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**Supporting information for article:**

**High-accuracy X-ray absorption spectra from mM solutions of nickel (II) complexes with multiple solutions using transmission XAS**

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## Supporting information - RV5033

Table S1. Measured X-ray mass attenuation coefficients  $[\mu]_S$  of the *bis*(N-i-propyl-salicylaldiminato) nickel(II) complex from the intensity measurements ( $I_0$  and  $I$ ) with a 15 mM solution of the complex, and its corresponding solvent. Several experimental systematics including energy calibration, dark-current, solvent attenuations, harmonic contamination and thickness-ratio (from the actual solvent attenuation and fitted background of the sample (solution) were corrected to obtain the final result. The first column lists calibrated energies (Section 4.3) in eV, and their associated uncertainties in parentheses. The second, third and fourth columns present corrected total X-ray mass attenuation coefficients  $[\mu]_S$  with associated relative and percentage uncertainties. The fifth column lists the absolute uncertainties including the uncertainty contributions from the thickness ratio  $t_{ratio}$  and column density  $[pt]_c$  measurements. The sixth and the seventh columns list the (effective) photoelectric absorption coefficient  $[\mu]_{pe}$  determined by subtracting the tabulated X-ray mass attenuations of the complex for the Rayleigh and Compton scattering from the total experimental X-ray mass attenuation coefficients  $[\mu]_S$  at measured energies, with their corresponding uncertainties. The eighth column lists the X-ray mass attenuations of Rayleigh and Compton scattering, where the corresponding uncertainty of  $[\mu]_{R+C}$  was determined from half of the variation between FFAST and XCOM tabulated values.

<i>Energy</i> (eV)	$[\mu]_S$ ( $cm^2/g$ )	$\sigma_{[\mu]_{rel}}$ ( $cm^2/g$ )	$\sigma_{[\mu]_{rel}}$ (%)	$\sigma_{[\mu]_{abs}}$ ( $cm^2/g$ )	$[\mu]_{pe}$ ( $cm^2/g$ )	$\sigma_{[\mu]_{pe}}$ ( $cm^2/g$ )	$[\mu]_{R+C}$ ( $cm^2/g$ )
7016.75(10)	21.5226	0.6013	2.79	0.6562	20.8524	0.6014	0.670(11)
7618.05(08)	14.8641	0.2674	1.80	0.3056	14.2368	0.2678	0.627(14)
8019.31(09)	12.4312	0.2454	1.97	0.2774	11.8503	0.2455	0.581(08)
8019.36(12)	13.4087	0.3431	2.56	0.3777	12.8278	0.3432	0.581(08)
8059.16(07)	13.4538	0.1749	1.30	0.2096	12.8818	0.1756	0.572(15)
8099.42(07)	12.7546	0.2021	1.58	0.2350	12.1916	0.2033	0.563(22)
8139.14(07)	12.9023	0.1640	1.27	0.1972	12.3479	0.1665	0.554(29)
8179.60(07)	10.7739	0.1630	1.51	0.1909	10.2290	0.1670	0.545(36)
8219.50(07)	11.6627	0.1525	1.31	0.1826	11.1280	0.1591	0.535(45)
8259.75(08)	11.6365	0.2348	2.02	0.2649	11.1113	0.2412	0.525(55)
8259.80(12)	11.0898	0.2378	2.14	0.2665	10.5647	0.2441	0.525(55)
8299.69(07)	12.1917	0.1382	1.13	0.1697	11.6760	0.1525	0.516(64)
8328.92(07)	13.0854	0.1353	1.03	0.1690	12.5592	0.1456	0.526(54)
8329.93(07)	13.1148	0.1287	0.98	0.1625	12.5849	0.1381	0.530(50)
8330.88(07)	13.6350	0.1367	1.00	0.1718	13.1015	0.1444	0.534(47)
8331.95(07)	13.4321	0.1420	1.06	0.1765	12.8946	0.1482	0.538(43)
8332.78(12)	13.5470	0.2232	1.65	0.2580	13.0065	0.2267	0.541(40)
8332.84(08)	13.6453	0.1582	1.16	0.1933	13.1045	0.1630	0.541(39)
8333.73(07)	14.1161	0.1316	0.93	0.1679	13.5771	0.1352	0.539(31)
8334.75(07)	14.5188	0.1273	0.88	0.1646	13.9762	0.1302	0.543(27)

8335.70(07)	14.7894	0.1555	1.05	0.1935	14.2434	0.1574	0.546(24)
8336.65(07)	14.7551	0.1332	0.90	0.1711	14.2058	0.1348	0.549(21)
8337.71(07)	14.6010	0.1266	0.87	0.1641	14.0481	0.1277	0.553(17)
8338.72(07)	15.3682	0.1310	0.85	0.1704	14.8119	0.1317	0.556(14)
8339.21(07)	15.4175	0.1297	0.84	0.1692	14.8596	0.1303	0.558(12)
8339.63(07)	15.7792	0.1323	0.84	0.1727	15.2200	0.1327	0.559(11)
8340.10(07)	16.2828	0.1353	0.83	0.1770	15.7220	0.1356	0.561(09)
8340.64(07)	17.2415	0.1331	0.77	0.1773	16.6791	0.1333	0.563(08)
8341.11(07)	17.9227	0.1334	0.74	0.1792	17.3588	0.1335	0.564(06)
8341.65(07)	19.4273	0.1291	0.66	0.1787	18.8618	0.1292	0.566(05)
8342.12(07)	20.5521	0.1233	0.60	0.1758	19.9852	0.1234	0.567(03)
8342.60(07)	21.9244	0.1209	0.55	0.1768	21.3561	0.1209	0.568(02)
8343.13(07)	23.8207	0.1322	0.55	0.1928	23.2509	0.1322	0.570(00)
8343.73(07)	26.0666	0.1338	0.51	0.2001	25.4951	0.1338	0.572(02)
8344.20(07)	28.8136	0.1365	0.47	0.2098	28.2408	0.1366	0.573(03)
8344.69(08)	32.4253	0.1787	0.55	0.2610	31.8512	0.1787	0.574(04)
8344.75(12)	32.4296	0.2346	0.72	0.3169	31.8554	0.2346	0.574(04)
8345.23(07)	35.3511	0.1262	0.36	0.2158	34.7757	0.1263	0.575(05)
8345.64(12)	39.1722	0.2157	0.55	0.3149	38.5958	0.2158	0.576(06)
8345.70(08)	39.1773	0.1620	0.41	0.2612	38.6007	0.1621	0.577(07)
8346.18(07)	42.7013	0.1275	0.30	0.2356	42.1235	0.1277	0.578(08)
8346.71(07)	46.9622	0.1311	0.28	0.2499	46.3833	0.1314	0.579(09)
8347.25(07)	51.2888	0.1239	0.24	0.2536	50.7087	0.1244	0.580(10)
8347.72(07)	56.6255	0.1597	0.28	0.3029	56.0444	0.1601	0.581(11)
8348.26(07)	61.1106	0.1254	0.21	0.2798	60.5284	0.1260	0.582(12)
8348.80(07)	65.9400	0.1305	0.20	0.2970	65.3568	0.1311	0.583(13)
8349.39(07)	70.2153	0.1241	0.18	0.3013	69.6311	0.1249	0.584(14)
8349.88(07)	73.7979	0.1271	0.17	0.3134	73.2128	0.1280	0.585(15)
8350.36(07)	76.1117	0.1342	0.18	0.3263	75.5259	0.1352	0.586(16)
8350.83(07)	77.8896	0.1229	0.16	0.3195	77.3032	0.1240	0.586(16)
8351.31(07)	78.5225	0.1256	0.16	0.3238	77.9354	0.1268	0.587(17)
8351.85(07)	78.9331	0.1277	0.16	0.3269	78.3455	0.1290	0.588(18)
8352.32(07)	78.7748	0.1275	0.16	0.3263	78.1867	0.1288	0.588(18)
8352.92(07)	79.0798	0.1280	0.16	0.3276	78.4911	0.1294	0.589(19)
8353.40(07)	78.4030	0.1299	0.17	0.3278	77.8140	0.1313	0.589(19)
8353.81(08)	77.4465	0.1663	0.21	0.3618	76.8572	0.1675	0.589(19)
8353.87(12)	77.4726	0.2153	0.28	0.4108	76.8834	0.2162	0.589(19)
8354.35(11)	76.8114	0.1996	0.26	0.3935	76.2219	0.2006	0.590(20)
8354.41(08)	76.7963	0.1536	0.20	0.3474	76.2068	0.1549	0.590(20)
8354.96(07)	75.8004	0.2431	0.32	0.4344	75.2107	0.2439	0.590(20)
8355.43(07)	75.6457	0.1676	0.22	0.3585	75.0561	0.1687	0.590(20)
8355.91(11)	73.8969	0.2174	0.29	0.4039	73.3073	0.2182	0.590(20)
8355.97(08)	74.1280	0.1601	0.22	0.3472	73.5384	0.1613	0.590(20)
8356.45(07)	73.0458	0.1318	0.18	0.3162	72.4564	0.1332	0.589(19)
8356.92(07)	71.7103	0.1272	0.18	0.3082	71.1211	0.1286	0.589(19)
8357.40(07)	70.4098	0.1397	0.20	0.3175	69.8210	0.1410	0.589(19)

8357.82(11)	69.6499	0.2141	0.31	0.3899	69.0614	0.2149	0.589(19)
8357.88(08)	69.6967	0.1501	0.22	0.3261	69.1083	0.1513	0.589(18)
8358.36(07)	68.4578	0.1323	0.19	0.3052	67.8698	0.1336	0.588(18)
8358.83(07)	66.8694	0.1308	0.20	0.2997	66.2821	0.1320	0.587(17)
8359.37(07)	66.4245	0.1245	0.19	0.2922	65.8379	0.1256	0.587(17)
8359.79(07)	65.0605	0.1301	0.20	0.2944	64.4747	0.1311	0.586(16)
8360.27(07)	64.0950	0.1381	0.22	0.3000	63.5101	0.1389	0.585(15)
8360.82(07)	62.9721	0.2144	0.34	0.3735	62.3883	0.2149	0.584(14)
8361.35(07)	62.9690	0.1239	0.20	0.2830	62.3865	0.1246	0.583(13)
8361.77(07)	61.5139	0.1411	0.23	0.2965	60.9325	0.1415	0.581(11)
8362.25(07)	60.7361	0.1252	0.21	0.2786	60.1561	0.1256	0.580(10)
8362.73(07)	60.4462	0.1273	0.21	0.2800	59.8678	0.1276	0.579(08)
8363.21(07)	59.8269	0.1398	0.23	0.2909	59.2501	0.1399	0.577(07)
8363.68(07)	58.6372	0.1299	0.22	0.2781	58.0621	0.1300	0.575(05)
8364.10(07)	57.9894	0.1467	0.25	0.2932	57.4160	0.1467	0.573(03)
8364.58(07)	58.0144	0.1262	0.22	0.2728	57.4430	0.1262	0.571(01)
8365.18(07)	56.9563	0.1258	0.22	0.2697	56.3877	0.1258	0.569(01)
8365.60(07)	56.2500	0.1321	0.23	0.2742	55.6834	0.1321	0.567(03)
8366.09(07)	55.2568	0.1351	0.24	0.2747	54.6927	0.1352	0.564(06)
8366.56(07)	54.5053	0.1260	0.23	0.2638	53.9438	0.1263	0.562(09)
8367.16(07)	53.8935	0.1323	0.25	0.2685	53.3355	0.1328	0.558(12)
8367.64(07)	54.2388	0.1253	0.23	0.2624	53.6839	0.1262	0.555(15)
8368.12(07)	53.2834	0.1233	0.23	0.2581	52.7316	0.1247	0.552(18)
8368.60(07)	52.5589	0.1253	0.24	0.2582	52.0105	0.1271	0.548(22)
8369.02(07)	51.9828	0.1300	0.25	0.2614	51.4375	0.1323	0.545(25)
8369.50(07)	51.5661	0.1202	0.23	0.2506	51.0246	0.1235	0.542(29)
8370.03(07)	51.0287	0.1381	0.27	0.2671	50.4915	0.1420	0.537(33)
8370.51(07)	50.8573	0.1340	0.26	0.2626	50.3242	0.1390	0.533(37)
8371.00(07)	49.8775	0.1400	0.28	0.2662	49.3488	0.1460	0.529(41)
8371.54(07)	50.2645	0.1570	0.31	0.2841	49.7408	0.1637	0.524(46)
8372.02(07)	49.3803	0.1256	0.25	0.2505	48.8614	0.1356	0.519(51)
8372.56(07)	48.6748	0.1253	0.26	0.2484	48.1615	0.1376	0.513(57)
8373.10(07)	48.3580	0.1224	0.25	0.2447	47.8507	0.1375	0.507(63)
8373.64(07)	48.2735	0.1253	0.26	0.2474	47.7724	0.1430	0.501(69)
8374.12(07)	47.9746	0.1281	0.27	0.2495	47.4793	0.1483	0.495(75)
8374.66(07)	47.4471	0.1431	0.30	0.2632	46.9558	0.1634	0.491(79)
8375.14(07)	47.2483	0.1242	0.26	0.2438	46.7563	0.1467	0.492(78)
8375.62(08)	47.1789	0.2747	0.58	0.3941	46.6864	0.2855	0.493(78)
8376.10(07)	47.9323	0.1291	0.27	0.2504	47.4391	0.1503	0.493(77)
8376.71(07)	47.3021	0.1701	0.36	0.2898	46.8082	0.1864	0.494(76)
8377.25(07)	47.5813	0.1632	0.34	0.2835	47.0868	0.1798	0.495(76)
8377.73(07)	47.1579	0.1419	0.30	0.2612	46.6627	0.1605	0.495(75)
8378.27(07)	47.4247	0.1345	0.28	0.2545	46.9289	0.1536	0.496(74)
8378.93(07)	48.0327	0.2302	0.48	0.3517	47.5361	0.2416	0.497(73)
8380.91(07)	49.5715	0.1263	0.25	0.2517	49.0724	0.1449	0.499(71)
8382.96(07)	51.8672	0.1206	0.23	0.2517	51.3655	0.1386	0.502(68)

8385.06(07)	54.2176	0.1216	0.22	0.2587	53.7133	0.1382	0.504(66)
8386.99(07)	56.8360	0.1191	0.21	0.2627	56.3293	0.1349	0.507(63)
8388.98(07)	57.8513	0.1290	0.22	0.2751	57.3422	0.1426	0.509(61)
8390.96(07)	58.7225	0.1174	0.20	0.2658	58.2110	0.1311	0.512(58)
8392.90(07)	59.2434	0.1589	0.27	0.3086	58.7295	0.1685	0.514(56)
8394.83(07)	60.3381	0.1257	0.21	0.2782	59.8218	0.1367	0.516(54)
8396.75(07)	60.6274	0.1353	0.22	0.2884	60.1087	0.1447	0.519(51)
8398.75(07)	61.4334	0.1279	0.21	0.2831	60.9122	0.1369	0.521(49)
8400.74(07)	61.3820	0.1273	0.21	0.2823	60.8584	0.1355	0.524(46)
8402.74(07)	60.6579	0.1271	0.21	0.2803	60.1318	0.1345	0.526(44)
8404.80(07)	61.2740	0.1117	0.18	0.2665	60.7454	0.1191	0.529(41)
8406.79(07)	59.9347	0.1218	0.20	0.2733	59.4037	0.1279	0.531(39)
8408.98(07)	59.3597	0.1250	0.21	0.2749	58.8260	0.1301	0.534(36)
8411.03(07)	58.5838	0.1252	0.21	0.2732	58.0476	0.1297	0.536(34)
8412.97(11)	57.5036	0.1967	0.34	0.3420	56.9650	0.1992	0.539(32)
8413.04(08)	57.5189	0.1510	0.26	0.2963	56.9803	0.1542	0.539(31)
8415.03(07)	57.5612	0.1255	0.22	0.2710	57.0202	0.1288	0.541(29)
8417.03(07)	56.9572	0.1191	0.21	0.2630	56.4137	0.1220	0.544(27)
8418.98(07)	56.1318	0.1289	0.23	0.2707	55.5860	0.1311	0.546(24)
8420.98(07)	56.0614	0.1135	0.20	0.2552	55.5132	0.1155	0.548(22)
8422.92(07)	56.3283	0.1168	0.21	0.2592	55.7777	0.1184	0.551(20)
8424.75(07)	55.5757	0.1189	0.21	0.2594	55.0229	0.1201	0.553(17)
8426.75(07)	55.3760	0.1202	0.22	0.2602	54.8208	0.1211	0.555(15)
8428.76(07)	56.0353	0.1148	0.20	0.2564	55.4777	0.1155	0.558(12)
8430.65(07)	55.3673	0.1159	0.21	0.2558	54.8075	0.1163	0.560(10)
8432.66(07)	55.1509	0.1170	0.21	0.2564	54.5886	0.1173	0.562(08)
8434.80(07)	54.3973	0.1199	0.22	0.2574	53.8325	0.1200	0.565(05)
8436.74(07)	54.3083	0.1187	0.22	0.2560	53.7412	0.1187	0.567(03)
8438.81(07)	54.5605	0.1201	0.22	0.2581	53.9908	0.1201	0.570(00)
8440.95(07)	54.9725	0.1261	0.23	0.2651	54.4004	0.1262	0.572(02)
8442.90(07)	54.7256	0.1166	0.21	0.2549	54.1512	0.1167	0.575(04)
8444.99(07)	54.9653	0.1142	0.21	0.2532	54.3884	0.1145	0.577(07)
8447.06(07)	55.1362	0.1182	0.21	0.2575	54.5568	0.1185	0.579(09)
8448.89(07)	55.2674	0.1257	0.23	0.2654	54.6871	0.1261	0.580(10)
8450.85(11)	55.4336	0.1906	0.34	0.3307	54.8536	0.1908	0.580(10)
8450.92(08)	55.8605	0.2589	0.46	0.4001	55.2805	0.2591	0.580(10)
8452.93(07)	55.6479	0.1202	0.22	0.2609	55.0681	0.1206	0.580(10)
8454.76(07)	56.7590	0.1196	0.21	0.2630	56.1795	0.1199	0.580(09)
8456.67(07)	56.1731	0.1213	0.22	0.2632	55.5938	0.1216	0.579(09)
8458.75(07)	56.1686	0.1222	0.22	0.2642	55.5896	0.1225	0.579(09)
8460.65(07)	56.3052	0.1147	0.20	0.2570	55.7265	0.1150	0.579(09)
8462.68(07)	56.3645	0.1211	0.21	0.2636	55.7860	0.1214	0.579(08)
8464.82(07)	56.4501	0.1173	0.21	0.2599	55.8719	0.1176	0.578(08)
8466.79(07)	56.6298	0.1155	0.20	0.2586	56.0518	0.1158	0.578(08)
8468.88(07)	56.5766	0.1207	0.21	0.2636	55.9990	0.1209	0.578(08)
8470.96(07)	56.4156	0.1154	0.20	0.2580	55.8382	0.1156	0.577(07)

8472.94(07)	56.3089	0.1176	0.21	0.2599	55.7318	0.1178	0.577(07)
8475.02(07)	56.2737	0.1097	0.19	0.2519	55.6968	0.1099	0.577(07)
8477.06(07)	56.4859	0.1133	0.20	0.2561	55.9093	0.1135	0.577(07)
8479.03(07)	56.4396	0.1141	0.20	0.2568	55.8632	0.1143	0.576(06)
8481.00(07)	56.6572	0.1147	0.20	0.2579	56.0811	0.1149	0.576(06)
8482.98(11)	56.8976	0.2103	0.37	0.3541	56.3218	0.2104	0.576(06)
8483.04(08)	56.7863	0.1437	0.25	0.2872	56.2104	0.1438	0.576(06)
8484.88(07)	56.9381	0.1164	0.20	0.2603	56.3625	0.1166	0.576(06)
8486.79(07)	56.9355	0.1206	0.21	0.2645	56.3601	0.1207	0.575(05)
8488.84(07)	57.1642	0.1096	0.19	0.2541	56.5891	0.1097	0.575(05)
8490.81(07)	57.0105	0.1163	0.20	0.2604	56.4356	0.1164	0.575(05)
8492.73(07)	57.0065	0.1150	0.20	0.2590	56.4318	0.1151	0.575(05)
8494.77(07)	57.0045	0.1116	0.20	0.2557	56.4301	0.1117	0.574(04)
8496.81(07)	56.7802	0.1155	0.20	0.2590	56.2061	0.1156	0.574(04)
8498.85(07)	56.7953	0.1204	0.21	0.2639	56.2215	0.1205	0.574(04)
8500.95(07)	56.4702	0.1094	0.19	0.2521	55.8965	0.1095	0.574(04)
8503.07(07)	56.2627	0.1143	0.20	0.2565	55.6891	0.1143	0.574(04)
8505.11(07)	55.9909	0.1106	0.20	0.2521	55.4173	0.1107	0.574(04)
8507.15(07)	55.6440	0.1135	0.20	0.2542	55.0705	0.1136	0.574(04)
8509.14(07)	55.4463	0.1112	0.20	0.2513	54.8730	0.1112	0.573(04)
8511.06(07)	55.1728	0.1056	0.19	0.2450	54.5995	0.1056	0.573(04)
8513.05(07)	55.2909	0.3193	0.58	0.4591	54.7176	0.3193	0.573(04)
8515.04(07)	55.1563	0.1192	0.22	0.2586	54.5832	0.1192	0.573(04)
8516.84(07)	54.6673	0.1125	0.21	0.2507	54.0942	0.1126	0.573(04)
8519.08(05)	54.2035	0.0840	0.15	0.2210	53.6305	0.0841	0.573(04)
8529.10(07)	53.2853	0.1096	0.21	0.2443	52.7127	0.1097	0.573(04)
8539.59(07)	53.5336	0.1164	0.22	0.2518	52.9615	0.1165	0.572(04)
8549.29(07)	53.5485	0.1125	0.21	0.2478	52.9767	0.1126	0.572(05)
8559.27(07)	53.4359	0.1210	0.23	0.2560	52.8645	0.1210	0.571(05)
8569.58(07)	53.7493	0.1153	0.21	0.2512	53.1783	0.1154	0.571(05)
8579.29(07)	53.1981	0.1147	0.22	0.2492	52.6275	0.1148	0.571(05)
8589.34(07)	53.0783	0.1230	0.23	0.2572	52.5081	0.1231	0.570(05)
8599.66(05)	52.3641	0.1045	0.20	0.2369	51.7944	0.1046	0.570(06)
8609.57(07)	51.9303	0.1190	0.23	0.2503	51.3610	0.1191	0.569(06)
8619.50(11)	52.0192	0.2446	0.47	0.3761	51.4503	0.2446	0.569(06)
8639.86(07)	51.2346	0.1095	0.21	0.2391	50.6666	0.1097	0.568(06)
8659.76(07)	50.0725	0.1152	0.23	0.2418	49.5053	0.1153	0.567(06)
8679.56(07)	50.3457	0.1106	0.22	0.2380	49.7794	0.1108	0.566(07)
8699.91(07)	49.5447	0.1132	0.23	0.2385	48.9793	0.1134	0.565(07)
8719.62(07)	50.0301	0.1177	0.24	0.2442	49.4655	0.1179	0.565(07)
8739.71(07)	48.7851	0.1292	0.26	0.2526	48.2215	0.1295	0.564(08)
8759.75(07)	48.4790	0.1124	0.23	0.2351	47.9163	0.1127	0.563(08)
8779.56(05)	48.0208	0.0903	0.19	0.2118	47.4590	0.0907	0.562(08)
8799.99(07)	48.1171	0.1860	0.39	0.3077	47.5563	0.1862	0.561(09)
8819.84(07)	47.2798	0.1134	0.24	0.2330	46.7199	0.1137	0.560(09)
8840.06(07)	47.7177	0.1169	0.24	0.2376	47.1588	0.1172	0.559(09)

8870.37(07)	46.9692	0.1497	0.32	0.2686	46.4116	0.1500	0.558(10)
8900.29(07)	47.0043	0.1167	0.25	0.2356	46.4482	0.1171	0.556(10)
8930.46(05)	46.9049	0.0853	0.18	0.2040	46.3503	0.0859	0.555(10)
8960.45(08)	46.0336	0.1406	0.31	0.2571	45.4805	0.1410	0.553(11)
8960.52(12)	46.1995	0.2094	0.45	0.3263	45.6464	0.2097	0.553(11)
8990.29(07)	46.1639	0.1181	0.26	0.2349	45.6123	0.1186	0.552(11)
9020.47(07)	46.1727	0.1197	0.26	0.2365	45.6225	0.1202	0.550(11)
9060.67(07)	45.8527	0.1148	0.25	0.2308	45.3041	0.1153	0.549(11)
9100.96(12)	45.3693	0.2017	0.44	0.3165	44.8224	0.2020	0.547(11)
9141.02(07)	44.1517	0.1169	0.26	0.2287	43.6066	0.1175	0.545(12)
9181.25(09)	43.5637	0.1455	0.33	0.2558	43.0203	0.1460	0.543(12)
9181.32(12)	43.3644	0.2063	0.48	0.3161	42.8210	0.2066	0.543(12)
9221.31(06)	43.4478	0.0930	0.21	0.2030	42.9062	0.0937	0.542(12)
9261.30(05)	42.9518	0.2084	0.49	0.3172	42.4120	0.2088	0.540(12)
9301.21(07)	43.2680	0.1242	0.29	0.2337	42.7300	0.1248	0.538(12)
9341.23(09)	42.6075	0.1549	0.36	0.2627	42.0714	0.1553	0.536(12)
9341.30(13)	42.3412	0.2201	0.52	0.3273	41.8051	0.2204	0.536(12)
9381.16(08)	42.7505	0.1298	0.30	0.2381	42.2163	0.1304	0.534(12)
9421.50(08)	42.4175	0.1344	0.32	0.2418	41.8851	0.1350	0.532(12)
9471.79(14)	42.8257	0.2412	0.56	0.3496	42.2957	0.2415	0.530(12)
9471.87(10)	42.8325	0.1709	0.40	0.2794	42.3026	0.1713	0.530(12)
9522.39(08)	42.8316	0.1457	0.34	0.2542	42.3041	0.1463	0.528(12)

Table S2. Measured X-ray mass attenuation coefficients  $[\mu]_S$  of the *bis*(N-i-propyl-salicylaldiminato) nickel(II) complex from the intensity measurements ( $I_0$  and  $I$ ) with a 1.5 mM solution of the complex, and its corresponding solvent. A number of experimental systematics including energy calibration, dark-current, solvent attenuations, harmonic contamination and thickness-ratio (from the actual solvent attenuation and fitted background of the sample (solution) were corrected to obtain the final result. The first column lists calibrated energies (Section 4.3) in eV, and their associated uncertainties in parentheses. The second, third and fourth columns present corrected total X-ray mass attenuation coefficients  $[\mu]_S$  with associated relative and percentage uncertainties. The fifth column lists the absolute uncertainties including the uncertainty contributions from the thickness ratio  $t_{ratio}$  and column density  $[\rho t]_c$  measurements. The sixth and the seventh columns list the (effective) photoelectric absorption coefficient  $[\mu]_{pe}$  determined by subtracting the tabulated X-ray mass attenuations of the complex for the Rayleigh and Compton scattering from the total experimental X-ray mass attenuation coefficients  $[\mu]_S$  at measured energies, with their corresponding uncertainties. The eighth column lists the X-ray mass attenuations of Rayleigh and Compton scattering, where the corresponding uncertainty of  $[\mu]_{R+C}$  was determined from half of the variation between FFAST and XCOM tabulated values.

<i>Energy</i> (eV)	$[\mu]_S$ ( $cm^2/g$ )	$\sigma_{[\mu]_S rel}$ ( $cm^2/g$ )	$\sigma_{[\mu]_S rel}$ (%)	$\sigma_{[\mu]_S abs}$ ( $cm^2/g$ )	$[\mu]_{pe}$ ( $cm^2/g$ )	$\sigma_{[\mu]_{pe}}$ ( $cm^2/g$ )	$[\mu]_{R+C}$ ( $cm^2/g$ )
8099.36(07)	36.8201	1.6698	4.53	1.7699	36.2571	1.6699	0.563(22)
8139.20(07)	24.6351	2.8668	11.6	2.9351	24.0807	2.8669	0.554(29)
8179.54(07)	26.3899	1.4862	5.63	1.5592	25.8450	1.4867	0.545(36)
8219.56(07)	14.2868	2.0371	14.2	2.0786	13.7521	2.0376	0.535(45)
8259.68(07)	23.1324	1.3674	5.91	1.4319	22.6072	1.3685	0.525(55)
8299.75(07)	13.4084	1.6295	12.2	1.6687	12.8928	1.6308	0.516(64)
8328.92(07)	18.7673	1.2302	6.56	1.2833	18.2411	1.2314	0.526(54)
8329.93(07)	20.3898	1.2591	6.18	1.3165	19.8599	1.2601	0.530(50)
8330.88(07)	19.2183	1.2664	6.59	1.3207	18.6848	1.2672	0.533(47)
8331.95(07)	21.2500	1.1905	5.60	1.2501	20.7125	1.1913	0.537(43)
8332.84(07)	18.2139	1.2140	6.67	1.2657	17.6732	1.2146	0.541(39)
8333.73(07)	21.3961	1.3173	6.16	1.3772	20.8571	1.3176	0.539(31)
8334.75(07)	21.0412	1.2631	6.00	1.3222	20.4986	1.2634	0.543(27)
8335.70(07)	22.5559	1.2547	5.56	1.3177	22.0099	1.2550	0.546(24)
8336.70(07)	23.2202	1.2484	5.38	1.3131	22.6707	1.2486	0.549(21)
8337.71(07)	22.0860	1.2646	5.73	1.3264	21.5331	1.2647	0.553(17)
8338.72(07)	21.0854	1.2806	6.07	1.3397	20.5291	1.2806	0.556(14)
8339.21(07)	22.1303	1.2761	5.77	1.3380	21.5725	1.2762	0.558(12)
8339.63(07)	21.7090	1.3003	5.99	1.3610	21.1497	1.3003	0.559(11)
8340.10(07)	23.6257	1.2924	5.47	1.3582	23.0649	1.2924	0.561(09)
8340.64(07)	25.2605	1.2718	5.03	1.3418	24.6980	1.2718	0.562(08)
8341.11(07)	26.6212	1.3845	5.20	1.4580	26.0573	1.3845	0.564(06)
8341.65(07)	26.5812	1.2639	4.75	1.3373	26.0157	1.2639	0.566(04)
8342.12(07)	29.5081	1.2332	4.18	1.3143	28.9412	1.2332	0.567(03)
8342.60(07)	29.6686	1.2208	4.11	1.3022	29.1002	1.2208	0.568(02)

8343.13(07)	32.5808	1.2454	3.82	1.3344	32.0109	1.2454	0.570(00)
8343.73(07)	33.9700	1.3099	3.86	1.4026	33.3985	1.3099	0.572(02)
8344.20(07)	37.5385	1.2379	3.30	1.3399	36.9657	1.2379	0.573(03)
8344.75(07)	40.3905	1.2714	3.15	1.3807	39.8163	1.2714	0.574(04)
8345.23(07)	46.1060	1.2319	2.67	1.3562	45.5306	1.2320	0.575(05)
8345.70(07)	48.6691	1.1919	2.45	1.3228	48.0925	1.1919	0.577(07)
8346.12(07)	53.8558	1.1712	2.17	1.3156	53.2782	1.1712	0.578(08)
8346.71(07)	56.6905	1.1872	2.09	1.3390	56.1115	1.1873	0.579(09)
8347.25(07)	62.3970	1.3015	2.09	1.4681	61.8169	1.3015	0.580(10)
8347.72(07)	65.3705	1.1849	1.81	1.3592	64.7894	1.1849	0.581(11)
8348.26(07)	73.6468	1.1839	1.61	1.3798	73.0646	1.1840	0.582(12)
8348.80(07)	77.6169	1.2166	1.57	1.4228	77.0337	1.2167	0.583(13)
8349.39(07)	83.2275	1.2775	1.53	1.4983	82.6433	1.2776	0.584(14)
8349.88(07)	84.6464	1.1817	1.40	1.4062	84.0614	1.1818	0.585(15)
8350.36(07)	89.4259	1.2367	1.38	1.4736	88.8401	1.2368	0.586(16)
8350.83(07)	88.7259	1.2723	1.43	1.5074	88.1395	1.2724	0.586(16)
8351.31(07)	92.1816	1.2068	1.31	1.4509	91.5946	1.2069	0.587(17)
8351.85(07)	91.0746	1.3127	1.44	1.5539	90.4869	1.3129	0.588(18)
8352.32(07)	91.7652	1.2537	1.37	1.4967	91.1771	1.2538	0.588(18)
8352.92(07)	90.7730	1.2374	1.36	1.4778	90.1843	1.2375	0.589(19)
8353.40(07)	88.6976	1.2258	1.38	1.4608	88.1086	1.2259	0.589(19)
8353.87(07)	90.9187	1.2680	1.39	1.5088	90.3294	1.2682	0.589(19)
8354.35(07)	88.4200	1.2682	1.43	1.5025	87.8305	1.2683	0.589(19)
8354.96(07)	87.1118	1.2182	1.40	1.4491	86.5222	1.2184	0.590(20)
8355.43(07)	86.1762	1.2732	1.48	1.5017	85.5866	1.2734	0.590(20)
8355.97(07)	84.6883	1.2437	1.47	1.4683	84.0987	1.2438	0.590(20)
8356.45(07)	85.1552	1.2510	1.47	1.4768	84.5658	1.2512	0.589(19)
8356.92(07)	84.7208	1.5755	1.86	1.8001	84.1316	1.5756	0.589(19)
8357.40(07)	81.5294	1.2262	1.50	1.4426	80.9405	1.2263	0.589(19)
8357.88(07)	80.1758	1.2960	1.62	1.5089	79.5873	1.2962	0.588(18)
8358.36(07)	80.0005	1.2598	1.57	1.4722	79.4125	1.2599	0.588(18)
8358.83(07)	77.9530	1.1855	1.52	1.3925	77.3657	1.1856	0.587(17)
8359.37(07)	77.2138	1.2133	1.57	1.4184	76.6273	1.2134	0.587(17)
8359.79(07)	76.1148	1.2178	1.60	1.4201	75.5289	1.2179	0.586(16)
8360.27(07)	74.8982	1.2296	1.64	1.4287	74.3133	1.2297	0.585(15)
8360.82(07)	74.0557	1.2609	1.70	1.4578	73.4719	1.2609	0.584(14)
8361.35(07)	73.2283	1.2497	1.71	1.4445	72.6458	1.2498	0.583(12)
8361.77(07)	72.6399	1.2015	1.65	1.3948	72.0585	1.2016	0.581(11)
8362.25(07)	70.9479	1.1698	1.65	1.3587	70.3679	1.1699	0.580(10)
8362.79(07)	69.6480	1.2151	1.74	1.4006	69.0697	1.2152	0.578(08)
8363.21(07)	69.2431	1.2000	1.73	1.3844	68.6662	1.2000	0.577(07)
8363.68(07)	69.4906	1.2508	1.80	1.4359	68.9156	1.2508	0.575(05)
8364.10(07)	67.3170	1.2547	1.86	1.4341	66.7436	1.2547	0.573(03)
8364.58(07)	65.9459	1.2072	1.83	1.3831	65.3745	1.2072	0.571(01)
8365.18(07)	65.3861	1.2928	1.98	1.4672	64.8175	1.2928	0.569(01)
8365.60(07)	65.6587	1.1522	1.75	1.3273	65.0921	1.1522	0.567(03)

8366.09(07)	63.8118	1.3465	2.11	1.5168	63.2477	1.3465	0.564(06)
8366.56(07)	61.0219	1.4998	2.46	1.6629	60.4604	1.4999	0.561(09)
8367.16(07)	61.5844	1.2386	2.01	1.4031	61.0265	1.2387	0.558(12)
8367.64(07)	61.1984	1.2298	2.01	1.3933	60.6435	1.2299	0.555(15)
8368.12(07)	61.1377	1.1726	1.92	1.3360	60.5860	1.1728	0.552(18)
8368.60(07)	57.5782	1.2211	2.12	1.3752	57.0298	1.2213	0.548(22)
8369.02(07)	58.5712	1.2394	2.12	1.3961	58.0260	1.2397	0.545(25)
8369.50(07)	57.4198	1.3116	2.28	1.4652	56.8782	1.3119	0.542(28)
8369.98(11)	56.3743	1.9821	3.52	2.1330	55.8367	1.9823	0.538(32)
8370.03(08)	56.8152	1.5918	2.80	1.7439	56.2780	1.5922	0.537(33)
8370.51(07)	54.6853	1.2314	2.25	1.3780	54.1522	1.2320	0.533(37)
8371.00(07)	55.5947	1.2621	2.27	1.4111	55.0659	1.2628	0.529(41)
8371.54(07)	55.1509	1.3258	2.40	1.4735	54.6273	1.3266	0.524(46)
8372.02(07)	52.9229	1.2654	2.39	1.4074	52.4041	1.2665	0.519(51)
8372.56(07)	52.7617	1.2587	2.39	1.4003	52.2485	1.2600	0.513(57)
8373.10(07)	51.9624	1.2309	2.37	1.3704	51.4551	1.2325	0.507(63)
8373.64(07)	52.3153	1.1675	2.23	1.3079	51.8142	1.1695	0.501(69)
8374.12(07)	52.6383	1.2267	2.33	1.3679	52.1430	1.2290	0.495(75)
8374.66(07)	51.9088	1.2087	2.33	1.3480	51.4174	1.2113	0.491(79)
8375.14(07)	50.6279	1.2691	2.51	1.4051	50.1359	1.2715	0.492(78)
8375.62(07)	50.2991	1.2485	2.48	1.3836	49.8065	1.2509	0.493(78)
8376.10(07)	48.5488	1.3552	2.79	1.4858	48.0556	1.3574	0.493(77)
8376.71(07)	48.7567	1.2117	2.49	1.3428	48.2628	1.2141	0.494(76)
8377.25(07)	48.9887	1.3718	2.80	1.5035	48.4942	1.3739	0.495(75)
8377.73(07)	48.4460	1.2173	2.51	1.3477	47.9509	1.2197	0.495(75)
8378.27(07)	49.5580	1.1988	2.42	1.3320	49.0622	1.2011	0.496(74)
8378.93(07)	49.6491	1.1988	2.41	1.3323	49.1525	1.2011	0.497(73)
8380.91(07)	50.0272	1.1565	2.31	1.2909	49.5281	1.1587	0.499(71)
8382.96(07)	52.0996	1.1851	2.27	1.3249	51.5980	1.1870	0.502(68)
8385.00(08)	54.9023	1.4512	2.64	1.5983	54.3981	1.4527	0.504(66)
8385.06(11)	54.1386	2.0900	3.86	2.2351	53.6343	2.0910	0.504(66)
8386.99(07)	59.2067	1.1865	2.00	1.3448	58.7000	1.1882	0.507(63)
8388.98(07)	59.3712	1.1451	1.93	1.3038	58.8621	1.1467	0.509(61)
8390.96(07)	61.7334	1.1786	1.91	1.3435	61.2218	1.1801	0.512(58)
8392.90(07)	59.9623	1.2133	2.02	1.3736	59.4483	1.2146	0.514(56)
8394.83(07)	59.6027	1.1038	1.85	1.2631	59.0864	1.1051	0.516(54)
8396.75(07)	62.0685	1.1308	1.82	1.2966	61.5498	1.1320	0.519(51)
8398.75(07)	63.5010	1.1425	1.80	1.3119	62.9799	1.1435	0.521(49)
8400.74(07)	60.9090	1.1577	1.90	1.3205	60.3854	1.1586	0.524(46)
8402.74(07)	61.6223	1.1259	1.83	1.2905	61.0963	1.1268	0.526(44)
8404.80(07)	60.7102	1.1304	1.86	1.2926	60.1817	1.1311	0.529(41)
8406.79(07)	58.7294	1.2704	2.16	1.4275	58.1984	1.2710	0.531(39)
8408.98(07)	59.1480	1.1370	1.92	1.2952	58.6143	1.1376	0.534(36)
8411.03(07)	56.2751	1.4833	2.64	1.6339	55.7389	1.4836	0.536(34)
8412.97(07)	54.6241	1.1249	2.06	1.2713	54.0855	1.1253	0.539(31)
8415.03(07)	55.6656	1.1544	2.07	1.3035	55.1245	1.1547	0.541(29)

8417.03(07)	55.8238	1.1069	1.98	1.2565	55.2804	1.1073	0.543(27)
8419.04(07)	55.9318	1.2176	2.18	1.3674	55.3859	1.2178	0.546(24)
8420.98(07)	54.5263	1.2023	2.21	1.3485	53.9781	1.2025	0.548(22)
8422.92(07)	55.3984	1.2376	2.23	1.3860	54.8478	1.2377	0.551(19)
8424.75(07)	52.7141	1.1811	2.24	1.3225	52.1613	1.1812	0.553(17)
8426.75(07)	52.1986	1.1812	2.26	1.3212	51.6435	1.1813	0.555(15)
8428.76(07)	52.1546	1.1472	2.20	1.2871	51.5970	1.1472	0.558(12)
8430.65(08)	50.6725	1.5808	3.12	1.7169	50.1126	1.5808	0.560(10)
8430.71(11)	52.8623	2.1120	4.00	2.2538	52.3023	2.1120	0.560(10)
8432.66(07)	50.3002	1.2577	2.50	1.3928	49.7379	1.2577	0.562(08)
8434.80(07)	50.4740	1.3249	2.62	1.4605	49.9092	1.3249	0.565(05)
8436.74(07)	50.1038	1.1770	2.35	1.3116	49.5367	1.1770	0.567(03)
8438.81(07)	50.5854	1.2194	2.41	1.3553	50.0158	1.2194	0.570(00)
8440.95(07)	52.1534	1.1757	2.25	1.3157	51.5813	1.1757	0.572(02)
8442.90(07)	49.6080	1.1898	2.40	1.3231	49.0335	1.1898	0.574(04)
8444.99(07)	49.3824	1.0897	2.21	1.2224	48.8055	1.0897	0.577(07)
8447.06(07)	51.0791	1.1351	2.22	1.2723	50.4997	1.1352	0.579(09)
8448.89(07)	50.3459	1.2240	2.43	1.3592	49.7657	1.2240	0.580(10)
8450.92(07)	51.2372	1.1220	2.19	1.2596	50.6572	1.1220	0.580(10)
8452.93(07)	53.0569	1.1567	2.18	1.2990	52.4772	1.1567	0.580(10)
8454.76(07)	52.1036	1.1136	2.14	1.2535	51.5241	1.1137	0.579(09)
8456.67(07)	52.1788	1.1048	2.12	1.2449	51.5995	1.1049	0.579(09)
8458.75(07)	51.8489	1.1347	2.19	1.2739	51.2699	1.1348	0.579(09)
8460.65(07)	51.3717	1.1658	2.27	1.3037	50.7930	1.1658	0.579(09)
8462.68(07)	53.8418	1.1257	2.09	1.2701	53.2633	1.1258	0.578(08)
8464.82(07)	52.6958	1.2733	2.42	1.4146	52.1176	1.2733	0.578(08)
8466.79(07)	51.9342	1.1461	2.21	1.2855	51.3562	1.1462	0.578(08)
8468.88(07)	52.6604	1.1812	2.24	1.3225	52.0828	1.1812	0.578(08)
8470.96(07)	51.8862	1.1302	2.18	1.2695	51.3088	1.1302	0.577(07)
8472.94(07)	52.1731	1.1276	2.16	1.2676	51.5960	1.1276	0.577(07)
8475.02(07)	53.7014	1.1416	2.13	1.2856	53.1245	1.1416	0.577(07)
8477.06(07)	52.9416	1.1852	2.24	1.3272	52.3650	1.1852	0.577(07)
8479.03(07)	53.5673	1.0639	1.99	1.2075	52.9910	1.0639	0.576(06)
8481.00(07)	54.1463	1.1300	2.09	1.2751	53.5702	1.1300	0.576(06)
8483.04(07)	55.0475	1.1343	2.06	1.2818	54.4717	1.1343	0.576(06)
8484.88(07)	53.1032	1.1573	2.18	1.2998	52.5276	1.1573	0.576(06)
8486.79(07)	54.3096	1.0653	1.96	1.2109	53.7342	1.0653	0.575(05)
8488.84(07)	53.6157	1.1532	2.15	1.2970	53.0406	1.1532	0.575(05)
8490.81(07)	53.2181	1.1131	2.09	1.2559	52.6432	1.1131	0.575(05)
8492.73(07)	52.7469	1.1834	2.24	1.3249	52.1723	1.1834	0.575(05)
8494.77(07)	54.6618	1.1297	2.07	1.2762	54.0874	1.1297	0.574(04)
8496.81(07)	53.4991	1.1404	2.13	1.2838	52.9250	1.1404	0.574(04)
8498.85(07)	54.5962	1.1192	2.05	1.2655	54.0224	1.1192	0.574(04)
8500.95(07)	55.3497	1.1205	2.02	1.2688	54.7760	1.1205	0.574(04)
8503.07(07)	54.9742	1.1260	2.05	1.2733	54.4006	1.1260	0.574(04)
8505.05(07)	53.7822	1.1181	2.08	1.2623	53.2086	1.1181	0.574(04)

8507.15(07)	55.7045	1.3394	2.40	1.4886	55.1311	1.3394	0.573(04)
8509.14(07)	54.4228	1.0569	1.94	1.2028	53.8494	1.0569	0.573(04)
8511.06(07)	53.8470	1.1001	2.04	1.2444	53.2736	1.1001	0.573(04)
8513.05(07)	52.3176	1.1236	2.15	1.2640	51.7443	1.1236	0.573(04)
8515.04(07)	53.6173	1.0595	1.98	1.2033	53.0442	1.0595	0.573(04)
8516.84(07)	53.9073	1.1218	2.08	1.2663	53.3343	1.1218	0.573(04)
8519.08(05)	53.7852	0.8248	1.53	0.9690	53.2122	0.8248	0.573(04)
8529.10(07)	48.2038	1.2008	2.49	1.3305	47.6312	1.2008	0.573(04)
8539.59(07)	54.8657	1.0352	1.89	1.1822	54.2935	1.0352	0.572(04)
8549.29(07)	42.3568	1.0655	2.52	1.1800	41.7850	1.0655	0.572(05)
8559.27(07)	46.6855	1.0645	2.28	1.1902	46.1141	1.0645	0.571(05)
8569.58(07)	44.7834	1.1368	2.54	1.2576	44.2124	1.1368	0.571(05)
8579.29(07)	48.3248	1.1274	2.33	1.2574	47.7542	1.1274	0.571(05)
8589.34(07)	48.6735	1.0830	2.23	1.2140	48.1034	1.0831	0.570(05)
8599.66(05)	53.8066	0.8024	1.49	0.9466	53.2369	0.8024	0.570(05)
8609.57(07)	42.2109	1.4014	3.32	1.5155	41.6416	1.4014	0.569(06)
8619.50(07)	46.9062	1.1391	2.43	1.2654	46.3373	1.1391	0.569(06)
8639.86(07)	39.6496	1.0536	2.66	1.1611	39.0816	1.0536	0.568(06)
8659.76(07)	45.2057	1.0719	2.37	1.1938	44.6385	1.0719	0.567(06)
8679.56(11)	44.5396	1.9369	4.35	2.0571	43.9733	1.9369	0.566(07)
8679.63(08)	42.3320	1.3253	3.13	1.4397	41.7657	1.3253	0.566(07)
8699.91(07)	49.0839	1.0717	2.18	1.2037	48.5184	1.0718	0.565(07)
8719.62(07)	44.2130	1.0692	2.42	1.1885	43.6485	1.0692	0.565(07)
8739.71(07)	49.8887	1.1325	2.27	1.2666	49.3250	1.1326	0.564(08)
8759.82(07)	47.9584	1.1484	2.39	1.2774	47.3957	1.1484	0.563(08)
8779.56(05)	52.5678	0.8076	1.54	0.9486	52.0060	0.8076	0.562(08)
8799.99(07)	46.6305	1.1166	2.39	1.2422	46.0697	1.1166	0.561(09)
8819.84(07)	51.5817	1.0752	2.08	1.2137	51.0218	1.0753	0.560(09)
8840.06(07)	44.4631	1.6648	3.74	1.7847	43.9041	1.6648	0.559(09)
8870.37(07)	52.7547	1.0818	2.05	1.2233	52.1972	1.0818	0.558(09)
8900.35(08)	56.5121	1.4510	2.57	1.6023	55.9560	1.4510	0.556(10)
8930.46(05)	56.2608	2.4498	4.35	2.6005	55.7062	2.4498	0.555(10)
8960.45(07)	56.7287	1.2394	2.18	1.3913	56.1756	1.2395	0.553(11)
8990.29(12)	55.1360	1.9125	3.47	2.0602	54.5844	1.9125	0.552(11)
8990.36(08)	49.9196	1.4712	2.95	1.6053	49.3680	1.4712	0.552(11)
9020.47(07)	63.1531	1.2094	1.91	1.3779	62.6029	1.2094	0.550(11)

Table S3. Measured X-ray mass attenuation coefficients  $[\mu/\rho]_S$  of the *bis*(N-n-propyl-salicylaldiminato) nickel(II) complex determined from the intensity measurements ( $I_0$  and  $I$ ) with a 15 mM solution of the complex, and its corresponding solvent. A number of experimental systematics including energy calibration, dark-current, solvent attenuations, harmonic contamination and thickness-ratio (from the actual solvent attenuation and fitted background of the sample (solution)) were corrected to obtain the final result (weighted mean of multiple measurements at each energy). The first column lists calibrated energies (Section 4.3) in eV, and their associated uncertainties in parentheses. The second, third and fourth columns present corrected total X-ray mass attenuation coefficients  $[\mu/\rho]_S$  with associated relative and percentage uncertainties. The fifth column lists the absolute uncertainties including the uncertainty contributions from the thickness ratio  $t_{ratio}$  and column density  $[\rho t]_c$  measurements. The sixth and the seventh columns list the (effective) photoelectric absorption coefficient  $[\mu/\rho]_{pe}$  determined by subtracting the tabulated X-ray mass attenuations of the complex for the Rayleigh and Compton scattering from the total experimental X-ray mass attenuation coefficients  $[\mu/\rho]_S$  at measured energies, with their corresponding uncertainties. The eighth column lists the X-ray mass attenuations of Rayleigh and Compton scattering, where the corresponding uncertainty of  $[\mu/\rho]_{R+C}$  was determined from half of the variation between FFAST and XCOM tabulated values.

<i>Energy</i> (eV)	$[\mu/\rho]_S$ ( $cm^2/g$ )	$\sigma_{[\mu/\rho]_S rel}$ ( $cm^2/g$ )	$\sigma_{[\mu/\rho]_S}(rel)$ (%)	$\sigma_{[\mu/\rho]_{abs}}$ ( $cm^2/g$ )	$[\mu/\rho]_{pe}$ ( $cm^2/g$ )	$\sigma_{[\mu/\rho]_{pe}}$ ( $cm^2/g$ )	$[\mu/\rho]_{R+C}$ ( $cm^2/g$ )
7918.60(11)	15.0026	0.3439	2.29	0.3566	14.3975	0.3440	0.605(10)
7958.94(10)	14.4521	0.1280	0.89	0.1404	13.8570	0.1280	0.595(02)
7998.73(10)	12.9877	0.2331	1.79	0.2446	12.4021	0.2331	0.586(05)
8039.15(10)	13.4378	0.1575	1.17	0.1693	12.8614	0.1579	0.576(12)
8078.88(12)	12.1499	0.2654	2.18	0.2765	11.5823	0.2661	0.568(19)
8078.93(17)	11.3425	0.2010	1.77	0.2117	10.7749	0.2019	0.568(19)
8119.13(10)	11.8420	0.1011	0.85	0.1120	11.2833	0.1043	0.559(26)
8159.17(09)	11.3740	0.1753	1.54	0.1859	10.8239	0.1782	0.550(32)
8199.09(09)	11.9725	0.1063	0.89	0.1173	11.4329	0.1137	0.540(40)
8239.54(09)	9.8658	0.2582	2.62	0.2680	9.3359	0.2631	0.530(50)
8278.65(09)	11.1380	0.0897	0.81	0.1002	10.6173	0.1075	0.521(59)
8283.63(09)	10.9600	0.1474	1.34	0.1578	10.4404	0.1593	0.520(60)
8288.75(09)	11.4219	0.0855	0.75	0.0962	10.9036	0.1055	0.518(62)
8293.87(09)	10.9533	0.1427	1.30	0.1532	10.4362	0.1560	0.517(63)
8298.76(09)	11.3262	0.0912	0.81	0.1018	10.8103	0.1115	0.516(64)
8303.65(05)	11.9663	0.0625	0.52	0.0735	11.4517	0.0905	0.515(65)
8308.43(09)	12.0490	0.0994	0.82	0.1104	11.5356	0.1197	0.513(67)
8309.38(09)	12.2179	0.0853	0.70	0.0965	11.7047	0.1084	0.513(67)
8310.32(09)	11.9839	0.0917	0.77	0.1027	11.4710	0.1136	0.513(67)
8311.34(09)	12.2849	0.0927	0.75	0.1039	11.7723	0.1146	0.513(67)
8312.34(09)	12.2484	0.1002	0.82	0.1113	11.7360	0.1208	0.512(68)
8313.46(09)	12.6040	0.0935	0.74	0.1049	12.0918	0.1156	0.512(68)
8314.46(09)	12.5348	0.0891	0.71	0.1004	12.0229	0.1122	0.512(68)
8315.41(09)	12.5665	0.0851	0.68	0.0965	12.0549	0.1092	0.512(68)

8316.42(09)	12.6117	0.0943	0.75	0.1057	12.1003	0.1166	0.511(69)
8317.49(09)	12.7160	0.0884	0.70	0.0998	12.2049	0.1121	0.511(69)
8318.49(09)	12.8593	0.0867	0.67	0.0982	12.3484	0.1109	0.511(69)
8319.02(09)	13.2490	0.0919	0.69	0.1036	12.7383	0.1151	0.511(69)
8319.62(09)	13.3094	0.0805	0.60	0.0922	12.7988	0.1063	0.511(69)
8320.09(09)	13.1921	0.0964	0.73	0.1081	12.6816	0.1189	0.510(70)
8320.62(09)	13.0655	0.1029	0.79	0.1145	12.5552	0.1243	0.510(70)
8321.10(09)	12.9936	0.1003	0.77	0.1119	12.4834	0.1222	0.510(70)
8321.58(09)	13.2144	0.1411	1.07	0.1528	12.7043	0.1575	0.510(70)
8322.05(09)	13.5160	0.0928	0.69	0.1047	13.0060	0.1163	0.510(70)
8322.58(09)	13.2740	0.1103	0.83	0.1220	12.7641	0.1307	0.510(70)
8323.12(09)	13.2916	0.0993	0.75	0.1110	12.7819	0.1217	0.510(70)
8323.59(09)	13.1612	0.0988	0.75	0.1104	12.6516	0.1213	0.510(70)
8324.12(09)	13.1028	0.0902	0.69	0.1019	12.5933	0.1145	0.509(71)
8324.65(09)	13.0729	0.0946	0.72	0.1062	12.5628	0.1177	0.510(70)
8325.13(09)	12.7662	0.0912	0.71	0.1026	12.2543	0.1138	0.512(68)
8325.66(09)	12.6681	0.1017	0.80	0.1131	12.1542	0.1214	0.514(66)
8326.15(09)	12.9941	0.0868	0.67	0.0983	12.4784	0.1080	0.516(64)
8326.62(09)	13.3032	0.0842	0.63	0.0960	12.7858	0.1049	0.517(63)
8327.15(09)	12.9793	0.0863	0.66	0.0979	12.4599	0.1054	0.519(61)
8327.57(09)	12.7948	0.0924	0.72	0.1039	12.2737	0.1096	0.521(59)
8328.04(09)	12.7191	0.0907	0.71	0.1021	12.1963	0.1072	0.523(57)
8328.57(09)	12.5894	0.0968	0.77	0.1082	12.0645	0.1114	0.525(55)
8329.05(09)	12.9246	0.0853	0.66	0.0968	12.3979	0.1006	0.527(53)
8329.52(09)	12.7369	0.0904	0.71	0.1018	12.2085	0.1041	0.528(52)
8330.00(09)	12.7613	0.1239	0.97	0.1353	12.2310	0.1335	0.530(50)
8330.47(09)	12.9064	0.1028	0.80	0.1143	12.3744	0.1135	0.532(48)
8331.07(09)	12.9967	0.0939	0.72	0.1055	12.4626	0.1045	0.534(46)
8331.55(09)	13.1421	0.0943	0.72	0.1060	12.6062	0.1041	0.536(44)
8331.96(09)	12.9859	0.0871	0.67	0.0987	12.4484	0.0969	0.537(43)
8332.50(09)	13.2308	0.0871	0.66	0.0988	12.6913	0.0960	0.539(41)
8332.91(09)	13.2972	0.0848	0.64	0.0965	12.7562	0.0933	0.541(39)
8333.45(09)	13.4960	0.0815	0.60	0.0933	12.9581	0.0875	0.538(32)
8333.86(09)	13.7092	0.0983	0.72	0.1102	13.1698	0.1029	0.539(31)
8334.34(09)	13.8201	0.0883	0.64	0.1003	13.2789	0.0929	0.541(29)
8334.87(09)	13.8094	0.1021	0.74	0.1141	13.2664	0.1056	0.543(27)
8335.29(09)	13.9741	0.0879	0.63	0.1000	13.4296	0.0915	0.545(25)
8335.82(09)	14.1363	0.0855	0.60	0.0977	13.5899	0.0887	0.546(24)
8336.31(09)	14.0868	0.0850	0.60	0.0972	13.5387	0.0878	0.548(22)
8336.84(09)	14.2042	0.1017	0.72	0.1140	13.6542	0.1037	0.550(20)
8337.38(09)	14.4006	0.0889	0.62	0.1012	13.8488	0.0907	0.552(18)
8337.85(09)	14.8022	0.0926	0.63	0.1052	14.2488	0.0941	0.553(17)
8338.33(09)	15.4063	0.0885	0.57	0.1015	14.8512	0.0898	0.555(15)
8338.80(09)	15.8844	0.0924	0.58	0.1057	15.3278	0.0934	0.557(13)
8339.28(09)	16.5746	0.0839	0.51	0.0975	16.0164	0.0847	0.558(12)
8339.75(09)	17.1886	0.0850	0.49	0.0990	16.6289	0.0857	0.560(10)

8340.23(09)	17.9072	0.0882	0.49	0.1025	17.3460	0.0886	0.561(09)
8340.76(09)	18.8303	0.0964	0.51	0.1113	18.2675	0.0966	0.563(07)
8341.30(09)	20.0802	0.0859	0.43	0.1015	19.5157	0.0861	0.565(06)
8341.72(09)	20.9746	0.0879	0.42	0.1041	20.4088	0.0880	0.566(04)
8342.26(09)	22.3591	0.0869	0.39	0.1038	21.7918	0.0870	0.567(03)
8342.85(09)	24.1739	0.0978	0.40	0.1158	23.6048	0.0978	0.569(01)
8343.39(09)	26.6625	0.0865	0.32	0.1059	26.0919	0.0865	0.571(01)
8343.86(09)	28.6822	0.0880	0.31	0.1085	28.1103	0.0880	0.572(02)
8344.40(09)	31.8424	0.0945	0.30	0.1168	31.2691	0.0946	0.573(03)
8344.88(09)	34.6921	0.0834	0.24	0.1074	34.1175	0.0836	0.575(05)
8345.35(09)	38.6115	0.0930	0.24	0.1192	38.0358	0.0932	0.576(06)
8345.83(09)	42.3968	0.0798	0.19	0.1081	41.8199	0.0801	0.577(07)
8346.42(09)	47.0804	0.0929	0.20	0.1239	46.5021	0.0933	0.578(08)
8346.91(09)	51.3041	0.0932	0.18	0.1266	50.7247	0.0936	0.579(09)
8347.44(09)	56.3805	0.0962	0.17	0.1325	55.7999	0.0968	0.581(11)
8348.52(09)	70.4395	0.0918	0.13	0.1361	69.8568	0.0927	0.583(13)
8350.60(09)	76.0340	0.0945	0.12	0.1420	75.4479	0.0958	0.586(16)
8352.64(09)	75.0248	0.0917	0.12	0.1386	74.4364	0.0935	0.588(18)
8354.67(09)	72.4205	0.0935	0.13	0.1389	71.8309	0.0955	0.590(20)
8356.70(09)	68.0119	0.0848	0.12	0.1278	67.4226	0.0870	0.589(19)
8358.61(09)	64.6053	0.1025	0.16	0.1434	64.0177	0.1040	0.588(18)
8360.59(08)	61.3634	0.0921	0.15	0.1313	60.7791	0.0932	0.584(14)
8362.57(08)	58.7797	0.0828	0.14	0.1204	58.2007	0.0833	0.579(09)
8364.36(08)	55.9661	0.0913	0.16	0.1274	55.3938	0.0914	0.572(02)
8366.39(08)	54.2395	0.0904	0.17	0.1254	53.6771	0.0907	0.562(08)
8368.38(08)	52.1884	0.0836	0.16	0.1175	51.6385	0.0860	0.550(20)
8370.29(08)	50.6032	0.0935	0.18	0.1265	50.0682	0.0998	0.535(35)
8372.34(08)	48.6696	0.0872	0.18	0.1191	48.1540	0.1028	0.516(54)
8374.38(08)	47.8563	0.1010	0.21	0.1325	47.3642	0.1276	0.492(78)
8376.42(08)	47.2438	0.0976	0.21	0.1287	46.7503	0.1240	0.494(77)
8378.53(08)	47.8057	0.1334	0.28	0.1648	47.3096	0.1525	0.496(74)
8380.57(08)	49.1540	0.0861	0.18	0.1183	48.6553	0.1118	0.499(71)
8382.62(08)	51.1068	0.0931	0.18	0.1264	50.6055	0.1157	0.501(69)
8384.66(08)	52.9162	0.0932	0.18	0.1275	52.4124	0.1143	0.504(66)
8386.64(08)	54.2970	0.1060	0.20	0.1411	53.7908	0.1237	0.506(64)
8388.58(08)	56.0695	0.0917	0.16	0.1278	55.5608	0.1103	0.509(61)
8390.56(08)	56.9979	0.0924	0.16	0.1290	56.4868	0.1096	0.511(59)
8392.56(08)	58.0661	0.0770	0.13	0.1142	57.5525	0.0955	0.514(56)
8394.43(08)	58.5039	0.1424	0.24	0.1799	57.9881	0.1524	0.516(54)
8396.35(08)	59.0096	0.1540	0.26	0.1918	58.4913	0.1624	0.518(52)
8398.35(08)	59.7412	0.0887	0.15	0.1269	59.2205	0.1015	0.521(49)
8400.34(08)	59.7195	0.1038	0.17	0.1420	59.1963	0.1139	0.523(47)
8402.33(08)	60.3301	0.0926	0.15	0.1311	59.8045	0.1027	0.526(44)
8404.40(08)	59.6788	0.1113	0.19	0.1494	59.1507	0.1189	0.528(42)
8406.45(08)	59.6471	0.0840	0.14	0.1222	59.1165	0.0928	0.531(39)
8408.51(08)	58.4479	0.1612	0.28	0.1987	57.9148	0.1654	0.533(37)

8410.63(08)	58.2696	0.1199	0.21	0.1573	57.7339	0.1247	0.536(34)
8412.64(08)	57.2181	0.1248	0.22	0.1616	56.6799	0.1288	0.538(32)
8414.69(08)	56.5993	0.1021	0.18	0.1385	56.0587	0.1063	0.541(29)
8416.69(08)	56.1816	0.1064	0.19	0.1426	55.6385	0.1098	0.543(27)
8418.58(08)	56.0481	0.1152	0.21	0.1513	55.5027	0.1178	0.545(25)
8420.58(08)	55.9638	0.0862	0.15	0.1223	55.4160	0.0891	0.548(22)
8422.53(08)	55.6392	0.1167	0.21	0.1525	55.0891	0.1183	0.550(20)
8424.35(08)	55.2355	0.0901	0.16	0.1257	54.6832	0.0918	0.552(18)
8426.35(08)	55.3025	0.1011	0.18	0.1368	54.7478	0.1023	0.555(15)
8428.37(08)	55.1096	0.0855	0.16	0.1210	54.5525	0.0864	0.557(13)
8430.25(08)	55.0282	0.0775	0.14	0.1130	54.4688	0.0783	0.559(11)
8432.26(08)	54.6509	0.2067	0.38	0.2420	54.0891	0.2069	0.562(08)
8434.39(08)	54.3352	0.0880	0.16	0.1231	53.7708	0.0882	0.564(06)
8436.34(08)	54.2761	0.0850	0.16	0.1201	53.7094	0.0850	0.567(03)
8438.54(08)	53.9127	0.0847	0.16	0.1196	53.3434	0.0847	0.569(01)
8440.61(08)	53.7910	0.0895	0.17	0.1244	53.2192	0.0896	0.572(02)
8442.56(08)	53.9991	0.0908	0.17	0.1258	53.4250	0.0909	0.574(04)
8444.65(08)	54.2086	0.0798	0.15	0.1149	53.6321	0.0801	0.577(06)
8446.72(08)	54.3395	0.0918	0.17	0.1270	53.7605	0.0923	0.579(09)
8448.62(08)	54.3923	0.0799	0.15	0.1150	53.8120	0.0805	0.580(10)
8450.57(08)	54.6064	0.0851	0.16	0.1204	54.0264	0.0857	0.580(10)
8452.59(08)	54.8616	0.1052	0.19	0.1406	54.2818	0.1056	0.580(10)
8454.49(08)	54.9462	0.1724	0.31	0.2079	54.3667	0.1727	0.580(09)
8456.39(08)	54.5410	0.0880	0.16	0.1232	53.9618	0.0885	0.579(09)
8458.48(08)	54.6889	0.0854	0.16	0.1207	54.1099	0.0858	0.579(09)
8460.38(08)	54.7483	0.0945	0.17	0.1298	54.1696	0.0949	0.579(09)
8462.40(08)	54.5447	0.0899	0.16	0.1252	53.9662	0.0903	0.579(08)
8464.49(08)	54.8027	0.0854	0.16	0.1208	54.2245	0.0858	0.578(08)
8466.45(07)	54.7076	0.0721	0.13	0.1074	54.1296	0.0725	0.578(08)
8468.85(08)	54.7508	0.0916	0.17	0.1270	54.1731	0.0919	0.578(08)
8479.07(08)	54.5002	0.0816	0.15	0.1169	53.9239	0.0819	0.576(06)
8488.88(08)	54.4326	0.0819	0.15	0.1170	53.8575	0.0820	0.575(05)
8498.89(08)	54.5378	0.1453	0.27	0.1806	53.9639	0.1454	0.574(04)
8509.12(08)	52.9093	0.1244	0.24	0.1587	52.3359	0.1244	0.573(04)
8518.93(08)	52.5364	0.0781	0.15	0.1122	51.9634	0.0782	0.573(04)
8528.96(08)	51.8447	0.1144	0.22	0.1481	51.2721	0.1145	0.573(04)
8539.26(08)	51.9105	0.0792	0.15	0.1129	51.3383	0.0793	0.572(04)
8548.96(08)	51.3640	0.0799	0.16	0.1134	50.7922	0.0801	0.572(05)
8559.00(06)	51.8442	0.0583	0.11	0.0920	51.2728	0.0585	0.571(05)
8569.31(08)	51.0806	0.1135	0.22	0.1468	50.5096	0.1136	0.571(05)
8579.02(08)	51.1984	0.0893	0.17	0.1226	50.6278	0.0894	0.571(05)
8589.07(08)	50.4235	0.0918	0.18	0.1247	49.8533	0.0920	0.570(05)
8599.33(08)	50.5602	0.0902	0.18	0.1232	49.9905	0.0904	0.570(05)
8609.30(06)	50.0431	0.0840	0.17	0.1167	49.4738	0.0842	0.569(06)
8619.42(07)	50.2759	0.0648	0.13	0.0976	49.7070	0.0650	0.569(06)
8639.67(13)	48.9375	0.1421	0.29	0.1742	48.3695	0.1423	0.568(06)

8639.73(09)	48.8728	0.1747	0.36	0.2067	48.3048	0.1748	0.568(06)
8659.63(08)	48.8465	0.1009	0.21	0.1329	48.2793	0.1011	0.567(06)
8679.37(09)	47.7008	0.1902	0.40	0.2216	47.1344	0.1903	0.566(07)
8679.43(13)	47.3296	0.1504	0.32	0.1816	46.7633	0.1506	0.566(07)
8699.71(08)	48.0933	0.0890	0.19	0.1205	47.5279	0.0892	0.565(07)
8719.44(13)	47.7475	0.1449	0.30	0.1763	47.1829	0.1451	0.565(07)
8719.50(09)	47.2965	0.0964	0.20	0.1275	46.7319	0.0967	0.565(07)
8739.52(07)	47.6887	0.0833	0.17	0.1146	47.1250	0.0836	0.564(08)
8759.70(07)	46.6689	0.0770	0.16	0.1078	46.1062	0.0774	0.563(08)
8779.37(07)	47.0756	0.0775	0.16	0.1085	46.5138	0.0780	0.562(08)
8799.67(07)	46.0529	0.0904	0.20	0.1208	45.4920	0.0908	0.561(09)
8819.54(07)	46.1991	0.0774	0.17	0.1079	45.6392	0.0779	0.560(09)
8839.82(05)	45.6728	0.1019	0.22	0.1321	45.1138	0.1023	0.559(09)
8870.07(05)	46.0757	0.0560	0.12	0.0864	45.5182	0.0568	0.558(09)
8900.11(05)	45.0012	0.1369	0.30	0.1667	44.4451	0.1372	0.556(10)
8930.22(05)	45.5676	0.0544	0.12	0.0845	45.0130	0.0553	0.555(10)
8960.14(09)	44.7945	0.1007	0.22	0.1304	44.2414	0.1012	0.553(11)
8960.21(06)	44.3669	0.0903	0.20	0.1198	43.8138	0.0909	0.553(11)
8990.12(05)	44.9562	0.0591	0.13	0.0889	44.4046	0.0601	0.552(11)
9020.24(07)	44.1507	0.1894	0.43	0.2187	43.6004	0.1897	0.550(11)
9060.44(06)	44.4859	0.0624	0.14	0.0919	43.9373	0.0634	0.549(11)
9100.87(07)	42.6163	0.1483	0.35	0.1767	42.0694	0.1487	0.547(11)
9140.95(08)	42.8422	0.0780	0.18	0.1066	42.2971	0.0788	0.545(11)
9181.03(08)	41.6936	0.1522	0.37	0.1801	41.1502	0.1526	0.543(12)
9221.10(08)	41.8914	0.0770	0.18	0.1050	41.3498	0.0779	0.542(12)
9261.02(10)	41.0080	0.2142	0.52	0.2417	40.4682	0.2145	0.540(12)
9261.09(14)	40.5252	0.1467	0.36	0.1740	39.9854	0.1472	0.540(12)
9301.07(10)	41.5239	0.1076	0.26	0.1354	40.9859	0.1082	0.538(12)
9341.17(08)	40.3366	0.1159	0.29	0.1431	39.8005	0.1166	0.536(12)
9380.95(08)	40.7612	0.0887	0.22	0.1161	40.2269	0.0896	0.534(12)
9471.67(09)	40.6914	0.0795	0.20	0.1068	40.1615	0.0804	0.530(12)
9521.81(09)	40.2717	0.1644	0.41	0.1915	39.7442	0.1648	0.528(12)