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Supplementary Material

Theoretical study on oxidative cleavage of olefin to carbonyls catalysed by Fe(III)-PyBisulidine

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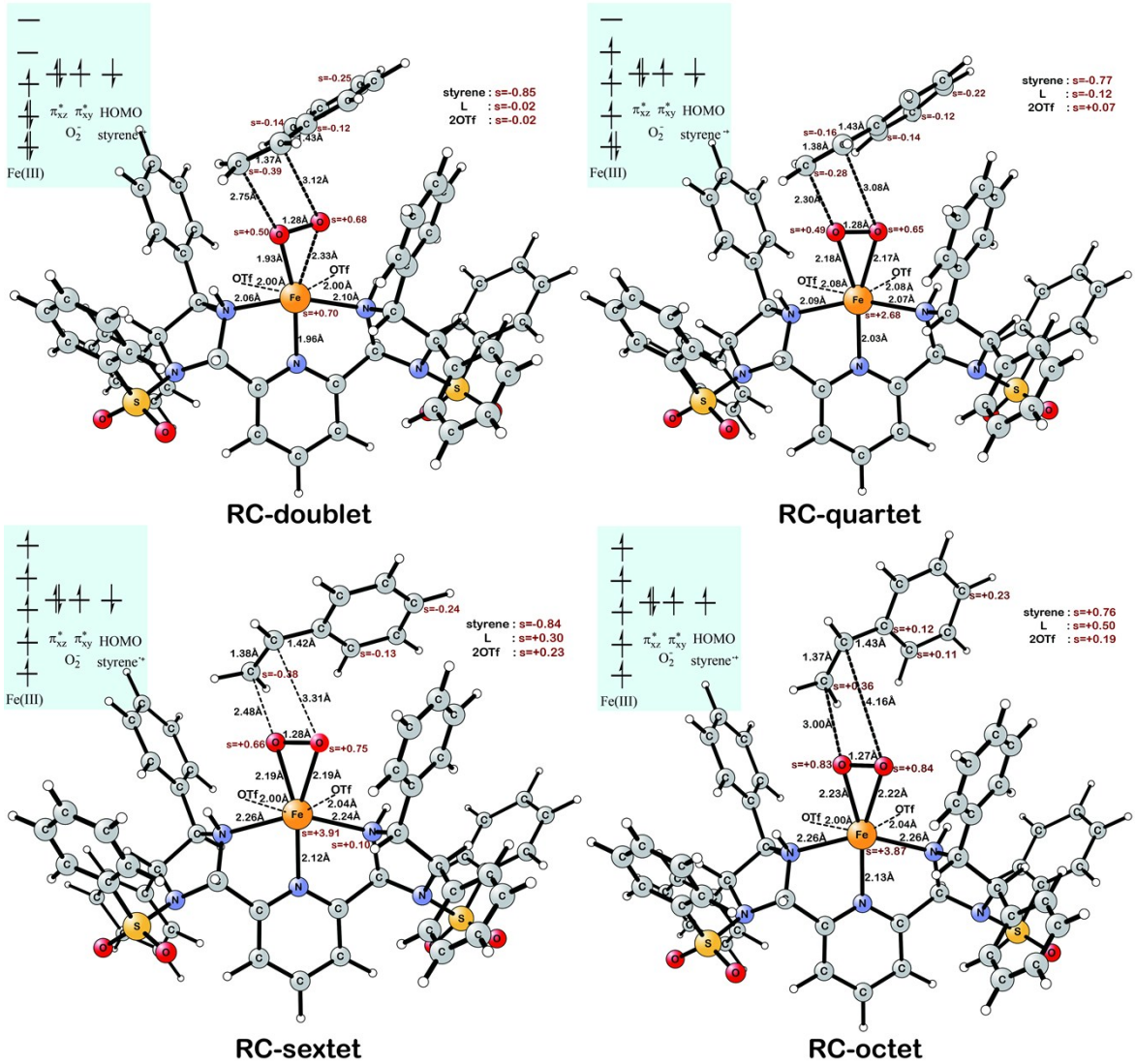

Figure S1. Different spin density and Structures information of RC along the reaction path of dioxygen ligation mechanism. Red data denotes the spin density of atoms and black data denotes key bond distance. OTf denotes triflate ion.

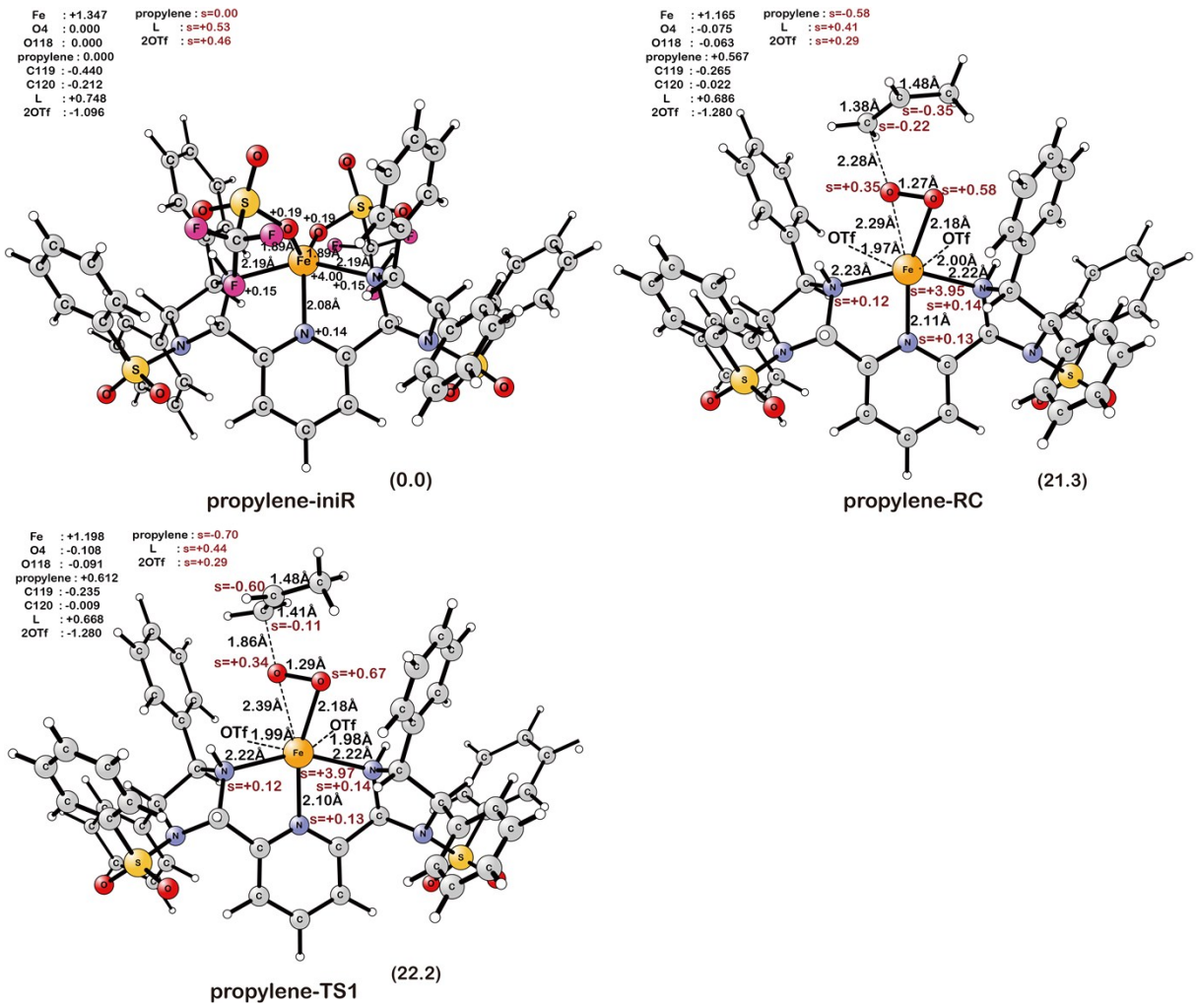

Figure S2. Structures and spin density information of iniR, RC and TS1 for propylene along the reaction path of dioxygen ligation mechanism. Red data denotes the spin density of atoms and black data in upper-left corner denotes the NPA charge. OTf denotes triflate ion. O_2 and propylene in iniR are not shown. The energy data of iniR, RC and TS1 are shown in parentheses.

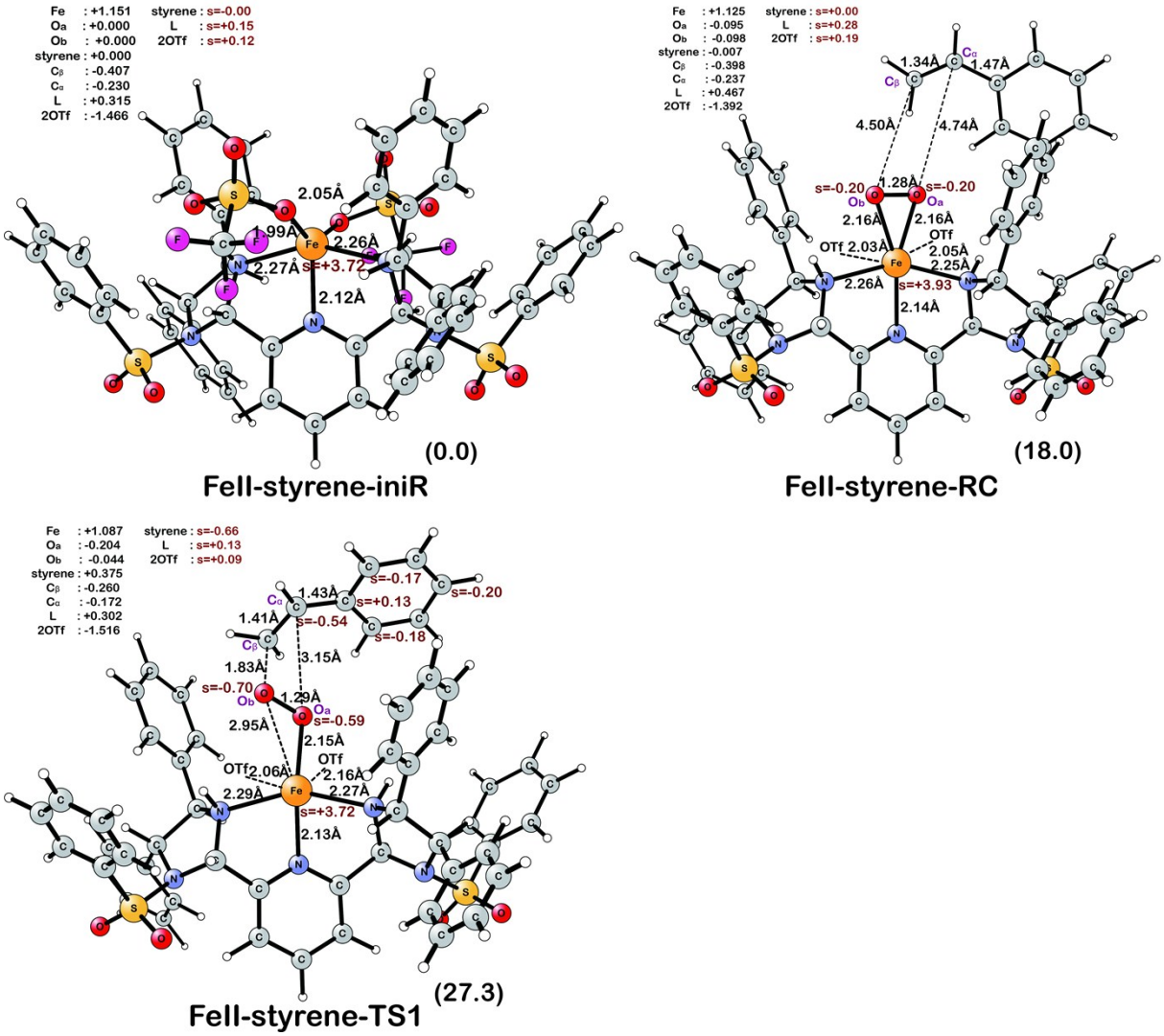

Figure S3. Structures and spin density information of iniR, RC and TS1 for Fe(II)-PyBisulidine along the reaction path of dioxygen ligation mechanism. Red data denotes the spin density of atoms and black data in upper-left corner denotes the NPA charge. OTf denotes triflate ion. The energy data of iniR, RC and TS1 are shown in parentheses.

Table S1. Spin density of the stationary points along the reaction path of the dioxygen ligation mechanism.

spin density	^{8}iniR †	^{6}RC	^{6}TS1	^{6}INT1	^{6}TS2	^{6}INT2	^{6}TS3	^{6}P
Fe	4.001	3.910	3.922	4.029	4.042	4.058	4.050	4.058
O_a	1.000	0.746	0.673	0.306	0.136	0.062	0.606	0.087
O_b	1.000	0.659	0.428	0.066	0.044	0.008	-0.103	0.064
styrene	0.000	-0.838	-0.605	0.011	0.053	0.016	-0.077	
L	0.534	0.299	0.349	0.372	0.454	0.500	0.238	0.405
2OTf	0.464	0.225	0.233	0.217	0.270	0.355	0.286	0.295
C_β	0.000	-0.378	-0.174	0.000	0.003	0.001	0.041	-0.011
C_α	0.000	-0.082	-0.228	0.004	0.017	0.003	-0.040	-0.009

† The superscript in Table denotes the spin state of the stationary point. The atom names in Table are labelled in Figure 1a.

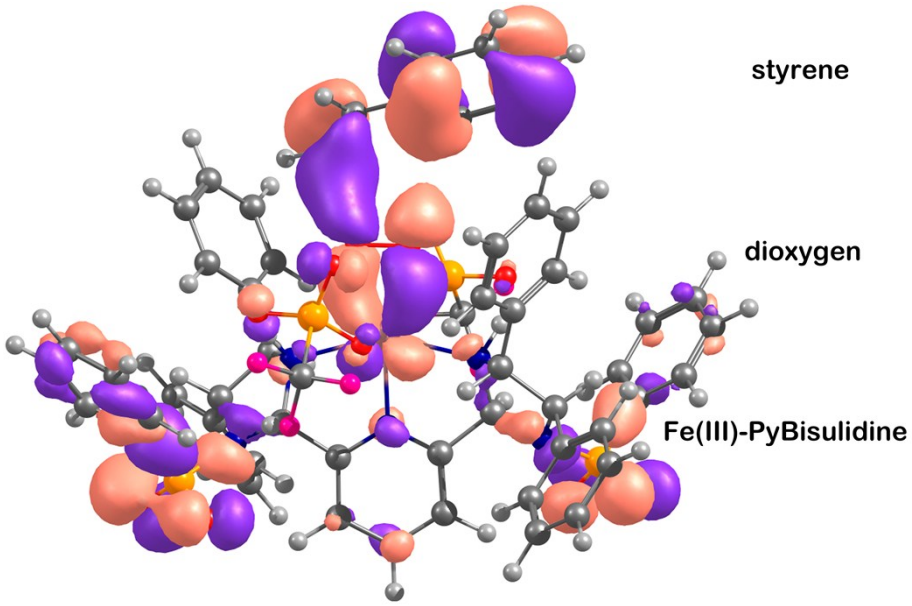

Figure S4. Molecular orbital beta 306 of RC complex, in which the orbital interaction among the styrene, dioxygen and iron are clearly shown.

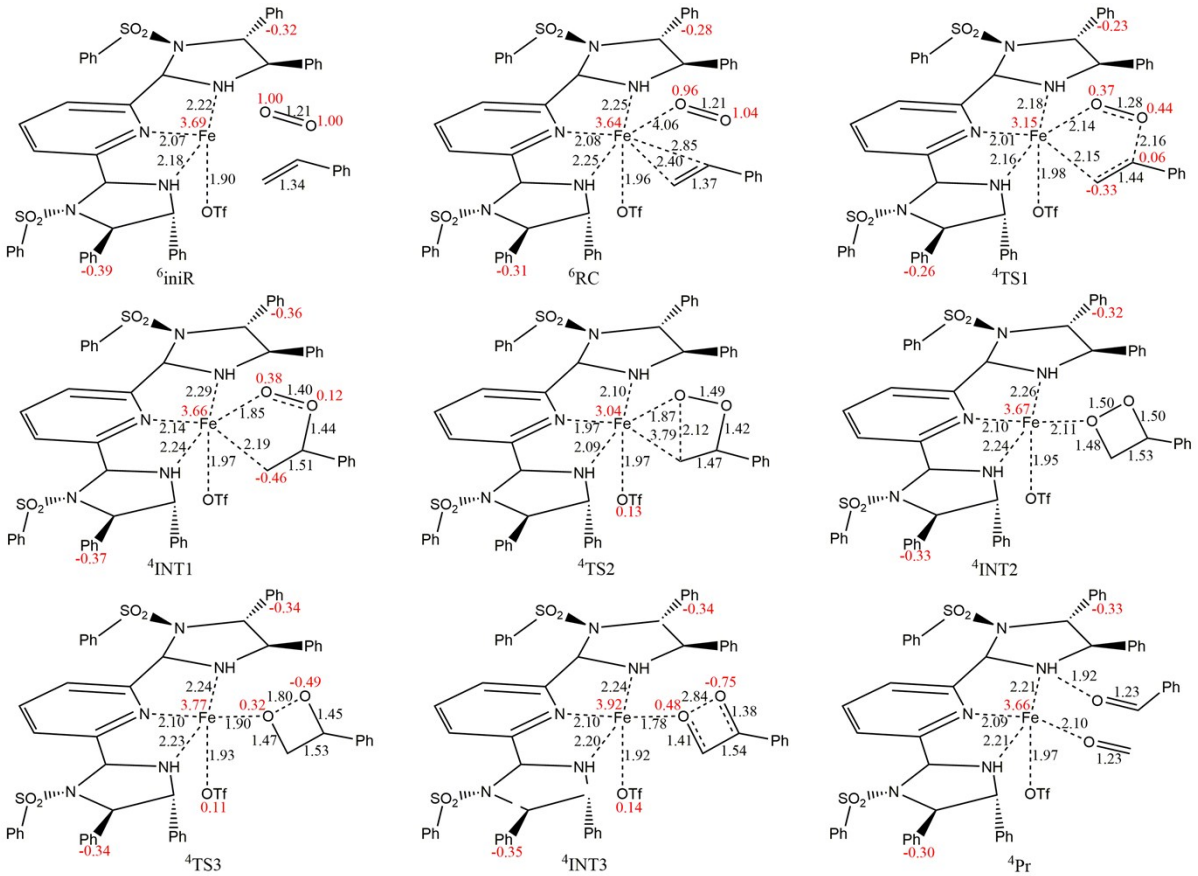

Figure S5. Structures and spin density of the stationary points along the reaction path of olefin ligation mechanism. Red number denotes the spin density of atoms and black number denotes the key bond distance. OTf denotes triflate ion. The structures shown here are the lowest energy state relative to the other two spin states. The structures of iniR and RC are sextet and the other structures are quartet.

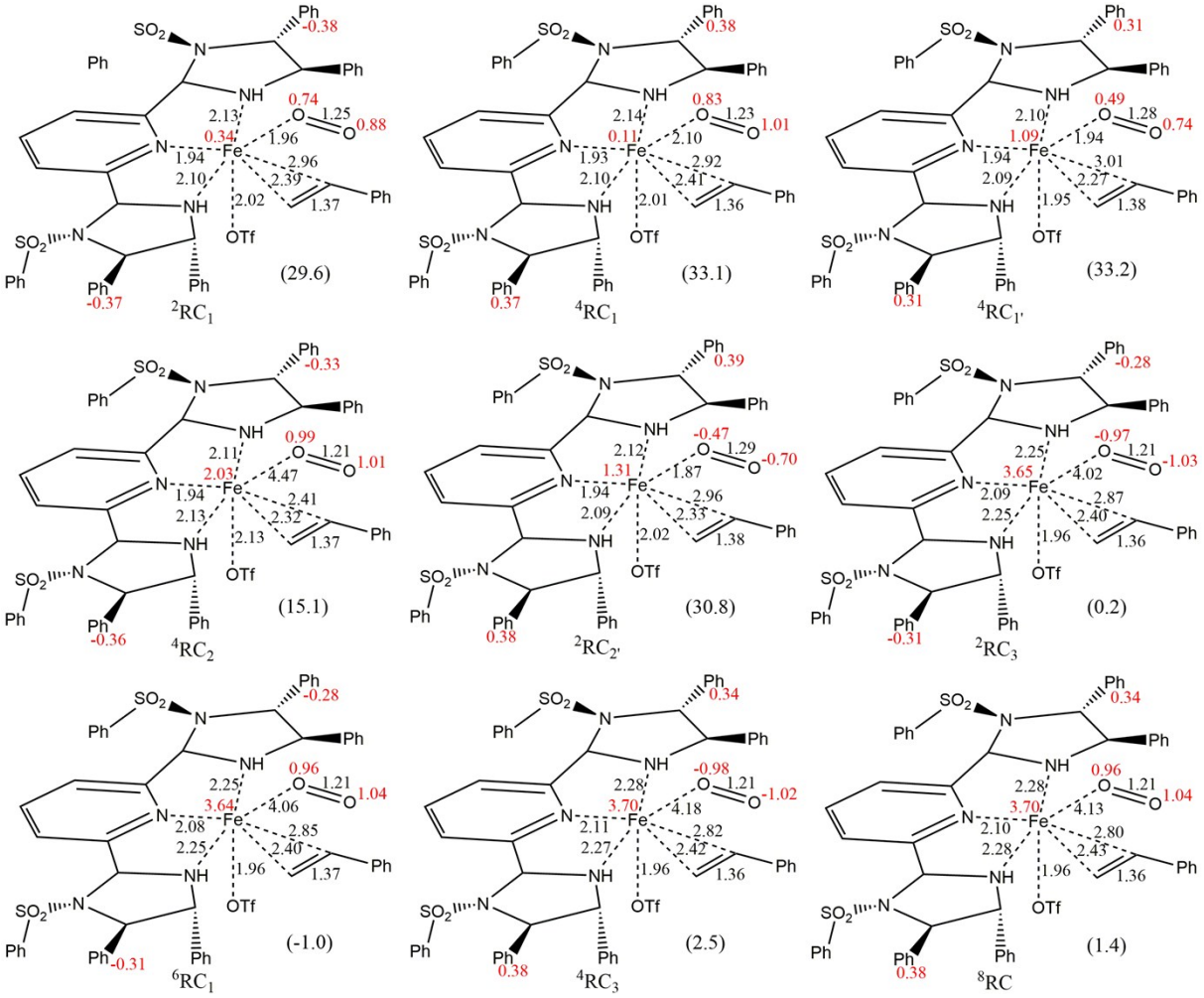

Figure S6. The structures and spin density of all the possible R states of olefin coordination way. The energy data including BS2 correction, solvation correction, zero-point energy correction, entropy and dispersion energy correction are shown in parentheses.

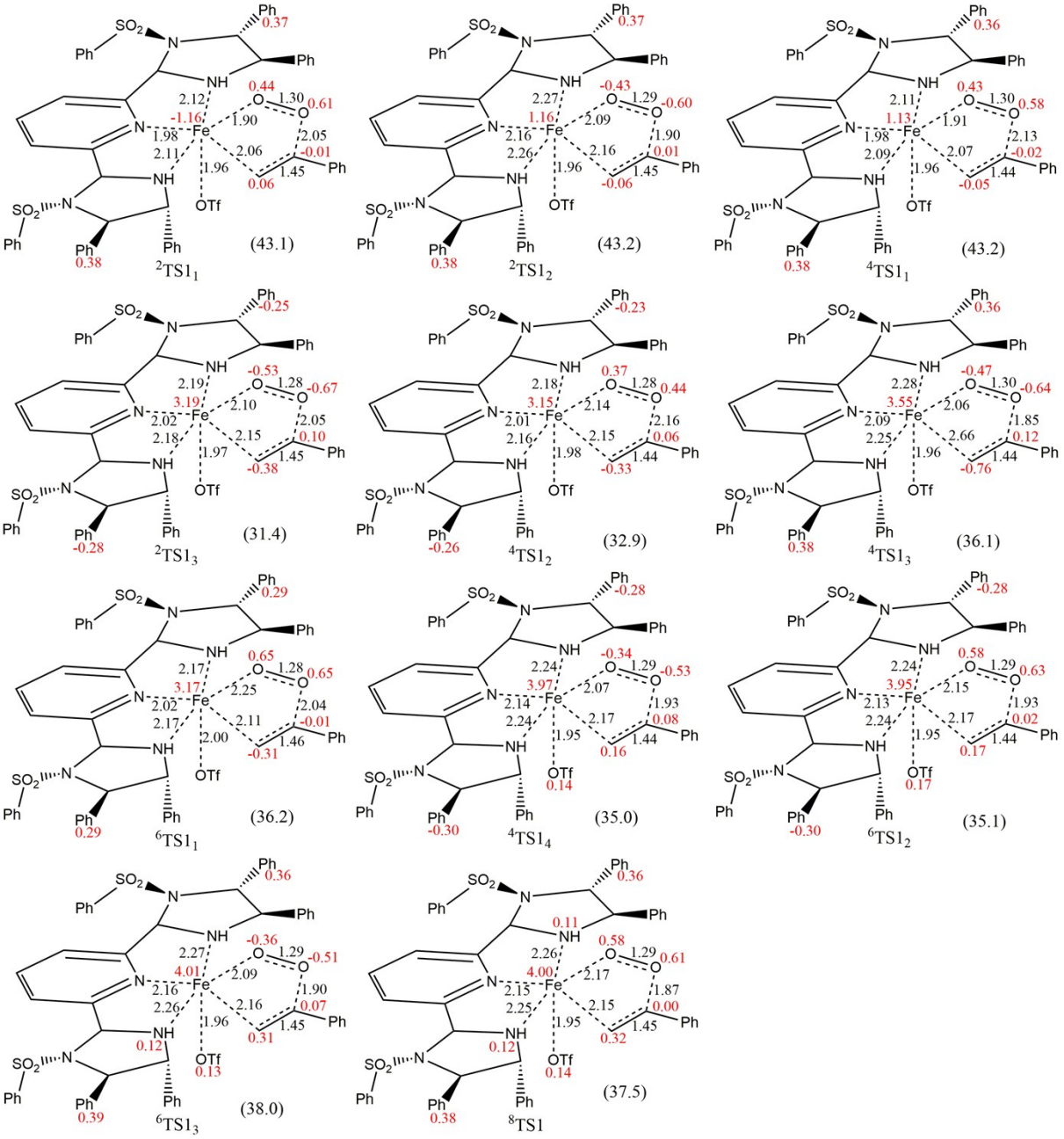

Figure S7. The structures and spin density of all the possible TS1 states of olefin coordination way. The energy data including BS2 correction, solvation correction, zero-point energy correction, entropy and dispersion energy correction are shown in parentheses.

Cartesian coordinates of stationary points

Dioxygen ligation pathway

Fe(III)_styrene-iniR-sextet: (without O_2 and styrene)

Fe1	-0.000399	0.000123	0.676711
S2	4.662899	1.271216	-2.373722
S3	-1.091552	-2.611440	2.273254
N4	-0.000388	-0.000247	-1.402602
O5	-0.059255	-1.680185	1.534076
O6	5.704116	0.495895	-3.033558
O7	-0.617588	-3.000885	3.584826
F8	-1.985575	-4.941733	1.487564
F9	0.166262	-4.713225	1.261424
C10	3.895314	-1.049512	2.451889
H11	4.121117	-0.003291	2.260456
O12	3.750622	2.165047	-3.096870
C13	3.967779	-2.934445	3.968691
H14	4.232762	-3.353392	4.934870
C15	-1.008473	-4.105831	1.152759
N16	2.129927	-0.013698	0.166032
H17	2.523807	0.606253	0.887407
F18	-1.184590	-3.711568	-0.123206
C19	3.361396	-3.735129	3.000214
H20	3.153040	-4.780480	3.207280
C21	3.013436	-3.191753	1.763297
H22	2.538885	-3.817315	1.013614
C23	4.152502	-0.926513	-0.768509
H24	4.909652	-0.477976	-0.111691
O25	-2.452602	-2.084232	2.089932
N26	3.598565	0.113643	-1.674035
C27	1.142936	0.276234	-2.060244
C28	5.395978	2.180081	-1.018042
C29	5.302219	3.974011	0.582222
H30	4.800041	4.843851	0.993604
C31	2.918025	-1.296500	0.117590
H32	2.313814	-2.024972	-0.430843
C33	3.271425	-1.845574	1.478577
C34	4.746607	-2.132089	-1.464448
C35	2.324316	0.622913	-1.159923
H36	2.342748	1.708804	-1.029262
C37	6.510153	3.532937	1.129525
C38	4.233511	-1.591075	3.691856
H39	4.706858	-0.962763	4.440498
C40	4.738476	3.303437	-0.502790
H41	3.824533	3.663183	-0.962218
C42	6.612255	1.734417	-0.487812
H43	7.122063	0.887796	-0.935434
C44	7.166653	2.422504	0.592172
H45	8.115794	2.096342	1.006455
C46	5.815284	-4.445149	-2.633230
H47	6.232446	-5.337274	-3.091179
C48	4.699710	-3.823093	-3.200313
H49	4.250832	-4.228675	-4.102575
C50	1.175596	0.295424	-3.449650
H51	2.095964	0.551637	-3.960214
C52	5.865073	-2.758237	-0.902568
H53	6.323226	-2.344502	-0.007458
C54	6.397040	-3.910624	-1.483064
H55	7.268580	-4.384208	-1.040678
C56	4.166147	-2.674298	-2.618124
H57	3.314193	-2.180156	-3.076752
C58	-0.000495	-0.000602	-4.143738
H59	-0.000532	-0.000746	-5.229563
S60	-4.663750	-1.271878	-2.373038
O61	-5.705365	-0.496744	-3.032458
C62	-3.896148	1.050776	2.451706
H63	-4.122683	0.004659	2.260549
O64	-3.751558	-2.165527	-3.096481
C65	-3.967523	2.936144	3.968006
H66	-4.232273	3.355505	4.934070
N67	-2.130585	0.013608	0.166223
H68	-2.524905	-0.605892	0.887642
C69	-3.360717	3.736227	2.999302
H70	-3.151808	4.781527	3.206075
C71	-3.013069	3.192321	1.762522
H72	-2.538161	3.817419	1.012672
C73	-4.153182	0.926337	-0.768517
H74	-4.910315	0.478022	-0.111522
N75	-3.599342	-0.114069	-1.673789
C76	-5.396020	-2.180799	-1.016961
C77	-5.300929	-3.974286	0.583734
H78	-4.798225	-4.843804	0.995149
C79	-2.918659	1.296561	0.117342
H80	-2.314357	2.024701	-0.431424
C81	-3.271757	1.846204	1.478187
C82	-4.747292	2.131795	-1.464684
C83	-6.508825	-3.533552	1.131396
C84	-4.234034	1.592852	3.691530
H85	-4.707751	0.965020	4.440338
C86	-4.737883	-3.303772	-0.501681
H87	-3.823996	-3.663283	-0.961412
C88	-6.612266	-1.735482	-0.486364
H89	-7.122592	-0.889180	-0.933998
C90	-7.165977	-2.423522	0.594007
H91	-8.115091	-2.097634	1.008567
C92	-5.815934	4.444717	-2.633757
H93	-6.233082	5.336790	-3.091818
C94	-4.700597	3.822361	-3.200969
H95	-4.251889	4.227654	-4.103446
C96	-5.865532	2.758235	-0.902674
H97	-6.323535	2.344776	-0.007360
C98	-6.397478	3.910556	-1.483312
H99	-7.268839	4.384373	-1.040820
C100	-4.167044	2.673629	-2.618635
H101	-3.315261	2.179267	-3.077337
C102	-1.143766	-0.276859	-2.060097
C103	-2.325107	-0.623268	-1.159646
H104	-2.343576	-1.709125	-1.028807
C105	-1.176547	-0.296424	-3.449488
H106	-2.096969	-0.552732	-3.959912
S107	1.092356	2.611514	2.272445
O108	0.059635	1.681557	1.532492
O109	0.618936	2.999991	3.584505
F110	1.986910	4.942383	1.489155
F111	-0.164774	4.714032	1.261524
C112	1.010049	4.106727	1.153096
F113	1.186935	3.713342	-0.122967
O114	2.453215	2.083685	2.088594
H115	-6.945280	-4.064625	1.972079
H116	6.947149	4.064056	1.969899

Fe(III)_styrene-RC-sextet:

Fe1	6.651086	6.495126	0.019984
S2	11.990560	5.893617	-2.087812
S3	4.007480	7.359713	-1.647105
O4	5.705930	4.540381	-0.229621
N5	8.026096	8.097104	-0.121996
O6	5.530534	7.158039	-1.492196
O7	12.563355	6.032868	-3.421386
O8	3.337374	6.223385	-2.267752
F9	2.777979	9.156383	-3.114126
F10	4.555634	8.306989	-4.046407
C11	7.633283	3.227061	-3.069621
H12	8.550719	2.991327	-2.533863
O13	12.448429	6.674904	-0.934081
C14	5.679987	2.460094	-4.274624
H15	5.078645	1.647375	-4.672913
C16	4.023310	8.735276	-2.901248
N17	8.289356	5.687539	-1.283547
H18	8.417406	4.727569	-0.947929
F19	4.757442	9.761709	-2.437365
C20	5.290755	3.783812	-4.479419
H21	4.379838	4.009405	-5.025542
C22	6.071039	4.828438	-3.980936
H23	5.759103	5.855458	-4.138821
C24	9.555480	5.717958	-3.351666
H25	9.873904	4.678807	-3.500308
O26	3.424650	7.952128	-0.427661
N27	10.344962	6.322979	-2.249547
C28	9.241332	7.882040	-0.652799
C29	12.046116	4.158773	-1.635536

C30	12.007670	2.442378	0.050345
H31	11.956899	2.151195	1.095092
C32	8.102893	5.705208	-2.769956
H33	7.622722	6.654048	-3.019670
C34	7.248532	4.562123	-3.272736
C35	9.640482	6.450607	-4.675648
C36	9.542132	6.431805	-1.021131
H37	10.049622	5.970098	-0.169796
C38	12.102348	1.471983	-0.950235
C39	6.852890	2.183631	-3.565946
H40	7.170595	1.155614	-3.413677
C41	11.986495	3.795739	-0.286050
H42	11.951746	4.556239	0.485214
C43	12.152883	3.197749	-2.647446
H44	12.250016	3.509729	-3.681881
C45	12.180538	1.847841	-2.294248
H46	12.279267	1.092277	-3.068079
C47	9.656435	7.759070	-7.156517
H48	9.669470	8.266701	-8.116739
C49	9.706800	8.498295	-5.971949
H50	9.762093	9.582673	-6.009217
C51	10.166340	8.915141	-0.775373
H52	11.150071	8.712257	-1.180224
C53	9.593629	5.715951	-5.865525
H54	9.554026	4.629776	-5.827689
C55	9.599561	6.365909	-7.100805
H56	9.568679	5.783292	-8.017122
C57	9.696636	7.848400	-4.738388
H58	9.758216	8.426268	-3.820770
C59	9.793009	10.189853	-0.345974
H60	10.490654	11.017217	-0.435191
S61	5.400556	11.878028	1.685978
O62	5.635611	12.639723	2.907024
C63	3.595781	7.347676	3.410494
H64	3.170020	8.076051	2.723654
O65	5.922907	12.285195	0.377604
C66	3.254964	5.651257	5.105500
H67	2.585341	5.064957	5.728722
N68	5.734342	8.117032	1.297219
H69	4.738423	8.055726	1.058837
C70	4.638085	5.495454	5.219615
H71	5.051710	4.781470	5.925897
C72	5.498398	6.267034	4.434434
H73	6.572410	6.142493	4.530861
C74	5.791100	9.621507	3.203948
H75	4.740307	9.802119	3.462556
N76	6.122383	10.350857	1.956935
C77	3.635354	11.609467	1.525405
C78	1.728104	11.049552	0.169616
H79	1.304236	10.790319	-0.795579
C80	5.935422	8.118331	2.777837
H81	6.964833	7.803904	2.963415
C82	4.988986	7.206711	3.529570
C83	6.654993	9.969022	4.399514
C84	0.909794	11.151540	1.297469
C85	2.735382	6.574900	4.191923
H86	1.660887	6.707946	4.100217
C87	3.098637	11.285442	0.274900
H88	3.734307	11.241974	-0.601494
C89	2.825943	11.726855	2.661316
H90	3.261740	12.027592	3.608116
C91	1.455288	11.495229	2.537691
H92	0.812996	11.596765	3.407494
C93	8.231897	10.476707	6.663763
H94	8.842157	10.680723	7.538885
C95	8.808573	10.477849	5.390913
H96	9.868437	10.686156	5.274094
C97	6.083082	9.973474	5.676812
H98	5.018130	9.785124	5.791881
C99	6.866699	10.223966	6.804403
H100	6.408293	10.231211	7.789206
C101	8.025866	10.223137	4.265619
H102	8.474690	10.246841	3.276755
C103	7.660946	9.317489	0.302212
C104	6.228139	9.429074	0.816042
H105	5.601033	9.752679	-0.018348
C106	8.525760	10.403832	0.198165
H107	8.199488	11.384994	0.519845
S108	8.099365	4.261862	1.922982
O109	7.631060	5.686603	1.620744
O110	7.131394	3.493651	2.718839
F111	10.142966	3.488279	3.374635
F112	9.100954	5.234172	4.160038
C113	9.531282	4.626699	3.053926
F114	10.400632	5.430326	2.422550
O115	8.682832	3.602401	0.740826
H116	-0.158263	10.975689	1.207276
H117	12.131290	0.419923	-0.681197
O118	4.972550	5.201907	0.582657
C119	3.832873	3.639479	2.139376
C120	3.280940	2.796218	1.193965
H121	4.841327	3.522299	2.522752
H122	3.235467	4.432541	2.575361
H123	2.245960	2.969085	0.905103
C124	3.956986	1.738415	0.521530
C125	3.232953	0.979755	-0.449401
C126	5.329296	1.411533	0.771218
C127	3.843321	-0.052203	-1.131119
H128	2.193975	1.229923	-0.643137
C129	5.928679	0.376410	0.078469
H130	5.904396	1.974588	1.498265
C131	5.194219	-0.357678	-0.868159
H132	3.289844	-0.629157	-1.864898
H133	6.968964	0.132878	0.267655
H134	5.670680	-1.174894	-1.402347

Fe(III)_styrene-TS1-sextet:

Fe1	6.709338	6.559824	0.025953
S2	12.045988	5.992602	-2.101635
S3	4.039519	7.382877	-1.626908
O4	5.775998	4.595728	-0.231096
N5	8.074428	8.166066	-0.127674
O6	5.565374	7.196620	-1.474062
O7	12.612775	6.135841	-3.437165
O8	3.377549	6.236400	-2.236891
F9	2.787324	9.160743	-3.095375
F10	4.567870	8.323522	-4.032999
C11	7.660993	3.279208	-3.000888
H12	8.570331	3.047615	-2.449535
O13	12.494296	6.786931	-0.952740
C14	5.709570	2.501568	-4.200807
H15	5.100354	1.684815	-4.578089
C16	4.037481	8.752605	-2.887923
N17	8.347914	5.756954	-1.274415
H18	8.484812	4.800938	-0.931228
F19	4.764746	9.787015	-2.431376
C20	5.338858	3.823353	-4.448181
H21	4.435623	4.043583	-5.009089
C22	6.126076	4.872652	-3.970868
H23	5.826729	5.898634	-4.158355
C24	9.602994	5.762616	-3.345841
H25	9.923501	4.720510	-3.469525
O26	3.456692	7.974504	-0.406454
N27	10.392548	6.397178	-2.259778
C28	9.289043	7.959356	-0.663613
C29	12.129274	4.261271	-1.642165
C30	12.124619	2.550861	0.049839
H31	12.084575	2.261981	1.095680
C32	8.152962	5.759087	-2.760007
H33	7.674545	6.706845	-3.017851
C34	7.293030	4.612474	-3.243893
C35	9.680561	6.463675	-4.687253
C36	9.598278	6.509727	-1.025994
H37	10.113935	6.055997	-0.175132
C38	12.228898	1.578369	-0.947794
C39	6.871877	2.231284	-3.473287
H40	7.171370	1.204346	-3.282589
C41	12.080925	3.902569	-0.290904
H42	12.037212	4.665274	0.477981
C43	12.246234	3.298366	-2.651162
H44	12.333534	3.608134	-3.687138
C45	12.295352	1.950360	-2.293420
H46	12.400790	1.193484	-3.065018
C47	9.680348	7.712193	-7.198679
H48	9.687391	8.196709	-8.170833

C49	9.749852	8.478881	-6.032723
H50	9.814316	9.561526	-6.096483
C51	10.203778	9.000306	-0.795056
H52	11.187189	8.804476	-1.204082
C53	9.614330	5.701087	-5.858604
H54	9.565126	4.616562	-5.794271
C55	9.612164	6.321435	-7.109099
H56	9.566034	5.717367	-8.010769
C57	9.747591	7.858773	-4.783759
H58	9.824794	8.457612	-3.880927
C59	9.821276	10.273089	-0.367961
H60	10.511098	11.106246	-0.463696
S61	5.418794	11.932934	1.664711
O62	5.661868	12.708351	2.875276
C63	3.621961	7.413676	3.377282
H64	3.206402	8.164308	2.708344
O65	5.927503	12.328168	0.347266
C66	3.255902	5.655250	5.002433
H67	2.576968	5.042388	5.588711
N68	5.781873	8.171990	1.292293
H69	4.786905	8.104293	1.049937
C70	4.636661	5.499896	5.137085
H71	5.039636	4.761463	5.824065
C72	5.509170	6.299656	4.394141
H73	6.581481	6.172979	4.504395
C74	5.819580	9.685357	3.194240
H75	4.768075	9.864956	3.450438
N76	6.150206	10.411250	1.944479
C77	3.653509	11.654212	1.524540
C78	1.735977	11.066403	0.195315
H79	1.303820	10.792747	-0.762207
C80	5.969513	8.182120	2.776347
H81	6.996784	7.868539	2.974006
C82	5.013351	7.266130	3.510627
C83	6.680308	10.040073	4.390559
C84	0.928107	11.179971	1.329664
C85	2.749828	6.612521	4.116412
H86	1.676809	6.746892	4.011229
C87	3.106299	11.310287	0.283899
H88	3.733354	11.258453	-0.598210
C89	2.854578	11.783395	2.666603
H90	3.298182	12.098621	3.605038
C91	1.483909	11.543504	2.559604
H92	0.849666	11.653883	3.434203
C93	8.250890	10.558461	6.656619
H94	8.858783	10.766747	7.532377
C95	8.829271	10.561665	5.384660
H96	9.888086	10.775987	5.269074
C97	6.106385	10.043008	5.666759
H98	5.042217	9.849284	5.780639
C99	6.887131	10.298621	6.795447
H100	6.427094	10.304298	7.779500
C101	8.049594	10.301589	4.258292
H102	8.499767	10.327538	3.270045
C103	7.699714	9.385161	0.293531
C104	6.266529	9.487114	0.807487
H105	5.638428	9.802880	-0.029216
C106	8.554817	10.478103	0.181751
H107	8.221549	11.457704	0.501019
S108	8.179194	4.350549	1.940426
O109	7.636017	5.751857	1.641667
O110	7.240903	3.539391	2.728594
F111	10.233297	3.675064	3.423677
F112	9.127424	5.400215	4.166054
C113	9.587801	4.785415	3.076326
F114	10.433228	5.605177	2.433823
O115	8.800395	3.724793	0.760490
H116	-0.139929	10.998000	1.252302
H117	12.274032	0.527862	-0.675133
O118	4.911001	5.180866	0.537066
C119	4.128268	4.042043	1.784207
C120	3.454197	3.060283	1.015888
H121	5.056006	3.806155	2.296989
H122	3.533861	4.827725	2.238379
H123	2.429506	3.281092	0.723715
C124	4.013868	1.862181	0.523374
C125	3.203319	1.026830	-0.307614
C126	5.353316	1.450865	0.813787
C127	3.705012	-0.151199	-0.824083
H128	2.186429	1.336899	-0.530713
C129	5.842457	0.269447	0.284122
H130	5.986689	2.053065	1.455862
C131	5.026308	-0.532414	-0.528940
H132	3.085045	-0.781999	-1.452993
H133	6.858170	-0.040693	0.507368
H134	5.416653	-1.463652	-0.929769

Fe(III)_styrene-INT1-sextet:

Fe1	6.663662	6.550986	-0.110054
S2	12.045775	5.943281	-2.197932
S3	4.113009	7.662971	-1.787286
O4	5.844008	4.845656	-0.456958
N5	8.112088	8.132301	-0.158926
O6	5.629815	7.492798	-1.583137
O7	12.652268	6.258233	-3.486023
O8	3.471955	6.547971	-2.474688
F9	2.903020	9.504040	-3.219919
F10	4.700168	8.686439	-4.143389
C11	7.643082	3.415422	-3.273784
H12	8.561366	3.143810	-2.756404
O13	12.489835	6.551780	-0.939064
C14	5.663399	2.727047	-4.481968
H15	5.042607	1.939596	-4.901224
C16	4.145893	9.078887	-2.995236
N17	8.343151	5.782506	-1.392980
H18	8.432549	4.808444	-1.089071
F19	4.867958	10.094809	-2.490259
C20	5.299213	4.064575	-4.639323
H21	4.387619	4.326656	-5.167885
C22	6.104030	5.076843	-4.113634
H23	5.807656	6.113798	-4.230267
C24	9.605354	5.894046	-3.461352
H25	9.904108	4.859650	-3.672113
O26	3.480597	8.205670	-0.566317
N27	10.410182	6.416290	-2.329147
C28	9.340574	7.912336	-0.650487
C29	12.069607	4.160731	-1.997966
C30	11.930313	2.216084	-0.589807
H31	11.822987	1.772673	0.395299
C32	8.153264	5.871156	-2.877285
H33	7.684418	6.836866	-3.079178
C34	7.281263	4.763419	-3.426347
C35	9.698333	6.700641	-4.741401
C36	9.612220	6.479182	-1.094221
H37	10.111391	5.964588	-0.270101
C38	12.082845	1.402406	-1.715698
C39	6.837667	2.403763	-3.795637
H40	7.135693	1.365061	-3.679626
C41	11.927909	3.604597	-0.721960
H42	11.839390	4.241829	0.150480
C43	12.233846	3.358300	-3.132715
H44	12.386072	3.819060	-4.102898
C45	12.238600	1.970924	-2.982596
H46	12.377312	1.336901	-3.853275
C47	9.722640	8.148840	-7.143115
H48	9.738473	8.710490	-8.072769
C49	9.833783	8.814501	-5.919800
H50	9.939740	9.895502	-5.896205
C51	10.303628	8.917943	-0.668848
H52	11.296522	8.706801	-1.046481
C53	9.591433	6.039026	-5.969959
H54	9.499925	4.955508	-5.992848
C55	9.601287	6.758925	-7.165833
H56	9.522356	6.232674	-8.112918
C57	9.819787	8.095248	-4.725213
H58	9.929725	8.614406	-3.777650
C59	9.954111	10.173627	-0.171657
H60	10.680599	10.980690	-0.177320
S61	5.546133	11.904115	1.739339
O62	5.786992	12.608476	2.993463
C63	3.560750	7.162356	3.055842
H64	3.161745	7.878898	2.341580
O65	6.131421	12.329450	0.463731
C66	3.157422	5.372420	4.639810
H67	2.466648	4.712907	5.158129

N68	5.779983	8.138604	1.190767
H69	4.793763	8.116239	0.903591
C70	4.524731	5.317709	4.916280
H71	4.907876	4.611827	5.647797
C72	5.408997	6.177737	4.259663
H73	6.472063	6.122357	4.471970
C74	5.720128	9.553849	3.152755
H75	4.647756	9.726850	3.315711
N76	6.174730	10.328754	1.972083
C77	3.773785	11.745623	1.521940
C78	1.877005	11.350761	0.096188
H79	1.467306	11.147816	-0.888424
C80	5.905893	8.075957	2.677273
H81	6.928612	7.765806	2.900105
C82	4.937703	7.109762	3.325946
C83	6.467826	9.849172	4.437275
C84	1.033406	11.469954	1.203436
C85	2.677556	6.295002	3.703077
H86	1.613936	6.354515	3.489148
C87	3.255814	11.495752	0.247044
H88	3.912968	11.436989	-0.612038
C89	2.940129	11.877656	2.638505
H90	3.366165	12.117685	3.606865
C91	1.562067	11.738301	2.469194
H92	0.901812	11.851577	3.323973
C93	7.828015	10.266700	6.854676
H94	8.354904	10.436114	7.789369
C95	8.530646	10.249980	5.646711
H96	9.605328	10.409246	5.640058
C97	5.769970	9.870373	5.649474
H98	4.691310	9.730588	5.653940
C99	6.445929	10.076541	6.853710
H100	5.890731	10.098025	7.787226
C101	7.855238	10.040516	4.445438
H102	8.401738	10.051607	3.506510
C103	7.768333	9.335764	0.330955
C104	6.318834	9.461429	0.790772
H105	5.734293	9.833598	-0.053697
C106	8.672067	10.394719	0.334385
H107	8.365282	11.364127	0.706173
S108	8.226542	4.436741	1.883209
O109	7.657770	5.818009	1.569869
O110	7.314735	3.613799	2.697035
F111	10.202947	3.817764	3.498127
F112	9.150011	5.649131	4.032547
C113	9.618648	4.914137	3.020424
F114	10.520079	5.633550	2.337387
O115	8.865151	3.797787	0.719383
H116	-0.040415	11.365018	1.077817
H117	12.094251	0.321949	-1.603664
O118	4.713417	5.276147	0.361415
C119	4.518586	4.221512	1.283231
C120	4.266873	2.978237	0.519614
H121	5.364559	4.137423	1.975474
H122	3.622840	4.484244	1.874340
H123	3.874924	3.140221	-0.484527
C124	4.434847	1.668280	0.958842
C125	3.959765	0.607250	0.119862
C126	5.051731	1.350015	2.213633
C127	4.058147	-0.705178	0.535662
H128	3.511463	0.854986	-0.837996
C129	5.148305	0.029984	2.609474
H130	5.485277	2.137989	2.818753
C131	4.649001	-0.989401	1.779628
H132	3.690683	-1.512178	-0.089314
H133	5.622966	-0.223891	3.551382
H134	4.734158	-2.023873	2.101415

Fe(III)_styrene-TS2-sextet:

Fe1	6.694309	6.538119	-0.004844
S2	12.017685	5.914339	-2.165853
S3	4.090139	7.489107	-1.680225
O4	5.703485	4.796711	-0.289712
N5	8.090975	8.140138	-0.152581
O6	5.618466	7.359643	-1.478799
O7	12.572489	6.075841	-3.504155
O8	3.476173	6.305239	-2.272293
F9	2.843147	9.111283	-3.323059
F10	4.756374	8.385195	-4.071272
C11	7.636622	3.316587	-3.139092
H12	8.542590	3.067196	-2.590075
O13	12.496914	6.667861	-1.002455
C14	5.718497	2.578681	-4.417001
H15	5.135243	1.776146	-4.861006
C16	4.095590	8.811108	-2.992052
N17	8.322046	5.752578	-1.314732
H18	8.427721	4.789585	-0.976846
F19	4.702230	9.910900	-2.516600
C20	5.327992	3.906930	-4.590963
H21	4.431923	4.145671	-5.155933
C22	6.093188	4.939366	-4.044903
H23	5.783438	5.969300	-4.184713
C24	9.560637	5.799254	-3.400186
H25	9.864059	4.759986	-3.575392
O26	3.462336	8.113645	-0.500373
N27	10.373954	6.369079	-2.297762
C28	9.309195	7.918358	-0.670981
C29	12.055804	4.171038	-1.749810
C30	12.022991	2.421010	-0.099517
H31	11.987855	2.108008	0.939446
C32	8.114232	5.788438	-2.800044
H33	7.635693	6.742944	-3.029176
C34	7.255418	4.656151	-3.319093
C35	9.634544	6.558623	-4.709644
C36	9.592535	6.472561	-1.058858
H37	10.103372	5.992368	-0.220541
C38	12.088838	1.470510	-1.121326
C39	6.872523	2.284987	-3.683574
H40	7.187696	1.254124	-3.548604
C41	12.012370	3.781355	-0.407011
H42	11.996789	4.526015	0.380413
C43	12.134878	3.230164	-2.783237
H44	12.220488	3.562020	-3.812503
C45	12.150092	1.873029	-2.458429
H46	12.226079	1.132482	-3.249093
C47	9.632417	7.917246	-7.162852
H48	9.638392	8.444433	-8.112516
C49	9.704258	8.631652	-5.964181
H50	9.769427	9.715969	-5.980086
C51	10.248240	8.941172	-0.767860
H52	11.233784	8.729695	-1.164468
C53	9.566416	5.848702	-5.913449
H54	9.517559	4.762371	-5.897328
C55	9.563356	6.523946	-7.135151
H56	9.516073	5.960649	-8.062735
C57	9.703045	7.956732	-4.744108
H58	9.782188	8.515293	-3.815851
C59	9.885438	10.213968	-0.324904
H60	10.593890	11.034008	-0.393373
S61	5.504928	11.932096	1.670592
O62	5.833671	12.710444	2.858694
C63	3.617945	7.310516	3.238166
H64	3.207454	8.061685	2.566518
O65	5.981550	12.288995	0.329807
C66	3.239621	5.497964	4.798048
H67	2.556095	4.846405	5.335344
N68	5.803596	8.159307	1.245408
H69	4.811923	8.091321	0.986380
C70	4.616918	5.386234	4.994717
H71	5.013554	4.643947	5.681251
C72	5.494481	6.231547	4.311065
H73	6.564564	6.133800	4.463804
C74	5.798755	9.638263	3.165039
H75	4.736906	9.811772	3.381809
N76	6.178565	10.379915	1.937383
C77	3.725064	11.733025	1.610074
C78	1.724708	11.204526	0.384348
H79	1.234828	10.928579	-0.544225
C80	5.966071	8.142534	2.733552
H81	6.992641	7.834434	2.941163
C82	5.005485	7.201033	3.427666
C83	6.613061	9.978205	4.397060
C84	0.974428	11.393224	1.548087
C85	2.741766	6.461120	3.914675
H86	1.670764	6.561850	3.762367

C87	3.108365	11.378856	0.405248
H88	3.691478	11.262927	-0.500750
C89	2.985447	11.934839	2.781142
H90	3.486750	12.249340	3.690320
C91	1.601399	11.762052	2.741281
H92	1.013460	11.927072	3.639238
C93	8.097119	10.471829	6.725579
H94	8.671656	10.670412	7.625769
C95	8.723902	10.484567	5.476699
H96	9.786887	10.696889	5.403679
C97	5.990580	9.970451	5.650301
H98	4.922872	9.775973	5.721608
C99	6.728526	10.214150	6.810132
H100	6.231629	10.211183	7.776095
C101	7.987181	10.236782	4.319345
H102	8.474308	10.270928	3.348994
C103	7.733587	9.359506	0.285075
C104	6.298374	9.477613	0.784449
H105	5.681827	9.811446	-0.053537
C106	8.613796	10.434901	0.206110
H107	8.295161	11.415337	0.537468
S108	8.201495	4.421540	1.931929
O109	7.690732	5.832978	1.601702
O110	7.277752	3.666388	2.783654
F111	10.284845	3.758662	3.380587
F112	9.232654	5.532605	4.086410
C113	9.651910	4.868793	3.009484
F114	10.498154	5.647187	2.316513
O115	8.770761	3.749975	0.750377
H116	-0.103743	11.264193	1.521887
H117	12.107983	0.412878	-0.874512
O118	4.715094	5.424020	0.622820
C119	4.308679	4.204610	1.250619
C120	4.472675	3.301095	0.053791
H121	4.969435	3.962619	2.085380
H122	3.272448	4.303755	1.591932
H123	3.887176	3.614831	-0.806993
C124	4.939423	1.959205	0.057013
C125	4.635834	1.151645	-1.072153
C126	5.623444	1.384431	1.161585
C127	4.968222	-0.193999	-1.079675
H128	4.130741	1.599421	-1.922549
C129	5.958433	0.039077	1.137602
H130	5.914839	1.999634	2.004859
C131	5.626172	-0.748693	0.026366
H132	4.719604	-0.814991	-1.934322
H133	6.481963	-0.403202	1.979036
H134	5.887387	-1.803332	0.020347

Fe(III)_styrene-INT2-sextet:

Fe1	-0.287441	-0.207178	0.106348
S2	5.002501	-0.602146	-2.148144
S3	-2.913131	0.578047	-1.700915
O4	-1.140128	-2.448398	0.108911
N5	0.997451	1.458628	-0.130346
O6	-1.435391	0.203672	-1.440078
O7	5.564392	-0.253515	-3.447057
O8	-3.641869	-0.499252	-2.361497
F9	-3.867816	2.388118	-3.336647
F10	-1.998551	1.484216	-4.000463
C11	0.661064	-3.498980	-2.849637
H12	1.520835	-3.682187	-2.208066
O13	5.388432	0.080932	-0.907926
C14	-1.144786	-4.386999	-4.192692
H15	-1.690183	-5.238434	-4.589586
C16	-2.679292	1.941787	-2.950363
N17	1.311707	-0.957850	-1.243034
H18	1.473662	-1.901635	-0.871655
F19	-1.989302	2.946057	-2.385804
C20	-1.528500	-3.088437	-4.530624
H21	-2.376332	-2.921050	-5.188407
C22	-0.819256	-1.995149	-4.027652
H23	-1.122289	-0.987916	-4.294446
C24	2.537478	-0.961121	-3.331533
H25	2.885992	-1.997041	-3.432203
O26	-3.514282	1.213614	-0.513702
N27	3.321353	-0.279689	-2.273135
C28	2.211918	1.269247	-0.675870
C29	5.192302	-2.367594	-1.912970
C30	5.246117	-4.285772	-0.464387
H31	5.183436	-4.718240	0.529289
C32	1.093630	-0.998425	-2.725964
H33	0.578886	-0.075169	-2.999611
C34	0.283352	-2.188903	-3.187303
C35	2.575840	-0.292938	-4.690779
C36	2.553079	-0.173431	-1.027758
H37	3.097667	-0.599268	-0.181852
C38	5.478823	-5.102943	-1.574117
C39	-0.052136	-4.590135	-3.344878
H40	0.249229	-5.597512	-3.073846
C41	5.105570	-2.907450	-0.624833
H42	4.954514	-2.264503	0.234605
C43	5.433903	-3.172063	-3.032365
H44	5.536303	-2.719121	-4.012671
C45	5.576544	-4.548365	-2.852955
H46	5.776058	-5.183930	-3.710467
C47	2.513190	0.890722	-7.232186
H48	2.496527	1.350371	-8.216170
C49	2.575038	1.688739	-6.086714
H50	2.610961	2.770622	-6.178798
C51	3.104992	2.327409	-0.815980
H52	4.088599	2.147368	-1.231554
C53	2.517355	-1.087159	-5.841768
H54	2.498949	-2.170606	-5.749692
C55	2.484260	-0.498712	-7.107284
H56	2.444909	-1.126273	-7.993012
C57	2.603704	1.100775	-4.822874
H58	2.677644	1.723812	-3.936258
C59	2.707138	3.593901	-0.385571
H60	3.382937	4.437684	-0.487006
S61	-1.689133	5.159170	1.730971
O62	-1.435914	5.926666	2.943298
C63	-3.394894	0.488156	3.305471
H64	-3.836285	1.268757	2.688212
O65	-1.192568	5.562866	0.410778
C66	-3.698538	-1.415330	4.768942
H67	-4.354956	-2.116354	5.276622
N68	-1.255910	1.405804	1.291683
H69	-2.246913	1.302691	1.047447
C70	-2.315993	-1.498566	4.940694
H71	-1.888857	-2.269340	5.575040
C72	-1.472574	-0.594389	4.292815
H73	-0.398021	-0.674477	4.419785
C74	-1.289009	2.875057	3.219199
H75	-2.353509	3.012671	3.446838
N76	-0.946057	3.634749	1.990234
C77	-3.452550	4.869706	1.604360
C78	-5.385079	4.310463	0.285629
H79	-5.833731	4.067251	-0.672524
C80	-1.077276	1.386985	2.783658
H81	-0.038933	1.110825	2.978707
C82	-2.001708	0.404809	3.468601
C83	-0.472835	3.237113	4.443239
C84	-6.178577	4.393746	1.433005
C85	-4.237480	-0.419605	3.948568
H86	-5.313313	-0.340508	3.819574
C87	-4.013562	4.552697	0.362054
H88	-3.396419	4.524245	-0.528937
C89	-4.237234	4.969905	2.759164
H90	-3.782948	5.264670	3.699179
C91	-5.608232	4.727454	2.664423
H92	-6.231281	4.813676	3.549564
C93	1.021030	3.765965	6.756428
H94	1.599262	3.977757	7.651141
C95	1.629083	3.821352	5.499530
H96	2.680701	4.080417	5.414912
C97	-1.077203	3.186959	5.704410
H98	-2.134166	2.944742	5.788060
C99	-0.333938	3.448334	6.856739
H100	-0.816163	3.411781	7.829328
C101	0.887464	3.555973	4.349212
H102	1.358618	3.623826	3.372736
C103	0.607279	2.672167	0.297608
C104	-0.817256	2.743984	0.831138
H105	-1.464924	3.060324	0.010002

C106	1.443564	3.777413	0.178135
H107	1.095587	4.749969	0.503732
S108	1.380965	-2.284415	1.981881
O109	0.759578	-0.909788	1.599335
O110	0.512903	-3.081034	2.837814
F111	3.434058	-2.690780	3.561814
F112	2.283940	-0.900475	4.033102
C113	2.773677	-1.658617	3.050488
F114	3.610237	-0.921100	2.303819
O115	2.019182	-2.901713	0.806479
H116	-7.247235	4.212459	1.364233
H117	5.596171	-6.174318	-1.439755
O118	-1.851493	-1.531842	1.041882
C119	-3.150242	-2.115501	0.661661
C120	-2.456678	-3.006238	-0.379395
H121	-3.558428	-2.635855	1.528488
H122	-3.833833	-1.354059	0.287224
H123	-2.614757	-2.678911	-1.407803
C124	-2.527143	-4.488709	-0.226883
C125	-3.152133	-5.248245	-1.225055
C126	-2.027038	-5.121897	0.922895
C127	-3.297347	-6.626927	-1.068024
H128	-3.528164	-4.759215	-2.119646
C129	-2.156590	-6.502053	1.064160
H130	-1.515342	-4.542891	1.687070
C131	-2.797581	-7.254349	0.074800
H132	-3.792631	-7.209868	-1.838999
H133	-1.758267	-6.991722	1.947886
H134	-2.902899	-8.328941	0.193595

Fe(III)_styrene-TS3-sextet:

Fe1	6.738130	6.449028	0.175369
S2	12.035603	5.972247	-2.123494
S3	4.078175	7.327572	-1.555544
O4	6.131286	4.411980	0.122802
N5	8.071006	8.141777	-0.113029
O6	5.564538	6.971233	-1.366762
O7	12.593070	6.278526	-3.435352
O8	3.315365	6.248038	-2.174748
F9	3.025223	9.182159	-3.083011
F10	4.776043	8.205693	-3.939426
C11	7.695258	3.203888	-2.877681
H12	8.570242	3.003343	-2.262362
O13	12.470766	6.649838	-0.897095
C14	5.874815	2.358494	-4.227147
H15	5.329357	1.520207	-4.650925
C16	4.230470	8.685308	-2.822848
N17	8.358588	5.710742	-1.192913
H18	8.508529	4.762674	-0.831012
F19	5.014747	9.663745	-2.339433
C20	5.472899	3.667137	-4.500960
H21	4.611599	3.854170	-5.135576
C22	6.181695	4.744352	-3.964665
H23	5.867191	5.759901	-4.183299
C24	9.557898	5.740011	-3.301293
H25	9.888248	4.704374	-3.450072
O26	3.523092	7.971831	-0.347086
N27	10.371307	6.364656	-2.231577
C28	9.288963	7.926410	-0.634645
C29	12.150723	4.202460	-1.869029
C30	12.128326	2.300685	-0.397966
H31	12.056606	1.884201	0.601866
C32	8.122043	5.698996	-2.671693
H33	7.608990	6.630730	-2.919019
C34	7.301655	4.524314	-3.153494
C35	9.583782	6.460370	-4.634304
C36	9.607919	6.479383	-0.982711
H37	10.151177	6.047327	-0.139809
C38	12.302213	1.459699	-1.500574
C39	6.983835	2.128896	-3.408196
H40	7.298269	1.113440	-3.186668
C41	12.056770	3.682555	-0.573401
H42	11.949908	4.342005	0.280027
C43	12.335402	3.373517	-2.981571
H44	12.447599	3.809253	-3.968587
C45	12.410352	1.993815	-2.787346
H46	12.565216	1.339065	-3.639701
C47	9.498132	7.743334	-7.126701
H48	9.472545	8.241255	-8.091725
C49	9.603872	8.494228	-5.953063
H50	9.664806	9.577735	-6.004208
C51	10.217735	8.957681	-0.756473
H52	11.202384	8.747854	-1.155816
C53	9.481686	5.713421	-5.813627
H54	9.439297	4.627914	-5.762952
C55	9.437015	6.351150	-7.054593
H56	9.364014	5.759628	-7.962741
C57	9.644133	7.856987	-4.713506
H58	9.751840	8.442998	-3.805466
C59	9.852802	10.233124	-0.327510
H60	10.554993	11.056932	-0.412691
S61	5.461263	11.907099	1.740108
O62	5.661534	12.647641	2.979177
C63	3.937399	6.765259	3.125428
H64	3.436158	7.323028	2.339475
O65	6.034168	12.325655	0.456820
C66	3.783348	5.141169	4.912875
H67	3.220469	4.399292	5.470979
N68	5.848849	8.142145	1.311659
H69	4.855720	8.051473	1.076038
C70	5.109154	5.434485	5.274723
H71	5.572333	4.905346	6.101884
C72	5.843254	6.392885	4.575119
H73	6.873085	6.591803	4.852017
C74	5.760314	9.601414	3.221576
H75	4.675310	9.691508	3.376110
N76	6.163483	10.364035	2.010196
C77	3.702583	11.652560	1.512006
C78	1.836755	11.163038	0.074513
H79	1.440497	10.946951	-0.912843
C80	6.070344	8.132229	2.781414
H81	7.133440	7.944776	2.947910
C82	5.270534	7.075007	3.501183
C83	6.480973	9.997155	4.492504
C84	0.982374	11.234077	1.177804
C85	3.200302	5.806920	3.843171
H86	2.172726	5.600813	3.558740
C87	3.205475	11.378872	0.233049
H88	3.870669	11.362503	-0.622652
C89	2.856955	11.739043	2.624055
H90	3.263655	12.003095	3.594572
C91	1.489235	11.526863	2.447014
H92	0.818897	11.604713	3.297784
C93	7.801396	10.606705	6.889381
H94	8.312856	10.849790	7.816190
C95	8.513930	10.557530	5.687905
H96	9.580024	10.765636	5.678649
C97	5.772775	10.051397	5.697687
H98	4.701235	9.863925	5.704354
C99	6.429381	10.353685	6.892304
H100	5.866989	10.400554	7.820384
C101	7.858401	10.252806	4.496243
H102	8.411153	10.240502	3.560848
C103	7.717794	9.366962	0.316862
C104	6.294472	9.470040	0.845093
H105	5.646988	9.786410	0.024026
C106	8.586311	10.448798	0.218248
H107	8.262387	11.428268	0.547756
S108	8.483257	4.552971	2.125574
O109	7.908469	5.925570	1.691854
O110	7.598390	3.808452	3.014984
F111	10.512919	4.141030	3.738050
F112	9.438229	5.998710	4.115168
C113	9.896634	5.171897	3.169311
F114	10.766632	5.836883	2.394757
O115	9.107765	3.865125	0.982279
H116	-0.083809	11.074539	1.045820
H117	12.365949	0.385226	-1.354834
O118	5.114870	5.448931	1.334276
C119	4.038454	4.620012	0.850606
C120	4.816104	3.910230	-0.277981
H121	3.741269	3.931679	1.644334
H122	3.188591	5.217620	0.511195
H123	4.559686	4.314277	-1.260204
C124	4.799592	2.416561	-0.270845

C125	4.023093	1.730182	-1.219722
C126	5.496050	1.693077	0.716869
C127	3.932345	0.341568	-1.177015
H128	3.493589	2.289691	-1.985949
C129	5.416598	0.303227	0.741601
H130	6.100375	2.220416	1.449100
C131	4.632569	-0.374220	-0.198915
H132	3.324005	-0.185231	-1.906344
H133	5.961240	-0.254172	1.497966
H134	4.566594	-1.458153	-0.170333

Fe(III)_styrene-Pr-sextet:

Fe1	6.596708	6.271713	0.164291
S2	12.081054	5.913877	-1.842513
S3	3.973132	7.162164	-1.566288
O4	6.192781	4.168073	-0.298342
N5	7.950855	7.984061	-0.059167
O6	5.480555	6.879498	-1.338112
O7	12.731426	6.287724	-3.092843
O8	3.281465	5.999623	-2.118429
F9	2.882151	8.764433	-3.326958
F10	4.793277	7.935642	-3.962202
C11	7.875316	3.197981	-3.181728
H12	8.730475	2.958597	-2.552674
O13	12.413295	6.534599	-0.555749
C14	6.124593	2.445264	-4.673554
H15	5.618012	1.640173	-5.198068
C16	4.104161	8.426918	-2.929920
N17	8.340275	5.602381	-1.207796
H18	8.464753	4.636662	-0.889429
F19	4.735623	9.514445	-2.462944
C20	5.697973	3.764185	-4.831460
H21	4.855732	3.993721	-5.477725
C22	6.358508	4.799787	-4.164775
H23	6.022681	5.823284	-4.293842
C24	9.698693	5.744635	-3.219591
H25	10.039842	4.719073	-3.405544
O26	3.383873	7.886531	-0.431130
N27	10.428088	6.295739	-2.056211
C28	9.194745	7.796463	-0.534902
C29	12.203198	4.134687	-1.666298
C30	12.138098	2.166826	-0.286574
H31	12.026476	1.703379	0.688741
C32	8.218570	5.671293	-2.702791
H33	7.722071	6.616078	-2.936044
C34	7.453781	4.529320	-3.336372
C35	9.824127	6.537477	-4.504874
C36	9.563899	6.362235	-0.872677
H37	10.043208	5.910745	-0.001967
C38	12.378210	1.379987	-1.416376
C39	7.212768	2.163946	-3.841943
H40	7.551608	1.139928	-3.714273
C41	12.052909	3.554147	-0.402541
H42	11.893053	4.174159	0.471808
C43	12.456052	3.360730	-2.804723
H44	12.614363	3.843558	-3.763105
C45	12.540823	1.974409	-2.670638
H46	12.748200	1.361873	-3.543007
C47	9.926903	7.948163	-6.927546
H48	9.973094	8.495859	-7.864396
C49	9.864076	8.638663	-5.714250
H50	9.864533	9.725031	-5.706093
C51	10.094075	8.850780	-0.667926
H52	11.098196	8.654074	-1.021685
C53	9.890834	5.852398	-5.723414
H54	9.906042	4.765019	-5.730742
C55	9.940384	6.553093	-6.929752
H56	9.997852	6.008582	-7.867902
C57	9.810801	7.937897	-4.510273
H58	9.782803	8.480609	-3.569819
C59	9.668795	10.135307	-0.334869
H60	10.342649	10.979713	-0.443482
S61	5.195417	11.823768	1.425824
O62	5.556857	12.754618	2.488465
C63	3.671654	7.534112	3.778821
H64	3.197640	8.279840	3.144606
O65	5.556085	12.041051	0.020971
C66	3.453060	5.786980	5.440635
H67	2.831007	5.185804	6.097549
N68	5.695044	8.053791	1.397211
H69	4.696350	7.919228	1.209725
C70	4.837497	5.605846	5.424450
H71	5.299548	4.861498	6.066351
C72	5.638224	6.388640	4.587014
H73	6.713305	6.240978	4.579209
C74	5.762528	9.748347	3.148507
H75	4.721367	9.915586	3.448193
N76	5.983678	10.357269	1.819025
C77	3.431288	11.527547	1.526487
C78	1.377203	10.797843	0.512470
H79	0.834166	10.416584	-0.346654
C80	5.948130	8.215209	2.870965
H81	6.995647	7.955353	3.040379
C82	5.065334	7.357500	3.754177
C83	6.667514	10.246885	4.258195
C84	0.705558	11.059772	1.709675
C85	2.871992	6.754245	4.614449
H86	1.796402	6.905673	4.624223
C87	2.748027	11.034590	0.409869
H88	3.271681	10.857453	-0.522207
C89	2.770016	11.806377	2.728349
H90	3.318661	12.232572	3.561495
C91	1.397969	11.566385	2.812916
H92	0.869302	11.789308	3.734909
C93	8.319848	11.035988	6.383946
H94	8.959074	11.348273	7.204714
C95	8.830088	10.966550	5.085083
H96	9.866912	11.228344	4.893325
C97	6.161633	10.322492	5.561306
H98	5.119251	10.076485	5.750291
C99	6.983183	10.712770	6.620097
H100	6.575884	10.772544	7.625320
C101	8.010014	10.571600	4.028754
H102	8.407157	10.539174	3.018734
C103	7.543047	9.219299	0.282289
C104	6.112069	9.330700	0.779377
H105	5.467614	9.547270	-0.074682
C106	8.371934	10.328408	0.137153
H107	7.995416	11.311959	0.387843
S108	8.289373	4.248103	2.056545
O109	7.633877	5.608752	1.720439
O110	7.400719	3.385780	2.837636
F111	10.304199	3.781191	3.662298
F112	9.109080	5.512172	4.228074
C113	9.634069	4.833594	3.205604
F114	10.469203	5.634552	2.529952
O115	8.994441	3.675039	0.899536
H116	-0.363584	10.880994	1.778672
H117	12.452255	0.300902	-1.316612
O118	4.648697	5.584802	1.236404
C119	4.506042	4.734177	2.103892
C120	5.305447	3.616397	-0.975356
H121	5.337705	4.103845	2.443586
H122	3.515551	4.590808	2.559313
H123	4.713843	4.214483	-1.679573
C124	4.976040	2.209163	-0.853977
C125	3.917824	1.703020	-1.634239
C126	5.669175	1.363805	0.038385
C127	3.554691	0.364371	-1.524593
H128	3.390440	2.364833	-2.316003
C129	5.301810	0.028367	0.138417
H130	6.478568	1.767324	0.638416
C131	4.247590	-0.469429	-0.640919
H132	2.737802	-0.030700	-2.120373
H133	5.828435	-0.630362	0.822170
H134	3.964184	-1.514757	-0.555179

Fe(III)_propylene-RC-sextet:

Fe1	6.663402	6.542345	0.028439
S2	11.979614	5.919722	-2.101791
S3	4.000144	7.386128	-1.622582
O4	5.746862	4.590124	-0.274686
N5	8.032999	8.134757	-0.125973
O6	5.528102	7.180303	-1.454624
O7	12.547744	6.058892	-3.436625
O8	3.337410	6.238347	-2.226290

F9	2.787010	9.143889	-3.142265
F10	4.605594	8.316774	-4.013478
C11	7.538017	3.244396	-2.925931
H12	8.436843	3.009802	-2.359061
O13	12.427910	6.715068	-0.953447
C14	5.578530	2.470031	-4.116755
H15	4.955214	1.654538	-4.472760
C16	4.031403	8.749212	-2.891641
N17	8.277028	5.736087	-1.268774
H18	8.396016	4.781025	-0.911977
F19	4.735253	9.788353	-2.411800
C20	5.239050	3.791090	-4.410396
H21	4.345465	4.011786	-4.986257
C22	6.045477	4.838244	-3.960834
H23	5.770077	5.863876	-4.184339
C24	9.528229	5.694021	-3.337383
H25	9.834065	4.645013	-3.438141
O26	3.423313	7.991316	-0.407090
N27	10.325448	6.340986	-2.263460
C28	9.245989	7.920616	-0.664911
C29	12.039041	4.189584	-1.639903
C30	11.994949	2.482216	0.054526
H31	11.943294	2.195084	1.100294
C32	8.077039	5.720202	-2.754527
H33	7.612731	6.671081	-3.025991
C34	7.200268	4.576854	-3.214937
C35	9.615623	6.366016	-4.692328
C36	9.540915	6.469948	-1.027623
H37	10.051311	6.010588	-0.176198
C38	12.084544	1.506589	-0.941610
C39	6.729636	2.198179	-3.370871
H40	7.007285	1.171667	-3.148015
C41	11.978861	3.834019	-0.288035
H42	11.948138	4.598493	0.479674
C43	12.142408	3.223503	-2.647540
H44	12.238678	3.529687	-3.683818
C45	12.164876	1.875436	-2.287384
H46	12.258416	1.115397	-3.057288
C47	9.637486	7.561718	-7.228608
H48	9.653396	8.025677	-8.210577
C49	9.718825	8.351509	-6.078797
H50	9.801782	9.431269	-6.165249
C51	10.166169	8.956157	-0.794023
H52	11.147788	8.754068	-1.204747
C53	9.537362	5.579966	-5.847589
H54	9.470842	4.497962	-5.760949
C55	9.546222	6.174283	-7.110503
H56	9.490947	5.552620	-7.999516
C57	9.705275	7.757729	-4.817308
H58	9.792579	8.373791	-3.927012
C59	9.792216	10.229928	-0.361562
H60	10.486981	11.059092	-0.455615
S61	5.422803	11.899477	1.725132
O62	5.708916	12.661017	2.934447
C63	3.574830	7.347254	3.335637
H64	3.169099	8.097457	2.660059
O65	5.914117	12.290284	0.399495
C66	3.183695	5.600541	4.966519
H67	2.495720	4.994982	5.549850
N68	5.749457	8.136219	1.288478
H69	4.754392	8.072548	1.042753
C70	4.562396	5.440276	5.118452
H71	4.954053	4.704750	5.814960
C72	5.446509	6.232473	4.381819
H73	6.516906	6.103197	4.506315
C74	5.791278	9.614744	3.215150
H75	4.739676	9.795730	3.469919
N76	6.130940	10.359370	1.978534
C77	3.650821	11.654550	1.621699
C78	1.693300	11.106536	0.335226
H79	1.232560	10.845134	-0.612341
C80	5.931953	8.116040	2.774773
H81	6.956093	7.791691	2.969708
C82	4.963915	7.196800	3.488431
C83	6.650180	9.944455	4.419229
C84	0.912851	11.238015	1.486953
C85	2.691486	6.552967	4.067750
H86	1.620292	6.690975	3.949570
C87	3.070274	11.320384	0.393192
H88	3.676380	11.254055	-0.502780
C89	2.880031	11.801114	2.780876
H90	3.350628	12.106407	3.709413
C91	1.502695	11.589846	2.704155
H92	0.890281	11.713383	3.592353
C93	8.216172	10.420359	6.697080
H94	8.822337	10.612195	7.577709
C95	8.798472	10.441601	5.426977
H96	9.858335	10.653875	5.318007
C97	6.072285	9.928715	5.693720
H98	5.007169	9.736961	5.801641
C99	6.850942	10.163455	6.828260
H100	6.388449	10.155076	7.811068
C101	8.021042	10.202471	4.294609
H102	8.474010	10.243248	3.308097
C103	7.665947	9.354128	0.302459
C104	6.236995	9.459513	0.824452
H105	5.605633	9.793224	-0.002932
C106	8.528533	10.440919	0.192683
H107	8.202192	11.421117	0.517545
S108	8.045348	4.271284	1.895753
O109	7.579427	5.713223	1.601526
O110	7.057245	3.505756	2.656874
F111	10.072086	3.503846	3.371155
F112	9.016637	5.246758	4.145045
C113	9.463356	4.640048	3.045507
F114	10.335520	5.447120	2.422494
O115	8.651105	3.649735	0.705539
H116	-0.160279	11.079476	1.432647
H117	12.105663	0.455833	-0.667570
O118	4.937036	5.129279	0.547151
C119	3.802824	3.691645	1.898496
C120	3.512722	2.800267	0.882677
H121	4.714286	3.592372	2.481702
H122	3.084292	4.440733	2.213484
H123	2.555456	2.888069	0.370039
C124	4.477904	1.805833	0.376738
H125	3.986239	0.865162	0.100456
H126	4.912703	2.204660	-0.561678
H127	5.303093	1.626441	1.070149

Fe(III)_propylene-TS1-sextet:

Fe1	6.825890	6.554214	0.177465
S2	12.083905	6.070276	-2.115380
S3	4.049634	7.158010	-1.415199
O4	5.994101	4.543861	0.092346
N5	8.105820	8.199730	-0.111244
O6	5.583629	7.028894	-1.301304
O7	12.612950	6.214428	-3.465777
O8	3.411494	5.936446	-1.900988
F9	2.667966	8.719234	-2.999568
F10	4.496098	7.942377	-3.894805
C11	7.699846	3.191127	-2.691735
H12	8.585844	3.007504	-2.087234
O13	12.522275	6.905376	-0.991522
C14	5.810262	2.304910	-3.916388
H15	5.228762	1.455048	-4.262785
C16	3.944667	8.420715	-2.780505
N17	8.415857	5.765112	-1.161688
H18	8.586234	4.831279	-0.770270
F19	4.601091	9.529732	-2.406256
C20	5.438651	3.602044	-4.274169
H21	4.564266	3.769295	-4.896366
C22	6.194071	4.692790	-3.837984
H23	5.896183	5.699326	-4.113938
C24	9.608022	5.690771	-3.262689
H25	9.949598	4.649494	-3.324431
O26	3.482237	7.817762	-0.224294
N27	10.408073	6.414751	-2.242210
C28	9.312603	8.010780	-0.672038
C29	12.233136	4.351876	-1.631151
C30	12.292576	2.666419	0.084110
H31	12.270844	2.390347	1.133816
C32	8.173589	5.687826	-2.637557
H33	7.668476	6.612079	-2.928333
C34	7.331720	4.499265	-3.046265

C35	9.632673	6.302130	-4.648313
C36	9.655339	6.559060	-0.988485
H37	10.210142	6.155917	-0.136686
C38	12.409976	1.683072	-0.901535
C39	6.940306	2.102230	-3.118857
H40	7.239098	1.095845	-2.839787
C41	12.209876	4.011718	-0.274100
H42	12.154491	4.782935	0.485426
C43	12.364504	3.378683	-2.628627
H44	12.429223	3.676128	-3.669875
C45	12.452963	2.037756	-2.252744
H46	12.567706	1.272778	-3.014844
C47	9.538899	7.379361	-7.235731
H48	9.510175	7.797679	-8.237716
C49	9.606470	8.224346	-6.124868
H50	9.634257	9.301729	-6.261672
C51	10.190307	9.074676	-0.856973
H52	11.168571	8.895571	-1.285929
C53	9.568321	5.460869	-5.764815
H54	9.557863	4.382030	-5.628060
C55	9.519721	5.996145	-7.053068
H56	9.476232	5.332128	-7.911624
C57	9.650527	7.689280	-4.838071
H58	9.727634	8.349112	-3.978624
C59	9.780906	10.346761	-0.452610
H60	10.442792	11.196715	-0.588761
S61	5.385883	11.919037	1.663577
O62	5.656191	12.742147	2.835347
C63	3.756449	7.335768	3.459921
H64	3.304951	8.090312	2.819122
O65	5.841368	12.274087	0.315089
C66	3.475355	5.497511	5.011551
H67	2.826610	4.829216	5.570933
N68	5.864944	8.159351	1.367146
H69	4.868284	8.043763	1.148661
C70	4.861664	5.403305	5.143484
H71	5.299920	4.654605	5.796397
C72	5.694382	6.273003	4.435804
H73	6.771007	6.188642	4.539349
C74	5.856397	9.707346	3.235312
H75	4.798265	9.850668	3.487346
N76	6.159096	10.419699	1.968301
C77	3.624345	11.597883	1.597936
C78	1.670772	10.926880	0.364760
H79	1.205527	10.617108	-0.565965
C80	6.066388	8.204022	2.852636
H81	7.107397	7.937535	3.046128
C82	5.152758	7.246870	3.588954
C83	6.703732	10.121057	4.421833
C84	0.904713	11.061452	1.525733
C85	2.923664	6.465526	4.165113
H86	1.845233	6.555301	4.066764
C87	3.038125	11.200513	0.391133
H88	3.631705	11.133298	-0.513260
C89	2.867130	11.748728	2.765510
H90	3.339547	12.103346	3.675433
C91	1.499101	11.476787	2.720512
H92	0.896939	11.602580	3.615356
C93	8.257927	10.739849	6.672786
H94	8.859453	10.986220	7.542967
C95	8.830261	10.754189	5.398129
H96	9.877458	11.015791	5.274925
C97	6.135045	10.113427	5.700391
H98	5.082028	9.869872	5.822143
C99	6.908241	10.419069	6.821764
H100	6.453182	10.414878	7.808058
C101	8.058696	10.444232	4.278951
H102	8.502184	10.479230	3.287928
C103	7.704802	9.417681	0.292086
C104	6.284530	9.483452	0.844670
H105	5.621987	9.757734	0.019277
C106	8.524652	10.530034	0.128709
H107	8.171973	11.507472	0.433648
S108	8.366256	4.452282	2.077791
O109	7.844507	5.871829	1.729873
O110	7.425356	3.695620	2.896046
F111	10.455825	3.839780	3.537124
F112	9.359108	5.587296	4.240038
C113	9.799904	4.934266	3.164686
F114	10.628304	5.733968	2.475105
O115	8.966393	3.811557	0.894176
H116	-0.161450	10.856251	1.495761
H117	12.481569	0.637895	-0.615029
O118	5.117293	5.046018	0.900045
C119	3.819335	3.817690	1.414144
C120	3.013470	3.660334	0.263649
H121	4.534901	3.042061	1.675738
H122	3.460541	4.426508	2.239496
H123	2.176758	4.341152	0.127945
C124	3.330850	2.726600	-0.834855
H125	4.083570	1.983265	-0.561436
H126	2.423711	2.226032	-1.198499
H127	3.710925	3.312087	-1.690097

Fe(II)_styrene-iniR-quintet: (without O_2 and styrene)

Fe1	-0.001201	-0.118024	0.776405
S2	4.674044	1.281528	-2.303955
S3	-1.129293	-2.844864	2.170017
N4	0.002438	0.005415	-1.342505
O5	-0.042582	-1.840591	1.777542
O6	5.758847	0.529563	-2.928870
O7	-0.861126	-3.518886	3.431477
F8	-1.877423	-5.043378	0.918667
F9	0.276240	-4.743116	0.942863
C10	4.159548	-0.912768	2.428182
H11	4.412321	0.103805	2.136234
O12	3.797562	2.178499	-3.066136
C13	4.235851	-2.669162	4.090671
H14	4.540537	-3.023534	5.071514
C15	-0.904565	-4.129261	0.838924
N16	2.195737	-0.017400	0.237427
H17	2.565878	0.634558	0.939016
F18	-0.973327	-3.548002	-0.380371
C19	3.517883	-3.505070	3.235316
H20	3.255417	-4.511889	3.546921
C21	3.118143	-3.044501	1.980161
H22	2.538886	-3.690556	1.328580
C23	4.193997	-0.934205	-0.767310
H24	5.002871	-0.504973	-0.162473
O25	-2.488212	-2.326557	1.912893
N26	3.617817	0.116200	-1.645313
C27	1.147944	0.274081	-1.991021
C28	5.359561	2.205856	-0.928238
C29	5.163891	3.951859	0.716825
H30	4.603704	4.773235	1.151025
C31	3.003557	-1.268570	0.193582
H32	2.392491	-2.040956	-0.284272
C33	3.433463	-1.746796	1.563692
C34	4.715296	-2.156355	-1.495816
C35	2.337473	0.606086	-1.087405
H36	2.350064	1.691328	-0.959680
C37	6.383813	3.554560	1.268707
C38	4.553480	-1.370747	3.685100
H39	5.104603	-0.710125	4.348443
C40	4.647755	3.285158	-0.393931
H41	3.716489	3.608813	-0.844052
C42	6.587173	1.803171	-0.389994
H43	7.135124	0.986433	-0.847514
C44	7.097520	2.489488	0.712387
H45	8.053389	2.192854	1.134367
C46	5.632843	-4.513409	-2.712783
H47	5.990222	-5.422928	-3.187861
C48	4.554502	-3.813223	-3.259208
H49	4.071842	-4.175566	-4.162960
C50	1.188429	0.332431	-3.381941
H51	2.114827	0.578953	-3.885365
C52	5.797264	-2.860659	-0.955595
H53	6.285232	-2.490501	-0.057161
C54	6.253326	-4.033986	-1.558554
H55	7.096505	-4.568088	-1.129027
C56	4.096980	-2.643164	-2.653681
H57	3.270511	-2.090895	-3.090948
C58	0.007274	0.093020	-4.086382
H59	0.009560	0.125744	-5.172077
S60	-4.686534	-1.147755	-2.386325

O61	-5.764700	-0.350877	-2.965105
C62	-4.199520	0.799114	2.419797
H63	-4.476923	-0.190449	2.063969
O64	-3.828970	-2.020621	-3.196669
C65	-4.267756	2.459455	4.178327
H66	-4.586790	2.766754	5.170462
N67	-2.202767	-0.025100	0.221531
H68	-2.605846	-0.695598	0.885443
C69	-3.504941	3.320165	3.388871
H70	-3.220275	4.298984	3.763593
C71	-3.086722	2.919820	2.119310
H72	-2.471384	3.583004	1.520927
C73	-4.164339	0.993651	-0.759368
H74	-4.994870	0.560978	-0.187871
N75	-3.608939	-0.033422	-1.678928
C76	-5.375965	-2.130111	-1.052854
C77	-5.200468	-3.968649	0.491331
H78	-4.654880	-4.825425	0.872713
C79	-2.980195	1.247165	0.235164
H80	-2.340177	2.028000	-0.185585
C81	-3.427585	1.657832	1.621764
C82	-4.638612	2.262609	-1.437994
C83	-6.406102	-3.577825	1.078183
C84	-4.612083	1.196404	3.691514
H85	-5.199202	0.516134	4.302157
C86	-4.681620	-3.251613	-0.586318
H87	-3.762880	-3.569714	-1.065946
C88	-6.589686	-1.733888	-0.479599
H89	-7.126198	-0.883282	-0.886039
C90	-7.102915	-2.469500	0.589290
H91	-8.048247	-2.177521	1.037384
C92	-5.467706	4.699758	-2.556642
H93	-5.790561	5.640765	-2.993588
C94	-4.398179	3.996492	-3.116245
H95	-3.887529	4.388255	-3.991896
C96	-5.711450	2.970500	-0.884398
H97	-6.226144	2.572177	-0.013368
C98	-6.123480	4.183569	-1.438396
H99	-6.959855	4.720280	-0.998933
C100	-3.984625	2.786621	-2.559352
H101	-3.163838	2.233917	-3.006584
C102	-1.142512	-0.213050	-2.010508
C103	-2.344707	-0.575932	-1.135194
H104	-2.379246	-1.665986	-1.066417
C105	-1.177428	-0.185267	-3.402535
H106	-2.103513	-0.394244	-3.923263
S107	1.029463	2.706745	2.180196
O108	-0.027946	1.759454	1.630161
O109	0.693785	3.279010	3.477886
F110	1.858616	5.014800	1.198821
F111	-0.288179	4.713280	1.029355
C112	0.902090	4.109190	0.961210
F113	1.067446	3.648710	-0.300067
O114	2.408971	2.209140	1.972302
H115	-6.805698	-4.141085	1.916566
H116	6.781168	4.078874	2.133062

Fe(II)_styrene-RC-quintet:

Fe1	6.350733	6.658729	0.161948
S2	11.583828	5.478549	-2.008224
S3	3.945820	7.947354	-1.653493
O4	5.189012	4.844098	0.008266
N5	7.909442	8.113622	-0.032043
O6	5.380993	7.450292	-1.430560
O7	12.141907	5.492005	-3.357429
O8	3.089393	6.994276	-2.346913
F9	3.162648	9.951722	-3.168425
F10	4.821500	8.805854	-3.996034
C11	6.801565	3.257967	-2.727538
H12	7.637674	2.915869	-2.121080
O13	12.147286	6.279447	-0.914904
C14	4.763549	2.734299	-3.916581
H15	4.021012	2.008426	-4.236686
C16	4.294657	9.305961	-2.875373
N17	7.889604	5.656373	-1.143390
H18	7.924182	4.702877	-0.768765
F19	5.165857	10.192513	-2.352688
C20	4.625414	4.077813	-4.265583
H21	3.773633	4.407511	-4.853107
C22	5.570976	5.012297	-3.841481
H23	5.444349	6.060132	-4.094291
C24	9.117431	5.423676	-3.206189
H25	9.305737	4.343129	-3.254885
O26	3.422960	8.645243	-0.462108
N27	9.982343	6.036319	-2.163698
C28	9.077757	7.758825	-0.589390
C29	11.519507	3.772099	-1.455502
C30	11.386984	2.164147	0.329762
H31	11.321600	1.941370	1.390182
C32	7.684362	5.638114	-2.622919
H33	7.341609	6.635091	-2.910945
C34	6.666915	4.612493	-3.068917
C35	9.274762	6.018960	-4.590602
C36	9.211653	6.273098	-0.922521
H37	9.682523	5.786244	-0.065276
C38	11.396724	1.132482	-0.612233
C39	5.852275	2.324734	-3.142599
H40	5.960950	1.284598	-2.850128
C41	11.455904	3.493360	-0.086726
H42	11.476782	4.297696	0.638932
C43	11.537277	2.748408	-2.409646
H44	11.629681	2.992394	-3.462527
C45	11.475938	1.423397	-1.977455
H46	11.498804	0.618857	-2.706706
C47	9.411303	7.093023	-7.179543
H48	9.469276	7.509393	-8.181515
C49	9.576579	7.919669	-6.065450
H50	9.766028	8.981438	-6.198549
C51	10.105911	8.683950	-0.755523
H52	11.049427	8.371214	-1.184408
C53	9.112691	5.195984	-5.710450
H54	8.931100	4.132508	-5.574582
C55	9.178370	5.729299	-6.998849
H56	9.052902	5.077273	-7.858961
C57	9.506529	7.386804	-4.778875
H58	9.653657	8.029253	-3.915609
C59	9.889141	9.994501	-0.328351
H60	10.672014	10.738177	-0.445869
S61	5.766141	12.179389	1.793112
O62	6.025733	12.896339	3.038516
C63	3.417068	7.801078	3.434925
H64	3.070733	8.612943	2.798431
O65	6.388412	12.561056	0.520185
C66	2.893317	5.969047	4.924649
H67	2.158915	5.356898	5.440937
N68	5.635474	8.414533	1.386551
H69	4.641738	8.465846	1.138943
C70	4.255036	5.708201	5.076540
H71	4.589565	4.888352	5.705268
C72	5.197422	6.489474	4.405842
H73	6.254312	6.268758	4.512814
C74	5.820111	9.891055	3.292400
H75	4.783766	10.182892	3.504083
N76	6.290275	10.579814	2.062842
C77	3.990556	12.126668	1.543562
C78	2.101229	11.799034	0.089826
H79	1.701373	11.591930	-0.897765
C80	5.822515	8.386628	2.867294
H81	6.817489	7.977584	3.057917
C82	4.789013	7.541129	3.578640
C83	6.665768	10.145627	4.523739
C84	1.245454	11.968843	1.180341
C85	2.475632	7.016848	4.100067
H86	1.416700	7.223164	3.971871
C87	3.482219	11.885577	0.263285
H88	4.151099	11.780347	-0.582471
C89	3.144145	12.310720	2.643050
H90	3.564527	12.539832	3.616424
C91	1.764381	12.231395	2.451456
H92	1.095589	12.380530	3.294191
C93	8.198047	10.469430	6.852587
H94	8.791987	10.599569	7.753099
C95	8.818379	10.437304	5.601128
H96	9.897094	10.544765	5.525155
C97	6.050352	10.182069	5.779790

H98	4.969752	10.084459	5.852483
C99	6.811425	10.340971	6.939166
H100	6.318951	10.370397	7.907311
C101	8.057540	10.274279	4.443969
H102	8.541195	10.268160	3.471472
C103	7.691962	9.370818	0.383458
C104	6.284930	9.650833	0.910731
H105	5.698905	10.053561	0.081768
C106	8.670984	10.353057	0.249439
H107	8.465338	11.366814	0.569501
S108	7.745571	4.407045	2.122586
O109	7.306567	5.830009	1.771960
O110	6.817619	3.694656	2.996879
F111	9.850437	3.668262	3.518944
F112	8.872520	5.466464	4.267119
C113	9.233867	4.799732	3.167534
F114	10.100320	5.559307	2.470377
O115	8.292535	3.695185	0.949483
H116	0.170522	11.902073	1.038707
H117	11.349809	0.098792	-0.281360
O118	4.531417	5.657727	0.743960
C119	3.805205	1.464695	2.192369
C120	3.896078	0.468160	1.301469
H121	4.638965	2.112215	2.449556
H122	2.865324	1.666637	2.698069
H123	3.005813	-0.130130	1.104444
C124	5.084184	0.065382	0.529837
C125	4.984956	-1.017618	-0.361338
C126	6.325984	0.719020	0.639821
C127	6.080748	-1.438070	-1.116161
H128	4.033221	-1.535438	-0.460440
C129	7.420485	0.302082	-0.112869
H130	6.440579	1.560513	1.314315
C131	7.305661	-0.778681	-0.995025
H132	5.977519	-2.280940	-1.795105
H133	8.365161	0.828992	-0.008037
H134	8.162956	-1.104159	-1.579183

Fe(II)_styrene-TS1-triplet:

Fe1	6.586841	6.628181	-0.002831
S2	11.922390	5.861628	-2.110878
S3	3.910328	7.628284	-1.663391
O4	5.425966	4.839159	0.243106
N5	8.030213	8.195830	-0.132401
O6	5.377724	7.233471	-1.561082
O7	12.492572	5.945464	-3.453387
O8	3.063538	6.633593	-2.315068
F9	2.863844	9.619734	-3.045713
F10	4.499534	8.593675	-4.054848
C11	7.434170	3.302131	-3.008371
H12	8.334486	3.024235	-2.464122
O13	12.436727	6.652066	-0.986726
C14	5.418366	2.628916	-4.162285
H15	4.751903	1.845172	-4.512233
C16	4.054651	9.032685	-2.873446
N17	8.242839	5.731387	-1.271801
H18	8.370335	4.776278	-0.924868
F19	4.918320	9.962443	-2.414109
C20	5.112172	3.968603	-4.401581
H21	4.203420	4.237844	-4.931766
C22	5.963119	4.974587	-3.941573
H23	5.706947	6.015705	-4.108005
C24	9.487421	5.716598	-3.345661
H25	9.778966	4.665682	-3.468229
O26	3.416736	8.265496	-0.423469
N27	10.297584	6.336722	-2.266045
C28	9.231612	7.939195	-0.669584
C29	11.935775	4.135147	-1.617421
C30	11.821040	2.459188	0.105693
H31	11.731767	2.198173	1.155507
C32	8.042853	5.754482	-2.747893
H33	7.597835	6.722200	-2.995040
C34	7.131273	4.652391	-3.241380
C35	9.578646	6.412917	-4.688783
C36	9.492898	6.471951	-1.026556
H37	10.003205	6.018185	-0.173911
C38	11.897633	1.463731	-0.870661
C39	6.580934	2.297187	-3.462326
H40	6.818126	1.257139	-3.258693
C41	11.848670	3.804254	-0.261993
H42	11.815686	4.580611	0.492633
C43	12.021380	3.147669	-2.605514
H44	12.130443	3.434006	-3.646046
C45	12.003526	1.806317	-2.221857
H46	12.079611	1.030149	-2.977983
C47	9.589532	7.661010	-7.203087
H48	9.598645	8.145083	-8.175901
C49	9.720827	8.422062	-6.039018
H50	9.834540	9.500913	-6.103772
C51	10.193464	8.940818	-0.790288
H52	11.167862	8.710485	-1.202823
C53	9.450310	5.656090	-5.858930
H54	9.344461	4.575938	-5.791204
C55	9.453539	6.275418	-7.109847
H56	9.355744	5.673815	-8.009512
C57	9.713549	7.802648	-4.789484
H58	9.833849	8.395585	-3.887768
C59	9.868864	10.221670	-0.340585
H60	10.595935	11.024370	-0.424713
S61	5.550509	12.050804	1.721715
O62	5.750804	12.790102	2.965876
C63	3.603363	7.525177	3.428635
H64	3.182451	8.295841	2.786528
O65	6.127073	12.488812	0.445688
C66	3.254172	5.701596	4.980898
H67	2.581122	5.062340	5.546458
N68	5.732015	8.291642	1.322700
H69	4.734148	8.273613	1.088049
C70	4.635884	5.534420	5.086561
H71	5.046989	4.758046	5.725464
C72	5.499973	6.360790	4.365165
H73	6.572562	6.214220	4.438669
C74	5.831958	9.785078	3.226650
H75	4.781766	9.994826	3.466437
N76	6.213049	10.507783	1.986901
C77	3.783409	11.842788	1.484672
C78	1.921630	11.331773	0.047658
H79	1.538476	11.073350	-0.934254
C80	5.944654	8.284181	2.794436
H81	6.970403	7.951250	2.970543
C82	4.994127	7.367007	3.534081
C83	6.685395	10.108561	4.436558
C84	1.060387	11.439790	1.141608
C85	2.739288	6.696448	4.144457
H86	1.665041	6.832233	4.052476
C87	3.290438	11.542700	0.211301
H88	3.960803	11.485958	-0.637657
C89	2.930447	11.963549	2.587656
H90	3.335436	12.238598	3.555621
C91	1.561701	11.762016	2.406139
H92	0.887181	11.862184	3.251704
C93	8.244502	10.560089	6.727408
H94	8.848349	10.739933	7.612727
C95	8.836437	10.560123	5.461885
H96	9.903017	10.741790	5.359623
C97	6.098706	10.113195	5.706820
H98	5.029261	9.942137	5.805641
C99	6.872708	10.335447	6.847125
H100	6.401343	10.339466	7.826264
C101	8.062764	10.333708	4.324082
H102	8.524134	10.351019	3.341045
C103	7.712248	9.418735	0.314245
C104	6.280651	9.572043	0.838899
H105	5.663057	9.920749	0.007759
C106	8.616664	10.475510	0.220935
H107	8.333717	11.463481	0.561727
S108	8.154555	4.450910	2.004026
O109	7.676950	5.851719	1.696022
O110	7.255836	3.678916	2.873720
F111	10.284175	3.696386	3.367834
F112	9.270840	5.441893	4.188921
C113	9.637909	4.826877	3.059788
F114	10.488838	5.631713	2.393227
O115	8.711434	3.753506	0.824334
H116	-0.005380	11.276913	1.008114

H117	11.881302	0.417472	-0.578164
O118	4.330168	4.962077	0.903951
C119	3.940417	3.453621	1.867380
C120	3.548205	2.418783	0.992650
H121	4.902020	3.406662	2.370245
H122	3.161187	3.955833	2.433303
H123	2.503749	2.393259	0.688112
C124	4.405408	1.427278	0.411371
C125	3.838133	0.457537	-0.457012
C126	5.798509	1.350695	0.677105
C127	4.616958	-0.541694	-1.022876
H128	2.773789	0.505648	-0.673715
C129	6.570908	0.350773	0.100748
H130	6.272059	2.072622	1.332172
C131	5.989257	-0.601721	-0.745731
H132	4.160907	-1.277436	-1.679737
H133	7.635399	0.315268	0.314255
H134	6.598794	-1.387516	-1.184136

Olefin ligation pathway

Fe(III)_styrene-iniR-quartet: (without O_2 and styrene)

Fe1	-0.089800	-0.513801	0.559331
S2	4.647657	1.076573	-2.401085
S3	-1.324343	-2.978945	2.119428
N4	-0.063724	-0.150054	-1.481975
O5	-0.183373	-1.967554	1.787329
O6	5.723627	0.226911	-2.893350
O7	-1.120542	-3.620444	3.401200
F8	-1.976761	-5.138342	0.759686
F9	0.169879	-4.832223	0.957328
C10	4.024381	-0.718884	2.487334
H11	4.366725	0.227151	2.068940
O12	3.772319	1.867828	-3.268857
C13	3.958394	-2.247869	4.360322
H14	4.219665	-2.488353	5.386317
C15	-1.006555	-4.237302	0.779648
N16	2.049541	-0.053385	0.189958
H17	2.424652	0.616153	0.864620
F18	-0.982983	-3.591013	-0.414476
C19	3.232880	-3.158508	3.590820
H20	2.921603	-4.107219	4.016608
C21	2.895697	-2.848346	2.272566
H22	2.312646	-3.552459	1.687299
C23	4.117660	-0.984215	-0.664754
H24	4.890066	-0.491369	-0.060306
O25	-2.638152	-2.404801	1.772853
N26	3.551547	-0.029751	-1.636138
C27	1.093794	0.130664	-2.107602
C28	5.286545	2.142848	-1.116527
C29	5.136539	4.170860	0.169494
H30	4.652252	5.118475	0.384670
C31	2.906246	-1.296964	0.285348
H32	2.330378	-2.118722	-0.150011
C33	3.283933	-1.626393	1.709492
C34	4.712171	-2.226026	-1.284854
C35	2.259056	0.497095	-1.180192
H36	2.284905	1.591246	-1.113831
C37	6.282873	3.793130	0.875311
C38	4.353375	-1.025781	3.806812
H39	4.924844	-0.318120	4.399767
C40	4.629629	3.348270	-0.837230
H41	3.778200	3.657980	-1.434297
C42	6.449395	1.762921	-0.434214
H43	6.980002	0.860735	-0.719607
C44	6.940853	2.597972	0.570449
H45	7.850859	2.326763	1.096687
C46	5.801605	-4.573028	-2.355517
H47	6.231583	-5.479708	-2.770051
C48	4.754860	-3.921369	-3.026572
H49	4.379060	-4.322555	-3.962330
C50	1.155071	0.186196	-3.496910
H51	2.085325	0.439879	-3.990956
C52	5.761198	-2.887436	-0.616335
H53	6.149651	-2.481146	0.313222
C54	6.301782	-4.050569	-1.144421
H55	7.114361	-4.556564	-0.632887
C56	4.212893	-2.759765	-2.497371
H57	3.419545	-2.236873	-3.020680
C58	-0.017509	-0.055756	-4.219442
H59	0.004080	-0.025058	-5.304763
S60	-4.840193	-0.998065	-2.556400
O61	-5.862308	-0.045203	-2.974337
C62	-3.647603	0.961021	2.519768
H63	-4.032866	-0.034438	2.311467
O64	-4.026505	-1.776803	-3.491756
C65	-3.310061	2.759589	4.105519
H66	-3.432526	3.164476	5.105494
N67	-2.187343	-0.173912	0.083451
H68	-2.653660	-0.808663	0.746953
C69	-2.673213	3.514187	3.117821
H70	-2.300077	4.508113	3.345474
C71	-2.518716	2.991140	1.833273
H72	-2.030714	3.586886	1.064611
C73	-4.131034	0.941995	-0.724671
H74	-4.863491	0.469003	-0.053526
N75	-3.658563	-0.013437	-1.741297
C76	-5.522472	-2.095259	-1.326037
C77	-5.429744	-4.164049	-0.103851
H78	-4.963653	-5.124863	0.089889
C79	-2.819512	1.176432	0.125612
H80	-2.179895	1.855466	-0.447871
C81	-3.001231	1.711091	1.521660
C82	-4.724095	2.201912	-1.288885
C83	-6.559009	-3.771127	0.619850
C84	-3.794668	1.482778	3.804386
H85	-4.289785	0.893453	4.570034
C86	-4.904642	-3.329947	-1.090627
H87	-4.060591	-3.646323	-1.694200
C88	-6.664035	-1.694096	-0.620688
H89	-7.158496	-0.760498	-0.867022
C90	-7.178826	-2.545887	0.357307
H91	-8.074253	-2.260466	0.900710
C92	-5.826159	4.577905	-2.278260
H93	-6.261269	5.496698	-2.659704
C94	-4.842061	3.905315	-3.022252
H95	-4.522010	4.302585	-3.980000
C96	-5.708191	2.889538	-0.545407
H97	-6.039723	2.487888	0.407777
C98	-6.255062	4.064374	-1.033277
H99	-7.018241	4.589508	-0.467895
C100	-4.292848	2.731622	-2.533741
H101	-3.546711	2.192033	-3.106414
C102	-1.206736	-0.356475	-2.166427
C103	-2.423251	-0.677594	-1.288224
H104	-2.546300	-1.764252	-1.245725
C105	-1.219145	-0.323344	-3.556977
H106	-2.138986	-0.522044	-4.095196
H107	-6.968316	-4.430096	1.379454
H108	6.679535	4.444851	1.647926

Fe(III)_styrene-RC-sextet:

Fe1	-0.525719	-0.639344	-0.037281
S2	1.429251	2.190074	-4.615068
N3	0.345424	1.246196	0.134194
O4	-2.599185	2.755244	0.769471
O5	0.957225	3.323487	-5.401045
C6	-3.064672	-1.009714	-3.597747
H7	-2.116812	-1.464475	-3.876459
O8	2.639783	2.229393	-3.791990
C9	-5.484755	-1.135404	-3.563682
H10	-6.400909	-1.666876	-3.802504
N11	-0.733063	0.221457	-2.101235
H12	-0.591475	-0.628761	-2.663300
C13	-5.540438	0.110323	-2.933958
H14	-6.499974	0.553551	-2.684617
C15	-4.360053	0.790063	-2.627755
H16	-4.408347	1.763925	-2.145455
C17	-1.205082	1.735730	-3.894183
H18	-1.237588	1.009595	-4.719816
N19	0.176660	1.933859	-3.433738
C20	0.755508	1.850953	-0.998313
C21	1.464331	0.739353	-5.653944
C22	2.238220	-1.496290	-6.079730
H23	2.829553	-2.359160	-5.790692
C24	-1.863311	1.023831	-2.639569
H25	-2.091707	1.803703	-1.906546

C26	-3.111038	0.236595	-2.950612
C27	-1.905188	2.996516	-4.314888
C28	0.470807	1.066643	-2.281032
H29	1.330360	0.418892	-2.478975
C30	1.491519	-1.515241	-7.260843
C31	-4.245919	-1.692304	-3.893595
H32	-4.197311	-2.657577	-4.388496
C33	2.236219	-0.362540	-5.267894
H34	2.844460	-0.323116	-4.372161
C35	0.718682	0.740694	-6.839129
H36	0.172585	1.628481	-7.139576
C37	0.740451	-0.399531	-7.642990
H38	0.184385	-0.409918	-8.575358
C39	-3.265755	5.316140	-5.097259
H40	-3.791022	6.214311	-5.407678
C41	-2.320443	5.378953	-4.061268
H42	-2.111914	6.326723	-3.575317
C43	1.456545	3.051522	-0.956383
H44	1.812032	3.503873	-1.874018
C45	-2.861236	2.942911	-5.349986
H46	-3.060860	1.998742	-5.848917
C47	-3.535130	4.090802	-5.739324
H48	-4.263214	4.050886	-6.543296
C49	-1.648307	4.231262	-3.670243
H50	-0.901733	4.272420	-2.884382
C51	1.712670	3.624340	0.291598
H52	2.252204	4.564556	0.355559
S53	0.751062	2.042113	4.998018
O54	2.053199	2.119299	5.646339
C55	-0.236619	-3.032402	3.904134
H56	-0.729948	-2.284219	4.522748
O57	0.090378	3.195878	4.379302
C58	0.123287	-5.364347	3.365993
H59	-0.091746	-6.413762	3.543234
N60	-0.211648	-0.413688	2.178191
H61	-1.029355	-0.737385	2.699967
C62	1.045668	-4.993201	2.387227
H63	1.546571	-5.750529	1.792545
C64	1.325776	-3.643592	2.162512
H65	2.037535	-3.364133	1.393298
C66	1.480619	-0.394234	3.919756
H67	0.973091	-0.815505	4.797326
N68	0.986072	0.969179	3.665656
C69	-0.395500	1.262698	6.127916
C70	-2.640250	0.959639	6.932521
H71	-3.700177	1.188782	6.879283
C72	0.990052	-1.191770	2.654327
H73	1.752372	-1.105875	1.876655
C74	0.683044	-2.649436	2.911345
C75	2.971514	-0.500370	4.130133
C76	-2.154600	0.116878	7.936810
C77	-0.516926	-4.380707	4.126964
H78	-1.222319	-4.665951	4.902089
C79	-1.762604	1.540601	6.016731
H80	-2.119895	2.235735	5.264574
C81	0.108445	0.435724	7.139550
H82	1.178336	0.288715	7.242597
C83	-0.785269	-0.142968	8.041442
H84	-0.409019	-0.774123	8.840597
C85	5.733302	-0.801334	4.485899
H86	6.803212	-0.917577	4.629343
C87	5.242331	0.228044	3.668198
H88	5.933124	0.910671	3.183583
C89	3.472446	-1.530560	4.949707
H90	2.782987	-2.207636	5.446635
C91	4.841007	-1.682253	5.125783
H92	5.224861	-2.474190	5.761099
C93	3.874507	0.377312	3.489184
H94	3.487183	1.183799	2.875931
C95	0.603758	1.779036	1.340900
C96	0.042737	1.006785	2.539414
H97	-0.899559	1.481738	2.831881
C98	1.284151	2.988476	1.458422
H99	1.453529	3.424213	2.435306
S100	0.915490	-2.914738	-1.764936
O101	0.823676	-1.961111	-0.545511
O102	0.571355	-4.286327	-1.425838
F103	3.059406	-3.490740	-3.169812
F104	3.396489	-3.365552	-1.019648
C105	2.754114	-2.833932	-2.056995
F106	3.122545	-1.546485	-2.187285
O107	0.294340	-2.291517	-2.953720
O108	-3.240253	3.733044	1.096006
C109	-2.296274	-2.252404	0.055471
H110	-1.864114	-2.917660	0.799694
C111	-3.260120	-1.332218	0.349734
H112	-3.691718	-0.785492	-0.487954
H113	1.505965	-2.397458	-7.893691
H114	-2.842038	-0.318890	8.655774
H115	-2.121099	-2.515028	-0.985721
C116	-3.827576	-1.001752	1.653774
C117	-3.555092	-1.748994	2.821542
C118	-4.735723	0.074192	1.734416
C119	-4.168076	-1.417912	4.025337
H120	-2.899302	-2.613384	2.775973
C121	-5.349600	0.401592	2.940804
H122	-4.970500	0.638483	0.835741
C123	-5.066838	-0.344410	4.087945
H124	-3.971202	-2.010689	4.913559
H125	-6.058147	1.223017	2.985009
H126	-5.561465	-0.106114	5.024897

Fe(III)_styrene-TS1-quartet:

Fe1	-0.578979	-0.268485	0.101948
S2	1.323265	2.065634	-4.720649
N3	0.596340	1.366028	0.121669
O4	-2.153135	1.038627	0.723410
O5	0.865808	3.192258	-5.523633
C6	-3.237849	-0.655738	-3.380968
H7	-2.336355	-1.128788	-3.765391
O8	2.612407	2.039953	-4.024887
C9	-5.649992	-0.679575	-3.161012
H10	-6.606831	-1.152611	-3.361395
N11	-0.761445	0.388038	-1.952636
H12	-0.736850	-0.494681	-2.480180
C13	-5.596251	0.530490	-2.464653
H14	-6.511082	1.006585	-2.123539
C15	-4.363860	1.140619	-2.215431
H16	-4.328131	2.080790	-1.671640
C17	-1.254433	1.920297	-3.736853
H18	-1.430861	1.218125	-4.564156
N19	0.183145	1.980080	-3.413696
C20	1.000328	1.877540	-1.055094
C21	1.145057	0.565485	-5.672417
C22	1.732389	-1.732751	-6.063207
H23	2.304133	-2.616852	-5.799172
C24	-1.863970	1.269860	-2.439153
H25	-1.997595	2.059002	-1.694753
C26	-3.173986	0.554669	-2.669529
C27	-1.872649	3.252277	-4.080626
C28	0.508137	1.110105	-2.277868
H29	1.267674	0.369044	-2.541532
C30	0.854966	-1.758700	-7.150711
C31	-4.467935	-1.272376	-3.615850
H32	-4.503561	-2.208080	-4.165685
C33	1.889553	-0.565128	-5.317221
H34	2.599441	-0.522189	-4.499828
C35	0.272028	0.559935	-6.767451
H36	-0.247823	1.467612	-7.055103
C37	0.132483	-0.615746	-7.505766
H38	-0.526078	-0.632848	-8.368726
C39	-3.094029	5.696217	-4.696955
H40	-3.564128	6.643271	-4.943856
C41	-2.061930	5.651446	-3.748110
H42	-1.731023	6.564805	-3.263948
C43	1.854931	2.974931	-1.092839
H44	2.205226	3.354252	-2.045272
C45	-2.910593	3.305664	-5.028966
H46	-3.230833	2.395834	-5.529316
C47	-3.517427	4.516783	-5.336047
H48	-4.310828	4.556822	-6.075758
C49	-1.456467	4.441017	-3.440739
H50	-0.639950	4.402409	-2.727082
C51	2.259535	3.538976	0.120150
H52	2.922492	4.398971	0.120032

S53	1.053246	2.268559	4.968966
O54	2.212896	2.037851	5.818920
C55	-0.381791	-2.669102	4.066145
H56	-0.796256	-1.846604	4.647929
O57	0.774681	3.539162	4.296078
C58	-0.227396	-5.052819	3.670037
H59	-0.524288	-6.067947	3.916047
N60	-0.102200	-0.138264	2.227930
H61	-0.935579	-0.334561	2.785337
C62	0.708383	-4.821517	2.661437
H63	1.135469	-5.652785	2.109615
C64	1.102022	-3.516970	2.354980
H65	1.832745	-3.348526	1.571527
C66	1.598578	-0.239416	3.957070
H67	1.058387	-0.570242	4.852377
N68	1.252148	1.163869	3.657798
C69	-0.419107	1.762775	5.850682
C70	-2.796118	1.913275	6.192405
H71	-3.759030	2.349123	5.943897
C72	1.015864	-1.023879	2.726345
H73	1.767785	-1.049980	1.935955
C74	0.559121	-2.428374	3.048735
C75	3.073576	-0.493707	4.163388
C76	-2.693569	0.980941	7.229160
C77	-0.771330	-3.973413	4.374217
H78	-1.481257	-4.148982	5.177761
C79	-1.655975	2.314976	5.494914
H80	-1.712517	3.080793	4.728415
C81	-0.298276	0.844389	6.901061
H82	0.680479	0.487011	7.203458
C83	-1.449482	0.452573	7.586195
H84	-1.369848	-0.243118	8.415971
C85	5.792799	-1.061498	4.522712
H86	6.846602	-1.278259	4.668588
C87	5.400471	-0.059339	3.623187
H88	6.151568	0.501646	3.075973
C89	3.475089	-1.497400	5.063235
H90	2.726545	-2.048749	5.625901
C91	4.823417	-1.781185	5.241906
H92	5.129575	-2.551157	5.943047
C93	4.052636	0.221663	3.442613
H94	3.746405	1.011609	2.764402
C95	0.972267	1.899937	1.295509
C96	0.330736	1.264766	2.526080
H97	-0.555715	1.854438	2.780645
C98	1.812210	3.008547	1.333653
H99	2.082569	3.449905	2.285648
S100	0.845394	-2.674555	-1.473205
O101	0.839549	-1.554905	-0.397560
O102	0.499653	-3.979035	-0.925979
F103	2.881396	-3.493101	-2.911384
F104	3.349325	-3.113537	-0.815465
C105	2.666490	-2.691289	-1.876741
F106	3.062148	-1.445852	-2.187948
O107	0.155905	-2.207286	-2.694748
O108	-3.316640	0.585084	0.996822
C109	-2.046064	-1.835629	0.140866
H110	-1.601797	-2.509151	0.870868
C111	-3.429216	-1.462257	0.313592
H112	-3.905498	-1.012759	-0.551717
H113	0.746453	-2.667895	-7.734397
H114	-3.582324	0.685968	7.779123
H115	-1.854609	-2.141441	-0.889598
C116	-4.326227	-1.983118	1.303343
C117	-5.716968	-1.735814	1.136709
C118	-3.894740	-2.761056	2.411764
C119	-6.637073	-2.243941	2.038194
H120	-6.047788	-1.144725	0.287535
C121	-4.821530	-3.265696	3.308519
H122	-2.841553	-2.976524	2.555756
C123	-6.190789	-3.011578	3.125245
H124	-7.697432	-2.055929	1.904494
H125	-4.492427	-3.869031	4.148481
H126	-6.911908	-3.418009	3.828477

Fe(III)_styrene-INT1-quartet:

Fe1	-0.777007	-0.271153	0.169141
S2	1.350879	1.957324	-4.745701
N3	0.589157	1.378189	0.130831
O4	-2.245916	0.660263	0.810426
O5	0.904244	3.064055	-5.584457
C6	-3.353154	-0.417066	-3.430940
H7	-2.488225	-0.903558	-3.877412
O8	2.650274	1.925269	-4.072208
C9	-5.752668	-0.349639	-3.108568
H10	-6.738201	-0.765366	-3.296996
N11	-0.803809	0.430716	-1.957121
H12	-0.838090	-0.451647	-2.483159
C13	-5.615326	0.803947	-2.332740
H14	-6.491508	1.284442	-1.907976
C15	-4.348482	1.344560	-2.102938
H16	-4.246608	2.239398	-1.494632
C17	-1.211621	1.985109	-3.736089
H18	-1.440877	1.290235	-4.556992
N19	0.224379	1.954687	-3.424437
C20	1.019635	1.837504	-1.057638
C21	1.117789	0.426260	-5.634578
C22	1.624171	-1.905491	-5.929331
H23	2.166594	-2.796702	-5.630100
C24	-1.855709	1.375913	-2.429038
H25	-1.936852	2.170625	-1.682590
C26	-3.207069	0.741610	-2.649475
C27	-1.735380	3.350251	-4.091966
C28	0.492595	1.076802	-2.272741
H29	1.218561	0.299204	-2.526276
C30	0.735950	-1.948875	-7.007189
C31	-4.618647	-0.961934	-3.652876
H32	-4.719827	-1.856381	-4.260362
C33	1.827578	-0.712555	-5.236172
H34	2.544571	-0.659669	-4.425248
C35	0.233822	0.402789	-6.720434
H36	-0.257387	1.314013	-7.044609
C37	0.048405	-0.798524	-7.405780
H38	-0.617773	-0.830562	-8.262434
C39	-2.768442	5.870793	-4.741227
H40	-3.169191	6.845997	-5.000663
C41	-1.713768	5.767599	-3.819230
H42	-1.298363	6.663516	-3.369317
C43	1.948470	2.871818	-1.139124
H44	2.309143	3.200082	-2.106479
C45	-2.798332	3.464336	-5.012633
H46	-3.207664	2.570536	-5.474562
C47	-3.310934	4.710463	-5.335278
H48	-4.123131	4.800023	-6.049618
C49	-1.202223	4.521682	-3.495191
H50	-0.376194	4.430280	-2.798265
C51	2.416533	3.435616	0.048932
H52	3.134838	4.249345	0.016865
S53	1.283641	2.382368	4.938728
O54	2.426607	2.092019	5.796155
C55	-0.360392	-2.540884	4.183556
H56	-0.734742	-1.691654	4.754319
O57	1.094992	3.652518	4.236686
C58	-0.336997	-4.931092	3.805626
H59	-0.694552	-5.925544	4.054940
N60	0.002234	-0.087227	2.313115
H61	-0.832160	-0.251307	2.878799
C62	0.614793	-4.760628	2.799529
H63	0.994727	-5.619301	2.255074
C64	1.078940	-3.482482	2.482530
H65	1.810394	-3.357330	1.691110
C66	1.711429	-0.169001	4.011774
H67	1.158678	-0.454047	4.916134
N68	1.414254	1.229593	3.657113
C69	-0.220649	1.995309	5.825399
C70	-2.586386	2.297573	6.142714
H71	-3.519678	2.782952	5.874313
C72	1.097037	-0.980933	2.808168
H73	1.839652	-1.048839	2.010179
C74	0.595659	-2.360658	3.167498
C75	3.174373	-0.454402	4.235038
C76	-2.549193	1.381476	7.197965
C77	-0.824958	-3.818145	4.497882
H78	-1.555888	-3.947031	5.290718
C79	-1.418329	2.615464	5.448033

H80	-1.423086	3.365155	4.663803
C81	-0.164081	1.092595	6.894838
H82	0.788455	0.682674	7.213690
C83	-1.342293	0.786209	7.577338
H84	-1.312124	0.103781	8.421247
C85	5.877693	-1.066704	4.634812
H86	6.924870	-1.303261	4.797030
C87	5.518390	-0.053221	3.730512
H88	6.289016	0.494280	3.197433
C89	3.544720	-1.472820	5.138446
H90	2.776699	-2.013802	5.683905
C91	4.881902	-1.777748	5.337182
H92	5.167182	-2.556142	6.037628
C93	4.181145	0.249811	3.529885
H94	3.893534	1.042250	2.847512
C95	1.052913	1.900986	1.279224
C96	0.448136	1.308532	2.550416
H97	-0.424960	1.910883	2.823341
C98	1.967665	2.950405	1.278830
H99	2.296763	3.381609	2.216474
S100	0.534245	-2.744745	-1.416887
O101	0.538482	-1.661688	-0.304971
O102	0.097188	-4.043974	-0.926117
F103	2.593097	-3.640832	-2.771022
F104	2.997801	-3.294192	-0.657959
C105	2.368907	-2.837179	-1.739516
F106	2.830289	-1.606969	-2.025796
O107	-0.061800	-2.212863	-2.658815
O108	-3.411401	0.023215	1.267122
C109	-2.224744	-1.885483	0.443000
H110	-1.797789	-2.210945	1.395313
C111	-3.556845	-1.182801	0.492205
H112	-3.883090	-0.904054	-0.513571
H113	0.590699	-2.878497	-7.549137
H114	-3.459311	1.150029	7.743219
H115	-2.102022	-2.628014	-0.343619
C116	-4.565244	-2.098836	1.144176
C117	-5.582037	-2.669020	0.362077
C118	-4.473484	-2.418819	2.510744
C119	-6.503961	-3.537128	0.941725
H120	-5.653809	-2.420223	-0.693213
C121	-5.406252	-3.276016	3.087673
H122	-3.689062	-1.980353	3.120631
C123	-6.418496	-3.839874	2.304370
H124	-7.293533	-3.971379	0.336275
H125	-5.346957	-3.508105	4.146690
H126	-7.140927	-4.513306	2.755641

Fe(III)_styrene-TS2-quartet:

Fe1	-1.476027	-0.510778	0.125326
S2	-5.882081	-3.937781	0.629319
N3	-1.359959	-2.363185	-0.541965
O4	-1.736335	1.246158	-0.459641
O5	-6.951663	-4.351463	-0.265113
C6	-5.491236	1.379571	-0.363540
H7	-5.693754	0.896185	0.588991
O8	-4.884809	-4.858371	1.184010
C9	-5.730661	3.324086	-1.790370
H10	-6.115682	4.325948	-1.957485
N11	-3.510848	-0.986820	0.004216
C12	-5.027607	2.664136	-2.801873
H13	-4.861529	3.150969	-3.758406
C14	-4.557859	1.365320	-2.594446
H15	-4.030043	0.850509	-3.393211
C16	-5.536967	-1.742141	-1.050796
H17	-6.292733	-1.260419	-0.415879
N18	-4.903240	-2.858510	-0.312457
C19	-2.433872	-3.160113	-0.378230
C20	-6.567802	-2.963520	1.959546
C21	-6.389085	-2.044486	4.174775
H22	-5.846970	-1.934134	5.108776
C23	-4.348099	-0.728433	-1.214792
H24	-3.759323	-1.037944	-2.082961
C25	-4.786167	0.709666	-1.377533
C26	-6.161325	-2.122639	-2.371450
C27	-3.625436	-2.459556	0.263841
H28	-3.589148	-2.623527	1.345893
C29	-7.629980	-1.424313	4.003245
C30	-5.958561	2.679669	-0.569424
H31	-6.516567	3.180385	0.216590
C32	-5.849787	-2.826995	3.154205
H33	-4.914918	-3.358011	3.297413
C34	-7.817959	-2.359605	1.777780
H35	-8.377531	-2.528887	0.863745
C36	-8.345002	-1.586743	2.813138
H37	-9.321920	-1.127651	2.696657
C38	-7.312687	-2.724074	-4.853301
H39	-7.762854	-2.964543	-5.811684
C40	-6.136623	-3.367758	-4.451326
H41	-5.677490	-4.111237	-5.095972
C42	-2.376819	-4.497624	-0.750263
H43	-3.234656	-5.138364	-0.580829
C44	-7.339049	-1.480546	-2.781008
H45	-7.813181	-0.752211	-2.127665
C46	-7.912442	-1.779497	-4.015650
H47	-8.830583	-1.286170	-4.319624
C48	-5.561959	-3.066882	-3.219663
H49	-4.664539	-3.587743	-2.898058
C50	-1.191644	-4.973532	-1.321096
H51	-1.121512	-6.013518	-1.625427
S52	3.204454	-2.482957	-2.400132
O53	4.321028	-3.248475	-1.870224
C54	2.514693	1.437578	1.105719
H55	2.779373	1.445887	0.049652
O56	2.255894	-3.007906	-3.388424
C57	2.599365	2.518118	3.268655
H58	2.913216	3.350371	3.892104
N59	0.569642	-0.597235	-0.330473
C60	1.920862	1.437399	3.833155
H61	1.693710	1.427577	4.894768
C62	1.540944	0.356480	3.035330
H63	1.017537	-0.482991	3.480519
C64	2.747734	-1.549167	0.182535
H65	3.446379	-0.752576	-0.100917
N66	2.187086	-2.167084	-1.040017
C67	3.805489	-0.899005	-2.972411
C68	3.584514	1.012857	-4.415456
H69	3.064334	1.541745	-5.208407
C70	1.495835	-0.874137	0.842534
H71	0.992601	-1.618458	1.464088
C72	1.834672	0.344614	1.667235
C73	3.447363	-2.504153	1.122775
C74	4.754420	1.546374	-3.866119
C75	2.890924	2.519287	1.900834
H76	3.427587	3.353141	1.458010
C77	3.100721	-0.218954	-3.973188
H78	2.228730	-0.673659	-4.431613
C79	4.988914	-0.386703	-2.426862
H80	5.549496	-0.964028	-1.699029
C81	5.456379	0.847928	-2.879588
H82	6.381492	1.251216	-2.479298
C83	4.730786	-4.198442	2.947417
H84	5.231894	-4.858793	3.648685
C85	3.595910	-4.640327	2.258672
H86	3.219173	-5.645640	2.421774
C87	4.584575	-2.067441	1.816163
H88	4.974428	-1.067420	1.642025
C89	5.223498	-2.910226	2.724770
H90	6.109050	-2.566580	3.250602
C91	2.955400	-3.797279	1.354229
H92	2.089982	-4.153593	0.802357
C93	-0.216558	-2.799492	-1.102903
C94	0.831925	-1.711131	-1.305240
H95	0.727600	-1.325521	-2.325777
C96	-0.099229	-4.120437	-1.516222
H97	0.813438	-4.456333	-1.994580
S98	-2.435217	0.432561	2.945311
O99	-1.533018	-0.497249	2.092770
O100	-1.883920	1.784348	3.065334
F101	-3.075977	0.247683	5.470152
F102	-1.045503	-0.402167	5.021990
C103	-2.310638	-0.406392	4.608810
F104	-2.738838	-1.664484	4.481651
O105	-3.845555	0.302036	2.525882
O106	-0.524466	2.104109	-0.444864

C107	-2.443301	3.148094	0.144747
H108	-2.361207	2.831244	1.181703
C109	-1.208374	3.342588	-0.618269
H110	-1.383664	3.543955	-1.679680
H111	-8.050473	-0.828157	4.807546
H112	5.134237	2.497887	-4.226208
H113	-3.402986	3.520058	-0.211392
C114	-0.691082	4.561199	0.110533
C115	-0.735399	5.815339	-0.537469
C116	-0.257476	4.469413	1.453836
C117	-0.324370	6.954864	0.139511
H118	-1.072064	5.882060	-1.568487
C119	0.160943	5.619418	2.116088
H120	-0.231669	3.507706	1.956042
C121	0.123169	6.857089	1.466127
H122	-0.343513	7.918993	-0.358524
H123	0.507068	5.553519	3.142478
H124	0.441324	7.752559	1.991760
H125	-3.908056	-0.489518	0.817491
H126	0.831110	0.298838	-0.750092

Fe(III)_styrene-INT2-quartet:

Fe1	-0.534219	-0.384095	0.096898
S2	1.307717	1.993744	-4.780940
N3	0.545584	1.412020	0.090488
O4	-2.547989	-0.681163	0.634034
O5	0.845373	3.086809	-5.627369
C6	-3.370535	-0.540824	-3.350865
H7	-2.513148	-1.039954	-3.795561
O8	2.597674	1.997723	-4.087565
C9	-5.762443	-0.482966	-2.968760
H10	-6.747778	-0.915600	-3.114696
N11	-0.780037	0.391875	-1.990771
H12	-0.799775	-0.489674	-2.521007
C13	-5.616363	0.698620	-2.237540
H14	-6.486975	1.190023	-1.813189
C15	-4.348073	1.256221	-2.058553
H16	-4.241049	2.180207	-1.495172
C17	-1.268633	1.912006	-3.776741
H18	-1.471617	1.187513	-4.578877
N19	0.170118	1.954024	-3.471539
C20	0.943370	1.906316	-1.097206
C21	1.121662	0.454431	-5.666415
C22	1.664173	-1.872758	-5.933907
H23	2.213317	-2.754386	-5.619825
C24	-1.866896	1.302766	-2.447100
H25	-1.942003	2.114261	-1.716357
C26	-3.214376	0.643806	-2.611534
C27	-1.859503	3.242763	-4.155583
C28	0.478441	1.099623	-2.313371
H29	1.249845	0.362342	-2.556565
C30	0.794940	-1.936179	-7.026490
C31	-4.636946	-1.101906	-3.521885
H32	-4.744959	-2.018485	-4.094060
C33	1.840207	-0.671901	-5.247143
H34	2.546165	-0.602386	-4.427230
C35	0.255814	0.409952	-6.765832
H36	-0.245271	1.311421	-7.102001
C37	0.098917	-0.798577	-7.445445
H38	-0.553273	-0.846553	-8.312051
C39	-3.019753	5.695092	-4.851312
H40	-3.467866	6.644526	-5.128216
C41	-1.968580	5.660045	-3.920670
H42	-1.603094	6.583105	-3.482143
C43	1.761852	3.029366	-1.168718
H44	2.107804	3.386048	-2.131491
C45	-2.919468	3.287949	-5.084522
H46	-3.278164	2.367256	-5.536004
C47	-3.494861	4.501238	-5.430482
H48	-4.304283	4.536035	-6.152750
C49	-1.394360	4.447117	-3.573780
H50	-0.568199	4.411273	-2.871686
C51	2.134316	3.652040	0.024989
H52	2.763228	4.536985	0.000272
S53	1.033421	2.515319	4.902277
O54	2.233164	2.414581	5.723492
C55	0.018679	-2.644791	4.063636
H56	-0.533072	-1.881702	4.610001
O57	0.638925	3.730435	4.186070
C58	0.503793	-4.986129	3.698837
H59	0.335509	-6.029743	3.946944
N60	0.031147	-0.080633	2.263926
H61	-0.783371	-0.360403	2.814409
C62	1.433688	-4.640379	2.716744
H63	1.985872	-5.412811	2.190382
C64	1.655536	-3.298356	2.407131
H65	2.369963	-3.036919	1.632650
C66	1.726235	0.013305	3.982362
H67	1.177852	-0.345504	4.863223
N68	1.289279	1.373490	3.629717
C69	-0.366758	1.933116	5.849108
C70	-2.735896	1.919952	6.265350
H71	-3.736508	2.272557	6.034495
C72	1.230198	-0.842605	2.748844
H73	1.989087	-0.778486	1.964033
C74	0.950822	-2.288102	3.074554
C75	3.203349	-0.119910	4.241819
C76	-2.531380	1.035589	7.328606
C77	-0.206942	-3.985065	4.369748
H78	-0.930428	-4.250275	5.134562
C79	-1.651828	2.378997	5.516287
H80	-1.789146	3.109158	4.725654
C81	-0.144205	1.064336	6.924733
H82	0.867254	0.789669	7.204901
C83	-1.240727	0.613871	7.661057
H84	-1.084002	-0.045819	8.508940
C85	5.945512	-0.452816	4.706837
H86	7.007140	-0.582528	4.893797
C87	5.504995	0.540380	3.818243
H88	6.226285	1.181748	3.322045
C89	3.655594	-1.117069	5.129871
H90	2.935602	-1.753000	5.637060
C91	5.012404	-1.283467	5.361359
H92	5.359469	-2.046636	6.050652
C93	4.148196	0.704994	3.584612
H94	3.797143	1.481720	2.914096
C95	0.910302	1.995786	1.246170
C96	0.334755	1.349189	2.510820
H97	-0.591142	1.873592	2.772142
C98	1.700532	3.141624	1.251261
H99	1.949388	3.623681	2.188980
S100	0.179630	-3.048276	-1.561251
O101	0.189139	-2.148485	-0.303751
O102	-0.276063	-4.396829	-1.264441
F103	2.226578	-3.784605	-3.038283
F104	2.651627	-3.707338	-0.903819
C105	2.009552	-3.118844	-1.910230
F106	2.475886	-1.859463	-2.044832
O107	-0.399872	-2.333084	-2.717173
O108	-2.643315	-1.317744	1.985330
C109	-3.568656	-1.624778	0.123029
H110	-3.098512	-2.390641	-0.495720
C111	-3.873242	-2.056413	1.559701
H112	-4.738671	-1.532947	1.976269
H113	0.671118	-2.871947	-7.563119
H114	-3.378126	0.693304	7.915972
H115	-4.340513	-1.083587	-0.422240
C116	-3.873247	-3.497539	1.940308
C117	-4.918833	-3.994657	2.732787
C118	-2.861679	-4.368667	1.502672
C119	-4.965983	-5.347227	3.071768
H120	-5.702974	-3.323699	3.075746
C121	-2.909793	-5.718096	1.846052
H122	-2.034859	-4.004228	0.899383
C123	-3.962274	-6.209280	2.626543
H124	-5.783952	-5.725781	3.676992
H125	-2.130637	-6.387884	1.495345
H126	-4.000467	-7.263886	2.883416

Fe(III)_styrene-TS3-quartet:

Fe1	-0.608503	-0.357265	0.047739
S2	1.443132	2.040490	-4.730340
N3	0.486096	1.432013	0.107286
O4	-2.437987	-0.642603	0.462769
O5	1.003616	3.116335	-5.610667
C6	-3.278694	-0.478338	-3.514130

H7	-2.409194	-0.941660	-3.973797
O8	2.707728	2.063216	-3.992272
C9	-5.670222	-0.492065	-3.129206
H10	-6.644788	-0.943520	-3.289595
N11	-0.741516	0.434451	-2.037209
H12	-0.740262	-0.437036	-2.585287
C13	-5.552033	0.664523	-2.354483
H14	-6.433602	1.117306	-1.910407
C15	-4.297941	1.245463	-2.155152
H16	-4.211969	2.147792	-1.554425
C17	-1.167125	1.968832	-3.822007
H18	-1.335505	1.248837	-4.635884
N19	0.259990	2.015122	-3.461159
C20	0.933889	1.942780	-1.055990
C21	1.294164	0.484133	-5.593335
C22	1.831902	-1.852269	-5.781904
H23	2.359571	-2.729922	-5.422421
C24	-1.815217	1.348805	-2.521630
H25	-1.917085	2.152052	-1.785134
C26	-3.150842	0.680770	-2.730280
C27	-1.748488	3.299469	-4.216515
C28	0.524771	1.150186	-2.299780
H29	1.308609	0.417682	-2.518745
C30	1.004341	-1.938537	-6.904754
C31	-4.531017	-1.062794	-3.706017
H32	-4.617662	-1.960738	-4.310333
C33	1.990486	-0.634972	-5.120373
H34	2.668688	-0.548036	-4.278956
C35	0.470171	0.416367	-6.723391
H36	-0.014096	1.311276	-7.099427
C37	0.333053	-0.807825	-7.379029
H38	-0.285638	-0.874063	-8.268678
C39	-2.893057	5.750133	-4.943136
H40	-3.335548	6.698591	-5.232158
C41	-1.856503	5.718644	-3.995979
H42	-1.496378	6.643457	-3.556837
C43	1.755125	3.065544	-1.077228
H44	2.140967	3.434921	-2.020047
C45	-2.793624	3.341133	-5.162807
H46	-3.146904	2.418606	-5.614631
C47	-3.361272	4.553130	-5.523834
H48	-4.159423	4.585750	-6.258597
C49	-1.290082	4.506755	-3.633746
H50	-0.475253	4.472428	-2.918721
C51	2.077481	3.670910	0.139978
H52	2.706214	4.556211	0.154193
S53	0.826923	2.417425	4.955567
O54	2.004898	2.297456	5.805642
C55	-0.128092	-2.735506	3.933135
H56	-0.707991	-1.997037	4.483310
O57	0.450095	3.649565	4.259228
C58	0.390400	-5.059694	3.503128
H59	0.225894	-6.112909	3.710509
N60	-0.080321	-0.112374	2.215941
H61	-0.920190	-0.418339	2.714782
C62	1.342866	-4.672830	2.558781
H63	1.914878	-5.421864	2.020071
C64	1.562609	-3.318933	2.304388
H65	2.299268	-3.024314	1.563494
C66	1.552619	-0.058507	3.991693
H67	0.974977	-0.444160	4.842151
N68	1.122630	1.309428	3.660839
C69	-0.596155	1.807614	5.848106
C70	-2.975767	1.774066	6.195860
H71	-3.971175	2.127039	5.944333
C72	1.107670	-0.880080	2.717469
H73	1.892676	-0.786359	1.961612
C74	0.830226	-2.337750	2.986291
C75	3.020504	-0.190933	4.300618
C76	-2.797220	0.864012	7.241861
C77	-0.348095	-4.087915	4.187577
H78	-1.091020	-4.384430	4.921514
C79	-1.873201	2.256575	5.489959
H80	-1.992025	3.004618	4.713237
C81	-0.399776	0.912622	6.907304
H82	0.604623	0.635025	7.209108
C83	-1.514567	0.439489	7.600597
H84	-1.378875	-0.240969	8.435594
C85	5.747246	-0.520928	4.850340
H86	6.802552	-0.650055	5.070579
C87	5.332632	0.485023	3.963564
H88	6.067471	1.136583	3.501764
C89	3.446895	-1.200699	5.187033
H90	2.713017	-1.847297	5.659520
C91	4.795912	-1.365791	5.460487
H92	5.123507	-2.138731	6.148424
C93	3.983768	0.648609	3.688468
H94	3.651288	1.434447	3.019072
C95	0.808912	1.994369	1.285945
C96	0.199997	1.311630	2.515245
H97	-0.738735	1.818676	2.764180
C98	1.597317	3.140167	1.340093
H99	1.812093	3.604375	2.295139
S100	0.113682	-2.969680	-1.609642
O101	0.374468	-1.938445	-0.475294
O102	-0.629585	-4.127712	-1.133391
F103	1.894212	-4.316439	-2.984314
F104	2.394777	-4.072119	-0.877511
C105	1.873629	-3.482839	-1.951839
F106	2.591935	-2.388709	-2.247140
O107	-0.336319	-2.280926	-2.835340
O108	-2.786368	-1.273795	2.117581
C109	-3.413256	-1.675781	0.084950
H110	-2.889229	-2.570688	-0.259140
C111	-3.984434	-1.803715	1.494490
H112	-4.813729	-1.101881	1.643068
H113	0.893909	-2.887082	-7.421498
H114	-3.658755	0.502709	7.795303
H115	-4.075215	-1.281310	-0.687048
C116	-4.317062	-3.146606	2.069000
C117	-5.551927	-3.341417	2.707187
C118	-3.406778	-4.215155	1.982623
C119	-5.886748	-4.589977	3.230226
H120	-6.254638	-2.515393	2.784394
C121	-3.744275	-5.461296	2.506900
H122	-2.442066	-4.076790	1.503160
C123	-4.983158	-5.650944	3.129211
H124	-6.848583	-4.735704	3.712261
H125	-3.044783	-6.287822	2.425182
H126	-5.243714	-6.624943	3.532862

Fe(III)_styrene-INT3-quartet:

Fe1	-0.310930	-0.394337	-0.267875
S2	1.623573	2.564957	-4.813550
N3	0.648269	1.460845	-0.074886
O4	-2.064411	-0.569625	-0.002436
O5	1.018211	3.594477	-5.650418
C6	-2.558838	-0.866976	-4.010498
H7	-1.589601	-1.126038	-4.429678
O8	2.833747	2.778386	-4.016676
C9	-4.919666	-1.360778	-3.801557
H10	-5.775503	-1.980050	-4.052969
N11	-0.338304	0.421661	-2.316527
H12	-0.161856	-0.424787	-2.876437
C13	-5.077697	-0.251828	-2.966343
H14	-6.057290	-0.003707	-2.568368
C15	-3.976185	0.543125	-2.646931
H16	-4.101974	1.404759	-1.995760
C17	-0.954222	1.947183	-4.053996
H18	-0.943749	1.259103	-4.911491
N19	0.419080	2.235668	-3.607603
C20	1.048193	2.108600	-1.187874
C21	1.813992	1.070567	-5.771932
C22	2.832578	-1.084991	-6.085795
H23	3.527227	-1.854760	-5.765442
C24	-1.544862	1.141412	-2.827965
H25	-1.842719	1.864094	-2.062696
C26	-2.707594	0.243621	-3.163394
C27	-1.756267	3.168398	-4.413778
C28	0.796208	1.352685	-2.492528
H29	1.693608	0.772211	-2.727830
C30	2.066965	-1.264237	-7.241306
C31	-3.657967	-1.667541	-4.319888
H32	-3.530081	-2.527861	-4.969711
C33	2.717867	0.090304	-5.343937

H34	3.342545	0.258789	-4.473873
C35	1.050436	0.911895	-6.935119
H36	0.401068	1.711483	-7.275500
C37	1.185920	-0.267171	-7.669278
H38	0.615491	-0.398828	-8.583525
C39	-3.309935	5.403123	-5.074153
H40	-3.911629	6.267442	-5.338444
C41	-2.307242	5.517126	-4.098463
H42	-2.130417	6.470951	-3.612003
C43	1.710641	3.328511	-1.108901
H44	2.056018	3.813788	-2.013923
C45	-2.769355	3.062661	-5.388852
H46	-2.939783	2.112538	-5.886891
C47	-3.539115	4.167412	-5.717398
H48	-4.313421	4.088926	-6.473918
C49	-1.538646	4.412029	-3.768221
H50	-0.747796	4.492502	-3.030621
C51	1.937663	3.876830	0.155640
H52	2.443484	4.833256	0.248298
S53	0.941329	2.140432	4.816513
O54	2.204352	2.197917	5.543243
C55	0.107918	-2.942666	3.482297
H56	-0.537486	-2.231277	3.992822
O57	0.316481	3.312782	4.197486
C58	0.726767	-5.244356	3.053592
H59	0.571047	-6.305856	3.220822
N60	0.186673	-0.283455	1.910203
H61	-0.672211	-0.643942	2.352333
C62	1.749573	-4.811262	2.207873
H63	2.386142	-5.533471	1.706487
C64	1.952620	-3.446844	1.999528
H65	2.741893	-3.116998	1.331948
C66	1.780102	-0.240821	3.723260
H67	1.224842	-0.696902	4.553880
N68	1.275682	1.115590	3.459681
C69	-0.264310	1.304756	5.835562
C70	-2.554270	0.835368	6.392318
H71	-3.615791	0.975326	6.214661
C72	1.385998	-1.028421	2.408883
H73	2.186383	-0.893011	1.676906
C74	1.133224	-2.499974	2.627611
C75	3.253684	-0.309674	4.027026
C76	-2.119148	0.021192	7.441690
C77	-0.093525	-4.306449	3.690271
H78	-0.881819	-4.638397	4.359767
C79	-1.627883	1.488962	5.580198
H80	-1.954902	2.156743	4.791176
C81	0.187596	0.503120	6.891291
H82	1.248954	0.424742	7.100882
C83	-0.754118	-0.141323	7.693946
H84	-0.421450	-0.752370	8.527342
C85	5.995971	-0.519738	4.559541
H86	7.057102	-0.603844	4.773564
C87	5.524964	0.513891	3.735809
H88	6.221275	1.233245	3.316993
C89	3.736673	-1.346571	4.850541
H90	3.040594	-2.060516	5.281512
C91	5.093477	-1.452480	5.115464
H92	5.465248	-2.246949	5.754768
C93	4.168549	0.618483	3.468789
H94	3.790719	1.424937	2.850053
C95	0.884683	1.968028	1.149933
C96	0.349828	1.132967	2.316391
H97	-0.629577	1.530578	2.602879
C98	1.523423	3.195829	1.302066
H99	1.669093	3.609773	2.292267
S100	1.153783	-2.750205	-1.932276
O101	0.864707	-1.855155	-0.684403
O102	0.928764	-4.155923	-1.657573
F103	3.437886	-3.039764	-3.188362
F104	3.626847	-2.982680	-1.020309
C105	2.994150	-2.472292	-2.074340
F106	3.235534	-1.147117	-2.126129
O107	0.586911	-2.131190	-3.144194
O108	-2.542877	-0.537104	2.791616
C109	-3.031772	-1.424387	0.568572
H110	-2.591657	-2.412227	0.750061
C111	-3.543911	-0.799761	1.878679
H112	-4.099164	0.123798	1.646069
H113	2.169839	-2.177401	-7.819623
H114	-2.847104	-0.473826	8.077485
H115	-3.861777	-1.536612	-0.140908
C116	-4.453200	-1.719103	2.699408
C117	-5.710599	-1.263617	3.130572
C118	-4.005302	-2.999318	3.078460
C119	-6.538923	-2.105117	3.865533
H120	-6.045728	-0.265430	2.863172
C121	-4.839124	-3.836055	3.817636
H122	-3.016569	-3.341416	2.789341
C123	-6.104760	-3.392769	4.210255
H124	-7.524850	-1.764861	4.167398
H125	-4.502957	-4.831851	4.090279
H126	-6.753551	-4.045313	4.786837

Fe(III)_styrene-Pr-quartet:

Fe1	-0.465171	-0.676472	-0.366718
S2	1.513957	2.406251	-4.747263
N3	0.278657	1.254392	-0.076012
O4	-2.181117	-1.877836	-0.347969
O5	0.952152	3.444357	-5.603033
C6	-2.722737	-1.058342	-4.141421
H7	-1.739000	-1.318955	-4.525157
O8	2.676298	2.613873	-3.881036
C9	-5.090650	-1.551379	-4.013259
H10	-5.937065	-2.172567	-4.290936
N11	-0.575173	0.224545	-2.387541
H12	-0.354470	-0.588815	-2.978050
C13	-5.278625	-0.434369	-3.197104
H14	-6.271657	-0.182120	-2.837022
C15	-4.189129	0.365677	-2.847590
H16	-4.341732	1.238550	-2.216809
C17	-1.104773	1.773532	-4.129264
H18	-1.055316	1.091372	-4.990622
N19	0.245773	2.053013	-3.613496
C20	0.738520	1.911831	-1.158172
C21	1.764961	0.925796	-5.713467
C22	2.798087	-1.227373	-5.993537
H23	3.461717	-2.008009	-5.635366
C24	-1.748114	0.956140	-2.936673
H25	-2.070600	1.679070	-2.180676
C26	-2.902770	0.062319	-3.313457
C27	-1.887175	2.997862	-4.513452
C28	0.563090	1.163767	-2.482775
H29	1.475219	0.588882	-2.672743
C30	2.119511	-1.380786	-7.205438
C31	-3.810550	-1.862438	-4.482517
H32	-3.659828	-2.726247	-5.123217
C33	2.632127	-0.066231	-5.239603
H34	3.190994	0.080502	-4.322238
C35	1.086325	0.791812	-6.931044
H36	0.464401	1.600037	-7.300849
C37	1.273418	-0.372612	-7.676621
H38	0.771034	-0.484523	-8.632517
C39	-3.408368	5.238418	-5.226004
H40	-3.995818	6.106674	-5.508867
C41	-2.468615	5.335309	-4.186992
H42	-2.327410	6.279670	-3.671108
C43	1.391886	3.132785	-1.030793
H44	1.787880	3.628541	-1.909117
C45	-2.837554	2.909371	-5.552346
H46	-2.970018	1.969519	-6.080776
C47	-3.591213	4.017803	-5.906361
H48	-4.315309	3.951620	-6.712186
C49	-1.716983	4.226529	-3.830486
H50	-0.974992	4.295349	-3.042373
C51	1.546746	3.665487	0.251388
H52	2.049177	4.619049	0.383746
S53	0.372221	1.907820	4.802426
O54	1.665107	2.037957	5.463397
C55	-0.686602	-3.231448	3.229584
H56	-1.372417	-2.534474	3.705232
O57	-0.307571	3.038888	4.161395
C58	-0.061668	-5.518365	2.731726
H59	-0.248200	-6.584327	2.822846
N60	-0.416747	-0.484849	1.839619

H61	-1.308252	-0.793763	2.249623
C62	1.045262	-5.059759	2.015460
H63	1.718493	-5.765515	1.538878
C64	1.287081	-3.689872	1.904321
H65	2.139235	-3.340173	1.329956
C66	1.036151	-0.569070	3.761549
H67	0.368508	-1.004474	4.517652
N68	0.652391	0.822738	3.480441
C69	-0.759505	1.120764	5.939978
C70	-2.999940	0.775931	6.736607
H71	-4.067112	0.959158	6.660830
C72	0.720202	-1.287457	2.393138
H73	1.579022	-1.134968	1.733676
C74	0.424685	-2.763507	2.506805
C75	2.464749	-0.753470	4.200120
C76	-2.494998	-0.009589	7.777001
C77	-0.928167	-4.601175	3.335622
H78	-1.787707	-4.954570	3.897958
C79	-2.133060	1.348538	5.805959
H80	-2.505687	1.995395	5.019702
C81	-0.237099	0.347688	6.983719
H82	0.835820	0.233458	7.095052
C83	-1.119419	-0.222958	7.901226
H84	-0.730350	-0.812165	8.725898
C85	5.121150	-1.197695	4.968645
H86	6.149151	-1.371673	5.271747
C87	4.811991	-0.125414	4.118666
H88	5.599975	0.533971	3.769182
C89	2.784937	-1.829043	5.052288
H90	1.996136	-2.485418	5.409136
C91	4.100532	-2.051337	5.433185
H92	4.346121	-2.878169	6.092149
C93	3.497556	0.094954	3.734017
H94	3.245783	0.933255	3.093777
C95	0.429293	1.752050	1.164449
C96	-0.204466	0.914620	2.282193
H97	-1.176122	1.354413	2.530177
C98	1.061261	2.977233	1.365419
H99	1.147198	3.388621	2.363203
S100	1.008471	-2.914070	-2.094080
O101	0.925148	-1.980913	-0.865364
O102	0.432926	-4.229181	-1.820919
F103	3.152352	-3.842969	-3.281939
F104	3.340151	-3.651150	-1.118784
C105	2.857222	-3.093084	-2.227226
F106	3.394624	-1.874618	-2.380647
O107	0.592060	-2.207946	-3.323409
O108	-3.027896	-0.763193	3.113758
C109	-2.429630	-3.062291	-0.555528
H110	-1.649947	-3.767981	-0.875520
C111	-4.223031	-0.537646	2.918737
H112	-4.528733	0.066370	2.040223
H113	2.262083	-2.282877	-7.792716
H114	-3.174539	-0.439511	8.506968
H115	-3.458230	-3.426270	-0.424387
C116	-5.321890	-1.001005	3.760198
C117	-5.083141	-1.780111	4.909377
C118	-6.639352	-0.658380	3.406019
C119	-6.152205	-2.209079	5.685772
H120	-4.061180	-2.031018	5.174564
C121	-7.707810	-1.088900	4.187981
H122	-6.819132	-0.054179	2.519527
C123	-7.462686	-1.864192	5.325284
H124	-5.976939	-2.812503	6.571353
H125	-8.725214	-0.824546	3.917496
H126	-8.294941	-2.202273	5.935856