

Supplementary information

Organic sulfur and organic matter redox processes contribute to electron flow in anoxic incubations of peat

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The following information is also included in a separate CSV file to facilitate data import into *Excel*, *R*, *Matlab* or other mathematical programs.

Table S1. XANES spectra of sulfur-bearing reference materials covering a broad range of sulfur oxidation states

For method details and measurement conditions, please refer to *Methods* section of manuscript

CAS number	(own reference material)	(own reference material)	7704-34-9	69-78-3	52-90-4	132-65-0	1193-82-4	67-71-0	2386-57-4	926-39-6	7757-82-6
Energy (eV)	FeS	Pyrite	Elemental S	5,5-Dithiobis (2-nitrobenzoic acid)	L-cysteine	Dibenzotriophene	Methyl phenyl sulfoxide	Dimethyl sulfone	Sodium Methanesulfonate	Sulfuric acid mono(2-aminoethyl) ester	Sodium sulfate
2406.428	0.00127	0.0338	0.0128	0.0314	0.0179	0.0944	0.0346	0.0318	0.1939812	0.00345	0.0106
2411.354	0.00398	0.029	0.0105	0.0257	0.0162	0.0805	0.0301	0.027	0.18163918	0.00427	0.00931
2416.4	0.00361	0.0247	0.00817	0.0199	0.0144	0.0663	0.0255	0.0222	0.16899855	0.00511	0.00797
2421.398	-0.00312	0.0199	0.00583	0.0142	0.0127	0.0523	0.021	0.0174	0.15647716	0.00595	0.00664
2426.401	0.00238	0.0185	0.00348	0.0084	0.0109	0.0382	0.0164	0.0126	0.14394551	0.00678	0.00532
2431.398	-0.00101	0.0139	0.00114	0.00265	0.0092	0.0242	0.0119	0.00784	0.13142763	0.00761	0.00399
2433.398	0.00241	0.0137	0.000198	-0.000169	0.00831	0.0184	0.0102	0.0066	0.12713396	0.00768	0.00346
2435.402	0.000426	0.0113	-0.000591	-0.00129	0.00697	0.0171	0.00811	0.00525	0.11691552	0.00616	0.00291
2437.391	-0.000911	0.00962	0.0000565	-0.00132	0.00615	0.0146	0.00746	0.00427	0.1131135	0.00694	0.00201
2439.401	-0.000567	0.0098	-0.00161	0.00258	0.00435	0.011	0.00718	0.00533	0.10696508	0.00436	0.00135
2441.39	-0.000663	0.00765	0.00189	-0.00444	0.00329	0.0122	0.00731	0.00376	0.0941	0.00514	0.00175
2443.399	-0.00192	0.00386	0.00182	-0.00681	0.00295	0.0067	0.00465	0.00225	0.0841	0.00193	0.00061
2445.39	-0.00169	0.00429	-0.00342	-0.0127	0.00113	0.00521	0.00352	0.00276	0.0773	0.00249	0.000522
2447.396	0.0013	0.00187	0.000563	0.0178	0.000305	0.00513	0.00241	0.00122	0.0716	0.00258	0.00078
2449.396	-0.00117	0.00183	0.00172	0.00613	-0.000393	0.000517	0.00215	0.00217	0.0626	0.0017	-0.00028
2451.392	-0.00226	-0.00079	-0.00109	0.0316	-0.00129	0.000527	0.00126	0.00235	0.0605	0.000125	-0.000429
2453.403	-0.00138	-0.000558	-0.000225	-0.0132	-0.00158	-0.00234	0.00278	0.00216	0.0512	0.00134	-0.000441
2455.394	-0.000416	-0.000836	0.0072	-0.0147	-0.00164	-0.00279	0.00156	0.00158	0.043	0.00207	-0.000531
2457.394	-0.000641	-0.00262	-0.000081	-0.0139	-0.0017	-0.00258	0.00106	0.0024	0.0412	0.00172	0.000369
2459.405	0.00611	0.00298	0.000461	-0.0119	-0.00113	-0.0042	-0.000127	0.00295	0.032	0.00102	0.000443
2461.396	0.00822	0.00547	0.0019	-0.00695	-0.00309	-0.00437	-0.000738	-0.00145	0.0164	-0.000792	-0.000923
2461.599	0.00904	0.00402	0.0112	-0.0066	-0.00414	-0.00448	-0.00324	-0.00236	0.016	-0.0014	-0.000733
2461.794	0.00595	0.00498	0.019	-0.00627	-0.00591	-0.00795	-0.00851	-0.00486	0.0155	-0.00069	-0.000663
2462.001	0.0123	0.00631	0.00365	-0.00481	-0.00465	-0.00935	-0.00824	-0.00345	0.00977	-0.00157	-0.000522
2462.195	0.014	0.00581	0.00428	-0.00381	-0.00388	-0.0116	-0.0111	-0.000926	0.00394	-0.00313	-0.000111
2462.398	0.0147	0.00942	0.0122	-0.00444	-0.00142	-0.0146	-0.000138	-0.000694	0.00302	-0.00435	0.000131
2462.603	0.0156	0.00779	0.0111	-0.00588	-0.00218	-0.0109	-0.00123	-0.00125	0.00419	-0.00455	-0.000626
2462.791	0.0131	0.0124	0.0075	-0.00194	-0.00215	-0.0103	-0.00398	-0.00045	0.00497	-0.00295	0.000503
2463.002	0.0184	0.0107	0.00675	-0.00262	-0.0021	-0.0119	-0.00386	-0.00266	0.00721	-0.00354	0.000839
2463.201	0.015	0.0116	0.00938	-0.00328	-0.0022	-0.00838	-0.0066	-0.00385	0.00352	-0.0023	0.00129
2463.394	0.0228	0.0137	0.0105	-0.0019	-0.0018	-0.0062	-0.00472	-0.00392	0.000975	-0.0044	0.00326
2463.603	0.0217	0.013	0.00488	0.00000975	-0.000514	-0.00702	-0.00401	-0.00261	-0.00128	-0.00402	0.00332
2463.792	0.0233	0.0129	0.00415	0.000569	-0.00136	-0.00861	0.000521	-0.00225	-0.00423	-0.00421	0.00295
2463.999	0.0244	0.0164	0.0042	0.00224	-0.00183	-0.00854	0.0000838	-0.00111	-0.00165	-0.00394	0.00264

CAS number	(own reference material)	(own reference material)	7704-34-9	69-78-3	52-90-4	132-65-0	1193-82-4	67-71-0	2386-57-4	926-39-6	7757-82-6
Energy (eV)											
	FeS	Pyrite	Elemental S	5,5-Dithiobis (2-nitrobenzoic acid)	L-cysteine	Dibenzotriophene	Methyl phenyl sulfoxide	Dimethyl sulfone	Sodium Methane-sulfonate	Sulfuric acid mono(2-aminoethyl) ester	Sodium sulfate
2464.202	0.0265	0.0178	0.00662	0.00511	0.000215	-0.00753	-0.00219	-0.00279	-0.00365	-0.00342	0.00244
2464.39	0.0295	0.0192	0.0069	0.00385	0.000819	-0.00525	-0.00445	-0.00316	-0.00256	-0.00251	0.00272
2464.601	0.0304	0.0229	0.0088	0.00598	0.000183	-0.00751	-0.00143	-0.00173	-0.000241	-0.000214	0.0029
2464.803	0.0298	0.0255	0.0105	0.0174	0.00117	-0.00992	-0.0000588	-0.00312	-0.000129	-0.000259	0.00306
2464.993	0.0355	0.0247	0.00928	0.0119	0.0041	-0.0074	-0.00271	-0.000753	-0.000675	-0.000563	0.00397
2465.202	0.04	0.0287	0.0101	0.0138	0.00266	-0.00689	0.00191	-0.00308	0.00916	-0.000987	0.00306
2465.396	0.0411	0.0315	0.0133	0.0164	0.00511	-0.00548	0.00281	-0.000722	0.00509	-0.00044	0.00307
2465.598	0.0456	0.0351	0.0158	0.018	0.00748	-0.00483	0.001	0.00107	-0.00185	-0.000567	0.00493
2465.804	0.0526	0.0377	0.0195	0.0211	0.00614	-0.00551	0.00406	0.00116	-0.00696	-0.00237	0.00446
2465.991	0.058	0.0402	0.0211	0.0221	0.00704	-0.00313	0.0035	0.000944	-0.00765	-0.00211	0.00502
2466.202	0.0645	0.0441	0.0149	0.0282	0.00837	-0.000575	-0.00136	-0.000882	-0.00511	-0.00218	0.00464
2466.399	0.0757	0.0503	0.0163	0.0354	0.0107	-0.000581	-0.0033	-0.000859	-0.0052	-0.00251	0.00454
2466.595	0.0837	0.0586	0.0256	0.0368	0.0132	0.00122	-0.000669	-0.00049	-0.00671	-0.00184	0.00516
2466.802	0.0986	0.0601	0.0258	0.0361	0.0146	0.00394	0.00725	-0.000658	-0.00574	-0.00106	0.00592
2466.993	0.11738427	0.0648	0.0411	0.0395	0.0151	0.00538	0.00711	0.000141	-0.00421	-0.000872	0.00683
2467.198	0.15037783	0.0739	0.0396	0.0493	0.0156	0.00503	0.00676	0.00154	-0.00758	-0.000386	0.00726
2467.405	0.18722387	0.0831	0.0487	0.0494	0.0216	0.0116	0.00733	0.00186	-0.0141	0.000807	0.00748
2467.593	0.24880331	0.0922	0.0572	0.0574	0.0268	0.0204	0.00749	0.00224	-0.0131	-0.00044	0.00638
2467.801	0.35363205	0.11273865	0.0552	0.0673	0.0301	0.0236	0.00818	0.00323	-0.00458	0.000225	0.0076
2467.999	0.49555373	0.12900003	0.0456	0.0759	0.0309	0.0201	0.0114	0.00403	0.0016	0.000732	0.00835
2468.194	0.68966668	0.15156301	0.0846	0.0828	0.0321	0.0284	0.00867	0.005	-0.00313	0.000969	0.00811
2468.403	0.92794156	0.18351621	0.0815	0.0889	0.0377	0.0318	0.0145	0.0029	-0.00308	0.00256	0.00906
2468.594	1.1839382	0.21976477	0.0802	0.10005264	0.0403	0.032	0.0124	0.00261	-0.00501	0.00283	0.00887
2468.8	1.3860677	0.26556962	0.0986	0.11288551	0.0483	0.0323	0.012	0.00331	-0.00721	0.00219	0.00927
2469.005	1.4933546	0.32233965	0.11703685	0.12296836	0.0571	0.0353	0.0161	0.00383	-0.00892	0.00306	0.0104
2469.191	1.5287853	0.3847712	0.13350768	0.13334077	0.0637	0.0433	0.0205	0.00395	-0.0101	0.00549	0.0112
2469.401	1.4988098	0.46929462	0.16222087	0.15747473	0.0728	0.0541	0.0213	0.0085	-0.00961	0.00716	0.0106
2469.598	1.4396208	0.57922426	0.210155	0.17547096	0.0896	0.0593	0.0178	0.00917	-0.00407	0.0114	0.0104
2469.796	1.3286168	0.7238272	0.27347948	0.20229221	0.10755223	0.0677	0.0234	0.00803	-0.000754	0.0132	0.0113
2470.005	1.2148157	0.92568212	0.3733175	0.24736468	0.12491866	0.0819	0.039	0.00796	-0.00594	0.0159	0.0116
2470.193	1.0735897	1.1299246	0.51321183	0.30936425	0.14828572	0.0978	0.0394	0.00855	-0.00801	0.0255	0.0137
2470.401	0.9596956	1.348836	0.75770272	0.40951379	0.18930652	0.12237114	0.0368	0.00968	-0.00569	0.0342	0.015
2470.6	0.87449101	1.4954094	1.1141094	0.58170707	0.24446124	0.15793046	0.0406	0.0123	-0.0024	0.0436	0.0149
2470.793	0.8093827	1.574859	1.6642944	0.84733856	0.32427434	0.20475657	0.0507	0.0143	-0.00425	0.0525	0.0148
2471.003	0.75756523	1.5958608	2.419568	1.233782	0.46200304	0.2822427	0.0553	0.0173	-0.0102	0.0552	0.0169
2471.197	0.7252218	1.56911	3.0777293	1.6585653	0.65669207	0.42270257	0.0634	0.019	-0.00192	0.0525	0.0183
2471.398	0.68631364	1.5275547	3.3689824	2.1040925	0.89576571	0.70804772	0.0758	0.0205	0.00556	0.0505	0.0197
2471.603	0.67121475	1.4534654	3.524038	2.4698203	1.284303	1.1822188	0.0856	0.0271	0.00643	0.0476	0.0217
2471.791	0.66200845	1.3885422	3.471952	2.5757138	1.7100729	1.675835	0.10107051	0.0324	0.00195	0.0491	0.0226
2472.001	0.65713777	1.3175097	3.2298785	2.4507875	2.1929858	2.0582669	0.13338645	0.0369	0.0000178	0.0537	0.025

CAS number	(own reference material)	(own reference material)	7704-34-9	69-78-3	52-90-4	132-65-0	1193-82-4	67-71-0	2386-57-4	926-39-6	7757-82-6
Energy (eV)	FeS	Pyrite	Elemental S	5,5-Dithiobis (2-nitrobenzoic acid)	L-cysteine	Dibenzot-hiophene	Methyl phenyl sulfoxide	Dimethyl sulfone	Sodium Methane-sulfonate	Sulfuric acid mono(2-aminoethyl) ester	Sodium sulfate
2472.199	0.67434819	1.2534418	2.8896349	2.2214429	2.5364688	2.020832	0.16333901	0.0404	0.00179	0.0596	0.029
2472.395	0.70511996	1.1691569	2.5660764	1.997181	2.6597298	1.8899969	0.18363007	0.0397	0.00232	0.0673	0.0293
2472.604	0.75485589	1.0857216	2.2958951	1.8286222	2.5552123	2.1027328	0.19952592	0.0404	-0.00489	0.0751	0.0313
2472.795	0.80727873	1.0168165	2.0737876	1.7709293	2.3689271	2.5921224	0.21948523	0.0423	0.000301	0.0765	0.0319
2473	0.87198439	0.92577864	1.8267715	1.7938168	2.1690197	3.1733451	0.24333823	0.0437	0.00243	0.0794	0.0337
2473.203	0.92689058	0.84154101	1.5904103	1.9377895	1.9392077	3.4746012	0.27123286	0.0457	0.00864	0.0797	0.0362
2473.393	0.99590535	0.76903961	1.3918231	2.0818579	1.6962692	3.147856	0.31579384	0.0489	0.0117	0.0799	0.0378
2473.601	1.0516234	0.69686261	1.1835073	2.1869187	1.4114434	2.5702946	0.39826449	0.0511	0.0122	0.0805	0.04
2473.797	1.0998514	0.64451482	1.0255564	2.1334767	1.1583806	1.9397652	0.51035564	0.0544	0.0172	0.0809	0.0419
2473.998	1.1358517	0.61392879	0.91192106	1.9725568	1.0048697	1.5074296	0.67791107	0.0575	0.0122	0.0793	0.0444
2474.203	1.1828753	0.57468948	0.81010336	1.7550809	0.96318207	1.3142759	1.0603415	0.061	0.0192	0.0859	0.0478
2474.39	1.2096554	0.55119572	0.73405176	1.5529839	1.0090182	1.3293756	1.5945881	0.0677	0.0275	0.0865	0.051
2474.602	1.2512267	0.53468168	0.68121057	1.3646521	1.0733014	1.452966	2.4431598	0.0814	0.0342	0.0889	0.0557
2474.798	1.2703948	0.53056401	0.65538708	1.2346545	1.1422814	1.5579652	3.3491581	0.0962	0.0367	0.0938	0.0585
2474.996	1.2934284	0.53958093	0.62764306	1.0927071	1.1945569	1.5904342	4.0854271	0.11637023	0.0426	0.096	0.068
2475.203	1.3203083	0.55127429	0.62844507	0.96324789	1.2235697	1.4744545	4.4370761	0.13373787	0.0533	0.1001408	0.0721
2475.395	1.3228749	0.56928294	0.63318319	0.8571967	1.2422348	1.3013969	4.2994937	0.15515095	0.0628	0.10775459	0.0746
2475.599	1.3529782	0.59610883	0.64924246	0.79136288	1.2589777	1.1561856	3.8636837	0.18710477	0.0671	0.1193746	0.0786
2475.803	1.3609725	0.64162709	0.68136869	0.77468082	1.2706836	1.0592316	3.2129361	0.23816875	0.0853	0.13196219	0.0847
2475.992	1.361527	0.69196193	0.71843793	0.77296715	1.285874	0.9979162	2.6051968	0.32012341	0.0967	0.13602371	0.0872
2476.202	1.3729166	0.7441052	0.77081465	0.78449912	1.3056356	0.95955506	2.1027422	0.48553646	0.11759582	0.14247793	0.0936
2476.396	1.3746442	0.79965541	0.82726709	0.77965783	1.3262007	0.97640406	1.8745426	0.72220695	0.13638569	0.1481986	0.0965
2476.597	1.3761762	0.8382448	0.85630943	0.79159851	1.3559093	0.99263221	1.7435646	0.96200425	0.15125984	0.15199493	0.10240519
2476.803	1.3474268	0.87538069	0.9130295	0.80045095	1.3750325	1.0466929	1.6206549	0.97883155	0.16960713	0.15578153	0.11630846
2476.995	1.335272	0.90127498	0.99301032	0.79942039	1.387388	1.0908897	1.4977629	0.87065602	0.18716509	0.17175264	0.12655389
2477.2	1.3266721	0.92955122	1.0373816	0.82103652	1.3974236	1.1322346	1.384042	0.75285662	0.21866185	0.19147288	0.13635806
2477.401	1.3075306	0.95675896	1.068832	0.87276924	1.4033398	1.1676956	1.3118143	0.8453845	0.24888851	0.21955399	0.14874789
2477.595	1.3016073	0.97116181	1.0972677	0.89835079	1.4035914	1.1840385	1.2816984	1.0367743	0.29275545	0.24992344	0.16336155
2477.804	1.2796051	0.9939716	1.1524464	0.95133528	1.3954417	1.1781966	1.2754527	1.3093368	0.37737087	0.28519126	0.18086688
2477.992	1.2647137	1.0146791	1.1842604	1.0261286	1.3910246	1.1818067	1.2966015	1.5738982	0.48506078	0.32326193	0.20366
2478.199	1.2444746	1.03298	1.2079472	1.1411969	1.3862163	1.1952534	1.3079137	1.8930882	0.61522226	0.39477897	0.22825235
2478.401	1.2306766	1.0567191	1.2426073	1.2328214	1.3861892	1.2467715	1.3204909	2.3849009	0.77938433	0.48752458	0.25966347
2478.593	1.2207806	1.0828625	1.2652892	1.306381	1.3772583	1.2924449	1.3176101	3.0468215	1.0817881	0.6266943	0.29178179
2478.801	1.2042735	1.0876039	1.2811061	1.3774356	1.3540426	1.3268652	1.3233845	3.8972427	1.6122323	0.87907689	0.34017034
2478.992	1.2116686	1.1077065	1.2711991	1.4175908	1.3252388	1.3539381	1.3377005	4.7118574	2.2018345	1.2184038	0.40213114
2479.198	1.2014617	1.1172712	1.3048894	1.4442707	1.309793	1.4000964	1.3404073	5.4370703	2.9882095	1.6651286	0.48360392
2479.402	1.1806558	1.1377119	1.3141411	1.4555	1.2874162	1.4177061	1.3597583	5.763985	3.8141069	2.1650319	0.60032426
2479.591	1.1995473	1.155323	1.3164826	1.4714277	1.2668045	1.441949	1.3616674	5.638016	4.3759351	2.5941918	0.74657096
2479.801	1.1908669	1.1878003	1.3042426	1.4981845	1.2454849	1.454763	1.3613611	5.1799246	4.8164199	2.9192866	0.97080597
2479.999	1.1861586	1.223609	1.2734956	1.5182241	1.2136944	1.4586988	1.3576952	4.5066124	4.9636625	3.0464006	1.2787617

CAS number	(own reference material)	(own reference material)	7704-34-9	69-78-3	52-90-4	132-65-0	1193-82-4	67-71-0	2386-57-4	926-39-6	7757-82-6
Energy (eV)	FeS	Pyrite	Elemental S	5,5-Dithiobis (2-nitrobenzoic acid)	L-cysteine	Dibenzotriophene	Methyl phenyl sulfoxide	Dimethyl sulfone	Sodium Methane-sulfonate	Sulfuric acid mono(2-aminoethyl) ester	Sodium sulfate
2480.198	1.1627702	1.2580704	1.2354355	1.4917424	1.1897254	1.4760913	1.3425336	3.7638845	4.9264808	3.0610093	1.6829156
2480.403	1.1456828	1.3262988	1.224783	1.4731871	1.1701462	1.5092509	1.3069968	3.145917	4.7297434	3.0008812	2.3161903
2480.594	1.1399025	1.3831952	1.2085241	1.4787579	1.1537204	1.5424891	1.2871846	2.9198744	4.4004413	2.9268982	2.8999015
2480.8	1.1274773	1.4463666	1.1693758	1.4667223	1.1382418	1.5648255	1.2637526	2.7639558	3.8966796	2.8826076	3.6593374
2481	1.1057516	1.5127361	1.1300504	1.4381906	1.1158223	1.593158	1.2514796	2.5576481	3.4810117	3.0017217	4.2588372
2481.195	1.1080853	1.5562829	1.1197122	1.4152682	1.0983343	1.6138146	1.2371148	2.2798448	3.0601242	3.269509	4.7867976
2481.403	1.0886697	1.5789635	1.1191727	1.3838939	1.0831304	1.6062165	1.2176686	1.913442	2.6808358	3.6113235	5.2417727
2481.595	1.0819348	1.5698096	1.1017611	1.3610187	1.075068	1.5867644	1.2109893	1.608057	2.3757103	3.8437862	5.4641283
2481.799	1.0830811	1.551981	1.0737052	1.314165	1.0713099	1.5560899	1.1975861	1.37096	2.1889737	3.8591233	5.3699008
2482.002	1.0736118	1.5157029	1.0585052	1.2756744	1.0552238	1.5115158	1.179567	1.1902708	2.0170595	3.6086735	5.0215399
2482.193	1.065366	1.4642711	1.0460415	1.253264	1.0497263	1.4614812	1.1716507	1.0424572	1.8381766	3.2087907	4.4658324
2482.404	1.0502767	1.4048645	1.0352784	1.2144817	1.0519847	1.4183119	1.1656031	0.95216774	1.6416377	2.7831367	3.8367935
2482.596	1.0596771	1.3462982	1.0405955	1.1801031	1.048745	1.3767169	1.1560005	0.89014874	1.4990764	2.4664878	3.2342006
2482.8	1.0664342	1.2853993	1.011934	1.1521971	1.0434167	1.3238522	1.1433839	0.84985587	1.3922435	2.1668246	2.6708508
2483.002	1.0631268	1.2310351	1.0213397	1.1263915	1.0496837	1.2733492	1.1436803	0.8366806	1.3102596	1.9154407	2.1445712
2483.194	1.0522945	1.1918779	1.0088117	1.1129488	1.052883	1.2451979	1.1331824	0.83653718	1.2448642	1.7267803	1.7972823
2483.401	1.0720222	1.1573243	1.0522625	1.0945804	1.056858	1.2082134	1.1238016	0.84771637	1.205953	1.5545166	1.5010368
2483.597	1.0689392	1.1338479	1.0399111	1.0790299	1.0579884	1.1884145	1.1195034	0.85906602	1.1910867	1.4130715	1.2984655
2483.798	1.070203	1.1108796	1.0362051	1.0699937	1.0649307	1.1694385	1.1219138	0.87311831	1.1399909	1.2944931	1.166018
2484.004	1.0600996	1.0912971	1.0381346	1.0676792	1.0685951	1.1589457	1.124673	0.8931267	1.1591439	1.189114	1.048948
2484.191	1.0585799	1.0856542	1.0260967	1.0678012	1.0708031	1.1568155	1.1168606	0.92079503	1.1499973	1.1031861	0.97490065
2484.402	1.0777843	1.0827856	1.0526212	1.0571886	1.0780919	1.1396608	1.1207535	0.96414233	1.1256879	1.0157458	0.90242572
2484.595	1.0830763	1.0841552	1.060448	1.055096	1.0894652	1.1428432	1.1243958	0.98325436	1.1114729	0.93739625	0.86316075
2484.799	1.0786872	1.0803881	1.060832	1.0440282	1.081832	1.1572492	1.1119667	0.9901477	1.1200395	0.8924715	0.85757986
2485.003	1.0766377	1.073136	1.0737929	1.033541	1.0753794	1.1648964	1.1171109	0.9990711	1.1342268	0.85556031	0.86477279
2485.193	1.0766255	1.0722337	1.0833709	1.0331106	1.0810006	1.1677649	1.1316572	1.016634	1.1255981	0.81909475	0.87112628
2485.401	1.0823001	1.0734848	1.0805211	1.0283603	1.0839307	1.1858921	1.1323067	1.0416933	1.1451496	0.7841918	0.88154584
2485.598	1.0989878	1.0743112	1.0753201	1.0216372	1.0778726	1.1916703	1.1357513	1.0404973	1.1744995	0.76934505	0.90697929
2485.797	1.0924683	1.0642264	1.0767767	1.0167224	1.0724035	1.1919093	1.1181544	1.0360151	1.1927142	0.7552463	0.89880672
2486.002	1.0988833	1.0646246	1.0888909	1.0232484	1.079443	1.2014329	1.1244469	1.0369958	1.1977897	0.74470807	0.88758105
2486.192	1.1000901	1.0604622	1.102997	1.0188732	1.081068	1.2072319	1.1332056	1.0412087	1.2074443	0.73427321	0.88417944
2486.402	1.0905977	1.0572437	1.1073744	1.0185783	1.0778079	1.219478	1.1295965	1.045234	1.2183204	0.72782257	0.87681601
2486.597	1.0927379	1.0517059	1.094852	1.0128509	1.0712413	1.228741	1.1368075	1.0439055	1.2305694	0.72227889	0.87491183
2486.795	1.1042445	1.047145	1.1009234	1.0034962	1.0661643	1.2290347	1.1374351	1.0522811	1.262161	0.72125219	0.87672821
2487	1.0931964	1.0544531	1.1136666	1.0120256	1.0723127	1.2263388	1.1371508	1.0573534	1.2842932	0.72505349	0.88087784
2487.191	1.0914312	1.0476642	1.0743482	1.0062175	1.0667749	1.236577	1.1491875	1.0796639	1.2899123	0.72832112	0.88399854
2487.402	1.0886204	1.0521925	1.08647	1.0148886	1.0685426	1.2383809	1.1675702	1.1050562	1.3032326	0.73154494	0.88693599
2487.599	1.0822158	1.0475009	1.0890298	1.0231907	1.063137	1.2334675	1.1769301	1.1281615	1.3317735	0.74319537	0.89317092
2487.795	1.070306	1.0454028	1.0744565	1.0226061	1.0591643	1.239891	1.1815823	1.1542732	1.3225468	0.75595713	0.90836569
2488.003	1.0865501	1.0507432	1.0522493	1.0141771	1.0674741	1.2438856	1.194045	1.1877912	1.3183494	0.76924549	0.92788588

CAS number	(own reference material)	(own reference material)	7704-34-9	69-78-3	52-90-4	132-65-0	1193-82-4	67-71-0	2386-57-4	926-39-6	7757-82-6
Energy (eV)											
	FeS	Pyrite	Elemental S	5,5-Dithiobis (2-nitrobenzoic acid)	L-cysteine	Dibenzot- hiophene	Methyl phenyl sulfoxide	Dimethyl sulfone	Sodium Methane- sulfonate	Sulfuric acid mono(2- aminoethyl) ester	Sodium sulfate
2488.191	1.0808093	1.0461233	1.0576549	1.0117863	1.0701922	1.2341508	1.1825554	1.2185484	1.2983845	0.78284601	0.96273065
2488.4	1.0730727	1.048515	1.0631599	1.0026003	1.0612122	1.230012	1.1967005	1.2440097	1.2809264	0.80212762	1.0008285
2488.6	1.0690149	1.0560774	1.064469	1.014278	1.0590439	1.2352893	1.214156	1.2658704	1.2835042	0.82271473	1.0352052
2488.793	1.0630601	1.0602773	1.0900947	1.0275037	1.0572056	1.2194823	1.2107389	1.2847292	1.2972971	0.84297886	1.0757109
2489.003	1.0623977	1.0596907	1.0650369	1.0155777	1.0567115	1.2178917	1.2004717	1.3029451	1.2599504	0.86948495	1.126586
2489.191	1.0566599	1.0584315	1.0607409	1.0196918	1.061687	1.2161484	1.1980736	1.3185982	1.2478505	0.89347848	1.1630803
2489.401	1.0548745	1.0624095	1.0605229	1.033245	1.0560637	1.2229853	1.2110853	1.309098	1.2489218	0.91353897	1.1822991
2489.601	1.0587525	1.0646734	1.0518166	1.0435826	1.0560042	1.2181008	1.2172173	1.2947923	1.2431266	0.92343272	1.2041535
2489.794	1.0485873	1.0680366	1.0632567	1.0394867	1.0535614	1.1935818	1.2267412	1.2795465	1.2290257	0.93250158	1.2387632
2490.002	1.0483684	1.0702886	1.0739567	1.0418603	1.0478776	1.1856668	1.2274578	1.2682142	1.2307322	0.94830781	1.2825029
2490.192	1.0358665	1.077202	1.0658593	1.0387421	1.0421302	1.1687344	1.2207876	1.2637584	1.2273988	0.96651878	1.3291095
2490.399	1.0403338	1.0784173	1.0708877	1.0467136	1.0391942	1.1582933	1.2238433	1.2404903	1.2398216	0.98302751	1.3623693
2490.597	1.0447892	1.0896563	1.0758007	1.0562976	1.0396647	1.1577176	1.2093119	1.2338849	1.2746749	0.98567425	1.3638652
2490.795	1.036578	1.0806876	1.0796723	1.0454288	1.0383999	1.1587756	1.2125348	1.2192264	1.2912937	0.98905419	1.3434696
2491.003	1.034295	1.0749699	1.0707395	1.0456412	1.0331814	1.1432042	1.2158301	1.2102643	1.3144942	0.99591079	1.304114
2491.196	1.0345834	1.0934208	1.0564284	1.0452701	1.0323021	1.1380406	1.216518	1.2091341	1.3347493	1.0055834	1.251543
2491.403	1.0370268	1.0858426	1.0507308	1.0460634	1.0300415	1.1300448	1.2043812	1.2054467	1.3444449	1.0176815	1.205162
2491.601	1.0343668	1.0863914	1.044649	1.0463009	1.0242802	1.124193	1.1901137	1.2088647	1.3366885	1.0282003	1.1728628
2491.795	1.0238144	1.0867171	1.0368504	1.0470335	1.0176737	1.1144876	1.1889519	1.210342	1.353304	1.0323682	1.1471548
2492.003	1.0163861	1.0803725	1.0302389	1.0615558	1.0200011	1.1045709	1.180844	1.2046066	1.3571951	1.0454298	1.1285277
2492.195	1.0204103	1.0892615	1.065448	1.0663958	1.0195295	1.1034577	1.1724537	1.1980072	1.3613921	1.0581928	1.1224013
2492.4	1.0248162	1.078806	1.060881	1.0650082	1.0179039	1.1041498	1.1562542	1.1965784	1.3803672	1.0694646	1.1227129
2492.602	1.0139095	1.0874279	1.0547028	1.0609486	1.0159523	1.0970816	1.141228	1.1971302	1.4149421	1.0967437	1.1252368
2492.792	1.0129647	1.0865009	1.0403105	1.0603807	1.0140141	1.0968263	1.1342253	1.1988671	1.4254131	1.1130177	1.1298898
2493.001	1.0215015	1.076073	1.0439719	1.0662445	1.0113795	1.0968145	1.1181241	1.2067025	1.4598412	1.1236609	1.1384651
2493.193	1.0198216	1.0858819	1.0416758	1.0588388	1.0144834	1.0969899	1.1061405	1.2113115	1.4932887	1.1448758	1.1299108
2493.398	1.0190767	1.0837086	1.0296817	1.0440814	1.0101597	1.0938849	1.0973105	1.2277887	1.5135465	1.1691052	1.1385394
2493.599	1.027324	1.0839492	1.0496647	1.0503806	1.0044299	1.0797441	1.0894424	1.23093	1.5111991	1.1759047	1.1289524
2493.796	1.02317	1.0849434	1.0562528	1.0507438	1.0028439	1.0702047	1.0807576	1.226578	1.534671	1.1875934	1.114616
2494.001	1.0237279	1.0737881	1.05416	1.0519275	1.007794	1.0713309	1.0798525	1.2391608	1.5723074	1.2122384	1.106611
2494.193	1.0243851	1.0754357	1.0600501	1.0466937	1.0060335	1.066283	1.05013	1.2376145	1.5690708	1.2427365	1.1119227
2494.399	1.0177649	1.0685113	1.0170986	1.0399196	1.0044048	1.0610892	1.0294417	1.2506505	1.5824538	1.2510866	1.1312317
2494.6	1.0145315	1.0647838	1.0328796	1.0487167	0.99911141	1.0684851	1.0138396	1.2613607	1.5873938	1.2623918	1.1822002
2494.795	1.0212952	1.0705364	1.0485465	1.0455639	1.000944	1.0676954	1.0029391	1.2643308	1.5911856	1.2691863	1.2338524
2495	1.0309795	1.0699348	1.0317334	1.0366433	1.0053801	1.0594257	1.0110926	1.261581	1.5980186	1.2770525	1.287522
2495.191	1.0207031	1.06399	1.0255439	1.0346658	1.0074451	1.0479341	1.0206132	1.2720722	1.6017899	1.2881055	1.3535471
2495.402	1.0240671	1.0622145	1.0175464	1.0348847	1.0057864	1.0466784	1.0021618	1.2715726	1.609955	1.2900769	1.4245187
2495.596	1.0152218	1.0681303	1.0071001	1.0289501	1.0060717	1.057425	0.98286097	1.2748425	1.6325569	1.2929001	1.4948345
2495.798	1.0241988	1.0653639	1.0074549	1.0287049	1.0124898	1.0526048	0.9764999	1.2814486	1.6272696	1.297379	1.5908699
2496.003	1.0268616	1.0632816	1.0049249	1.0195829	1.0091588	1.0452448	0.97193278	1.2824451	1.5971078	1.3067976	1.6928218

CAS number	(own reference material)	(own reference material)	7704-34-9	69-78-3	52-90-4	132-65-0	1193-82-4	67-71-0	2386-57-4	926-39-6	7757-82-6
Energy (eV)											
	FeS	Pyrite	Elemental S	5,5-Dithiobis (2-nitrobenzoic acid)	L-cysteine	Dibenzot- hiophene	Methyl phenyl sulfoxide	Dimethyl sulfone	Sodium Methane- sulfonate	Sulfuric acid mono(2- aminoethyl) ester	Sodium sulfate
2496.194	1.0265624	1.0532367	1.0085056	1.0183084	1.0077999	1.0305984	0.96487965	1.2677605	1.5783911	1.3165412	1.7760546
2496.4	1.0269551	1.0582515	1.0131937	1.0111565	1.0095883	1.020929	0.95475242	1.2669457	1.5828835	1.3142209	1.8464443
2496.597	1.0212103	1.0556194	1.0033027	0.99147142	1.0098643	1.0208852	0.96448085	1.2694475	1.5976691	1.3117926	1.8955903
2496.799	1.0303729	1.055307	1.0156028	0.99424925	1.0081825	1.01663	0.96560046	1.265596	1.5738349	1.3151113	1.9349966
2497.003	1.0238912	1.0454751	1.0119125	1.0005483	1.0000468	1.013396	0.96142942	1.2699452	1.5408165	1.3195003	1.9697257
2497.189	1.0264876	1.0444051	1.009631	0.99453538	0.99722653	1.0150183	0.95557322	1.2647684	1.5387867	1.3190567	1.9938153
2497.401	1.0247971	1.0423828	1.003443	0.99100302	0.99849788	1.0278083	0.94880253	1.2536065	1.558549	1.3103774	1.9912615
2497.596	1.041052	1.0390624	0.9843421	1.0024828	0.99808162	1.0329207	0.94075175	1.2567141	1.5515494	1.3184349	1.9856686
2497.796	1.0228293	1.0394906	0.97783207	1.013936	1.0051815	1.0216642	0.92155212	1.2588521	1.5331959	1.3146039	1.9811739
2498.002	1.0420361	1.0320597	0.98280408	1.0006655	1.0041006	1.0082266	0.92921147	1.2594751	1.5234332	1.3074247	1.9679025
2498.193	1.0435257	1.031556	0.97707814	0.98248192	1.0043439	1.004567	0.93247157	1.2546825	1.4959411	1.3009474	1.9374917
2498.401	1.0401537	1.0266438	0.99522404	0.98119341	1.003776	1.0049451	0.92115166	1.2457145	1.4827468	1.2938657	1.9001251
2498.597	1.0440312	1.0305786	1.0045152	0.97095722	1.0006399	1.0158103	0.91132601	1.2371528	1.4778849	1.2838337	1.859662
2498.797	1.0406229	1.0190271	1.0041414	0.96468859	1.0045619	1.0094237	0.91274003	1.2287225	1.4497583	1.279389	1.810143
2499.005	1.0441677	1.0195589	1.0073132	0.96043767	1.0052926	1.0006231	0.91583087	1.2239843	1.4449954	1.2808147	1.7584373
2499.19	1.0456086	1.0173086	0.99695237	0.95589304	1.0071017	0.99995887	0.91650466	1.2171313	1.4424691	1.2688548	1.7199101
2499.402	1.0502196	1.0069352	0.97628749	0.9726738	1.0105103	0.98840828	0.91324826	1.2087622	1.4316401	1.2647027	1.6961144
2499.593	1.0386559	1.0083013	0.96405619	0.96846533	1.0125758	0.98977387	0.90884005	1.2040028	1.4109223	1.2600349	1.6510594
2499.799	1.0581661	1.0066277	0.9851669	0.96837461	1.0080811	0.99222755	0.89005388	1.1920015	1.3779578	1.2479163	1.607616
2500.001	1.0608217	1.005121	0.97858926	0.96042557	1.0086733	0.98996492	0.88872273	1.1703502	1.357943	1.2294628	1.5757351
2500.192	1.0570933	0.99890768	0.96813023	0.94092431	1.0061818	0.98921272	0.90678852	1.1576893	1.3520667	1.2232097	1.5494883
2500.404	1.0666639	0.9963435	0.97224478	0.95679097	1.005333	0.99041655	0.89651837	1.153091	1.3532121	1.2104334	1.5171282
2500.593	1.0660749	0.99393947	0.97297072	0.94885849	1.0078933	0.99116011	0.89003395	1.1521299	1.3561953	1.1895674	1.4931197
2500.8	1.0708544	0.9898911	0.9677956	0.94884161	1.0105465	0.98986629	0.89335582	1.1424572	1.3579907	1.1637341	1.4701803
2501	1.0565806	0.98742615	0.95884433	0.9495791	1.0111256	0.99493065	0.89912998	1.1268072	1.3657213	1.1516697	1.4355577
2501.195	1.0671907	0.97950322	0.95224995	0.95123709	1.0052137	0.99588879	0.90283376	1.1172889	1.3459181	1.1391536	1.405354
2501.403	1.0638132	0.97438779	0.96299342	0.94861001	1.0051623	0.99205432	0.89853163	1.1061802	1.3231594	1.1279614	1.3746391
2501.404	1.0686517	0.97435333	0.9630658	0.94855958	1.0051652	0.9920012	0.89848256	1.1060829	1.3230234	1.12789	1.3744359
2502.272	1.0748076	0.97318721	0.97067232	0.95669859	1.0099862	0.9888837	0.89540722	1.0617846	1.2876864	1.0863931	1.279476
2503.183	1.0838348	0.95862855	0.96857891	0.94692295	1.0041915	0.97518168	0.9005711	0.9966594	1.2339765	1.0306737	1.1971287
2504.108	1.08539	0.95871251	0.96025165	0.95546803	1.0028648	0.96417512	0.90190486	0.94531284	1.1780102	0.98473275	1.1193245
2505.036	1.0866741	0.95905146	0.9662061	0.95400981	1.0004331	0.96386157	0.89997072	0.89606696	1.1208131	0.93938036	1.0566879
2505.999	1.0803488	0.95854275	0.97197702	0.96130726	0.99642075	0.96805191	0.90010484	0.85207607	1.0764945	0.90491405	1.0149271
2506.975	1.0647081	0.96469164	0.9593781	0.96445053	0.99475323	0.97527083	0.89692082	0.81718741	1.0226521	0.87395601	0.97314045
2507.973	1.0636942	0.96492312	0.97839879	0.97128152	0.99226477	0.97921541	0.89889519	0.79858061	0.99394053	0.85413225	0.93361525
2508.99	1.0595268	0.97226506	0.97049392	0.97839036	0.99123889	0.98355274	0.89839246	0.79021679	0.97801225	0.83856158	0.90892717
2510.022	1.0493609	0.98725861	0.97090592	0.98386333	0.98863452	0.99344013	0.89473275	0.78714348	0.96959493	0.83309554	0.90358326
2511.076	1.0340327	0.99585294	0.97278738	0.98928217	0.99164251	1.0062902	0.90571866	0.79722379	0.96278358	0.83013953	0.91893492
2512.149	1.0290454	1.0069918	0.97749819	1.0003637	0.99432334	1.0226567	0.90925009	0.80590864	0.96750825	0.82494241	0.93477902
2513.241	1.0173258	1.0268433	0.97976014	0.99981855	0.99847707	1.0334508	0.90379728	0.82036742	0.96628966	0.8197716	0.94516101

CAS number	(own reference material)	(own reference material)	7704-34-9	69-78-3	52-90-4	132-65-0	1193-82-4	67-71-0	2386-57-4	926-39-6	7757-82-6
Energy (eV)	FeS	Pyrite	Elemental S	5,5-Dithiobis (2-nitrobenzoic acid)	L-cysteine	Dibenzot-hiophene	Methyl phenyl sulfoxide	Dimethyl sulfone	Sodium Methane-sulfonate	Sulfuric acid mono(2-aminoethyl) ester	Sodium sulfate
2514.355	1.0161485	1.0456851	0.97991038	1.0018738	0.99665557	1.0447372	0.90557832	0.83496511	0.9711674	0.81778989	0.94542945
2515.479	1.0075669	1.0548342	0.97886906	1.0034823	0.99853452	1.0484997	0.91303522	0.84411192	0.9699218	0.81932464	0.94380941
2516.628	0.99870167	1.0578778	0.98568096	1.0038702	1.0004157	1.0609204	0.9183242	0.85474161	0.95226378	0.81332156	0.941775
2517.804	0.99909336	1.0527353	0.97570519	1.0076889	1.004373	1.0640354	0.91487633	0.86967249	0.94592171	0.81513414	0.93746975
2518.981	0.99722288	1.0407659	0.98277744	1.0105888	1.0025956	1.0536055	0.92482146	0.88603733	0.94916639	0.80759544	0.92944744
2520.192	0.98844686	1.0374617	1.0083871	1.0026238	1.0092762	1.048888	0.93677037	0.89721061	0.94468431	0.80750181	0.90691322
2521.415	0.9861058	1.0290728	0.99872365	1.0057321	1.0062028	1.0449237	0.92773943	0.89875883	0.93564438	0.80782427	0.89768279
2522.668	0.98861771	1.0204113	0.99986237	0.99851216	1.0079882	1.0348718	0.93659609	0.90201727	0.93670012	0.80846032	0.88928121
2523.92	0.99730754	1.0116118	1.0166039	0.99950969	1.0123176	1.0329373	0.94358021	0.89725136	0.92701233	0.80881369	0.91587605
2525.21	0.99136378	0.99765242	1.0013587	1.0032365	1.0100404	1.0268797	0.94690423	0.89295058	0.92497423	0.80799903	0.93349662
2526.515	1.009549	0.98757002	1.0105207	1.0141919	1.0079977	1.0275506	0.9509245	0.89003908	0.93332366	0.81402337	0.93549133
2527.822	1.0050065	0.97533372	1.0134826	1.0244432	1.0089772	1.0276407	0.95526583	0.88715066	0.94417233	0.82059856	0.93099254
2529.171	1.0001353	0.97037437	1.0133095	1.0205881	1.0105405	1.0317634	0.95992195	0.88712029	0.95115721	0.82010062	0.92559279
2530.529	1.0010356	0.95899607	1.0195196	1.0261165	1.0109612	1.0246708	0.96442251	0.89223612	0.94440898	0.82274683	0.91735762
2531.906	0.99976955	0.94946314	1.0415797	1.0302317	1.011274	1.0319453	0.96672255	0.89689999	0.94269577	0.82994686	0.92057165
2533.302	0.99705973	0.9449567	1.0299494	1.0278694	1.0075672	1.0349244	0.96885628	0.90075095	0.9466164	0.83086697	0.92290289
2534.715	0.99813437	0.94497765	1.0473788	1.03909	1.0070996	1.0391107	0.97237237	0.90509378	0.95015658	0.83945068	0.91244168
2536.152	0.98913983	0.94817274	1.0432788	1.0400447	1.0059044	1.0409056	0.9733326	0.90406299	0.95958653	0.84220851	0.89947993
2537.605	0.98817648	0.95578083	1.0431697	1.0424665	0.99997677	1.0533152	0.97604466	0.90359805	0.95228903	0.85428975	0.89572754
2539.075	0.99096137	0.96035663	1.0465723	1.0433775	1.0070534	1.0559839	0.98002254	0.90442267	0.96923662	0.86393714	0.90172537
2540.569	0.99450414	0.97049503	1.0410537	1.0470153	0.99409671	1.0574603	0.97721637	0.90288029	0.98017185	0.87011457	0.91690331
2542.082	0.99627575	0.97500716	1.0553998	1.0510776	0.9937259	1.0662099	0.98019587	0.90247213	0.98670276	0.88116628	0.94286278
2543.61	0.98715645	0.97660373	1.0551007	1.0450608	0.99280574	1.0722015	0.98462495	0.9038941	0.99045793	0.89024972	0.97079679
2545.156	0.99103869	0.98268714	1.0329734	1.0348365	0.99429087	1.0729805	0.98209809	0.91119061	1.0017931	0.8997337	0.98655551
2546.727	0.98916899	0.98926339	1.0201174	1.0370713	0.98927965	1.0763596	0.98591435	0.91649954	1.0029006	0.90621274	0.99465942
2548.312	0.99822207	0.99123245	1.0255254	1.0329567	0.9889441	1.0706023	0.98599346	0.92630942	1.0010139	0.91265039	0.98481652
2549.914	1.0039494	0.99614266	1.0085132	1.0213867	0.98814147	1.0609078	0.98561294	0.93387922	1.0137966	0.91829486	0.98744773
2551.545	1.0097354	1.0035322	1.0232813	1.0119528	0.98482947	1.0559387	0.97855646	0.93836315	1.0088404	0.92570529	0.99748788
2553.185	1.0195253	1.0085387	0.99369145	1.0126481	0.98504846	1.0438883	0.98129705	0.93581233	1.010118	0.93265863	1.0142452
2554.85	1.0246475	1.0160233	0.98427631	1.0060317	0.98440979	1.0419689	0.98280345	0.94431191	1.0192092	0.93971443	1.0198567
2556.534	1.0357636	1.0230295	0.98273033	0.99615776	0.9804698	1.0357769	0.97879682	0.94167277	1.0155434	0.94601877	1.0231207
2558.234	1.0375332	1.0201147	0.97509196	0.99329181	0.98119969	1.0262219	0.98002289	0.94325456	1.0362182	0.95161848	1.0205961
2559.954	1.0350599	1.0335503	0.97422189	0.99064732	0.97916039	1.0184201	0.97535221	0.94464898	1.0395117	0.95943009	1.0317082
2561.69	1.0337374	1.0286033	0.97318366	0.98410308	0.97873881	1.0136985	0.98056033	0.95054306	1.0333668	0.9707283	1.0584553
2563.444	1.0380275	1.0299281	0.96819265	0.98851086	0.97626321	1.0109369	0.97637157	0.94559248	1.0455985	0.97867841	1.0799581
2565.227	1.0405245	1.0300792	0.97375459	0.9891345	0.97742533	1.0110189	0.99520798	0.95583446	1.0563014	0.97871936	1.1103519
2567.027	1.0289593	1.0353516	0.9642662	0.9848277	0.97481171	1.0131947	0.98326009	0.95601976	1.065689	0.98344639	1.1353327
2568.842	1.0211075	1.0243525	0.96573947	0.97722114	0.9731274	1.0170416	0.99100286	0.95742798	1.0640082	0.9913771	1.1450947
2570.672	1.0169959	1.0172101	0.95108795	0.97111472	0.96963334	1.0112694	0.98367722	0.96605395	1.0618682	0.9917066	1.1406727
2572.527	1.0080365	1.0152766	0.95279923	0.97919799	0.97243068	1.0172715	0.98532785	0.97264539	1.0718924	0.99858479	1.1186585

CAS number	(own reference material)	(own reference material)	7704-34-9	69-78-3	52-90-4	132-65-0	1193-82-4	67-71-0	2386-57-4	926-39-6	7757-82-6
Energy (eV)	FeS	Pyrite	Elemental S	5,5-Dithiobis (2-nitrobenzoic acid)	L-cysteine	Dibenzotriophene	Methyl phenyl sulfoxide	Dimethyl sulfone	Sodium Methane-sulfonate	Sulfuric acid mono(2-aminoethyl) ester	Sodium sulfate
2574.394	0.99781601	1.0083396	0.96674162	0.97477831	0.97154343	1.0105978	0.98496485	0.97775507	1.0752665	1.0050941	1.0982358
2576.288	0.9970855	0.99580294	0.96092	0.97546075	0.96889932	1.0128839	0.97647093	0.9738471	1.0767033	1.0005582	1.0865863
2578.197	0.99046659	0.99332759	0.96876057	0.96843978	0.96773252	1.0124359	0.98421794	0.98731597	1.0701157	1.0064641	1.0873944
2580.124	0.98436853	0.98723779	0.97636216	0.97727924	0.96876877	1.0128105	0.98006202	0.98333122	1.0715948	1.0105796	1.0837559
2582.075	0.97666223	0.98492372	0.97033997	0.97795601	0.97055108	1.0071237	0.97605638	0.98797803	1.0749438	1.0118434	1.0750851
2584.042	0.97900725	0.98061203	0.97014736	0.97584172	0.97012633	1.0086742	0.97929876	0.98867384	1.0671615	1.0084112	1.0724323
2586.03	0.96840404	0.9844897	0.97677831	0.97929501	0.96846136	1.0017973	0.97613203	0.98939117	1.0589374	1.0102436	1.0740112
2588.034	0.96645127	0.98688147	0.98270293	0.97916075	0.97073054	1.0081866	0.98010666	0.98909502	1.0605836	1.0073034	1.0731651
2590.057	0.96518534	0.99500408	0.9959092	0.98255247	0.97093976	0.99813455	0.97558464	0.99028932	1.0590332	1.0060479	1.0705168
2592.103	0.97031712	0.9932652	0.97996142	0.9758684	0.97233038	1.0020508	0.97631779	0.99166333	1.0431156	1.0072616	1.0672863
2594.172	0.9714298	0.98882516	0.99495734	0.98469028	0.97091463	0.99411677	0.9787245	0.98588596	1.0402614	1.0030713	1.0649654
2596.249	0.96856868	0.99709047	0.98979369	0.98792171	0.97114049	0.9958772	0.97282227	0.98639421	1.0454382	1.0042067	1.0602106
2598.356	0.973497	0.98870199	1.0038746	0.98365326	0.97171019	0.9868699	0.96771301	0.97620545	1.033915	0.9999104	1.0565914
2600.47	0.97065237	0.99568374	1.0021507	0.98960407	0.9751489	0.98795932	0.96495435	0.9789076	1.0224215	0.99547776	1.046359
2602.616	0.97356674	0.99591169	1.0034132	0.98551672	0.97280973	0.98702795	0.96730582	0.96887296	1.0236061	0.9903365	1.0303136
2604.769	0.97952628	1.0005302	1.0017579	0.99606808	0.97415704	0.99197348	0.97185349	0.96643394	1.0184672	0.99673497	1.0243778
2606.95	0.99155498	0.99862973	1.0134655	0.99595046	0.97562697	0.98868013	0.96883623	0.96249473	1.0136001	0.98724368	1.020395
2609.139	0.99005402	1.0046247	1.0079648	1.0048773	0.97496452	0.98489748	0.97273737	0.96088133	1.0137378	0.98266535	1.0183583
2611.36	0.99579428	1.0044898	1.0226348	0.99789312	0.97950364	0.98369912	0.97525443	0.9568955	1.0010289	0.98201747	1.0172747
2613.598	1.0012672	1.0000245	1.0086582	1.0077891	0.97926425	0.98941794	0.96900968	0.95434725	0.99407519	0.97559906	1.0034847
2615.841	1.003461	1.0013443	1.0165917	1.0065911	0.9798034	0.98664864	0.97267416	0.96040283	0.98849897	0.97556408	0.98902386
2618.119	1.0126951	1.0028061	1.0159012	1.0125511	0.98205885	0.9939058	0.96096808	0.95849738	0.98941228	0.9663569	0.98174645
2620.41	1.0053817	1.0013864	1.0112491	1.0142125	0.97950725	0.99148138	0.97427862	0.9657197	0.9847537	0.96494166	0.97224076
2622.724	1.0121002	1.0021063	1.0233971	1.0163913	0.98467448	0.9942468	0.97510832	0.96745197	0.97448573	0.96425342	0.95667722
2625.045	1.0148065	0.99884166	1.0140138	1.0138041	0.98220661	0.99034551	0.9719991	0.97623236	0.97864807	0.95826549	0.9574841
2627.398	1.0161528	1.0055157	1.0080653	1.0174736	0.98307605	0.99853462	0.9831148	0.97482846	0.98029747	0.95906278	0.9517244
2629.766	1.0156392	1.0109945	1.0187765	1.0105119	0.97977774	0.9986165	0.98185936	0.98445871	0.9785961	0.95821656	0.94144321
2632.153	1.0235068	1.0081068	1.0160136	1.0098581	0.98341097	1.0072174	0.97812928	0.98085478	0.96281787	0.95965802	0.93831874
2634.561	1.0236974	1.0076745	1.0066056	1.0069153	0.98358775	1.0051466	0.97675481	0.97900531	0.95733337	0.96042069	0.94022512
2636.979	1.018416	1.0113806	1.0226841	1.0081971	0.98074628	1.0036255	0.9809826	0.97623788	0.9498419	0.959454	0.93961829
2639.424	1.0163339	1.0139707	0.99680301	1.0065283	0.98200222	1.0068934	0.97826107	0.97723972	0.95740845	0.95684457	0.94298161
2641.887	1.0141181	1.0160673	0.99615242	1.0066036	0.98391642	1.0080816	0.9788024	0.97080841	0.95921621	0.95963046	0.95061935
2644.372	1.0133892	1.0135872	1.0011133	1.0092332	0.98006892	1.0046692	0.98026467	0.97143592	0.95409402	0.9630169	0.95151165
2646.868	1.0088079	1.0150415	1.0088566	0.99809989	0.98309448	1.0100085	0.98501572	0.97492485	0.95799747	0.96667418	0.95460271
2649.387	1.0068019	1.0053948	0.99750759	0.99708937	0.98088839	1.0084131	0.98537205	0.97001502	0.95771617	0.96512387	0.94288271
2651.928	1.0019812	1.0043959	1.0010842	0.99663826	0.98434591	1.0074583	0.981257	0.97199026	0.95802174	0.96612947	0.95410199
2654.482	0.99965369	1.0060184	0.99074826	0.99641157	0.98338863	1.0094817	0.9801344	0.97751132	0.96469869	0.96919986	0.95056531
2657.054	0.99439362	0.99651377	0.99402647	0.99562363	0.98111314	1.0076808	0.9803319	0.97663287	0.95695176	0.97018639	0.95761483
2659.653	0.99043236	0.98960089	0.98602005	0.99428618	0.98433067	0.99949872	0.98140035	0.97522996	0.9662987	0.97622613	0.9517743
2662.266	0.98348372	0.99280696	0.98962977	0.9911	0.98180626	1.0001354	0.98031194	0.97693958	0.96263017	0.98304491	0.95933443

CAS number	(own reference material)	(own reference material)	7704-34-9	69-78-3	52-90-4	132-65-0	1193-82-4	67-71-0	2386-57-4	926-39-6	7757-82-6
Energy (eV)			Elemental S	5,5-Dithiobis (2-nitrobenzoic acid)	L-cysteine	Dibenzotriophene	Methyl phenyl sulfoxide	Dimethyl sulfone	Sodium Methanesulfonate	Sulfuric acid mono(2-aminoethyl) ester	Sodium sulfate
2664.91	0.98962115	0.99052588	0.99263842	0.99728197	0.98853924	1.0023289	0.98508816	0.98040615	0.97121197	0.9815878	0.95600196
2667.554	0.98545026	0.99234583	0.98894689	0.99344492	0.98481118	1.0007749	0.98759532	0.97687154	0.96493598	0.984361	0.95499745
2670.225	0.9857528	0.99491733	0.99202797	0.98951094	0.99213945	0.99853543	0.99064211	0.98214179	0.97354859	0.9876743	0.96322877
2672.928	0.98591928	0.99245865	1.000492	0.98927312	0.99300494	1.0008544	0.98530091	0.9877148	0.98084886	0.99060509	0.96535986
2675.631	0.98560636	0.99068972	0.99288039	0.99357573	0.99361497	0.99697734	0.98868825	0.98716714	0.97886215	0.98971413	0.97978692
2678.364	0.97579303	0.9939771	1.0050564	0.99585781	0.99559387	0.99150694	0.9924242	0.99063843	0.98901665	0.99471277	0.9894856
2681.113	0.98217128	0.99181473	1.003059	0.99472916	0.99905459	0.99401315	0.98727435	0.99557689	0.99690987	1.0083119	0.99315314
2683.884	0.98853425	0.99950744	1.0059998	1.0039404	1.0011575	0.9917273	1.0025511	1.0038656	0.99852291	1.0081132	0.997352
2686.673	0.99210102	0.9978038	1.0105099	0.99762864	1.0023871	0.99354001	1.014883	1.0046601	0.9985343	1.0126256	1.0086639
2689.476	0.99298561	1.0002627	1.0104952	0.99822753	1.0025561	0.99275	1.0026717	1.0091478	1.0101672	1.0097611	1.0059755
2692.305	1.002916	1.001348	1.0144174	0.99978565	1.0045379	0.99507918	1.0054132	1.0233823	1.0226616	1.0145875	1.0084371
2695.141	1.0054468	1.0011831	1.0161406	0.99459715	1.0038947	0.99350168	1.0033246	1.0204936	1.0382741	1.0326116	1.0356162
2698.008	1.0056683	1.0068722	1.0073415	1.0054142	1.0042711	0.99633011	1.0138847	1.0168645	1.0207953	1.0300619	1.0455171
2700.89	1.0077026	1.0025336	1.0159199	0.99849111	1.009318	0.98901484	1.0104399	1.0219767	1.0276449	1.0244352	1.026142