Supporting Information

UV-Visible Spectral Analysis for the Characterization of Titanium(IV)-4-(2-Pyridylazo)resorcinol Complex as a Reagent for Determining Hydrogen Peroxide

Kiyoko Takamura* and Takatoshi Matsumoto**

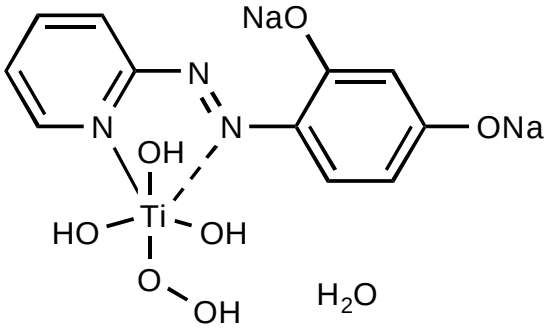
*Tokyo University of Pharmacy and Life Sciences,
1432-1, Horinouchi, Hachioji, Tokyo 192-0392, Japan
**Institute of Multidisciplinary Research for Advanced Materials, Tohoku University,
2-1-1, Katahira, Sendai 980-8577, Japan

Index

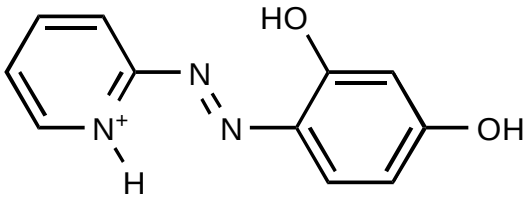
Table 1 Results of elementary analysis and mass spectrometry obtained for the colored species in the Ti(IV)-PAR-H_2O_2 system

	Calculated values	Observed values
Elemental analysis	32.30% C, 3.20% H, 10.27% N	32.75% C, 3.0% H, 10.2% N
Mass spectrometry(m/z)	216.07675	216

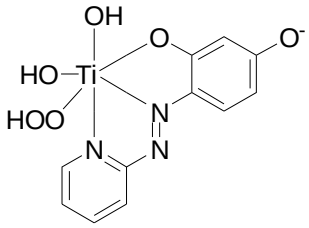
The Structure estimated from elemental analysis results

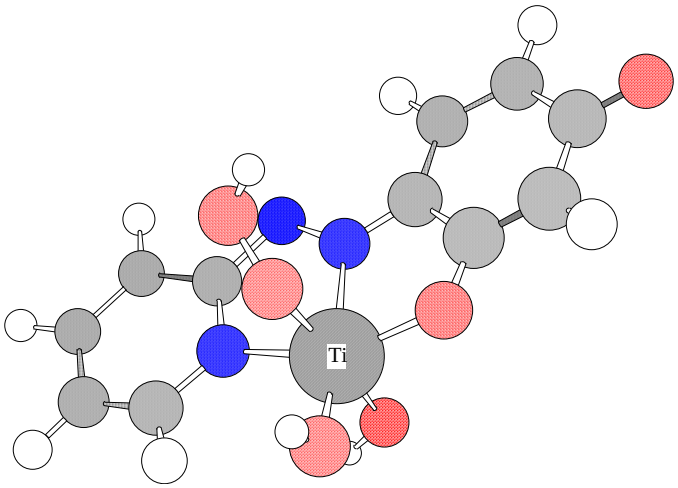


The structure estimated from mass spectrometry results



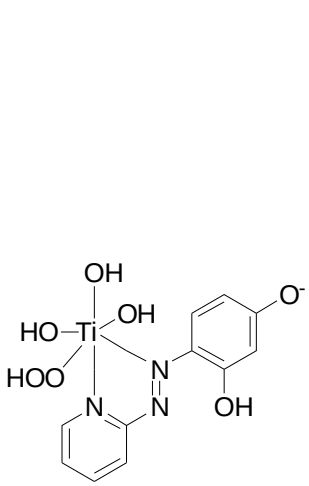
The species I to show the absorption peak at 508 nm in the previous paper (in Fig.3).

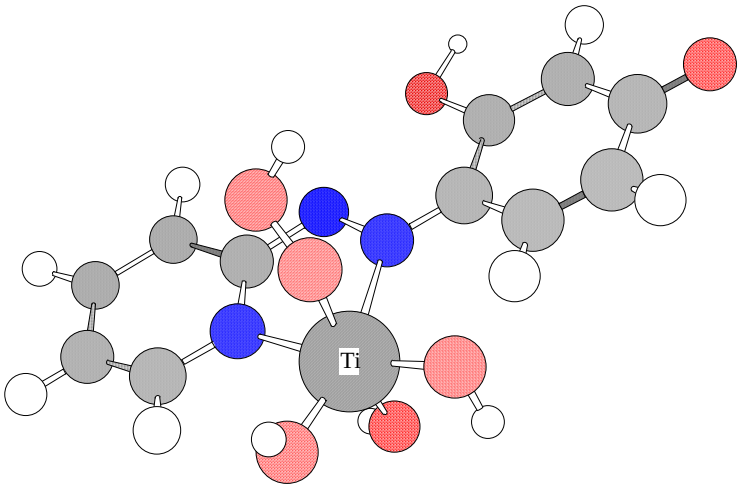




Atom	X	Y	Z	Atom	X	Y	Z
C	0.000000	0.000000	0.000000	H	-0.911934	0.003602	-0.577856
C	0.000000	0.000000	1.348887	H	-0.935337	0.001042	1.897833
C	1.229917	0.000000	2.062669	H	1.247059	0.003702	3.140046
C	2.383526	-0.002068	1.345027	H	3.352295	-0.003206	1.838731
N	2.441388	-0.012396	-0.024538	H	5.911153	0.064888	-5.421070
C	1.250078	0.002385	-0.727747	H	1.833344	0.008552	-7.047183
N	1.203963	-0.000384	-2.097787	H	0.906985	-0.007901	-4.756191
N	2.538381	0.033310	-2.526528	Ti	4.232621	0.022173	-1.188934
C	2.869930	0.029418	-3.784746	O	5.592817	0.171903	0.000558
C	4.357882	0.044836	-3.994623	H	5.863398	1.085620	0.233244
C	4.847697	0.055071	-5.248387	O	4.190400	-1.796787	-1.133276
C	3.968199	0.046954	-6.441932	H	3.686318	-2.283094	-0.448725
C	2.474529	0.019597	-6.174155	O	4.092336	1.923897	-1.075558
C	1.972603	0.010152	-4.951630	O	2.865577	2.536244	-1.357118
O	5.092236	0.046402	-2.870592	H	3.135259	3.228612	-2.031014
O	4.388433	0.059771	-7.603090				

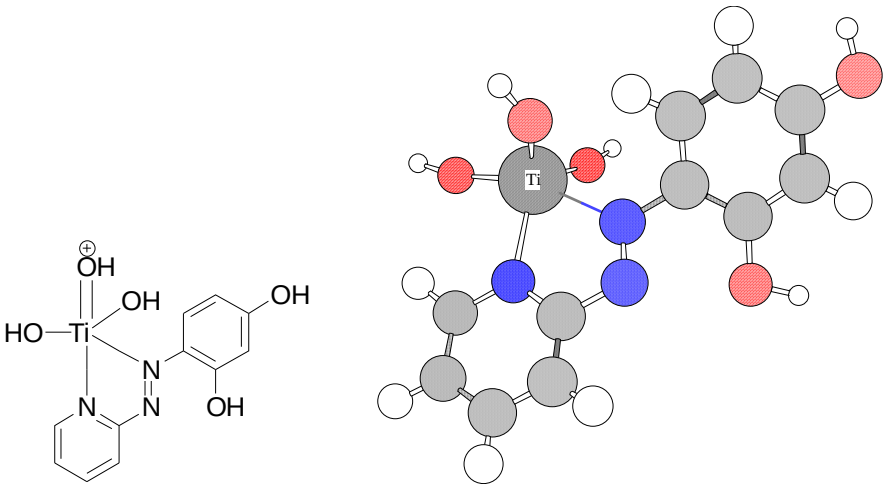
The species II based on the crystal structure found in CSD in this work (in Fig.3)..





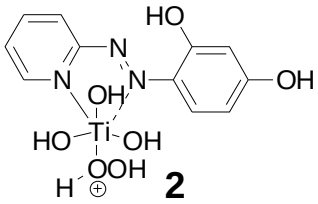
Atom	X	Y	Z	Atom	X	Y	Z
C	0.000000	0.000000	0.000000	H	-0.935325	-0.000794	1.902225
C	0.000000	0.000000	1.353380	H	1.247101	-0.000465	3.139793
C	1.227110	0.000000	2.062005	H	3.363769	-0.004475	1.810399
C	2.382781	0.000897	1.341114	H	0.697889	0.075219	-6.888901
N	2.427244	-0.002664	-0.025812	H	5.026942	0.284391	-6.332818
C	1.246902	0.003990	-0.718950	H	4.693441	0.171928	-3.892347
N	1.183027	-0.004601	-2.098291	H	-0.503634	-0.064592	-5.170877
N	2.457522	0.043673	-2.635029	Ti	4.252795	0.003160	-1.154030
C	2.527084	0.073525	-3.964367	O	5.221754	-0.014371	0.394593
C	1.368358	0.042837	-4.905156	H	5.674946	0.838037	0.577500
C	1.554036	0.101646	-6.229608	O	4.065194	-1.808651	-1.299007
C	2.892925	0.199555	-6.873286	H	3.220088	-2.254434	-1.085196
C	4.034944	0.218290	-5.908270	O	5.606680	0.073327	-2.401923
C	3.855860	0.158874	-4.597362	H	6.147611	-0.746277	-2.409883
O	0.085080	-0.057224	-4.372610	O	4.085131	1.874612	-1.281793
O	3.038680	0.257390	-8.098009	O	2.854144	2.521084	-1.149247
H	-0.910837	0.000879	-0.579724	H	2.849539	3.111181	-1.960041

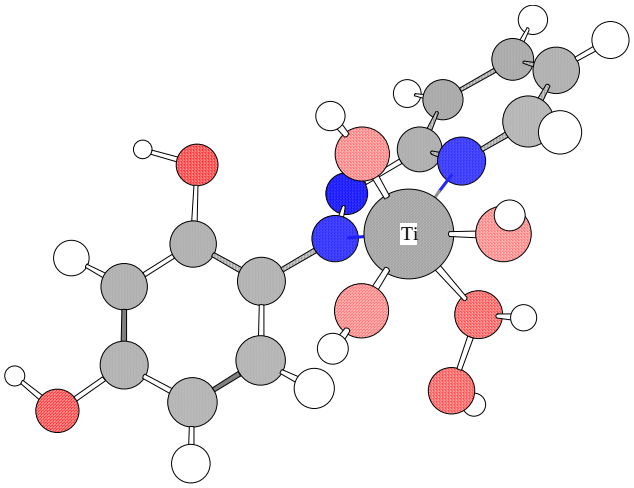
The precursor Ti-PAR (**3**) (in Fig.6)



Atom	X	Y	Z	Atom	X	Y	Z
C	0.000000	0.000000	0.000000	Ti	4.220192	-0.037051	-1.151247
C	0.000000	0.000000	1.394531	O	5.131881	-0.018452	0.291065
C	1.210863	0.000000	2.073101	O	4.676647	1.368668	-1.991437
C	2.395156	0.000613	1.346686	O	4.654919	-1.554289	-1.899928
N	2.418512	0.001021	-0.009274	H	-0.915626	0.001002	-0.579646
C	1.217283	-0.001931	-0.656410	H	-0.939138	0.000682	1.941398
N	1.230214	-0.001439	-2.124806	H	1.249510	0.001100	3.155310
N	2.431502	-0.078843	-2.562247	H	3.367758	0.001190	1.833093
C	2.542784	-0.034942	-4.017794	H	1.108340	1.217756	-6.833581
C	1.616958	0.668748	-4.821353	H	4.604156	-1.233015	-6.433346
C	1.797108	0.677548	-6.199415	H	4.305752	-1.234580	-3.968492
C	2.862599	-0.008324	-6.782776	H	0.112683	1.829262	-4.939038
C	3.779678	-0.702621	-5.978135	H	3.751378	-0.487194	-8.404188
C	3.616753	-0.700172	-4.613186	H	5.832482	0.112549	0.946835
O	0.590427	1.365389	-4.208476	H	5.135272	2.100737	-2.429685
O	2.956298	0.047072	-8.159361	H	5.312049	-2.253629	-1.738732

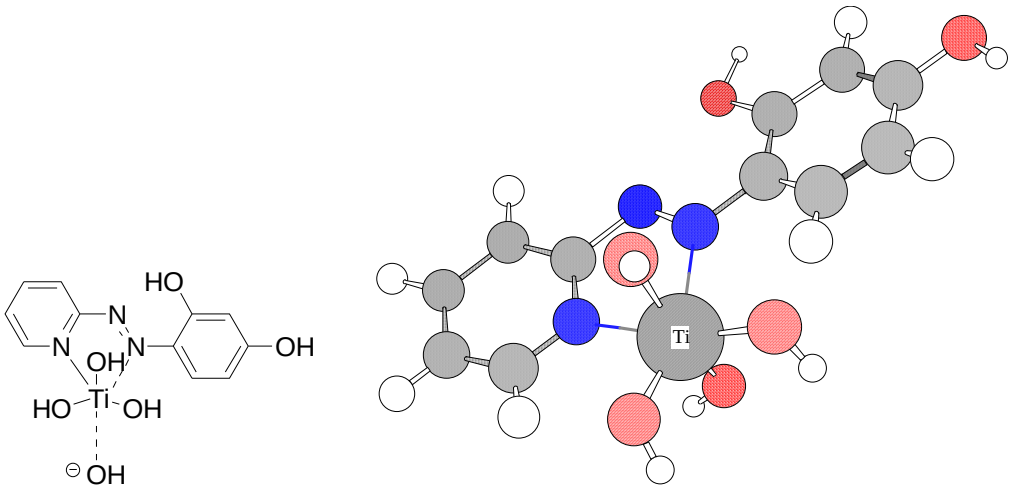
The species (**2**) when hydrogen peroxide approaches to the Ti atom of the Ti-PAR complex (**3**) (in Fig.7).





Atom	X	Y	Z	Atom	X	Y	Z
C	0.000000	0.000000	0.000000	H	1.245413	0.000885	3.155280
C	0.000000	0.000000	1.396071	H	3.374528	-0.001901	1.826168
C	1.208242	0.000000	2.072777	H	1.206495	-1.561800	-6.727137
C	2.398230	-0.004192	1.345050	H	4.160324	1.543596	-6.579541
N	2.416858	-0.005227	-0.002749	H	4.013286	1.551428	-4.098271
C	1.220566	-0.002698	-0.648221	H	0.447060	-2.293091	-4.754305
N	1.253922	0.007840	-2.118495	H	2.199545	-0.634711	-8.541758
N	2.455046	0.047671	-2.559586	Ti	4.234587	-0.203072	-1.227235
C	2.521512	0.016450	-4.029644	O	5.164751	0.252659	0.262256
C	1.714858	-0.867281	-4.763651	H	5.849534	-0.336808	0.631825
C	1.815304	-0.875605	-6.154364	O	4.070186	-1.896295	-1.155842
C	2.689629	-0.007893	-6.802516	H	4.113953	-2.859587	-1.241865
C	3.490114	0.875550	-6.057711	O	5.336140	0.062734	-2.497543
C	3.406475	0.873854	-4.687066	H	6.013707	0.094834	-3.187067
O	0.880399	-1.729152	-4.068502	O	3.999795	1.923592	-1.015871
O	2.826954	0.037049	-8.177422	O	4.369177	2.746642	-2.083376
H	-0.916372	0.001057	-0.578520	H	4.686535	2.065364	-0.307703
H	-0.938841	0.000788	1.941610	H	3.725229	3.509659	-1.974026

The species when hydroxyl ion approaches to the Ti atom of the Ti-PAR complex (**3**) (in Fig.8).



Atom	X	Y	Z	Atom	X	Y	Z
C	0.000000	0.000000	0.000000	H	-0.936427	0.003446	1.933767
C	0.000000	0.000000	1.386782	H	1.247122	0.005932	3.146753
C	1.210959	0.000000	2.065648	H	3.374261	0.006904	1.805622
C	2.392232	-0.004025	1.336912	H	0.633804	-0.127740	-6.961203
N	2.409023	-0.013062	-0.014059	H	4.837550	0.486447	-6.450319
C	1.221552	-0.001455	-0.664317	H	4.545671	0.369419	-3.959901
N	1.203192	0.009462	-2.134515	H	-0.552417	-0.374740	-5.163782
N	2.386007	0.058326	-2.622935	H	3.785908	0.386164	-8.440137
C	2.433895	0.083777	-4.083658	Ti	4.283226	0.149986	-1.190327
C	1.305825	-0.067805	-4.925370	O	5.230280	0.243962	0.347671
C	1.482972	-0.012375	-6.303484	H	5.911171	-0.442723	0.506869
C	2.747095	0.191284	-6.852727	O	3.749576	1.905242	-1.267133
C	3.858545	0.334105	-6.018930	H	4.495605	2.538658	-1.195897
C	3.695565	0.277348	-4.651366	O	5.525832	0.275528	-2.526546
O	0.047648	-0.281754	-4.382232	H	6.111015	-0.504482	-2.629638
O	2.830015	0.236215	-8.237380	O	4.158798	-1.666941	-1.369750
H	-0.914690	0.005069	-0.578080	H	3.605963	-2.226655	-0.787124