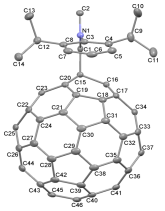
Numbering scheme of (**1**) (VT XRD experiment):



A_n			$U_{eq}(A_n,T)$								$\frac{U_{eq}(A_n,T)}{U_{eq}(A_n,T\text{-}50\ K)}$							$I(A_n,T)=\frac{U_{eq}(A_n,T)}{U_{eq}(A_n,T\text{-}50\ K)}\cdot n\cdot\left(\sum_n \frac{U_{eq}(A_n,T)}{U_{eq}(A_n,T\text{-}50\ K)}\right)^{-1}$							$I(A_n)$
Atom	**Distance *d* [Å]**		**80 K**	**130 K**	**180 K**	**230 K**	**280 K**	**330 K**	**380 K**	**430 K**	**130 K**	**180 K**	**230 K**	**280 K**	**330 K**	**380 K**	**430 K**	**130 K**	**180 K**	**230 K**	**280 K**	**330 K**	**380 K**	**430 K**	**Average**
C1	**0.000**		0.0131	0.0162	0.0192	0.0234	0.0284	0.0347	0.0437	0.0530	1.237	1.185	1.219	1.214	1.222	1.259	1.213	0.923	0.912	0.937	0.942	0.930	0.960	0.926	0.933
C2	**0.676**		0.0165	0.0207	0.0260	0.0319	0.0387	0.0476	0.0592	0.0727	1.255	1.256	1.227	1.213	1.230	1.244	1.228	0.936	0.967	0.943	0.942	0.936	0.948	0.938	0.944
C2	**0.676**		0.0165	0.0207	0.0260	0.0319	0.0387	0.0476	0.0592	0.0727	1.255	1.256	1.227	1.213	1.230	1.244	1.228	0.936	0.967	0.943	0.942	0.936	0.948	0.938	0.944
C3	**2.484**		0.0148	0.0186	0.0232	0.0280	0.0341	0.0424	0.0522	0.0640	1.257	1.247	1.207	1.218	1.243	1.231	1.226	0.938	0.960	0.928	0.946	0.946	0.938	0.936	0.942
C3	**2.484**		0.0148	0.0186	0.0232	0.0280	0.0341	0.0424	0.0522	0.0640	1.257	1.247	1.207	1.218	1.243	1.231	1.226	0.938	0.960	0.928	0.946	0.946	0.938	0.936	0.942
C4	**3.290**		0.0174	0.0225	0.0287	0.0358	0.0436	0.0548	0.0667	0.0810	1.293	1.276	1.247	1.218	1.257	1.217	1.214	0.965	0.982	0.959	0.946	0.957	0.928	0.927	0.952
C4	**3.290**		0.0174	0.0225	0.0287	0.0358	0.0436	0.0548	0.0667	0.0810	1.293	1.276	1.247	1.218	1.257	1.217	1.214	0.965	0.982	0.959	0.946	0.957	0.928	0.927	0.952
C5	**4.571**		0.0204	0.0279	0.0364	0.0463	0.0570	0.0692	0.0847	0.1030	1.368	1.305	1.272	1.231	1.214	1.224	1.216	1.021	1.004	0.978	0.956	0.924	0.933	0.929	0.963
C5	**4.571**		0.0204	0.0279	0.0364	0.0463	0.0570	0.0692	0.0847	0.1030	1.368	1.305	1.272	1.231	1.214	1.224	1.216	1.021	1.004	0.978	0.956	0.924	0.933	0.929	0.963
C6	**5.105**		0.0221	0.0303	0.0391	0.0492	0.0607	0.0746	0.0890	0.1100	1.371	1.290	1.258	1.234	1.229	1.193	1.236	1.023	0.993	0.967	0.958	0.935	0.909	0.944	0.961
C6	**5.105**		0.0221	0.0303	0.0391	0.0492	0.0607	0.0746	0.0890	0.1100	1.371	1.290	1.258	1.234	1.229	1.193	1.236	1.023	0.993	0.967	0.958	0.935	0.909	0.944	0.961
C7	**4.661**		0.0199	0.0266	0.0338	0.0422	0.0514	0.0627	0.0750	0.0930	1.337	1.271	1.249	1.218	1.220	1.196	1.240	0.998	0.978	0.960	0.946	0.928	0.912	0.947	0.953
C7	**4.661**		0.0199	0.0266	0.0338	0.0422	0.0514	0.0627	0.0750	0.0930	1.337	1.271	1.249	1.218	1.220	1.196	1.240	0.998	0.978	0.960	0.946	0.928	0.912	0.947	0.953
C8	**3.419**		0.0162	0.0206	0.0258	0.0316	0.0378	0.0464	0.0556	0.0683	1.272	1.252	1.225	1.196	1.228	1.198	1.228	0.949	0.964	0.941	0.929	0.934	0.913	0.938	0.938
C8	**3.419**		0.0162	0.0206	0.0258	0.0316	0.0378	0.0464	0.0556	0.0683	1.272	1.252	1.225	1.196	1.228	1.198	1.228	0.949	0.964	0.941	0.929	0.934	0.913	0.938	0.938
C9	**3.404**		0.0250	0.0337	0.0428	0.0532	0.0638	0.0788	0.0957	0.1143	1.348	1.270	1.243	1.199	1.235	1.214	1.194	1.006	0.977	0.955	0.931	0.940	0.926	0.912	0.950
C9	**3.404**		0.0250	0.0337	0.0428	0.0532	0.0638	0.0788	0.0957	0.1143	1.348	1.270	1.243	1.199	1.235	1.214	1.194	1.006	0.977	0.955	0.931	0.940	0.926	0.912	0.950
C10	**3.885**		0.0364	0.0497	0.0630	0.0787	0.0937	0.1133	0.1380	0.1590	1.365	1.268	1.249	1.191	1.209	1.218	1.152	1.019	0.976	0.960	0.925	0.920	0.928	0.880	0.944
C10	**3.885**		0.0364	0.0497	0.0630	0.0787	0.0937	0.1133	0.1380	0.1590	1.365	1.268	1.249	1.191	1.209	1.218	1.152	1.019	0.976	0.960	0.925	0.920	0.928	0.880	0.944
C11	**4.526**		0.0338	0.0457	0.0592	0.0754	0.0911	0.1123	0.1377	0.1753	1.352	1.295	1.274	1.208	1.233	1.226	1.273	1.009	0.997	0.979	0.938	0.938	0.935	0.972	0.967
C11	**4.526**		0.0338	0.0457	0.0592	0.0754	0.0911	0.1123	0.1377	0.1753	1.352	1.295	1.274	1.208	1.233	1.226	1.273	1.009	0.997	0.979	0.938	0.938	0.935	0.972	0.967
C12	**3.636**		0.0192	0.0255	0.0323	0.0400	0.0483	0.0595	0.0719	0.0850	1.328	1.267	1.238	1.208	1.232	1.208	1.182	0.991	0.975	0.952	0.938	0.938	0.921	0.903	0.945
C12	**3.636**		0.0192	0.0255	0.0323	0.0400	0.0483	0.0595	0.0719	0.0850	1.328	1.267	1.238	1.208	1.232	1.208	1.182	0.991	0.975	0.952	0.938	0.938	0.921	0.903	0.945
C13	**4.149**		0.0309	0.0433	0.0562	0.0731	0.0897	0.1107	0.1327	0.1600	1.401	1.298	1.301	1.227	1.234	1.199	1.206	1.046	0.999	1.000	0.953	0.939	0.914	0.921	0.967
C13	**4.149**		0.0309	0.0433	0.0562	0.0731	0.0897	0.1107	0.1327	0.1600	1.401	1.298	1.301	1.227	1.234	1.199	1.206	1.046	0.999	1.000	0.953	0.939	0.914	0.921	0.967
C14	**4.752**		0.0250	0.0342	0.0453	0.0571	0.0705	0.0843	0.1037	0.1253	1.368	1.325	1.260	1.235	1.196	1.230	1.208	1.021	1.019	0.969	0.959	0.910	0.938	0.923	0.963
C14	**4.752**		0.0250	0.0342	0.0453	0.0571	0.0705	0.0843	0.1037	0.1253	1.368	1.325	1.260	1.235	1.196	1.230	1.208	1.021	1.019	0.969	0.959	0.910	0.938	0.923	0.963
N1	**1.083**		0.0139	0.0178	0.0218	0.0263	0.0314	0.0389	0.0476	0.0576	1.281	1.225	1.206	1.194	1.239	1.224	1.210	0.956	0.943	0.927	0.927	0.943	0.933	0.924	0.936
N1	**1.083**		0.0139	0.0178	0.0218	0.0263	0.0314	0.0389	0.0476	0.0576	1.281	1.225	1.206	1.194	1.239	1.224	1.210	0.956	0.943	0.927	0.927	0.943	0.933	0.924	0.936
C15	**0.000**		0.0126	0.0162	0.0194	0.0233	0.0277	0.0339	0.0399	0.0487	1.286	1.198	1.201	1.189	1.224	1.177	1.221	0.960	0.922	0.923	0.923	0.931	0.897	0.932	0.927
C46	**0.127**		0.0178	0.0223	0.0280	0.0352	0.0422	0.0542	0.0673	0.0797	1.253	1.256	1.257	1.199	1.284	1.242	1.184	0.935	0.966	0.966	0.931	0.977	0.946	0.904	0.947
C40	**1.356**		0.0176	0.0231	0.0301	0.0384	0.0501	0.0655	0.0880	0.1127	1.313	1.303	1.276	1.305	1.307	1.344	1.281	0.980	1.003	0.980	1.013	0.995	1.024	0.978	0.996
C40	**1.356**		0.0176	0.0231	0.0301	0.0384	0.0501	0.0655	0.0880	0.1127	1.313	1.303	1.276	1.305	1.307	1.344	1.281	0.980	1.003	0.980	1.013	0.995	1.024	0.978	0.996
C20	**1.439**		0.0140	0.0175	0.0221	0.0287	0.0377	0.0524	0.0730	0.0970	1.250	1.263	1.299	1.314	1.390	1.393	1.329	0.933	0.972	0.998	1.020	1.058	1.062	1.015	1.008
C20	**1.439**		0.0140	0.0175	0.0221	0.0287	0.0377	0.0524	0.0730	0.0970	1.250	1.263	1.299	1.314	1.390	1.393	1.329	0.933	0.972	0.998	1.020	1.058	1.062	1.015	1.008
C16	**1.415**		0.0137	0.0175	0.0219	0.0284	0.0379	0.0518	0.0723	0.0930	1.277	1.251	1.297	1.335	1.367	1.396	1.286	0.953	0.963	0.997	1.036	1.040	1.064	0.982	1.005
C45	**1.492**		0.0181	0.0244	0.0310	0.0397	0.0521	0.0693	0.0907	0.1253	1.348	1.270	1.281	1.312	1.330	1.309	1.381	1.006	0.978	0.984	1.019	1.012	0.998	1.055	1.007
C41	**2.111**		0.0183	0.0243	0.0316	0.0408	0.0541	0.0720	0.0958	0.1260	1.328	1.300	1.291	1.326	1.331	1.331	1.315	0.991	1.001	0.992	1.030	1.013	1.014	1.004	1.006
C41	**2.111**		0.0183	0.0243	0.0316	0.0408	0.0541	0.0720	0.0958	0.1260	1.328	1.300	1.291	1.326	1.331	1.331	1.315	0.991	1.001	0.992	1.030	1.013	1.014	1.004	1.006
C23	**2.201**		0.0151	0.0200	0.0257	0.0343	0.0450	0.0612	0.0850	0.1187	1.325	1.285	1.335	1.312	1.360	1.389	1.396	0.989	0.989	1.026	1.019	1.035	1.059	1.066	1.026
C23	**2.201**		0.0151	0.0200	0.0257	0.0343	0.0450	0.0612	0.0850	0.1187	1.325	1.285	1.335	1.312	1.360	1.389	1.396	0.989	0.989	1.026	1.019	1.035	1.059	1.066	1.026
C19	**2.288**		0.0157	0.0201	0.0259	0.0342	0.0453	0.0638	0.0921	0.1353	1.280	1.289	1.320	1.325	1.408	1.444	1.469	0.955	0.992	1.015	1.029	1.072	1.100	1.122	1.041
C19	**2.288**		0.0157	0.0201	0.0259	0.0342	0.0453	0.0638	0.0921	0.1353	1.280	1.289	1.320	1.325	1.408	1.444	1.469	0.955	0.992	1.015	1.029	1.072	1.100	1.122	1.041
C39	**2.306**		0.0183	0.0252	0.0327	0.0435	0.0577	0.0794	0.1073	0.1483	1.377	1.298	1.330	1.326	1.376	1.351	1.382	1.028	0.999	1.022	1.030	1.047	1.030	1.055	1.030
C39	**2.306**		0.0183	0.0252	0.0327	0.0435	0.0577	0.0794	0.1073	0.1483	1.377	1.298	1.330	1.326	1.376	1.351	1.382	1.028	0.999	1.022	1.030	1.047	1.030	1.055	1.030
C17	**2.264**		0.0148	0.0194	0.0253	0.0341	0.0457	0.0656	0.0943	0.1277	1.311	1.304	1.348	1.340	1.435	1.438	1.354	0.978	1.004	1.036	1.041	1.092	1.096	1.034	1.040
C17	**2.264**		0.0148	0.0194	0.0253	0.0341	0.0457	0.0656	0.0943	0.1277	1.311	1.304	1.348	1.340	1.435	1.438	1.354	0.978	1.004	1.036	1.041	1.092	1.096	1.034	1.040
C43	**2.415**		0.0190	0.0251	0.0333	0.0448	0.0607	0.0853	0.1220	0.1673	1.321	1.327	1.345	1.355	1.405	1.430	1.371	0.986	1.021	1.034	1.052	1.069	1.090	1.047	1.043
C43	**2.415**		0.0190	0.0251	0.0333	0.0448	0.0607	0.0853	0.1220	0.1673	1.321	1.327	1.345	1.355	1.405	1.430	1.371	0.986	1.021	1.034	1.052	1.069	1.090	1.047	1.043
C18	**2.620**		0.0158	0.0209	0.0269	0.0363	0.0487	0.0660	0.0870	0.1177	1.323	1.287	1.349	1.342	1.355	1.318	1.353	0.987	0.991	1.037	1.042	1.031	1.005	1.033	1.018
C18	**2.620**		0.0158	0.0209	0.0269	0.0363	0.0487	0.0660	0.0870	0.1177	1.323	1.287	1.349	1.342	1.355	1.318	1.353	0.987	0.991	1.037	1.042	1.031	1.005	1.033	1.018
C42	**2.656**		0.0188	0.0255	0.0336	0.0449	0.0588	0.0793	0.1097	0.1570	1.356	1.318	1.336	1.310	1.349	1.383	1.431	1.012	1.014	1.027	1.017	1.026	1.054	1.093	1.035
C42	**2.656**		0.0188	0.0255	0.0336	0.0449	0.0588	0.0793	0.1097	0.1570	1.356	1.318	1.336	1.310	1.349	1.383	1.431	1.012	1.014	1.027	1.017	1.026	1.054	1.093	1.035
C36	**2.999**		0.0188	0.0257	0.0342	0.0453	0.0595	0.0793	0.1063	0.1393	1.367	1.331	1.325	1.313	1.333	1.340	1.310	1.020	1.024	1.018	1.020	1.014	1.022	1.001	1.017
C36	**2.999**		0.0188	0.0257	0.0342	0.0453	0.0595	0.0793	0.1063	0.1393	1.367	1.331	1.325	1.313	1.333	1.340	1.310	1.020	1.024	1.018	1.020	1.014	1.022	1.001	1.017
C22	**3.111**		0.0175	0.0235	0.0315	0.0422	0.0562	0.0768	0.1067	0.1453	1.343	1.340	1.340	1.332	1.367	1.389	1.362	1.002	1.032	1.030	1.034	1.040	1.059	1.040	1.034
C22	**3.111**		0.0175	0.0235	0.0315	0.0422	0.0562	0.0768	0.1067	0.1453	1.343	1.340	1.340	1.332	1.367	1.389	1.362	1.002	1.032	1.030	1.034	1.040	1.059	1.040	1.034
C34	**3.042**		0.0167	0.0229	0.0301	0.0403	0.0542	0.0741	0.1010	0.1390	1.371	1.314	1.339	1.345	1.367	1.363	1.376	1.023	1.012	1.029	1.044	1.040	1.039	1.051	1.034
C34	**3.042**		0.0167	0.0229	0.0301	0.0403	0.0542	0.0741	0.1010	0.1390	1.371	1.314	1.339	1.345	1.367	1.363	1.376	1.023	1.012	1.029	1.044	1.040	1.039	1.051	1.034
C44	**3.186**		0.0202	0.0272	0.0360	0.0486	0.0651	0.0890	0.1233	0.1920	1.347	1.324	1.350	1.340	1.367	1.385	1.557	1.005	1.019	1.038	1.040	1.040	1.056	1.189	1.055
C44	**3.186**		0.0202	0.0272	0.0360	0.0486	0.0651	0.0890	0.1233	0.1920	1.347	1.324	1.350	1.340	1.367	1.385	1.557	1.005	1.019	1.038	1.040	1.040	1.056	1.189	1.055
C21	**3.132**		0.0173	0.0234	0.0306	0.0414	0.0550	0.0760	0.0999	0.1340	1.353	1.308	1.353	1.329	1.382	1.314	1.341	1.009	1.006	1.040	1.032	1.052	1.002	1.024	1.024
C21	**3.132**		0.0173	0.0234	0.0306	0.0414	0.0550	0.0760	0.0999	0.1340	1.353	1.308	1.353	1.329	1.382	1.314	1.341	1.009	1.006	1.040	1.032	1.052	1.002	1.024	1.024
C38	**3.138**		0.0194	0.0262	0.0349	0.0465	0.0618	0.0832	0.1127	0.1543	1.351	1.332	1.332	1.329	1.346	1.355	1.369	1.008	1.025	1.024	1.032	1.025	1.032	1.046	1.027
C38	**3.138**		0.0194	0.0262	0.0349	0.0465	0.0618	0.0832	0.1127	0.1543	1.351	1.332	1.332	1.329	1.346	1.355	1.369	1.008	1.025	1.024	1.032	1.025	1.032	1.046	1.027
C35	**3.300**		0.0195	0.0266	0.0353	0.0470	0.0628	0.0837	0.1113	0.1457	1.364	1.327	1.331	1.336	1.333	1.330	1.309	1.018	1.021	1.023	1.038	1.014	1.014	1.000	1.018
C35	**3.300**		0.0195	0.0266	0.0353	0.0470	0.0628	0.0837	0.1113	0.1457	1.364	1.327	1.331	1.336	1.333	1.330	1.309	1.018	1.021	1.023	1.038	1.014	1.014	1.000	1.018
C24	**3.368**		0.0179	0.0243	0.0330	0.0446	0.0593	0.0793	0.1070	0.1400	1.358	1.358	1.352	1.330	1.337	1.349	1.308	1.013	1.045	1.039	1.032	1.018	1.028	0.999	1.025
C24	**3.368**		0.0179	0.0243	0.0330	0.0446	0.0593	0.0793	0.1070	0.1400	1.358	1.358	1.352	1.330	1.337	1.349	1.308	1.013	1.045	1.039	1.032	1.018	1.028	0.999	1.025
C31	**3.316**		0.0177	0.0244	0.0325	0.0438	0.0601	0.0811	0.1113	0.1693	1.379	1.332	1.348	1.372	1.349	1.372	1.521	1.029	1.025	1.036	1.065	1.027	1.046	1.162	1.056
C31	**3.316**		0.0177	0.0244	0.0325	0.0438	0.0601	0.0811	0.1113	0.1693	1.379	1.332	1.348	1.372	1.349	1.372	1.521	1.029	1.025	1.036	1.065	1.027	1.046	1.162	1.056
C28	**3.378**		0.0199	0.0273	0.0364	0.0490	0.0667	0.0931	0.1320	0.1870	1.372	1.333	1.346	1.361	1.396	1.418	1.417	1.024	1.026	1.035	1.057	1.062	1.081	1.082	1.052
C28	**3.378**		0.0199	0.0273	0.0364	0.0490	0.0667	0.0931	0.1320	0.1870	1.372	1.333	1.346	1.361	1.396	1.418	1.417	1.024	1.026	1.035	1.057	1.062	1.081	1.082	1.052
C30	**3.456**		0.0192	0.0261	0.0339	0.0451	0.0592	0.0782	0.1045	0.1417	1.359	1.299	1.330	1.313	1.321	1.336	1.356	1.015	1.000	1.022	1.019	1.005	1.019	1.036	1.016
C30	**3.456**		0.0192	0.0261	0.0339	0.0451	0.0592	0.0782	0.1045	0.1417	1.359	1.299	1.330	1.313	1.321	1.336	1.356	1.015	1.000	1.022	1.019	1.005	1.019	1.036	1.016
C29	**3.476**		0.0194	0.0270	0.0359	0.0471	0.0620	0.0834	0.1112	0.1520	1.392	1.330	1.312	1.316	1.345	1.333	1.367	1.039	1.023	1.008	1.022	1.024	1.016	1.044	1.025
C29	**3.476**		0.0194	0.0270	0.0359	0.0471	0.0620	0.0834	0.1112	0.1520	1.392	1.330	1.312	1.316	1.345	1.333	1.367	1.039	1.023	1.008	1.022	1.024	1.016	1.044	1.025
C37	**3.405**		0.0189	0.0263	0.0344	0.0455	0.0591	0.0777	0.1019	0.1343	1.392	1.308	1.323	1.299	1.315	1.311	1.318	1.039	1.007	1.017	1.009	1.001	1.000	1.006	1.011
C37	**3.405**		0.0189	0.0263	0.0344	0.0455	0.0591	0.0777	0.1019	0.1343	1.392	1.308	1.323	1.299	1.315	1.311	1.318	1.039	1.007	1.017	1.009	1.001	1.000	1.006	1.011
C25	**3.535**		0.0192	0.0263	0.0349	0.0462	0.0603	0.0812	0.1090	0.1433	1.370	1.327	1.324	1.305	1.347	1.342	1.315	1.022	1.021	1.017	1.013	1.025	1.023	1.004	1.018
C25	**3.535**		0.0192	0.0263	0.0349	0.0462	0.0603	0.0812	0.1090	0.1433	1.370	1.327	1.324	1.305	1.347	1.342	1.315	1.022	1.021	1.017	1.013	1.025	1.023	1.004	1.018
C33	**3.452**		0.0183	0.0256	0.0341	0.0459	0.0601	0.0808	0.1080	0.1383	1.399	1.332	1.346	1.309	1.344	1.337	1.281	1.044	1.025	1.034	1.017	1.023	1.019	0.978	1.020
C33	**3.452**		0.0183	0.0256	0.0341	0.0459	0.0601	0.0808	0.1080	0.1383	1.399	1.332	1.346	1.309	1.344	1.337	1.281	1.044	1.025	1.034	1.017	1.023	1.019	0.978	1.020
C26	**3.573**		0.0199	0.0276	0.0368	0.0490	0.0637	0.0860	0.1157	0.1507	1.387	1.333	1.332	1.300	1.350	1.345	1.303	1.035	1.026	1.023	1.009	1.027	1.025	0.995	1.020
C26	**3.573**		0.0199	0.0276	0.0368	0.0490	0.0637	0.0860	0.1157	0.1507	1.387	1.333	1.332	1.300	1.350	1.345	1.303	1.035	1.026	1.023	1.009	1.027	1.025	0.995	1.020
C32	**3.509**		0.0186	0.0259	0.0347	0.0469	0.0637	0.0873	0.1193	0.1550	1.392	1.340	1.352	1.358	1.370	1.367	1.299	1.039	1.031	1.039	1.055	1.043	1.042	0.992	1.034
C32	**3.509**		0.0186	0.0259	0.0347	0.0469	0.0637	0.0873	0.1193	0.1550	1.392	1.340	1.352	1.358	1.370	1.367	1.299	1.039	1.031	1.039	1.055	1.043	1.042	0.992	1.034
C27	**3.580**		0.0201	0.0272	0.0369	0.0500	0.0677	0.0930	0.1263	0.1670	1.353	1.357	1.355	1.354	1.374	1.358	1.322	1.010	1.044	1.041	1.051	1.045	1.035	1.010	1.034
C27	**3.580**		0.0201	0.0272	0.0369	0.0500	0.0677	0.0930	0.1263	0.1670	1.353	1.357	1.355	1.354	1.374	1.358	1.322	1.010	1.044	1.041	1.051	1.045	1.035	1.010	1.034

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0.064	0.937
1.398	1.002
1.454	1.006
2.156	1.016
2.297	1.035
2.339	1.041
2.638	1.026
3.055	1.025
3.114	1.045
3.135	1.025
3.334	1.022
3.347	1.054
3.466	1.021
3.470	1.015
3.513	1.020
3.545	1.034