Supplementary materials

Investigation of Corrosion Inhibition Potential of Triazolopyrimidinones via Density Functional Theory and Monte-Carlo Simulations

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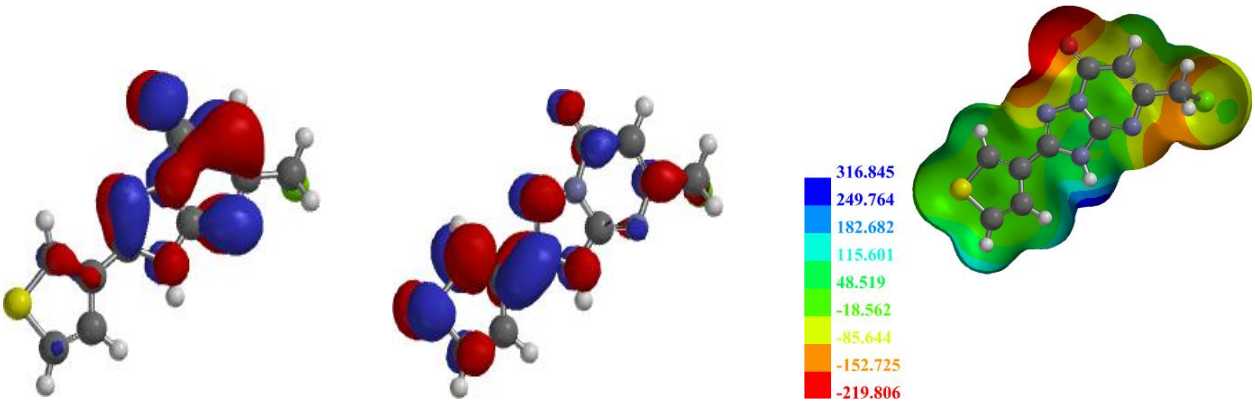
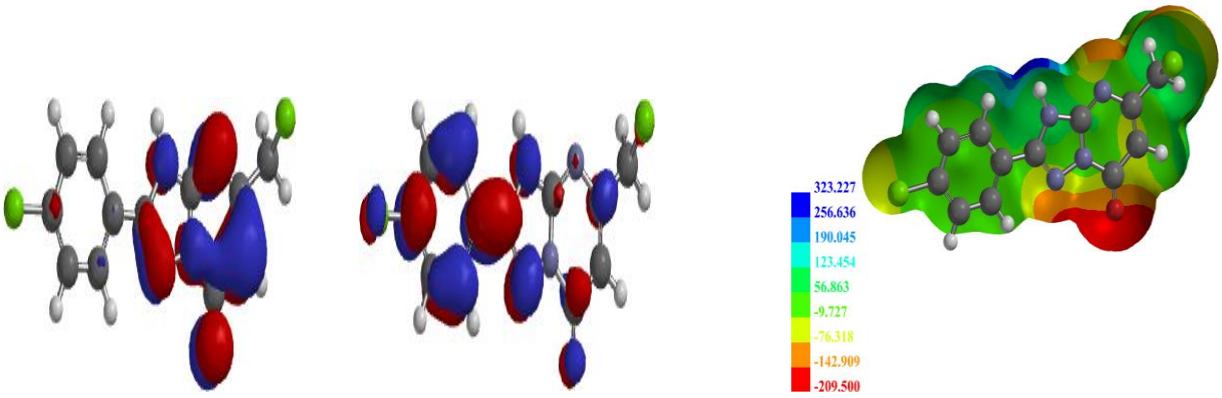


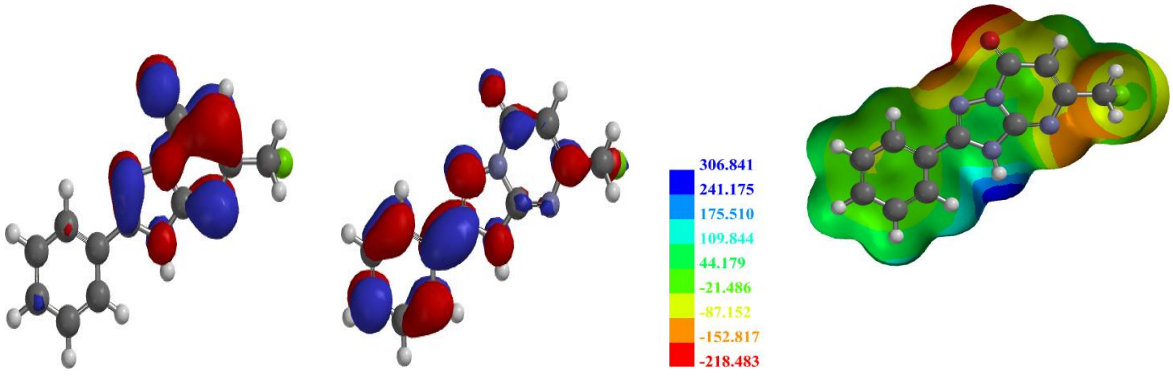
(a) (b) (c)

Fig. S1: (a) HOMO map (b) LUMO map (c) ESP of A2



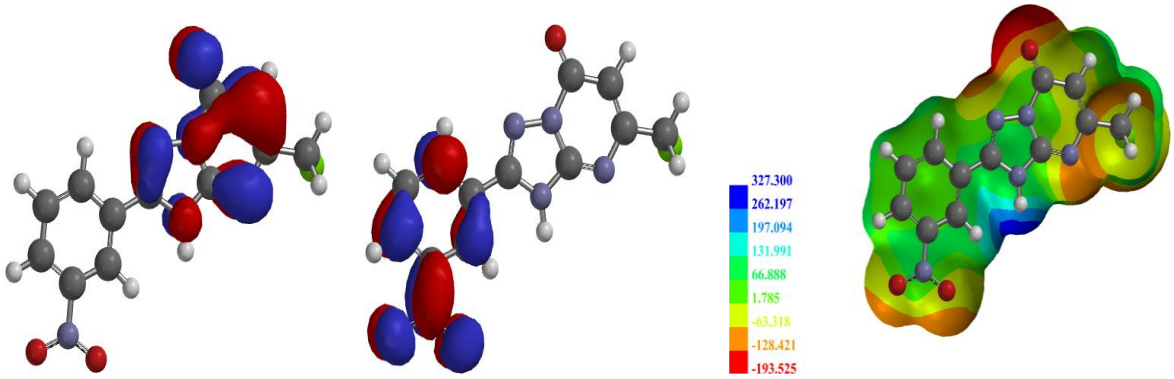
(a) (b) (c)

Fig. S2: (a) HOMO map (b) LUMO map (c) ESP of A3



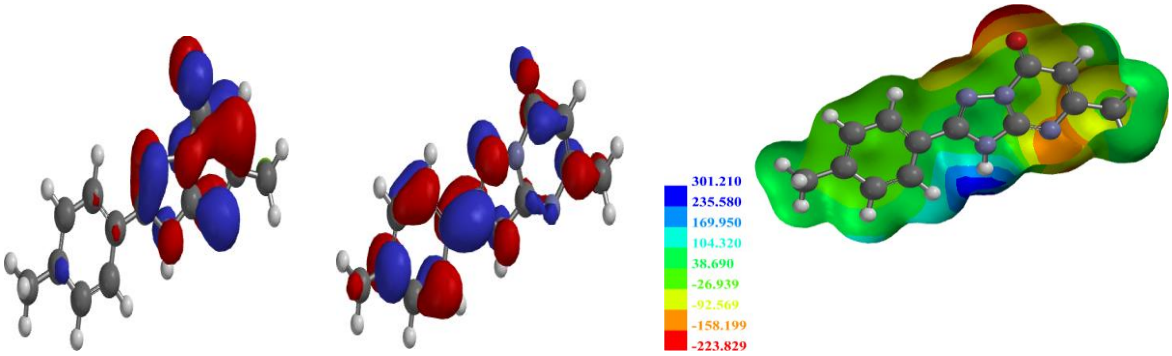
(a) (b) (c)

Fig. S3: (a) HOMO map (b) LUMO map (c) ESP of A4



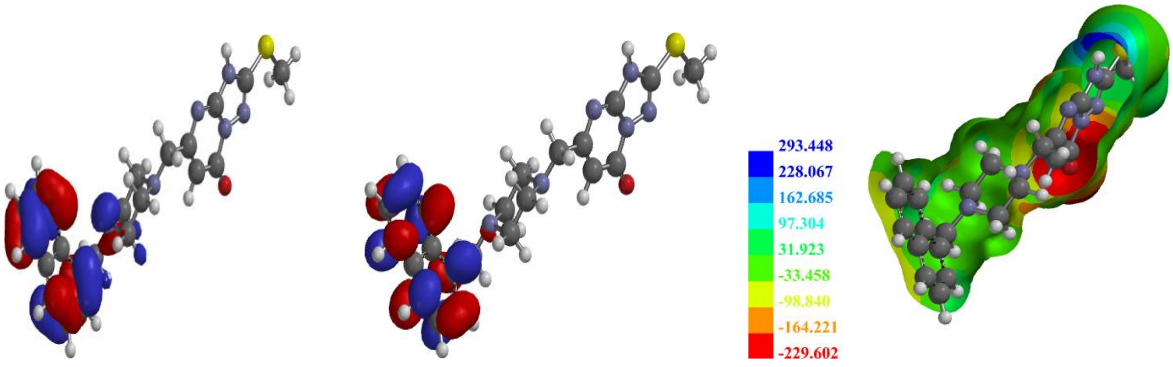
(a) (b) (c)

Fig. S4: (a) HOMO map (b) LUMO map (c) ESP of A5



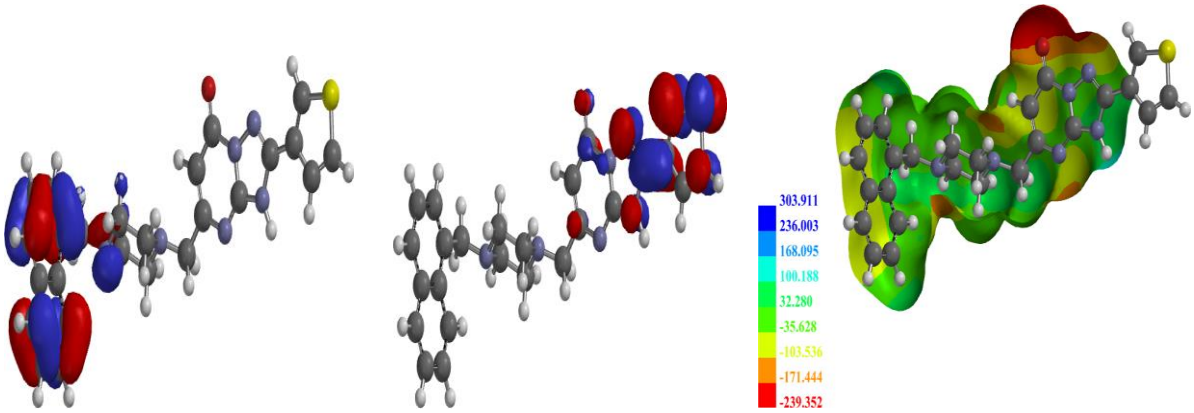
(a) (b) (c)

Fig. S5: (a) HOMO map (b) LUMO map (c) ESP of A6



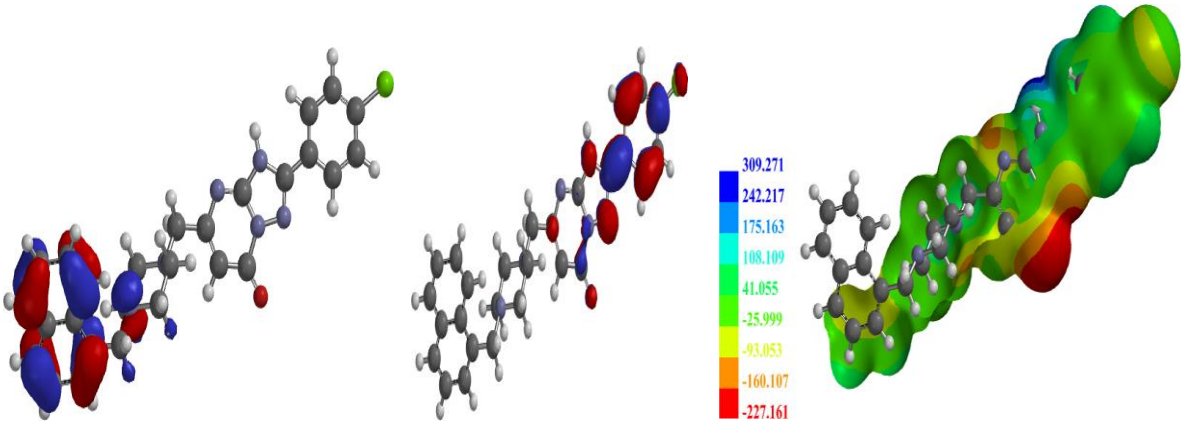
(a) (b) (c)

Fig. S6: (a) HOMO map (b) LUMO map (c) ESP of B1



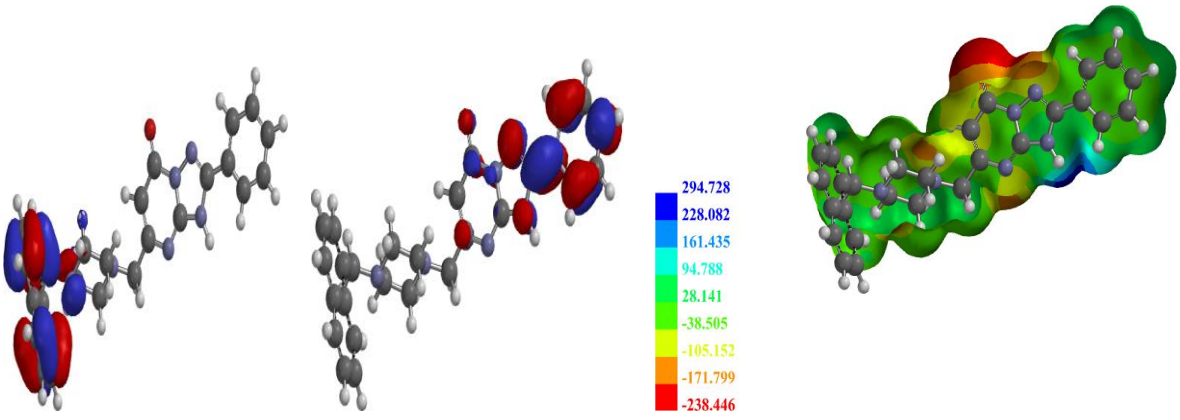
(a) (b) (c)

Fig. S7: (a) HOMO map (b) LUMO map (c) ESP of B2



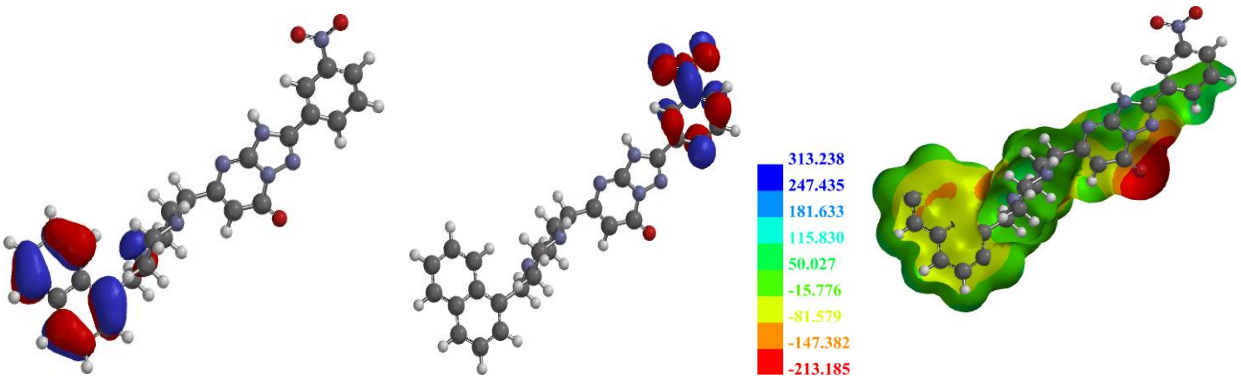
(a) (b) (c)

Fig. S8: (a) HOMO map (b) LUMO map (c) ESP of B3



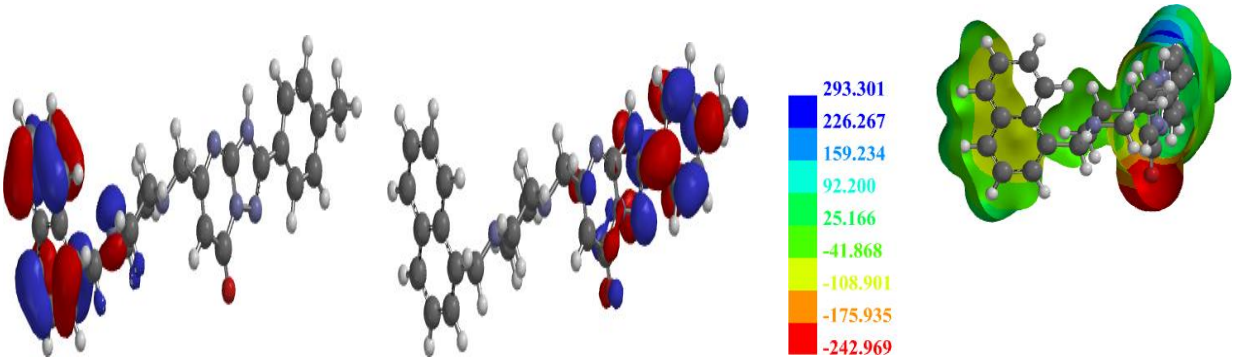
(a) (b) (c)

Fig. S9: (a) HOMO map (b) LUMO map (c) ESP of B4



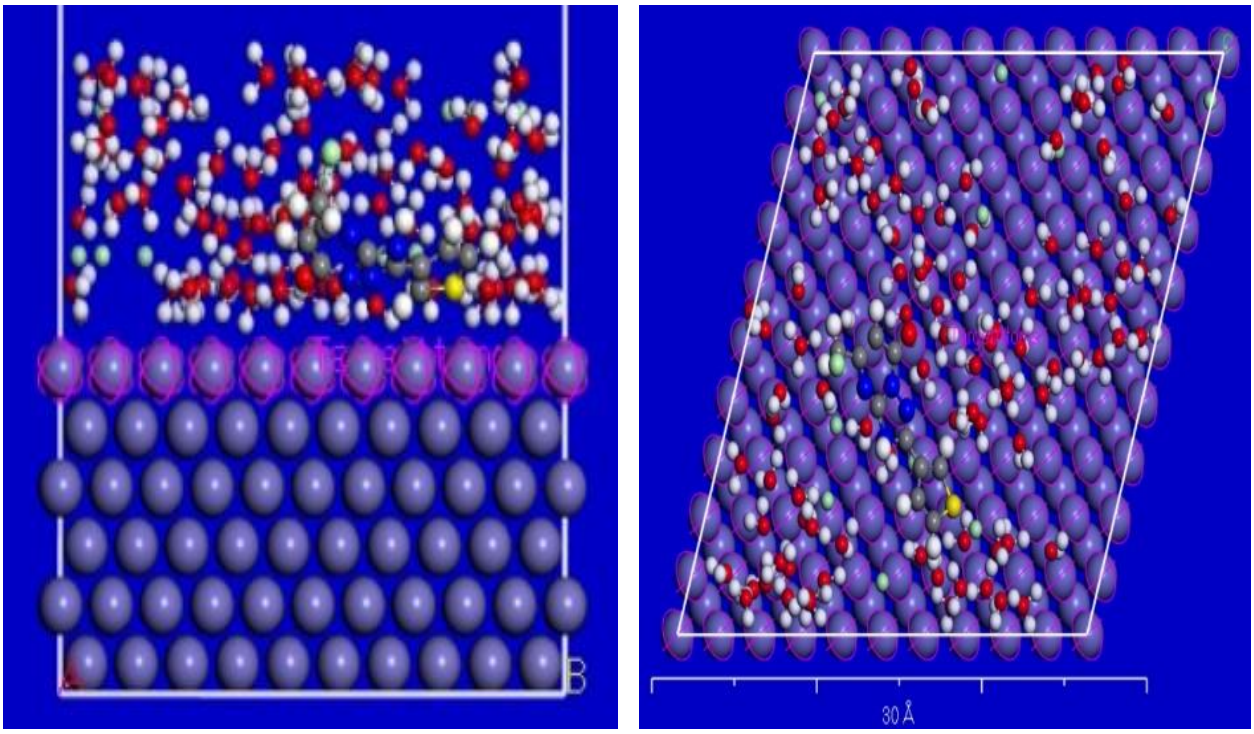
(a) (b) (c)

Fig. S10: (a) HOMO map (b) LUMO map (c) ESP of B5



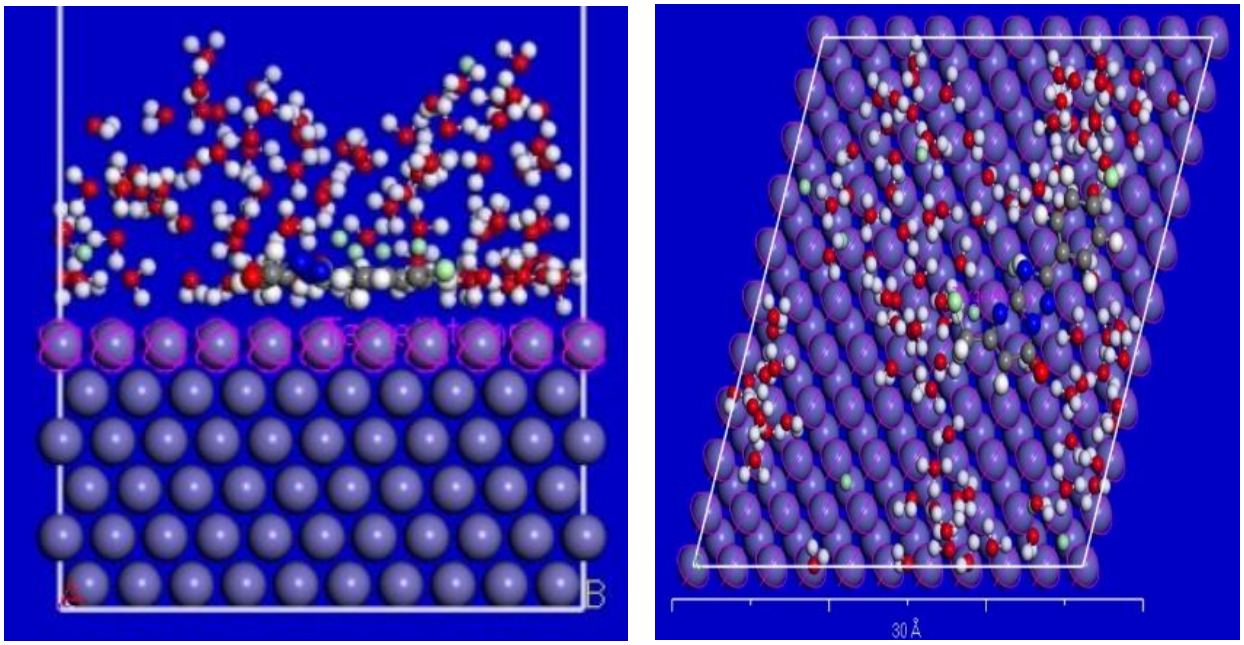
(a) (b) (c)

Fig. S11: (a) HOMO map (b) LUMO map (c) ESP of B6



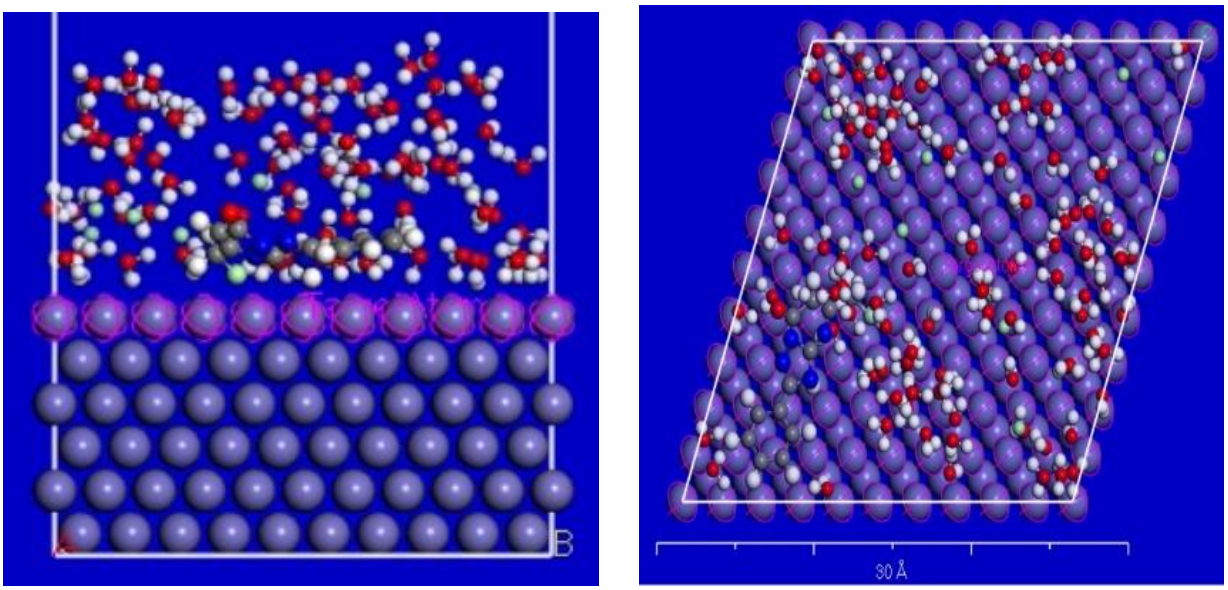
(a) (b)

Fig. S12: (a) Side view (b) Top view of adsorption of A2 on Fe(110).



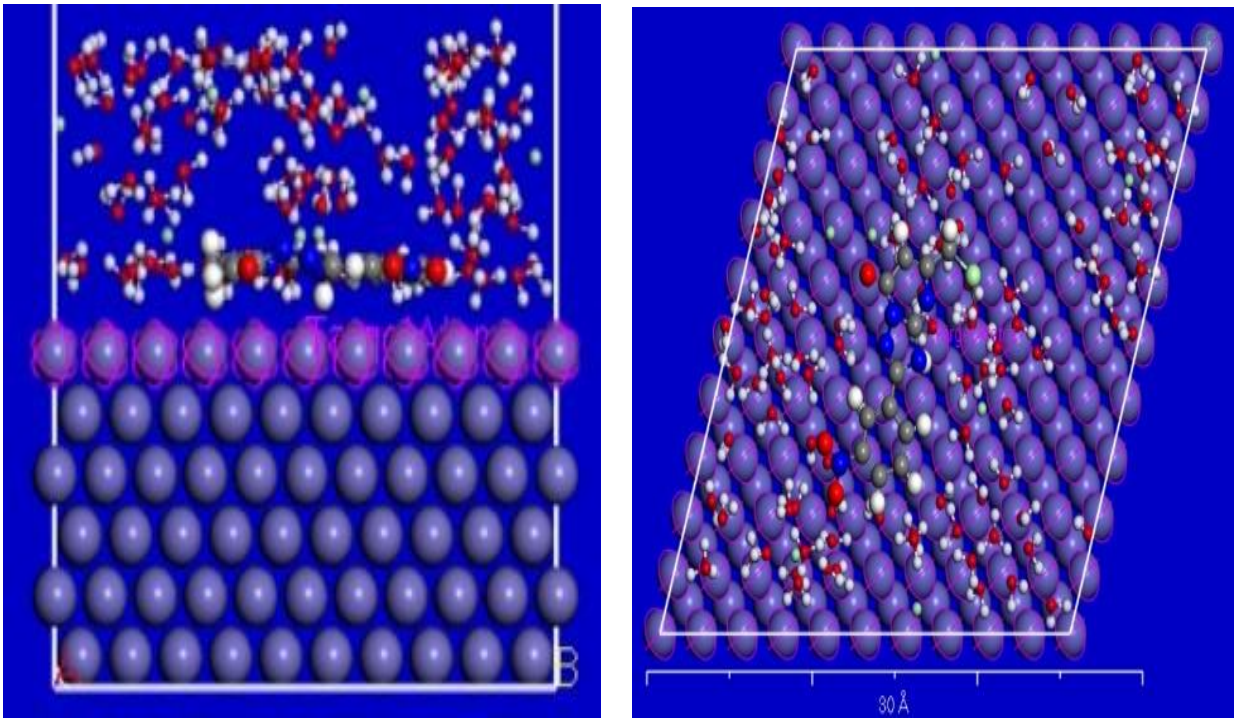
(a) (b)

Fig. S13: (a) Side view (b) Top view of adsorption of A3 on Fe(110).



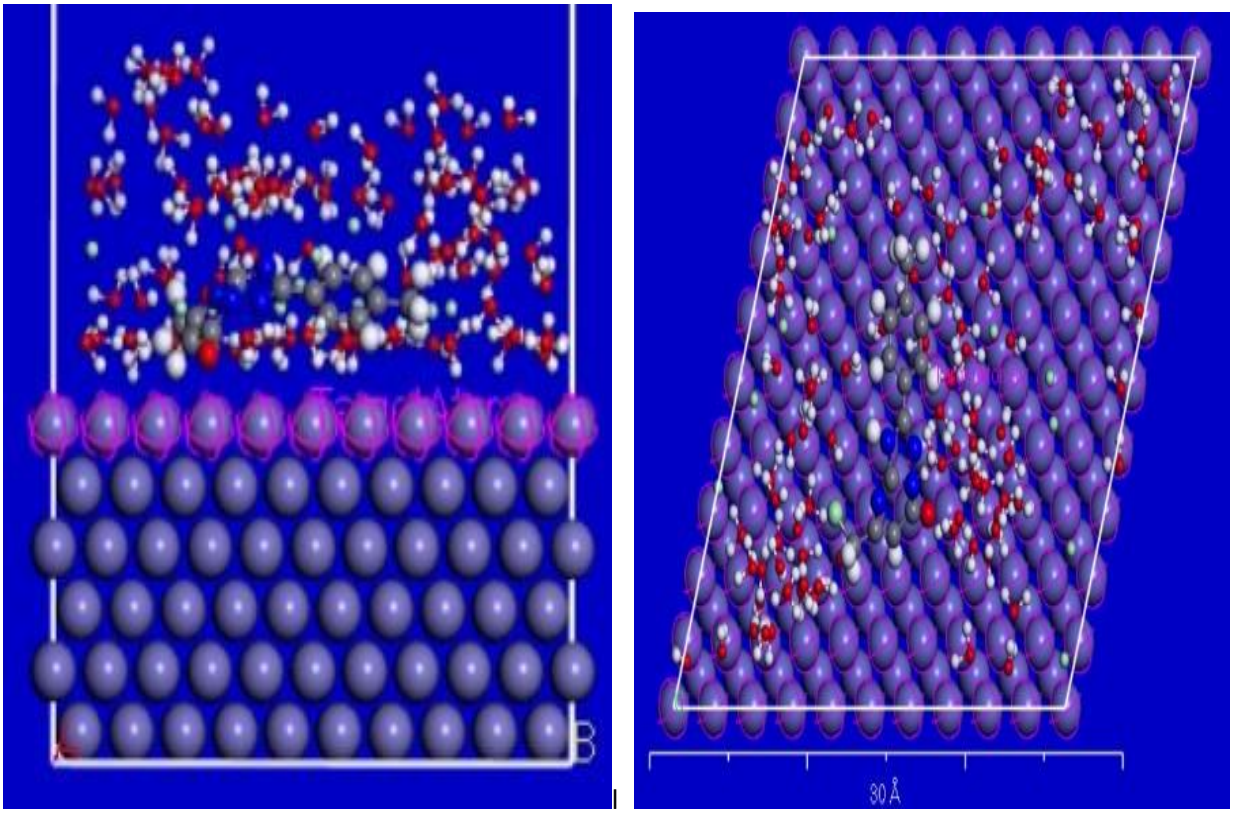
(a) (b)

Fig. S14: (a) Side view (b) Top view of adsorption of A4 on Fe(110).



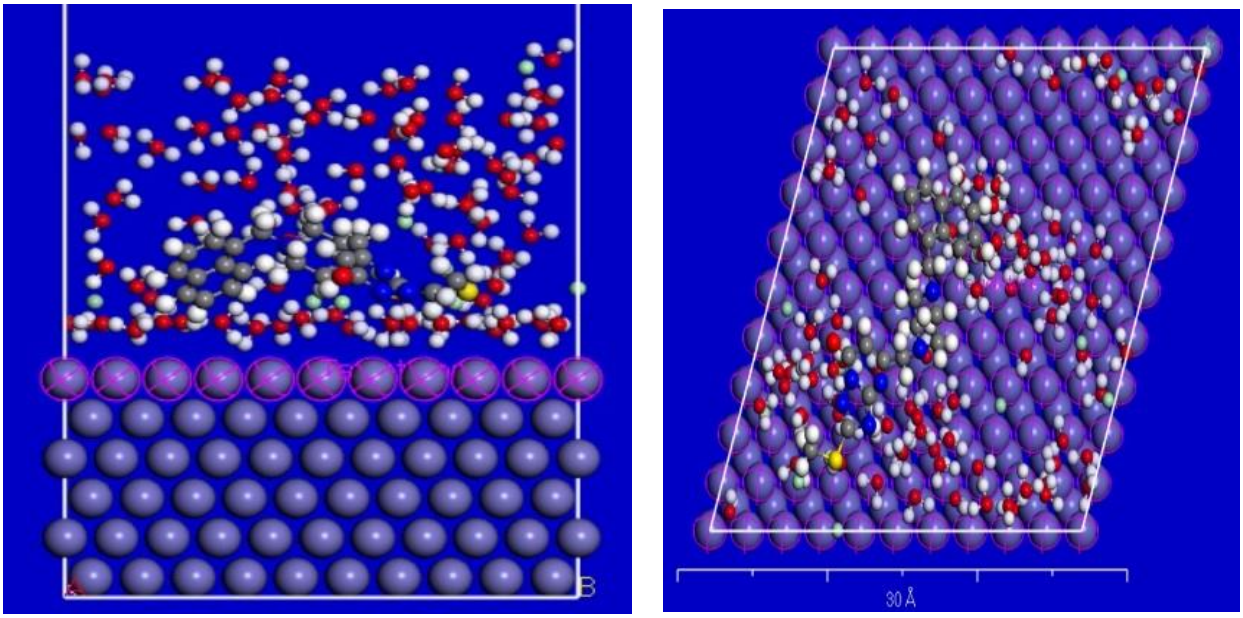
(a) (b)

Fig. S15: (a) Side view (b) Top view of adsorption of A5 on Fe(110).



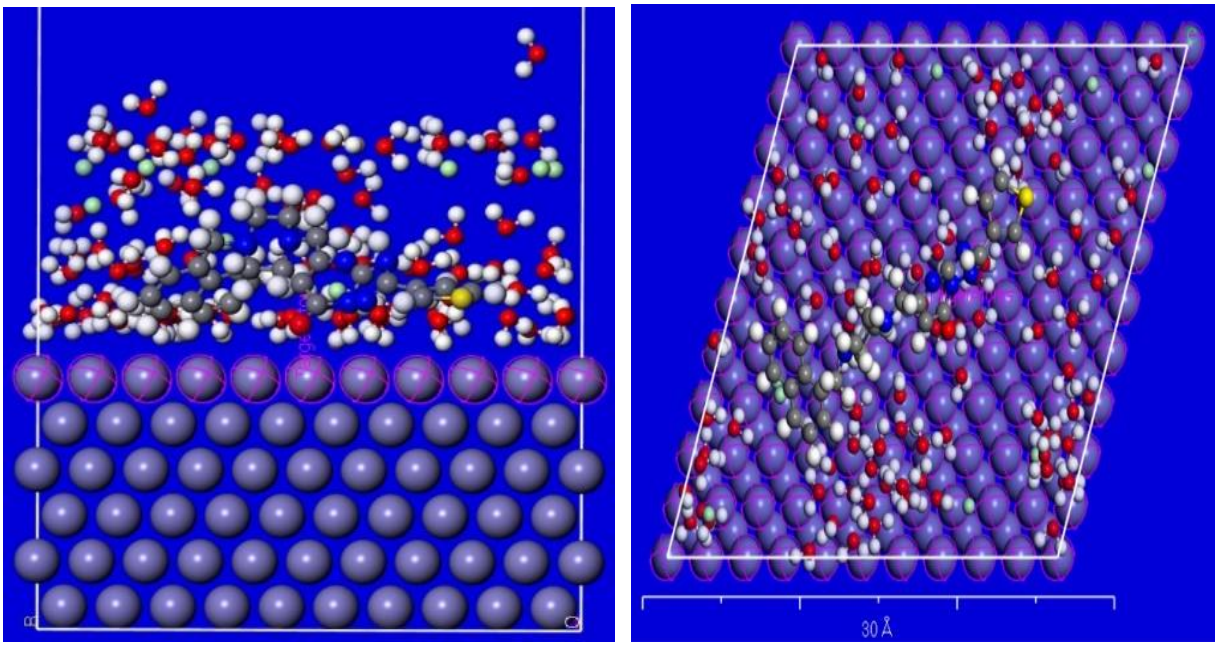
(a) (b)

Fig. S16: (a) Side view (b) Top view of adsorption of A6 on Fe(110).



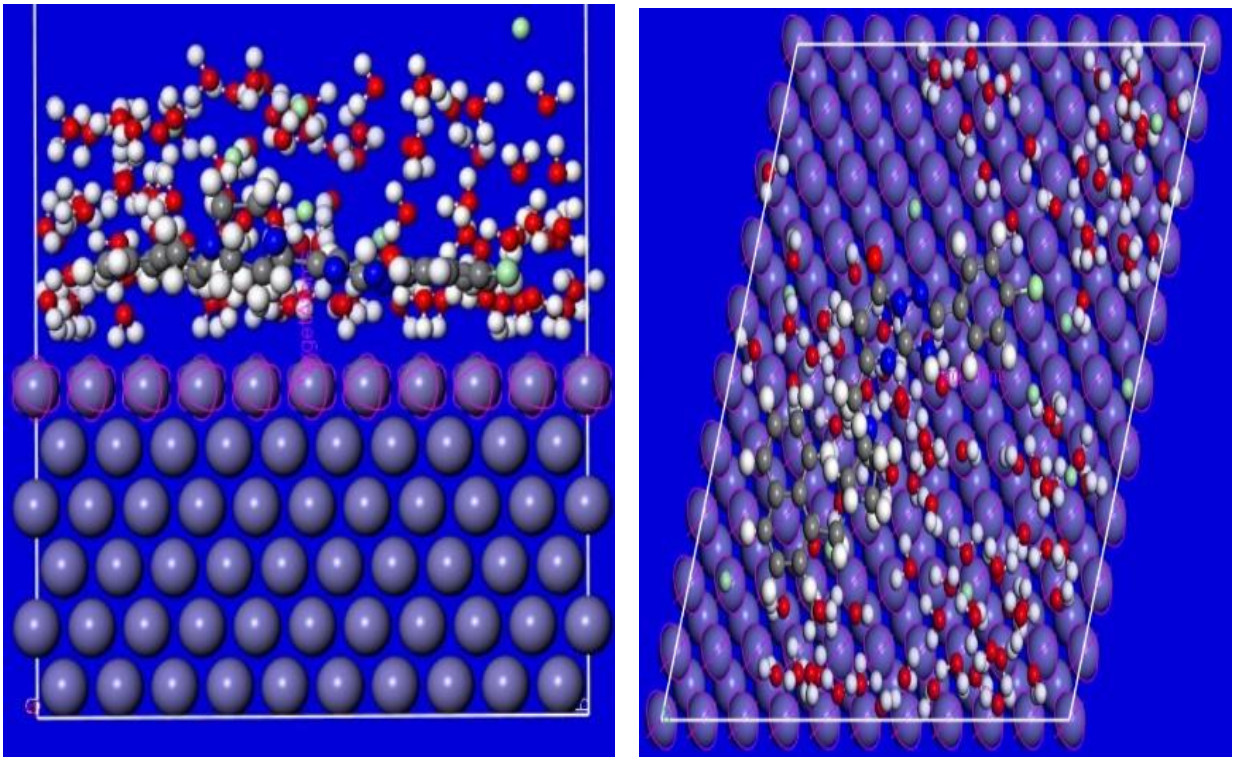
(a) (b)

Fig. S17: (a) Side view (b) Top view of adsorption of B1 on Fe(110).



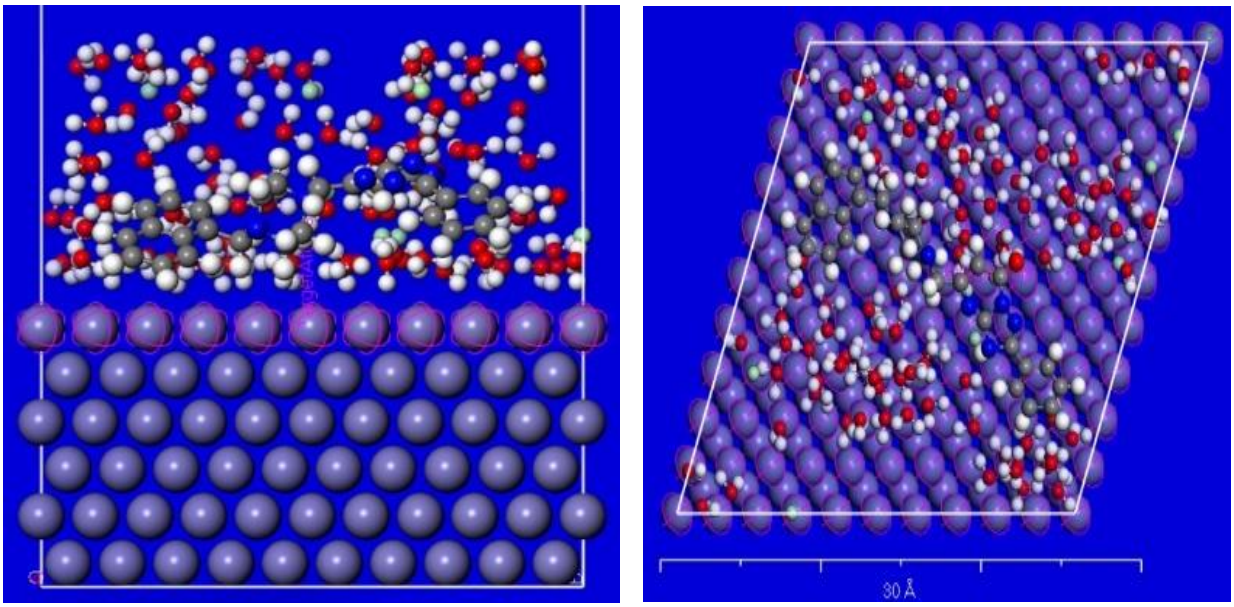
(a) (b)

Fig. S18: (a) Side view (b) Top view of adsorption of B2 on Fe(110).



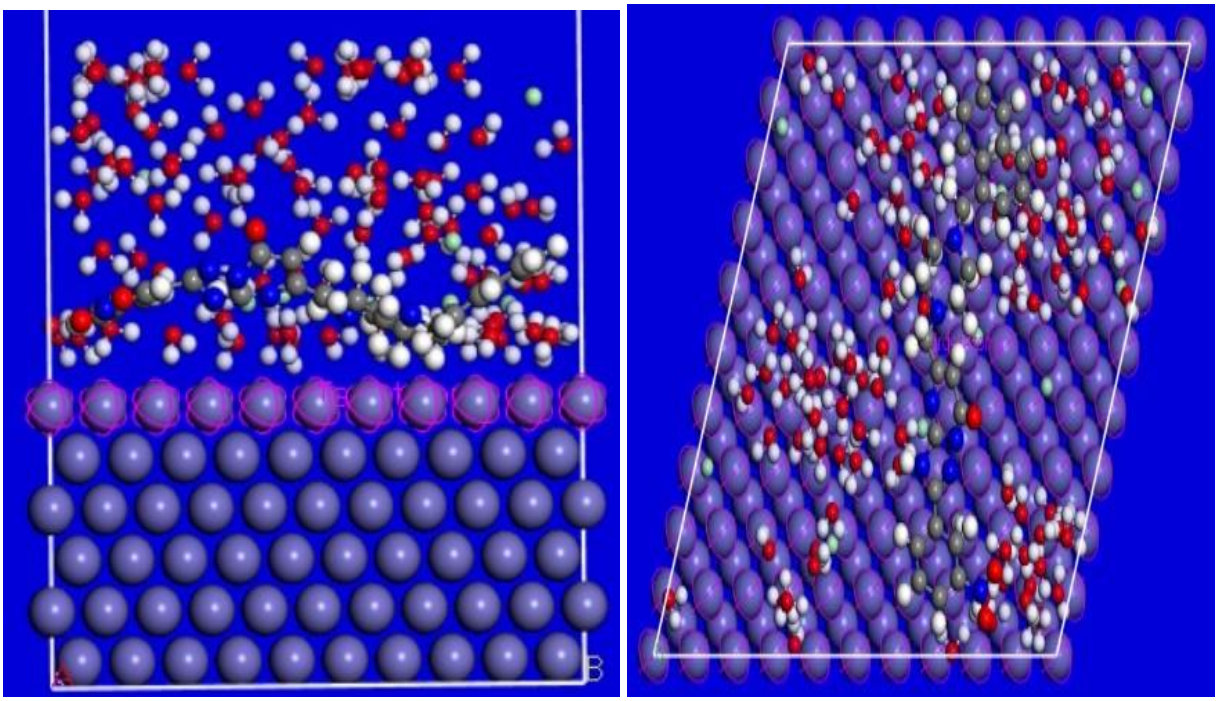
(a) (b)

Fig. S19: (a) Side view (b) Top view of adsorption of B3 on Fe(110).



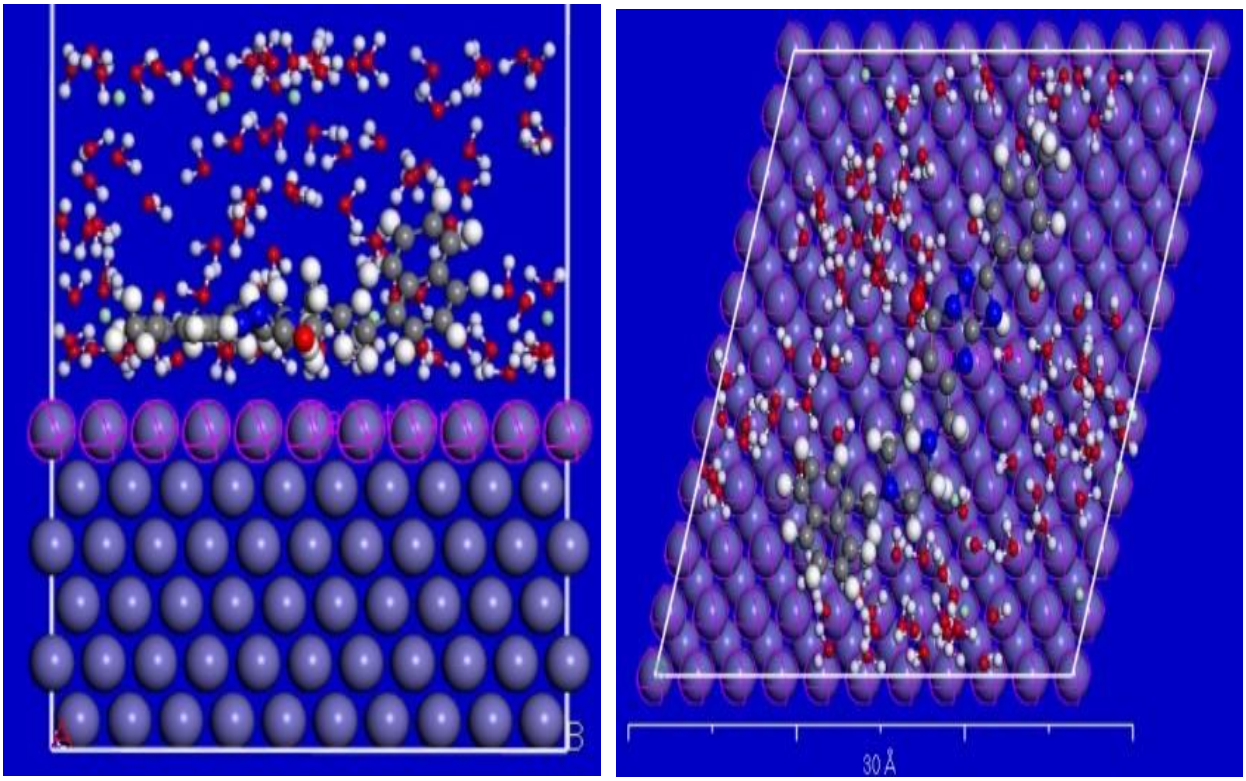
(a) (b)

Fig. S20: (a) Side view (b) Top view of adsorption of B4 on Fe(110).



(a) (b)

Fig. S21: (a) Side view (b) Top view of adsorption of B5 on Fe(110).



(a) (b)

Fig. S22: (a) Side view (b) Top view of adsorption of B6 on Fe(110).

Table S1: Fukui Parameters of A2

Atom	q_k (N+1)	q_k	q_k (N-1)	f_K^+	f_K^-	Δf_K
C1	0.369	0.324	0.311	0.045	0.013	0.032
C2	-0.304	-0.275	-0.209	-0.029	-0.066	0.037
C3	0.592	0.62	0.648	-0.028	-0.028	0
O1	-0.561	-0.493	-0.364	-0.068	-0.129	0.061
N1	-0.438	-0.434	-0.402	-0.004	-0.032	0.028
C4	0.802	0.833	0.863	-0.031	-0.03	-0.001
N2	-0.609	-0.574	-0.488	-0.035	-0.086	0.051
C5	-0.332	-0.436	-0.444	**0.104**	0.008	**0.096**
Cl1	-0.714	-0.076	0.001	-0.638	-0.077	-0.561
N3	-0.341	-0.334	-0.266	-0.007	-0.068	0.061
C6	0.513	0.54	0.566	-0.027	-0.026	-0.001
N4	-0.768	-0.762	-0.74	-0.006	-0.022	0.016
C7	0.131	0.121	0.098	0.01	**0.023**	**-0.013**
C8	-0.388	-0.377	-0.34	-0.011	-0.037	0.026
S1	0.25	0.309	0.433	-0.059	-0.124	0.065
C9	-0.113	-0.111	-0.089	-0.002	-0.022	0.02
C10	-0.36	-0.358	-0.351	-0.002	-0.007	0.005

Table S2: Fukui Parameters of A3

Atom	q_k (N+1)	q_k	q_k (N-1)	f_K^+	f_K^-	Δf_K
C1	0.369	0.324	0.313	0.045	0.011	0.034
C2	-0.302	-0.275	-0.208	-0.027	-0.067	0.04
C3	0.591	0.621	0.649	-0.03	-0.028	-0.002
O1	-0.56	-0.49	-0.363	-0.07	-0.127	0.057
N1	-0.433	-0.433	-0.401	0	-0.032	0.032
C4	0.805	0.837	0.867	-0.032	-0.03	-0.002
N2	-0.606	-0.572	-0.488	-0.034	-0.084	0.05
C5	-0.334	-0.437	-0.444	**0.103**	0.007	**0.096**
Cl1	-0.675	-0.074	0.002	-0.601	-0.076	-0.525
N3	-0.333	-0.328	-0.266	-0.005	-0.062	0.057
C6	0.499	0.53	0.554	-0.031	-0.024	-0.007
N4	-0.777	-0.771	-0.749	-0.006	-0.022	0.016
C7	0.128	0.126	0.116	0.002	**0.01**	**-0.008**
C8	-0.165	-0.158	-0.139	-0.007	-0.019	0.012
C9	-0.139	-0.136	-0.125	-0.003	-0.011	0.008
C10	-0.066	-0.061	-0.058	-0.005	-0.003	-0.002
C11	-0.137	-0.135	-0.123	-0.002	-0.012	0.01
C12	-0.185	-0.177	-0.154	-0.008	-0.023	0.015
Cl2	-0.049	0.003	0.116	-0.052	-0.113	0.061

Table S3: Fukui Parameters of A4

Atom	q_k (N+1)	q_k	q_k (N-1)	f_K^+	f_K^-	Δf_K
C1	0.369	0.324	0.315	0.045	0.009	0.036
C2	-0.304	-0.275	-0.197	-0.029	-0.078	0.049
C3	0.592	0.62	0.65	-0.028	-0.03	0.002
O1	-0.56	-0.492	-0.356	-0.068	-0.136	0.068
N1	-0.435	-0.432	-0.4	-0.003	-0.032	0.029
C4	0.804	0.836	0.867	-0.032	-0.031	-0.001
N2	-0.607	-0.574	-0.486	-0.033	-0.088	0.055
C5	-0.333	-0.437	-0.446	**0.104**	0.009	**0.095**
Cl1	-0.701	-0.076	0.005	-0.625	-0.081	-0.544
N3	-0.334	-0.329	-0.267	-0.005	-0.062	0.057
C6	0.497	0.525	0.549	-0.028	-0.024	-0.004
N4	-0.774	-0.769	-0.743	-0.005	-0.026	0.021
C7	0.128	0.127	0.12	0.001	**0.007**	**-0.006**
C8	-0.167	-0.163	-0.144	-0.004	-0.019	0.015
C9	-0.139	-0.136	-0.128	-0.003	-0.008	0.005
C10	-0.129	-0.119	-0.098	-0.01	-0.021	0.011
C11	-0.135	-0.134	-0.126	-0.001	-0.008	0.007
C12	-0.188	-0.181	-0.162	-0.007	-0.019	0.012

Table S4: Fukui Parameters of A5

Atom	q_k (N+1)	q_k	q_k (N-1)	f_K^+	f_K^-	Δf_K
C1	0.33	0.323	0.332	0.007	-0.009	0.016
C2	-0.283	0.274	-0.169	-0.557	**0.443**	**-1**
C3	0.611	0.621	0.654	-0.01	-0.033	0.023
O1	-0.523	-0.488	-0.341	-0.035	-0.147	0.112
N1	-0.423	-0.433	-0.402	0.01	-0.031	0.041
C4	0.828	0.841	0.874	-0.013	-0.033	0.02
N2	-0.588	-0.569	-0.493	-0.019	-0.076	0.057
C5	-0.434	-0.437	-0.459	0.003	0.022	-0.019
Cl1	-0.112	-0.071	0.019	-0.041	-0.09	0.049
N3	-0.367	-0.33	-0.285	-0.037	-0.045	0.008
C6	0.504	0.542	0.559	-0.038	-0.017	-0.021
N4	-0.767	-0.773	-0.739	0.006	-0.034	0.04
C7	0.118	0.113	0.11	0.005	0.003	0.002
C8	0.24	-0.207	-0.194	**0.447**	-0.013	**0.46**
C9	0.294	0.269	0.271	0.025	-0.002	0.027
C10	-0.186	-0.141	-0.121	-0.045	-0.02	-0.025
C11	-0.142	-0.144	-0.139	0.002	-0.005	0.007
C12	-0.201	-0.142	-0.133	-0.059	-0.009	-0.05
N5	0.271	0.387	0.402	-0.116	-0.015	-0.101
O2	-0.521	-0.384	-0.355	-0.137	-0.029	-0.108
O3	-0.537	-0.392	-0.379	-0.145	-0.013	-0.132

Table S5: Fukui Parameters of A6

Atom	q_k (N+1)	q_k	q_k (N-1)	f_K^+	f_K^-	Δf_K
C1	0.369	0.324	0.312	0.045	0.012	0.033
C2	-0.304	-0.275	-0.213	-0.029	-0.062	0.033
C3	0.592	0.62	0.648	-0.028	-0.028	0
O1	-0.561	-0.493	-0.368	-0.068	-0.125	0.057
N1	-0.435	-0.433	-0.401	-0.002	-0.032	0.03
C4	0.805	0.835	0.865	-0.03	-0.03	1.11E-16
N2	-0.608	-0.574	-0.491	-0.034	-0.083	0.049
C5	-0.332	-0.437	-0.443	**0.105**	0.006	**0.099**
Cl1	-0.706	-0.077	-0.002	-0.629	-0.075	-0.554
N3	-0.338	-0.329	-0.264	-0.009	-0.065	0.056
C6	0.502	0.521	0.552	-0.019	-0.031	0.012
N4	-0.777	-0.766	-0.75	-0.011	-0.016	0.005
C7	0.129	0.124	0.117	0.005	0.007	-0.002
C8	-0.168	-0.161	-0.142	-0.007	-0.019	0.012
C9	-0.188	-0.184	-0.171	-0.004	-0.013	0.009
C10	0.183	0.185	0.192	-0.002	-0.007	0.005
C11	-0.191	-0.187	-0.168	-0.004	-0.019	0.015
C12	-0.187	-0.18	-0.156	-0.007	-0.024	0.017
C13	-0.53	-0.533	-0.542	0.003	**0.009**	**-0.006**

Table S6: Fukui Parameters of B1

Atom	q_k (N+1)	q_k	q_k (N-1)	f_K^+	f_K^-	Δf_K
C1	0.271	0.278	0.309	-0.007	-0.031	0.024
C2	-0.286	-0.278	-0.295	-0.008	0.017	-0.025
C3	0.59	0.615	0.63	-0.025	-0.015	-0.01
O1	-0.547	-0.504	-0.46	-0.043	-0.044	0.001
N1	-0.419	-0.441	-0.439	**0.022**	-0.002	**0.024**
C4	0.787	0.818	0.828	-0.031	-0.01	-0.021
N2	-0.61	-0.588	-0.607	-0.022	0.019	-0.041
C5	-0.167	-0.172	-0.246	0.005	**0.074**	**-0.069**
N3	-0.294	-0.277	0.202	-0.017	-0.479	0.462
C6	0.22	0.327	0.327	-0.107	0	-0.107
N4	-0.689	-0.711	-0.708	**0.022**	-0.003	**0.025**
S1	0.017	0.174	0.208	-0.157	-0.034	-0.123
C7	-0.573	-0.586	-0.593	0.013	0.007	0.006
C8	-0.204	-0.203	-0.208	-0.001	0.005	-0.006
C9	0.083	0.106	0.103	-0.023	0.003	-0.026
C10	-0.22	-0.191	-0.179	-0.029	-0.012	-0.017
C11	0.074	0.071	0.083	0.003	-0.012	0.015
C12	-0.137	-0.131	-0.132	-0.006	0.001	-0.007
C13	0.151	0.138	0.131	0.013	0.007	0.006
C14	-0.212	-0.182	-0.215	-0.03	0.033	-0.063

C15	-0.145	-0.139	-0.129	-0.006	-0.01	0.004
C16	-0.134	-0.131	-0.129	-0.003	-0.002	-0.001
C17	-0.223	-0.197	-0.186	-0.026	-0.011	-0.015
C18	-0.204	-0.207	-0.274	0.003	0.067	-0.064
N5	-0.392	-0.399	-0.27	0.007	-0.129	0.136
C19	-0.117	-0.122	-0.188	0.005	0.066	-0.061
C20	-0.119	-0.126	-0.177	0.007	0.051	-0.044
C21	-0.117	-0.123	-0.18	0.006	0.057	-0.051
C22	-0.124	-0.13	-0.174	0.006	0.044	-0.038
N6	-0.4	-0.407	-0.277	0.007	-0.13	0.137

Table S7: Fukui Parameters of B2

Atom	q_k (N+1)	q_k	q_k (N-1)	f_K^+	f_K^-	Δf_K
C1	0.276	0.277	0.289	-0.001	-0.012	0.011
C2	-2.287	-0.276	-0.248	-2.011	-0.028	-1.983
C3	0.596	0.613	0.63	-0.017	-0.017	0
O1	-0.543	-0.502	-0.446	-0.041	-0.056	0.015
N1	-0.417	-0.432	-0.421	**0.015**	-0.011	**0.026**
C4	0.817	0.832	0.847	-0.015	-0.015	0
N2	-0.623	-0.602	-0.573	-0.021	-0.029	0.008
C5	-0.171	-0.174	-0.199	0.003	**0.025**	**-0.022**
N3	-0.39	-0.335	0.189	-0.055	-0.524	0.469
C6	0.475	0.536	0.545	-0.061	-0.009	-0.052
N4	-0.771	-0.765	-0.751	-0.006	-0.014	0.008
C7	0.125	0.122	0.112	0.003	0.01	-0.007
C8	-0.434	-0.378	-0.369	-0.056	-0.009	-0.047
S1	0.161	0.304	0.353	-0.143	-0.049	-0.094
C9	-0.117	-0.112	-0.108	-0.005	-0.004	-0.001
C10	-0.37	-0.358	-0.356	-0.012	-0.002	-0.01
C11	-0.204	-0.203	-0.188	-0.001	-0.015	0.014
C12	0.092	0.104	0.096	-0.012	0.008	-0.02
C13	-0.215	-0.19	-0.174	-0.025	-0.016	-0.009
C14	0.075	0.071	0.09	0.004	-0.019	0.023
C15	-0.136	-0.131	-0.126	-0.005	-0.005	0
C16	0.149	0.138	0.137	0.011	0.001	0.01
C17	-0.206	-0.183	-0.178	-0.023	-0.005	-0.018
C18	-0.144	-0.139	-0.126	-0.005	-0.013	0.008
C19	-0.134	-0.131	-0.122	-0.003	-0.009	0.006
C20	-0.218	-0.197	-0.182	-0.021	-0.015	-0.006
C21	-0.207	-0.207	-0.232	0	**0.025**	**-0.025**
N5	-0.391	-0.399	-0.362	0.008	-0.037	0.045
C22	-0.126	-0.126	-0.141	0	0.015	-0.015
C23	-0.114	-0.12	-0.141	0.006	0.021	-0.015

C24	-0.11	-0.121	-0.141	0.011	0.02	-0.009
C25	-0.129	-0.133	-0.143	0.004	0.01	-0.006
N6	-0.4	-0.404	-0.383	0.004	-0.021	0.025

Table S8: Fukui Parameters of B3

Atom	q_k (N+1)	q_k	q_k (N-1)	f_K^+	f_K^-	Δf_K
C1	0.281	0.276	0.306	0.005	-0.03	0.035
C2	-0.278	-0.274	-0.295	-0.004	0.021	-0.025
C3	0.592	0.614	0.63	-0.022	-0.016	-0.006
O1	-0.546	-0.5	-0.457	-0.046	-0.043	-0.003
N1	-0.411	-0.431	-0.431	**0.02**	0	**0.02**
C4	0.812	0.837	0.846	-0.025	-0.009	-0.016
N2	-0.605	-0.6	-0.621	-0.005	0.021	-0.026
C5	-0.185	-0.176	-0.241	-0.009	0.065	-0.074
N3	-0.394	-0.329	-0.317	-0.065	-0.012	-0.053
C6	0.457	0.527	0.529	-0.07	-0.002	-0.068
N4	-0.778	-0.773	-0.769	-0.005	-0.004	-0.001
C7	0.102	0.128	0.124	-0.026	0.004	-0.03
C8	-0.2	-0.178	-0.175	-0.022	-0.003	-0.019
C9	-0.138	-0.135	-0.133	-0.003	-0.002	-0.001
C10	-0.097	-0.061	-0.6	-0.036	**0.539**	**-0.575**
C11	-0.143	-0.136	-0.134	-0.007	-0.002	-0.005
C12	-0.182	-0.159	-0.155	-0.023	-0.004	-0.019
Cl2	-0.11	-0.001	0.034	-0.109	-0.035	-0.074
C13	-0.204	-0.203	-0.205	-0.001	0.002	-0.003
C14	0.101	0.108	0.095	-0.007	0.013	-0.02
C15	-0.207	0.19	-0.18	-0.397	0.37	-0.767
C16	0.071	0.073	0.089	-0.002	-0.016	0.014
C17	-0.134	-0.131	-0.133	-0.003	0.002	-0.005
C18	0.146	0.138	0.131	0.008	0.007	0.001
C19	-0.197	-0.182	-0.219	-0.015	0.037	-0.052
C20	-0.143	-0.139	-0.131	-0.004	-0.008	0.004
C21	-0.133	-0.131	-0.13	-0.002	-0.001	-0.001
C22	-0.211	-0.197	-0.187	-0.014	-0.01	-0.004
C23	-0.206	-0.211	-0.267	0.005	0.056	-0.051
N5	-0.394	-0.397	-0.271	0.003	-0.126	0.129
C24	-0.119	-0.127	-0.177	0.008	0.05	-0.042
C25	-0.122	-0.123	-0.186	0.001	0.063	-0.062
C26	-0.118	-0.129	-0.179	0.011	0.05	-0.039
C27	-0.116	-0.124	-0.184	0.008	0.06	-0.052
N6	-0.396	-0.404	-0.276	0.008	-0.128	0.136

Table S9: Fukui Parameters of B4

Atom	q_k (N+1)	q_k	q_k (N-1)	f_K^+	f_K^-	Δf_K
C1	0.275	0.277	0.306	-0.002	-0.029	0.027
C2	-0.287	-0.277	-0.296	-0.01	0.019	-0.029
C3	0.595	0.613	0.629	-0.018	-0.016	-0.002
O1	-0.545	-0.501	-0.457	-0.044	-0.044	-5.6E-17
N1	-0.414	-0.432	-0.43	**0.018**	-0.002	**0.02**
C4	0.818	0.836	0.845	-0.018	-0.009	-0.009
N2	-0.622	-0.601	-0.62	-0.021	0.019	-0.04
C5	-0.172	-0.173	-0.244	0.001	0.071	-0.07
N3	-0.391	-0.328	-0.317	-0.063	-0.011	-0.052
C6	0.456	0.521	0.524	-0.065	-0.003	-0.062
N4	-0.776	-0.771	-0.766	-0.005	-0.005	0
C7	0.106	0.127	0.125	-0.021	0.002	-0.023
C8	-0.184	-0.163	-0.159	-0.021	-0.004	-0.017
C9	-0.141	-0.136	-0.134	-0.005	-0.002	-0.003
C10	-0.161	-0.119	-0.114	-0.042	-0.005	-0.037
C11	-0.135	-0.134	-0.132	-0.001	-0.002	0.001
C12	-0.202	-0.182	-0.18	-0.02	-0.002	-0.018
C13	-0.204	-0.203	-0.179	-0.001	-0.024	0.023
C14	0.093	0.103	0.062	-0.01	0.041	-0.051
C15	-0.212	0.19	-0.179	-0.402	**0.369**	**-0.771**
C16	0.074	0.072	0.096	0.002	-0.024	0.026
C17	-0.135	-0.131	-0.134	-0.004	0.003	-0.007
C18	0.148	0.138	0.13	0.01	0.008	0.002
C19	-0.203	-0.183	-0.215	-0.02	0.032	-0.052
C20	-0.144	-0.139	-0.128	-0.005	-0.011	0.006
C21	-0.133	-0.131	-0.13	-0.002	-0.001	-0.001
C22	-0.216	-0.197	-0.187	-0.019	-0.01	-0.009
C23	-0.206	-0.206	-0.251	0	0.045	-0.045
N5	-0.392	-0.399	-0.277	0.007	-0.122	0.129
C24	-0.126	-0.127	-0.186	0.001	0.059	-0.058
C25	-0.115	-0.12	-0.177	0.005	0.057	-0.052
C26	-0.109	-0.119	-0.184	0.01	0.065	-0.055
C27	-0.128	-0.133	-0.179	0.005	0.046	-0.041
N6	-0.4	-0.405	-0.271	0.005	-0.134	0.139

Table S10: Fukui Parameters of B5

Atom	q_k (N+1)	q_k	q_k (N-1)	f_K^+	f_K^-	Δf_K
C1	0.284	0.276	0.302	0.008	-0.026	0.034
C2	-0.407	-0.275	-0.296	-0.132	0.021	-0.153
C3	0.94	0.614	0.626	0.326	-0.012	0.338
O1	-0.637	-0.498	-0.458	-0.139	-0.04	-0.099
N1	-0.894	-0.431	-0.43	-0.463	-0.001	-0.462
C4	1.276	0.84	0.845	0.436	-0.005	0.441
N2	-0.844	-0.597	-0.606	-0.247	0.009	-0.256
C5	-0.169	-0.174	-0.241	0.005	**0.067**	**-0.062**
N3	-0.345	-0.33	-0.319	-0.015	-0.011	-0.004
C6	0.806	0.539	0.539	0.267	0	0.267
N4	-1.049	-0.776	-0.763	-0.273	-0.013	-0.26
C7	-0.145	0.114	0.112	-0.259	0.002	-0.261
C8	-0.228	-0.208	-0.207	-0.02	-0.001	-0.019
C9	0.378	0.269	0.271	**0.109**	-0.002	**0.111**
C10	-0.213	-0.142	-0.135	-0.071	-0.007	-0.064
C11	-0.237	-0.145	-0.144	-0.092	-0.001	-0.091
C12	-0.217	-0.142	-0.138	-0.075	-0.004	-0.071
N5	-0.14	0.387	0.392	-0.527	-0.005	-0.522
O2	-0.532	-0.385	-0.369	-0.147	-0.016	-0.131
O3	-0.57	-0.393	-0.392	-0.177	-0.001	-0.176
C13	-0.236	-0.204	-0.204	-0.032	0	-0.032
C14	-0.026	0.105	0.095	-0.131	0.01	-0.141
C15	-0.2	-0.19	-0.179	-0.01	-0.011	0.001
C16	-0.103	0.07	0.088	-0.173	-0.018	-0.155
C17	-0.232	-0.131	-0.133	-0.101	0.002	-0.103
C18	-0.088	0.139	0.13	-0.227	0.009	-0.236
C19	-0.2	-0.184	-0.215	-0.016	0.031	-0.047
C20	-0.242	-0.139	-0.132	-0.103	-0.007	-0.096
C21	-0.237	-0.131	-0.129	-0.106	-0.002	-0.104
C22	-0.199	-0.197	-0.186	-0.002	-0.011	0.009
C23	-0.163	-0.208	-0.266	0.045	0.058	-0.013
N6	-0.688	-0.399	-0.266	-0.289	-0.133	-0.156
C24	-0.178	-0.126	-0.183	-0.052	0.057	-0.109
C25	-0.179	-0.12	-0.185	-0.059	0.065	-0.124
C26	-0.175	-0.132	-0.183	-0.043	0.051	-0.094
C27	-0.167	-0.125	-0.18	-0.042	0.055	-0.097
N7	-0.705	-0.406	-0.281	-0.299	-0.125	-0.174

Table S11: Fukui Parameters of B6

Atom	q_k (N+1)	q_k	q_k (N-1)	f_K^+	f_K^-	Δf_K
C1	0.275	0.277	0.305	-0.002	-0.028	0.026
C2	-0.287	-0.278	-0.299	-0.009	0.021	-0.03
C3	0.595	0.613	0.624	-0.018	-0.011	-0.007
O1	-0.545	-0.502	-0.463	-0.043	-0.039	-0.004
N1	-0.414	-0.431	-0.428	**0.017**	-0.003	**0.02**
C4	0.818	0.836	0.841	-0.018	-0.005	-0.013
N2	-0.622	-0.602	-0.611	-0.02	0.009	-0.029
C5	-0.172	-0.173	-0.247	0.001	0.074	-0.073
N3	-0.392	0.161	-0.322	-0.553	**0.483**	**-1.036**
C6	0.458	0.523	0.525	-0.065	-0.002	-0.063
N4	-0.777	-0.771	-0.764	-0.006	-0.007	0.001
C7	0.106	0.126	0.123	-0.02	0.003	-0.023
C8	-0.182	-0.163	-0.16	-0.019	-0.003	-0.016
C9	-0.193	-0.185	-0.181	-0.008	-0.004	-0.004
C10	0.163	0.185	0.185	-0.022	0	-0.022
C11	-0.19	-0.186	-0.184	-0.004	-0.002	-0.002
C12	-0.203	-0.181	-0.179	-0.022	-0.002	-0.02
C13	-0.526	-0.533	-0.535	0.007	0.002	0.005
C14	-0.204	-0.203	-0.19	-0.001	-0.013	0.012
C15	0.093	0.105	0.053	-0.012	0.052	-0.064
C16	-0.212	-0.19	-0.178	-0.022	-0.012	-0.01
C17	0.073	0.072	0.103	0.001	-0.031	0.032
C18	-0.135	-0.131	-0.133	-0.004	0.002	-0.006
C19	0.148	0.138	0.13	0.01	0.008	0.002
C20	-0.204	-0.183	-0.219	-0.021	0.036	-0.057
C21	-0.144	-0.139	-0.13	-0.005	-0.009	0.004
C22	-0.133	-0.131	-0.13	-0.002	-0.001	-0.001
C23	-0.216	-0.197	-0.186	-0.019	-0.011	-0.008
C24	-0.206	-0.207	-0.239	0.001	0.032	-0.031
N5	-0.392	-0.399	-0.28	0.007	-0.119	0.126
C25	-0.126	-0.127	-0.184	0.001	0.057	-0.056
C26	-0.115	-0.121	-0.184	0.006	0.063	-0.057
C27	-0.109	-0.118	-0.178	0.009	0.06	-0.051
C28	-0.129	0.151	-0.178	-0.28	0.329	-0.609
N6	-0.4	-0.406	-0.283	0.006	-0.123	0.129