Corrosion inhibition studies of ferrocenyl Schiff bases in mild acidic medium through experimental methods and DFT calculations

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Supplementary Information

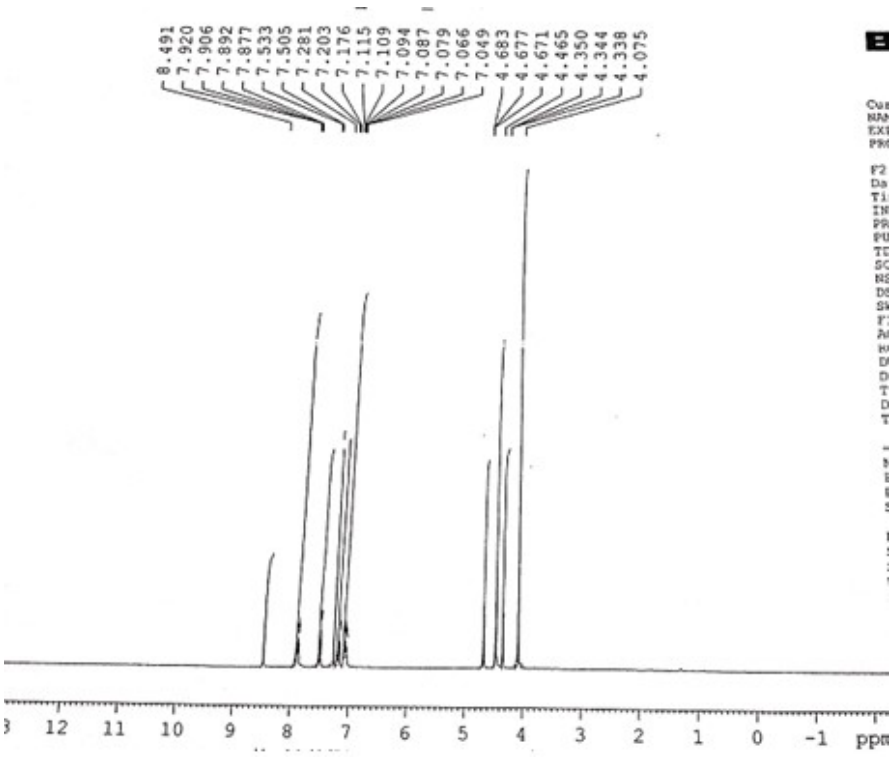

Fig. S1. ^{1}H NMR spectrum of FcA in $CDCl_3$

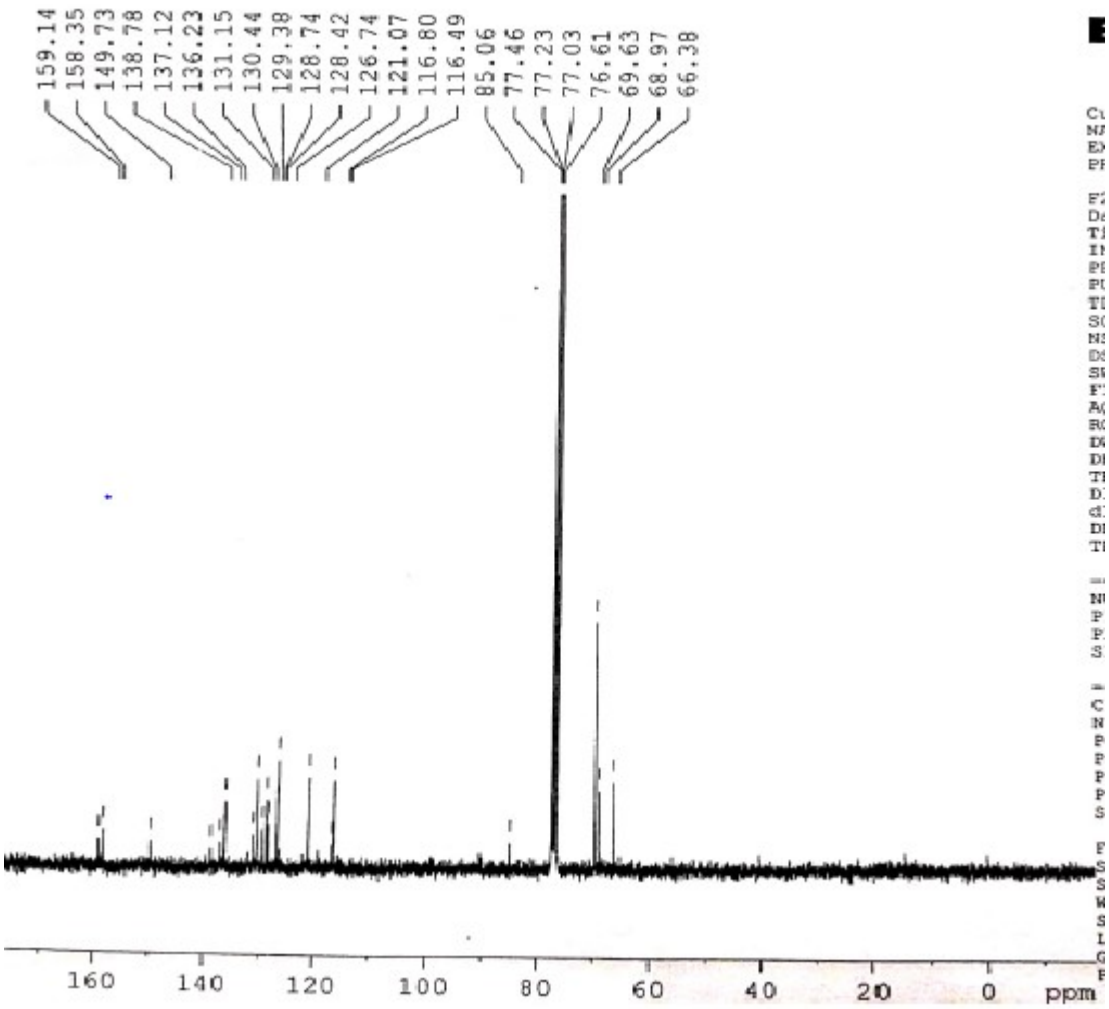

Fig. S2. ^{13}C NMR spectrum of FcA $CDCl_3$

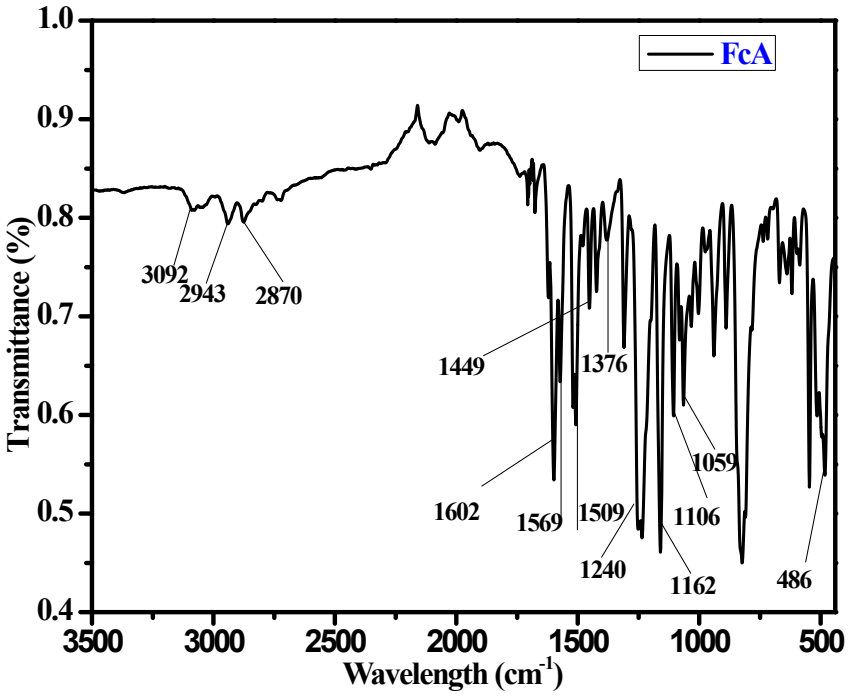

Fig. S3. FT-IR spectrum of FcA

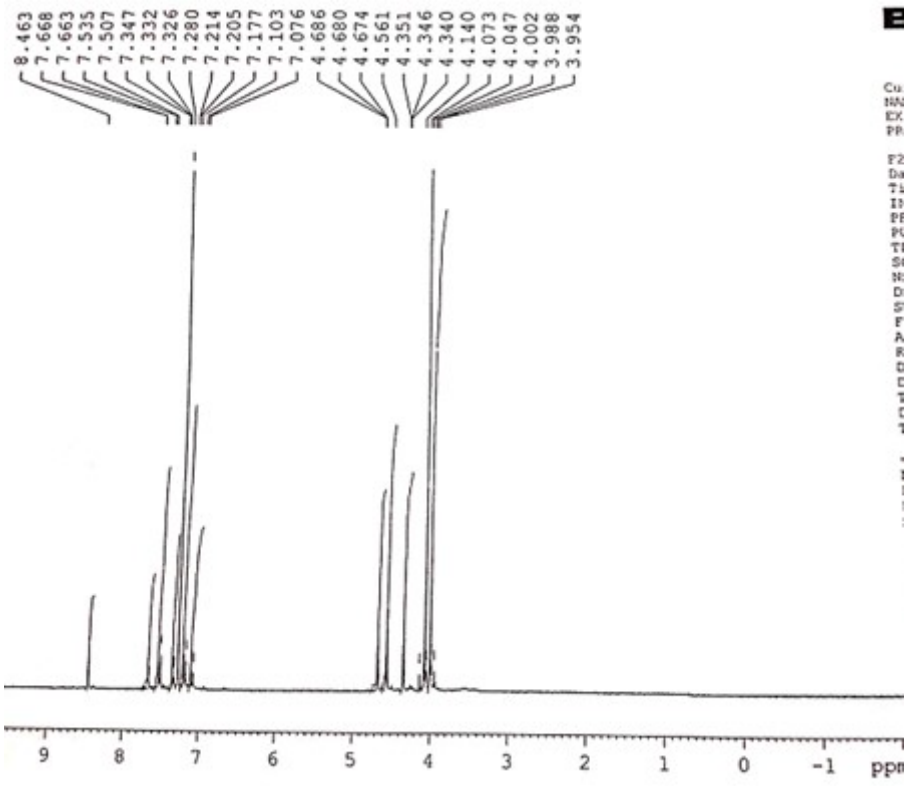

Fig. S4. ^{1}H NMR spectrum of FcB in $CDCl_3$

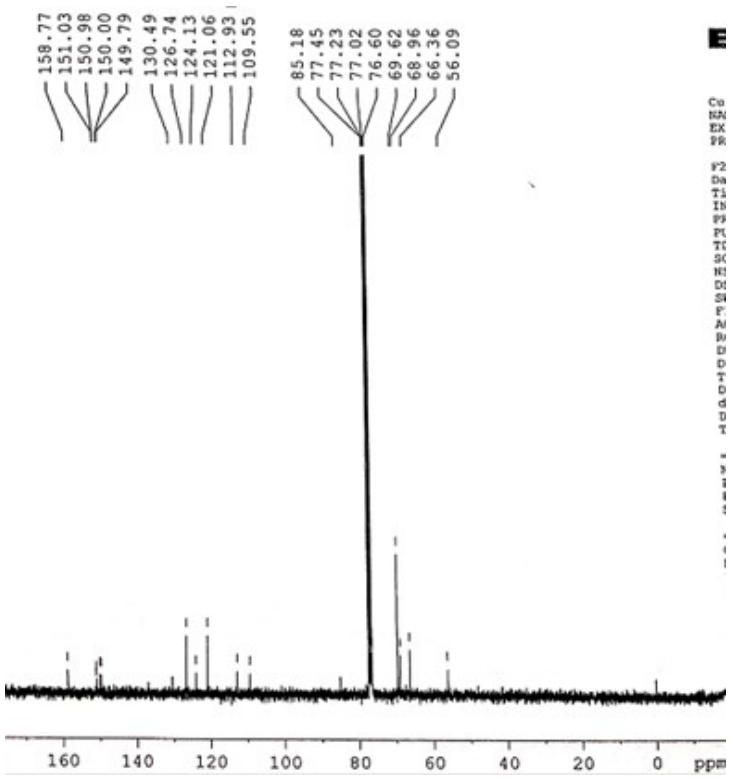

Fig. S5. ^{13}C NMR spectrum of FcB $CDCl_3$

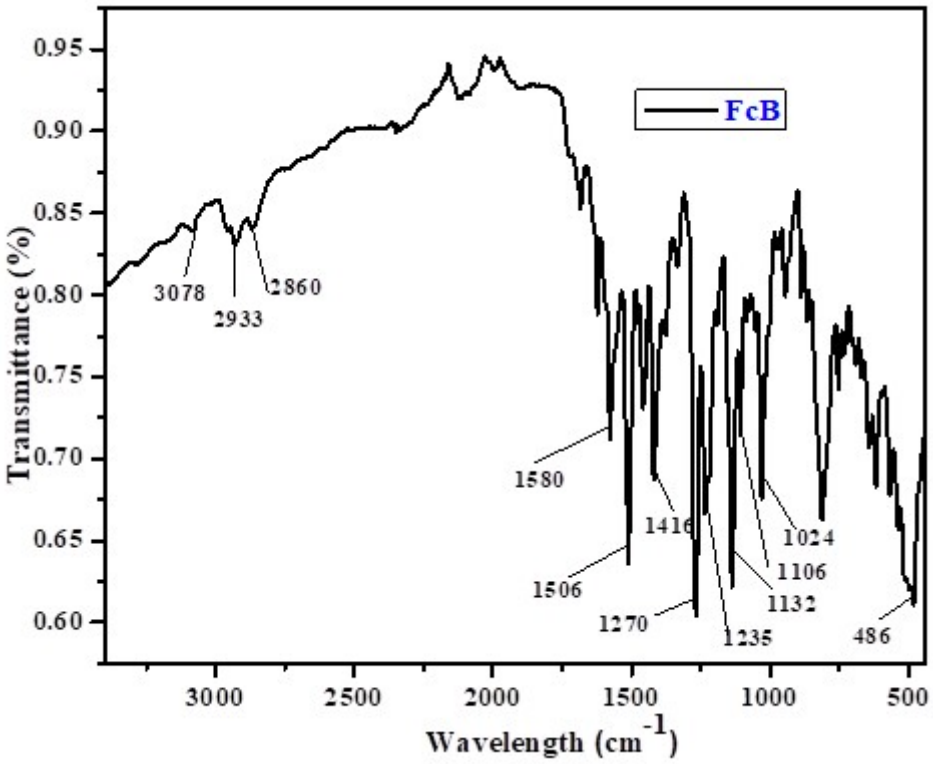

Fig. S6. FT-IR spectrum of FcB

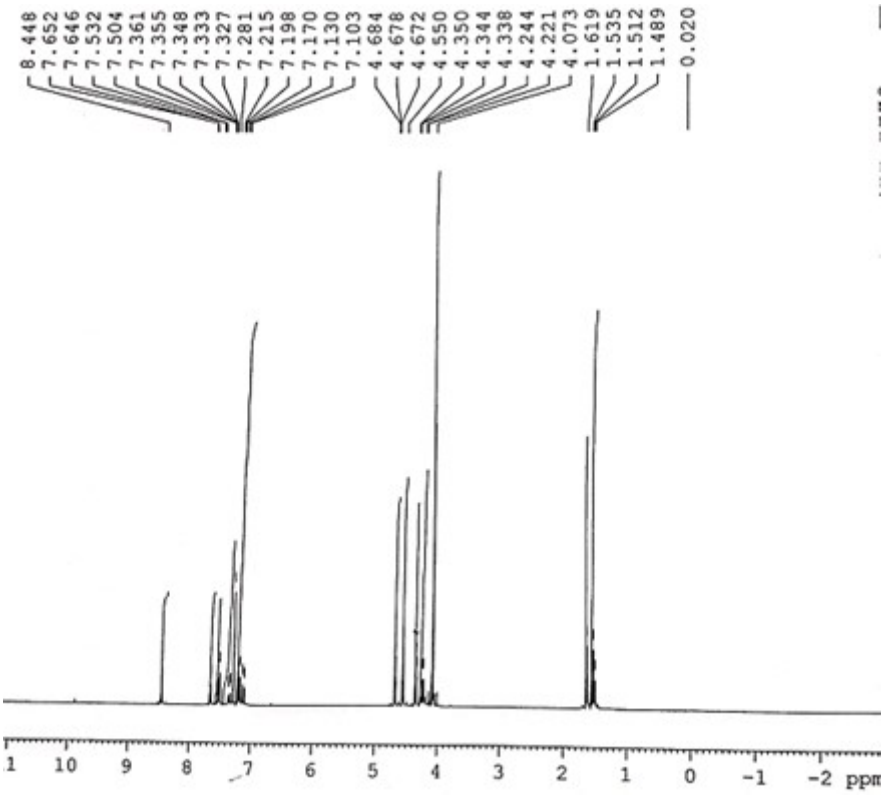

Fig. S7. ^{1}H NMR spectrum of FcC in $CDCl_3$

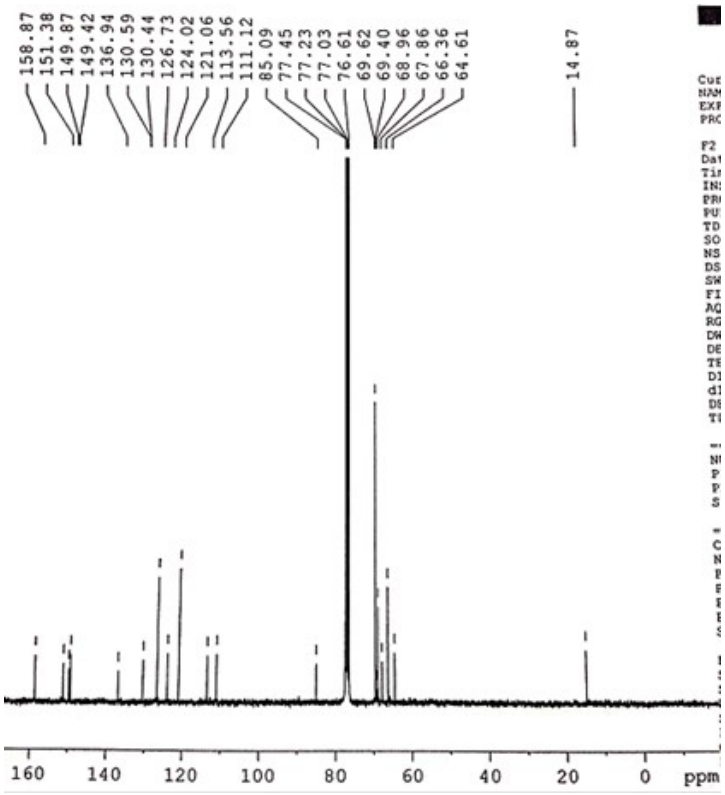

Fig. S8. ^{13}C NMR spectrum of FcC in $CDCl_3$

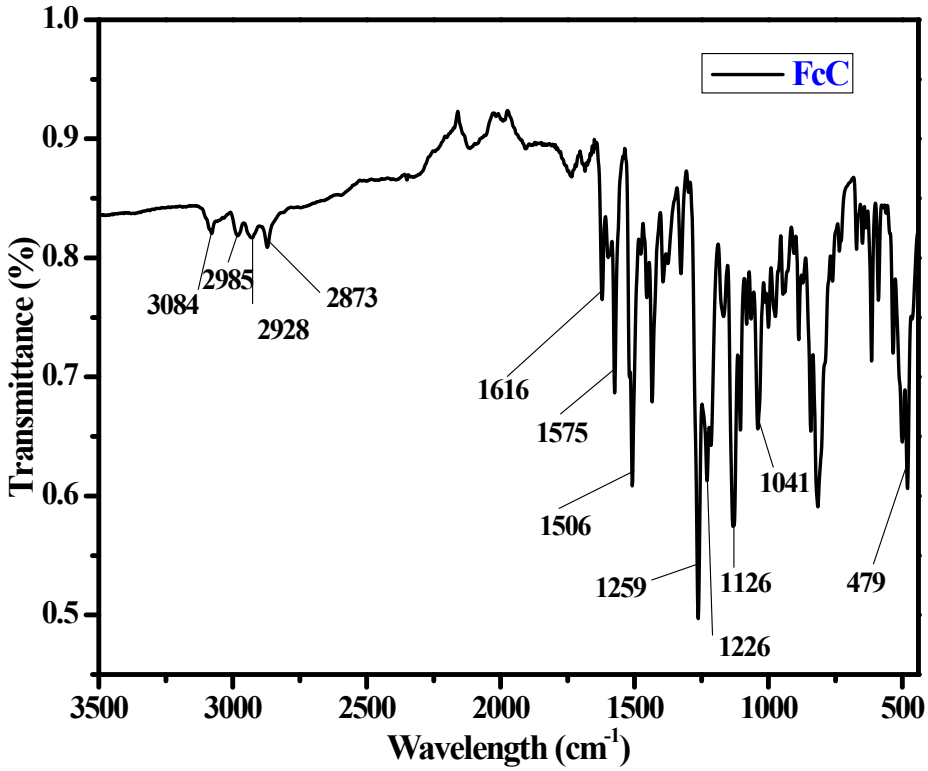

Fig. S9. FT-IR spectrum of FcC

Table S1. Selected Mulliken atomic charges on the corrosion inhibitors FcA, FcB and FcC calculated at GGA/PBE with a DZ basis set

Atomic charges (e)	Compounds		
	FcA	**FcB**	**FcC**
$q_{Fe\ (12)}$	0.4328	0.4233	0.4365
q_c	-0.3126	-0.3121	-0.3127
q_c	-0.3452	-0.3129	-0.3306
q_c	-0.2897	-0.2944	-0.2917
q_c	-0.0993	-0.1100	-0.1032
$q_{N\ (23)}$	-0.3831	-0.3962	-0.3920
q_c	-0.0863	-0.0597	-0.0568
q_c	-0.1522	-0.1390	-0.1476
$q_{O\ (35)}$	-0.5903	-0.5864	-0.5976
q_c	-0.1517	-0.0906	-0.0673
$q_{O\ (39)}$	-0.5976	-0.5708	-0.6137
q_c	0.2222	0.2402	0.2619
q_c	-0.3089	0.2612	0.1778
q_c	-0.0814	-0.0579	-0.0656
$q_{N\ (50)}$	-0.3794	-0.3860	-0.3886
q_c	-0.0177	-0.0448	-0.0380
q_c	-0.2455	-0.2582	-0.2425
$q_{Fe\ (73)}$	0.4646	0.4463	0.3928
q_c	-0.3101	-0.3144	-0.3183
q_c	-0.3321	-0.3561	-0.3088
q_c	-0.3277	-0.3295	-0.3074
$q_{O\ (89)}$	-----	-0.6063	-0.5929
$q_{O\ (90)}$	-----	-0.6009	-0.5737
q_c	-----	-0.5616	-0.3657

q_c	----	-0.5258	-0.3372
q_c	----	---	-0.8215
q_c	---	---	-0.7842

APPENDIX I

Computational output data obtained from ADF software at GGA/PBE level of theory with a DZ basis set.

Coordinates of Optimized Compound 1 (FcA)

Atom	angstrom X	Y	Z
1 Fe	-7.304069499331	11.055934759635	-1.022428270545
2 C	-8.648924971795	10.939642595774	0.549854924065
3 C	-7.490492257419	9.282327940959	-2.094823840164
4 C	-8.929461141325	12.103473686998	-0.253516542039
5 C	-7.295129013373	11.050982292499	1.066576939684
6 C	-6.136680935612	9.441557513710	-1.619844586142
7 C	-7.802970548438	10.411511294918	-2.940602739509
8 C	-7.751781232757	12.937578540018	-0.256462766947
9 C	-6.743250018678	12.291311154310	0.546427599885
10 C	-5.610842363190	10.668610895247	-2.171588104144
11 C	-6.640731889035	11.267198603311	-2.990256018390
12 H	-9.341379112881	10.120669044051	0.731726127359
13 H	-8.157192977595	8.453839014858	-1.861454031529
14 H	-9.867317526580	12.317041705546	-0.762918492724
15 H	-2.220799843733	3.006983498732	-0.644945397884
16 H	-5.614301847612	8.769903724753	-0.939763426217
17 H	-8.744462652717	10.580932193304	-3.459994970840
18 H	-7.646320026514	13.897003826098	-0.760137201035
19 H	-0.723233283776	3.204954308095	-1.698875181912

20	H	-4.609259066819	11.065337664867	-2.014058450022
21	H	-6.553029935432	12.194876414032	-3.553481342825
22	C	-6.609863335936	10.070507178027	1.924413108849
23	C	-7.350802592154	9.114786072923	2.660676430818
24	C	-6.717827244975	8.197898095202	3.504275256115
25	C	-5.311296354682	8.180597206714	3.611639202807
26	C	-4.556680364839	9.140507601428	2.896962665324
27	C	-5.200638719759	10.069046686368	2.074532372601
28	H	-8.441253232165	9.124029716227	2.612506036872
29	H	-7.296414820968	7.498822105764	4.111199995577
30	H	-5.758781993850	12.698079950969	0.768460683399
31	H	-3.470406645412	9.162931803631	3.012760674098
32	H	-4.599299731729	10.803339513924	1.534832560575
33	N	-4.719399298238	7.297977795169	4.552228800294
34	C	-3.733222962338	6.488424705124	4.317683398196
35	C	-3.071045050425	6.114069870555	3.045357363182
36	C	-3.703657205149	6.189020295945	1.782171602293
37	C	-3.042028961991	5.740766305929	0.632692224361
38	C	-1.746333798675	5.218801530817	0.742549835909
39	C	-1.093282240470	5.138186406736	1.976996729719
40	C	-1.765684844375	5.576540874262	3.124114846347
41	H	-4.716892931020	6.584545591506	1.701667633627
42	H	-3.513235949138	5.802164171238	-0.350266650751
43	O	-1.073362777161	4.782181408953	-0.443450452352
44	H	-0.081775645418	4.733187283392	2.033270187700
45	H	-1.271927661266	5.502953621229	4.097010742203
46	C	-1.177110540603	3.339268554256	-0.708494602949
47	O	-0.498374393918	2.528038816292	0.296865101841
48	C	0.916694691021	2.566621436181	0.361262735745
49	C	1.492093782966	1.560165711130	1.158031972387

50	C	2.877354469058	1.499792176897	1.301733453339
51	C	3.711312699681	2.448195390102	0.658469832487
52	C	3.105220348283	3.471048278334	-0.101110332700
53	C	1.712246699711	3.538816302824	-0.263265806215
54	H	0.832984873062	0.841951900299	1.648068573788
55	H	3.319025836671	0.718718635800	1.921584278846
56	C	5.185567697095	2.452762273471	0.797147475036
57	H	3.731133240253	4.231796957858	-0.575927482775
58	H	1.265450490741	4.358190477286	-0.826278002696
59	N	6.001980867603	1.466318101865	1.019675826930
60	C	5.620773138076	0.096659176131	1.004494107700
61	C	6.003956547397	-0.728896405593	2.083041367504
62	C	5.689556179130	-2.090264813938	2.074836665928
63	C	5.026412695174	-2.685571628084	0.973746621352
64	C	4.703027824253	-1.855859023052	-0.126233295633
65	C	4.982948063463	-0.486437590183	-0.112749161946
66	H	6.551957840264	-0.282581764524	2.915189897486
67	H	5.970095645630	-2.702912231393	2.933348154135
68	H	4.735775333871	0.137161692947	-0.974811058503
69	H	4.249684403742	-2.294247025712	-1.017070351399
70	Fe	3.181100864606	-5.025600518123	2.050774810774
71	C	3.758087998841	-4.784256539893	0.076658856098
72	C	1.291618678825	-4.166684866667	2.231980387429
73	C	3.728450419274	-6.186797241394	0.409761761830
74	C	4.706590864147	-4.121906576231	0.956583237761
75	C	2.237155786870	-3.488086167355	3.085993957410
76	C	1.247914075606	-5.555776030386	2.629024781581
77	C	4.644385497581	-6.405391286583	1.503098899665
78	C	5.240840846495	-5.138513211586	1.847306568186
79	C	2.776555572906	-4.455029632875	4.012025091724

80	C	2.163624301473	-5.733667201021	3.730994635267
81	H	3.165029837315	-4.312334378179	-0.703551200893
82	H	0.709085313457	-3.711366739287	1.432967018833
83	H	3.124071484592	-6.946783164285	-0.082499438789
84	H	-3.335415901985	5.971270473456	5.202254084355
85	H	2.518320697016	-2.437728151801	3.023481412893
86	H	0.622328470834	-6.328917146878	2.185959667074
87	H	4.860688697485	-7.361487479413	1.976588812027
88	H	6.002551146207	-4.987397437910	2.608925942821
89	H	3.505314083084	-4.253750670818	4.795212337189
90	H	2.351379897917	-6.664738260423	4.263230320658
91	H	5.655982384670	3.442694295962	0.716780272568

Coordinates of Optimized Compound 2 (FcB)

Atom	angstrom		
	X	Y	Z
1 Fe	-7.547434	10.123398	-1.294159
2 C	-8.671483	9.264950	0.219626
3 C	-6.627499	8.558191	-2.310685
4 C	-9.526258	10.030327	-0.654878
5 C	-7.675124	10.157217	0.789031
6 C	-5.634927	9.445089	-1.752150
7 C	-7.451025	9.324336	-3.219639
8 C	-9.063217	11.396781	-0.646218
9 C	-7.920788	11.476320	0.230022
10 C	-5.845189	10.759132	-2.311879
11 C	-6.967689	10.684865	-3.218949
12 H	-8.770607	8.200080	0.416544
13 H	-6.733085	7.496994	-2.092057
14 H	-10.376545	9.644885	-1.214733
15 H	-1.841596	2.562872	1.261089

16 H	-4.882233	9.180520	-1.011045
17 H	-8.283663	8.942171	-3.807782
18 H	-9.505320	12.227210	-1.194043
19 H	-0.815166	2.412005	-0.264991
20 H	-5.252998	11.647492	-2.098515
21 H	-7.369897	11.507272	-3.808338
22 C	-6.601069	9.785425	1.725471
23 C	-6.613727	8.537407	2.393137
24 C	-5.611680	8.185651	3.302734
25 C	-4.565185	9.089763	3.593696
26 C	-4.555360	10.351136	2.958807
27 C	-5.545377	10.679635	2.028754
28 H	-7.436407	7.841103	2.222322
29 H	-5.651469	7.230362	3.830878
30 H	-7.377673	12.387994	0.468800
31 H	-3.771660	11.065117	3.220264
32 H	-5.505143	11.654408	1.539557
33 N	-3.629303	8.818328	4.624317
34 C	-2.748896	7.863041	4.628161
35 C	-2.323773	6.932367	3.558391
36 C	-2.678645	7.062707	2.189065
37 C	-2.184559	6.155253	1.249973
38 C	-1.327331	5.114095	1.639896
39 C	-0.948027	5.007641	2.987820
40 C	-1.438255	5.900170	3.936355
41 H	-3.326625	7.873911	1.859505
42 H	-2.431045	6.243735	0.190381
43 O	-0.811261	4.283006	0.581632
44 O	-0.016506	4.020628	3.437996
45 H	-1.014310	5.760824	4.943533

46 C	-0.919160	2.844737	0.735858
47 O	0.174419	2.318438	1.594155
48 C	1.473999	2.126411	0.994742
49 C	2.225935	1.070265	1.509723
50 C	3.521066	0.878048	1.015724
51 C	4.064220	1.707670	0.010549
52 C	3.256336	2.773029	-0.479459
53 C	1.960483	3.000348	0.017876
54 H	1.803006	0.432134	2.285586
55 H	4.130047	0.075040	1.430602
56 C	5.464753	1.602200	-0.464416
57 O	3.845960	3.562140	-1.468719
58 H	1.360960	3.852344	-0.297719
59 N	6.236859	0.553024	-0.498919
60 C	5.741669	-0.755124	-0.231063
61 C	6.319402	-1.515442	0.804989
62 C	5.789736	-2.770730	1.128907
63 C	4.706395	-3.318179	0.403057
64 C	4.211006	-2.586776	-0.703755
65 C	4.714888	-1.323652	-1.018413
66 H	7.169199	-1.102614	1.352169
67 H	6.241563	-3.350789	1.936240
68 H	4.317418	-0.756331	-1.863028
69 H	3.396677	-3.002103	-1.301193
70 Fe	2.151309	-4.871131	1.442003
71 C	3.405885	-5.537565	-0.070124
72 C	0.513716	-3.937899	0.556395
73 C	2.962618	-6.651791	0.730015
74 C	4.115332	-4.609519	0.793222
75 C	1.252648	-2.995364	1.364505

76	C	0.068164	-5.010998	1.415406
77	C	3.382853	-6.422715	2.091383
78	C	4.085499	-5.164211	2.134991
79	C	1.265902	-3.486807	2.722161
80	C	0.535480	-4.733735	2.753028
81	H	3.286661	-5.440140	-1.147435
82	H	0.311961	-3.849900	-0.509915
83	H	2.422088	-7.523318	0.364860
84	H	-2.190558	7.747040	5.566613
85	H	1.739486	-2.090274	1.003564
86	H	-0.524869	-5.871394	1.110242
87	H	3.202587	-7.083836	2.937100
88	H	4.509576	-4.704946	3.025653
89	H	1.740444	-3.004331	3.574977
90	H	0.355499	-5.348040	3.633634
91	H	5.910123	2.542678	-0.803442
92	H	0.604999	3.293993	5.322723
93	H	1.802499	4.371501	4.458313
94	H	0.161972	3.232853	2.772138
95	C	3.098459	4.734881	-1.977137
96	C	0.762610	4.282447	4.840436
97	H	3.780572	5.183116	-2.707678
98	H	2.170181	4.406874	-2.470116
99	H	2.891262	5.441895	-1.159000

Coordinates of Optimized Compound 3 (FcC)

Atom	angstrom		
	X	Y	Z
1 Fe	-5.437895	8.100568	-0.310547
2 C	-7.173713	6.961226	-0.291804

3	C	-4.008045	7.009951	-1.365366
4	C	-7.436142	8.248115	-0.887178
5	C	-6.702260	7.171141	1.063741
6	C	-3.552412	7.265753	-0.018398
7	C	-4.234509	8.283356	-2.010498
8	C	-7.120980	9.263915	0.088748
9	C	-6.661789	8.605932	1.287403
10	C	-3.499034	8.698706	0.168075
11	C	-3.917791	9.326515	-1.065064
12	H	-7.299150	5.996695	-0.780522
13	H	-4.156869	6.030742	-1.817655
14	H	-7.812742	8.421111	-1.893664
15	H	-0.967064	6.015956	-0.798783
16	H	-3.329123	6.513796	0.737506
17	H	-4.576390	8.430031	-3.033513
18	H	-7.227104	10.338913	-0.047328
19	H	0.797956	5.803354	-1.298361
20	H	-3.183528	9.216831	1.072197
21	H	-3.980098	10.397756	-1.248847
22	C	-6.268820	6.119295	1.998230
23	C	-6.816403	4.817820	1.941629
24	C	-6.323606	3.788561	2.755278
25	C	-5.237644	4.035494	3.614505
26	C	-4.751479	5.354208	3.755586
27	C	-5.266167	6.377317	2.962055
28	H	-7.652103	4.615754	1.267720
29	H	-6.756470	2.786570	2.720295
30	H	-6.391053	9.097411	2.219791
31	H	-3.953888	5.550384	4.475114
32	H	-4.856738	7.385556	3.054054

33 N	-4.651623	2.966986	4.362406
34 C	-3.393420	2.670124	4.196803
35 C	-2.464755	3.236604	3.186862
36 C	-2.870979	3.478195	1.857443
37 C	-1.971424	3.994357	0.916157
38 C	-0.657655	4.306807	1.299893
39 C	-0.231247	4.055567	2.626851
40 C	-1.129303	3.510633	3.550047
41 H	-3.888269	3.241816	1.543326
42 H	-2.280523	4.112788	-0.121387
43 O	0.320117	4.843222	0.427217
44 O	1.110028	4.239336	3.015188
45 H	-0.763246	3.292999	4.554950
46 C	-0.103149	5.343778	-0.878881
47 O	-0.576703	4.247229	-1.744748
48 C	0.399637	3.268746	-2.064651
49 C	0.170665	1.953210	-1.641633
50 C	1.076946	0.941647	-1.969510
51 C	2.234166	1.241486	-2.725488
52 C	2.445594	2.569110	-3.155476
53 C	1.540044	3.582129	-2.822736
54 H	-0.727417	1.743302	-1.058143
55 H	0.889423	-0.080010	-1.638129
56 C	3.212911	0.196075	-3.119264
57 O	1.771034	4.932218	-3.186325
58 N	3.572314	-0.874940	-2.476924
59 C	3.182373	-1.135468	-1.129136
60 C	3.504489	-0.227661	-0.095300
61 C	3.165823	-0.521915	1.227221
62 C	2.482725	-1.716223	1.559318

63 C	2.188509	-2.626435	0.517388
64 C	2.555552	-2.356001	-0.808342
65 H	4.023822	0.700858	-0.342910
66 H	3.405904	0.194572	2.015860
67 H	2.371225	-3.081552	-1.603256
68 H	1.715966	-3.581054	0.759497
69 Fe	0.989469	-0.860169	4.260450
70 C	0.959359	-2.757624	3.406624
71 C	-0.772877	0.097564	3.686148
72 C	1.013515	-2.859354	4.844887
73 C	2.128704	-2.027057	2.955705
74 C	0.371301	0.822420	3.192361
75 C	-0.678290	0.041338	5.127926
76 C	2.210674	-2.189211	5.294833
77 C	2.895857	-1.669884	4.136824
78 C	1.177869	1.213859	4.321573
79 C	0.528187	0.735231	5.521629
80 H	0.168261	-3.147630	2.768788
81 H	-1.573070	-0.324032	3.080588
82 H	0.281313	-3.357611	5.477935
83 H	-2.960966	1.947078	4.900300
84 H	0.592598	1.036224	2.148105
85 H	-1.388176	-0.440343	5.798304
86 H	2.548586	-2.105331	6.326315
87 H	3.854324	-1.154466	4.135639
88 H	2.084503	1.811530	4.274615
89 H	0.883374	0.870307	6.541896
90 H	3.677780	0.336712	-4.104760
91 C	1.623724	5.654128	2.942914
92 H	3.196893	5.134138	1.560420

93 H	3.601667	4.880545	3.293287
94 C	1.573792	5.216605	-4.652794
95 C	0.107574	5.087481	-5.046364
96 C	3.100987	5.554413	2.574754
97 H	1.464939	6.092258	3.942782
98 H	1.055501	6.212121	2.186022
99 H	3.588933	6.544944	2.617900
100 H	2.210987	4.524285	-5.228958
101 H	1.951061	6.242735	-4.755947
102 H	-0.509945	5.772273	-4.445863
103 H	-0.252327	4.057887	-4.884938
104 H	-0.015351	5.335415	-6.114796
105 H	3.343595	2.831936	-3.720422

APPENDIX II

Computational output data obtained from Gaussian 09 software at DFT/B3LYP/6-31G

Table S2. Computed quantum mechanical parameters and reactivity descriptors of ferrocenyl Schiff bases computed in Gaussian 09 at DFT/B3LYP/6-31G level in gas phase

Corrosion Inhibitors	**E_{HOMO} / eV**	**E_{LUMO} / eV**	**ΔE /eV**	**I / eV**	**A /eV**	**η / eV**	**χ / eV**	**σ /eV^{-1}**	**μ /D**
FcA	-5.200	-1.684	3.515	5.200	1.684	1.757	3.442	0.569	2.388
FcB	-5.210	-1.697	3.510	5.210	1.697	1.755	3.455	0.569	3.437
FcC	-5.200	-1.697	3.502	5.200	1.697	1.749	3.428	0.571	3.397

Table S3. Selected Mulliken atomic charges on the corrosion inhibitors FcA, FcB and FcC calculated at DFT/B3LYP with a 6-31G basis set

Atomic charges (e)	Compounds		
	FcA	**FcB**	**FcC**
q_{Fe}	0.6247 (12)	0.6239 (12)	0.6243 (12)
q_c	-0.20656 (1)	-0.2065(1)	-0.2063 (1)
q_c	-0.2092 (3)	-0.2065(3)	-0.2063 (3)
q_c	-0.2101 (4)	-0.2099(4)	-0.2100 (4)
q_c	-0.2132(5)	-0.2128(5)	-0.2128 (5)
q_N	-0.4244 (23)	-0.4173 (23)	-0.4182 (23)
q_c	-0.1644(14)	-0.1645(14)	-0.1645(14)
q_c	-0.1174(15)	-0.1172(15)	-0.1179(15)
q_O	-0.5465 (35)	-0.5560 (35)	-0.5588 (35)
q_c	0.2295(36)	0.2387(36)	0.2379(36)
q_O	-0.5473(39)	-0.5599(39)	-0.5557(39)
q_c	0.2777(40)	0.2978(40)	0.2914(40)
q_c	-0.1292(41)	0.2573(41)	0.2594(41)
q_c	-0.1639(42)	-0.1710(42)	-0.1691(42)
q_N	-0.4252(50)	-0.4256(50)	-0.4256(50)
q_c	0.1388(52)	0.1367(52)	0.1376(52)
q_c	-0.1761(53)	-0.1767(53)	-0.1766(53)
q_{Fe}	0.6249(73)	0.6241(73)	0.6243(73)
q_c	-0.2098(72)	-0.2099(72)	-0.2099(72)
q_c	-0.2096(71)	-0.2094(71)	-0.2093(71)
q_O	-----	-0.5601(90)	-0.5614(90)
q_O	-----	-0.5516(91)	-0.5601(91)
q_c	-----	-0.1841(92)	-0.0179(92)
q_c	----	-0.1778(93)	-0.0329(93)

Coordinates of Compound 1 (FcA)

Center	Atomic nr	X	Y	Z
1	6	-12.847296	-1.924934	1.950903
2	1	-11.861446	-1.560931	2.194681
3	6	-14.081137	-1.222027	2.157913
4	6	-15.151414	-2.055717	1.688006
5	6	-13.154551	-3.193601	1.353738
6	6	-14.578947	-3.274597	1.191211
7	6	-12.550755	-0.557131	-1.116626
8	6	-13.786701	0.155430	-0.894400
9	6	-14.872339	-0.655598	-1.359444
10	6	-12.901299	-1.827067	-1.710241
11	6	-14.324653	-1.881793	-1.863587
12	26	-13.825136	-1.645836	0.136672
13	6	-11.190873	-0.055970	-0.862942
14	6	-10.936898	1.326989	-0.752189
15	6	-9.653024	1.808086	-0.509120
16	6	-8.562939	0.926045	-0.401345
17	6	-8.806713	-0.459373	-0.501457
18	6	-10.097081	-0.935654	-0.722196
19	1	-11.754364	2.030129	-0.869305
20	1	-9.463249	2.871382	-0.414518
21	1	-7.991741	-1.163176	-0.365165
22	1	-10.264852	-2.007041	-0.766226
23	7	-7.290210	1.486335	-0.156546
24	6	-6.199089	0.939924	-0.582550
25	1	-6.209365	0.042224	-1.217065
26	6	-4.877258	1.479737	-0.269084
27	6	-4.722220	2.626877	0.542656

28	6	-3.460519	3.123748	0.832487
29	6	-2.321028	2.481367	0.317098
30	6	-2.448380	1.344620	-0.491667
31	6	-3.726875	0.854661	-0.776968
32	1	-5.613362	3.105868	0.931024
33	1	-1.580846	0.840412	-0.900272
34	1	-3.829749	-0.026712	-1.404022
35	8	-1.104960	3.058395	0.672547
36	6	0.108494	2.453438	0.218457
37	1	0.180353	1.413054	0.566611
38	1	0.177210	2.493184	-0.878011
39	8	1.123861	3.260702	0.820694
40	6	2.459777	2.914657	0.635602
41	6	3.387213	3.728081	1.302060
42	6	4.745872	3.458469	1.180475
43	6	5.205738	2.379565	0.396310
44	6	4.258891	1.577238	-0.266657
45	6	2.893498	1.836734	-0.153786
46	1	5.464881	4.087446	1.697732
47	1	4.617343	0.750416	-0.869148
48	1	2.187320	1.202870	-0.677055
49	6	6.639335	2.112485	0.290576
50	7	7.116750	1.158509	-0.439605
51	1	7.293115	2.783330	0.865607
52	6	11.245114	0.160215	-0.682797
53	6	10.703945	0.650249	0.524329
54	6	9.359051	0.997537	0.628851
55	6	8.495291	0.855191	-0.476729
56	6	9.020408	0.340363	-1.675543
57	6	10.370709	0.017181	-1.780493

58	1	11.341541	0.740750	1.397761
59	1	8.966200	1.340826	1.580686
60	1	8.349712	0.217589	-2.518607
61	1	10.757534	-0.343217	-2.727479
62	6	12.668405	-0.195690	-0.795229
63	6	13.739345	0.262347	0.060084
64	6	14.977817	-0.253915	-0.441915
65	6	13.274001	-1.015089	-1.818808
66	6	14.690320	-1.043304	-1.604463
67	6	12.324977	-2.936961	1.133888
68	1	11.272774	-2.719946	1.231715
69	6	13.368242	-2.463906	1.998664
70	6	14.616987	-2.976721	1.509668
71	6	12.928137	-3.742670	0.111047
72	6	14.344903	-3.767207	0.342945
73	26	13.696771	-1.810236	0.050512
74	1	15.075297	-4.297329	-0.248000
75	1	15.587464	-2.809314	1.950009
76	1	13.236662	-1.843321	2.871192
77	1	12.406430	-4.248390	-0.686182
78	1	13.631944	0.918946	0.908990
79	1	15.955662	-0.068022	-0.026222
80	1	15.413013	-1.563664	-2.213198
81	1	12.750991	-1.520747	-2.615188
82	1	-14.883808	-2.696195	-2.296801
83	1	-12.204985	-2.587368	-2.027351
84	1	-15.917291	-0.388599	-1.337834
85	1	-15.124002	-4.109586	0.779659
86	1	-16.202407	-1.814072	1.715483
87	1	-14.185867	-0.242638	2.597688

88	1	-12.442175	-3.958319	1.086558
89	1	3.019108	4.551723	1.901515
90	1	-3.321492	4.000754	1.453200
91	1	-13.879905	1.134978	-0.452466

Coordinates of Compound 2 (FcB)

Center	Atomic nr	X	Y	Z
1	6	-11.759679	-3.729283	0.546077
2	1	-10.737457	-3.399916	0.647710
3	6	-12.746319	-3.746745	1.588066
4	6	-13.972206	-4.244243	1.030115
5	6	-12.374956	-4.215899	-0.655798
6	6	-13.743012	-4.533768	-0.356676
7	6	-12.651302	-0.579569	-0.270350
8	6	-13.633973	-0.608634	0.787048
9	6	-14.868427	-1.100429	0.251383
10	6	-13.303056	-1.078049	-1.459964
11	6	-14.663572	-1.390788	-1.138125
12	26	-13.370884	-2.521882	0.026429
13	6	-11.273837	-0.071315	-0.174133
14	6	-10.907735	0.845348	0.833716
15	6	-9.612090	1.349207	0.915087
16	6	-8.622669	0.938297	0.004456
17	6	-8.982900	0.038786	-1.020102
18	6	-10.283046	-0.453768	-1.102561
19	1	-11.656178	1.187701	1.540164
20	1	-9.337957	2.067075	1.679932
21	1	-8.251440	-0.251598	-1.767612
22	1	-10.535564	-1.147735	-1.897766

23	7	-7.331905	1.491970	0.148875
24	6	-6.263534	0.850978	-0.192142
25	1	-6.299561	-0.185957	-0.555183
26	6	-4.928851	1.443313	-0.107403
27	6	-4.739821	2.764428	0.346473
28	6	-3.470386	3.323211	0.422368
29	6	-2.347435	2.550717	0.038262
30	6	-2.523850	1.242079	-0.425313
31	6	-3.807362	0.693239	-0.495041
32	1	-5.595481	3.354615	0.649535
33	1	-1.674388	0.639945	-0.724631
34	1	-3.934564	-0.325052	-0.849936
35	8	-1.103939	3.169112	0.162810
36	6	0.072210	2.410025	-0.132884
37	1	0.136422	1.521857	0.510383
38	1	0.087909	2.118222	-1.192466
39	8	1.132224	3.324563	0.157883
40	6	2.451797	2.897140	-0.001460
41	6	3.458278	3.803722	0.396536
42	6	4.793539	3.417218	0.291176
43	6	5.157647	2.152987	-0.206178
44	6	4.144494	1.267527	-0.614513
45	6	2.805123	1.638929	-0.514146
46	1	5.546887	4.127281	0.615331
47	1	4.426232	0.296142	-1.002542
48	1	2.039664	0.938207	-0.826143
49	6	6.572284	1.787980	-0.288433
50	7	6.967517	0.652347	-0.761480
51	1	7.281918	2.546954	0.068975
52	6	11.025067	-0.615517	-0.897864

53	6	10.577671	0.215025	0.150975
54	6	9.258125	0.656114	0.214446
55	6	8.326974	0.270245	-0.771851
56	6	8.757341	-0.581700	-1.804405
57	6	10.083316	-1.001498	-1.874877
58	1	11.269405	0.500884	0.936761
59	1	8.936795	1.266873	1.052136
60	1	8.033698	-0.888269	-2.551399
61	1	10.399593	-1.628159	-2.701753
62	6	12.423365	-1.068050	-0.972556
63	6	13.569245	-0.415843	-0.381181
64	6	14.749490	-1.133134	-0.762070
65	6	12.923822	-2.205207	-1.708387
66	6	14.350368	-2.239634	-1.582765
67	6	12.150399	-2.979250	1.786050
68	1	11.126814	-2.654910	1.890477
69	6	13.300785	-2.344124	2.363092
70	6	14.463421	-3.087832	1.968814
71	6	12.601503	-4.116117	1.035299
72	6	14.031324	-4.183184	1.147803
73	26	13.460618	-2.374521	0.289648
74	1	14.667463	-4.933061	0.704163
75	1	15.481675	-2.869527	2.250160
76	1	13.292585	-1.468634	2.993263
77	1	11.975146	-4.804160	0.489511
78	1	13.544982	0.487111	0.208389
79	1	15.761262	-0.874519	-0.492002
80	1	15.008520	-2.967771	-2.030304
81	1	12.324929	-2.911946	-2.261011
82	1	-15.407058	-1.763471	-1.825115

83	1	-12.854658	-1.157374	-2.437541
84	1	-15.790773	-1.225529	0.796612
85	1	-14.467286	-4.934202	-1.048731
86	1	-14.899243	-4.387016	1.562940
87	1	-12.590717	-3.447855	2.612761
88	1	-11.891838	-4.335375	-1.612732
89	1	-13.468784	-0.309757	1.810252
90	8	3.208433	5.043276	0.973528
91	8	-3.355115	4.601695	0.959495
92	6	-2.700421	5.644632	0.160604
93	6	2.258010	5.966138	0.340974
94	1	-1.642124	5.421965	0.019206
95	1	-3.199853	5.750908	-0.809587
96	1	-2.825907	6.557671	0.742261
97	1	2.488089	6.082656	-0.724386
98	1	1.233349	5.617462	0.466020
99	1	2.411348	6.913153	0.858518

Coordinates of Compound 3 (FcC)

Center	Atomic nr	X	Y	Z
1	6	-11.731383	-3.968533	0.585418
2	1	-10.712678	-3.630115	0.693020
3	6	-12.718997	-4.014656	1.625493
4	6	-13.938093	-4.517866	1.057952
5	6	-12.339323	-4.443090	-0.625089
6	6	-13.703610	-4.782727	-0.333110
7	6	-12.651409	-0.825133	-0.218279
8	6	-13.606556	-0.865611	0.863858

9	6	-14.852798	-1.357500	0.356534
10	6	-13.331781	-1.318062	-1.394028
11	6	-14.682622	-1.637401	-1.039840
12	26	-13.356838	-2.772455	0.083307
13	6	-11.273218	-0.314158	-0.153650
14	6	-10.868842	0.554996	0.881167
15	6	-9.571853	1.058955	0.934728
16	6	-8.618703	0.697356	-0.034164
17	6	-9.018074	-0.154560	-1.084665
18	6	-10.319018	-0.649221	-1.137245
19	1	-11.588583	0.860421	1.632852
20	1	-9.268306	1.740328	1.721501
21	1	-8.317652	-0.406469	-1.874582
22	1	-10.601159	-1.307065	-1.953007
23	7	-7.325216	1.251159	0.086296
24	6	-6.268400	0.645636	-0.344515
25	1	-6.312188	-0.364657	-0.775219
26	6	-4.935702	1.245110	-0.280160
27	6	-4.734995	2.529640	0.264429
28	6	-3.466826	3.095004	0.325006
29	6	-2.359495	2.364149	-0.173386
30	6	-2.547990	1.093487	-0.726301
31	6	-3.829581	0.537285	-0.776407
32	1	-5.579189	3.083275	0.655480
33	1	-1.709107	0.526153	-1.111601
34	1	-3.967046	-0.451981	-1.202321
35	8	-1.116112	2.989298	-0.066261
36	6	0.057657	2.244515	-0.401525
37	1	0.133830	1.340554	0.217924
38	1	0.060605	1.979900	-1.468196

39	8	1.120566	3.156209	-0.106804
40	6	2.436831	2.709685	-0.229371
41	6	3.443522	3.615391	0.169802
42	6	4.776803	3.216640	0.101185
43	6	5.139213	1.937574	-0.360540
44	6	4.125827	1.054312	-0.772639
45	6	2.787320	1.438697	-0.709212
46	1	5.530656	3.925847	0.426450
47	1	4.406636	0.072882	-1.135474
48	1	2.022716	0.739522	-1.026993
49	6	6.551334	1.557383	-0.406085
50	7	6.945569	0.409994	-0.851201
51	1	7.260714	2.315545	-0.046478
52	6	10.992949	-0.898253	-0.876636
53	6	10.530142	-0.047529	0.149140
54	6	9.213804	0.406987	0.176362
55	6	8.300965	0.014249	-0.824292
56	6	8.746490	-0.857411	-1.834012
57	6	10.069653	-1.290020	-1.868457
58	1	11.206441	0.243748	0.946242
59	1	8.880042	1.033924	0.997083
60	1	8.036663	-1.169569	-2.591867
61	1	10.397719	-1.932542	-2.678379
62	6	12.387520	-1.365917	-0.912665
63	6	13.522595	-0.731300	-0.282757
64	6	14.705701	-1.458419	-0.634625
65	6	12.896790	-2.503478	-1.641813
66	6	14.318921	-2.554336	-1.475446
67	6	12.014810	-3.303829	1.819981
68	1	10.990119	-2.975426	1.897525

69	6	13.150538	-2.679533	2.436877
70	6	14.320946	-3.426791	2.071779
71	6	12.482632	-4.436974	1.073913
72	6	13.907995	-4.512972	1.229108
73	26	13.373852	-2.694390	0.369055
74	1	14.553732	-5.262590	0.799170
75	1	15.331234	-3.216695	2.386197
76	1	13.127742	-1.809958	3.074845
77	1	11.869049	-5.117165	0.504331
78	1	13.491388	0.166148	0.314772
79	1	15.712052	-1.213985	-0.332830
80	1	14.981963	-3.285788	-1.910216
81	1	12.307812	-3.199837	-2.217658
82	1	-15.441969	-2.007595	-1.710628
83	1	-12.908706	-1.390428	-2.383423
84	1	-15.760427	-1.488980	0.924489
85	1	-14.422253	-5.180008	-1.032744
86	1	-14.864016	-4.680651	1.586962
87	1	-12.568612	-3.729424	2.654867
88	1	-11.853608	-4.540113	-1.583393
89	1	-13.416831	-0.573303	1.884666
90	8	3.167708	4.868360	0.707154
91	8	-3.326265	4.316113	0.967423
92	6	-2.635658	5.444014	0.297098
93	6	2.400796	5.840420	-0.105272
94	1	-2.177216	5.097919	-0.631944
95	1	1.388096	5.460962	-0.255428
96	6	2.412349	7.144576	0.671040
97	6	-1.599710	6.006982	1.253393
98	1	-3.415263	6.177455	0.062547

99	1	-2.065715	6.270319	2.208211
100	1	-0.815822	5.267175	1.435396
101	1	-1.145325	6.911826	0.831090
102	1	3.437323	7.494181	0.828273
103	1	1.860287	7.916167	0.121972
104	1	1.940758	7.009268	1.649048
105	1	2.895304	5.944310	-1.080168