SUPPLEMENTARY INFORMATION

1) de Mello method for the calculation of the absolute quantum efficiency of a compound

DE MELLO's method for integrating spheres.

The emission spectra described in Fig. SI1 are recorded, and corrected for the response of the sensor, The integrals of the spectra are calculated and used in the equation in Fig.SI1 to calculate the absolute emission quantum yield.

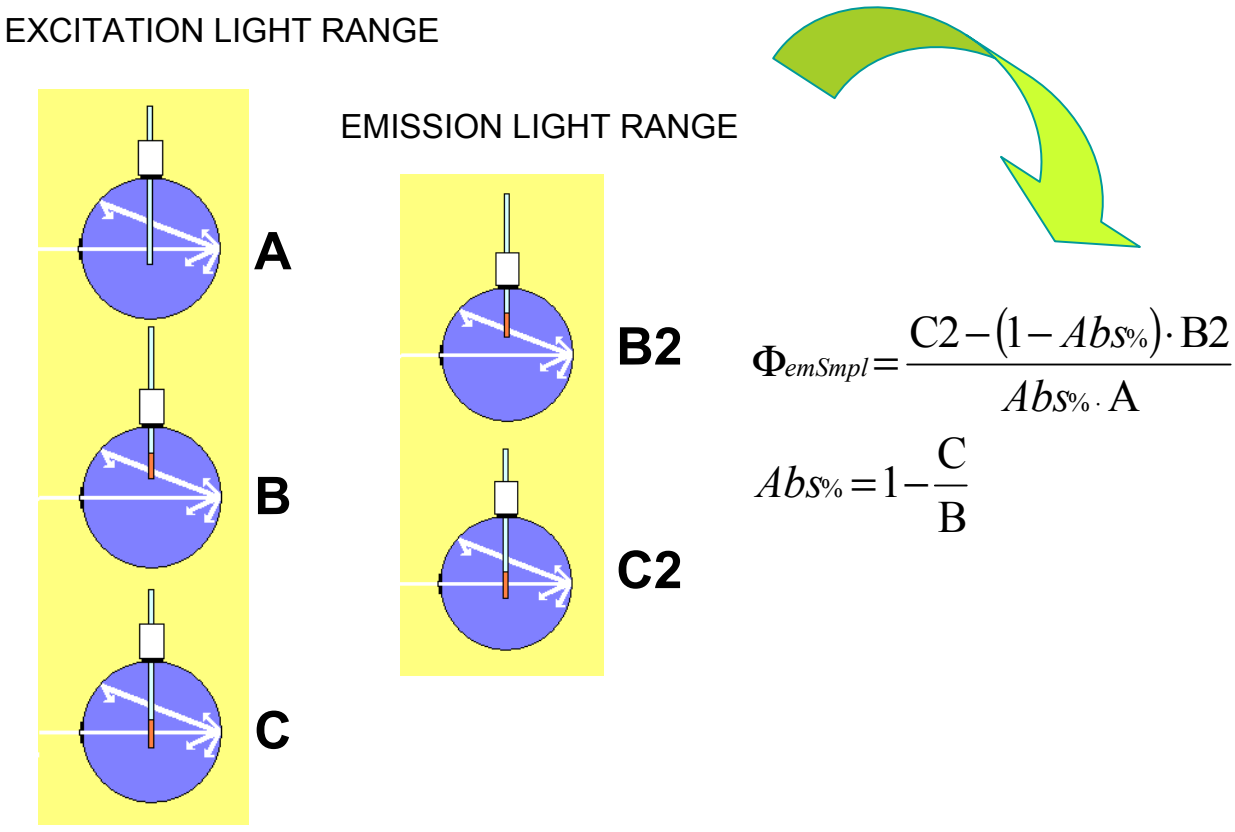

Fig. SI1 Description of the method for the determination of the absolute emission quantum yield proposed by De Mello et al. *J. C. De Mello, H. F. Wittmann and R. H. Friend, Advanced Materials, 1997, 9, 230.*

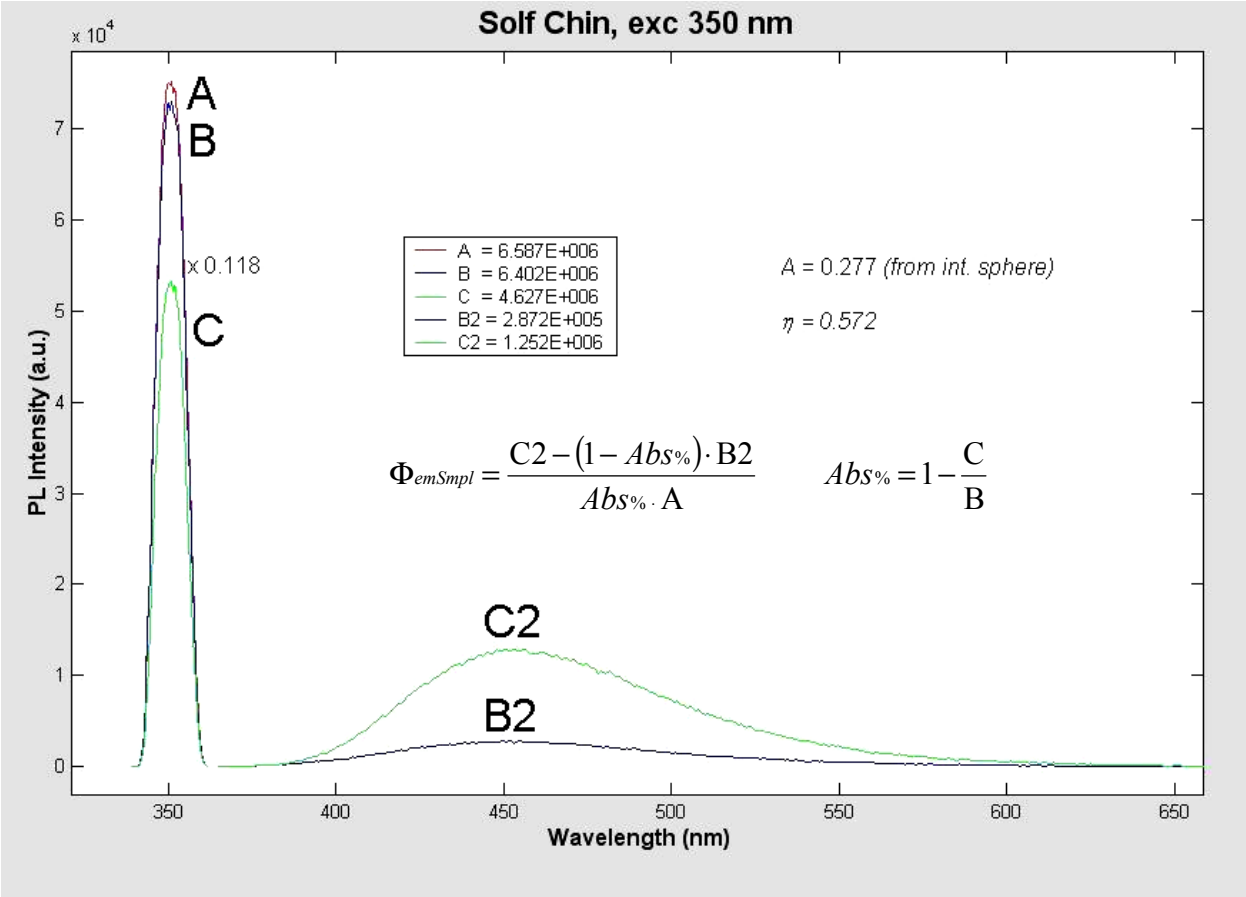

Fig. SI2 Example of the determination of the emission quantum yield of a sample of quinine sulphate using the De Mello's method. This experiment was undertaken in our lab in order to verify the confidence of the technique.

Raw data of the emission spectra recorded to calculate the emission quantum yield of the **Cuprorivaite** are listed below (**left column** = nm ; **right column** = emission intensity). The name of the spectrum refers to the experimental conditions described in Fig. SI1.

A

580	2173.2485
580.5	440.5207
581	2177.1625
581.5	3717.3215
582	159.2998
582.5	4822.048
583	7140.1145
583.5	11585.44
584	8162.647
584.5	15753.85
585	24061.315
585.5	38406.125
586	56449.665
586.5	77458.06
587	69258.23
587.5	137381.4
588	176912.8
588.5	230338.9
589	282297.25
589.5	346193.3
590	344138.45
590.5	520659.85
591	596982.85
591.5	668609.05
592	665967.1
592.5	857361.7
593	825560.45
593.5	1.0284E6
594	1.0196E6
594.5	1.11948E6
595	1.24396E6
595.5	1.3047E6
596	1.37505E6
596.5	1.42858E6
597	1.46706E6
597.5	1.49893E6
598	1.54885E6
598.5	1.59575E6
599	1.56448E6
599.5	1.58433E6
600	1.60477E6
600.5	1.62642E6
601	1.61921E6

601.5	1.62161E6
602	1.62823E6
602.5	1.62342E6
603	1.61259E6
603.5	1.62342E6
604	1.60898E6
604.5	1.59996E6
605	1.59816E6
605.5	1.58794E6
606	1.55486E6
606.5	1.54223E6
607	1.50615E6
607.5	1.45143E6
608	1.41294E6
608.5	1.3516E6
609	1.27042E6
609.5	1.2016E6
610	1.1321E6
610.5	1.04112E6
611	942686.9
611.5	841510
612	856089.65
612.5	682601.6
613	677219.85
613.5	490913.45
614	488662.9
614.5	338658.85
615	336701.85
615.5	221825.95
616	204017.25
616.5	127400.7
617	112527.5
617.5	63602.5
618	57154.185
618.5	31811.035
619	29482.205
619.5	22378.295
620	14716.64
620.5	11458.235
621	10558.015
621.5	11086.405
622	7214.4805
622.5	8612.757
623	6031.474
623.5	5770.2145
624	9548.203
624.5	4613.6275
625	5647.902

B

580	227.8
580.5	4277
581	3226
581.5	1899
582	4830
582.5	9213
583	-951.8
583.5	6385
584	8445
584.5	16400
585	22140
585.5	26950
586	46500
586.5	70250
587	92710
587.5	118300
588	150800
588.5	205400
589	242800
589.5	310000
590	377800
590.5	453700
591	522400
591.5	585700
592	680200
592.5	770500
593	838300
593.5	914900
594	1.012E6
594.5	1.076E6
595	1.14E6
595.5	1.193E6
596	1.241E6
596.5	1.299E6
597	1.286E6
597.5	1.353E6
598	1.359E6
598.5	1.391E6
599	1.405E6
599.5	1.417E6
600	1.44E6
600.5	1.456E6
601	1.459E6
601.5	1.481E6
602	1.468E6
602.5	1.496E6
603	1.478E6

603.5	1.471E6
604	1.471E6
604.5	1.468E6
605	1.454E6
605.5	1.446E6
606	1.443E6
606.5	1.38E6
607	1.41E6
607.5	1.33E6
608	1.271E6
608.5	1.222E6
609	1.215E6
609.5	1.075E6
610	1.072E6
610.5	924100
611	822800
611.5	751000
612	763800
612.5	607000
613	602600
613.5	461000
614	432000
614.5	304200
615	279400
615.5	241400
616	175200
616.5	128400
617	103500
617.5	80790
618	52290
618.5	31880
619	26050
619.5	19690
620	13990
620.5	12840
621	6736
621.5	7827
622	8733
622.5	9103
623	5412
623.5	8112
624	5627
624.5	5998
625	7051

B2

740	352.8

741	122.4
742	-32.424
743	507.12
744	-343.68
745	-460.2
746	-173.28
747	187.68
748	535.32
749	438.48
750	389.28
751	90.996
752	693.96
753	45.036
754	164.16
755	59.304
756	-176.76
757	-102.468
758	728.28
759	717.96
760	-7.2156
761	379.92
762	-64.032
763	346.32
764	337.56
765	315
766	369
767	560.64
768	-96.3
769	143.64
770	-455.52
771	-168.96
772	867
773	267.72
774	-226.8
775	39.888
776	-304.2
777	-308.88
778	111.048
779	292.44
780	181.08
781	-147.96
782	-204.96
783	994.2
784	6.3432
785	-113.58
786	125.64
787	707.04
788	-93.612
789	37.32
790	99.108
791	536.4

792	85.98
793	48.948
794	573.12
795	613.68
796	284.52
797	524.4
798	456.12
799	-29.904
800	232.44
801	296.76
802	5.9016
803	510.72
804	444.24
805	134.04
806	-313.8
807	115.776
808	51.876
809	-11.4756
810	79.968
811	79.608
812	232.08
813	118.332
814	-100.98
815	558.36
816	105.528
817	254.04
818	598.8
819	584.64
820	396.6
821	340.32
822	381
823	69.24
824	142.68
825	618.72
826	312
827	613.68
828	286.2
829	754.56
830	300.96
831	784.92
832	521.88
833	717.48
834	498.48
835	383.76
836	679.8
837	729.96
838	508.44
839	476.04
840	622.8
841	784.68
842	157.08

843	359.88
844	356.16
845	796.92
846	815.64
847	796.2
848	624.12
849	837.48
850	646.2
851	739.2
852	839.16
853	730.56
854	1251.6
855	865.92
856	755.52
857	846.96
858	827.76
859	890.04
860	879.48
861	939.12
862	1085.76
863	794.04
864	621
865	1145.64
866	621.36
867	944.28
868	1174.56
869	912.6
870	1302
871	1113.96
872	1201.2
873	1357.2
874	927.24
875	1341.6
876	1038.6
877	1032.84
878	1043.64
879	1557.6
880	1020.12
881	1136.52
882	1302
883	1060.2
884	1263.6
885	1449.6
886	1095.84
887	936.36
888	1575.6
889	1007.64
890	1140.24
891	1315.2
892	1186.8
893	1323.6

894	1220.4
895	1657.2
896	1315.2
897	1260
898	1698
899	1548
900	1321.2
901	1274.4
902	1425.6
903	1133.52
904	1596
905	1378.8
906	1187.28
907	1480.8
908	1422
909	1184.28
910	1453.2
911	1288.8
912	1203.6
913	1318.8
914	1378.8
915	1508.4
916	1334.4
917	1345.2
918	1464
919	1384.8
920	1383.6
921	1501.2
922	1242
923	1173.96
924	1183.08
925	1140.48
926	1303.2
927	1129.32
928	1236
929	1125.72
930	1178.4
931	1202.4
932	997.44
933	1220.4
934	1258.8
935	1123.32
936	1165.44
937	1300.8
938	1256.4
939	1021.56
940	1176.24
941	1363.2
942	1120.8
943	1106.28
944	1233.6

945	1037.64
946	1368
947	1074.84
948	1077.24
949	1055.04
950	979.8
951	1094.64
952	1007.04
953	946.44
954	1033.32
955	860.04
956	1014.12
957	927.24
958	841.44
959	932.52
960	918.6
961	897.96
962	804.96
963	1066.08
964	1123.68
965	725.76
966	904.68
967	867
968	914.16
969	914.04
970	798
971	705.96
972	660.72
973	818.64
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978	585.24
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980	641.76
981	654
982	785.28
983	479.28
984	572.64
985	661.92
986	584.28
987	530.52
988	676.56
989	488.64
990	745.56
991	672.24
992	556.08
993	669.12
994	699.48
995	592.8

996	468.12
997	663.6
998	453
999	561
1000	421.8
1001	544.8
1002	472.56
1003	581.28
1004	511.92
1005	435.24
1006	552.72
1007	360
1008	472.68
1009	515.28
1010	460.8
1011	391.56
1012	405
1013	483.48
1014	494.04
1015	408.6
1016	449.76
1017	425.16
1018	390.96
1019	310.92
1020	304.32
1021	351.48
1022	315.48
1023	369.12
1024	200.52
1025	369.24
1026	381.24
1027	189.36
1028	336.84
1029	375
1030	297.12
1031	163.8
1032	291.84
1033	274.44
1034	360.24
1035	238.2
1036	402
1037	337.08
1038	266.16
1039	264.36
1040	191.04
1041	294.72
1042	276.24
1043	321.12
1044	273.84
1045	216.6
1046	215.04

1047	239.88
1048	285.96
1049	196.68
1050	115.176
1051	271.32
1052	268.32
1053	144.6
1054	306.12
1055	248.52
1056	276.72
1057	166.08
1058	248.88
1059	183
1060	231
1061	321.96
1062	167.52
1063	206.76
1064	143.88
1065	230.88
1066	228.24
1067	122.52
1068	234.96
1069	189.36
1070	124.56
1071	242.76
1072	113.376
1073	144.96
1074	181.32
1075	211.44
1076	230.64
1077	276.36
1078	142.92
1079	112.56
1080	245.52
1081	131.76
1082	188.52
1083	117.156
1084	193.08
1085	240
1086	119.328
1087	15.66
1088	65.004
1089	128.76
1090	116.628
1091	194.64
1092	191.04
1093	177.84
1094	139.44
1095	145.32
1096	160.92
1097	189.72

1098	201.72
1099	-4.8012
1100	21.6
1101	183.6
1102	133.2
1103	57.648
1104	194.64
1105	185.04
1106	99.72
1107	18.024
1108	111.816
1109	174.48
1110	95.1
1111	55.428
1112	26.52
1113	211.08
1114	97.848
1115	133.08
1116	122.52
1117	82.596
1118	114.324
1119	108.372
1120	128.04
1121	191.76
1122	182.16
1123	149.28
1124	44.064
1125	25.704
1126	108.996
1127	115.2
1128	116.52
1129	71.136
1130	49.02
1131	109.08
1132	-18.42
1133	139.32
1134	112.62
1135	101.616
1136	172.08
1137	103.788
1138	181.44
1139	148.2
1140	-3.708
1141	125.04
1142	96.636
1143	93.06
1144	8.7024
1145	112.128
1146	150.96
1147	153.72
1148	33.756

1149	116.316
1150	8.7624
1151	-35.088
1152	90.3
1153	12.552
1154	26.364
1155	121.92
1156	106.92
1157	70.488
1158	194.04
1159	79.5
1160	36.648
1161	98.7
1162	100.068
1163	74.844
1164	21.6
1165	72.564
1166	116.004
1167	190.2
1168	123.96
1169	39.672
1170	170.4
1171	61.632
1172	9.0084
1173	91.596
1174	62.064
1175	94.572
1176	83.076
1177	157.32
1178	108.12
1179	241.44
1180	109.884
1181	99.684
1182	56.568
1183	65.94
1184	140.04
1185	-15.876
1186	152.4
1187	15.912
1188	3.9816
1189	50.52
1190	-18.648
1191	101.328
1192	46.68
1193	44.016
1194	6.6708
1195	161.64
1196	-20.064
1197	139.2
1198	33.492
1199	139.44

1200	177.12
1201	131.76
1202	60.588
1203	176.64
1204	83.736
1205	55.464
1206	117.9
1207	119.412
1208	119.532
1209	82.932
1210	63.984
1211	80.448
1212	88.74
1213	131.28
1214	-8.2116
1215	76.752
1216	108.42
1217	1.374
1218	100.344
1219	52.296
1220	75.804
1221	104.928
1222	4.1484
1223	1.3848
1224	63.78
1225	133.2
1226	69.468
1227	286.44
1228	135
1229	19.524
1230	53.088
1231	116.172
1232	91.164
1233	23.904
1234	97.26
1235	-52.284
1236	172.92
1237	66.768
1238	31.332
1239	122.76
1240	160.32
1241	238.32
1242	175.68
1243	37.524
1244	72.3
1245	101.376
1246	98.628
1247	77.004
1248	17.46
1249	58.284
1250	-18.96

1251	40.884
1252	144.72
1253	102.42
1254	172.8
1255	23.448
1256	154.08
1257	69.036
1258	24.996
1259	142.68
1260	-26.508
1261	95.856
1262	177.24
1263	85.74
1264	168.6
1265	192.48
1266	137.76
1267	146.88
1268	310.56
1269	154.8
1270	101.352
1271	210.36
1272	174.72
1273	89.736
1274	-14.988
1275	175.68
1276	255.72
1277	277.08
1278	131.16
1279	101.064
1280	126.84
1281	92.184
1282	231.6
1283	42.468
1284	24.312
1285	53.244
1286	41.112
1287	-44.196
1288	141.96
1289	-10.7028
1290	79.608
1291	128.64
1292	59.748
1293	292.92
1294	41.484
1295	-6.1596
1296	132.72
1297	236.52
1298	43.344
1299	142.56
1300	119.46
1301	158.52

1302	42.012
1303	51.444
1304	204.6
1305	37.536
1306	61.08
1307	244.68
1308	157.08
1309	105.432
1310	156
1311	138.96
1312	93.3
1313	71.292
1314	85.728
1315	116.136
1316	31.884
1317	108.636
1318	48.024
1319	171.6
1320	221.88
1321	198.24
1322	43.608
1323	82.536
1324	144.36
1325	209.64
1326	159.72
1327	248.28
1328	70.452
1329	146.28
1330	148.44
1331	87.72
1332	31.56
1333	84.996
1334	33.444
1335	142.56
1336	296.28
1337	45.6
1338	166.08
1339	32.304
1340	196.32
1341	130.32
1342	74.004
1343	8.6412
1344	257.04
1345	20.964
1346	31.692
1347	104.88
1348	172.32
1349	123
1350	12.744
1351	78.84
1352	214.32

1353 167.88
1354 175.56
1355 250.08
1356 246
1357 113.592
1358 237.12
1359 97.032
1360 88.56
1361 -110.16
1362 111.408
1363 111.3
1364 68.328
1365 203.76
1366 93.612
1367 333
1368 206.52
1369 210
1370 138.12
1371 128.64
1372 273
1373 173.4
1374 14.604
1375 102.132
1376 279.84
1377 160.2
1378 86.472
1379 53.46
1380 215.52
1381 79.2
1382 46.224
1383 118.188
1384 327.12
1385 305.04
1386 -110.316
1387 282.48
1388 164.04
1389 445.08
1390 156.84
1391 229.32
1392 -123
1393 -220.8
1394 22.008
1395 124.44
1396 169.44
1397 83.136
1398 190.8
1399 200.64
1400 339.24

C

580	2849.0
580.5	5043.5
581	7360.0
581.5	7577.8
582	1582.9
582.5	-55.8
583	7935.2
583.5	4883.1
584	2897.9
584.5	14234.4
585	10754.0
585.5	20778.5
586	29042.0
586.5	39274.9
587	65555.5
587.5	79758.7
588	112020.6
588.5	129006.0
589	187127.5
589.5	213811.6
590	287934.1
590.5	340709.3
591	388147.6
591.5	441515.8
592	526904.9
592.5	602806.3
593	644314.9
593.5	739784.7
594	809756.3
594.5	805012.5
595	983499.4
595.5	939618.9
596	1.1E6
596.5	1.1E6
597	1.1E6
597.5	1.1E6
598	1.2E6
598.5	1.2E6
599	1.2E6
599.5	1.2E6
600	1.3E6
600.5	1.3E6
601	1.3E6
601.5	1.3E6
602	1.3E6
602.5	1.3E6
603	1.3E6
603.5	1.3E6
604	1.3E6
604.5	1.3E6

605	1.3E6
605.5	1.2E6
606	1.2E6
606.5	1.2E6
607	1.1E6
607.5	1.1E6
608	990615.1
608.5	982313.4
609	898703.3
609.5	818651.0
610	796710.7
610.5	628304.5
611	614665.9
611.5	532241.7
612	519196.2
612.5	430249.2
613	414238.8
613.5	319362.0
614	279039.4
614.5	210846.7
615	197156.2
615.5	122024.3
616	85833.8
616.5	68035.6
617	69004.7
617.5	35388.1
618	41473.7
618.5	21591.3
619	15860.0
619.5	8895.0
620	13161.1
620.5	7345.4
621	9718.2
621.5	6360.7
622	7841.4
622.5	5874.0
623	4042.1
623.5	6830.7
624	6425.3
624.5	6374.2
625	4123.4

C2

740	131.28
741	823.92
742	980.76
743	-24.144

744	583.44
745	-23.808
746	661.68
747	742.92
748	46.548
749	838.56
750	526.68
751	-318.48
752	226.32
753	-517.8
754	149.28
755	541.2
756	139.92
757	878.28
758	-254.88
759	681.72
760	230.88
761	788.52
762	256.2
763	431.16
764	527.52
765	483
766	403.8
767	-186.84
768	268.32
769	506.04
770	1209.6
771	195.96
772	-47.04
773	247.68
774	713.88
775	232.68
776	-72.744
777	834.72
778	163.32
779	298.92
780	-58.2
781	-83.664
782	-44.82
783	312.24
784	393.24
785	-246.12
786	885.36
787	18.768
788	293.28
789	503.88
790	-111.492
791	413.04
792	835.2
793	666.96
794	103.656

795	42.54
796	54.492
797	-277.32
798	1116.24
799	287.04
800	202.68
801	546
802	784.92
803	322.8
804	485.16
805	553.56
806	598.44
807	735.24
808	414.96
809	625.44
810	679.68
811	369.6
812	718.8
813	608.52
814	594.72
815	457.92
816	449.88
817	585.48
818	824.04
819	524.52
820	483.6
821	691.44
822	1834.8
823	990.72
824	1078.2
825	665.88
826	1617.6
827	1134.48
828	930.24
829	1038.24
830	1620
831	1251.6
832	1861.2
833	1683.6
834	1693.2
835	2130
836	1926
837	1779.6
838	1819.2
839	2343.6
840	1626
841	1945.2
842	2020.8
843	1897.2
844	2506.8
845	2469.6

846	1951.2
847	2346
848	2530.8
849	2904
850	2542.8
851	2865.6
852	2436
853	3198
854	2882.4
855	2625.6
856	3591.6
857	2972.4
858	3850.8
859	2828.4
860	3142.8
861	3498
862	3745.2
863	4011.6
864	4014
865	4069.2
866	3694.8
867	3916.8
868	4041.6
869	4244.4
870	4408.8
871	4381.2
872	4616.4
873	4653.6
874	4542
875	4870.8
876	4798.8
877	4759.2
878	4544.4
879	4768.8
880	5397.6
881	5228.4
882	4767.6
883	4896
884	5283.6
885	5196
886	5019.6
887	5074.8
888	5656.8
889	5413.2
890	5569.2
891	5463.6
892	5580
893	5365.2
894	5521.2
895	5608.8
896	5850

897	5533.2
898	5463.6
899	6078
900	5786.4
901	5618.4
902	5479.2
903	5620.8
904	5578.8
905	5546.4
906	5739.6
907	5792.4
908	5661.6
909	5311.2
910	5490
911	5422.8
912	5896.8
913	5600.4
914	5518.8
915	5420.4
916	5392.8
917	5653.2
918	5386.8
919	5257.2
920	5278.8
921	5536.8
922	5548.8
923	5130
924	5437.2
925	5382
926	5355.6
927	5181.6
928	5097.6
929	5268
930	5280
931	5300.4
932	4900.8
933	4837.2
934	5023.2
935	4875.6
936	4920
937	5244
938	4898.4
939	4990.8
940	4719.6
941	4575.6
942	4705.2
943	4580.4
944	4626
945	4473.6
946	4623.6
947	4358.4

948	4497.6
949	4422
950	4261.2
951	4216.8
952	4326
953	4335.6
954	4131.6
955	4089.6
956	4004.4
957	3824.4
958	3831.6
959	3733.2
960	3942
961	3838.8
962	3608.4
963	3880.8
964	3615.6
965	3532.8
966	3688.8
967	3446.4
968	3265.2
969	3376.8
970	3183.6
971	4014
972	3262.8
973	3136.8
974	3350.4
975	3201.6
976	3026.4
977	2876.4
978	2859.6
979	3055.2
980	2986.8
981	2721.6
982	2907.6
983	2817.6
984	2653.2
985	2816.4
986	2620.8
987	2450.4
988	2401.2
989	2416.8
990	2265.6
991	2329.2
992	2133.6
993	2324.4
994	2490
995	2370
996	2256
997	2103.6
998	2175.6

999	2107.2
1000	1954.8
1001	1996.8
1002	2023.2
1003	1996.8
1004	1702.8
1005	1869.6
1006	1629.6
1007	1693.2
1008	1753.2
1009	1634.4
1010	1636.8
1011	1612.8
1012	1539.6
1013	1473.6
1014	1418.4
1015	1389.6
1016	1276.8
1017	1326
1018	1292.4
1019	1364.4
1020	1305.6
1021	1263.6
1022	1261.2
1023	1197.96
1024	1212
1025	1139.52
1026	1071.12
1027	1195.32
1028	972.6
1029	1106.76
1030	1011.12
1031	950.28
1032	962.52
1033	929.28
1034	1039.32
1035	963.24
1036	931.2
1037	757.44
1038	821.4
1039	887.52
1040	840.84
1041	697.44
1042	913.56
1043	810.36
1044	850.44
1045	720.48
1046	801.12
1047	801.12
1048	709.92
1049	711.72

1050	746.16
1051	807.6
1052	745.2
1053	661.8
1054	625.92
1055	702
1056	555.84
1057	612.24
1058	542.16
1059	539.16
1060	554.52
1061	750.12
1062	671.52
1063	600.6
1064	617.16
1065	384.48
1066	615.96
1067	504.84
1068	464.88
1069	421.56
1070	355.32
1071	481.92
1072	471.84
1073	492.12
1074	432
1075	278.28
1076	490.32
1077	395.28
1078	419.04
1079	545.88
1080	417.24
1081	303.48
1082	542.64
1083	396.12
1084	349.92
1085	458.28
1086	464.04
1087	365.04
1088	412.92
1089	317.64
1090	381.12
1091	359.28
1092	360.36
1093	309.96
1094	267.96
1095	362.76
1096	236.52
1097	289.32
1098	246.12
1099	216
1100	273.6

1101	267.6
1102	307.32
1103	157.32
1104	161.04
1105	350.76
1106	141.72
1107	183.84
1108	336.6
1109	340.44
1110	191.4
1111	237.36
1112	337.56
1113	200.28
1114	167.88
1115	183.96
1116	332.28
1117	187.08
1118	313.8
1119	314.16
1120	91.464
1121	180.72
1122	217.68
1123	127.32
1124	107.712
1125	324.48
1126	215.52
1127	85.788
1128	138.6
1129	229.32
1130	127.44
1131	189.96
1132	189.12
1133	72.732
1134	169.56
1135	275.04
1136	169.56
1137	248.4
1138	248.16
1139	139.56
1140	105.072
1141	183.12
1142	195.72
1143	233.28
1144	154.2
1145	113.376
1146	186
1147	174.96
1148	151.2
1149	242.64
1150	117.66
1151	93.972

1152	116.628
1153	233.4
1154	203.4
1155	125.64
1156	98.112
1157	81.816
1158	191.52
1159	137.52
1160	309.6
1161	153.12
1162	221.64
1163	44.4
1164	147.36
1165	212.64
1166	108.348
1167	148.08
1168	125.28
1169	60.144
1170	111.504
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1172	137.76
1173	150.96
1174	80.16
1175	110.124
1176	131.16
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1178	36.48
1179	141
1180	184.44
1181	13.116
1182	89.448
1183	63.3
1184	112.308
1185	27.792
1186	105.984
1187	21.216
1188	156.6
1189	143.52
1190	71.916
1191	207.96
1192	270.72
1193	-25.344
1194	113.412
1195	148.2
1196	155.16
1197	127.2
1198	-73.692
1199	119.316
1200	-38.916
1201	-16.128
1202	92.892

1203	74.16
1204	153.96
1205	113.64
1206	90.792
1207	86.844
1208	43.464
1209	69.336
1210	-13.62
1211	140.4
1212	114.684
1213	60.144
1214	135.48
1215	174.12
1216	96.072
1217	125.04
1218	-81.108
1219	64.68
1220	92.34
1221	-27.612
1222	102.336
1223	164.76
1224	84.576
1225	68.016
1226	50.016
1227	207.12
1228	73.788
1229	0
1230	188.64
1231	15.396
1232	178.08
1233	-32.34
1234	163.56
1235	98.928
1236	109.104
1237	120.72
1238	54.12
1239	225.6
1240	104.508
1241	162.24
1242	87.84
1243	274.2
1244	101.208
1245	172.32
1246	-10.1532
1247	204.84
1248	37.836
1249	93.264
1250	147.36
1251	131.4
1252	62.844
1253	52.668

1254	224.04
1255	99.672
1256	-921.6
1257	67.572
1258	49.98
1259	-22.068
1260	0
1261	-39.816
1262	184.56
1263	44.352
1264	156.84
1265	4.4412
1266	16.296
1267	164.76
1268	-46.068
1269	147.36
1270	128.16
1271	85.044
1272	37.344
1273	-5.982
1274	77.928
1275	66.072
1276	178.92
1277	-25.596
1278	173.28
1279	110.112
1280	64.92
1281	-30.228
1282	48.432
1283	77.34
1284	19.752
1285	-4.5636
1286	44.16
1287	-111.264
1288	82.428
1289	134.52
1290	52.044
1291	42.876
1292	117.96
1293	39.876
1294	81.42
1295	46.188
1296	10.8048
1297	162.36
1298	58.824
1299	51.132
1300	-10.86
1301	65.256
1302	17.112
1303	57.684
1304	28.104

1305	28.152
1306	32.892
1307	-128.64
1308	117.852
1309	61.368
1310	-18.912
1311	195.72
1312	33.204
1313	166.32
1314	163.56
1315	163.92
1316	39.864
1317	83.076
1318	169.68
1319	12.828
1320	152.76
1321	35.46
1322	130.8
1323	101.964
1324	131.4
1325	113.784
1326	4.8876
1327	169.92
1328	158.88
1329	47.664
1330	16.488
1331	122.52
1332	210.96
1333	23.328
1334	185.64
1335	23.484
1336	215.52
1337	155.4
1338	-98.268
1339	139.44
1340	174.12
1341	41.136
1342	84.324
1343	195.36
1344	66
1345	103.104
1346	125.04
1347	5.3328
1348	208.2
1349	86.82
1350	30.96
1351	-77.004
1352	73.908
1353	100.728
1354	135.84
1355	30.552

1356	101.868
1357	173.28
1358	113.76
1359	97.032
1360	120
1361	-12.012
1362	123.6
1363	-36.432
1364	98.472
1365	67.944
1366	69.708
1367	338.88
1368	-78.216
1369	240.24
1370	215.28
1371	73.524
1372	137.52
1373	101.148
1374	22.956
1375	-21.276
1376	37.164
1377	74.46
1378	-60.768
1379	308.64
1380	48.168
1381	-23.76
1382	358.92
1383	-19.236
1384	-79.068
1385	-45.492
1386	105.06
1387	191.76
1388	51.276
1389	83.448
1390	67.236
1391	-73.98
1392	-71.304
1393	159.48
1394	264.12
1395	114.636
1396	29.04
1397	64.128
1398	-18.612
1399	156.84
1400	115.38

2) XRD analysis of a sample of cuprorivaite

X-ray powder diffraction data have been used to detect the crystalline phases contained in the sample.

X-ray powder diffraction data were collected in theta-theta reflection geometry with the CuKα radiation on a PANalytical X'PERT PRO diffractometer, PW3050 goniometer equipped with an X'Celerator detector. The LFF tube operated at 40KV, 40mA. Data were collected using a step size of 0.017° and a count time of 10s per step.

The data were analysed using a PANAlytical X'PERT HighScore V.2.2b program. The position of the experimental 2theta peaks was determined using the minimum 2nd derivative method; the processed data were then used in the search and match procedure implemented in the program, which makes use of the ICDD PDF2 database (see Table 2).

The final result of this investigation determined the presence of cuprorivaite.

Scan Parameters

Dataset Name:	bludegitto
File name:	D:\riccardo\documenti\x\aldo\bludegitto.xrdml
Comment:	Configuration=BRACKET, Owner=User-1, Creation date=1/9/2008 12:11:56 PM Goniometer=PW3050/60 (Theta/Theta); Minimum step size 2Theta:0.001; Minimum step size Omega:0.001 Sample stage=PW3071/xx Bracket Diffractometer system=XPERT-PRO Measurement program=RIC, Owner=User-1, Creation date=1/16/2008 10:35:32 AM bracket
Operator:	labin
Raw Data Origin:	XRD measurement (*.XRDML)
Scan Axis:	Gonio
Start Position [°2Th.]:	4.0054
End Position [°2Th.]:	79.9784
Step Size [°2Th.]:	0.0170
Scan Step Time [s]:	10.3373
Scan Type:	Continuous
PSD Mode:	Scanning
PSD Length [°2Th.]:	2.12
Offset [°2Th.]:	0.0000
Divergence Slit Type:	Fixed
Divergence Slit Size [°]:	0.4785
Specimen Length [mm]:	10.00
Measurement Temperature [°C]:	25.00
Anode Material:	Cu
K-Alpha1 [Å]:	1.54060
K-Alpha2 [Å]:	1.54443
K-Beta [Å]:	1.39225
K-A2 / K-A1 Ratio:	0.50000
Generator Settings:	40 mA, 40 kV

Diffractometer Type:	0000000011029761
Diffractometer Number:	0
Goniometer Radius [mm]:	240.00
Dist. Focus-Diverg. Slit [mm]:	91.00
Incident Beam Monochromator:	No
Spinning:	No

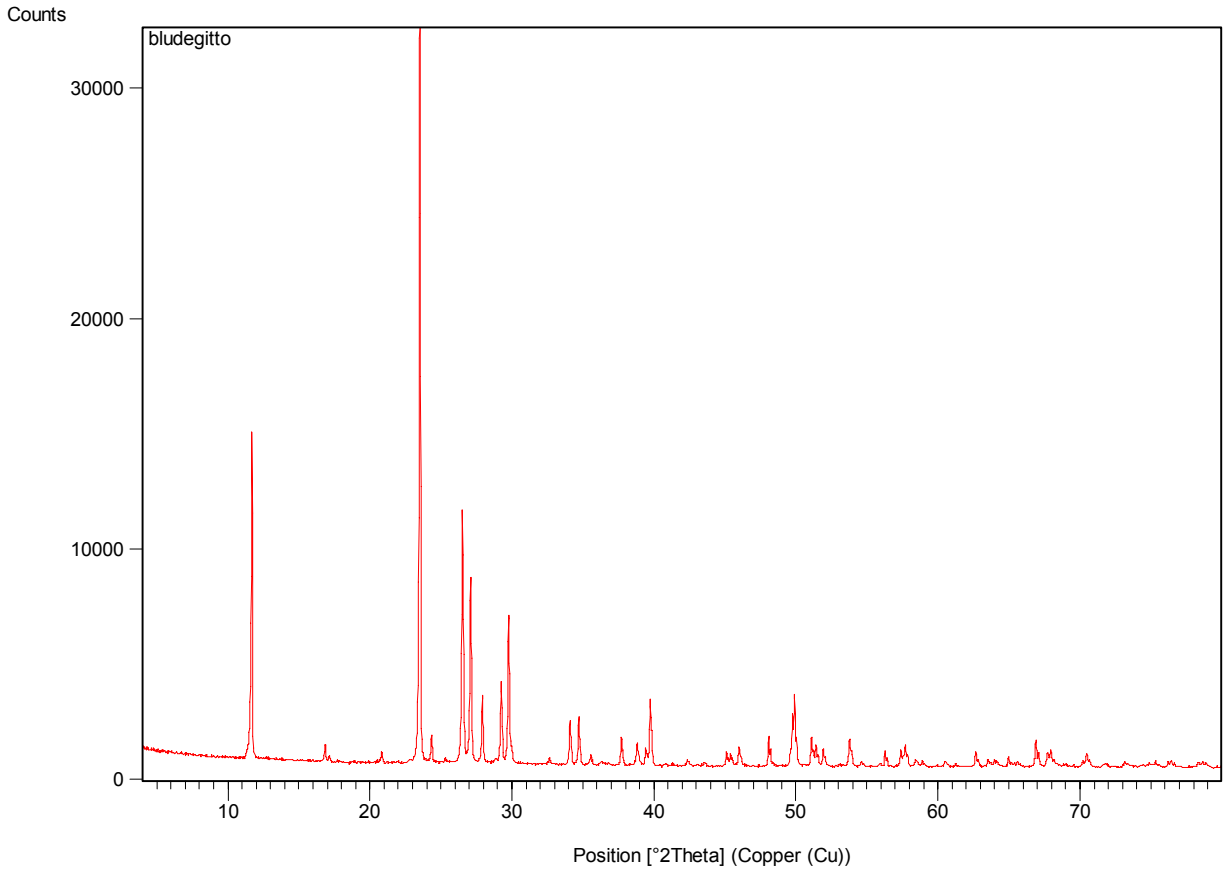

Fig. SI3 X-ray powder diffraction pattern of Egyptian blue

Table 1: Phase matching results

Ref.Code	Score	Compound Name	Displ.[°2Th]	Scale Fac.	Chem. Formula
01-074-0828	79	Calcium Copper Silicate	-0.036	0.270	Ca Cu (Si4 O10)

Document History

Insert Measurement:
- File name = "bludegitto.xrdml"

Default properties:
- Measurement step axis = "None"
- Internal wavelengths used from anode material: Copper (Cu)
- Original K-Alpha1 wavelength = "1.54060"
- Used K-Alpha1 wavelength = "1.54060"
- Original K-Alpha2 wavelength = "1.54443"
- Used K-Alpha2 wavelength = "1.54443"
- Original K-Beta wavelength = "1.39225"
- Used K-Beta wavelength = "1.39225"
- Incident beam monochromator = "No"
- Dist. focus to div. slit = "91.00000"
- Irradiated length = "10.00000"
- Spinner used = "No"
- Receiving slit size = "0.10000"
- Step axis value = "0.00000"
- Offset = "0.00000"
- Sample length = "10.00000"

Interpolate Step Size:
- Step Size = "Derived"

Determine Background:
- Correction method = "Automatic"
- Bending factor = "0"
- Use smoothed input data = "Yes"
- Granularity = "21"
- Add to net scan = "Nothing"

Search Peaks:
- Minimum significance = "1.00"
- Minimum tip width = "0.05"
- Maximum tip width = "3.00"
- Peak base width = "5.00"
- Method = "Minimum 2nd derivative"

Search & Match:
- Data source = "Peak list"
- Restriction = "None"
- Scoring schema = "Multi phase"
- Auto residue = "Yes"
- Match intensity = "Yes"
- Demote unmatched strong = "Yes"
- Allow pattern shift = "Yes"
- Two theta shift = "0"
- Identify = "No"

Table 2: Peak position, intensity and phase matching for the pattern shown in Fig. SI3.

No.	Pos. [°2Th.]	d-spacing [Å]	Rel. Int. [%]	Area [cts*°2Th.]	Height [cts]	Matched by
1	11.7046	7.56087	44.49	946.12	14334.01	01-074-0828
2	16.8696	5.25577	2.20	46.89	710.45	01-074-0828
3	17.1594	5.16765	0.86	18.26	276.68	01-074-0828
4	20.8408	4.26241	1.45	23.07	466.04	01-074-0828
5	23.5077	3.78453	100.00	3190.20	32221.67	01-074-0828
6	24.3568	3.65448	3.82	121.74	1229.64	01-074-0828
7	25.3047	3.51970	0.76	16.10	243.92	
8	26.5169	3.36149	33.81	1078.71	10895.19	01-074-0828
9	27.0898	3.29169	24.99	664.32	8051.72	01-074-0828
10	27.9160	3.19612	9.27	246.55	2988.22	01-074-0828
11	29.2400	3.05434	10.71	284.71	3450.75	01-074-0828
12	29.7640	3.00175	19.98	531.30	6439.47	01-074-0828
13	32.6369	2.74378	1.00	16.03	323.76	01-074-0828
14	34.0976	2.62952	6.03	128.31	1943.96	01-074-0828
15	34.7079	2.58467	6.57	139.67	2116.07	01-074-0828
16	35.5765	2.52352	1.42	30.30	459.09	01-074-0828
17	36.3360	2.47250	0.56	35.95	181.54	01-074-0828
18	37.7132	2.38532	3.74	79.44	1203.61	01-074-0828
19	38.8180	2.31994	2.98	63.38	960.18	01-074-0828
20	39.4325	2.28519	2.33	37.18	751.14	01-074-0828
21	39.7513	2.26572	8.89	311.60	2863.99	01-074-0828
22	40.8044	2.20964	0.29	25.38	93.30	01-074-0828
23	41.2978	2.18438	0.25	26.37	80.78	
24	42.3438	2.13280	0.84	29.47	270.86	01-074-0828
25	43.0312	2.10031	0.21	21.64	66.31	01-074-0828
26	43.5801	2.07512	0.66	17.40	213.17	01-074-0828
27	45.1148	2.00803	1.96	68.84	632.71	01-074-0828
28	45.4010	1.99604	1.67	73.14	537.79	01-074-0828
29	46.0057	1.97120	2.68	117.34	862.79	01-074-0828
30	48.0882	1.89058	4.09	143.44	1318.36	01-074-0828
31	49.6088	1.83614	2.09	73.33	674.00	01-074-0828
32	49.7713	1.83052	7.10	248.93	2287.95	01-074-0828
33	49.9083	1.82582	9.68	339.24	3118.02	01-074-0828
34	51.1084	1.78573	3.99	174.83	1285.51	01-074-0828
35	51.4284	1.77536	3.01	105.46	969.26	01-074-0828
36	51.9301	1.75938	2.35	82.49	758.16	01-074-0828
37	53.7812	1.70311	3.73	163.65	1203.28	01-074-0828
38	54.5972	1.67957	0.61	21.38	196.49	01-074-0828
39	55.8589	1.64459	0.45	23.47	143.82	01-074-0828
40	56.2818	1.63323	2.11	73.89	679.16	01-074-0828
41	57.3941	1.60419	2.19	96.07	706.40	01-074-0828
42	57.7032	1.59633	3.00	105.21	966.98	01-074-0828
43	58.4300	1.57820	1.02	26.80	328.41	01-074-0828
44	58.9101	1.56647	0.83	29.10	267.42	01-074-0828
45	60.5175	1.52866	0.76	53.07	243.89	01-074-0828
46	61.2513	1.51209	0.43	18.99	139.61	01-074-0828
47	62.6725	1.48118	2.06	90.25	663.63	01-074-0828
48	63.5239	1.46336	1.01	53.16	325.71	01-074-0828
49	63.9851	1.45392	0.97	34.03	312.76	01-074-0828
50	64.1722	1.45013	0.78	41.24	252.72	01-074-0828
51	64.9746	1.43415	1.28	44.76	411.41	01-074-0828
52	65.3942	1.42596	0.65	16.98	208.11	01-074-0828
53	65.5996	1.42199	0.73	32.10	236.06	01-074-0828
54	66.8945	1.39757	3.47	152.10	1118.41	01-074-0828
55	67.7355	1.38225	1.98	86.58	636.62	01-074-0828
56	67.9636	1.37817	2.01	105.56	646.81	01-074-0828
57	68.9323	1.36115	0.27	37.29	85.69	01-074-0828
58	69.5417	1.35070	0.36	18.71	114.65	01-074-0828
59	70.1998	1.33964	0.61	31.96	195.85	01-074-0828
60	70.4860	1.33490	1.97	103.50	634.21	01-074-0828
61	71.7623	1.31427	0.43	60.30	138.55	01-074-0828
62	73.1450	1.29280	0.81	28.42	261.24	01-074-0828

63	74.4776	1.27293	0.37	19.63	120.25	01-074-0828
64	74.8520	1.26749	0.59	41.44	190.42	01-074-0828
65	75.3470	1.26039	0.88	23.08	282.87	01-074-0828
66	76.2151	1.24818	0.76	26.57	244.22	01-074-0828
67	76.4418	1.24504	0.94	49.48	303.19	01-074-0828
68	78.3945	1.21884	0.59	36.26	190.46	01-074-0828

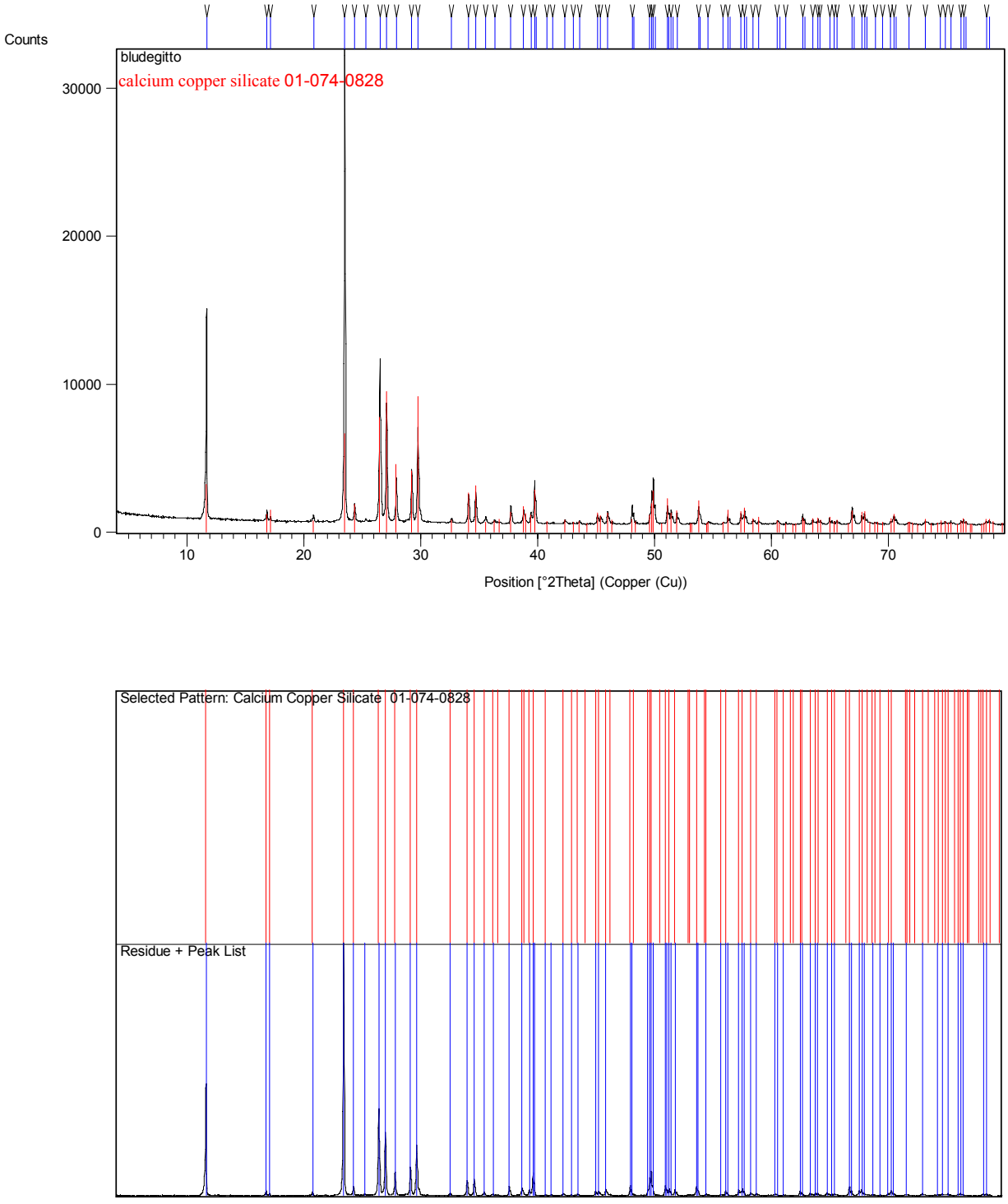

Fig. SI4: Comparison between the experimental peaks (blue) and those relative to the matched calcium copper silicate phase (red, PDF number: 01-074-0828). The experimental pattern is also shown (black).

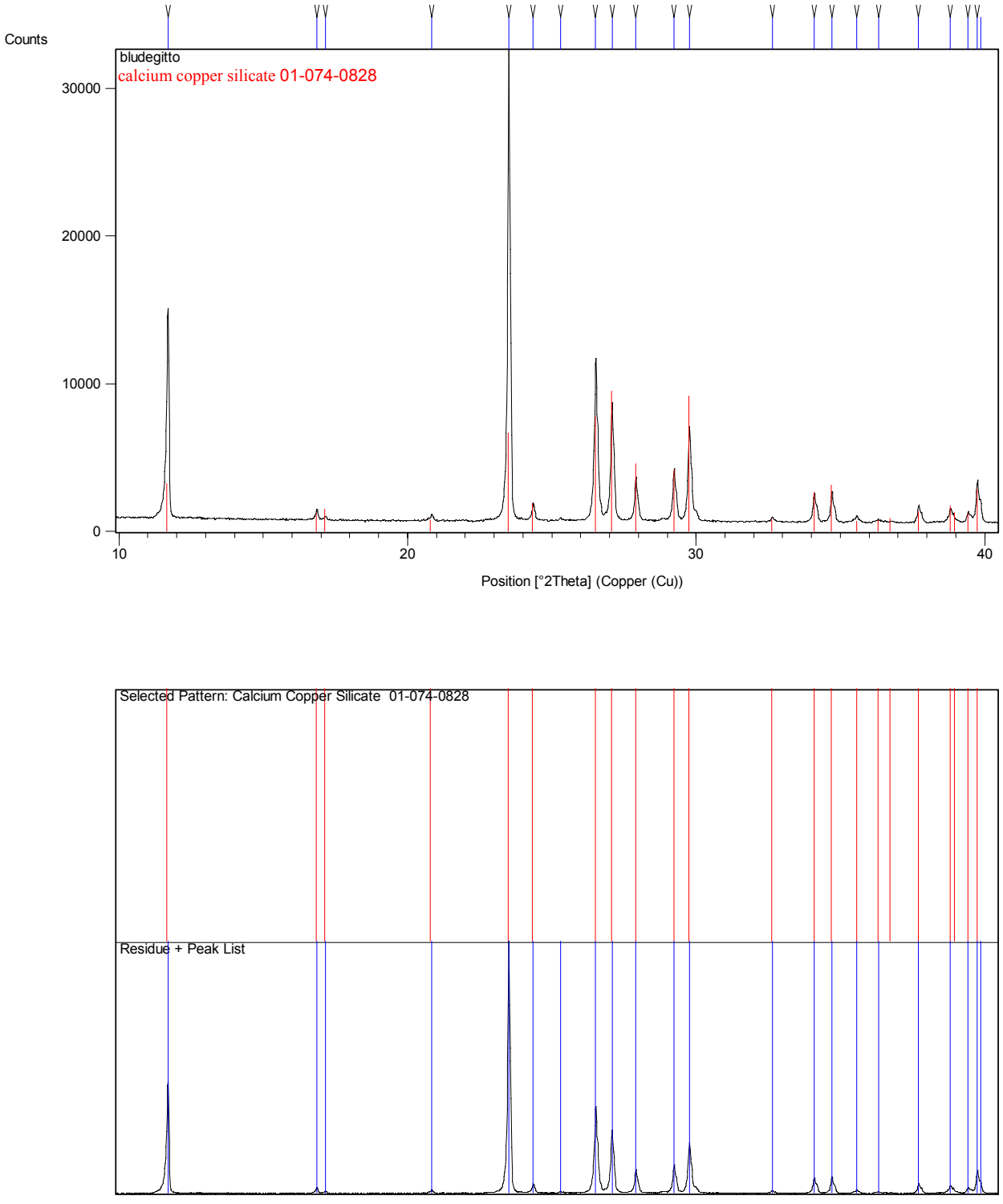

Fig. SI5: Enlargement of Fig. SI4 in the 10-40° 2theta range

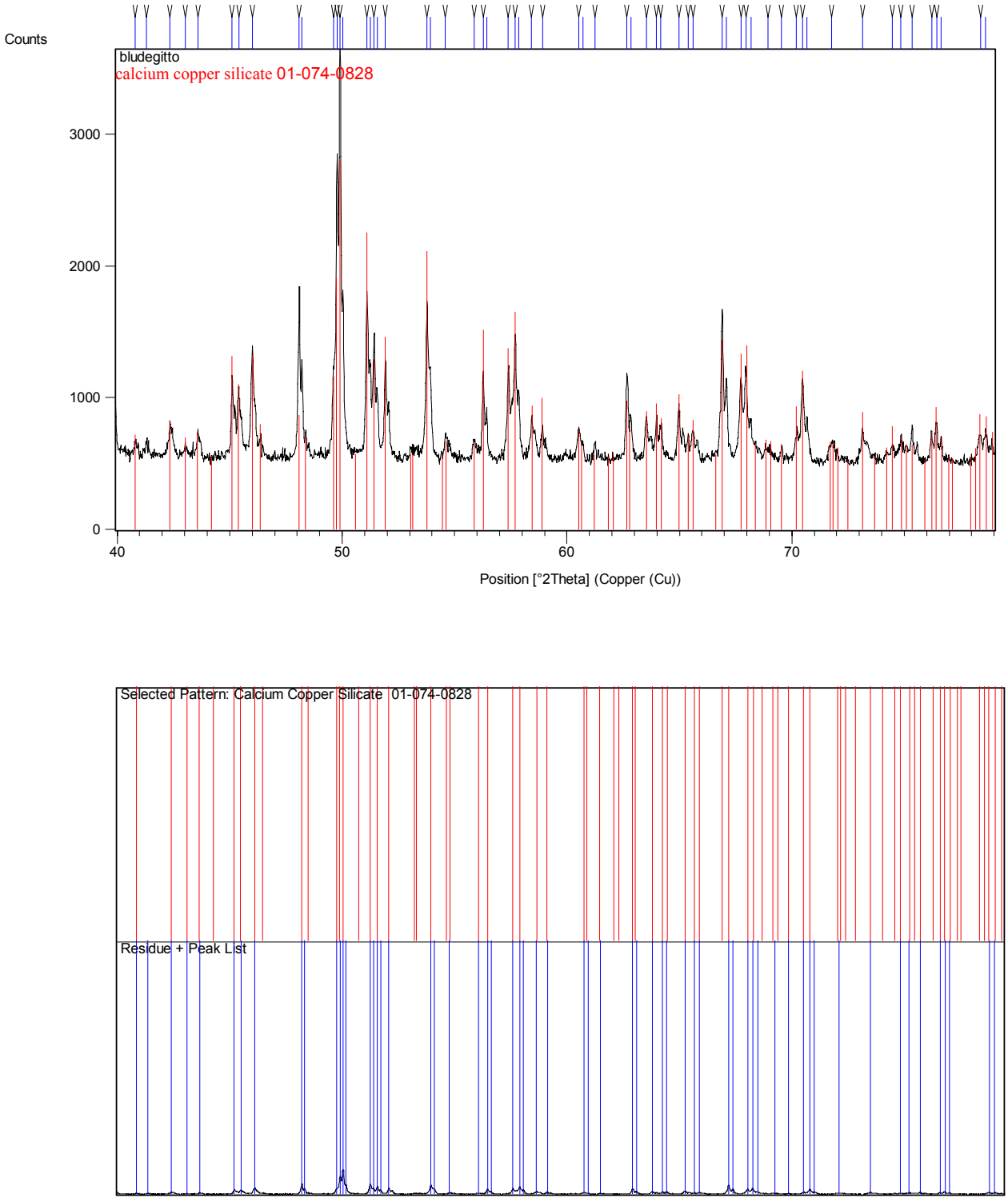

Fig. SI6: Enlargement of Fig. SI4 in the 40-80° 2theta range.

Details of Calcium Copper Silicate, Ref. Code 01-074-0828

Name and formula

Reference code: 01-074-0828

ICSD name: Calcium Copper Silicate

Empirical formula: $CaCuO_{10}Si_4$
Chemical formula: $CaCu (Si_4O_{10})$

Crystallographic parameters

Crystal system: Tetragonal
Space group: P4/ncc
Space group number: 130

a (Å): 7.3000
b (Å): 7.3000
c (Å): 15.1200
Alpha (°): 90.0000
Beta (°): 90.0000
Gamma (°): 90.0000

Calculated density (g/cm^3): 3.10
Measured density (g/cm^3): 3.06
Volume of cell (10^6 pm^3): 805.74
Z: 4.00

RIR: 1.21

Subfiles and Quality

Subfiles: Inorganic
Corrosion
Modelled additional pattern
Quality: Calculated (C)

Comments

Additional pattern: See PDF 12-512.
See PDF 12-512.
ICSD collection code: 026502

References

Primary reference: *Calculated from ICSD using POWD-12++*, (1997)
Structure: Pabst, A., *Acta Crystallogr.*, **12**, 733, (1959)

Peak list

No.	h	k	l	d [A]	2Theta[deg]	I [%]
1	0	0	2	7.56000	11.696	26.3
2	1	0	2	5.25139	16.870	5.1
3	1	1	0	5.16188	17.164	8.3
4	1	1	2	4.26296	20.821	0.8
5	0	0	4	3.78000	23.517	67.5

6	2	0	0	3.65000	24.367	13.3
7	1	0	4	3.35669	26.533	80.3
8	2	0	2	3.28695	27.107	100.0
9	2	1	1	3.19112	27.937	44.5
10	1	1	4	3.04973	29.260	39.6
11	2	1	2	2.99714	29.786	96.6
12	2	1	3	2.74005	32.655	2.2
13	2	0	4	2.62570	34.120	22.9
14	2	2	0	2.58094	34.730	28.7
15	0	0	6	2.52000	35.598	0.6
16	2	1	4	2.47073	36.332	1.7
17	2	2	2	2.44252	36.766	3.1
18	1	0	6	2.38206	37.734	8.4
19	3	0	2	2.31631	38.848	13.2
20	3	1	0	2.30846	38.985	7.7
21	3	1	1	2.28202	39.456	6.5
22	1	1	6	2.26455	39.773	25.8
23	3	1	2	2.20783	40.839	1.7
24	2	2	4	2.13148	42.371	3.0
25	3	1	3	2.09878	43.064	1.6
26	2	0	6	2.07376	43.610	2.1
27	3	0	4	2.04605	44.232	0.1
28	3	2	1	2.00674	45.146	8.7
29	2	1	6	1.99483	45.430	6.3
30	3	1	4	1.97013	46.032	8.8
31	3	2	2	1.95573	46.391	2.9
32	0	0	8	1.89000	48.104	3.7
33	3	2	3	1.87873	48.411	1.9
34	3	1	5	1.83492	49.644	7.1
35	1	0	8	1.82967	49.796	15.5
36	4	0	0	1.82500	49.932	25.6
37	2	2	6	1.80140	50.632	0.4
38	3	2	4	1.78476	51.138	19.4
39	1	1	8	1.77478	51.447	8.5
40	4	1	1	1.75850	51.958	10.5
41	4	1	2	1.72387	53.083	0.4
42	3	3	0	1.72063	53.190	0.4
43	3	1	6	1.70221	53.812	17.9
44	3	2	5	1.68239	54.498	0.3
45	2	0	8	1.67834	54.641	1.6
46	4	0	4	1.64348	55.900	1.4
47	4	2	0	1.63233	56.316	11.2
48	4	1	4	1.60335	57.427	9.6
49	4	2	2	1.59556	57.734	12.7
50	3	2	6	1.57723	58.469	4.7
51	3	3	4	1.56602	58.929	5.4
52	4	1	5	1.52790	60.551	2.6
53	2	2	8	1.52486	60.684	1.4
54	0	0	10	1.51200	61.255	0.5
55	4	2	4	1.49857	61.864	0.3
56	2	1	9	1.49381	62.083	0.6
57	1	0	10	1.48058	62.701	5.1
58	4	0	6	1.47810	62.818	2.7
59	3	1	8	1.46239	63.571	4.2
60	4	3	1	1.45324	64.019	4.9
61	4	1	6	1.44870	64.243	3.6
62	5	0	2	1.43351	65.007	5.7
63	5	1	1	1.42527	65.430	2.1
64	3	3	6	1.42099	65.652	3.5
65	4	3	3	1.40235	66.637	0.5
66	2	0	10	1.39689	66.932	10.4
67	3	2	8	1.38159	67.773	9.2
68	5	1	3	1.37716	68.020	9.9

69	4	2	6	1.37002	68.424	1.5
70	5	0	4	1.36194	68.887	1.8
71	3	1	9	1.35836	69.094	1.7
72	5	2	1	1.35016	69.574	1.5
73	5	1	4	1.33884	70.248	4.7
74	5	2	2	1.33430	70.523	7.8
75	4	3	5	1.31478	71.730	1.7
76	4	0	8	1.31285	71.852	1.6
77	5	2	3	1.30905	72.093	1.2
78	4	2	7	1.30229	72.527	0.1
79	3	2	9	1.29212	73.190	4.3
80	3	0	10	1.28426	73.711	0.5
81	5	2	4	1.27601	74.268	1.3
82	3	3	8	1.27234	74.518	3.1
83	2	1	11	1.26684	74.897	2.2
84	5	0	6	1.26329	75.144	1.6
85	0	0	12	1.26000	75.374	1.5
86	5	3	0	1.25194	75.945	0.2
87	5	3	1	1.24767	76.252	2.2
88	5	1	6	1.24479	76.460	4.8
89	1	0	12	1.24164	76.689	2.2
90	5	2	5	1.23698	77.031	0.5
91	4	2	8	1.23512	77.168	0.4
92	1	1	12	1.22406	77.997	0.2
93	4	4	4	1.22126	78.210	1.0
94	4	1	9	1.21868	78.407	3.9
95	5	3	3	1.21502	78.689	3.6
96	3	2	10	1.21146	78.965	2.2
97	6	0	2	1.20121	79.773	0.6
98	5	2	6	1.19333	80.407	6.8
99	2	0	12	1.19103	80.594	3.8
100	5	3	4	1.18845	80.805	1.1
101	6	1	2	1.18527	81.067	2.9
102	3	1	11	1.18103	81.419	0.9
103	2	1	12	1.17549	81.885	0.6
104	6	1	3	1.16747	82.570	1.6
105	4	0	10	1.16432	82.842	0.9
106	6	0	4	1.15815	83.382	0.6
107	5	3	5	1.15673	83.507	0.7
108	5	0	8	1.15541	83.624	1.5
109	6	2	0	1.15423	83.729	1.0
110	4	1	10	1.14978	84.127	2.7
111	6	1	4	1.14385	84.664	0.3
112	5	1	8	1.14101	84.924	3.9
113	3	2	11	1.13684	85.310	2.8
114	2	2	12	1.13227	85.736	3.8
115	5	3	6	1.12120	86.791	4.4
116	3	0	12	1.11890	87.014	2.6
117	6	1	5	1.11548	87.348	0.5
118	5	4	3	1.11197	87.694	0.4
119	4	2	10	1.10925	87.964	2.3
120	3	1	12	1.10598	88.292	1.2
121	6	2	4	1.10391	88.500	0.8
122	4	3	9	1.10201	88.693	1.7
123	6	0	6	1.09562	89.348	0.1
124	5	4	4	1.09150	89.776	0.5
125	5	1	9	1.08966	89.969	0.4