

Corrected Supporting information for

**The corrosion inhibition of stainless steel by ferrocene-polyoxometalate hybrid  
molecular materials – experimental and first principles studies**

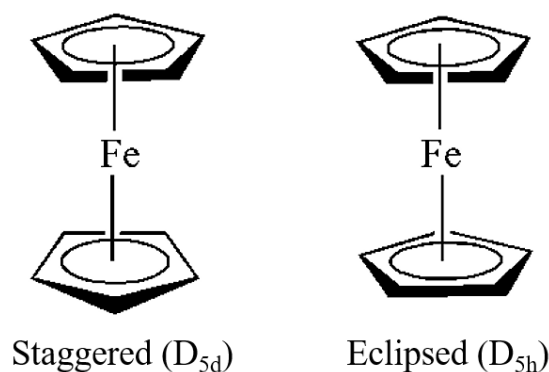
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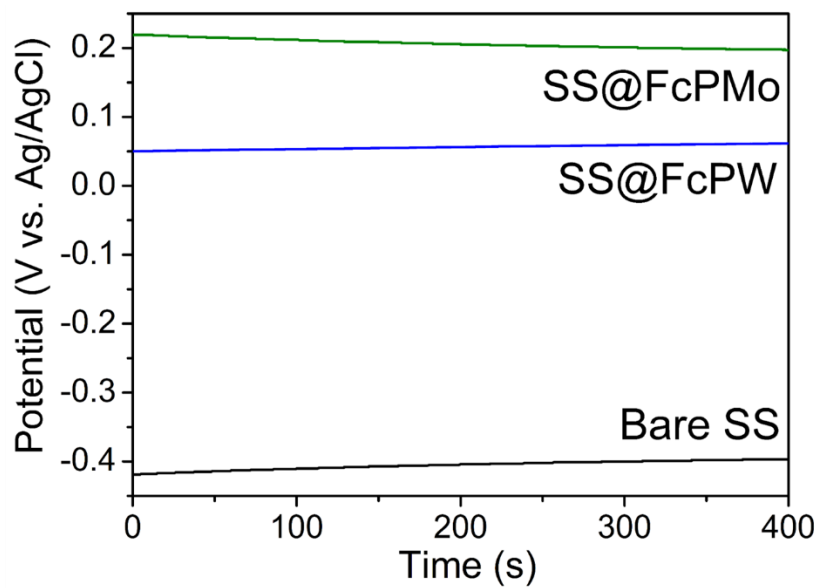


**Figure S1** Staggered and eclipsed forms of ferrocene.

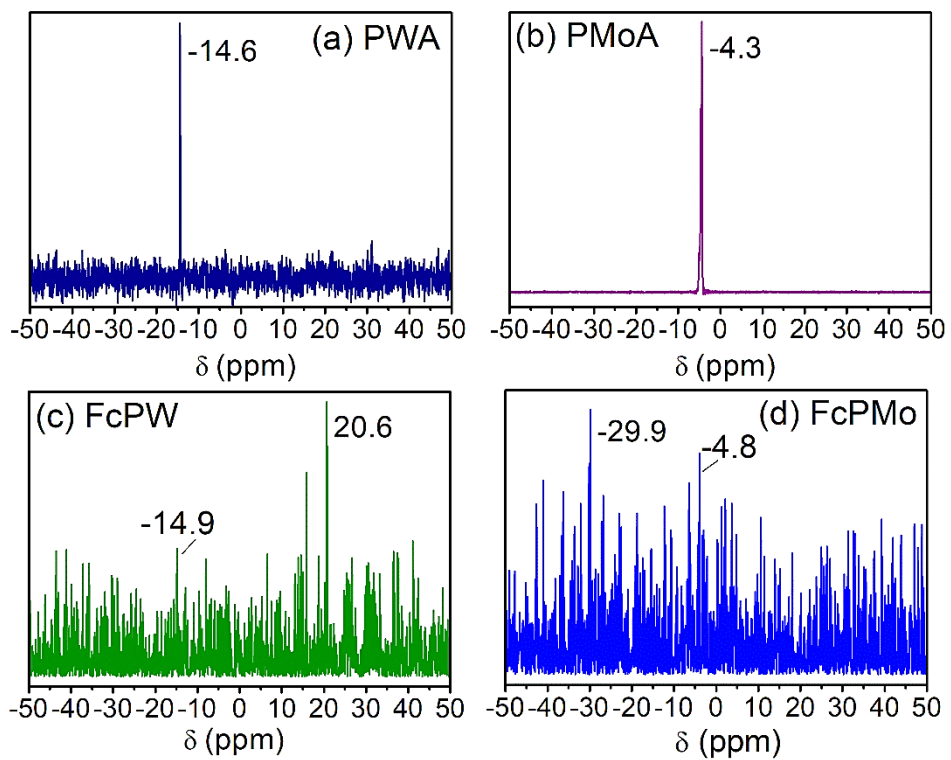
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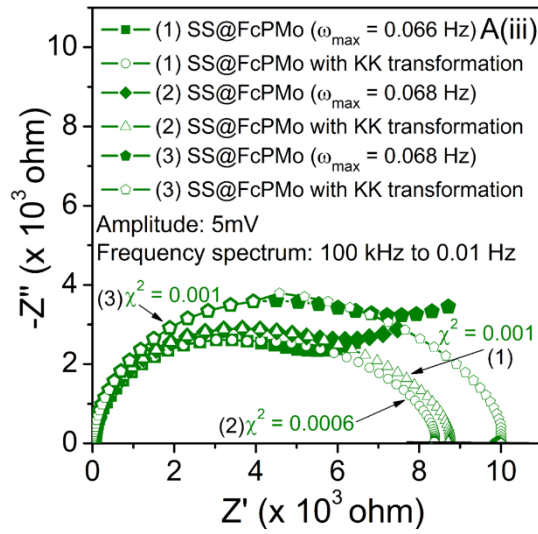
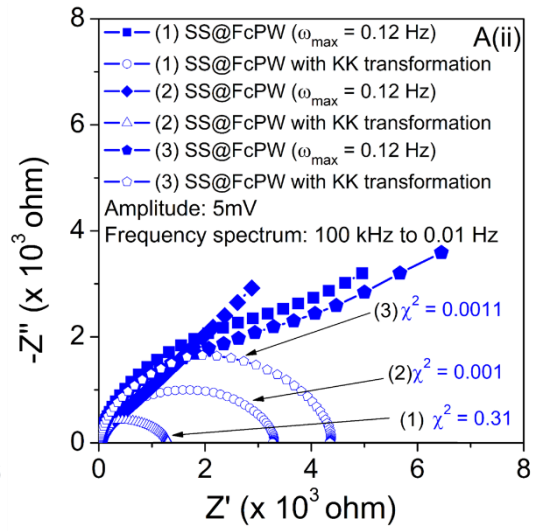
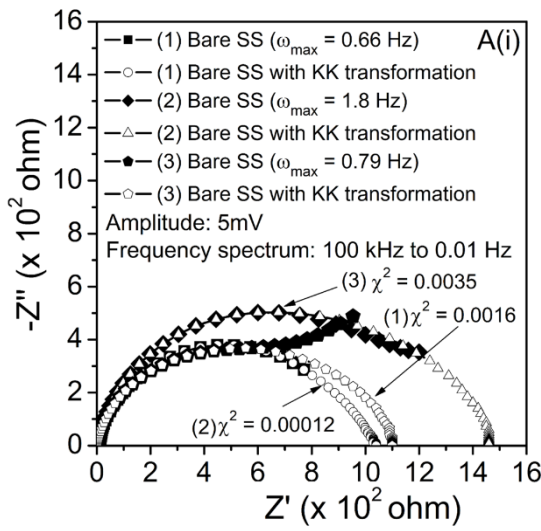
[grrao@iitm.ac.in](mailto:grrao@iitm.ac.in) (G. Ranga Rao).

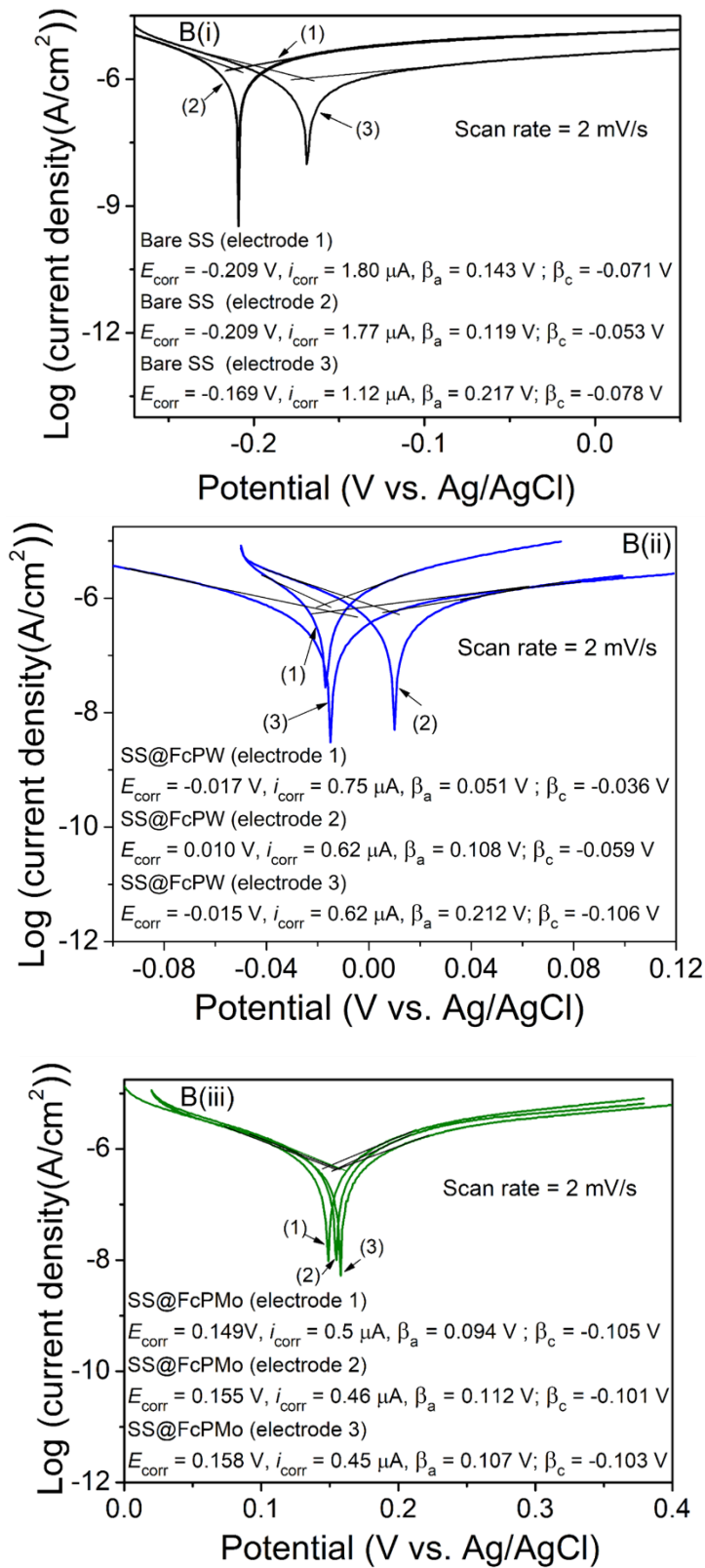


**Figure S2** Steady state open circuit potential vs. time for bare SS, SS@FcPW and SS@FcPMo.

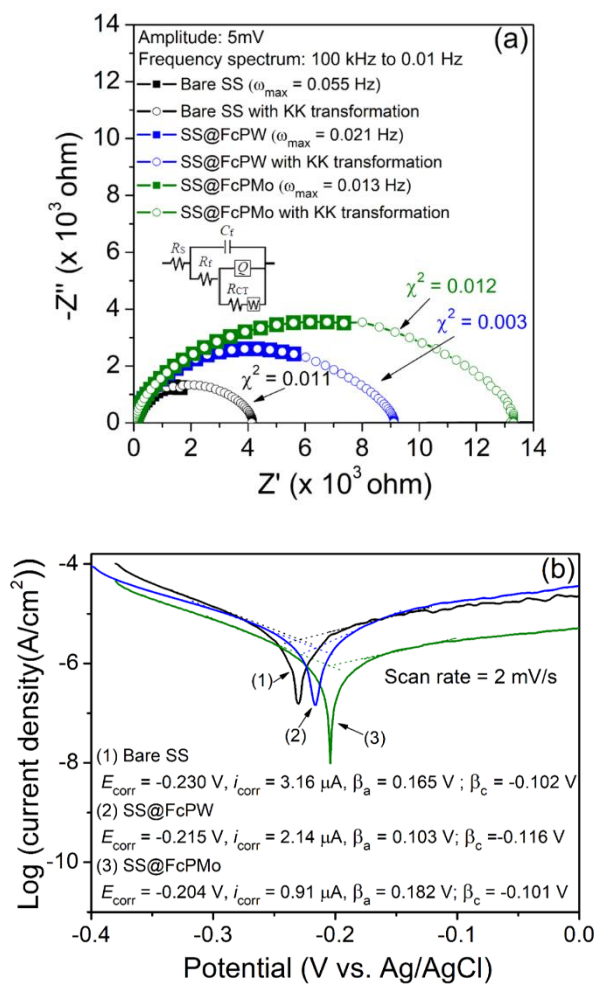


**Figure S3**  $^{31}\text{P}$  MAS spectra of (a) PWA, (b) PMoA, (c) FcPW and (d) FcPMo.

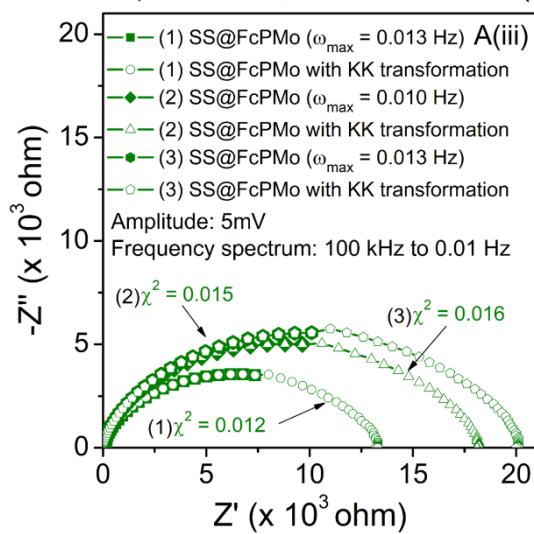
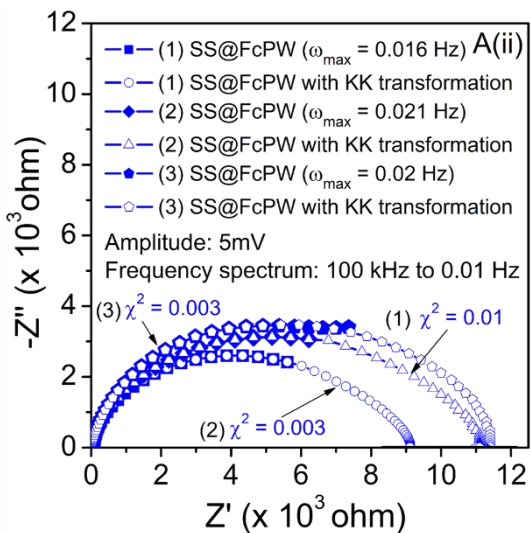
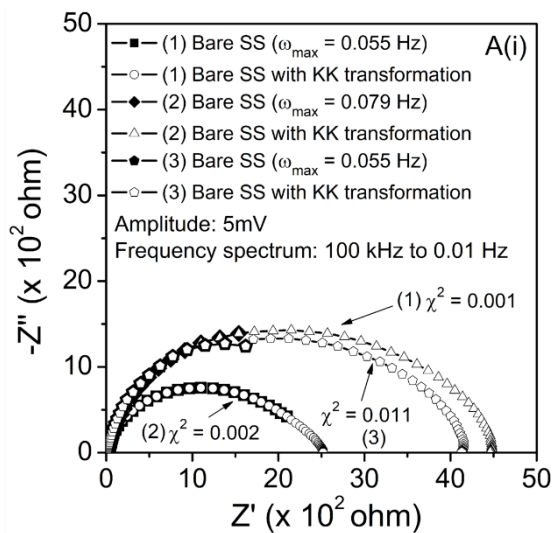


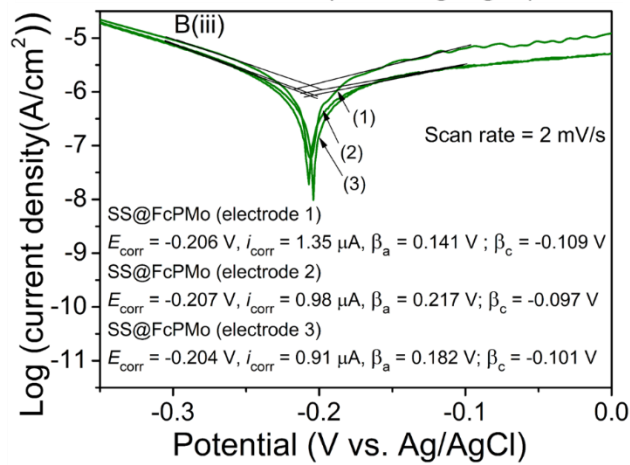
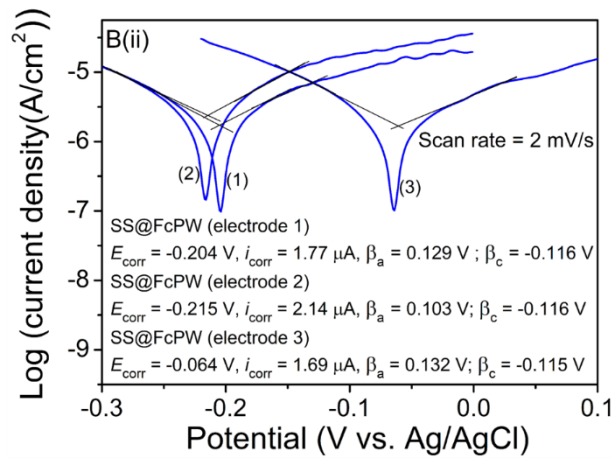
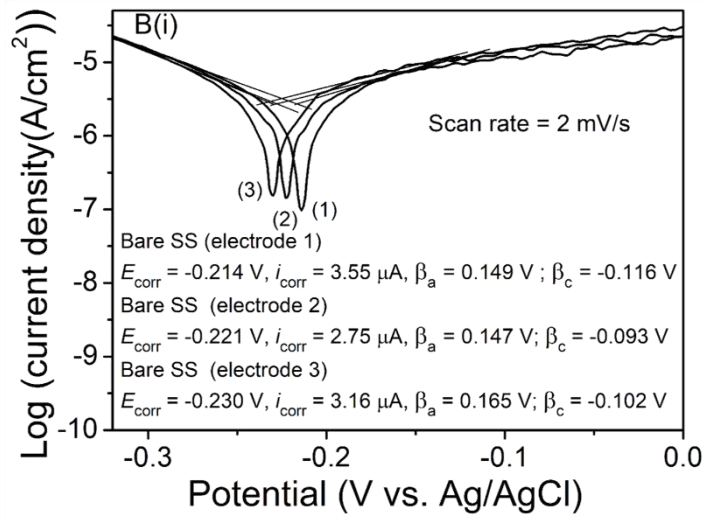


**Figure S4** (A) Nyquist and (B) Tafel plots for repeated corrosion test experiments each for (i) bare SS, (ii) SS@FcPW and (iii) SS@FcPMo in 0.5 M  $\text{H}_2\text{SO}_4$ .

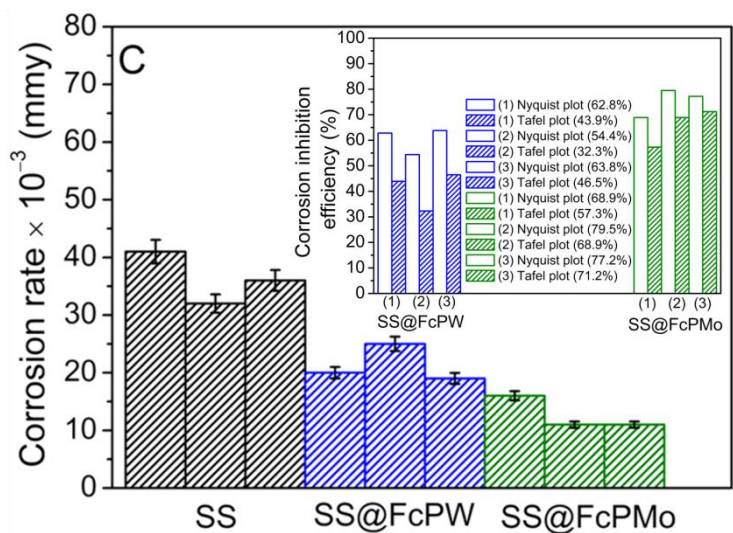


**Figure S5** (a) EIS of SS, SS@FcPW, SS@FcPMo and (b) Tafel plots of SS, SS@FcPW and SS@FcPMo with Ringer's solution as electrolyte.









**Figure S6** (A) Nyquist, (B) Tafel plots of triplicate experiments on corrosion studies of bare SS, SS@FcPMo and SS@FcPW in Ringer's solution. (C) Reproducibility tests with error bars [Fig. S6(C) is corrected, but the inset of the figure S6(C) has no change].

**Table S1** Pore size and pore volume from BET

<b>Hybrid material</b>	<b>Pore size</b>	<b>Pore volume</b>
FcPW	$4.2 \pm 0.025 \text{ m}^2/\text{g}$	Total pore volume of pores less than 1032.3 Å radius at $P/P_0 = 0.99$ was $0.013 \text{ cm}^3/\text{g}$
FcPMo	$6.8 \pm 0.094 \text{ m}^2/\text{g}$	Total pore volume of pores less than 1191.8 Å radius at $P/P_0 = 0.99$ was $0.047 \text{ cm}^3/\text{g}$

**Table S2** Parameters obtained from triplicate experiments for corrosion study in 0.5 M H<sub>2</sub>SO<sub>4</sub>

Electrode	$E_{\text{corr}}$ (V)	$i_{\text{corr}}$ ( $\mu\text{A}$ )	$R_{\text{CT}}$ (ohm $\text{cm}^2$ ) $\eta$ (%) w.r.t. SS2 (cal.)	$R_p$ (ohm $\text{cm}^2$ )	Rate (mmy) from Tafel extrapolation method	Standard deviation	Corrosion inhibition efficiency $\eta$ (%) w.r.t. SS2 (cal.)
SS1 <sup>a</sup>	#Instr.: - 0.209 *Calc.: - 0.209	Instr.: 2.1 Calc.: 1.8	1102	Instr.: 9192 Calc.: 11445	0.0209	0.0045	–
SS2 <sup>a</sup>	Instr.: - 0.209 Calc.: - 0.209	Instr.: 2.1 Calc.: 1.77	1040	Instr.: 8804 Calc.: 8995	0.0205		–
SS3 <sup>a</sup>	Instr.: - 0.169 Calc.: - 0.169	Instr.: 0.93 Calc.: 1.12	1458	Instr.: 25800 Calc.: 22244	0.0130		–
SS@FcPW1 <sup>b</sup>	Instr.: - 0.017 Calc.: - 0.017	Instr.: 0.68 Calc.: 0.75	1309	Instr.: 11961 Calc.: 12218	0.0087	0.00087	EIS: 20.5 Tafel: 57.6
SS@FcPW2 <sup>b</sup>	Instr.: 0.010 Calc.: 0.010	Instr.: 0.62 Calc.: 0.62	3285	Instr.: 26222 Calc.: 26722	0.0072		EIS: 68.3 Tafel: 64.9
SS@FcPW3 <sup>b</sup>	Instr.: - 0.015 Calc.: - 0.015	Instr.: 0.62 Calc.: 0.62	4355	Instr.: 38079 Calc.: 49491	0.0072		EIS: 76.1 Tafel: 64.9
SS@FcPMo1 <sup>c</sup>	Instr.: 0.149 Calc.: 0.149	Instr.: 0.49 Calc.: 0.50	8702	Instr.: 34544 Calc.: 43072	0.0058	0.00032	EIS: 88.0 Tafel: 71.7
SS@FcPMo2 <sup>c</sup>	Instr.: 0.155 Calc.: 0.155	Instr.: 0.56 Calc.: 0.46	8375	Instr.: 33344 Calc.: 37194	0.0053		EIS: 87.6 Tafel: 74.0
SS@FcPMo3 <sup>c</sup>	Instr.: 0.158 Calc.: 0.158	Instr.: 0.54 Calc.: 0.45	9958	Instr.: 39269 Calc.: 49539	0.0052		EIS: 89.5 Tafel: 74.5

<sup>#</sup>Instr. From CH Instrument software

\*Calc. From Tafel extrapolation method

<sup>a</sup>Relative error (%): 14.2%, std. dev. = 0.0045

<sup>b</sup>Relative error (%): 6.5%, std. dev. = 0.00087

<sup>c</sup>Relative error (%): 3.4%, std. dev. = 0.00032

**Table S3** Parameters obtained from Nyquist plot for corrosion studies in Ringer's solution

<b>Electrode</b>	$R_s$ (ohm $\text{cm}^2$ )	$C_f$ ( $\mu\text{F}/\text{cm}^2$ )	$R_f$ (ohm $\text{cm}^2$ )	$Q_{dl}$ ( $\mu\text{F}/\text{cm}^2$ )	$R_{CT}$ (ohm $\text{cm}^2$ )	$\omega_{max}$ (Hz)
Bare Steel (SS) (316 grade)	0.01	-	12.6	496.5	4155	0.055
SS@FcPW	12.2	271.5	0.0013	263.3	9115	0.021
SS@FcPMo	11.9	166.3	0.0089	239.2	13357	0.013

**Table S4** Calculation from Tafel plots of electrodes immersed in Ringer's solution using Tafel extrapolation method

<b>Electrode</b>	$E_{corr}$ (V)	$i_{corr}$ ( $\mu\text{A}/\text{cm}^2$ )	$R_p$ (ohm $\text{cm}^2$ )	<b>Corrosion rate (mmy)</b>	<b>%Corrosion inhibition</b>
SS	-0.230	3.16	7709	0.036	-
SS@FcPW	-0.215	2.14	11070	0.025	32.3
SS@FcPMo	-0.204	0.91	30993	0.011	71.2

**Table S5** Experimental errors and standard deviations from triplicate experiments for corrosion study in Ringer's solution

Electrode	Tafel plot parameters					Nyquist plots	
	$E_{\text{corr}}$ (V)	$i_{\text{corr}}$ ( $\mu\text{A}$ )	Corrosion rate (mmy)	$\eta$ (%) w.r.t. SS3 (calc.)	$R_p$ (ohm $\text{cm}^2$ )	$R_{\text{CT}}$ (ohm $\text{cm}^2$ )	$\eta$ (%) w.r.t. SS3
SS 1 <sup>a</sup>	-0.214	#Instr.: 3.47 *Calc.: 3.55	Instr.: 0.040 Calc.: 0.041	-	Instr.: 7946 Calc.: 8962	4494	-
SS 2 <sup>a</sup>	-0.223	Instr.: 3.6 Calc.: 2.75	Instr.: 0.042 Calc.: 0.032	-	Instr.: 6710 Calc.: 8994	2514	-
SS 3 <sup>a</sup>	-0.230	Instr.: 3.6 Calc.: 3.16	Instr.: 0.042 Calc.: 0.036	-	Instr.: 7642 Calc.: 7709	4155	-
SS@FcPW1 <sup>b</sup>	-0.204	Instr.: 3.55 Calc.: 1.77	Instr.: 0.041 Calc.: 0.020	43.9	Instr.: 10490 Calc.: 14983	11174	62.8
SS@FcPW2 <sup>b</sup>	-0.215	Instr.: 2.85 Calc.: 2.14	Instr.: 0.033 Calc.: 0.025	32.3	Instr.: 8428 Calc.: 11070	9115	54.4
SS@FcPW3 <sup>b</sup>	-0.064	Instr.: 2.32 Calc.: 1.69	Instr.: 0.027 Calc.: 0.019	46.5	Instr.: 11367 Calc.: 15790	11479	63.8
SS@FcPMo1 <sup>c</sup>	-0.206	Instr.: 1.68 Calc.: 1.35	Instr.: 0.019 Calc.: 0.016	57.3	Instr.: 15996 Calc.: 19773	13357	68.9
SS@FcPMo2 <sup>c</sup>	-0.207	Instr.: 1.13 Calc.: 0.98	Instr.: 0.013 Calc.: 0.011	68.9	Instr.: 24840 Calc.: 29701	20281	79.5
SS@FcPMo3 <sup>c</sup>	-0.204	Instr.: 1.16 Calc.: 0.91	Instr.: 0.013 Calc.: 0.011	71.2	Instr.: 24781 Calc.: 30993	18211	77.2

#Instr.. From CH Instrument software

\*Calc. From Tafel extrapolation method

<sup>a</sup>Relative error (%): 7.2%, std. dev. = 0.0045

<sup>b</sup>Relative error (%): 8.7%, std. dev. = 0.0032

<sup>c</sup>Relative error (%): 13.2%, std. dev. = 0.0029

**Table S6** Bond angles between atoms in FcPW optimized structure in aqueous phase

Atoms	Bond length (Å)	Atoms	Bond length (Å)	Atoms	Bond length (Å)	Atoms	Bond length (Å)
W1-O18	1.718	W8-O39	1.8895	C56-H66	1.0848	C83-H92	1.0864
W1-O19	1.906	W8-O53	1.7321	C57-C58	1.4289	C84-C85	1.4321
W1-O21	1.943	W9-O16	1.9338	C57-H67	1.0855	C84-H93	1.0867
W1-O26	1.929	W9-O20	1.9146	C58-C59	1.4238	C85-H94	1.0861
W1-O37	2.4	W9-O28	1.9348	C58-H68	1.0878	C96-Fe97	2.1298
W1-O39	1.962	W9-O32	1.9128	C59-H69	1.0868	C96-C98	1.4225
W2-O14	1.92	W9-O42	2.488	C60-C61	1.4373	C96-C99	1.4265
W2-O20	1.917	W9-O44	1.7174	C60-C64	1.4308	C96-H107	1.0859
W2-O22	2.497	W10-O14	1.9496	C60-H70	1.087	Fe97-C98	2.1109
W2-O25	1.917	W10-O22	2.4762	C61-C62	1.4377	Fe97-C99	2.0712
W2-O38	1.967	W10-O24	1.9306	C61-H71	1.0864	Fe97-C100	2.0284
W2-O48	1.724	W10-O31	1.9299	C62-C63	1.4291	Fe97-C101	2.0495
W3-O17	1.908	W10-O34	1.9101	C62-H72	1.0863	Fe97-C102	2.0632
W3-O19	1.958	W10-O52	1.726	C63-C64	1.4256	Fe97-C103	2.0597
W3-O30	1.929	W11-O27	1.9052	C63-H73	1.0865	Fe97-C104	2.0874
W3-O33	2.464	W11-O30	1.929	C64-H74	1.0866	Fe97-C105	2.0996
W3-O40	1.962	W11-O31	1.9672	C75-Fe76	2.0539	Fe97-C106	2.0836
W3-O46	1.709	W11-O33	2.4345	C75-C77	1.4369	C98-C101	1.4307
W4-O26	1.925	W11-O41	1.9232	C75-C78	1.4338	C98-H108	1.0849
W4-O29	1.896	W11-O49	1.7254	C75-H86	1.0861	C99-C100	1.4359
W4-O35	1.94	W12-O35	1.9221	Fe76-C77	2.0371	C99-H109	1.0841
W4-O36	1.929	W12-O40	1.9033	Fe76-C78	2.0958	C100-C101	1.4366
W4-O51	1.73	W12-O41	1.943	Fe76-C79	2.1061	C100-H110	1.0847
W5-O17	1.941	W12-O45	1.7217	Fe76-C80	2.0642	C101-H111	1.085
W5-O21	1.929	W12-O47	1.9423	Fe76-C81	2.1045	C102-C103	1.4358
W5-O22	2.452	P13-O22	1.5471	Fe76-C82	2.0559	C102-C106	1.4305
W5-O25	1.932	P13-O33	1.5492	Fe76-C83	2.0346	C102-H112	1.0859
W5-O34	1.954	P13-O37	1.5526	Fe76-C84	2.0597	C103-C104	1.4323
W5-O50	1.709	P13-O42	1.5392	Fe76-C85	2.1019	C103-H113	1.0847
W6-O16	1.963	C54-Fe55	2.0346	C77-C80	1.435	C104-C105	1.4269
W6-O23	1.883	C54-C56	1.4377	C77-H87	1.0869	C104-H114	1.0843
W6-O29	1.961	C54-C57	1.4382	C78-C79	1.425	C105-C106	1.4275
W6-O43	1.717	C54-H65	1.0862	C78-H88	1.0872	C105-H115	1.0845
W6-O47	1.898	Fe55-C56	2.0469	C79-C80	1.4274	C106-H116	1.0864
W7-O15	1.711	Fe55-C57	2.0738	C79-H89	1.0862	O117-H118	0.9684
W7-O23	1.955	Fe55-C58	2.1231	C80-H90	1.0856	O117-H119	0.9705
W7-O24	1.904	Fe55-C59	2.1031	C81-C82	1.429	O120-H121	0.9722
W7-O27	1.929	Fe55-C60	2.0584	C81-C85	1.4246	O120-H122	0.9706

W7-O32	1.927	Fe55-C61	2.04	C81-H95	1.0864	O123-H124	0.9684
W7-O42	2.481	Fe55-C62	2.0675	C82-C83	1.4374	O123-H125	0.9697
W8-O28	1.914	Fe55-C63	2.1094	C82-H91	1.0856	O126-H127	0.9693
W8-O36	1.975	Fe55-C64	2.1029	C83-C84	1.4374	O126-H128	0.9698
W8-O38	1.92	C56-C59	1.4315				

**Table S7** Bond lengths between atoms in FcPMo optimized structure in aqueous phase

Atoms	Bond length (Å)	Atoms	Bond length (Å)	Atoms	Bond length (Å)	Atoms	Bond length (Å)
Mo1-O18	1.6804	Mo8-O38	1.8544	C56-H66	1.0843	C84-H93	1.0856
Mo1-O19	1.8735	Mo8-O39	1.8576	C57-C58	1.4283	C85-H94	1.0868
Mo1-O21	1.9799	Mo8-O53	1.7064	C57-H67	1.0863	C96-Fe97	2.1113
Mo1-O26	1.8977	Mo9-O16	1.8731	C58-C59	1.4243	C96-C98	1.4234
Mo1-O37	2.3819	Mo9-O20	1.9576	C58-H68	1.0869	C96-C99	1.4294
Mo1-O39	2.0029	Mo9-O28	1.8972	C59-H69	1.0866	C96-H107	1.0868
Mo2-O14	1.8594	Mo9-O32	1.948	C60-C61	1.4372	Fe97-C98	2.1079
Mo2-O20	1.8748	Mo9-O42	2.4752	C60-C64	1.4319	Fe97-C99	2.0553
Mo2-O22	2.4908	Mo9-O44	1.6907	C60-H70	1.0872	Fe97-C100	2.0283
Mo2-O25	1.9492	Mo10-O14	2.0096	C61-C62	1.4372	Fe97-C101	2.0562
Mo2-O38	2.0381	Mo10-O22	2.4857	C61-H71	1.0868	Fe97-C102	2.0507
Mo2-O48	1.6952	Mo10-O24	1.964	C62-C63	1.4284	Fe97-C103	2.0604
Mo3-O17	1.8711	Mo10-O31	1.8645	C62-H72	1.0862	Fe97-C104	2.0908
Mo3-O19	1.9818	Mo10-O34	1.8673	C63-C64	1.4248	Fe97-C105	2.0901
Mo3-O30	1.8987	Mo10-O52	1.7001	C63-H73	1.0855	Fe97-C106	2.0657
Mo3-O33	2.4196	Mo11-O27	1.8651	C64-H74	1.0862	C98-C101	1.4302
Mo3-O40	1.9939	Mo11-O30	1.9582	C75-Fe76	2.0529	C98-H108	1.0863
Mo3-O46	1.6839	Mo11-O31	2.0286	C75-C77	1.4369	C99-C100	1.4372
Mo4-O26	1.9435	Mo11-O33	2.4677	C75-C78	1.4331	C99-H109	1.0856
Mo4-O29	1.8532	Mo11-O41	1.8538	C75-H86	1.0871	C100-C101	1.4375
Mo4-O35	2.0281	Mo11-O49	1.7015	Fe76-C77	2.0363	C100-H110	1.0866
Mo4-O36	1.8651	Mo12-O33	2.5073	Fe76-C78	2.0948	C101-H111	1.0856
Mo4-O37	2.5092	Mo12-O35	1.8564	Fe76-C79	2.1049	C102-C103	1.4366
Mo4-O51	1.7035	Mo12-O40	1.8758	Fe76-C80	2.0628	C102-C106	1.4337
Mo5-O17	1.9793	Mo12-O41	2.0147	Fe76-C81	2.1014	C102-H112	1.086
Mo5-O21	1.8747	Mo12-O45	1.6954	Fe76-C82	2.0551	C103-C104	1.4315
Mo5-O22	2.4145	Mo12-O47	1.9712	Fe76-C83	2.0345	C103-H113	1.0859
Mo5-O25	1.8952	P13-O22	1.5499	Fe76-C84	2.0601	C104-C105	1.4256
Mo5-O34	2.003	P13-O33	1.5498	Fe76-C85	2.1015	C104-H114	1.0862
Mo5-O50	1.6807	P13-O37	1.5524	C77-C80	1.4364	C105-C106	1.4292
Mo6-O16	1.969	P13-O42	1.5393	C77-H87	1.0862	C105-H115	1.0861
Mo6-O23	1.8621	C54-Fe55	2.0357	C78-C79	1.4255	C106-H116	1.087
Mo6-O29	1.9947	C54-C56	1.4378	C78-H88	1.0859	O117-H118	0.9693
Mo6-O42	2.495	C54-C57	1.4377	C79-C80	1.4283	O117-H119	0.9701
Mo6-O43	1.6895	C54-H65	1.0871	C79-H89	1.0863	O120-H121	0.9736
Mo6-O47	1.8634	Fe55-C56	2.0456	C80-H90	1.0858	O120-H122	0.9708
Mo7-O15	1.6852	Fe55-C57	2.0764	C81-C82	1.4297	O123-H124	0.9698
Mo7-O23	1.9848	Fe55-C58	2.12	C81-C85	1.4236	O123-H125	0.9701
Mo7-O24	1.868	Fe55-C59	2.0963	C81-H95	1.0872	O126-H127	0.9698
Mo7-O27	1.9717	Fe55-C60	2.0555	C82-C83	1.437	O126-H128	0.9713
Mo7-O32	1.8889	Fe55-C61	2.0376	C82-H91	1.0864	O129-H130	0.9715
Mo7-O42	2.4498	Fe55-C62	2.0659	C83-C84	1.4367	O129-H131	0.9748
Mo8-O28	1.9321	Fe55-C63	2.1075	C83-H92	1.0866	O132-H133	0.9709
Mo8-O36	2.0508	Fe55-C64	2.0986	C84-C85	1.4311	O132-H134	0.9718
Mo8-O37	2.5086	C56-C59	1.4321				



**Table S8** Bond angles between atoms in FcPW optimized structure in aqueous phase

Atoms	Angle (deg.)	Atoms	Angle (deg.)	Atoms	Angle (deg.)	Atoms	Angle (deg.)
O18-W1-O19	105.19	O24-W10-O52	102.98	C54-C57-H67	126.63	C81-C82-C83	108.1
O18-W1-O21	105.51	O31-W10-O34	91.26	Fe55-C57-C58	71.96	C81-C82-H91	124.67
O18-W1-O26	96.08	O31-W10-O52	101.68	Fe55-C57-H67	124.37	C83-C82-H91	127.19
O18-W1-O37	163.26	O34-W10-O52	102.35	C58-C57-H67	125.27	Fe76-C83-C82	70.23
O18-W1-O39	95.76	O27-W11-O30	155.77	Fe55-C58-C57	68.25	Fe76-C83-C84	70.39
O19-W1-O21	85.35	O27-W11-O31	83.88	Fe55-C58-C59	69.56	Fe76-C83-H92	124.06
O19-W1-O26	92.77	O27-W11-O33	84.75	Fe55-C58-H68	124.52	C82-C83-C84	107.63
O19-W1-O37	87.84	O27-W11-O41	91.64	C57-C58-C59	108.2	C82-C83-H92	126.37
O19-W1-O39	158.97	O27-W11-O49	103.26	C57-C58-H68	126.11	C84-C83-H92	125.99
O21-W1-O26	158.07	O30-W11-O31	86.82	C59-C58-H68	125.55	Fe76-C84-C83	68.51
O21-W1-O37	85.67	O30-W11-O33	71.92	Fe55-C59-C56	67.72	Fe76-C84-C85	71.47
O21-W1-O39	87.29	O30-W11-O41	87.84	Fe55-C59-C58	71.07	Fe76-C84-H93	125.26
O26-W1-O37	72.42	O30-W11-O49	100.52	Fe55-C59-H69	123.63	C83-C84-C85	107.78
O26-W1-O39	86.77	O31-W11-O33	83.05	C56-C59-C58	108.29	C83-C84-H93	125.92
O37-W1-O39	71.95	O31-W11-O41	156.05	C56-C59-H69	126.5	C85-C84-H93	126.3
O14-W2-O20	90.2	O31-W11-O49	101.7	C58-C59-H69	125.07	Fe76-C85-C81	70.3
O14-W2-O22	71.31	O33-W11-O41	73.11	Fe55-C60-C61	68.78	Fe76-C85-C84	68.29
O14-W2-O25	87.91	O33-W11-O49	171	Fe55-C60-C64	71.57	Fe76-C85-H94	125.31
O14-W2-O38	155.1	O41-W11-O49	102.22	Fe55-C60-H70	123.28	C81-C85-C84	108.38
O14-W2-O48	103.8	O35-W12-O40	89.99	C61-C60-C64	107.82	C81-C85-H94	125.05
O20-W2-O22	84.41	O35-W12-O41	153.33	C61-C60-H70	125.52	C84-C85-H94	126.53
O20-W2-O25	154.2	O35-W12-O45	101.28	C64-C60-H70	126.62	Fe97-C96-C98	69.69
O20-W2-O38	83.97	O35-W12-O47	84.81	Fe55-C61-C60	70.16	Fe97-C96-C99	67.95
O20-W2-O48	102.3	O40-W12-O41	87.51	Fe55-C61-C62	70.54	Fe97-C96-H107	125.27
O22-W2-O25	70.58	O40-W12-O45	103.11	Fe55-C61-H71	124.68	C98-C96-C99	108.11
O22-W2-O38	83.99	O40-W12-O47	154.21	C60-C61-C62	107.77	C98-C96-H107	126
O22-W2-O48	171.9	O41-W12-O45	105.14	C60-C61-H71	125.43	C99-C96-H107	125.8
O25-W2-O38	86.96	O41-W12-O47	85.99	C62-C61-H71	126.81	C96-Fe97-C98	39.19

O25-W2-O48	103.2	O45-W12-O47	102.68	Fe55-C62-C61	68.49	C96-Fe97-C99	39.67
O38-W2-O48	101.1	O22-P13-O33	109.97	Fe55-C62-C63	71.58	C96-Fe97-C100	67.7
O17-W3-O19	84.54	O22-P13-O37	109.28	Fe55-C62-H72	123.85	C96-Fe97-C101	67.22
O17-W3-O30	91.53	O22-P13-O42	109.61	C61-C62-C63	107.86	C96-Fe97-C102	146.28
O17-W3-O33	84.07	O33-P13-O37	109.64	C61-C62-H72	126.92	C96-Fe97-C103	115.54
O17-W3-O40	154.3	O33-P13-O42	109.31	C63-C62-H72	125.19	C96-Fe97-C104	110.88
O17-W3-O46	105.4	O37-P13-O42	109.02	Fe55-C63-C62	68.42	C96-Fe97-C105	134.4
O19-W3-O30	156.3	W2-O14-W10	128.29	Fe55-C63-C64	69.97	C96-Fe97-C106	172.82
O19-W3-O33	85.15	W6-O16-W9	131.4	Fe55-C63-H73	123.27	C98-Fe97-C99	66.93
O19-W3-O40	86.4	W3-O17-W5	152.55	C62-C63-C64	108.3	C98-Fe97-C100	68
O19-W3-O46	104.7	W1-O19-W3	149.09	C62-C63-H73	125.58	C98-Fe97-C101	40.19
O30-W3-O33	71.23	W2-O20-W9	152.43	C64-C63-H73	125.91	C98-Fe97-C102	116.99
O30-W3-O40	87.22	W1-O21-W5	149.2	Fe55-C64-C60	68.23	C98-Fe97-C103	112.13
O30-W3-O46	98.86	W2-O22-W5	89.05	Fe55-C64-C63	70.47	C98-Fe97-C104	135.73
O33-W3-O40	71.22	W2-O22-W10	88.88	Fe55-C64-H74	122.95	C98-Fe97-C105	173.33
O33-W3-O46	166.7	W2-O22-P13	126.61	C60-C64-C63	108.25	C98-Fe97-C106	146.67
O40-W3-O46	100.1	W5-O22-W10	89.39	C60-C64-H74	126.96	C99-Fe97-C100	40.99
O26-W4-O29	154.7	W5-O22-P13	125.78	C63-C64-H74	124.58	C99-Fe97-C101	68.46
O26-W4-O35	84.96	W10-O22-P13	125.28	Fe76-C75-C77	68.81	C99-Fe97-C102	173.88
O26-W4-O36	87.21	W6-O23-W7	130.29	Fe76-C75-C78	71.37	C99-Fe97-C103	143.59
O26-W4-O51	101.3	W7-O24-W10	152.05	Fe76-C75-H86	125.63	C99-Fe97-C104	113.06
O29-W4-O35	84.68	W2-O25-W5	128.75	C77-C75-C78	107.84	C99-Fe97-C105	109.06
O29-W4-O36	91.91	W1-O26-W4	128	C77-C75-H86	125.83	C99-Fe97-C106	133.84
O29-W4-O51	103.6	W7-O27-W11	152.13	C78-C75-H86	126.33	C100-Fe97-C101	41.25
O35-W4-O36	153.6	W8-O28-W9	152	C75-Fe76-C77	41.12	C100-Fe97-C102	134.76
O35-W4-O51	103	W4-O29-W6	151.08	C75-Fe76-C78	40.41	C100-Fe97-C103	175.37
O36-W4-O51	103.3	W3-O30-W11	127.04	C75-Fe76-C79	67.63	C100-Fe97-C104	142.67
O17-W5-O21	84.78	W10-O31-W11	152.07	C75-Fe76-C80	68.49	C100-Fe97-C105	112.86
O17-W5-O22	83.41	W7-O32-W9	129.45	C75-Fe76-C81	156.11	C100-Fe97-C106	109.17
O17-W5-O25	154.7	W3-O33-W11	89.66	C75-Fe76-C82	163.08	C101-Fe97-C102	111.13
O17-W5-O34	87.45	W3-O33-P13	125.51	C75-Fe76-C83	126.44	C101-Fe97-C103	135.94
O17-W5-O50	105.2	W11-O33-P13	126.8	C75-Fe76-C84	109.59	C101-Fe97-C104	175.32
O21-W5-O22	85.4	W5-O34-W10	127.5	C75-Fe76-C85	122.79	C101-Fe97-C105	144.5
O21-W5-O25	90.44	W4-O35-W12	153.32	C77-Fe76-C78	68.29	C101-Fe97-C106	115.09
O21-W5-O34	156.32	W4-O36-W8	127.23	C77-Fe76-C79	68.05	C102-Fe97-C103	40.76
O21-W5-O50	104.13	W1-O37-P13	126.09	C77-Fe76-C80	40.95	C102-Fe97-C104	67.87
O22-W5-O25	71.43	W2-O38-W8	151.02	C77-Fe76-C81	161.58	C102-Fe97-C105	67.49
O22-W5-O34	71.48	W1-O39-W8	127.89	C77-Fe76-C82	124.05	C102-Fe97-C106	40.35
O22-W5-O50	167.52	W3-O40-W12	128.96	C77-Fe76-C83	105.86	C103-Fe97-C104	40.4
O25-W5-O34	87.09	W11-O41-W12	127.21	C77-Fe76-C84	120.15	C103-Fe97-C105	67.59
O25-W5-O50	100.08	W7-O42-W9	88.64	C77-Fe76-C85	156.21	C103-Fe97-C106	68.01
O34-W5-O50	99.49	W7-O42-P13	125.44	C78-Fe76-C79	39.65	C104-Fe97-C105	39.85

O16-W6-O23	87.8	W9-O42-P13	125.8	C78-Fe76-C80	67.45	C104-Fe97-C106	67.35
O16-W6-O29	82.26	W6-O47-W12	151.46	C78-Fe76-C81	121.59	C105-Fe97-C106	39.9
O16-W6-O43	103.11	Fe55-C54-C56	69.83	C78-Fe76-C82	153.4	C96-C98-Fe97	71.12
O16-W6-O47	151.82	Fe55-C54-C57	70.98	C78-Fe76-C83	165.22	C96-C98-C101	108.42
O23-W6-O29	154.73	Fe55-C54-H65	124.01	C78-Fe76-C84	128.96	C96-C98-H108	125.31
O23-W6-O43	102.14	C56-C54-C57	107.51	C78-Fe76-C85	111.38	Fe97-C98-C101	67.59
O23-W6-O47	93.02	C56-C54-H65	125.89	C79-Fe76-C80	40.02	Fe97-C98-H108	124.24
O29-W6-O43	102.72	C57-C54-H65	126.6	C79-Fe76-C81	108.67	C101-C98-H108	126.17
O29-W6-O47	85.22	C54-Fe55-C56	41.25	C79-Fe76-C82	118.45	C96-C99-Fe97	72.38
O43-W6-O47	104.23	C54-Fe55-C57	40.97	C79-Fe76-C83	152.4	C96-C99-C100	108.13
O15-W7-O23	104.34	C54-Fe55-C58	67.82	C79-Fe76-C84	165.24	C96-C99-H109	125.33
O15-W7-O24	101.56	C54-Fe55-C59	68.19	C79-Fe76-C85	127.96	Fe97-C99-C100	67.91
O15-W7-O27	102.61	C54-Fe55-C60	122.04	C80-Fe76-C81	124.92	Fe97-C99-H109	125.26
O15-W7-O32	103.56	C54-Fe55-C61	107.24	C80-Fe76-C82	105.33	C100-C99-H109	126.53
O15-W7-O42	172.36	C54-Fe55-C62	124.11	C80-Fe76-C83	117.69	Fe97-C100-C99	71.1
O23-W7-O24	154.04	C54-Fe55-C63	160.65	C80-Fe76-C84	153.98	Fe97-C100-C101	70.16
O23-W7-O27	86.47	C54-Fe55-C64	157.91	C80-Fe76-C85	162.58	Fe97-C100-H110	124.35
O23-W7-O32	84.82	C56-Fe55-C57	68.5	C81-Fe76-C82	40.16	C99-C100-C101	107.61
O23-W7-O42	70.32	C56-Fe55-C58	67.39	C81-Fe76-C83	68.17	C99-C100-H110	125.92
O24-W7-O27	86.18	C56-Fe55-C59	40.33	C81-Fe76-C84	67.6	C101-C100-H110	126.47
O24-W7-O32	90.92	C56-Fe55-C60	106.27	C81-Fe76-C85	39.59	Fe97-C101-C98	72.21
O24-W7-O42	84.07	C56-Fe55-C61	122.68	C82-Fe76-C83	41.14	Fe97-C101-C100	68.59
O27-W7-O32	153.73	C56-Fe55-C62	160.24	C82-Fe76-C84	68.64	Fe97-C101-H111	124.63
O27-W7-O42	82.79	C56-Fe55-C63	157.34	C82-Fe76-C85	67.5	C98-C101-C100	107.73
O32-W7-O42	70.94	C56-Fe55-C64	121.71	C83-Fe76-C84	41.1	C98-C101-H111	125.91
O28-W8-O36	86.92	C57-Fe55-C58	39.79	C83-Fe76-C85	68.15	C100-C101-H111	126.36
O28-W8-O38	84.63	C57-Fe55-C59	67.17	C84-Fe76-C85	40.24	Fe97-C102-C103	69.49
O28-W8-O39	153.71	C57-Fe55-C60	159.42	C75-C77-Fe76	70.06	Fe97-C102-C106	70.59
O28-W8-O53	104.11	C57-Fe55-C61	123.76	C75-C77-C80	107.59	Fe97-C102-H112	126.32
O36-W8-O38	156.46	C57-Fe55-C62	109.3	C75-C77-H87	125.99	C103-C102-C106	107.9
O36-W8-O39	87.2	C57-Fe55-C63	124.92	Fe76-C77-C80	70.54	C103-C102-H112	126.04
O36-W8-O53	100.86	C57-Fe55-C64	159.52	Fe76-C77-H87	124.18	C106-C102-H112	126.05
O38-W8-O39	90.71	C58-Fe55-C59	39.37	C80-C77-H87	126.41	Fe97-C103-C102	69.75
O38-W8-O53	102.49	C58-Fe55-C60	158.33	C75-C78-Fe76	68.22	Fe97-C103-C104	70.84
O39-W8-O53	102.16	C58-Fe55-C61	159.87	C75-C78-C79	108.19	Fe97-C103-H113	125.75
O16-W9-O20	152.65	C58-Fe55-C62	124.35	C75-C78-H88	126.53	C102-C103-C104	107.78
O16-W9-O28	85.85	C58-Fe55-C63	109.92	Fe76-C78-C79	70.57	C102-C103-H113	126.51
O16-W9-O32	87.85	C58-Fe55-C64	123.97	Fe76-C78-H88	125.43	C104-C103-H113	125.7
O16-W9-O42	68.71	C59-Fe55-C60	122.53	C79-C78-H88	125.25	Fe97-C104-C103	68.76
O16-W9-O44	102.92	C59-Fe55-C61	158.92	Fe76-C79-C78	69.79	Fe97-C104-C105	70.53
O20-W9-O28	84.88	C59-Fe55-C62	158.53	Fe76-C79-C80	68.41	Fe97-C104-H114	123.52
O20-W9-O32	89.75	C59-Fe55-C63	123.17	Fe76-C79-H89	124.76	C103-C104-C105	108.04

O20-W9-O42	84.77	C59-Fe55-C64	108.03	C78-C79-C80	108.15	C103-C104-H114	126.17
O20-W9-O44	104.15	C60-Fe55-C61	41.06	C78-C79-H89	126.09	C105-C104-H114	125.69
O28-W9-O32	154.94	C60-Fe55-C62	68.51	C80-C79-H89	125.67	Fe97-C105-C104	69.62
O28-W9-O42	84.15	C60-Fe55-C63	67.45	Fe76-C80-C77	68.51	Fe97-C105-C106	69.45
O28-W9-O44	101.94	C60-Fe55-C64	40.2	Fe76-C80-C79	71.57	Fe97-C105-H115	122.58
O32-W9-O42	70.97	C61-Fe55-C62	40.97	Fe76-C80-H90	123.66	C104-C105-C106	108.25
O32-W9-O44	103.11	C61-Fe55-C63	67.87	C77-C80-C79	108.22	C104-C105-H115	125.42
O42-W9-O44	169.51	C61-Fe55-C64	68.02	C77-C80-H90	126.49	C106-C105-H115	126.13
O14-W10-O22	71.36	C62-Fe55-C63	40	C79-C80-H90	125.24	Fe97-C106-C102	69.06
O14-W10-O24	86.62	C62-Fe55-C64	67.4	Fe76-C81-C82	68.09	Fe97-C106-C105	70.65
O14-W10-O31	154.85	C63-Fe55-C64	39.56	Fe76-C81-C85	70.11	Fe97-C106-H116	123.03
O14-W10-O34	87.08	C54-C56-Fe55	68.92	Fe76-C81-H95	124.88	C102-C106-C105	108.03
O14-W10-O52	103.19	C54-C56-C59	107.92	C82-C81-C85	108.11	C102-C106-H116	125.76
O22-W10-O24	83.18	C54-C56-H66	125.68	C82-C81-H95	125.89	C105-C106-H116	126.11
O22-W10-O31	84.3	Fe55-C56-C59	71.95	C85-C81-H95	125.92	H118-O117-H119	104.75
O22-W10-O34	71.55	Fe55-C56-H66	121.71	Fe76-C82-C81	71.75	H121-O120-H122	103.9
O22-W10-O52	171.72	C59-C56-H66	126.29	Fe76-C82-C83	68.63	H124-O123-H125	104.37
O24-W10-O31	84.23	C54-C57-Fe55	68.05	Fe76-C82-H91	123.41	H127-O126-H128	104.35
O24-W10-O34	154.66	C54-C57-C58	108.08				

**Table S9** Bond angles between atoms in FcPMo optimized structure in aqueous phase

Atoms	Angle (deg.)	Atoms	Angle (deg.)	Atoms	Angle (deg.)	Atoms	Angle (deg.)
O18-Mo1-O19	106.4	O14-Mo10-O52	101.5	C60-Fe55-C64	40.31	C82-C81-C85	108.1
O18-Mo1-O21	104.9	O22-Mo10-O24	81.92	C61-Fe55-C62	41	C82-C81-H95	125.8
O18-Mo1-O26	96.41	O22-Mo10-O31	85.91	C61-Fe55-C63	67.97	C85-C81-H95	126
O18-Mo1-O37	163.4	O22-Mo10-O34	71.66	C61-Fe55-C64	68.14	Fe76-C82-C81	71.64
O18-Mo1-O39	94.65	O22-Mo10-O52	170.8	C62-Fe55-C63	40.01	Fe76-C82-C83	68.66
O19-Mo1-O21	84.77	O24-Mo10-O31	84.8	C62-Fe55-C64	67.43	Fe76-C82-H91	123.6
O19-Mo1-O26	95.45	O24-Mo10-O34	153.5	C63-Fe55-C64	39.6	C81-C82-C83	108
O19-Mo1-O37	88.15	O24-Mo10-O52	102.3	C54-C56-Fe55	69	C81-C82-H91	124.8
O19-Mo1-O39	158.2	O31-Mo10-O34	95.72	C54-C56-C59	107.8	C83-C82-H91	127.2
O21-Mo1-O26	157.7	O31-Mo10-O52	102.6	C54-C56-H66	125.9	Fe76-C83-C82	70.2
O21-Mo1-O37	83.81	O34-Mo10-O52	103.5	Fe55-C56-C59	71.68	Fe76-C83-C84	70.42
O21-Mo1-O39	84.62	O27-Mo11-O30	154.1	Fe55-C56-H66	121.9	Fe76-C83-H92	124.2
O26-Mo1-O37	73.93	O27-Mo11-O31	82.62	C59-C56-H66	126.1	C82-C83-C84	107.7
O26-Mo1-O39	87.34	O27-Mo11-O33	85.86	C54-C57-Fe55	68.02	C82-C83-H92	126.3
O37-Mo1-O39	71.85	O27-Mo11-O41	96.18	C54-C57-C58	108.1	C84-C83-H92	126
O14-Mo2-O20	95.33	O27-Mo11-O49	103.4	C54-C57-H67	126.6	Fe76-C84-C83	68.51
O14-Mo2-O22	72.7	O30-Mo11-O31	82.8	Fe55-C57-C58	71.76	Fe76-C84-C85	71.45
O14-Mo2-O25	88.47	O30-Mo11-O33	70.97	Fe55-C57-H67	124.8	Fe76-C84-H93	125.1
O14-Mo2-O38	155.4	O30-Mo11-O41	88.31	C58-C57-H67	125.3	C83-C84-C85	107.8
O14-Mo2-O48	104.5	O30-Mo11-O49	100.3	Fe55-C58-C57	68.47	C83-C84-H93	125.9
O20-Mo2-O22	84.97	O31-Mo11-O33	82.05	Fe55-C58-C59	69.36	C85-C84-H93	126.3
O20-Mo2-O25	152.8	O31-Mo11-O41	155.3	Fe55-C58-H68	124.4	Fe76-C85-C81	70.2
O20-Mo2-O38	82.7	O31-Mo11-O49	100.7	C57-C58-C59	108.2	Fe76-C85-C84	68.34
O20-Mo2-O48	103.4	O33-Mo11-O41	73.29	C57-C58-H68	126.3	Fe76-C85-H94	125.5
O22-Mo2-O25	70.47	O33-Mo11-O49	170.6	C59-C58-H68	125.4	C81-C85-C84	108.4
O22-Mo2-O38	82.66	O41-Mo11-O49	103.6	Fe55-C59-C56	67.88	C81-C85-H94	125.2
O22-Mo2-O48	171.5	O33-Mo12-O35	86.08	Fe55-C59-C58	71.16	C84-C85-H94	126.4
O25-Mo2-O38	82.78	O33-Mo12-O40	71.14	Fe55-C59-H69	123.6	Fe97-C96-C98	70.16
O25-Mo2-O48	101.7	O33-Mo12-O41	70.03	C56-C59-C58	108.3	Fe97-C96-C99	67.84
O38-Mo2-O48	99.8	O33-Mo12-O45	170.5	C56-C59-H69	126.4	Fe97-C96-H107	125.3
O17-Mo3-O19	84.39	O33-Mo12-O47	82.28	C58-C59-H69	125.2	C98-C96-C99	108.1
O17-Mo3-O30	94.67	O35-Mo12-O40	96.02	Fe55-C60-C61	68.77	C98-C96-H107	126
O17-Mo3-O33	85.54	O35-Mo12-O41	154.3	Fe55-C60-C64	71.47	C99-C96-H107	125.9
O17-Mo3-O40	155.3	O35-Mo12-O45	102.4	Fe55-C60-H70	123.2	C96-Fe97-C98	39.43
O17-Mo3-O46	105.4	O35-Mo12-O47	85.46	C61-C60-C64	107.8	C96-Fe97-C99	40.1
O19-Mo3-O30	155.6	O40-Mo12-O41	85.28	C61-C60-H70	125.6	C96-Fe97-C100	68.13
O19-Mo3-O33	82.66	O40-Mo12-O45	103.2	C64-C60-H70	126.6	C96-Fe97-C101	67.5
O19-Mo3-O40	83.85	O40-Mo12-O47	153.2	Fe55-C61-C60	70.12	C96-Fe97-C102	145.6
O19-Mo3-O46	104.3	O41-Mo12-O45	102.3	Fe55-C61-C62	70.56	C96-Fe97-C103	115
O30-Mo3-O33	72.99	O41-Mo12-O47	82.25	Fe55-C61-H71	124.5	C96-Fe97-C104	110.6

O30-Mo3-O40	87.28	O45-Mo12-O47	102.6	C60-C61-C62	107.7	C96-Fe97-C105	134.3
O30-Mo3-O46	99.43	O22-P13-O33	110.1	C60-C61-H71	125.6	C96-Fe97-C106	173.1
O33-Mo3-O40	71.47	O22-P13-O37	109.5	C62-C61-H71	126.7	C98-Fe97-C99	67.36
O33-Mo3-O46	167.4	O22-P13-O42	109.2	Fe55-C62-C61	68.44	C98-Fe97-C100	68.08
O40-Mo3-O46	98.5	O33-P13-O37	109.6	Fe55-C62-C63	71.56	C98-Fe97-C101	40.15
O26-Mo4-O29	152.4	O33-P13-O42	109	Fe55-C62-H72	123.9	C98-Fe97-C102	116.2
O26-Mo4-O35	81.88	O37-P13-O42	109.4	C61-C62-C63	108	C98-Fe97-C103	111.6
O26-Mo4-O36	88.52	Mo2-O14-Mo10	127.9	C61-C62-H72	126.8	C98-Fe97-C104	135.5
O26-Mo4-O37	70.22	Mo6-O16-Mo9	131.8	C63-C62-H72	125.2	C98-Fe97-C105	173.4
O26-Mo4-O51	101.4	Mo3-O17-Mo5	152.2	Fe55-C63-C62	68.43	C98-Fe97-C106	146.2
O29-Mo4-O35	81.99	Mo1-O19-Mo3	150.2	Fe55-C63-C64	69.86	C99-Fe97-C100	41.21
O29-Mo4-O36	96.64	Mo2-O20-Mo9	154.2	Fe55-C63-H73	123.6	C99-Fe97-C101	68.72
O29-Mo4-O37	85.46	Mo1-O21-Mo5	150.4	C62-C63-C64	108.2	C99-Fe97-C102	174
O29-Mo4-O51	103.6	Mo2-O22-Mo5	89.13	C62-C63-H73	125.7	C99-Fe97-C103	143.6
O35-Mo4-O36	154.5	Mo2-O22-Mo10	88.63	C64-C63-H73	125.9	C99-Fe97-C104	113.2
O35-Mo4-O37	81.74	Mo2-O22-P13	126.6	Fe55-C64-C60	68.23	C99-Fe97-C105	109
O35-Mo4-O51	101.4	Mo5-O22-Mo10	89.96	Fe55-C64-C63	70.54	C99-Fe97-C106	133.7
O36-Mo4-O37	72.74	Mo5-O22-P13	125.8	Fe55-C64-H74	123.2	C100-Fe97-C101	41.21
O36-Mo4-O51	103.7	Mo10-O22-P13	125	C60-C64-C63	108.3	C100-Fe97-C102	134.4
O37-Mo4-O51	170.7	Mo6-O23-Mo7	128.8	C60-C64-H74	126.9	C100-Fe97-C103	175.1
O17-Mo5-O21	84.49	Mo7-O24-Mo10	151.3	C63-C64-H74	124.6	C100-Fe97-C104	143.3
O17-Mo5-O22	82.3	Mo2-O25-Mo5	127.1	Fe76-C75-C77	68.81	C100-Fe97-C105	113.2
O17-Mo5-O25	155.3	Mo1-O26-Mo4	126.6	Fe76-C75-C78	71.36	C100-Fe97-C106	109
O17-Mo5-O34	83.93	Mo7-O27-Mo11	152.9	Fe76-C75-H86	125.7	C101-Fe97-C102	110.5
O17-Mo5-O50	103.3	Mo8-O28-Mo9	151.4	C77-C75-C78	107.9	C101-Fe97-C103	135.5
O21-Mo5-O22	86.23	Mo4-O29-Mo6	154.1	C77-C75-H86	125.8	C101-Fe97-C104	174.9
O21-Mo5-O25	95.04	Mo3-O30-Mo11	126.3	C78-C75-H86	126.3	C101-Fe97-C105	144.8
O21-Mo5-O34	155.9	Mo10-O31-Mo11	152.3	C75-Fe76-C77	41.14	C101-Fe97-C106	114.8
O21-Mo5-O50	105.3	Mo7-O32-Mo9	128.4	C75-Fe76-C78	40.41	C102-Fe97-C103	40.91
O22-Mo5-O25	73.08	Mo3-O33-Mo11	89.5	C75-Fe76-C79	67.67	C102-Fe97-C104	68.1
O22-Mo5-O34	71.33	Mo3-O33-Mo12	89.66	C75-Fe76-C80	68.55	C102-Fe97-C105	67.98
O22-Mo5-O50	167.6	Mo3-O33-P13	126	C75-Fe76-C81	155.9	C102-Fe97-C106	40.76
O25-Mo5-O34	86.9	Mo11-O33-Mo12	88.68	C75-Fe76-C82	163.2	C103-Fe97-C104	40.34
O25-Mo5-O50	100.7	Mo11-O33-P13	125.8	C75-Fe76-C83	126.5	C103-Fe97-C105	67.71
O34-Mo5-O50	97.94	Mo12-O33-P13	125.5	C75-Fe76-C84	109.6	C103-Fe97-C106	68.38
O16-Mo6-O23	87.31	Mo5-O34-Mo10	127	C75-Fe76-C85	122.6	C104-Fe97-C105	39.87
O16-Mo6-O29	80.63	Mo4-O35-Mo12	152.2	C77-Fe76-C78	68.34	C104-Fe97-C106	67.67
O16-Mo6-O42	68	Mo4-O36-Mo8	128	C77-Fe76-C79	68.13	C105-Fe97-C106	40.23
O16-Mo6-O43	102.9	Mo1-O37-Mo4	89.06	C77-Fe76-C80	41.02	C96-C98-Fe97	70.41
O16-Mo6-O47	151.6	Mo1-O37-Mo8	89.96	C77-Fe76-C81	161.8	C96-C98-C101	108.5
O23-Mo6-O29	154.2	Mo1-O37-P13	125.3	C77-Fe76-C82	124.2	C96-C98-H108	125.4
O23-Mo6-O42	71.41	Mo4-O37-Mo8	89.1	C77-Fe76-C83	106.1	Fe97-C98-C101	67.98
O23-Mo6-O43	103.8	Mo4-O37-P13	126.4	C77-Fe76-C84	120.3	Fe97-C98-H108	124.6

O23-Mo6-O47	96.23	Mo8-O37-P13	125.5	C77-Fe76-C85	156.2	C101-C98-H108	126
O29-Mo6-O42	82.95	Mo2-O38-Mo8	150.2	C78-Fe76-C79	39.68	C96-C99-Fe97	72.06
O29-Mo6-O43	101.1	Mo1-O39-Mo8	127.2	C78-Fe76-C80	67.53	C96-C99-C100	108
O29-Mo6-O47	84.34	Mo3-O40-Mo12	127.7	C78-Fe76-C81	121.4	C96-C99-H109	125.3
O42-Mo6-O43	169.5	Mo11-O41-Mo12	128	C78-Fe76-C82	153.4	Fe97-C99-C100	68.39
O42-Mo6-O47	86.37	Mo6-O42-Mo7	89.1	C78-Fe76-C83	165.2	Fe97-C99-H109	124.5
O43-Mo6-O47	103.6	Mo6-O42-Mo9	89.76	C78-Fe76-C84	128.8	C100-C99-H109	126.6
O15-Mo7-O23	101.7	Mo6-O42-P13	125.4	C78-Fe76-C85	111.1	Fe97-C100-C99	70.4
O15-Mo7-O24	102.6	Mo7-O42-Mo9	89.08	C79-Fe76-C80	40.07	Fe97-C100-C101	70.44
O15-Mo7-O27	101.2	Mo7-O42-P13	126.8	C79-Fe76-C81	108.5	Fe97-C100-H110	124.1
O15-Mo7-O32	104.3	Mo9-O42-P13	125	C79-Fe76-C82	118.5	C99-C100-C101	107.7
O15-Mo7-O42	171.6	Mo6-O47-Mo12	150.9	C79-Fe76-C83	152.6	C99-C100-H110	126
O23-Mo7-O24	155	Fe55-C54-C56	69.75	C79-Fe76-C84	165	C101-C100-H110	126.4
O23-Mo7-O27	83.75	Fe55-C54-C57	71.06	C79-Fe76-C85	127.7	Fe97-C101-C98	71.87
O23-Mo7-O32	85.22	Fe55-C54-H65	124.1	C80-Fe76-C81	124.9	Fe97-C101-C100	68.36
O23-Mo7-O42	70.72	C56-C54-C57	107.6	C80-Fe76-C82	105.4	Fe97-C101-H111	124.6
O24-Mo7-O27	85.84	C56-C54-H65	125.9	C80-Fe76-C83	117.9	C98-C101-C100	107.7
O24-Mo7-O32	94.41	C57-C54-H65	126.6	C80-Fe76-C84	154.2	C98-C101-H111	125.9
O24-Mo7-O42	85.34	C54-Fe55-C56	41.25	C80-Fe76-C85	162.5	C100-C101-H111	126.4
O27-Mo7-O32	153.8	C54-Fe55-C57	40.91	C81-Fe76-C82	40.22	Fe97-C102-C103	69.91
O27-Mo7-O42	81.91	C54-Fe55-C58	67.84	C81-Fe76-C83	68.2	Fe97-C102-C106	70.18
O32-Mo7-O42	71.98	C54-Fe55-C59	68.28	C81-Fe76-C84	67.6	Fe97-C102-H112	125.4
O28-Mo8-O36	82.5	C54-Fe55-C60	121.9	C81-Fe76-C85	39.6	C103-C102-C106	107.8
O28-Mo8-O37	81.67	C54-Fe55-C61	107.1	C82-Fe76-C83	41.14	C103-C102-H112	126.2
O28-Mo8-O38	86.26	C54-Fe55-C62	124.1	C82-Fe76-C84	68.64	C106-C102-H112	126.1
O28-Mo8-O39	152.4	C54-Fe55-C63	160.6	C82-Fe76-C85	67.52	Fe97-C103-C102	69.18
O28-Mo8-O53	103	C54-Fe55-C64	157.9	C83-Fe76-C84	41.08	Fe97-C103-C104	70.97
O36-Mo8-O37	70.1	C56-Fe55-C57	68.49	C83-Fe76-C85	68.12	Fe97-C103-H113	124.7
O36-Mo8-O38	155.5	C56-Fe55-C58	67.51	C84-Fe76-C85	40.21	C102-C103-C104	107.9
O36-Mo8-O39	84.72	C56-Fe55-C59	40.43	C75-C77-Fe76	70.05	C102-C103-H113	126.4
O36-Mo8-O53	100	C56-Fe55-C60	106.2	C75-C77-C80	107.6	C104-C103-H113	125.7
O37-Mo8-O38	86.8	C56-Fe55-C61	122.6	C75-C77-H87	126	Fe97-C104-C103	68.69
O37-Mo8-O39	71.02	C56-Fe55-C62	160.2	Fe76-C77-C80	70.48	Fe97-C104-C105	70.04
O37-Mo8-O53	168.7	C56-Fe55-C63	157.4	Fe76-C77-H87	124.3	Fe97-C104-H114	123.5
O38-Mo8-O39	95.68	C56-Fe55-C64	121.7	C80-C77-H87	126.4	C103-C104-C105	108.1
O38-Mo8-O53	103.7	C57-Fe55-C58	39.78	C75-C78-Fe76	68.22	C103-C104-H114	126.1
O39-Mo8-O53	103.3	C57-Fe55-C59	67.24	C75-C78-C79	108.2	C105-C104-H114	125.7
O16-Mo9-O20	152.6	C57-Fe55-C60	159.3	C75-C78-H88	126.5	Fe97-C105-C104	70.09
O16-Mo9-O28	91.21	C57-Fe55-C61	123.6	Fe76-C78-C79	70.54	Fe97-C105-C106	68.97
O16-Mo9-O32	87.86	C57-Fe55-C62	109.3	Fe76-C78-H88	125.4	Fe97-C105-H115	123.3
O16-Mo9-O42	69.72	C57-Fe55-C63	125	C79-C78-H88	125.3	C104-C105-C106	108.3
O16-Mo9-O44	104.4	C57-Fe55-C64	159.6	Fe76-C79-C78	69.78	C104-C105-H115	125.7
O20-Mo9-O28	84.16	C58-Fe55-C59	39.48	Fe76-C79-C80	68.38	C106-C105-H115	125.9

O20-Mo9-O32	85.64	C58-Fe55-C60	158.5	Fe76-C79-H89	124.6	Fe97-C106-C102	69.06
O20-Mo9-O42	83.05	C58-Fe55-C61	159.7	C78-C79-C80	108.2	Fe97-C106-C105	70.81
O20-Mo9-O44	103	C58-Fe55-C62	124.3	C78-C79-H89	126.1	Fe97-C106-H116	123.7
O28-Mo9-O32	155.9	C58-Fe55-C63	109.9	C80-C79-H89	125.6	C102-C106-C105	107.9
O28-Mo9-O42	86.55	C58-Fe55-C64	124	Fe76-C80-C77	68.5	C102-C106-H116	125.8
O28-Mo9-O44	101.8	C59-Fe55-C60	122.5	Fe76-C80-C79	71.55	C105-C106-H116	126.2
O32-Mo9-O42	70.52	C59-Fe55-C61	158.9	Fe76-C80-H90	123.8	H118-O117-H119	104.3
O32-Mo9-O44	101.7	C59-Fe55-C62	158.5	C77-C80-C79	108.2	H121-O120-H122	103.1
O42-Mo9-O44	170	C59-Fe55-C63	123.1	C77-C80-H90	126.6	H124-O123-H125	103.7
O14-Mo10-O22	70.65	C59-Fe55-C64	107.9	C79-C80-H90	125.2	H127-O126-H128	103
O14-Mo10-O24	82.5	C60-Fe55-C61	41.11	Fe76-C81-C82	68.14	H130-O129-H131	105.4
O14-Mo10-O31	154.6	C60-Fe55-C62	68.56	Fe76-C81-C85	70.2	H133-O132-H134	106.9
O14-Mo10-O34	86.19	C60-Fe55-C63	67.57	Fe76-C81-H95	124.6		



**Table S10** Torsional angles between atoms in FcPW optimized structure in aqueous phase

Atoms	Torsion	Atoms	Torsion	Atoms	Torsion	Atoms	Torsion
O18-W1-O19-W3	-145.3	O22-P13-O42-W7	59.32	C62-C63-C64-H74	174.95	H93-C84-C85-C81	-179.7
O21-W1-O19-W3	-40.47	O22-P13-O42-W9	-59.19	H73-C63-C64-Fe55	-117.2	H93-C84-C85-H94	-1.98
O26-W1-O19-W3	117.6	O33-P13-O42-W7	-61.28	H73-C63-C64-C60	-175.1	C98-C96-Fe97-C99	120.5
O37-W1-O19-W3	45.35	O33-P13-O42-W9	-179.8	H73-C63-C64-H74	-0.04	C98-C96-Fe97-C100	82.08
O39-W1-O19-W3	29.44	O37-P13-O42-W7	178.9	C77-C75-Fe76-C78	118.52	C98-C96-Fe97-C101	37.25
O18-W1-O21-W5	143	O37-P13-O42-W9	60.39	C77-C75-Fe76-C79	81.76	C98-C96-Fe97-C102	-57.06
O19-W1-O21-W5	38.46	C56-C54-Fe55-C57	117.75	C77-C75-Fe76-C80	38.47	C98-C96-Fe97-C103	-94.29
O26-W1-O21-W5	-47.4	C56-C54-Fe55-C58	80.51	C77-C75-Fe76-C81	167.5	C98-C96-Fe97-C104	-138.2
O37-W1-O21-W5	-49.73	C56-C54-Fe55-C59	37.91	C77-C75-Fe76-C82	-32.91	C98-C96-Fe97-C105	-177.2
O39-W1-O21-W5	-121.8	C56-C54-Fe55-C60	-77.73	C77-C75-Fe76-C83	-70.78	C98-C96-Fe97-C106	147.49
O18-W1-O26-W4	164.1	C56-C54-Fe55-C61	-120.2	C77-C75-Fe76-C84	-113.8	C99-C96-Fe97-C98	-120.5
O19-W1-O26-W4	-90.31	C56-C54-Fe55-C62	-162.1	C77-C75-Fe76-C85	-156.5	C99-C96-Fe97-C100	-38.42
O21-W1-O26-W4	-5.88	C56-C54-Fe55-C63	167.62	C78-C75-Fe76-C77	-118.5	C99-C96-Fe97-C101	-83.26
O37-W1-O26-W4	-3.45	C56-C54-Fe55-C64	-46.36	C78-C75-Fe76-C79	-36.76	C99-C96-Fe97-C102	-177.6
O39-W1-O26-W4	68.63	C57-C54-Fe55-C56	-117.8	C78-C75-Fe76-C80	-80.05	C99-C96-Fe97-C103	145.2
O18-W1-O37-P13	177.7	C57-C54-Fe55-C58	-37.23	C78-C75-Fe76-C81	48.98	C99-C96-Fe97-C104	101.35
O19-W1-O37-P13	-40.56	C57-C54-Fe55-C59	-79.84	C78-C75-Fe76-C82	-151.4	C99-C96-Fe97-C105	62.3
O21-W1-O37-P13	44.94	C57-C54-Fe55-C60	164.52	C78-C75-Fe76-C83	170.7	C99-C96-Fe97-C106	26.98
O26-W1-O37-P13	-134.2	C57-C54-Fe55-C61	122.02	C78-C75-Fe76-C84	127.71	H107-C96-Fe97-C98	120.38
O39-W1-O37-P13	133.5	C57-C54-Fe55-C62	80.14	C78-C75-Fe76-C85	84.98	H107-C96-Fe97-C99	-119.1
O18-W1-O39-W8	-165	C57-C54-Fe55-C63	49.87	H86-C75-Fe76-C77	119.64	H107-C96-Fe97-C100	-157.5
O19-W1-O39-W8	20.13	C57-C54-Fe55-C64	-164.1	H86-C75-Fe76-C78	-121.8	H107-C96-Fe97-C101	157.63
O21-W1-O39-W8	89.71	H65-C54-Fe55-C56	120.37	H86-C75-Fe76-C79	-158.6	H107-C96-Fe97-C102	63.32
O26-W1-O39-W8	-69.16	H65-C54-Fe55-C57	-121.9	H86-C75-Fe76-C80	158.11	H107-C96-Fe97-C103	26.09
O37-W1-O39-W8	3.39	H65-C54-Fe55-C58	-159.1	H86-C75-Fe76-C81	-72.86	H107-C96-Fe97-C104	-17.77
O20-W2-O14-W10	-87.98	H65-C54-Fe55-C59	158.28	H86-C75-Fe76-C82	86.73	H107-C96-Fe97-C105	-56.81

O22-W2-O14-W10	-3.94	H65-C54-Fe55-C60	42.64	H86-C75-Fe76-C83	48.86	H107-C96-Fe97-C106	-92.13
O25-W2-O14-W10	66.25	H65-C54-Fe55-C61	0.13	H86-C75-Fe76-C84	5.87	Fe97-C96-C98-C101	-57.42
O38-W2-O14-W10	-11.96	H65-C54-Fe55-C62	-41.74	H86-C75-Fe76-C85	-36.86	Fe97-C96-C98-H108	119.11
O48-W2-O14-W10	169.3	H65-C54-Fe55-C63	-72.01	Fe76-C75-C77-C80	-60.87	C99-C96-C98-Fe97	57.16
O14-W2-O20-W9	121.9	H65-C54-Fe55-C64	74.01	Fe76-C75-C77-H87	118.37	C99-C96-C98-C101	-0.25
O22-W2-O20-W9	50.65	Fe55-C54-C56-C59	-61.73	C78-C75-C77-Fe76	61	C99-C96-C98-H108	176.27
O25-W2-O20-W9	36.23	Fe55-C54-C56-H66	114.63	C78-C75-C77-C80	0.14	H107-C96-C98-Fe97	-119.5
O38-W2-O20-W9	-33.87	C57-C54-C56-Fe55	61.32	C78-C75-C77-H87	179.37	H107-C96-C98-C101	-176.9
O48-W2-O20-W9	-134	C57-C54-C56-C59	-0.4	H86-C75-C77-Fe76	-119.4	H107-C96-C98-H108	-0.36
O14-W2-O22-W5	91.84	C57-C54-C56-H66	175.96	H86-C75-C77-C80	179.74	Fe97-C96-C99-C100	58.72
O14-W2-O22-W10	2.44	H65-C54-C56-Fe55	-118	H86-C75-C77-H87	-1.02	Fe97-C96-C99-H109	-121.2
O14-W2-O22-P13	-132.4	H65-C54-C56-C59	-179.8	Fe76-C75-C78-C79	59.44	C98-C96-C99-Fe97	-58.22
O20-W2-O22-W5	-176.1	H65-C54-C56-H66	-3.39	Fe76-C75-C78-H88	-118.8	C98-C96-C99-C100	0.5
O20-W2-O22-W10	94.55	Fe55-C54-C57-C58	61.13	C77-C75-C78-Fe76	-59.39	C98-C96-C99-H109	-179.4
O20-W2-O22-P13	-40.3	Fe55-C54-C57-H67	-117.3	C77-C75-C78-C79	0.05	H107-C96-C99-Fe97	118.42
O25-W2-O22-W5	-2.66	C56-C54-C57-Fe55	-60.59	C77-C75-C78-H88	-178.1	H107-C96-C99-C100	177.14
O25-W2-O22-W10	-92.07	C56-C54-C57-C58	0.54	H86-C75-C78-Fe76	121.01	H107-C96-C99-H109	-2.73
O25-W2-O22-P13	133.1	C56-C54-C57-H67	-177.9	H86-C75-C78-C79	-179.6	C96-Fe97-C98-C101	120.15
O38-W2-O22-W5	-91.55	H65-C54-C57-Fe55	118.75	H86-C75-C78-H88	2.26	C96-Fe97-C98-H108	-120.4
O38-W2-O22-W10	179.1	H65-C54-C57-C58	179.88	C75-Fe76-C77-C80	117.98	C99-Fe97-C98-C96	-36.71
O38-W2-O22-P13	44.2	H65-C54-C57-H67	1.44	C75-Fe76-C77-H87	-120.6	C99-Fe97-C98-C101	83.44
O48-W2-O22-W5	37.84	C54-Fe55-C56-C59	118.19	C78-Fe76-C77-C75	-37.81	C99-Fe97-C98-H108	-157.1
O48-W2-O22-W10	-51.57	C54-Fe55-C56-H66	-119.8	C78-Fe76-C77-C80	80.17	C100-Fe97-C98-C96	-81.25
O48-W2-O22-P13	173.6	C57-Fe55-C56-C54	-38.58	C78-Fe76-C77-H87	-158.4	C100-Fe97-C98-C101	38.9
O14-W2-O25-W5	-66.57	C57-Fe55-C56-C59	79.61	C79-Fe76-C77-C75	-80.67	C100-Fe97-C98-H108	158.34
O20-W2-O25-W5	19.57	C57-Fe55-C56-H66	-158.4	C79-Fe76-C77-C80	37.31	C101-Fe97-C98-C96	-120.2
O22-W2-O25-W5	4.33	C58-Fe55-C56-C54	-81.65	C79-Fe76-C77-H87	158.71	C101-Fe97-C98-H108	119.44
O38-W2-O25-W5	89.02	C58-Fe55-C56-C59	36.55	C80-Fe76-C77-C75	-118	C102-Fe97-C98-C96	148.47
O48-W2-O25-W5	-170.3	C58-Fe55-C56-H66	158.58	C80-Fe76-C77-H87	121.4	C102-Fe97-C98-C101	-91.38
O14-W2-O38-W8	-43.8	C59-Fe55-C56-C54	-118.2	C81-Fe76-C77-C75	-163.9	C102-Fe97-C98-H108	28.06

O20-W2-O38-W8	33.56	C59-Fe55-C56-H66	122.04	C81-Fe76-C77-C80	-45.92	C103-Fe97-C98-C96	103.75
O22-W2-O38-W8	-51.43	C60-Fe55-C56-C54	120.36	C81-Fe76-C77-H87	75.48	C103-Fe97-C98-C101	-136.1
O25-W2-O38-W8	-122.2	C60-Fe55-C56-C59	-121.4	C82-Fe76-C77-C75	169	C103-Fe97-C98-H108	-16.66
O48-W2-O38-W8	134.9	C60-Fe55-C56-H66	0.59	C82-Fe76-C77-C80	-73.02	C104-Fe97-C98-C96	63.25
O19-W3-O17-W5	-32.21	C61-Fe55-C56-C54	78.61	C82-Fe76-C77-H87	48.37	C104-Fe97-C98-C101	-176.6
O30-W3-O17-W5	124.4	C61-Fe55-C56-C59	-163.2	C83-Fe76-C77-C75	127.84	C104-Fe97-C98-H108	-57.16
O33-W3-O17-W5	53.46	C61-Fe55-C56-H66	-41.16	C83-Fe76-C77-C80	-114.2	C105-Fe97-C98-C96	17.49
O40-W3-O17-W5	37.65	C62-Fe55-C56-C54	48.79	C83-Fe76-C77-H87	7.22	C105-Fe97-C98-C101	137.64
O46-W3-O17-W5	-136	C62-Fe55-C56-C59	166.99	C84-Fe76-C77-C75	85.65	C105-Fe97-C98-H108	-102.9
O17-W3-O19-W1	38.29	C62-Fe55-C56-H66	-70.98	C84-Fe76-C77-C80	-156.4	C106-Fe97-C98-C96	-173
O30-W3-O19-W1	-43	C63-Fe55-C56-C54	-169.4	C84-Fe76-C77-H87	-34.97	C106-Fe97-C98-C101	-52.82
O33-W3-O19-W1	-46.2	C63-Fe55-C56-C59	-51.18	C85-Fe76-C77-C75	56.18	C106-Fe97-C98-H108	66.62
O40-W3-O19-W1	-117.6	C63-Fe55-C56-H66	70.86	C85-Fe76-C77-C80	174.16	C96-Fe97-C99-C100	-118.8
O46-W3-O19-W1	142.8	C64-Fe55-C56-C54	161.35	C85-Fe76-C77-H87	-64.45	C96-Fe97-C99-H109	121.24
O17-W3-O30-W11	-87.04	C64-Fe55-C56-C59	-80.46	C75-Fe76-C78-C79	-119.8	C98-Fe97-C99-C96	36.28
O19-W3-O30-W11	-7.2	C64-Fe55-C56-H66	41.58	C75-Fe76-C78-H88	120.16	C98-Fe97-C99-C100	-82.49
O33-W3-O30-W11	-3.83	C54-Fe55-C57-C58	-118.9	C77-Fe76-C78-C75	38.46	C98-Fe97-C99-H109	157.53
O40-W3-O30-W11	67.27	C54-Fe55-C57-H67	120.24	C77-Fe76-C78-C79	-81.37	C100-Fe97-C99-C96	118.77
O46-W3-O30-W11	167.1	C56-Fe55-C57-C54	38.84	C77-Fe76-C78-H88	158.62	C100-Fe97-C99-H109	-120
O17-W3-O33-W11	96.07	C56-Fe55-C57-C58	-80.06	C79-Fe76-C78-C75	119.83	C101-Fe97-C99-C96	79.86
O17-W3-O33-P13	-40.96	C56-Fe55-C57-H67	159.08	C79-Fe76-C78-H88	-120	C101-Fe97-C99-C100	-38.91
O19-W3-O33-W11	-178.9	C58-Fe55-C57-C54	118.9	C80-Fe76-C78-C75	82.83	C101-Fe97-C99-H109	-158.9
O19-W3-O33-P13	44.03	C58-Fe55-C57-H67	-120.9	C80-Fe76-C78-C79	-37	C102-Fe97-C99-C96	167.24
O30-W3-O33-W11	2.42	C59-Fe55-C57-C54	82.52	C80-Fe76-C78-H88	-157	C102-Fe97-C99-C100	48.47
O30-W3-O33-P13	-134.6	C59-Fe55-C57-C58	-36.37	C81-Fe76-C78-C75	-159	C102-Fe97-C99-H109	-71.52
O40-W3-O33-W11	-91.1	C59-Fe55-C57-H67	-157.2	C81-Fe76-C78-C79	81.19	C103-Fe97-C99-C96	-60.18

O40-W3-O33-P13	131.9	C60-Fe55-C57-C54	-40.07	C81-Fe76-C78-H88	-38.82	C103-Fe97-C99-C100	-179
O46-W3-O33-W11	-40.44	C60-Fe55-C57-C58	-159	C82-Fe76-C78-C75	161.89	C103-Fe97-C99-H109	61.06
O46-W3-O33-P13	-177.5	C60-Fe55-C57-H67	80.18	C82-Fe76-C78-C79	42.05	C104-Fe97-C99-C96	-95.36
O17-W3-O40-W12	20.66	C61-Fe55-C57-C54	-76.93	C82-Fe76-C78-H88	-77.95	C104-Fe97-C99-C100	145.87
O19-W3-O40-W12	90.12	C61-Fe55-C57-C58	164.18	C83-Fe76-C78-C75	-30.66	C104-Fe97-C99-H109	25.88
O30-W3-O40-W12	-67.08	C61-Fe55-C57-H67	43.31	C83-Fe76-C78-C79	-150.5	C105-Fe97-C99-C96	-138
O33-W3-O40-W12	4.03	C62-Fe55-C57-C54	-120.2	C83-Fe76-C78-H88	89.5	C105-Fe97-C99-C100	103.24
O46-W3-O40-W12	-165.6	C62-Fe55-C57-C58	120.91	C84-Fe76-C78-C75	-73.45	C105-Fe97-C99-H109	-16.75
O29-W4-O26-W1	19.55	C62-Fe55-C57-H67	0.05	C84-Fe76-C78-C79	166.71	C106-Fe97-C99-C96	-175.5
O35-W4-O26-W1	85.72	C63-Fe55-C57-C54	-162	C84-Fe76-C78-H88	46.7	C106-Fe97-C99-C100	65.74
O36-W4-O26-W1	-69.03	C63-Fe55-C57-C58	79.11	C85-Fe76-C78-C75	-115.9	C106-Fe97-C99-H109	-54.25
O51-W4-O26-W1	-172	C63-Fe55-C57-H67	-41.76	C85-Fe76-C78-C79	124.24	C96-Fe97-C100-C99	37.21
O26-W4-O29-W6	34.69	C64-Fe55-C57-C54	162.89	C85-Fe76-C78-H88	4.23	C96-Fe97-C100-C101	-80.39
O35-W4-O29-W6	-31.53	C64-Fe55-C57-C58	44	C75-Fe76-C79-C78	37.45	C96-Fe97-C100-H110	158.36
O36-W4-O29-W6	122.2	C64-Fe55-C57-H67	-76.87	C75-Fe76-C79-C80	-82.73	C98-Fe97-C100-C99	79.68
O51-W4-O29-W6	-133.6	C54-Fe55-C58-C57	38.31	C75-Fe76-C79-H89	158.01	C98-Fe97-C100-C101	-37.93
O26-W4-O35-W12	-132.1	C54-Fe55-C58-C59	-82.19	C77-Fe76-C79-C78	82.02	C98-Fe97-C100-H110	-159.2
O29-W4-O35-W12	24.74	C54-Fe55-C58-H68	158.02	C77-Fe76-C79-C80	-38.16	C99-Fe97-C100-C101	-117.6
O36-W4-O35-W12	-58.83	C56-Fe55-C58-C57	83.09	C77-Fe76-C79-H89	-157.4	C99-Fe97-C100-H110	121.14
O51-W4-O35-W12	127.5	C56-Fe55-C58-C59	-37.41	C78-Fe76-C79-C80	-120.2	C101-Fe97-C100-C99	117.6
O26-W4-O36-W8	66.85	C56-Fe55-C58-H68	-157.2	C78-Fe76-C79-H89	120.56	C101-Fe97-C100-H110	-121.3
O29-W4-O36-W8	-87.82	C57-Fe55-C58-C59	-120.5	C80-Fe76-C79-C78	120.18	C102-Fe97-C100-C99	-173.6
O35-W4-O36-W8	-5.94	C57-Fe55-C58-H68	119.71	C80-Fe76-C79-H89	-119.3	C102-Fe97-C100-C101	68.85
O51-W4-O36-W8	167.8	C59-Fe55-C58-C57	120.5	C81-Fe76-C79-C78	-117.3	C102-Fe97-C100-H110	-52.41
O21-W5-O17-W3	31.68	C59-Fe55-C58-H68	-119.8	C81-Fe76-C79-C80	122.5	C103-Fe97-C100-C99	172.25
O22-W5-O17-W3	-54.28	C60-Fe55-C58-C57	160.02	C81-Fe76-C79-H89	3.24	C103-Fe97-C100-C101	54.65

O25-W5-O17-W3	-48.23	C60-Fe55-C58-C59	39.53	C82-Fe76-C79-C78	-160.1	C103-Fe97-C100-H110	-66.61
O34-W5-O17-W3	-125.9	C60-Fe55-C58-H68	-80.26	C82-Fe76-C79-C80	79.76	C104-Fe97-C100-C99	-58.37
O50-W5-O17-W3	134.9	C61-Fe55-C58-C57	-41.2	C82-Fe76-C79-H89	-39.49	C104-Fe97-C100-C101	-176
O17-W5-O21-W1	-35.26	C61-Fe55-C58-C59	-161.7	C83-Fe76-C79-C78	164.26	C104-Fe97-C100-H110	62.78
O22-W5-O21-W1	48.52	C61-Fe55-C58-H68	78.51	C83-Fe76-C79-C80	44.08	C105-Fe97-C100-C99	-93.17
O25-W5-O21-W1	119.9	C62-Fe55-C58-C57	-78.75	C83-Fe76-C79-H89	-75.18	C105-Fe97-C100-C101	149.23
O34-W5-O21-W1	36.09	C62-Fe55-C58-C59	160.75	C84-Fe76-C79-C78	-44.56	C105-Fe97-C100-H110	27.98
O50-W5-O21-W1	-139.6	C62-Fe55-C58-H68	40.96	C84-Fe76-C79-C80	-164.7	C106-Fe97-C100-C99	-135.9
O17-W5-O22-W2	179.9	C63-Fe55-C58-C57	-121.1	C84-Fe76-C79-H89	76	C106-Fe97-C100-C101	106.52
O17-W5-O22-W10	-91.21	C63-Fe55-C58-C59	118.42	C85-Fe76-C79-C78	-77.49	C106-Fe97-C100-H110	-14.73
O17-W5-O22-P13	43.57	C63-Fe55-C58-H68	-1.37	C85-Fe76-C79-C80	162.32	C96-Fe97-C101-C98	-36.35
O21-W5-O22-W2	94.64	C64-Fe55-C58-C57	-163	C85-Fe76-C79-H89	43.07	C96-Fe97-C101-C100	81.64
O21-W5-O22-W10	-176.5	C64-Fe55-C58-C59	76.55	C75-Fe76-C80-C77	-38.63	C96-Fe97-C101-H111	-158.2
O21-W5-O22-P13	-41.69	C64-Fe55-C58-H68	-43.24	C75-Fe76-C80-C79	80.41	C98-Fe97-C101-C100	117.98
O25-W5-O22-W2	2.62	C54-Fe55-C59-C56	-38.75	C75-Fe76-C80-H90	-159	C98-Fe97-C101-H111	-121.8
O25-W5-O22-W10	91.52	C54-Fe55-C59-C58	81.19	C77-Fe76-C80-C79	119.04	C99-Fe97-C101-C98	-79.31
O25-W5-O22-P13	-133.7	C54-Fe55-C59-H69	-158.7	C77-Fe76-C80-H90	-120.4	C99-Fe97-C101-C100	38.67
O34-W5-O22-W2	-90.59	C56-Fe55-C59-C58	119.94	C78-Fe76-C80-C77	-82.37	C99-Fe97-C101-H111	158.88
O34-W5-O22-W10	-1.69	C56-Fe55-C59-H69	-120	C78-Fe76-C80-C79	36.67	C100-Fe97-C101-C98	-118
O34-W5-O22-P13	133.1	C57-Fe55-C59-C56	-83.19	C78-Fe76-C80-H90	157.25	C100-Fe97-C101-H111	120.21
O50-W5-O22-W2	-45.75	C57-Fe55-C59-C58	36.75	C79-Fe76-C80-C77	-119	C102-Fe97-C101-C98	107.24
O50-W5-O22-W10	43.14	C57-Fe55-C59-H69	156.84	C79-Fe76-C80-H90	120.58	C102-Fe97-C101-C100	-134.8
O50-W5-O22-P13	177.9	C58-Fe55-C59-C56	-119.9	C81-Fe76-C80-C77	163.93	C102-Fe97-C101-H111	-14.57
O17-W5-O25-W2	-10.72	C58-Fe55-C59-H69	120.09	C81-Fe76-C80-C79	-77.03	C103-Fe97-C101-C98	67.45
O21-W5-O25-W2	-89.38	C60-Fe55-C59-C56	76.25	C81-Fe76-C80-H90	43.55	C103-Fe97-C101-C100	-174.6
O22-W5-O25-W2	-4.39	C60-Fe55-C59-C58	-163.8	C82-Fe76-C80-C77	124.75	C103-Fe97-C101-H111	-54.36

O34-W5-O25-W2	67.05	C60-Fe55-C59-H69	-43.72	C82-Fe76-C80-C79	-116.2	C104-Fe97-C101-C98	30.53
O50-W5-O25-W2	166.2	C61-Fe55-C59-C56	42.57	C82-Fe76-C80-H90	4.37	C104-Fe97-C101-C100	148.51
O17-W5-O34-W10	86.67	C61-Fe55-C59-C58	162.51	C83-Fe76-C80-C77	82.31	C104-Fe97-C101-H111	-91.28
O21-W5-O34-W10	15.84	C61-Fe55-C59-H69	-77.39	C83-Fe76-C80-C79	-158.7	C105-Fe97-C101-C98	-172.3
O22-W5-O34-W10	2.77	C62-Fe55-C59-C56	-168	C83-Fe76-C80-H90	-38.07	C105-Fe97-C101-C100	-54.27
O25-W5-O34-W10	-68.61	C62-Fe55-C59-C58	-48.05	C84-Fe76-C80-C77	52.18	C105-Fe97-C101-H111	65.94
O50-W5-O34-W10	-168.4	C62-Fe55-C59-H69	72.04	C84-Fe76-C80-C79	171.21	C106-Fe97-C101-C98	151.09
O23-W6-O16-W9	-58.92	C63-Fe55-C59-C56	158.98	C84-Fe76-C80-H90	-68.2	C106-Fe97-C101-C100	-90.92
O29-W6-O16-W9	97.79	C63-Fe55-C59-C58	-81.08	C85-Fe76-C80-C77	-172.1	C106-Fe97-C101-H111	29.29
O43-W6-O16-W9	-160.9	C63-Fe55-C59-H69	39.02	C85-Fe76-C80-C79	-53.08	C96-Fe97-C102-C103	-56.73
O47-W6-O16-W9	33.36	C64-Fe55-C59-C56	118.08	C85-Fe76-C80-H90	67.5	C96-Fe97-C102-C106	-175.4
O16-W6-O23-W7	66.68	C64-Fe55-C59-C58	-122	C75-Fe76-C81-C82	170.94	C96-Fe97-C102-H112	63.58
O29-W6-O23-W7	0.07	C64-Fe55-C59-H69	-1.89	C75-Fe76-C81-C85	50.82	C98-Fe97-C102-C103	-93.26
O43-W6-O23-W7	169.62	C54-Fe55-C60-C61	-79.26	C75-Fe76-C81-H95	-69.73	C98-Fe97-C102-C106	148.07
O47-W6-O23-W7	-85.12	C54-Fe55-C60-C64	162.35	C77-Fe76-C81-C82	-35.83	C98-Fe97-C102-H112	27.05
O16-W6-O29-W4	-120.7	C54-Fe55-C60-H70	40.12	C77-Fe76-C81-C85	-156	C99-Fe97-C102-C103	137.99
O23-W6-O29-W4	-52.91	C56-Fe55-C60-C61	-121.4	C77-Fe76-C81-H95	83.5	C99-Fe97-C102-C106	19.32
O43-W6-O29-W4	137.57	C56-Fe55-C60-C64	120.19	C78-Fe76-C81-C82	-154	C99-Fe97-C102-H112	-101.7
O47-W6-O29-W4	34.03	C56-Fe55-C60-H70	-2.04	C78-Fe76-C81-C85	85.87	C100-Fe97-C102-C103	-178.3
O16-W6-O47-W12	31.08	C57-Fe55-C60-C61	-49.4	C78-Fe76-C81-H95	-34.68	C100-Fe97-C102-C106	63.07
O23-W6-O47-W12	122.04	C57-Fe55-C60-C64	-167.8	C79-Fe76-C81-C82	-112.3	C100-Fe97-C102-H112	-57.96
O29-W6-O47-W12	-32.69	C57-Fe55-C60-H70	69.98	C79-Fe76-C81-C85	127.59	C101-Fe97-C102-C103	-137
O43-W6-O47-W12	-134.6	C58-Fe55-C60-C61	169.07	C79-Fe76-C81-H95	7.04	C101-Fe97-C102-C106	104.31
O15-W7-O23-W6	-173.5	C58-Fe55-C60-C64	50.68	C80-Fe76-C81-C82	-70.88	C101-Fe97-C102-H112	-16.71
O24-W7-O23-W6	10.55	C58-Fe55-C60-H70	-71.55	C80-Fe76-C81-C85	169	C103-Fe97-C102-C106	-118.7
O27-W7-O23-W6	84.34	C59-Fe55-C60-C61	-162.3	C80-Fe76-C81-H95	48.45	C103-Fe97-C102-H112	120.31

O32-W7-O23-W6	-70.85	C59-Fe55-C60-C64	79.29	C82-Fe76-C81-C85	-120.1	C104-Fe97-C102-C103	38.07
O42-W7-O23-W6	0.74	C59-Fe55-C60-H70	-42.94	C82-Fe76-C81-H95	119.33	C104-Fe97-C102-C106	-80.61
O15-W7-O24-W10	-129.8	C61-Fe55-C60-C64	-118.4	C83-Fe76-C81-C82	38.44	C104-Fe97-C102-H112	158.37
O23-W7-O24-W10	46.17	C61-Fe55-C60-H70	119.38	C83-Fe76-C81-C85	-81.68	C105-Fe97-C102-C103	81.3
O27-W7-O24-W10	-27.69	C62-Fe55-C60-C61	38.42	C83-Fe76-C81-H95	157.77	C105-Fe97-C102-C106	-37.37
O32-W7-O24-W10	126.18	C62-Fe55-C60-C64	-79.97	C84-Fe76-C81-C82	82.97	C105-Fe97-C102-H112	-158.4
O42-W7-O24-W10	55.45	C62-Fe55-C60-H70	157.8	C84-Fe76-C81-C85	-37.15	C106-Fe97-C102-C103	118.67
O15-W7-O27-W11	130.25	C63-Fe55-C60-C61	81.7	C84-Fe76-C81-H95	-157.7	C106-Fe97-C102-H112	-121
O23-W7-O27-W11	-125.8	C63-Fe55-C60-C64	-36.69	C85-Fe76-C81-C82	120.12	C96-Fe97-C103-C102	149.04
O24-W7-O27-W11	29.25	C63-Fe55-C60-H70	-158.9	C85-Fe76-C81-H95	-120.6	C96-Fe97-C103-C104	-92.75
O32-W7-O27-W11	-55.07	C64-Fe55-C60-C61	118.39	C75-Fe76-C82-C81	-167.4	C96-Fe97-C103-H113	27.99
O42-W7-O27-W11	-55.24	C64-Fe55-C60-H70	-122.2	C75-Fe76-C82-C83	-48.65	C98-Fe97-C103-C102	106.17
O15-W7-O32-W9	174.32	C54-Fe55-C61-C60	119.31	C75-Fe76-C82-H91	72.64	C98-Fe97-C103-C104	-135.6
O23-W7-O32-W9	70.79	C54-Fe55-C61-C62	-122.6	C77-Fe76-C82-C81	167.1	C98-Fe97-C103-H113	-14.88
O24-W7-O32-W9	-83.56	C54-Fe55-C61-H71	-0.67	C77-Fe76-C82-C83	-74.2	C99-Fe97-C103-C102	-173.1
O27-W7-O32-W9	-0.33	C56-Fe55-C61-C60	76.72	C77-Fe76-C82-H91	47.09	C99-Fe97-C103-C104	-54.89
O42-W7-O32-W9	-0.15	C56-Fe55-C61-C62	-165.2	C78-Fe76-C82-C81	56.47	C99-Fe97-C103-H113	65.85
O15-W7-O42-W9	-44.64	C56-Fe55-C61-H71	-43.26	C78-Fe76-C82-C83	175.17	C100-Fe97-C103-C102	15.47
O15-W7-O42-P13	-179.2	C57-Fe55-C61-C60	161.28	C78-Fe76-C82-H91	-63.54	C100-Fe97-C103-C104	133.68
O23-W7-O42-W9	-91.17	C57-Fe55-C61-C62	-80.59	C79-Fe76-C82-C81	85.56	C100-Fe97-C103-H113	-105.6
O23-W7-O42-P13	134.3	C57-Fe55-C61-H71	41.3	C79-Fe76-C82-C83	-155.8	C101-Fe97-C103-C102	66.12
O24-W7-O42-W9	93.12	C58-Fe55-C61-C60	-168.3	C79-Fe76-C82-H91	-34.45	C101-Fe97-C103-C104	-175.7
O24-W7-O42-P13	-41.4	C58-Fe55-C61-C62	-50.12	C80-Fe76-C82-C81	126.56	C101-Fe97-C103-H113	-54.93
O27-W7-O42-W9	-180	C58-Fe55-C61-H71	71.76	C80-Fe76-C82-C83	-114.7	C102-Fe97-C103-C104	118.21
O27-W7-O42-P13	45.48	C59-Fe55-C61-C60	45.38	C80-Fe76-C82-H91	6.55	C102-Fe97-C103-H113	-121.1
O32-W7-O42-W9	0.09	C59-Fe55-C61-C62	163.51	C81-Fe76-C82-C83	118.7	C104-Fe97-C103-C102	-118.2

O32-W7-O42-P13	-134.4	C59-Fe55-C61-H71	-74.6	C81-Fe76-C82-H91	-120	C104-Fe97-C103-H113	120.74
O36-W8-O28-W9	-127.2	C60-Fe55-C61-C62	118.13	C83-Fe76-C82-C81	-118.7	C105-Fe97-C103-C102	-81.03
O38-W8-O28-W9	30.77	C60-Fe55-C61-H71	-120	C83-Fe76-C82-H91	121.29	C105-Fe97-C103-C104	37.18
O39-W8-O28-W9	-49.9	C62-Fe55-C61-C60	-118.1	C84-Fe76-C82-C81	-80.15	C105-Fe97-C103-H113	157.92
O53-W8-O28-W9	132.32	C62-Fe55-C61-H71	121.89	C84-Fe76-C82-C83	38.55	C106-Fe97-C103-C102	-37.78
O28-W8-O36-W4	86.9	C63-Fe55-C61-C60	-80.6	C84-Fe76-C82-H91	159.84	C106-Fe97-C103-C104	80.43
O38-W8-O36-W4	17.9	C63-Fe55-C61-C62	37.53	C85-Fe76-C82-C81	-36.63	C106-Fe97-C103-H113	-158.8
O39-W8-O36-W4	-67.46	C63-Fe55-C61-H71	159.42	C85-Fe76-C82-C83	82.06	C96-Fe97-C104-C103	105.29
O53-W8-O36-W4	-169.3	C64-Fe55-C61-C60	-37.76	C85-Fe76-C82-H91	-156.6	C96-Fe97-C104-C105	-135.4
O28-W8-O38-W2	-32.96	C64-Fe55-C61-C62	80.37	C75-Fe76-C83-C82	164.24	C96-Fe97-C104-H114	-14.84
O36-W8-O38-W2	36.49	C64-Fe55-C61-H71	-157.7	C75-Fe76-C83-C84	-77.74	C98-Fe97-C104-C103	68.14
O39-W8-O38-W2	121.11	C54-Fe55-C62-C61	76.47	C75-Fe76-C83-H92	43.06	C98-Fe97-C104-C105	-172.5
O53-W8-O38-W2	-136.3	C54-Fe55-C62-C63	-164.9	C77-Fe76-C83-C82	124.03	C98-Fe97-C104-H114	-52
O28-W8-O39-W1	-8.74	C54-Fe55-C62-H72	-44.4	C77-Fe76-C83-C84	-118	C99-Fe97-C104-C103	148.15
O36-W8-O39-W1	68.53	C56-Fe55-C62-C61	39.66	C77-Fe76-C83-H92	2.85	C99-Fe97-C104-C105	-92.52
O38-W8-O39-W1	-88.01	C56-Fe55-C62-C63	158.26	C78-Fe76-C83-C82	-171.5	C99-Fe97-C104-H114	28.02
O53-W8-O39-W1	169.05	C56-Fe55-C62-H72	-81.2	C78-Fe76-C83-C84	-53.48	C100-Fe97-C104-C103	-174.5
O20-W9-O16-W6	-26.13	C57-Fe55-C62-C61	119.66	C78-Fe76-C83-H92	67.32	C100-Fe97-C104-C105	-55.15
O28-W9-O16-W6	-96.56	C57-Fe55-C62-C63	-121.7	C79-Fe76-C83-C82	51.21	C100-Fe97-C104-H114	65.39
O32-W9-O16-W6	59.16	C57-Fe55-C62-H72	-1.21	C79-Fe76-C83-C84	169.24	C101-Fe97-C104-C103	40.13
O42-W9-O16-W6	-11.23	C58-Fe55-C62-C61	161.34	C79-Fe76-C83-H92	-69.96	C101-Fe97-C104-C105	159.46
O44-W9-O16-W6	162.12	C58-Fe55-C62-C63	-80.06	C80-Fe76-C83-C82	81.55	C101-Fe97-C104-H114	-80.01
O16-W9-O20-W2	-37.63	C58-Fe55-C62-H72	40.48	C80-Fe76-C83-C84	-160.4	C102-Fe97-C104-C103	-38.4
O28-W9-O20-W2	33.02	C59-Fe55-C62-C61	-163.8	C80-Fe76-C83-H92	-39.62	C102-Fe97-C104-C105	80.93
O32-W9-O20-W2	-122.5	C59-Fe55-C62-C63	-45.21	C81-Fe76-C83-C82	-37.54	C102-Fe97-C104-H114	-158.5
O42-W9-O20-W2	-51.55	C59-Fe55-C62-H72	75.33	C81-Fe76-C83-C84	80.48	C103-Fe97-C104-C105	119.33



O44-W9-O20-W2	134.07	C60-Fe55-C62-C61	-38.5	C81-Fe76-C83-H92	-158.7	C103-Fe97-C104-H114	-120.1
O16-W9-O28-W8	123.85	C60-Fe55-C62-C63	80.1	C82-Fe76-C83-C84	118.02	C105-Fe97-C104-C103	-119.3
O20-W9-O28-W8	-30.39	C60-Fe55-C62-H72	-159.4	C82-Fe76-C83-H92	-121.2	C105-Fe97-C104-H114	120.54
O32-W9-O28-W8	47.96	C61-Fe55-C62-C63	118.6	C84-Fe76-C83-C82	-118	C106-Fe97-C104-C103	-82.2
O42-W9-O28-W8	54.85	C61-Fe55-C62-H72	-120.9	C84-Fe76-C83-H92	120.8	C106-Fe97-C104-C105	37.12
O44-W9-O28-W8	-133.8	C63-Fe55-C62-C61	-118.6	C85-Fe76-C83-C82	-80.34	C106-Fe97-C104-H114	157.66
O16-W9-O32-W7	-68.05	C63-Fe55-C62-H72	120.53	C85-Fe76-C83-C84	37.68	C96-Fe97-C105-C104	66.73
O20-W9-O32-W7	84.7	C64-Fe55-C62-C61	-82.01	C85-Fe76-C83-H92	158.48	C96-Fe97-C105-C106	-173.5
O28-W9-O32-W7	7.4	C64-Fe55-C62-C63	36.59	C75-Fe76-C84-C83	123.44	C96-Fe97-C105-H115	-53.03
O42-W9-O32-W7	0.15	C64-Fe55-C62-H72	157.12	C75-Fe76-C84-C85	-118	C98-Fe97-C105-C104	51.31
O44-W9-O32-W7	-170.8	C54-Fe55-C63-C62	40.49	C75-Fe76-C84-H93	3.85	C98-Fe97-C105-C106	171.05
O16-W9-O42-W7	95.17	C54-Fe55-C63-C64	160.74	C77-Fe76-C84-C83	79.33	C98-Fe97-C105-H115	-68.44
O16-W9-O42-P13	-130.6	C54-Fe55-C63-H73	-78.77	C77-Fe76-C84-C85	-162.1	C99-Fe97-C105-C104	103.45
O20-W9-O42-W7	-91.64	C56-Fe55-C63-C62	-161	C77-Fe76-C84-H93	-40.26	C99-Fe97-C105-C106	-136.8
O20-W9-O42-P13	42.63	C56-Fe55-C63-C64	-40.79	C78-Fe76-C84-C83	164.71	C99-Fe97-C105-H115	-16.3
O28-W9-O42-W7	-177	C56-Fe55-C63-H73	79.7	C78-Fe76-C84-C85	-76.72	C100-Fe97-C105-C104	147.31
O28-W9-O42-P13	-42.75	C57-Fe55-C63-C62	78.18	C78-Fe76-C84-H93	45.12	C100-Fe97-C105-C106	-92.95
O32-W9-O42-W7	-0.09	C57-Fe55-C63-C64	-161.6	C79-Fe76-C84-C83	-160.1	C100-Fe97-C105-H115	27.56
O32-W9-O42-P13	134.17	C57-Fe55-C63-H73	-41.08	C79-Fe76-C84-C85	-41.57	C101-Fe97-C105-C104	-177.2
O44-W9-O42-W7	56.93	C58-Fe55-C63-C62	120.12	C79-Fe76-C84-H93	80.27	C101-Fe97-C105-C106	-57.44
O44-W9-O42-P13	-168.8	C58-Fe55-C63-C64	-119.6	C80-Fe76-C84-C83	42.55	C101-Fe97-C105-H115	63.07
O22-W10-O14-W2	3.98	C58-Fe55-C63-H73	0.86	C80-Fe76-C84-C85	161.11	C102-Fe97-C105-C104	-81.96
O24-W10-O14-W2	87.91	C59-Fe55-C63-C62	161.93	C80-Fe76-C84-H93	-77.04	C102-Fe97-C105-C106	37.79
O31-W10-O14-W2	19.19	C59-Fe55-C63-C64	-77.83	C81-Fe76-C84-C83	-82	C102-Fe97-C105-H115	158.29
O34-W10-O14-W2	-67.53	C59-Fe55-C63-H73	42.66	C81-Fe76-C84-C85	36.57	C103-Fe97-C105-C104	-37.68
O52-W10-O14-W2	-169.5	C60-Fe55-C63-C62	-82.98	C81-Fe76-C84-H93	158.41	C103-Fe97-C105-C106	82.06

O14-W10-O22-W2	-2.4	C60-Fe55-C63-C64	37.26	C82-Fe76-C84-C83	-38.58	C103-Fe97-C105-H115	-157.4
O14-W10-O22-W5	-91.46	C60-Fe55-C63-H73	157.76	C82-Fe76-C84-C85	79.98	C104-Fe97-C105-C106	119.74
O14-W10-O22-P13	133.4	C61-Fe55-C63-C62	-38.42	C82-Fe76-C84-H93	-158.2	C104-Fe97-C105-H115	-119.8
O24-W10-O22-W2	-91.12	C61-Fe55-C63-C64	81.82	C83-Fe76-C84-C85	118.56	C106-Fe97-C105-C104	-119.7
O24-W10-O22-W5	179.82	C61-Fe55-C63-H73	-157.7	C83-Fe76-C84-H93	-119.6	C106-Fe97-C105-H115	120.51
O24-W10-O22-P13	44.68	C62-Fe55-C63-C64	120.24	C85-Fe76-C84-C83	-118.6	C96-Fe97-C106-C102	159.13
O31-W10-O22-W2	-176	C62-Fe55-C63-H73	-119.3	C85-Fe76-C84-H93	121.84	C96-Fe97-C106-C105	40.07
O31-W10-O22-W5	94.97	C64-Fe55-C63-C62	-120.2	C75-Fe76-C85-C81	-158.1	C96-Fe97-C106-H116	-81.03
O31-W10-O22-P13	-40.16	C64-Fe55-C63-H73	120.49	C75-Fe76-C85-C84	81.73	C98-Fe97-C106-C102	-59.06
O34-W10-O22-W2	90.8	C54-Fe55-C64-C60	-43.12	C75-Fe76-C85-H94	-38.48	C98-Fe97-C106-C105	-178.1
O34-W10-O22-W5	1.73	C54-Fe55-C64-C63	-163.1	C77-Fe76-C85-C81	161.39	C98-Fe97-C106-H116	60.78
O34-W10-O22-P13	-133.4	C54-Fe55-C64-H74	77.72	C77-Fe76-C85-C84	41.19	C99-Fe97-C106-C102	-177.2
O52-W10-O22-W2	47.42	C56-Fe55-C64-C60	-77.24	C77-Fe76-C85-H94	-79.01	C99-Fe97-C106-C105	63.75
O52-W10-O22-W5	-41.64	C56-Fe55-C64-C63	162.79	C78-Fe76-C85-C81	-114.2	C99-Fe97-C106-H116	-57.36
O52-W10-O22-P13	-176.8	C56-Fe55-C64-H74	43.6	C78-Fe76-C85-C84	125.64	C100-Fe97-C106-C102	-137.9
O14-W10-O24-W7	-128.2	C57-Fe55-C64-C60	167.74	C78-Fe76-C85-H94	5.43	C100-Fe97-C106-C105	103.02
O22-W10-O24-W7	-56.55	C57-Fe55-C64-C63	47.77	C79-Fe76-C85-C81	-72.18	C100-Fe97-C106-H116	-18.08
O31-W10-O24-W7	28.37	C57-Fe55-C64-H74	-71.42	C79-Fe76-C85-C84	167.62	C101-Fe97-C106-C102	-93.66
O34-W10-O24-W7	-52.3	C58-Fe55-C64-C60	-159.9	C79-Fe76-C85-H94	47.42	C101-Fe97-C106-C105	147.29
O52-W10-O24-W7	129.06	C58-Fe55-C64-C63	80.18	C80-Fe76-C85-C81	-31.49	C101-Fe97-C106-H116	26.18
O14-W10-O31-W11	37.08	C58-Fe55-C64-H74	-39.01	C80-Fe76-C85-C84	-151.7	C102-Fe97-C106-C105	-119.1
O22-W10-O31-W11	51.56	C59-Fe55-C64-C60	-119.4	C80-Fe76-C85-H94	88.11	C102-Fe97-C106-H116	119.84
O24-W10-O31-W11	-32.14	C59-Fe55-C64-C63	120.63	C81-Fe76-C85-C84	-120.2	C103-Fe97-C106-C102	38.15
O34-W10-O31-W11	122.87	C59-Fe55-C64-H74	1.44	C81-Fe76-C85-H94	119.6	C103-Fe97-C106-C105	-80.9
O52-W10-O31-W11	-134.2	C60-Fe55-C64-C63	-120	C82-Fe76-C85-C81	37.14	C103-Fe97-C106-H116	157.99
O14-W10-O34-W5	68.58	C60-Fe55-C64-H74	120.84	C82-Fe76-C85-C84	-83.06	C104-Fe97-C106-C102	81.98

O22-W10-O34-W5	-2.74	C61-Fe55-C64-C60	38.54	C82-Fe76-C85-H94	156.74	C104-Fe97-C106-C105	-37.07
O24-W10-O34-W5	-7.19	C61-Fe55-C64-C63	-81.42	C83-Fe76-C85-C81	81.73	C104-Fe97-C106-H116	-158.2
O31-W10-O34-W5	-86.31	C61-Fe55-C64-H74	159.39	C83-Fe76-C85-C84	-38.47	C105-Fe97-C106-C102	119.06
O52-W10-O34-W5	171.45	C62-Fe55-C64-C60	82.99	C83-Fe76-C85-H94	-158.7	C105-Fe97-C106-H116	-121.1
O30-W11-O27-W7	37.97	C62-Fe55-C64-C63	-36.98	C84-Fe76-C85-C81	120.2	C96-C98-C101-Fe97	59.59
O31-W11-O27-W7	-30.07	C62-Fe55-C64-H74	-156.2	C84-Fe76-C85-H94	-120.2	C96-C98-C101-C100	-0.08
O33-W11-O27-W7	53.47	C63-Fe55-C64-C60	119.97	C75-C77-C80-Fe76	60.57	C96-C98-C101-H111	179.89
O41-W11-O27-W7	126.34	C63-Fe55-C64-H74	-119.2	C75-C77-C80-C79	-0.27	Fe97-C98-C101-C100	-59.67
O49-W11-O27-W7	-130.7	C54-C56-C59-Fe55	59.8	C75-C77-C80-H90	177.29	Fe97-C98-C101-H111	120.3
O27-W11-O30-W3	20.11	C54-C56-C59-C58	0.11	Fe76-C77-C80-C79	-60.84	H108-C98-C101-Fe97	-116.9
O31-W11-O30-W3	87.58	C54-C56-C59-H69	175.99	Fe76-C77-C80-H90	116.72	H108-C98-C101-C100	-176.6
O33-W11-O30-W3	3.86	Fe55-C56-C59-C58	-59.69	H87-C77-C80-Fe76	-118.7	H108-C98-C101-H111	3.4
O41-W11-O30-W3	-69.07	Fe55-C56-C59-H69	116.19	H87-C77-C80-C79	-179.5	C96-C99-C100-Fe97	-61.53
O49-W11-O30-W3	-171.1	H66-C56-C59-Fe55	-116.5	H87-C77-C80-H90	-1.95	C96-C99-C100-C101	-0.54
O27-W11-O31-W10	32.64	H66-C56-C59-C58	-176.2	C75-C78-C79-Fe76	-57.99	C96-C99-C100-H110	179.23
O30-W11-O31-W10	-125	H66-C56-C59-H69	-0.34	C75-C78-C79-C80	-0.22	Fe97-C99-C100-C101	60.99
O33-W11-O31-W10	-52.79	C54-C57-C58-Fe55	-58.68	C75-C78-C79-H89	-176.9	Fe97-C99-C100-H110	-119.2
O41-W11-O31-W10	-47.54	C54-C57-C58-C59	-0.48	Fe76-C78-C79-C80	57.77	H109-C99-C100-Fe97	118.34
O49-W11-O31-W10	134.95	C54-C57-C58-H68	-176.3	Fe76-C78-C79-H89	-118.9	H109-C99-C100-C101	179.33
O27-W11-O33-W3	-175.8	Fe55-C57-C58-C59	58.2	H88-C78-C79-Fe76	120.23	H109-C99-C100-H110	-0.9
O27-W11-O33-P13	-39.65	Fe55-C57-C58-H68	-117.7	H88-C78-C79-C80	177.99	Fe97-C100-C101-C98	61.98
O30-W11-O33-W3	-2.41	H67-C57-C58-Fe55	119.79	H88-C78-C79-H89	1.31	Fe97-C100-C101-H111	-118
O30-W11-O33-P13	133.73	H67-C57-C58-C59	177.99	Fe76-C79-C80-C77	58.92	C99-C100-C101-Fe97	-61.59
O31-W11-O33-W3	-91.33	H67-C57-C58-H68	2.13	Fe76-C79-C80-H90	-118.7	C99-C100-C101-C98	0.39
O31-W11-O33-P13	44.81	Fe55-C58-C59-C56	57.62	C78-C79-C80-Fe76	-58.61	C99-C100-C101-H111	-179.6
O41-W11-O33-W3	90.9	Fe55-C58-C59-H69	-118.3	C78-C79-C80-C77	0.31	H110-C100-C101-Fe97	118.64
O41-W11-O33-P13	-133	C57-C58-C59-Fe55	-57.4	C78-C79-C80-H90	-177.3	H110-C100-C101-C98	-179.4
O49-W11-O33-W3	31.13	C57-C58-C59-C56	0.23	H89-C79-C80-Fe76	118.09	H110-C100-C101-H111	0.65
O49-W11-O33-P13	167.27	C57-C58-C59-H69	-175.7	H89-C79-C80-C77	177.01	Fe97-C102-C103-C104	-60.94

O27-W11-O41-W12	-87.28	H68-C58-C59-Fe55	118.49	H89-C79-C80-H90	-0.59	Fe97-C102-C103-H113	120.11
O30-W11-O41-W12	68.48	H68-C58-C59-C56	176.12	Fe76-C81-C82-C83	-59.25	C106-C102-C103-Fe97	60.41
O31-W11-O41-W12	-8.72	H68-C58-C59-H69	0.16	Fe76-C81-C82-H91	118.49	C106-C102-C103-C104	-0.53
O33-W11-O41-W12	-3.27	Fe55-C60-C61-C62	-60.82	C85-C81-C82-Fe76	58.84	C106-C102-C103-H113	-179.5
O49-W11-O41-W12	168.78	Fe55-C60-C61-H71	119.06	C85-C81-C82-C83	-0.4	H112-C102-C103-Fe97	-120.7
O40-W12-O35-W4	130.61	C64-C60-C61-Fe55	61.25	C85-C81-C82-H91	177.33	H112-C102-C103-C104	178.4
O41-W12-O35-W4	46.21	C64-C60-C61-C62	0.42	H95-C81-C82-Fe76	-118	H112-C102-C103-H113	-0.54
O45-W12-O35-W4	-126	C64-C60-C61-H71	-179.7	H95-C81-C82-C83	-177.3	Fe97-C102-C106-C105	60.15
O47-W12-O35-W4	-24.09	H70-C60-C61-Fe55	-116.5	H95-C81-C82-H91	0.46	Fe97-C102-C106-H116	-116.3
O35-W12-O40-W3	-86.83	H70-C60-C61-C62	-177.3	Fe76-C81-C85-C84	57.79	C103-C102-C106-Fe97	-59.72
O41-W12-O40-W3	66.61	H70-C60-C61-H71	2.56	Fe76-C81-C85-H94	-119.9	C103-C102-C106-C105	0.43
O45-W12-O40-W3	171.58	Fe55-C60-C64-C63	59.28	C82-C81-C85-Fe76	-57.6	C103-C102-C106-H116	-176.1
O47-W12-O40-W3	-8.86	Fe55-C60-C64-H74	-115.6	C82-C81-C85-C84	0.19	H112-C102-C106-Fe97	121.35
O35-W12-O41-W11	17.69	C61-C60-C64-Fe55	-59.48	C82-C81-C85-H94	-177.5	H112-C102-C106-C105	-178.5
O40-W12-O41-W11	-67.3	C61-C60-C64-C63	-0.2	H95-C81-C85-Fe76	119.26	H112-C102-C106-H116	5.02
O45-W12-O41-W11	-170.2	C61-C60-C64-H74	-175.1	H95-C81-C85-C84	177.06	Fe97-C103-C104-C105	-59.83
O47-W12-O41-W11	87.72	H70-C60-C64-Fe55	118.23	H95-C81-C85-H94	-0.65	Fe97-C103-C104-H114	116.73
O35-W12-O47-W6	30.11	H70-C60-C64-C63	177.51	Fe76-C82-C83-C84	-60.75	C102-C103-C104-Fe97	60.25
O40-W12-O47-W6	-49.03	H70-C60-C64-H74	2.61	Fe76-C82-C83-H92	118.32	C102-C103-C104-C105	0.42
O41-W12-O47-W6	-124.8	Fe55-C61-C62-C63	-61.07	C81-C82-C83-Fe76	61.21	C102-C103-C104-H114	176.98
O45-W12-O47-W6	130.53	Fe55-C61-C62-H72	116.91	C81-C82-C83-C84	0.46	H113-C103-C104-Fe97	-120.8
O33-P13-O22-W2	178.2	C60-C61-C62-Fe55	60.58	C81-C82-C83-H92	179.53	H113-C103-C104-C105	179.38
O33-P13-O22-W5	-61.13	C60-C61-C62-C63	-0.48	H91-C82-C83-Fe76	-116.5	H113-C103-C104-H114	-4.06
O33-P13-O22-W10	58.47	C60-C61-C62-H72	177.5	H91-C82-C83-C84	-177.2	Fe97-C104-C105-C106	-58.88
O37-P13-O22-W2	-61.41	H71-C61-C62-Fe55	-119.3	H91-C82-C83-H92	1.87	Fe97-C104-C105-H115	116.15
O37-P13-O22-W5	59.26	H71-C61-C62-C63	179.63	Fe76-C83-C84-C85	-60.99	C103-C104-C105-Fe97	58.72
O37-P13-O22-W10	178.86	H71-C61-C62-H72	-2.38	Fe76-C83-C84-H93	118.75	C103-C104-C105-C106	-0.15
O42-P13-O22-W2	58.01	Fe55-C62-C63-C64	-58.75	C82-C83-C84-Fe76	60.65	C103-C104-C105-H115	174.87
O42-P13-O22-W5	178.68	Fe55-C62-C63-H73	116.26	C82-C83-C84-C85	-0.34	H114-C104-C105-Fe97	-117.9
O42-P13-O22-W10	-61.72	C61-C62-C63-Fe55	59.11	C82-C83-C84-H93	179.4	H114-C104-C105-C106	-176.7
O22-P13-O33-W3	59.06	C61-C62-C63-C64	0.36	H92-C83-C84-Fe76	-118.4	H114-C104-C105-H115	-1.71

O22-P13-O33-W11	-62.59	C61-C62-C63-H73	175.37	H92-C83-C84-C85	-179.4	Fe97-C105-C106-C102	-59.16
O37-P13-O33-W3	-61.11	H72-C62-C63-Fe55	-118.9	H92-C83-C84-H93	0.32	Fe97-C105-C106-H116	117.31
O37-P13-O33-W11	177.23	H72-C62-C63-C64	-177.7	Fe76-C84-C85-C81	-59.03	C104-C105-C106-Fe97	58.98
O42-P13-O33-W3	179.44	H72-C62-C63-H73	-2.65	Fe76-C84-C85-H94	118.64	C104-C105-C106-C102	-0.17
O42-P13-O33-W11	57.79	Fe55-C63-C64-C60	-57.9	C83-C84-C85-Fe76	59.12	C104-C105-C106-H116	176.29
O22-P13-O37-W1	-61.8	Fe55-C63-C64-H74	117.15	C83-C84-C85-C81	0.09	H115-C105-C106-Fe97	-116
O33-P13-O37-W1	58.79	C62-C63-C64-Fe55	57.8	C83-C84-C85-H94	177.76	H115-C105-C106-C102	-175.2
O42-P13-O37-W1	178.41	C62-C63-C64-C60	-0.1	H93-C84-C85-Fe76	-120.6	H115-C105-C106-H116	1.31

\*torsional angles closer to 0° or 180°.

**Table S11** Torsional angles between atoms in FcPMo optimized structure in aqueous phase

Atom1	Torsional angle (deg.)	Atom1	Torsional angle (deg.)	Atom1	Torsional angle (deg.)	Atom1	Torsional angle (deg.)
O18-Mo1-O19-Mo3	-141.7	O33-Mo11-O31-Mo10	-52.82	C54-C56-C59-H69	176.05	Fe76-C81-C85-H94	-120.04
O21-Mo1-O19-Mo3	-37.65	O41-Mo11-O31-Mo10	-54.74	Fe55-C56-C59-C58	-59.89	C82-C81-C85-Fe76	-57.71
O26-Mo1-O19-Mo3	119.96	O49-Mo11-O31-Mo10	136.36	Fe55-C56-C59-H69	116.25	C82-C81-C85-C84*	0.07
O37-Mo1-O19-Mo3	46.3	O27-Mo11-O33-Mo3	-171.31	H66-C56-C59-Fe55	-116.57	C82-C81-C85-H94	-177.76
O39-Mo1-O19-Mo3	23.46	O27-Mo11-O33-Mo12	99.02	H66-C56-C59-C58	-176.46	H95-C81-C85-Fe76	118.96
O18-Mo1-O21-Mo5	143.16	O27-Mo11-O33-P13	-35.37	H66-C56-C59-H69*	-0.32	H95-C81-C85-C84	176.74
O19-Mo1-O21-Mo5	37.52	O30-Mo11-O33-Mo3	-3.11	C54-C57-C58-Fe55	-58.51	H95-C81-C85-H94	-1.09
O26-Mo1-O21-Mo5	-54.08	O30-Mo11-O33-Mo12	-92.78	C54-C57-C58-C59*	-0.4	Fe76-C82-C83-C84	-60.75
O37-Mo1-O21-Mo5	-51.18	O30-Mo11-O33-P13	132.84	C54-C57-C58-H68	-176.19	Fe76-C82-C83-H92	118.44
O39-Mo1-O21-Mo5	-123.45	O31-Mo11-O33-Mo3	-88.2	Fe55-C57-C58-C59	58.1	C81-C82-C83-Fe76	61.14
O18-Mo1-O26-Mo4	161.47	O31-Mo11-O33-Mo12	-177.87	Fe55-C57-C58-H68	-117.69	C81-C82-C83-C84*	0.39
O19-Mo1-O26-Mo4	-91.28	O31-Mo11-O33-P13	47.75	H67-C57-C58-Fe55	120.19	C81-C82-C83-H92*	179.59
O21-Mo1-O26-Mo4	-1.79	O41-Mo11-O33-Mo3	90.97	H67-C57-C58-C59	178.29	H91-C82-C83-Fe76	-116.64
O37-Mo1-O26-Mo4	-4.79	O41-Mo11-O33-Mo12	1.3	H67-C57-C58-H68	2.5	H91-C82-C83-C84	-177.39
O39-Mo1-O26-Mo4	67.09	O41-Mo11-O33-P13	-133.09	Fe55-C58-C59-C56	57.86	H91-C82-C83-H92	1.8
O18-Mo1-O37-Mo4	-52.92	O49-Mo11-O33-Mo3	19.07	Fe55-C58-C59-H69	-118.34	Fe76-C83-C84-C85	-60.96
O18-Mo1-O37-Mo8	36.19	O49-Mo11-O33-Mo12	-70.6	C57-C58-C59-Fe55	-57.55	Fe76-C83-C84-H93	118.56
O18-Mo1-O37-P13	171.47	O49-Mo11-O33-P13	155.02	C57-C58-C59-C56*	0.31	C82-C83-C84-Fe76	60.61
O19-Mo1-O37-Mo4	99.18	O27-Mo11-O41-Mo12	-85.83	C57-C58-C59-H69	-175.89	C82-C83-C84-C85	-0.35
O19-Mo1-O37-Mo8	-171.71	O30-Mo11-O41-Mo12	68.57	H68-C58-C59-Fe55	118.28	C82-C83-C84-H93*	179.16
O19-Mo1-O37-P13	-36.43	O31-Mo11-O41-Mo12*	-0.06	H68-C58-C59-C56	176.14	H92-C83-C84-Fe76	-118.59
O21-Mo1-O37-Mo4	-175.88	O33-Mo11-O41-Mo12	-2.05	H68-C58-C59-H69*	-0.06	H92-C83-C84-C85*	-179.55
O21-Mo1-O37-Mo8	-86.78	O49-Mo11-O41-Mo12	168.72	Fe55-C60-C61-C62	-60.85	H92-C83-C84-H93*	-0.03
O21-Mo1-O37-P13	48.51	O35-Mo12-O33-Mo3	98.81	Fe55-C60-C61-H71	118.75	Fe76-C84-C85-C81	-58.92
O26-Mo1-O37-Mo4	2.98	O35-Mo12-O33-Mo11	-171.68	C64-C60-C61-Fe55	61.14	Fe76-C84-C85-H94	118.87
O26-Mo1-O37-Mo8	92.08	O35-Mo12-O33-P13	-37.07	C64-C60-C61-C62*	0.29	C83-C84-C85-Fe76	59.1
O26-Mo1-O37-P13	-132.63	O40-Mo12-O33-Mo3	1.09	C64-C60-C61-H71*	179.89	C83-C84-C85-C81*	0.18
O39-Mo1-O37-Mo4	-89.53	O40-Mo12-O33-Mo11	90.59	H70-C60-C61-Fe55	-116.37	C83-C84-C85-H94	177.97
O39-Mo1-O37-Mo8*	-0.42	O40-Mo12-O33-P13	-134.8	H70-C60-C61-C62	-177.22	H93-C84-C85-Fe76	-120.41
O39-Mo1-O37-P13	134.86	O41-Mo12-O33-Mo3	-90.72	H70-C60-C61-H71	2.38	H93-C84-C85-C81*	-179.33
O18-Mo1-O39-Mo8	-169.46	O41-Mo12-O33-Mo11	-1.22	Fe55-C60-C64-C63	59.34	H93-C84-C85-H94	-1.55
O19-Mo1-O39-Mo8	24.82	O41-Mo12-O33-P13	133.39	Fe55-C60-C64-H74	-115.98	C98-C96-Fe97-C99	120.22
O21-Mo1-O39-Mo8	85.95	O45-Mo12-O33-Mo3	-53.66	C61-C60-C64-Fe55	-59.44	C98-C96-Fe97-C100	81.65
O26-Mo1-O39-Mo8	-73.23	O45-Mo12-O33-Mo11	35.84	C61-C60-C64-C63*	-0.09	C98-C96-Fe97-C101	36.99
O37-Mo1-O39-Mo8*	0.72	O45-Mo12-O33-P13	170.45	C61-C60-C64-H74	-175.42	C98-C96-Fe97-C102	-56.82
O20-Mo2-O14-Mo10	-86.31	O47-Mo12-O33-Mo3	-175.24	H70-C60-C64-Fe55	118.04	C98-C96-Fe97-C103	-94.18
O22-Mo2-O14-Mo10	-3.28	O47-Mo12-O33-Mo11	-85.73	H70-C60-C64-C63	177.39	C98-C96-Fe97-C104	-137.87

O25-Mo2-O14-Mo10	66.73	O47-Mo12-O33-P13	48.88	H70-C60-C64-H74	2.07	C98-C96-Fe97-C105	-176.74
O38-Mo2-O14-Mo10	-2.2	O33-Mo12-O35-Mo4	51.42	Fe55-C61-C62-C63	-60.95	C98-C96-Fe97-C106	147.71
O48-Mo2-O14-Mo10	168.38	O40-Mo12-O35-Mo4	121.97	Fe55-C61-C62-H72	117	C99-C96-Fe97-C98	-120.22
O14-Mo2-O20-Mo9	119.25	O41-Mo12-O35-Mo4	30.35	C60-C61-C62-Fe55	60.57	C99-C96-Fe97-C100	-38.57
O22-Mo2-O20-Mo9	47.2	O45-Mo12-O35-Mo4	-133.08	C60-C61-C62-C63*	-0.38	C99-C96-Fe97-C101	-83.23
O25-Mo2-O20-Mo9	22.19	O47-Mo12-O35-Mo4	-31.12	C60-C61-C62-H72	177.57	C99-C96-Fe97-C102	-177.04
O38-Mo2-O20-Mo9	-36.02	O33-Mo12-O40-Mo3	-1.67	H71-C61-C62-Fe55	-119.02	C99-C96-Fe97-C103	145.6
O48-Mo2-O20-Mo9	-134.41	O35-Mo12-O40-Mo3	-85.43	H71-C61-C62-C63	-179.97	C99-C96-Fe97-C104	101.91
O14-Mo2-O22-Mo5	92.07	O41-Mo12-O40-Mo3	68.83	H71-C61-C62-H72	-2.02	C99-C96-Fe97-C105	63.04
O14-Mo2-O22-Mo10	2.09	O45-Mo12-O40-Mo3	170.33	Fe55-C62-C63-C64	-58.66	C99-C96-Fe97-C106	27.49
O14-Mo2-O22-P13	-132.1	O47-Mo12-O40-Mo3	6.42	Fe55-C62-C63-H73	116.61	H107-C96-Fe97-C98	120.63
O20-Mo2-O22-Mo5	-170.74	O33-Mo12-O41-Mo11	2.05	C61-C62-C63-Fe55	58.98	H107-C96-Fe97-C99	-119.15
O20-Mo2-O22-Mo10	99.27	O35-Mo12-O41-Mo11	24.49	C61-C62-C63-C64*	0.33	H107-C96-Fe97-C100	-157.72
O20-Mo2-O22-P13	-34.92	O40-Mo12-O41-Mo11	-69.58	C61-C62-C63-H73	175.59	H107-C96-Fe97-C101	157.61
O25-Mo2-O22-Mo5	-2.56	O45-Mo12-O41-Mo11	-172.07	H72-C62-C63-Fe55	-119.01	H107-C96-Fe97-C102	63.81
O25-Mo2-O22-Mo10	-92.55	O47-Mo12-O41-Mo11	86.61	H72-C62-C63-C64	-177.67	H107-C96-Fe97-C103	26.44
O25-Mo2-O22-P13	133.26	O33-Mo12-O47-Mo6	-56.3	H72-C62-C63-H73	-2.4	H107-C96-Fe97-C104	-17.24
O38-Mo2-O22-Mo5	-87.47	O35-Mo12-O47-Mo6	30.35	Fe55-C63-C64-C60	-57.92	H107-C96-Fe97-C105	-56.11
O38-Mo2-O22-Mo10	-177.46	O40-Mo12-O47-Mo6	-64.02	Fe55-C63-C64-H74	117.54	H107-C96-Fe97-C106	-91.66
O38-Mo2-O22-P13	48.35	O41-Mo12-O47-Mo6	-127.07	C62-C63-C64-Fe55	57.77	Fe97-C96-C98-C101	-57.41
O48-Mo2-O22-Mo5	19.94	O45-Mo12-O47-Mo6	132.03	C62-C63-C64-C60*	-0.14	Fe97-C96-C98-H108	119.06
O48-Mo2-O22-Mo10	-70.05	O33-P13-O22-Mo2	175.53	C62-C63-C64-H74	175.31	C99-C96-C98-Fe97	57.34
O48-Mo2-O22-P13	155.76	O33-P13-O22-Mo5	-63.63	H73-C63-C64-Fe55	-117.48	C99-C96-C98-C101*	-0.07
O14-Mo2-O25-Mo5	-68.07	O33-P13-O22-Mo10	56.57	H73-C63-C64-C60	-175.4	C99-C96-C98-H108	176.4
O20-Mo2-O25-Mo5	30.64	O37-P13-O22-Mo2	-63.86	H73-C63-C64-H74*	0.06	H107-C96-C98-Fe97	-119.77
O22-Mo2-O25-Mo5	4.1	O37-P13-O22-Mo5	56.97	C77-C75-Fe76-C78	118.62	H107-C96-C98-C101	-177.18
O38-Mo2-O25-Mo5	88.83	O37-P13-O22-Mo10	177.18	C77-C75-Fe76-C79	81.84	H107-C96-C98-H108*	-0.72
O48-Mo2-O25-Mo5	-172.59	O42-P13-O22-Mo2	55.86	C77-C75-Fe76-C80	38.52	Fe97-C96-C99-C100	59.17
O14-Mo2-O38-Mo8	-54.52	O42-P13-O22-Mo5	176.69	C77-C75-Fe76-C81	167.37	Fe97-C96-C99-H109	-120.06
O20-Mo2-O38-Mo8	32.35	O42-P13-O22-Mo10	-63.1	C77-C75-Fe76-C82	-33.26	C98-C96-C99-Fe97	-58.76
O22-Mo2-O38-Mo8	-53.49	O22-P13-O33-Mo3	55.41	C77-C75-Fe76-C83	-71.06	C98-C96-C99-C100*	0.41
O25-Mo2-O38-Mo8	-124.62	O22-P13-O33-Mo11	-65.33	C77-C75-Fe76-C84	-113.97	C98-C96-C99-H109	-178.82
O48-Mo2-O38-Mo8	134.73	O22-P13-O33-Mo12	176.02	C77-C75-Fe76-C85	-156.67	H107-C96-C99-Fe97	118.35
O19-Mo3-O17-Mo5	-32.44	O37-P13-O33-Mo3	-65.1	C78-C75-Fe76-C77	-118.62	H107-C96-C99-C100	177.52
O30-Mo3-O17-Mo5	123.1	O37-P13-O33-Mo11	174.17	C78-C75-Fe76-C79	-36.78	H107-C96-C99-H109	-1.71
O33-Mo3-O17-Mo5	50.6	O37-P13-O33-Mo12	55.52	C78-C75-Fe76-C80	-80.1	C96-Fe97-C98-C101	120.46
O40-Mo3-O17-Mo5	29.45	O42-P13-O33-Mo3	175.18	C78-C75-Fe76-C81	48.74	C96-Fe97-C98-H108	-120.11
O46-Mo3-O17-Mo5	-135.76	O42-P13-O33-Mo11	54.45	C78-C75-Fe76-C82	-151.88	C99-Fe97-C98-C96	-37.09
O17-Mo3-O19-Mo1	36.63	O42-P13-O33-Mo12	-64.2	C78-C75-Fe76-C83	170.31	C99-Fe97-C98-C101	83.37
O30-Mo3-O19-Mo1	-52.31	O22-P13-O37-Mo1	-65.08	C78-C75-Fe76-C84	127.41	C99-Fe97-C98-H108	-157.2
O33-Mo3-O19-Mo1	-49.57	O22-P13-O37-Mo4	175.22	C78-C75-Fe76-C85	84.71	C100-Fe97-C98-C96	-81.78
O40-Mo3-O19-Mo1	-121.61	O22-P13-O37-Mo8	55.12	H86-C75-Fe76-C77	119.6	C100-Fe97-C98-C101	38.68
O46-Mo3-O19-Mo1	141.15	O33-P13-O37-Mo1	55.82	H86-C75-Fe76-C78	-121.77	C100-Fe97-C98-H108	158.1

O17-Mo3-O30-Mo11	-88.84	O33-P13-O37-Mo4	-63.88	H86-C75-Fe76-C79	-158.56	C101-Fe97-C98-C96	-120.46
O19-Mo3-O30-Mo11	-2.12	O33-P13-O37-Mo8	176.02	H86-C75-Fe76-C80	158.12	C101-Fe97-C98-H108	119.43
O33-Mo3-O30-Mo11	-4.96	O42-P13-O37-Mo1	175.32	H86-C75-Fe76-C81	-73.03	C102-Fe97-C98-C96	148.2
O40-Mo3-O30-Mo11	66.49	O42-P13-O37-Mo4	55.62	H86-C75-Fe76-C82	86.35	C102-Fe97-C98-C101	-91.34
O46-Mo3-O30-Mo11	164.66	O42-P13-O37-Mo8	-64.48	H86-C75-Fe76-C83	48.54	C102-Fe97-C98-H108	28.09
O17-Mo3-O33-Mo11	99.45	O22-P13-O42-Mo6	176.42	H86-C75-Fe76-C84	5.64	C103-Fe97-C98-C96	103.52
O17-Mo3-O33-Mo12	-171.87	O22-P13-O42-Mo7	55.88	H86-C75-Fe76-C85	-37.07	C103-Fe97-C98-C101	-136.01
O17-Mo3-O33-P13	-36.35	O22-P13-O42-Mo9	-64.09	Fe76-C75-C77-C80	-60.82	C103-Fe97-C98-H108	-16.59
O19-Mo3-O33-Mo11	-175.64	O33-P13-O42-Mo6	56.07	Fe76-C75-C77-H87	118.47	C104-Fe97-C98-C96	63.55
O19-Mo3-O33-Mo12	-86.96	O33-P13-O42-Mo7	-64.47	C78-C75-C77-Fe76	60.95	C104-Fe97-C98-C101	-175.99
O19-Mo3-O33-P13	48.55	O33-P13-O42-Mo9	175.56	C78-C75-C77-C80	0.13	C104-Fe97-C98-H108	-56.56
O30-Mo3-O33-Mo11	3.17	O37-P13-O42-Mo6	-63.81	C78-C75-C77-H87*	179.42	C105-Fe97-C98-C96	20.67
O30-Mo3-O33-Mo12	91.85	O37-P13-O42-Mo7	175.65	H86-C75-C77-Fe76	-119.51	C105-Fe97-C98-C101	141.13
O30-Mo3-O33-P13	-132.63	O37-P13-O42-Mo9	55.68	H86-C75-C77-C80*	179.68	C105-Fe97-C98-H108	-99.44
O40-Mo3-O33-Mo11	-89.7	C56-C54-Fe55-C57	117.81	H86-C75-C77-H87	-1.03	C106-Fe97-C98-C96	-173.38
O40-Mo3-O33-Mo12	-1.02	C56-C54-Fe55-C58	80.67	Fe76-C75-C78-C79	59.41	C106-Fe97-C98-C101	-52.92
O40-Mo3-O33-P13	134.5	C56-C54-Fe55-C59	37.97	Fe76-C75-C78-H88	-118.72	C106-Fe97-C98-H108	66.51
O46-Mo3-O33-Mo11	-51.26	C56-C54-Fe55-C60	-77.69	C77-C75-C78-Fe76	-59.33	C96-Fe97-C99-C100	-118.57
O46-Mo3-O33-Mo12	37.42	C56-C54-Fe55-C61	-120.21	C77-C75-C78-C79*	0.07	C96-Fe97-C99-H109	121.02
O46-Mo3-O33-P13	172.94	C56-C54-Fe55-C62	-162.03	C77-C75-C78-H88	-178.06	C98-Fe97-C99-C96	36.49
O17-Mo3-O40-Mo12	24.02	C56-C54-Fe55-C63	167.71	H86-C75-C78-Fe76	121.12	C98-Fe97-C99-C100	-82.08
O19-Mo3-O40-Mo12	86.01	C56-C54-Fe55-C64	-46.31	H86-C75-C78-C79*	-179.47	C98-Fe97-C99-H109	157.51
O30-Mo3-O40-Mo12	-71.24	C57-C54-Fe55-C56	-117.81	H86-C75-C78-H88	2.4	C100-Fe97-C99-C96	118.57
O33-Mo3-O40-Mo12	1.72	C57-C54-Fe55-C58	-37.14	C75-Fe76-C77-C80	117.97	C100-Fe97-C99-H109	-120.41
O46-Mo3-O40-Mo12	-170.38	C57-C54-Fe55-C59	-79.85	C75-Fe76-C77-H87	-120.67	C101-Fe97-C99-C96	79.91
O29-Mo4-O26-Mo1	34.04	C57-C54-Fe55-C60	164.49	C78-Fe76-C77-C75	-37.76	C101-Fe97-C99-C100	-38.66
O35-Mo4-O26-Mo1	88.73	C57-C54-Fe55-C61	121.98	C78-Fe76-C77-C80	80.22	C101-Fe97-C99-H109	-159.07
O36-Mo4-O26-Mo1	-67.53	C57-C54-Fe55-C62	80.15	C78-Fe76-C77-H87	-158.43	C102-Fe97-C99-C96	163.7
O37-Mo4-O26-Mo1	4.64	C57-C54-Fe55-C63	49.9	C79-Fe76-C77-C75	-80.63	C102-Fe97-C99-C100	45.13
O51-Mo4-O26-Mo1	-171.23	C57-C54-Fe55-C64	-164.13	C79-Fe76-C77-C80	37.34	C102-Fe97-C99-H109	-75.29
O26-Mo4-O29-Mo6	18.87	H65-C54-Fe55-C56	120.29	C79-Fe76-C77-H87	158.7	C103-Fe97-C99-C96	-59.66
O35-Mo4-O29-Mo6	-35.81	H65-C54-Fe55-C57	-121.9	C80-Fe76-C77-C75	-117.97	C103-Fe97-C99-C100	-178.23
O36-Mo4-O29-Mo6	118.47	H65-C54-Fe55-C58	-159.04	C80-Fe76-C77-H87	121.35	C103-Fe97-C99-H109	61.36
O37-Mo4-O29-Mo6	46.47	H65-C54-Fe55-C59	158.25	C81-Fe76-C77-C75	-163.42	C104-Fe97-C99-C96	-94.94
O51-Mo4-O29-Mo6	-135.64	H65-C54-Fe55-C60	42.6	C81-Fe76-C77-C80	-45.45	C104-Fe97-C99-C100	146.49
O26-Mo4-O35-Mo12	-125.56	H65-C54-Fe55-C61*	0.08	C81-Fe76-C77-H87	75.91	C104-Fe97-C99-H109	26.07
O29-Mo4-O35-Mo12	32.03	H65-C54-Fe55-C62	-41.75	C82-Fe76-C77-C75	168.97	C105-Fe97-C99-C96	-137.59
O36-Mo4-O35-Mo12	-56.6	H65-C54-Fe55-C63	-72	C82-Fe76-C77-C80	-73.06	C105-Fe97-C99-C100	103.84
O37-Mo4-O35-Mo12	-54.51	H65-C54-Fe55-C64	73.98	C82-Fe76-C77-H87	48.3	C105-Fe97-C99-H109	-16.58
O51-Mo4-O35-Mo12	134.36	Fe55-C54-C56-C59	-61.5	C83-Fe76-C77-C75	127.73	C106-Fe97-C99-C96	-175.61
O26-Mo4-O36-Mo8	66.9	Fe55-C54-C56-H66	114.88	C83-Fe76-C77-C80	-114.3	C106-Fe97-C99-C100	65.82
O29-Mo4-O36-Mo8	-85.96	C57-C54-C56-Fe55	61.34	C83-Fe76-C77-H87	7.05	C106-Fe97-C99-H109	-54.59
O35-Mo4-O36-Mo8*	-0.66	C57-C54-C56-C59*	-0.16	C84-Fe76-C77-C75	85.48	C96-Fe97-C100-C99	37.56



O37-Mo4-O36-Mo8	-2.83	C57-C54-C56-H66	176.22	C84-Fe76-C77-C80	-156.55	C96-Fe97-C100-C101	-80.36
O51-Mo4-O36-Mo8	168.28	H65-C54-C56-Fe55	-118.03	C84-Fe76-C77-H87	-35.2	C96-Fe97-C100-H110	158.34
O26-Mo4-O37-Mo1	-2.97	H65-C54-C56-C59	-179.53	C85-Fe76-C77-C75	55.67	C98-Fe97-C100-C99	80.2
O26-Mo4-O37-Mo8	-92.94	H65-C54-C56-H66	-3.15	C85-Fe76-C77-C80	173.64	C98-Fe97-C100-C101	-37.71
O26-Mo4-O37-P13	131.84	Fe55-C54-C57-C58	60.84	C85-Fe76-C77-H87	-65.01	C98-Fe97-C100-H110	-159.02
O29-Mo4-O37-Mo1	-169.8	Fe55-C54-C57-H67	-117.83	C75-Fe76-C78-C79	-119.85	C99-Fe97-C100-C101	-117.91
O29-Mo4-O37-Mo8	100.23	C56-C54-C57-Fe55	-60.5	C75-Fe76-C78-H88	120.08	C99-Fe97-C100-H110	120.78
O29-Mo4-O37-P13	-34.99	C56-C54-C57-C58*	0.35	C77-Fe76-C78-C75	38.42	C101-Fe97-C100-C99	117.91
O35-Mo4-O37-Mo1	-87.26	C56-C54-C57-H67	-178.33	C77-Fe76-C78-C79	-81.43	C101-Fe97-C100-H110	-121.3
O35-Mo4-O37-Mo8	-177.23	H65-C54-C57-Fe55	118.87	C77-Fe76-C78-H88	158.5	C102-Fe97-C100-C99	-174.08
O35-Mo4-O37-P13	47.55	H65-C54-C57-C58*	179.71	C79-Fe76-C78-C75	119.85	C102-Fe97-C100-C101	68
O36-Mo4-O37-Mo1	91.79	H65-C54-C57-H67	1.04	C79-Fe76-C78-H88	-120.07	C102-Fe97-C100-H110	-53.3
O36-Mo4-O37-Mo8	1.82	C54-Fe55-C56-C59	118.21	C80-Fe76-C78-C75	82.84	C103-Fe97-C100-C99	167.71
O36-Mo4-O37-P13	-133.4	C54-Fe55-C56-H66	-120.07	C80-Fe76-C78-C79	-37.01	C103-Fe97-C100-C101	49.8
O51-Mo4-O37-Mo1	23.02	C57-Fe55-C56-C54	-38.51	C80-Fe76-C78-H88	-157.08	C103-Fe97-C100-H110	-71.5
O51-Mo4-O37-Mo8	-66.95	C57-Fe55-C56-C59	79.7	C81-Fe76-C78-C75	-158.92	C104-Fe97-C100-C99	-58.01
O51-Mo4-O37-P13	157.83	C57-Fe55-C56-H66	-158.58	C81-Fe76-C78-C79	81.23	C104-Fe97-C100-C101	-175.92
O21-Mo5-O17-Mo3	32.73	C58-Fe55-C56-C54	-81.55	C81-Fe76-C78-H88	-38.84	C104-Fe97-C100-H110	62.78
O22-Mo5-O17-Mo3	-54.2	C58-Fe55-C56-C59	36.66	C82-Fe76-C78-C75	162.34	C105-Fe97-C100-C99	-92.77
O25-Mo5-O17-Mo3	-57.34	C58-Fe55-C56-H66	158.38	C82-Fe76-C78-C79	42.49	C105-Fe97-C100-C101	149.32
O34-Mo5-O17-Mo3	-126.11	C59-Fe55-C56-C54	-118.21	C82-Fe76-C78-H88	-77.58	C105-Fe97-C100-H110	28.02
O50-Mo5-O17-Mo3	137.13	C59-Fe55-C56-H66	121.72	C83-Fe76-C78-C75	-31.91	C106-Fe97-C100-C99	-135.79
O17-Mo5-O21-Mo1	-35.22	C60-Fe55-C56-C54	120.3	C83-Fe76-C78-C79	-151.76	C106-Fe97-C100-C101	106.3
O22-Mo5-O21-Mo1	47.4	C60-Fe55-C56-C59	-121.48	C83-Fe76-C78-H88	88.17	C106-Fe97-C100-H110	-15
O25-Mo5-O21-Mo1	120.02	C60-Fe55-C56-H66*	0.24	C84-Fe76-C78-C75	-73.69	C96-Fe97-C101-C98	-36.34
O34-Mo5-O21-Mo1	26.35	C61-Fe55-C56-C54	78.53	C84-Fe76-C78-C79	166.46	C96-Fe97-C101-C100	82.01
O50-Mo5-O21-Mo1	-137.48	C61-Fe55-C56-C59	-163.26	C84-Fe76-C78-H88	46.39	C96-Fe97-C101-H111	-157.91
O17-Mo5-O22-Mo2	-176.03	C61-Fe55-C56-H66	-41.54	C85-Fe76-C78-C75	-115.97	C98-Fe97-C101-C100	118.35
O17-Mo5-O22-Mo10	-87.4	C62-Fe55-C56-C54	48.89	C85-Fe76-C78-C79	124.18	C98-Fe97-C101-H111	-121.57
O17-Mo5-O22-P13	47.52	C62-Fe55-C56-C59	167.1	C85-Fe76-C78-H88	4.1	C99-Fe97-C101-C98	-79.69
O21-Mo5-O22-Mo2	99.03	C62-Fe55-C56-H66	-71.18	C75-Fe76-C79-C78	37.44	C99-Fe97-C101-C100	38.66
O21-Mo5-O22-Mo10	-172.34	C63-Fe55-C56-C54	-169.43	C75-Fe76-C79-C80	-82.77	C99-Fe97-C101-H111	158.74
O21-Mo5-O22-P13	-37.41	C63-Fe55-C56-C59	-51.22	C75-Fe76-C79-H89	158.06	C100-Fe97-C101-C98	-118.35
O25-Mo5-O22-Mo2	2.6	C63-Fe55-C56-H66	70.5	C77-Fe76-C79-C78	82	C100-Fe97-C101-H111	120.08
O25-Mo5-O22-Mo10	91.23	C64-Fe55-C56-C54	161.35	C77-Fe76-C79-C80	-38.21	C102-Fe97-C101-C98	106.64
O25-Mo5-O22-P13	-133.85	C64-Fe55-C56-C59	-80.44	C77-Fe76-C79-H89	-157.37	C102-Fe97-C101-C100	-135.01
O34-Mo5-O22-Mo2	-89.87	C64-Fe55-C56-H66	41.28	C78-Fe76-C79-C80	-120.21	C102-Fe97-C101-H111	-14.92
O34-Mo5-O22-Mo10	-1.24	C54-Fe55-C57-C58	-119.08	C78-Fe76-C79-H89	120.63	C103-Fe97-C101-C98	67.03
O34-Mo5-O22-P13	133.68	C54-Fe55-C57-H67	120.19	C80-Fe76-C79-C78	120.21	C103-Fe97-C101-C100	-174.62
O50-Mo5-O22-Mo2	-58.61	C56-Fe55-C57-C54	38.82	C80-Fe76-C79-H89	-119.16	C103-Fe97-C101-H111	-54.54
O50-Mo5-O22-Mo10	30.03	C56-Fe55-C57-C58	-80.26	C81-Fe76-C79-C78	-117.12	C104-Fe97-C101-C98	33.26
O50-Mo5-O22-P13	164.95	C56-Fe55-C57-H67	159.01	C81-Fe76-C79-C80	122.67	C104-Fe97-C101-C100	151.61
O17-Mo5-O25-Mo2*	-0.91	C58-Fe55-C57-C54	119.08	C81-Fe76-C79-H89	3.5	C104-Fe97-C101-H111	-88.31

O21-Mo5-O25-Mo2	-88.67	C58-Fe55-C57-H67	-120.74	C82-Fe76-C79-C78	-159.85	C105-Fe97-C101-C98	-172.79
O22-Mo5-O25-Mo2	-4.17	C59-Fe55-C57-C54	82.61	C82-Fe76-C79-C80	79.94	C105-Fe97-C101-C100	-54.44
O34-Mo5-O25-Mo2	67.26	C59-Fe55-C57-C58	-36.47	C82-Fe76-C79-H89	-39.23	C105-Fe97-C101-H111	65.64
O50-Mo5-O25-Mo2	164.76	C59-Fe55-C57-H67	-157.2	C83-Fe76-C79-C78	164.75	C106-Fe97-C101-C98	150.76
O17-Mo5-O34-Mo10	85.96	C60-Fe55-C57-C54	-39.86	C83-Fe76-C79-C80	44.54	C106-Fe97-C101-C100	-90.89
O21-Mo5-O34-Mo10	24.29	C60-Fe55-C57-C58	-158.93	C83-Fe76-C79-H89	-74.63	C106-Fe97-C101-H111	29.19
O22-Mo5-O34-Mo10	2.06	C60-Fe55-C57-H67	80.33	C84-Fe76-C79-C78	-44.81	C96-Fe97-C102-C103	-57.13
O25-Mo5-O34-Mo10	-71.11	C61-Fe55-C57-C54	-76.82	C84-Fe76-C79-C80	-165.02	C96-Fe97-C102-C106	-175.63
O50-Mo5-O34-Mo10	-171.45	C61-Fe55-C57-C58	164.1	C84-Fe76-C79-H89	75.82	C96-Fe97-C102-H112	63.59
O23-Mo6-O16-Mo9	-62.16	C61-Fe55-C57-H67	43.37	C85-Fe76-C79-C78	-77.34	C98-Fe97-C102-C103	-93.45
O29-Mo6-O16-Mo9	94.98	C62-Fe55-C57-C54	-120.14	C85-Fe76-C79-C80	162.45	C98-Fe97-C102-C106	148.06
O42-Mo6-O16-Mo9	8.86	C62-Fe55-C57-C58	120.78	C85-Fe76-C79-H89	43.29	C98-Fe97-C102-H112	27.27
O43-Mo6-O16-Mo9	-165.71	C62-Fe55-C57-H67*	0.04	C75-Fe76-C80-C77	-38.63	C99-Fe97-C102-C103	141.53
O47-Mo6-O16-Mo9	35.97	C63-Fe55-C57-C54	-161.96	C75-Fe76-C80-C79	80.38	C99-Fe97-C102-C106	23.04
O16-Mo6-O23-Mo7	66.64	C63-Fe55-C57-C58	78.96	C75-Fe76-C80-H90	-159.06	C99-Fe97-C102-H112	-97.75
O29-Mo6-O23-Mo7	4.8	C63-Fe55-C57-H67	-41.77	C77-Fe76-C80-C79	119.01	C100-Fe97-C102-C103	-177.65
O42-Mo6-O23-Mo7	-1.04	C64-Fe55-C57-C54	162.83	C77-Fe76-C80-H90	-120.43	C100-Fe97-C102-C106	63.86
O43-Mo6-O23-Mo7	169.26	C64-Fe55-C57-C58	43.76	C78-Fe76-C80-C77	-82.34	C100-Fe97-C102-H112	-56.93
O47-Mo6-O23-Mo7	-85.07	C64-Fe55-C57-H67	-76.98	C78-Fe76-C80-C79	36.67	C101-Fe97-C102-C103	-136.94
O16-Mo6-O29-Mo4	-119.17	C54-Fe55-C58-C57	38.17	C78-Fe76-C80-H90	157.22	C101-Fe97-C102-C106	104.56
O23-Mo6-O29-Mo4	-55.98	C54-Fe55-C58-C59	-82.29	C79-Fe76-C80-C77	-119.01	C101-Fe97-C102-H112	-16.22
O42-Mo6-O29-Mo4	-50.4	C54-Fe55-C58-H68	158.18	C79-Fe76-C80-H90	120.56	C103-Fe97-C102-C106	-118.5
O43-Mo6-O29-Mo4	139.4	C56-Fe55-C58-C57	82.94	C81-Fe76-C80-C77	164.21	C103-Fe97-C102-H112	120.72
O47-Mo6-O29-Mo4	36.62	C56-Fe55-C58-C59	-37.52	C81-Fe76-C80-C79	-76.78	C104-Fe97-C102-C103	37.75
O16-Mo6-O42-Mo7	-94.07	C56-Fe55-C58-H68	-157.05	C81-Fe76-C80-H90	43.77	C104-Fe97-C102-C106	-80.74
O16-Mo6-O42-Mo9	-4.99	C57-Fe55-C58-C59	-120.46	C82-Fe76-C80-C77	124.86	C104-Fe97-C102-H112	158.47
O16-Mo6-O42-P13	129.55	C57-Fe55-C58-H68	120.01	C82-Fe76-C80-C79	-116.13	C105-Fe97-C102-C103	80.9
O23-Mo6-O42-Mo7*	0.66	C59-Fe55-C58-C57	120.46	C82-Fe76-C80-H90	4.42	C105-Fe97-C102-C106	-37.6
O23-Mo6-O42-Mo9	89.75	C59-Fe55-C58-H68	-119.53	C83-Fe76-C80-C77	82.41	C105-Fe97-C102-H112	-158.39
O23-Mo6-O42-P13	-135.72	C60-Fe55-C58-C57	159.72	C83-Fe76-C80-C79	-158.58	C106-Fe97-C102-C103	118.5
O29-Mo6-O42-Mo7	-176.79	C60-Fe55-C58-C59	39.26	C83-Fe76-C80-H90	-38.02	C106-Fe97-C102-H112	-120.78
O29-Mo6-O42-Mo9	-87.7	C60-Fe55-C58-H68	-80.27	C84-Fe76-C80-C77	52.14	C96-Fe97-C103-C102	148.42
O29-Mo6-O42-P13	46.83	C61-Fe55-C58-C57	-41.13	C84-Fe76-C80-C79	171.15	C96-Fe97-C103-C104	-92.95
O43-Mo6-O42-Mo7	-63.57	C61-Fe55-C58-C59	-161.59	C84-Fe76-C80-H90	-68.29	C96-Fe97-C103-H113	27.87
O43-Mo6-O42-Mo9	25.51	C61-Fe55-C58-H68	78.88	C85-Fe76-C80-C77	-171.44	C98-Fe97-C103-C102	105.46
O43-Mo6-O42-P13	160.04	C62-Fe55-C58-C57	-78.86	C85-Fe76-C80-C79	-52.43	C98-Fe97-C103-C104	-135.9
O47-Mo6-O42-Mo7	98.48	C62-Fe55-C58-C59	160.68	C85-Fe76-C80-H90	68.12	C98-Fe97-C103-H113	-15.09
O47-Mo6-O42-Mo9	-172.43	C62-Fe55-C58-H68	41.15	C75-Fe76-C81-C82	170.95	C99-Fe97-C103-C102	-173.75
O47-Mo6-O42-P13	-37.9	C63-Fe55-C58-C57	-121.2	C75-Fe76-C81-C85	50.9	C99-Fe97-C103-C104	-55.11
O16-Mo6-O47-Mo12	28.01	C63-Fe55-C58-C59	118.34	C75-Fe76-C81-H95	-69.84	C99-Fe97-C103-H113	65.7
O23-Mo6-O47-Mo12	123.89	C63-Fe55-C58-H68	-1.19	C77-Fe76-C81-C82	-36.4	C100-Fe97-C103-C102	19.92
O29-Mo6-O47-Mo12	-30.2	C64-Fe55-C58-C57	-163.09	C77-Fe76-C81-C85	-156.45	C100-Fe97-C103-C104	138.56
O42-Mo6-O47-Mo12	53.06	C64-Fe55-C58-C59	76.45	C77-Fe76-C81-H95	82.81	C100-Fe97-C103-H113	-100.63

O43-Mo6-O47-Mo12	-130.25	C64-Fe55-C58-H68	-43.08	C78-Fe76-C81-C82	-154.26	C101-Fe97-C103-C102	65.77
O15-Mo7-O23-Mo6	-175.18	C54-Fe55-C59-C56	-38.72	C78-Fe76-C81-C85	85.7	C101-Fe97-C103-C104	-175.59
O24-Mo7-O23-Mo6	18.7	C54-Fe55-C59-C58	81.09	C78-Fe76-C81-H95	-35.04	C101-Fe97-C103-H113	-54.78
O27-Mo7-O23-Mo6	84.66	C54-Fe55-C59-H69	-158.63	C79-Fe76-C81-C82	-112.54	C102-Fe97-C103-C104	118.64
O32-Mo7-O23-Mo6	-71.5	C56-Fe55-C59-C58	119.81	C79-Fe76-C81-C85	127.42	C102-Fe97-C103-H113	-120.55
O42-Mo7-O23-Mo6	1.06	C56-Fe55-C59-H69	-119.92	C79-Fe76-C81-H95	6.68	C104-Fe97-C103-C102	-118.64
O15-Mo7-O24-Mo10	-127.95	C57-Fe55-C59-C56	-83.07	C80-Fe76-C81-C82	-71.18	C104-Fe97-C103-H113	120.81
O23-Mo7-O24-Mo10	38.13	C57-Fe55-C59-C58	36.73	C80-Fe76-C81-C85	168.78	C105-Fe97-C103-C102	-81.63
O27-Mo7-O24-Mo10	-27.41	C57-Fe55-C59-H69	157.01	C80-Fe76-C81-H95	48.04	C105-Fe97-C103-C104	37
O32-Mo7-O24-Mo10	126.28	C58-Fe55-C59-C56	-119.81	C82-Fe76-C81-C85	-120.04	C105-Fe97-C103-H113	157.81
O42-Mo7-O24-Mo10	54.8	C58-Fe55-C59-H69	120.28	C82-Fe76-C81-H95	119.21	C106-Fe97-C103-C102	-38.12
O15-Mo7-O27-Mo11	134.5	C60-Fe55-C59-C56	76.19	C83-Fe76-C81-C82	38.45	C106-Fe97-C103-C104	80.52
O23-Mo7-O27-Mo11	-124.75	C60-Fe55-C59-C58	-164.01	C83-Fe76-C81-C85	-81.59	C106-Fe97-C103-H113	-158.67
O24-Mo7-O27-Mo11	32.47	C60-Fe55-C59-H69	-43.73	C83-Fe76-C81-H95	157.67	C96-Fe97-C104-C103	104.74
O32-Mo7-O27-Mo11	-59.07	C61-Fe55-C59-C56	42.47	C84-Fe76-C81-C82	82.95	C96-Fe97-C104-C105	-135.55
O42-Mo7-O27-Mo11	-53.41	C61-Fe55-C59-C58	162.27	C84-Fe76-C81-C85	-37.1	C96-Fe97-C104-H114	-15.24
O15-Mo7-O32-Mo9	170.84	C61-Fe55-C59-H69	-77.45	C84-Fe76-C81-H95	-157.84	C98-Fe97-C104-C103	67.32
O23-Mo7-O32-Mo9	69.95	C62-Fe55-C59-C56	-168.08	C85-Fe76-C81-C82	120.04	C98-Fe97-C104-C105	-172.97
O24-Mo7-O32-Mo9	-84.95	C62-Fe55-C59-C58	-48.27	C85-Fe76-C81-H95	-120.74	C98-Fe97-C104-H114	-52.66
O27-Mo7-O32-Mo9	4.59	C62-Fe55-C59-H69	72	C75-Fe76-C82-C81	-167.12	C99-Fe97-C104-C103	148.03
O42-Mo7-O32-Mo9	-1.31	C63-Fe55-C59-C56	159.01	C75-Fe76-C82-C83	-48.48	C99-Fe97-C104-C105	-92.26
O15-Mo7-O42-Mo6	25.47	C63-Fe55-C59-C58	-81.18	C75-Fe76-C82-H91	72.81	C99-Fe97-C104-H114	28.05
O15-Mo7-O42-Mo9	-64.3	C63-Fe55-C59-H69	39.1	C77-Fe76-C82-C81	167.01	C100-Fe97-C104-C103	-174.54
O15-Mo7-O42-P13	160.9	C64-Fe55-C59-C56	118.11	C77-Fe76-C82-C83	-74.35	C100-Fe97-C104-C105	-54.83
O23-Mo7-O42-Mo6*	-0.62	C64-Fe55-C59-C58	-122.09	C77-Fe76-C82-H91	46.94	C100-Fe97-C104-H114	65.49
O23-Mo7-O42-Mo9	-90.39	C64-Fe55-C59-H69	-1.81	C78-Fe76-C82-C81	55.87	C101-Fe97-C104-C103	37.03
O23-Mo7-O42-P13	134.81	C54-Fe55-C60-C61	-79.23	C78-Fe76-C82-C83	174.51	C101-Fe97-C104-C105	156.74
O24-Mo7-O42-Mo6	-173.24	C54-Fe55-C60-C64	162.37	C78-Fe76-C82-H91	-64.2	C101-Fe97-C104-H114	-82.95
O24-Mo7-O42-Mo9	96.99	C54-Fe55-C60-H70	40.26	C79-Fe76-C82-C81	85.26	C102-Fe97-C104-C103	-38.27
O24-Mo7-O42-P13	-37.81	C56-Fe55-C60-C61	-121.35	C79-Fe76-C82-C83	-156.1	C102-Fe97-C104-C105	81.43
O27-Mo7-O42-Mo6	-86.79	C56-Fe55-C60-C64	120.25	C79-Fe76-C82-H91	-34.81	C102-Fe97-C104-H114	-158.25
O27-Mo7-O42-Mo9	-176.56	C56-Fe55-C60-H70	-1.86	C80-Fe76-C82-C81	126.37	C103-Fe97-C104-C105	119.71
O27-Mo7-O42-P13	48.64	C57-Fe55-C60-C61	-49.6	C80-Fe76-C82-C83	-114.99	C103-Fe97-C104-H114	-119.98
O32-Mo7-O42-Mo6	90.58	C57-Fe55-C60-C64	-168	C80-Fe76-C82-H91	6.3	C105-Fe97-C104-C103	-119.71
O32-Mo7-O42-Mo9*	0.81	C57-Fe55-C60-H70	69.9	C81-Fe76-C82-C83	118.64	C105-Fe97-C104-H114	120.32
O32-Mo7-O42-P13	-133.99	C58-Fe55-C60-C61	169.18	C81-Fe76-C82-H91	-120.07	C106-Fe97-C104-C103	-82.44
O36-Mo8-O28-Mo9	-127.76	C58-Fe55-C60-C64	50.78	C83-Fe76-C82-C81	-118.64	C106-Fe97-C104-C105	37.27
O37-Mo8-O28-Mo9	-56.89	C58-Fe55-C60-H70	-71.33	C83-Fe76-C82-H91	121.29	C106-Fe97-C104-H114	157.59
O38-Mo8-O28-Mo9	30.41	C59-Fe55-C60-C61	-162.33	C84-Fe76-C82-C81	-80.15	C96-Fe97-C105-C104	66.36
O39-Mo8-O28-Mo9	-64.7	C59-Fe55-C60-C64	79.27	C84-Fe76-C82-C83	38.5	C96-Fe97-C105-C106	-173.8
O53-Mo8-O28-Mo9	133.6	C59-Fe55-C60-H70	-42.83	C84-Fe76-C82-H91	159.79	C96-Fe97-C105-H115	-53.9
O28-Mo8-O36-Mo4	86.69	C61-Fe55-C60-C64	-118.4	C85-Fe76-C82-C81	-36.66	C98-Fe97-C105-C104	48.09
O37-Mo8-O36-Mo4	2.87	C61-Fe55-C60-H70	119.49	C85-Fe76-C82-C83	81.98	C98-Fe97-C105-C106	167.93

O38-Mo8-O36-Mo4	23.27	C62-Fe55-C60-C61	38.44	C85-Fe76-C82-H91	-156.73	C98-Fe97-C105-H115	-72.17
O39-Mo8-O36-Mo4	-68.84	C62-Fe55-C60-C64	-79.96	C75-Fe76-C83-C82	164.41	C99-Fe97-C105-C104	103.75
O53-Mo8-O36-Mo4	-171.4	C62-Fe55-C60-H70	157.94	C75-Fe76-C83-C84	-77.51	C99-Fe97-C105-C106	-136.41
O28-Mo8-O37-Mo1	-175.73	C63-Fe55-C60-C61	81.72	C75-Fe76-C83-H92	43.33	C99-Fe97-C105-H115	-16.51
O28-Mo8-O37-Mo4	-86.67	C63-Fe55-C60-C64	-36.68	C77-Fe76-C83-C82	124.05	C100-Fe97-C105-C104	147.85
O28-Mo8-O37-P13	49.16	C63-Fe55-C60-H70	-158.79	C77-Fe76-C83-C84	-117.87	C100-Fe97-C105-C106	-92.31
O36-Mo8-O37-Mo1	-90.74	C64-Fe55-C60-C61	118.4	C77-Fe76-C83-H92	2.97	C100-Fe97-C105-H115	27.59
O36-Mo8-O37-Mo4	-1.68	C64-Fe55-C60-H70	-122.11	C78-Fe76-C83-C82	-170.35	C101-Fe97-C105-C104	-176.48
O36-Mo8-O37-P13	134.15	C54-Fe55-C61-C60	119.26	C78-Fe76-C83-C84	-52.27	C101-Fe97-C105-C106	-56.64
O38-Mo8-O37-Mo1	97.58	C54-Fe55-C61-C62	-122.65	C78-Fe76-C83-H92	68.57	C101-Fe97-C105-H115	63.26
O38-Mo8-O37-Mo4	-173.36	C54-Fe55-C61-H71*	-0.88	C79-Fe76-C83-C82	50.71	C102-Fe97-C105-C104	-81.75
O38-Mo8-O37-P13	-37.52	C56-Fe55-C61-C60	76.72	C79-Fe76-C83-C84	168.78	C102-Fe97-C105-C106	38.09
O39-Mo8-O37-Mo1*	0.46	C56-Fe55-C61-C62	-165.19	C79-Fe76-C83-H92	-70.37	C102-Fe97-C105-H115	157.99
O39-Mo8-O37-Mo4	89.52	C56-Fe55-C61-H71	-43.42	C80-Fe76-C83-C82	81.44	C103-Fe97-C105-C104	-37.42
O39-Mo8-O37-P13	-134.65	C57-Fe55-C61-C60	161.11	C80-Fe76-C83-C84	-160.49	C103-Fe97-C105-C106	82.42
O53-Mo8-O37-Mo1	-60.66	C57-Fe55-C61-C62	-80.8	C80-Fe76-C83-H92	-39.65	C103-Fe97-C105-H115	-157.68
O53-Mo8-O37-Mo4	28.4	C57-Fe55-C61-H71	40.97	C81-Fe76-C83-C82	-37.62	C104-Fe97-C105-C106	119.84
O53-Mo8-O37-P13	164.24	C58-Fe55-C61-C60	-168.53	C81-Fe76-C83-C84	80.46	C104-Fe97-C105-H115	-120.26
O28-Mo8-O38-Mo2	-31.55	C58-Fe55-C61-C62	-50.44	C81-Fe76-C83-H92	-158.7	C106-Fe97-C105-C104	-119.84
O36-Mo8-O38-Mo2	31.14	C58-Fe55-C61-H71	71.34	C82-Fe76-C83-C84	118.08	C106-Fe97-C105-H115	119.9
O37-Mo8-O38-Mo2	50.3	C59-Fe55-C61-C60	45.41	C82-Fe76-C83-H92	-121.08	C96-Fe97-C106-C102	158.94
O39-Mo8-O38-Mo2	120.86	C59-Fe55-C61-C62	163.51	C84-Fe76-C83-C82	-118.08	C96-Fe97-C106-C105	40.09
O53-Mo8-O38-Mo2	-133.98	C59-Fe55-C61-H71	-74.72	C84-Fe76-C83-H92	120.84	C96-Fe97-C106-H116	-81.2
O28-Mo8-O39-Mo1	7.49	C60-Fe55-C61-C62	118.09	C85-Fe76-C83-C82	-80.42	C98-Fe97-C106-C102	-58.67
O36-Mo8-O39-Mo1	70.07	C60-Fe55-C61-H71	-120.13	C85-Fe76-C83-C84	37.66	C98-Fe97-C106-C105	-177.52
O37-Mo8-O39-Mo1*	-0.68	C62-Fe55-C61-C60	-118.09	C85-Fe76-C83-H92	158.5	C98-Fe97-C106-H116	61.19
O38-Mo8-O39-Mo1	-85.32	C62-Fe55-C61-H71	121.77	C75-Fe76-C84-C83	123.64	C99-Fe97-C106-C102	-176.78
O53-Mo8-O39-Mo1	169.17	C63-Fe55-C61-C60	-80.65	C75-Fe76-C84-C85	-117.77	C99-Fe97-C106-C105	64.38
O20-Mo9-O16-Mo6	-15.08	C63-Fe55-C61-C62	37.44	C75-Fe76-C84-H93	4.1	C99-Fe97-C106-H116	-56.92
O28-Mo9-O16-Mo6	-94.7	C63-Fe55-C61-H71	159.22	C77-Fe76-C84-C83	79.54	C100-Fe97-C106-C102	-137.33
O32-Mo9-O16-Mo6	61.18	C64-Fe55-C61-C60	-37.81	C77-Fe76-C84-C85	-161.88	C100-Fe97-C106-C105	103.83
O42-Mo9-O16-Mo6	-8.82	C64-Fe55-C61-C62	80.28	C77-Fe76-C84-H93	-40.01	C100-Fe97-C106-H116	-17.47
O44-Mo9-O16-Mo6	162.75	C64-Fe55-C61-H71	-157.95	C78-Fe76-C84-C83	164.96	C101-Fe97-C106-C102	-93.19
O16-Mo9-O20-Mo2	-45.53	C54-Fe55-C62-C61	76.3	C78-Fe76-C84-C85	-76.45	C101-Fe97-C106-C105	147.97
O28-Mo9-O20-Mo2	35.78	C54-Fe55-C62-C63	-164.93	C78-Fe76-C84-H93	45.42	C101-Fe97-C106-H116	26.67
O32-Mo9-O20-Mo2	-122.31	C54-Fe55-C62-H72	-44.45	C79-Fe76-C84-C83	-159.79	C102-Fe97-C106-C105	-118.85
O42-Mo9-O20-Mo2	-51.44	C56-Fe55-C62-C61	39.44	C79-Fe76-C84-C85	-41.21	C102-Fe97-C106-H116	119.86
O44-Mo9-O20-Mo2	136.62	C56-Fe55-C62-C63	158.22	C79-Fe76-C84-H93	80.66	C103-Fe97-C106-C102	38.25
O16-Mo9-O28-Mo8	123.32	C56-Fe55-C62-H72	-81.3	C80-Fe76-C84-C83	42.68	C103-Fe97-C106-C105	-80.6
O20-Mo9-O28-Mo8	-29.64	C57-Fe55-C62-C61	119.43	C80-Fe76-C84-C85	161.26	C103-Fe97-C106-H116	158.1
O32-Mo9-O28-Mo8	35.85	C57-Fe55-C62-C63	-121.8	C80-Fe76-C84-H93	-76.87	C104-Fe97-C106-C102	81.89
O42-Mo9-O28-Mo8	53.72	C57-Fe55-C62-H72	-1.31	C81-Fe76-C84-C83	-82.04	C104-Fe97-C106-C105	-36.96
O44-Mo9-O28-Mo8	-131.72	C58-Fe55-C62-C61	161.13	C81-Fe76-C84-C85	36.54	C104-Fe97-C106-H116	-158.25

O16-Mo9-O32-Mo7	-67.92	C58-Fe55-C62-C63	-80.1	C81-Fe76-C84-H93	158.42	C105-Fe97-C106-C102	118.85
O20-Mo9-O32-Mo7	85.47	C58-Fe55-C62-H72	40.38	C82-Fe76-C84-C83	-38.56	C105-Fe97-C106-H116	-121.3
O28-Mo9-O32-Mo7	20.27	C59-Fe55-C62-C61	-163.83	C82-Fe76-C84-C85	80.03	C96-C98-C101-Fe97	58.9
O42-Mo9-O32-Mo7	1.31	C59-Fe55-C62-C63	-45.06	C82-Fe76-C84-H93	-158.1	C96-C98-C101-C100*	-0.29
O44-Mo9-O32-Mo7	-172.16	C59-Fe55-C62-H72	75.43	C83-Fe76-C84-C85	118.58	C96-C98-C101-H111	178.87
O16-Mo9-O42-Mo6	5.18	C60-Fe55-C62-C61	-38.55	C83-Fe76-C84-H93	-119.55	Fe97-C98-C101-C100	-59.19
O16-Mo9-O42-Mo7	94.29	C60-Fe55-C62-C63	80.22	C85-Fe76-C84-C83	-118.58	Fe97-C98-C101-H111	119.98
O16-Mo9-O42-P13	-129.65	C60-Fe55-C62-H72	-159.29	C85-Fe76-C84-H93	121.87	H108-C98-C101-Fe97	-117.54
O20-Mo9-O42-Mo6	-177.71	C61-Fe55-C62-C63	118.77	C75-Fe76-C85-C81	-157.88	H108-C98-C101-C100	-176.73
O20-Mo9-O42-Mo7	-88.61	C61-Fe55-C62-H72	-120.74	C75-Fe76-C85-C84	81.86	H108-C98-C101-H111	2.43
O20-Mo9-O42-P13	47.46	C63-Fe55-C62-C61	-118.77	C75-Fe76-C85-H94	-38.19	C96-C99-C100-Fe97	-61.48
O28-Mo9-O42-Mo6	97.75	C63-Fe55-C62-H72	120.48	C77-Fe76-C85-C81	161.95	C96-C99-C100-C101*	-0.58
O28-Mo9-O42-Mo7	-173.14	C64-Fe55-C62-C61	-82.16	C77-Fe76-C85-C84	41.69	C96-C99-C100-H110	-179.92
O28-Mo9-O42-P13	-37.08	C64-Fe55-C62-C63	36.61	C77-Fe76-C85-H94	-78.36	Fe97-C99-C100-C101	60.9
O32-Mo9-O42-Mo6	-89.9	C64-Fe55-C62-H72	157.09	C78-Fe76-C85-C81	-114.1	Fe97-C99-C100-H110	-118.43
O32-Mo9-O42-Mo7*	-0.79	C54-Fe55-C63-C62	40.47	C78-Fe76-C85-C84	125.64	H109-C99-C100-Fe97	117.73
O32-Mo9-O42-P13	135.27	C54-Fe55-C63-C64	160.71	C78-Fe76-C85-H94	5.59	H109-C99-C100-C101	178.63
O44-Mo9-O42-Mo6	-49.83	C54-Fe55-C63-H73	-78.9	C79-Fe76-C85-C81	-72.2	H109-C99-C100-H110*	-0.7
O44-Mo9-O42-Mo7	39.28	C56-Fe55-C63-C62	-160.91	C79-Fe76-C85-C84	167.54	Fe97-C100-C101-C98	61.42
O44-Mo9-O42-P13	175.34	C56-Fe55-C63-C64	-40.67	C79-Fe76-C85-H94	47.49	Fe97-C100-C101-H111	-117.74
O22-Mo10-O14-Mo2	3.32	C56-Fe55-C63-H73	79.72	C80-Fe76-C85-C81	-32.04	C99-C100-C101-Fe97	-60.88
O24-Mo10-O14-Mo2	87.35	C57-Fe55-C63-C62	78.15	C80-Fe76-C85-C84	-152.3	C99-C100-C101-C98*	0.54
O31-Mo10-O14-Mo2	26.75	C57-Fe55-C63-C64	-161.61	C80-Fe76-C85-H94	87.65	C99-C100-C101-H111	-178.62
O34-Mo10-O14-Mo2	-68.57	C57-Fe55-C63-H73	-41.22	C81-Fe76-C85-C84	-120.26	H110-C100-C101-Fe97	118.45
O52-Mo10-O14-Mo2	-171.59	C58-Fe55-C63-C62	120.04	C81-Fe76-C85-H94	119.69	H110-C100-C101-C98*	179.87
O14-Mo10-O22-Mo2	-1.96	C58-Fe55-C63-C64	-119.72	C82-Fe76-C85-C81	37.22	H110-C100-C101-H111*	0.71
O14-Mo10-O22-Mo5	-91.09	C58-Fe55-C63-H73*	0.68	C82-Fe76-C85-C84	-83.04	Fe97-C102-C103-C104	-60.69
O14-Mo10-O22-P13	133.44	C59-Fe55-C63-C62	161.96	C82-Fe76-C85-H94	156.91	Fe97-C102-C103-H113	118.42
O24-Mo10-O22-Mo2	-86.81	C59-Fe55-C63-C64	-77.8	C83-Fe76-C85-C81	81.81	C106-C102-C103-Fe97	60.25
O24-Mo10-O22-Mo5	-175.94	C59-Fe55-C63-H73	42.6	C83-Fe76-C85-C84	-38.45	C106-C102-C103-C104*	-0.45
O24-Mo10-O22-P13	48.59	C60-Fe55-C63-C62	-82.92	C83-Fe76-C85-H94	-158.5	C106-C102-C103-H113	178.67
O31-Mo10-O22-Mo2	-172.13	C60-Fe55-C63-C64	37.32	C84-Fe76-C85-C81	120.26	H112-C102-C103-Fe97	-119.82
O31-Mo10-O22-Mo5	98.74	C60-Fe55-C63-H73	157.72	C84-Fe76-C85-H94	-120.05	H112-C102-C103-C104	179.49
O31-Mo10-O22-P13	-36.73	C61-Fe55-C63-C62	-38.34	C75-C77-C80-Fe76	60.54	H112-C102-C103-H113	-1.39
O34-Mo10-O22-Mo2	90.46	C61-Fe55-C63-C64	81.9	C75-C77-C80-C79*	-0.29	Fe97-C102-C106-C105	60.4
O34-Mo10-O22-Mo5	1.33	C61-Fe55-C63-H73	-157.71	C75-C77-C80-H90	177.46	Fe97-C102-C106-H116	-117.14
O34-Mo10-O22-P13	-134.15	C62-Fe55-C63-C64	120.24	Fe76-C77-C80-C79	-60.83	C103-C102-C106-Fe97	-60.08
O52-Mo10-O22-Mo2	30.83	C62-Fe55-C63-H73	-119.37	Fe76-C77-C80-H90	116.92	C103-C102-C106-C105*	0.33
O52-Mo10-O22-Mo5	-58.3	C64-Fe55-C63-C62	-120.24	H87-C77-C80-Fe76	-118.74	C103-C102-C106-H116	-177.22
O52-Mo10-O22-P13	166.23	C64-Fe55-C63-H73	120.4	H87-C77-C80-C79	-179.58	H112-C102-C106-Fe97	119.99
O14-Mo10-O24-Mo7	-129.8	C54-Fe55-C64-C60	-43.1	H87-C77-C80-H90	-1.82	H112-C102-C106-C105	-179.61
O22-Mo10-O24-Mo7	-58.39	C54-Fe55-C64-C63	-163.07	C75-C78-C79-Fe76	-57.98	H112-C102-C106-H116	2.84

O31-Mo10-O24-Mo7	28.2	C54-Fe55-C64-H74	77.69	C75-C78-C79-C80*	-0.26	Fe97-C103-C104-C105	-59.17
O34-Mo10-O24-Mo7	-64.21	C56-Fe55-C64-C60	-77.17	C75-C78-C79-H89	-176.7	Fe97-C103-C104-H114	116.65
O52-Mo10-O24-Mo7	129.96	C56-Fe55-C64-C63	162.86	Fe76-C78-C79-C80	57.72	C102-C103-C104-Fe97	59.56
O14-Mo10-O31-Mo11	27.33	C56-Fe55-C64-H74	43.62	Fe76-C78-C79-H89	-118.73	C102-C103-C104-C105*	0.4
O22-Mo10-O31-Mo11	49.43	C57-Fe55-C64-C60	167.81	H88-C78-C79-Fe76	120.18	C102-C103-C104-H114	176.22
O24-Mo10-O31-Mo11	-32.82	C57-Fe55-C64-C63	47.84	H88-C78-C79-C80	177.9	H113-C103-C104-Fe97	-119.56
O34-Mo10-O31-Mo11	120.51	C57-Fe55-C64-H74	-71.4	H88-C78-C79-H89	1.46	H113-C103-C104-C105	-178.73
O52-Mo10-O31-Mo11	-134.25	C58-Fe55-C64-C60	-159.93	Fe76-C79-C80-C77	58.92	H113-C103-C104-H114	-2.91
O14-Mo10-O34-Mo5	68.86	C58-Fe55-C64-C63	80.1	Fe76-C79-C80-H90	-118.87	Fe97-C104-C105-C106	-58.53
O22-Mo10-O34-Mo5	-2	C58-Fe55-C64-H74	-39.15	C78-C79-C80-Fe76	-58.58	Fe97-C104-C105-H115	117.26
O24-Mo10-O34-Mo5	4.06	C59-Fe55-C64-C60	-119.41	C78-C79-C80-C77*	0.34	C103-C104-C105-Fe97	58.33
O31-Mo10-O34-Mo5	-85.75	C59-Fe55-C64-C63	120.62	C78-C79-C80-H90	-177.45	C103-C104-C105-C106*	-0.2
O52-Mo10-O34-Mo5	169.82	C59-Fe55-C64-H74	1.37	H89-C79-C80-Fe76	117.89	C103-C104-C105-H115	175.59
O30-Mo11-O27-Mo7	23.38	C60-Fe55-C64-C63	-119.97	H89-C79-C80-C77	176.81	H114-C104-C105-Fe97	-117.5
O31-Mo11-O27-Mo7	-32.87	C60-Fe55-C64-H74	120.79	H89-C79-C80-H90*	-0.98	H114-C104-C105-C106	-176.03
O33-Mo11-O27-Mo7	49.63	C61-Fe55-C64-C60	38.55	Fe76-C81-C82-C83	-59.27	H114-C104-C105-H115*	-0.25
O41-Mo11-O27-Mo7	122.3	C61-Fe55-C64-C63	-81.42	Fe76-C81-C82-H91	118.58	Fe97-C105-C106-C102	-59.3
O49-Mo11-O27-Mo7	-132.11	C61-Fe55-C64-H74	159.33	C85-C81-C82-Fe76	58.98	Fe97-C105-C106-H116	118.23
O27-Mo11-O30-Mo3	32.73	C62-Fe55-C64-C60	82.99	C85-C81-C82-C83*	-0.29	C104-C105-C106-Fe97	59.22
O31-Mo11-O30-Mo3	88.96	C62-Fe55-C64-C63	-36.98	C85-C81-C82-H91	177.56	C104-C105-C106-C102*	-0.08
O33-Mo11-O30-Mo3	4.92	C62-Fe55-C64-H74	-156.22	H95-C81-C82-Fe76	-117.7	C104-C105-C106-H116	177.45
O41-Mo11-O30-Mo3	-67.97	C63-Fe55-C64-C60	119.97	H95-C81-C82-C83	-176.97	H115-C105-C106-Fe97	-116.55
O49-Mo11-O30-Mo3	-171.47	C63-Fe55-C64-H74	-119.24	H95-C81-C82-H91*	0.88	H115-C105-C106-C102	-175.86
O27-Mo11-O31-Mo10	34.01	C54-C56-C59-Fe55	59.8	Fe76-C81-C85-C84	57.78	H115-C105-C106-H116	1.68
O30-Mo11-O31-Mo10	-124.5	C54-C56-C59-C58*	-0.09				

torsional angles closer to 0° or 180°.