.4069	0.6569	0.75	1
O232	O	0.9069	0.5931	0	1
O233	O	0.9069	0.0931	0.5	1
O234	O	0.3431	0.0931	0.75	1
O235	O	0.1569	0.25	0.4069	1
O236	O	0.6569	0	0.3431	1
O237	O	0.0931	0.75	0.3431	1
O238	O	0.0931	0.25	0.8431	1
O239	O	0.5931	0	0.9069	1
O240	O	0.5931	0.5	0.4069	1
O241	O	0.9069	0	0.5931	1
O242	O	0.9069	0.5	0.0931	1
O243	O	0.4069	0	0.0931	1
O244	O	0.3431	0.75	0.0931	1
O245	O	0.3431	0.25	0.5931	1
O246	O	0.8431	0.5	0.6569	1
O247	O	0.8431	0	0.1569	1
O248	O	0.4069	0.25	0.1569	1
O249	O	0.4069	0.75	0.6569	1

O250	O	0.9069	0.75	0.1569	1
O251	O	0.5931	0.9069	0	1
O252	O	0.5931	0.4069	0.5	1
O253	O	0.0931	0.4069	0	1
O254	O	0.0931	0.3431	0.75	1
O255	O	0.0931	0.8431	0.25	1
O256	O	0.5931	0.3431	0.25	1
O257	O	0.6569	0.8431	0.5	1
O258	O	0.6569	0.3431	0	1
O259	O	0.1569	0.4069	0.25	1
O260	O	0.1569	0.9069	0.75	1
O261	O	0	0.5931	0.9069	1
O262	O	0	0.0931	0.4069	1
O263	O	0.5	0.5931	0.4069	1
O264	O	0.75	0.0931	0.3431	1
O265	O	0.25	0.0931	0.8431	1
O266	O	0.25	0.5931	0.3431	1
O267	O	0.5	0.6569	0.8431	1
O268	O	0	0.6569	0.3431	1
O269	O	0.25	0.1569	0.4069	1
O270	O	0.75	0.1569	0.9069	1
O271	O	0.25	0.6569	0.9069	1
O272	O	0.75	0.6569	0.4069	1
O273	O	0.5	0.0931	0.9069	1
O274	O	0.75	0.5931	0.8431	1
O275	O	0.5	0.1569	0.3431	1
O276	O	0	0.1569	0.8431	1
O277	O	0.1569	0.3431	0.5	1
O278	O	0.1569	0.8431	0	1
O279	O	0.5931	0.8431	0.75	1
O280	O	0.0931	0.9069	0.5	1
O281	O	0.6569	0.9069	0.25	1
O282	O	0.6569	0.4069	0.75	1
O283	O	0.8431	0.75	0.5931	1
O284	O	0.8431	0.25	0.0931	1
O285	O	0.3431	0.5	0.1569	1
O286	O	0.3431	0	0.6569	1
O287	O	0.9069	0.25	0.6569	1
O288	O	0.4069	0.5	0.5931	1
O289	O	0.125	0.125	0.3721	1
O290	O	0.125	0.625	0.8721	1
O291	O	0.625	0.125	0.8721	1
O292	O	0.625	0.625	0.3721	1
O293	O	0.125	0.625	0.3779	1
O294	O	0.125	0.125	0.8779	1
O295	O	0.625	0.625	0.8779	1

O296	O	0.3721	0.125	0.125	1
O297	O	0.3721	0.625	0.625	1
O298	O	0.8721	0.125	0.625	1
O299	O	0.8721	0.625	0.125	1
O300	O	0.3779	0.125	0.625	1
O301	O	0.8779	0.625	0.625	1
O302	O	0.8779	0.125	0.125	1
O303	O	0.125	0.3721	0.125	1
O304	O	0.125	0.8721	0.625	1
O305	O	0.625	0.8721	0.125	1
O306	O	0.625	0.3721	0.625	1
O307	O	0.625	0.3779	0.125	1
O308	O	0.625	0.8779	0.625	1
O309	O	0.875	0.375	0.1279	1
O310	O	0.875	0.875	0.6279	1
O311	O	0.375	0.375	0.1221	1
O312	O	0.875	0.875	0.1221	1
O313	O	0.375	0.875	0.6221	1
O314	O	0.875	0.6221	0.375	1
O315	O	0.875	0.1221	0.875	1
O316	O	0.375	0.1221	0.375	1
O317	O	0.875	0.6279	0.875	1
O318	O	0.375	0.1279	0.875	1
O319	O	0.375	0.6279	0.375	1
O320	O	0.1221	0.375	0.375	1
O321	O	0.1221	0.875	0.875	1
O322	O	0.6221	0.375	0.875	1
O323	O	0.1279	0.875	0.375	1
O324	O	0.6279	0.875	0.875	1
O325	O	0.6279	0.375	0.375	1
O326	O	0.375	0.875	0.1279	1
O327	O	0.375	0.375	0.6279	1
O328	O	0.875	0.375	0.6221	1
O329	O	0.1279	0.375	0.875	1
O330	O	0.6221	0.875	0.375	1
O331	O	0.875	0.1279	0.375	1
O332	O	0.375	0.6221	0.875	1
O333	O	0.625	0.125	0.3779	1
O334	O	0.125	0.3779	0.625	1
O335	O	0.125	0.8779	0.125	1
O336	O	0.3779	0.625	0.125	1
O337	O	0.1716	0.1716	0.1716	1
Si338	Si	0.2181	0.2181	0.2181	1
O339	O	0.1716	0.6716	0.6716	1
Si340	Si	0.2181	0.7181	0.7181	1
O341	O	0.6716	0.1716	0.6716	1

Si342	Si	0.7181	0.2181	0.7181	1
O343	O	0.6716	0.6716	0.1716	1
Si344	Si	0.7181	0.7181	0.2181	1
O345	O	0.5784	0.0784	0.6716	1
Si346	Si	0.5319	0.0319	0.7181	1
O347	O	0.5784	0.5784	0.1716	1
Si348	Si	0.5319	0.5319	0.2181	1
O349	O	0.0784	0.6716	0.5784	1
Si350	Si	0.0319	0.7181	0.5319	1
O351	O	0.0784	0.1716	0.0784	1
Si352	Si	0.0319	0.2181	0.0319	1
O353	O	0.5784	0.1716	0.5784	1
Si354	Si	0.5319	0.2181	0.5319	1
O355	O	0.6716	0.5784	0.0784	1
Si356	Si	0.7181	0.5319	0.0319	1
O357	O	0.1716	0.5784	0.5784	1
Si358	Si	0.2181	0.5319	0.5319	1
O359	O	0.9216	0.4216	0.3284	1
Si360	Si	0.9681	0.4681	0.2819	1
O361	O	0.9216	0.9216	0.8284	1
Si362	Si	0.9681	0.9681	0.7819	1
O363	O	0.8284	0.8284	0.8284	1
Si364	Si	0.7819	0.7819	0.7819	1
O365	O	0.8284	0.3284	0.3284	1
Si366	Si	0.7819	0.2819	0.2819	1
O367	O	0.3284	0.8284	0.3284	1
Si368	Si	0.2819	0.7819	0.2819	1
O369	O	0.3284	0.3284	0.8284	1
Si370	Si	0.2819	0.2819	0.7819	1
O371	O	0.4216	0.3284	0.9216	1
Si372	Si	0.4681	0.2819	0.9681	1
O373	O	0.4216	0.8284	0.4216	1
Si374	Si	0.4681	0.7819	0.4681	1
O375	O	0.9216	0.8284	0.9216	1
Si376	Si	0.9681	0.7819	0.9681	1
O377	O	0.3284	0.9216	0.4216	1
Si378	Si	0.2819	0.9681	0.4681	1
O379	O	0.8284	0.9216	0.9216	1
Si380	Si	0.7819	0.9681	0.9681	1
O381	O	0.4216	0.9216	0.3284	1
Si382	Si	0.4681	0.9681	0.2819	1
O383	O	0.4216	0.4216	0.8284	1
Si384	Si	0.4681	0.4681	0.7819	1
O385	O	0.9216	0.3284	0.4216	1
Si386	Si	0.9681	0.2819	0.4681	1
O387	O	0.3284	0.4216	0.9216	1

Si388	Si	0.2819	0.4681	0.9681	1
O389	O	0.8284	0.4216	0.4216	1
Si390	Si	0.7819	0.4681	0.4681	1
O391	O	0.0784	0.5784	0.6716	1
Si392	Si	0.0319	0.5319	0.7181	1
O393	O	0.0784	0.0784	0.1716	1
Si394	Si	0.0319	0.0319	0.2181	1
O395	O	0.5784	0.6716	0.0784	1
Si396	Si	0.5319	0.7181	0.0319	1
O397	O	0.6716	0.0784	0.5784	1
Si398	Si	0.7181	0.0319	0.5319	1
O399	O	0.1716	0.0784	0.0784	1
Si400	Si	0.2181	0.0319	0.0319	1
Si401	Si	0.125	0.125	0.125	1
Si402	Si	0.125	0.625	0.625	1
Si403	Si	0.625	0.125	0.625	1
Si404	Si	0.625	0.625	0.125	1
Si405	Si	0.875	0.375	0.375	1
Si406	Si	0.875	0.875	0.875	1
Si407	Si	0.375	0.375	0.875	1
Si408	Si	0.375	0.875	0.375	1
C409	C	0.71195	0.12587	0.12721	1
N410	N	0.66852	0.16799	0.08373	1
C411	C	0.6264	0.12489	0.0394	1
N412	N	0.58238	0.08177	0.08182	1
C413	C	0.62333	0.03734	0.12538	1
N414	N	0.66639	0.08195	0.1704	1
C415	C	0.62118	0.1263	0.21353	1
C416	C	0.62423	0.21154	0.12545	1
N417	N	0.58023	0.16815	0.16755	1
C418	C	0.53781	0.12501	0.12357	1
H419	H	0.74413	0.15759	0.16166	1
H420	H	0.74556	0.09191	0.09647	1
H421	H	0.65922	0.09283	0.00565	1
H422	H	0.59459	0.15739	0.00504	1
H423	H	0.65789	0.00421	0.0948	1
H424	H	0.59074	0.00464	0.1585	1
H425	H	0.65417	0.15819	0.24704	1
H426	H	0.58871	0.09271	0.24586	1
H427	H	0.59244	0.245	0.092	1
H428	H	0.65536	0.24617	0.15823	1
H429	H	0.50264	0.09306	0.15495	1
H430	H	0.50495	0.15746	0.09018	1
H431	H	0.69546	0.05214	0.20122	1
C432	C	0.31249	0.40245	0.43076	1
N433	N	0.3583	0.44467	0.39004	1

C434	C	0.42972	0.42978	0.40652	1
N435	N	0.44393	0.358	0.39092	1
C436	C	0.40062	0.31316	0.43162	1
N437	N	0.32762	0.32907	0.41432	1
C438	C	0.31552	0.31639	0.33966	1
C439	C	0.34681	0.43292	0.31703	1
N440	N	0.36124	0.36114	0.30163	1
C441	C	0.43268	0.34599	0.3179	1
H442	H	0.258	0.41281	0.41852	1
H443	H	0.3207	0.41043	0.48639	1
H444	H	0.44071	0.44124	0.4612	1
H445	H	0.46399	0.46337	0.37594	1
H446	H	0.40816	0.32176	0.48725	1
H447	H	0.41038	0.25842	0.41999	1
H448	H	0.26099	0.32743	0.32821	1
H449	H	0.32597	0.26162	0.32886	1
H450	H	0.3811	0.46647	0.28645	1
H451	H	0.29353	0.44663	0.30227	1
H452	H	0.44585	0.29241	0.30374	1
H453	H	0.46693	0.37955	0.28731	1
H454	H	0.29637	0.29845	0.442	1
C455	C	0.06597	0.09442	0.68672	1
N456	N	0.1089	0.05428	0.64098	1
C457	C	0.09374	0.07031	0.5695	1
N458	N	0.10802	0.14272	0.5573	1
C459	C	0.0649	0.18545	0.60047	1
N460	N	0.0809	0.16846	0.67352	1
C461	C	0.15488	0.18269	0.68786	1
C462	C	0.18127	0.06753	0.65472	1
N463	N	0.19534	0.13998	0.64218	1
C464	C	0.18035	0.15618	0.57072	1
H465	H	0.07725	0.08324	0.74126	1
H466	H	0.01077	0.08526	0.67701	1
H467	H	0.0396	0.05789	0.55694	1
H468	H	0.1259	0.0382	0.53524	1
H469	H	0.00974	0.17544	0.59133	1
H470	H	0.07521	0.24068	0.59216	1
H471	H	0.16526	0.17077	0.74242	1
H472	H	0.16456	0.23793	0.67887	1
H473	H	0.21359	0.03538	0.62067	1
H474	H	0.19487	0.05305	0.70812	1
H475	H	0.19338	0.21037	0.55908	1
H476	H	0.21264	0.1242	0.53647	1
H477	H	0.05157	0.19762	0.70472	1
C478	C	0.56354	0.59919	0.68515	1
N479	N	0.5803	0.67024	0.67008	1

C480	C	0.65256	0.68362	0.68423	1
N481	N	0.6945	0.64003	0.64026	1
C482	C	0.68117	0.56806	0.65434	1
N483	N	0.60694	0.55496	0.6401	1
C484	C	0.59201	0.5703	0.56644	1
C485	C	0.56536	0.68573	0.59838	1
N486	N	0.60779	0.64218	0.55487	1
C487	C	0.68013	0.65533	0.56846	1
H488	H	0.50899	0.58766	0.67427	1
H489	H	0.57473	0.58596	0.73925	1
H490	H	0.66442	0.67393	0.73908	1
H491	H	0.66463	0.73846	0.67458	1
H492	H	0.69198	0.55459	0.70847	1
H493	H	0.71182	0.53432	0.62057	1
H494	H	0.53742	0.5585	0.55605	1
H495	H	0.62449	0.53656	0.53445	1
H496	H	0.57602	0.74061	0.58739	1
H497	H	0.51017	0.67745	0.58707	1
H498	H	0.71269	0.62336	0.53453	1
H499	H	0.693	0.70957	0.55668	1
H500	H	0.59622	0.50523	0.64968	1
C501	C	0.84384	0.31932	0.93352	1
N502	N	0.85865	0.30587	0.86171	1
C503	C	0.81504	0.34776	0.81769	1
N504	N	0.82918	0.42002	0.83114	1
C505	C	0.81348	0.43682	0.90205	1
N506	N	0.85816	0.3935	0.94668	1
C507	C	0.93196	0.40838	0.93199	1
C508	C	0.93058	0.32017	0.84708	1
N509	N	0.94419	0.39252	0.86019	1
C510	C	0.90102	0.4349	0.81622	1
H511	H	0.87721	0.28865	0.96761	1
H512	H	0.78954	0.30865	0.94646	1
H513	H	0.76011	0.33594	0.82696	1
H514	H	0.8251	0.33562	0.76294	1
H515	H	0.75928	0.42559	0.91482	1
H516	H	0.82427	0.49138	0.91361	1
H517	H	0.9636	0.3759	0.96605	1
H518	H	0.94228	0.46297	0.94386	1
H519	H	0.94277	0.3072	0.79296	1
H520	H	0.96418	0.2876	0.87939	1
H521	H	0.91228	0.4901	0.82447	1
H522	H	0.9124	0.42416	0.76143	1
H523	H	0.84812	0.40431	0.99633	1
C524	C	0.09772	0.68119	0.18268	1
N525	N	0.11009	0.60872	0.19476	1

C526	C	0.06532	0.56675	0.15206	1
N527	N	0.07978	0.58109	0.08003	1
C528	C	0.06643	0.65277	0.06453	1
N529	N	0.11236	0.69525	0.10873	1
C530	C	0.18568	0.67853	0.09371	1
C531	C	0.18159	0.59199	0.18031	1
N532	N	0.19557	0.60615	0.1082	1
C533	C	0.15118	0.56423	0.06504	1
H534	H	0.13223	0.71358	0.21396	1
H535	H	0.04388	0.69572	0.19365	1
H536	H	0.01067	0.57728	0.1641	1
H537	H	0.07393	0.51154	0.16323	1
H538	H	0.01262	0.667	0.07586	1
H539	H	0.07765	0.66496	0.01019	1
H540	H	0.21833	0.71091	0.12692	1
H541	H	0.19648	0.69111	0.03937	1
H542	H	0.19213	0.53729	0.1923	1
H543	H	0.21615	0.62259	0.21349	1
H544	H	0.16284	0.57305	0.01001	1
H545	H	0.16096	0.50898	0.07496	1
H546	H	0.10398	0.74537	0.09884	1
C547	C	0.93693	0.81184	0.39953	1
N548	N	0.92023	0.83005	0.32918	1
C549	C	0.84816	0.81559	0.31503	1
N550	N	0.80573	0.8573	0.36034	1
C551	C	0.81896	0.83998	0.43161	1
N552	N	0.89298	0.85442	0.44558	1
C553	C	0.90729	0.9288	0.43359	1
C554	C	0.93441	0.9025	0.3169	1
N555	N	0.89151	0.94367	0.36228	1
C556	C	0.81936	0.92983	0.34834	1
H557	H	0.99132	0.82275	0.41175	1
H558	H	0.92618	0.75712	0.41026	1
H559	H	0.8369	0.76028	0.32254	1
H560	H	0.83604	0.82727	0.26061	1
H561	H	0.8087	0.78518	0.4425	1
H562	H	0.78785	0.87179	0.46677	1
H563	H	0.96179	0.93909	0.44591	1
H564	H	0.87452	0.95893	0.46874	1
H565	H	0.92368	0.91568	0.26252	1
H566	H	0.9895	0.91398	0.32567	1
H567	H	0.78626	0.96193	0.38165	1
H568	H	0.8065	0.94379	0.29461	1
H569	H	0.90371	0.84259	0.49485	1
C570	C	0.43112	0.81958	0.84142	1
N571	N	0.35979	0.8054	0.85763	1

C572	C	0.34663	0.81839	0.9301	1
N573	N	0.3596	0.89062	0.94461	1
C574	C	0.43092	0.90729	0.93089	1
N575	N	0.44411	0.89364	0.85657	1
C576	C	0.39814	0.93729	0.81357	1
C577	C	0.3145	0.84764	0.8157	1
N578	N	0.32781	0.91973	0.83077	1
C579	C	0.31439	0.93335	0.90311	1
H580	H	0.44287	0.80985	0.7867	1
H581	H	0.46619	0.7886	0.87348	1
H582	H	0.37986	0.78545	0.96243	1
H583	H	0.29286	0.80483	0.94326	1
H584	H	0.46602	0.87472	0.9613	1
H585	H	0.44251	0.96185	0.94172	1
H586	H	0.40969	0.92691	0.75894	1
H587	H	0.40962	0.99176	0.82484	1
H588	H	0.26007	0.83494	0.82673	1
H589	H	0.32269	0.83683	0.76039	1
H590	H	0.32255	0.98844	0.91501	1
H591	H	0.25994	0.92207	0.91548	1
H592	H	0.4934	0.90498	0.84553	1