Supplementary Materials: Cr (III) Removal Capacity in Aqueous Solution in Relation to the Functional Groups Present in the Orange Peel (Citrus Sinensis)

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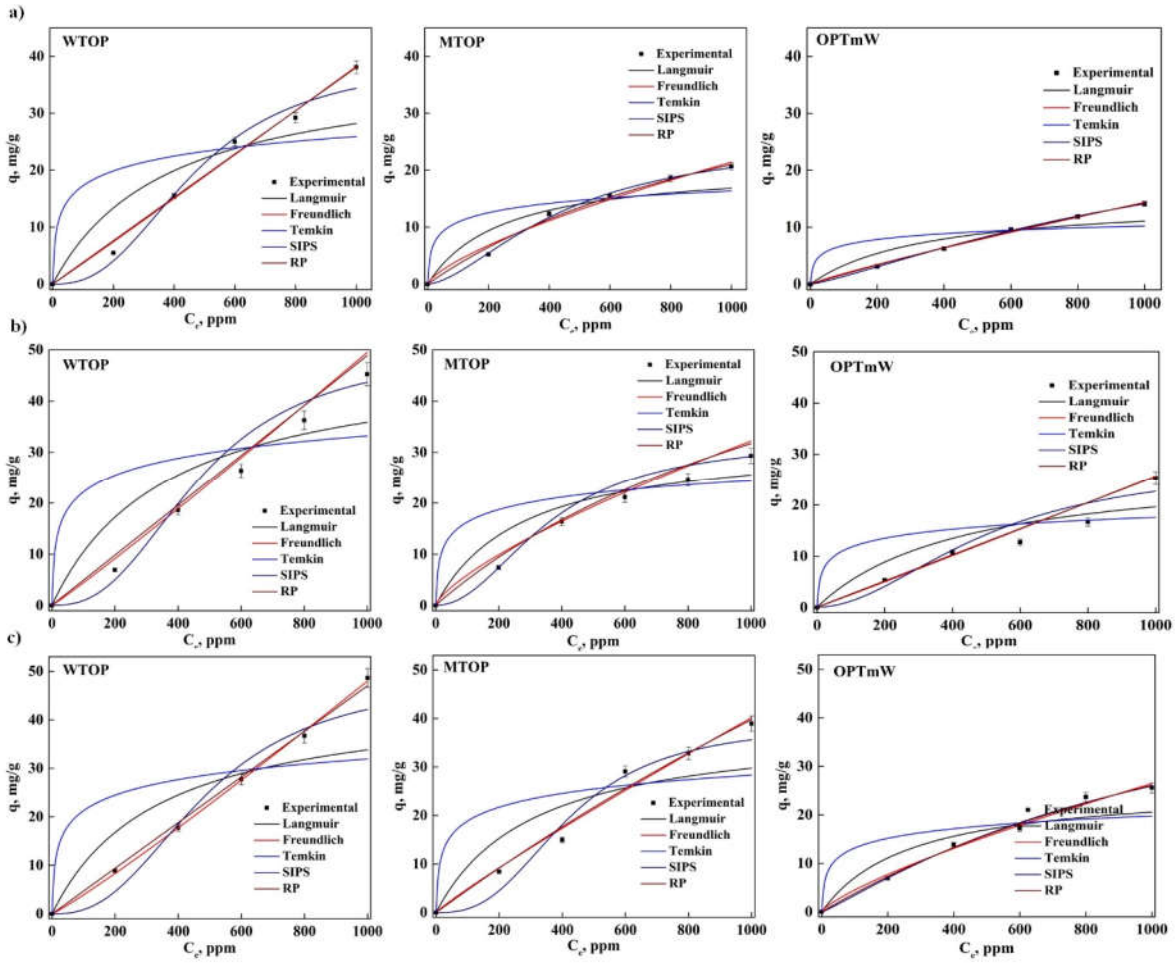

Figure S1. Adjustment of experimental data with the adsorption isotherms of WTOP, MTOP and OPTmW with different pH, a) 0.91, b) 1.78 y c) 2.72.

Table S1. Kinetic data of Cr (III) removal using WTOP.

Model	Parameter	4 g/L			8 g/L			12 g/L			16 g/L			20 g/L		
		0.91	**1.78**	**2.72**	**0.91**	**1.78**	**2.72**	**0.91**	**1.78**	**2.72**	**0.91**	**1.78**	**2.72**	**0.91**	**1.78**	**2.72**
PFO	q_{max}	35.26	46.09	57.83	49.58	30.22	32.79	28.05	23.78	27.83	15.77	19.11	21.60	13.85	21.28	16.50
	k_1	0.262	0.392	0.343	0.071	0.604	0.973	0.096	0.309	0.457	0.115	0.237	0.364	0.079	0.124	0.432
	R^2	0.915	0.989	0.989	0.991	0.969	0.946	0.984	0.992	0.981	0.996	0.988	0.983	0.984	0.988	0.977
	Δq, %	3.132	0.663	3.329	34.71	1.317	2.798	20.92	1.501	4.381	16.56	3.812	1.104	31.56	15.411	2.68
PSO	q_{max}	40.22	46.00	54.01	50.00	32.00	34.01	25.00	22.01	24.01	11.55	18.01	20.01	8.003	15.01	14.01
	k_2	0.009	0.019	0.016	0.002	0.038	0.071	0.007	0.039	0.054	0.030	0.030	0.054	0.003	0.029	0.146
	R^2	0.862	0.930	0.899	0.978	0.979	0.961	0.953	0.904	0.943	0.920	0.920	0.921	0.849	0.850	0.805
	Δq, %	1.396	0.592	0.607	35.32	0.693	1.506	14.80	1.251	1.416	2.676	1.548	5.368	3.339	0.446	3.244
Elovich	α	16.08	43.53	49.09	9.673	35.69	38.69	7.284	17.80	36.40	4.637	10.31	21.41	2.858	6.596	16.30
	β	0.061	0.074	0.057	0.094	0.112	0.093	0.141	0.138	0.156	0.228	0.161	0.162	0.293	0.162	0.197
	R^2	0.972	0.975	0.976	0.966	0.961	0.994	0.967	0.988	0.995	0.981	0.989	0.992	0.974	0.973	0.951
	Δq, %	0.548	0.605	2.405	0.613	0.100	0.373	1.456	1.109	0.476	0.561	1.062	0.394	0.543	0.073	1.506
ID	k_{id}	11.47	15.80	19.78	7.147	11.19	13.51	5.105	7.674	9.201	3.207	5.634	7.556	2.181	4.552	6.035
	R^2	0.944	0.928	0.928	0.927	0.868	0.820	0.945	0.970	0.958	0.960	0.979	0.982	0.910	0.950	0.903
	Δq, %	1.399	4.653	7.794	2.622	5.475	5.453	2.166	3.185	4.038	1.130	2.062	3.028	1.177	0.162	6.153
ED	k_{ext}	0.032	0.058	0.082	0.042	0.094	0.132	0.045	0.099	0.136	0.036	0.096	0.159	0.030	0.097	0.163
	R^2	0.975	0.692	0.842	0.987	0.576	0.569	0.975	0.867	0.827	0.973	0.829	0.812	0.975	0.853	0.846
	Δq, %	3.101	9.030	18.06	2.086	8.860	10.16	2.353	5.206	11.01	3.874	13.34	5.080	4.285	10.35	17.54

Table S2. Kinetic data of Cr (III) removal using MTOP

Model	Parameter	4 g/L			8 g/L			12 g/L			16 g/L			20 g/L		
		0.91	**1.78**	**2.72**	**0.91**	**1.78**	**2.72**	**0.91**	**1.78**	**2.72**	**0.91**	**1.78**	**2.72**	**0.91**	**1.78**	**2.72**
PFO	q_{max}	25.02	36.29	45.06	56.28	31.81	31.06	23.33	28.83	30.17	9.212	14.50	16.00	8.536	11.43	12.06
	k_1	0.321	0.191	0.250	0.055	0.152	0.260	0.137	0.154	0.126	0.430	0.381	0.516	0.329	0.336	0.257
	R^2	0.997	0.997	0.975	0.994	0.999	0.893	0.996	0.998	0.986	0.962	0.996	0.861	0.990	0.964	0.853
	Δq, %	2.248	7.453	0.385	68.78	11.99	1.886	18.46	17.65	24.22	1.623	11.61	1.133	2.615	11.61	24.34
PSO	q_{max}	24.01	30.01	42.69	20.01	35.01	32.69	18.01	23.02	19.69	10.01	13.02	15.69	8.905	10.03	11.69
	k_2	0.030	0.017	0.012	0.021	0.022	0.012	0.014	0.013	0.022	0.071	0.081	0.022	0.101	0.109	0.040
	R^2	0.941	0.907	0.876	0.836	0.875	0.800	0.954	0.944	0.868	0.967	0.879	0.737	0.930	0.882	0.712
	Δq, %	0.628	0.041	0.150	1.979	16.75	0.160	5.633	6.961	11.10	1.490	9.563	0.319	4.834	9.563	24.67
Elovich	α	19.40	17.98	21.79	9.498	12.90	14.03	8.992	10.42	8.992	12.25	12.46	6.259	7.367	11.33	5.314
	β	0.129	0.094	0.054	0.117	0.113	0.061	0.170	0.137	0.111	0.409	0.220	0.108	0.398	0.320	0.139
	R^2	0.999	0.989	0.988	0.972	0.985	0.969	0.976	0.985	0.996	0.986	0.985	0.981	0.991	0.976	0.967
	Δq, %	0.179	0.784	0.036	0.442	0.977	0.102	1.783	0.566	1.152	0.492	2.623	0.542	0.086	2.623	23.89
ID	k_{id}	8.541	9.730	14.16	6.301	7.546	10.25	5.168	6.165	6.232	3.416	5.074	4.791	3.227	36.88	4.009
	R^2	0.994	0.980	0.857	0.909	0.965	0.877	0.964	0.960	0.826	0.980	0.953	0.801	0.986	0.982	0.832
	Δq, %	1.470	0.353	0.173	3.525	1.101	14.49	5.858	0.787	2.106	0.727	4.532	5.852	6.084	4.532	25.16
ED	k_{ext}	0.030	0.034	0.057	0.049	0.058	0.091	0.062	0.076	0.081	0.052	0.086	0.084	0.056	0.080	0.089
	R^2	0.847	0.835	0.979	0.894	0.876	0.977	0.885	0.882	0.982	0.765	0.822	0.942	0.862	0.837	0.958
	Δq, %	4.777	4.918	0.350	1.231	3.529	12.38	2.245	3.398	0.935	4.811	8.661	1.516	6.236	8.661	23.97

Table S3. Kinetic data of Cr (III) removal using OPTmW

Model	Parameter	4 g/L			8 g/L			12 g/L			16 g/L			20 g/L		
		0.91	**1.78**	**2.72**	**0.91**	**1.78**	**2.72**	**0.91**	**1.78**	**2.72**	**0.91**	**1.78**	**2.72**	**0.91**	**1.78**	**2.72**
PPO	q_{max}	15.69	24.63	39.51	10.95	19.52	30.60	8.156	16.86	23.94	8.626	15.08	13.16	9.919	13.94	11.58
	k_1	0.544	0.246	0.207	0.240	0.343	0.183	0.619	0.346	0.150	0.296	0.172	0.260	0.171	0.170	0.263
	R^2	0.980	0.996	0.989	0.979	0.999	0.954	0.987	0.994	0.992	0.986	0.993	0.902	0.995	0.993	0.901
	Δq, %	0.309	4.772	12.34	2.099	1.871	8.286	0.244	2.138	20.97	4.018	12.26	0.827	14.84	8.853	0.667
PSO	q_{max}	15.69	25.01	31.01	10.69	25.72	25.01	8.690	16.83	15.01	6.690	12.01	14.01	7.000	10.01	10.01
	k_2	0.081	0.018	0.020	0.043	0.012	0.017	0.129	0.048	0.044	0.204	0.039	0.028	0.089	0.059	0.066
	R^2	0.956	0.963	0.868	0.945	0.998	0.802	0.981	0.914	0.817	0.824	0.889	0.814	0.847	0.841	0.710
	Δq, %	0.321	5.486	0.911	1.762	15.44	0.672	2.933	2.044	2.066	6.048	1.483	1.779	1.545	2.372	6.089
Elovich	α	28.01	15.41	17.61	7.312	15.56	11.27	17.82	12.92	8.263	6.841	6.515	6.007	4.163	5.860	5.277
	β	0.253	0.135	0.072	0.323	0.156	0.079	0.510	0.184	0.132	0.398	0.222	0.147	0.332	0.237	0.163
	R^2	0.996	0.992	0.995	0.971	0.998	0.973	0.995	0.988	0.998	0.986	0.984	0.965	0.996	0.989	0.975
	Δq, %	0.726	0.161	0.532	0.179	0.714	0.031	0.202	0.023	0.227	0.157	0.564	1.078	0.044	0.004	0.456
ID	k_{id}	6.117	7.434	11.09	3.304	6.812	8.125	3.245	5.739	5.551	2.839	3.823	4.339	3.504	3.503	3.840
	R^2	0.954	0.991	0.957	0.987	0.993	0.947	0.923	0.960	0.944	0.995	0.956	0.970	0.953	0.952	0.946
	Δq, %	4.534	1.147	0.730	0.213	4.620	10.38	6.110	12.10	0.419	1.564	1.288	4.103	20.80	0.195	3.749
ED	k_{ext}	0.021	0.025	0.043	0.023	0.049	0.068	0.034	0.068	0.070	0.042	0.059	0.074	0.048	0.071	0.084
	R^2	0.604	0.876	0.934	0.888	0.813	0.992	0.553	0.833	0.979	0.870	0.961	0.985	0.966	0.959	0.983
	Δq, %	9.610	7.523	6.566	11.02	8.811	9.180	11.02	9.034	4.064	6.560	5.763	1.271	0.094	5.383	0.631

Table S4. Linear regression of the adjust of the data that are part of the external transport process.

WTOP									
	0.91			**1.78**			**2.72**		
C_{ads}, g/L	$k_{externa}$	**Ln (C_0)**	**R^2**	$k_{externa}$	**Ln (C_0)**	**R^2**	$k_{externa}$	**Ln (C_0)**	**R^2**
4	-0.0339	6.3910	0.9827	-0.1097	6.3908	0.9977	-0.0394	6.3962	0.9995
8	-0.0456	6.3964	0.9827	-0.1545	6.2227	0.9964	-0.0447	6.3955	0.9887
12	-0.0498	6.3903	0.9827	-0.1292	6.1918	0.9599	-0.0576	6.3982	0.9994
16	-0.0399	6.3908	0.9827	-0.1428	6.2222	0.9965	-0.0411	6.3921	0.9814
20	-0.0231	6.3966	0.9827	-0.0875	6.1981	0.9526	-0-0306	6.3973	0.9998
MTOP									
4	-0.0484	6.2105	0.9905	-0.0397	6.2046	0.9772	-0.0632	6.2121	0.9992
8	-0.0523	6.2206	0.99830	-0.0638	6.2073	0.9963	-0.0898	6.2297	0.9870
12	-0.0720	6.2091	0.9923	-0.0829	6.2115	0.9992	-0.0937	6.2328	0.9827
16	-0.0626	6.1975	0.9091	-0.1144	6.1959	0.9894	-0.0745	6.2295	0.9763
20	-0.0768	6.1955	0.9234	-0.0839	6.1950	0.9616	-0.0475	6.2071	0.9663
OPTmW									
4	-0.0271	6.2098	0.9900	-0.0303	6.2037	0.9645	-0.0501	6.2147	0.9881
8	-0.0220	6.2044	0.9403	-0.0642	6.1957	0.9759	-0.0647	6.2177	0.9983
12	-0.0494	6.2042	0.9738	-0.0961	6.2057	0.9966	-0.0785	6.2217	0.9950
16	-0.0516	6.2128	0.9825	-0.0666	6.2114	0.9990	-0.0658	6.2145	0.9986
20	-0.0573	6.2172	0.9957	-0.0784	6.2140	0.9984	-0.0767	6.2210	0.9961

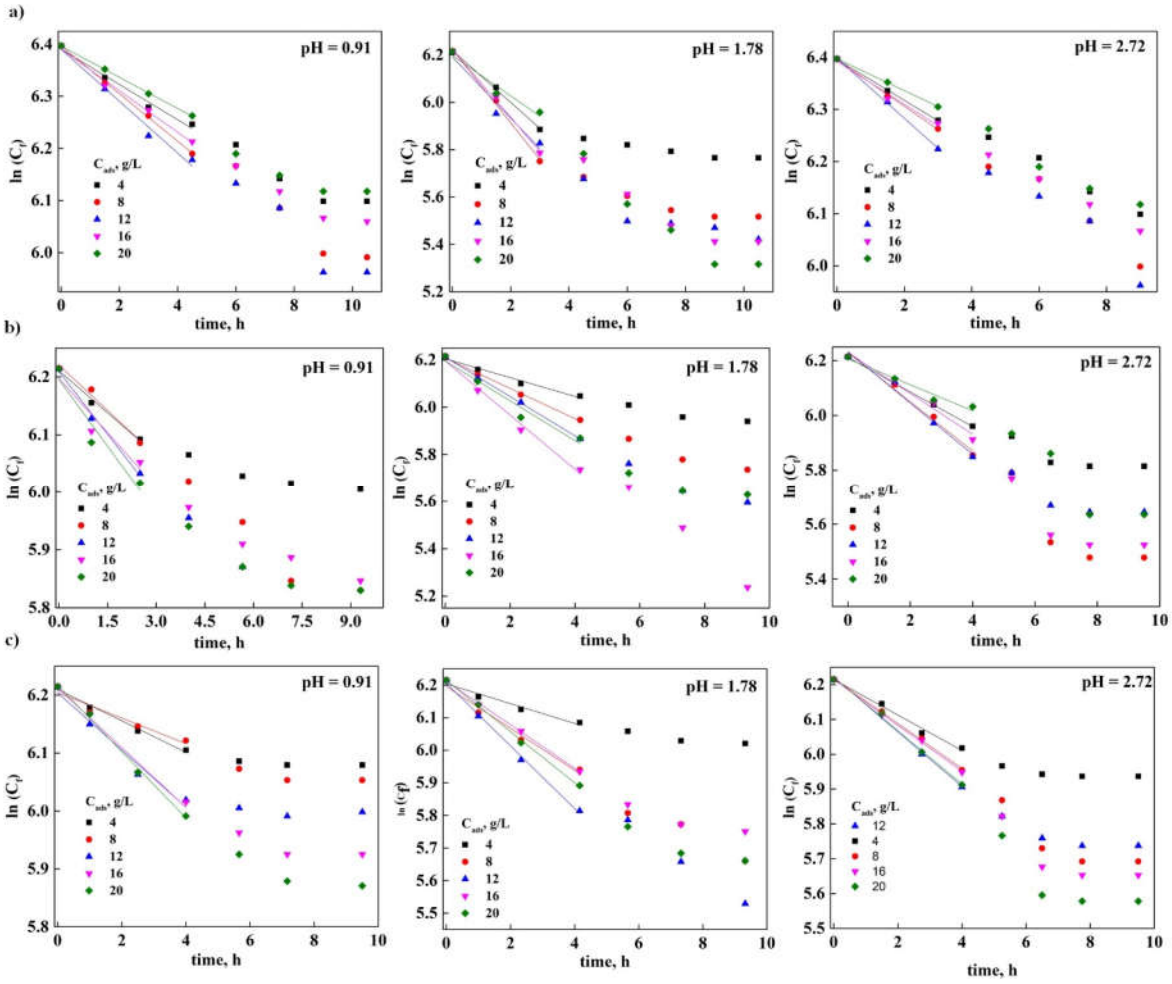

Figure S2. Analysis of internal mass transport with different pH a) WTOP, b) MTOP y c) OPTmW.

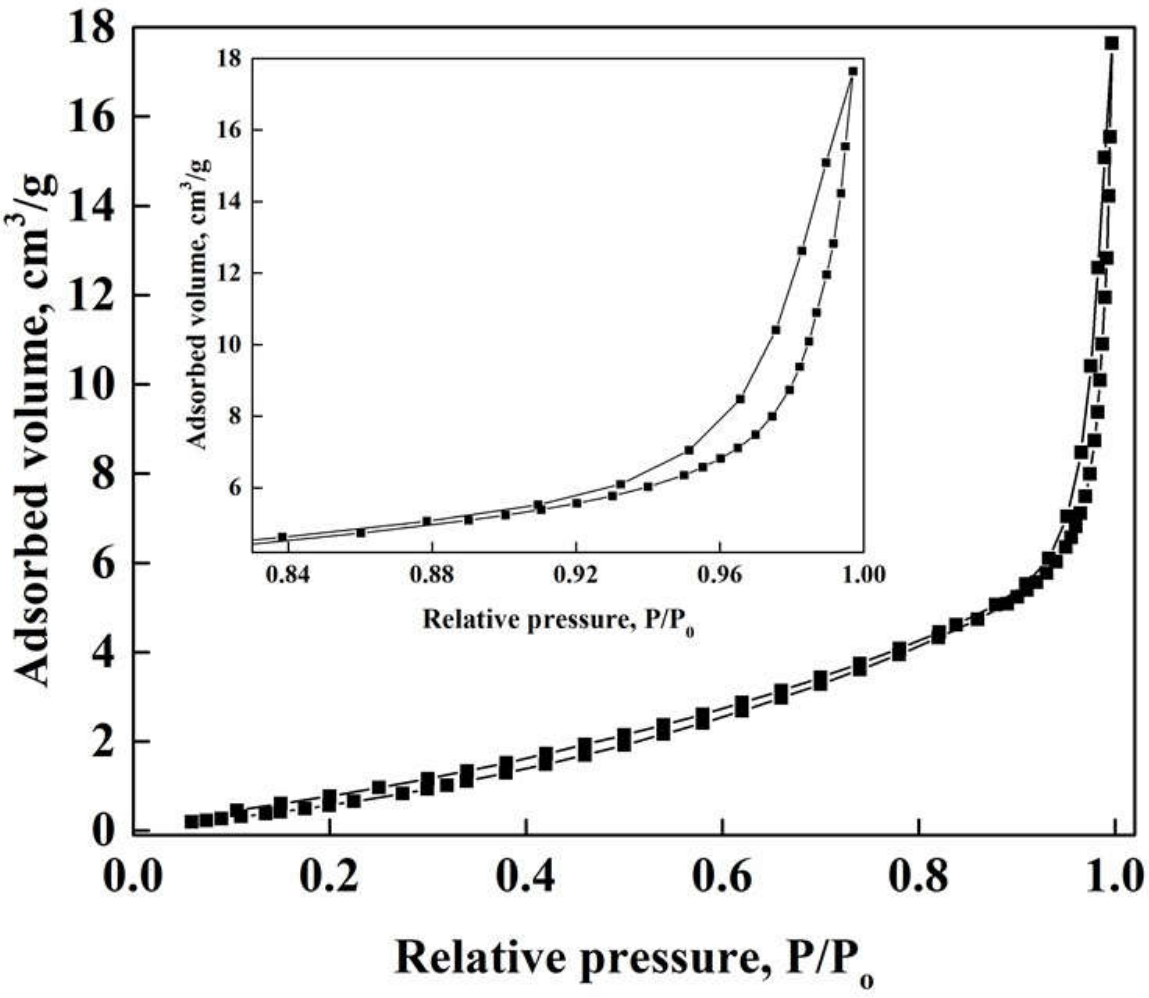

Figure S3. Adsorption-Desorption Isotherm of WTOP.

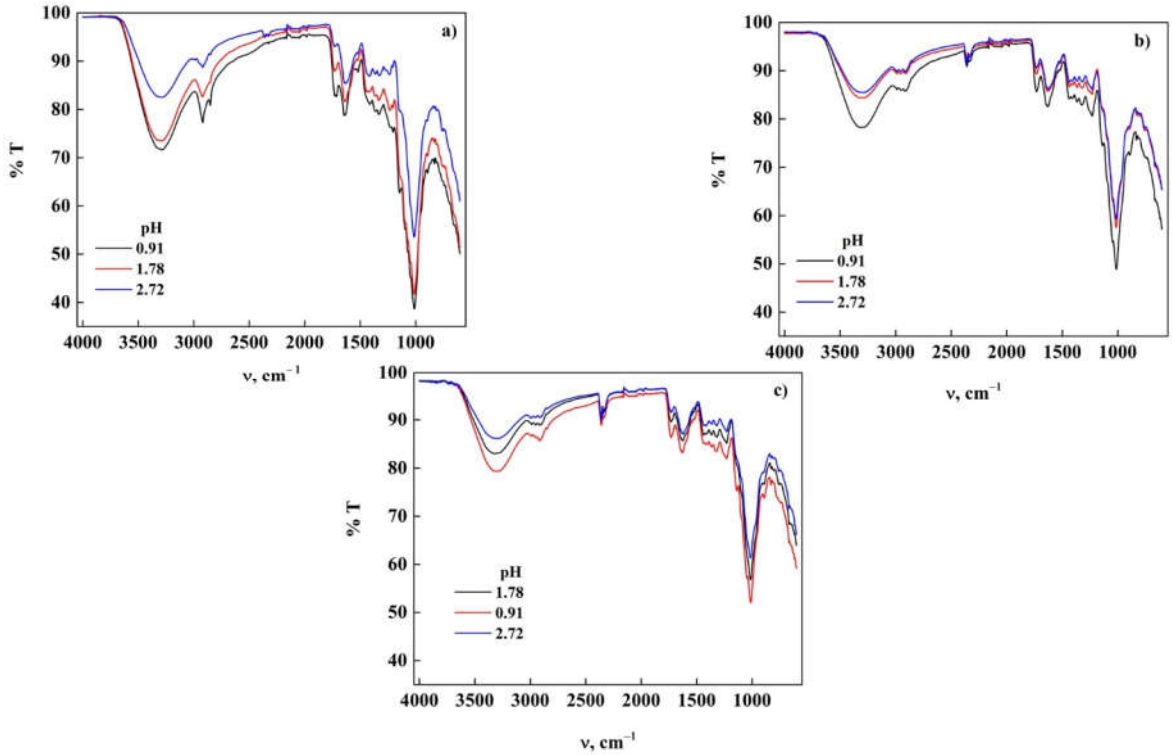

Figure S4. FT-IR spectra of OP in Cr (III) adsorption with different treatments: a) WTOP, b) MTOP y c) OPTmW.