

Bader Charges Analysis for Al/Ga-doped (6,0) SWSiCNTs at Si/C sites

Table 1. Bader Charges Analysis for Al-doped (6,0) SWSiCNTs at Si site

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# Item: 0
# File: D:/Y-Bader-ED-LSDA-SiCNT-(6.0)-Al(Si)-115-50Ha-0.001.hdf5
# Title: Y-Bader-ED-LSDA-SiCNT-(6.0)-Al(Si)-115-50Ha-0.001.hdf5 - BaderCharges_0
# Type: BaderCharges
+-----+
| |
| Bader Charges Analysis |
| |
+-----+
+-----+
| | Bader charge analysis only makes sense on an all electron density. |
| | If a pseudo-potential DFT calculation was used to generate this charge |
| | density then the core electron density must be included in order to get |
| | meaningful results. |
| |
| | Additionally, a fine electron density grid mesh should be used in order |
| | to correctly reproduce the total charge. |
+-----+
| | Electron Density Grid: 427 x 439 x 152 |
| | Identified 545 charge maxima |
+-----+
| | Bader Charge Volumes |
+-----+
| | # x y z Charge Atom Distance |
+-----+
| 0 0.0002 -0.0000 0.1847 0.0000 10 8.3543 |
| 1 0.0745 0.0371 0.3325 0.0000 18 8.2728 |
| 2 -0.0149 16.2702 0.6644 0.0000 10 8.2486 |
| 3 -0.0144 16.2702 1.1076 0.0000 10 8.1967 |
| 4 15.6906 0.0216 1.4956 0.0000 18 8.3127 |
| 5 15.7495 16.2174 1.7539 0.0000 10 8.1979 |
| 6 15.7497 16.1431 1.9016 0.0000 10 8.1507 |
| 7 15.6913 0.0216 2.1235 0.0000 18 8.3083 |
| 8 15.7875 16.2545 2.5664 0.0000 10 8.2216 |
| 9 0.0034 -0.0001 2.9545 0.0000 10 8.2611 |
| 10 0.0776 0.1484 3.1023 0.0000 18 8.1582 |
| 11 0.1153 0.0370 3.5455 0.0000 15 8.2760 |
| 12 0.1899 -0.0003 3.8410 0.0000 7 8.2260 |
| 13 15.6936 0.0958 4.1916 0.0000 19 8.3524 |
| 14 15.7311 0.0958 4.5240 0.0000 19 8.4081 |
| 15 15.6572 0.1330 4.8194 0.0000 20 8.3406 |
| 16 15.8060 0.0586 5.1150 0.0000 15 8.4875 |
| 17 0.0431 0.1856 5.3920 0.0000 18 8.3287 |
| 18 0.2289 -0.0003 5.5399 0.0000 10 8.2440 |
| 19 15.6897 0.1702 0.8309 0.0000 18 8.2774 |
| 20 15.7273 0.1701 1.2741 0.0000 18 8.2045 |
| 21 15.7651 0.2072 1.9758 0.0000 18 8.1316 |
| 22 0.1902 0.2226 4.2842 0.0000 15 8.1234 |
| 23 15.8017 0.2444 1.6066 0.0000 18 8.0830 |
| 24 15.7656 0.2072 2.3821 0.0000 18 8.1470 |
| 25 0.1905 0.5198 4.8012 0.0000 15 7.9960 |
| 26 0.1118 0.1485 0.5910 0.0000 18 8.1309 |
| 27 15.7999 0.4301 0.1662 0.0000 18 8.1455 |
| 28 0.2280 0.2226 4.9490 0.0000 15 8.1728 |
| 29 15.8022 0.4301 2.1236 0.0000 18 7.9697 |
| 30 15.6925 0.3187 3.4530 0.0000 19 8.1963 |
| 31 15.7263 0.3559 0.6093 0.0000 18 8.1672 |
| 32 15.6180 0.2074 3.0836 0.0000 19 8.2279 |
| 33 15.7673 0.4301 4.0809 0.0000 15 8.1755 |
| 34 15.7299 0.4301 3.7854 0.0000 19 8.1536 |
| 35 0.0788 0.5570 4.5057 0.0000 15 8.0247 |
| 36 15.8056 0.4672 5.1519 0.0000 20 8.1957 |
| 37 15.7689 0.5043 5.5212 0.0000 20 8.1757 |
| 38 0.4820 0.5196 0.2591 0.0000 18 7.6777 |
| 39 0.2603 0.5569 1.0713 0.0000 18 7.7019 |
| 40 0.1500 0.5570 1.8836 0.0000 18 7.7508 |
| 41 15.6905 0.5045 1.8649 0.0000 18 8.0106 |
| 42 0.0769 0.9285 3.1023 0.0000 18 7.6954 |
| 43 -0.0003 0.6686 0.3324 0.0000 18 7.9497 |
| 44 0.1495 0.5942 1.5143 0.0000 18 7.7356 |
| 45 0.1113 0.8542 0.7387 0.0000 18 7.6858 |
| 46 0.0021 0.7057 2.4005 0.0000 18 7.8012 |
| 47 15.6913 0.5045 2.5297 0.0000 18 8.0378 |
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	48	0.4479	0.5567	2.8811	0.0000	18	7.5873	
	49	0.1139	0.7799	2.9546	0.0000	18	7.7275	
	50	0.0748	0.7800	1.1819	0.0000	18	7.7073	
	51	0.1526	0.6313	4.2472	0.0000	15	7.8982	
	52	15.6563	0.8388	4.6347	0.0000	20	7.8024	
	53	0.0026	0.8915	2.9914	0.0000	18	7.7593	
	54	15.6922	0.7645	3.5638	0.0000	19	7.9205	
	55	15.6558	0.8017	4.1546	0.0000	20	7.8438	
	56	0.4133	0.8167	5.3185	0.0000	18	7.6922	
	57	15.6512	0.8017	0.1661	0.0000	20	7.9150	
	58	15.6938	0.8759	5.0041	0.0000	20	7.8094	
	59	15.4348	0.8390	5.5208	0.0000	20	7.7068	
	60	0.1105	1.0028	0.1848	0.0000	18	7.7025	
	61	0.1146	0.8913	3.6194	0.0000	15	7.7537	
	62	15.6163	1.3589	2.5665	0.0000	22	7.5191	
	63	0.0419	1.1885	5.1704	0.0000	20	7.7355	
	64	0.7063	0.8165	2.0689	0.0000	18	7.1555	
	65	0.0775	1.1885	3.8409	0.0000	15	7.6194	
	66	0.0407	1.1514	4.1363	0.0000	15	7.6832	
	67	0.0422	1.1885	5.4658	0.0000	18	7.7416	
	68	15.6897	1.0617	1.6433	0.0000	18	7.6987	
	69	15.7641	1.2102	1.9758	0.0000	18	7.5540	
	70	15.5073	1.5447	4.6345	0.0000	20	7.1892	
	71	5.5996	6.6064	4.7336	8.2560	12	0.0177	
	72	15.6518	0.9132	0.8308	0.0000	22	7.8262	
	73	15.4663	1.1362	0.9045	0.0000	22	7.5388	
	74	0.1142	1.2999	3.6193	0.0000	15	7.5258	
	75	15.5407	1.2104	1.2000	0.0000	22	7.5274	
	76	15.7995	1.2845	0.4986	0.0000	18	7.6069	
	77	0.1109	1.6715	1.0711	0.0000	18	7.2070	
	78	15.7654	1.2473	3.1207	0.0000	18	7.6368	
	79	6.3023	5.2314	1.8538	8.3311	18	0.0264	
	80	0.1128	1.6714	2.7330	0.0000	18	7.2190	
	81	6.4526	5.3798	3.6636	11.6908	15	0.0192	
	82	0.1479	1.4857	0.8126	0.0000	18	7.3015	
	83	15.6901	1.3960	2.2342	0.0000	18	7.5287	
	84	15.5055	1.1733	2.7880	0.0000	22	7.5555	
	85	0.0371	1.7087	1.4034	0.0000	18	7.2247	
	86	5.4841	6.6066	1.0034	11.6831	17	0.0156	
	87	15.5434	1.6190	3.8960	0.0000	20	7.2003	
	88	15.5809	1.5818	4.2284	0.0000	20	7.2269	
	89	15.5080	1.5819	5.2993	0.0000	20	7.1950	
	90	0.4127	1.6711	5.5032	0.0000	17	7.1643	
	91	0.0038	1.9687	4.9857	0.0000	20	7.1677	
	92	15.5446	1.5447	4.8931	0.0000	20	7.2207	
	93	0.0034	2.0058	4.6533	0.0000	20	7.1335	
	94	10.3055	6.6390	0.8614	11.6510	23	0.0187	
	95	15.7260	1.9160	1.6064	0.0000	23	7.2212	
	96	15.5787	2.0276	2.6403	0.0000	22	7.1536	
	97	15.5769	2.0276	1.0892	0.0000	23	7.0009	
	98	5.2612	8.1670	2.0003	8.3677	14	0.0209	
	99	10.4211	6.6017	4.6285	8.3033	20	0.0180	
	100	10.7873	8.1244	1.8221	8.3628	2	0.0199	
	101	5.3375	8.1669	3.8469	10.7628	11	0.0236	
	102	10.7153	8.1244	3.6686	11.6690	0	0.0166	
	103	5.5595	9.7268	4.7335	8.2365	8	0.0248	
	104	10.3811	9.6477	4.6284	8.3043	1	0.0207	
	105	5.4440	9.6898	1.0033	11.6594	13	0.0211	
	106	10.3026	9.6479	0.8613	11.6376	5	0.0216	
	107	0.0246	13.9670	0.8492	0.0000	13	6.8972	
	108	15.5323	13.9145	4.4866	0.0000	1	6.6701	
	109	15.4953	13.9517	4.5604	0.0000	1	6.6643	
	110	15.7918	14.2485	4.6346	0.0000	1	7.0820	
	111	6.4102	10.9518	3.6635	11.6726	7	0.0213	
	112	15.5669	14.2859	2.6401	0.0000	6	7.1858	
	113	15.7140	14.3601	1.6431	0.0000	10	7.2116	
	114	0.0247	14.6357	1.4401	0.0000	10	7.2130	
	115	0.0633	14.6356	2.7327	0.0000	10	7.2234	
	116	0.1353	14.6356	0.8862	0.0000	10	7.1697	
	117	0.0242	14.6728	1.0338	0.0000	10	7.2657	
	118	15.5309	14.6574	3.8588	0.0000	1	7.2051	
	119	15.5326	14.6945	5.3729	0.0000	1	7.2297	
	120	0.1377	14.7841	3.0652	0.0000	10	7.2827	
	121	15.5318	14.6946	4.6712	0.0000	1	7.1907	
	122	0.3230	15.0440	3.1762	0.0000	10	7.2848	
	123	0.0289	15.1185	5.4655	0.0000	10	7.7149	
	124	0.0285	15.1185	5.1701	0.0000	1	7.7355	
	125	0.0641	15.1185	3.8406	0.0000	7	7.5995	
	126	0.0645	15.1185	4.2099	0.0000	7	7.6175	
	127	0.1764	15.0069	4.6902	0.0000	7	7.5148	

128	-0.0123	15.1186	1.9570	0.0000	10	7.4840
129	15.6772	14.8430	2.2340	0.0000	10	7.4826
130	15.6033	14.9546	2.5663	0.0000	6	7.5525
131	0.0975	15.3042	0.8492	0.0000	10	7.5593
132	15.4904	15.0661	1.2366	0.0000	6	7.5067
133	15.4551	15.0661	2.7877	0.0000	6	7.5175
134	15.5288	15.0661	2.4184	0.0000	6	7.5395
135	15.4908	14.3232	1.0150	0.0000	5	6.9896
136	15.6390	15.2146	1.5692	0.0000	6	7.6947
137	-0.0114	15.4529	2.9911	0.0000	10	7.7536
138	0.0230	15.4158	0.5906	0.0000	10	7.7205
139	15.5282	15.2518	2.0861	0.0000	6	7.6261
140	0.0618	15.4528	2.1418	0.0000	10	7.6138
141	0.1337	15.3414	0.0737	0.0000	10	7.6910
142	0.0608	15.5272	1.3293	0.0000	10	7.6687
143	0.3951	15.0439	1.3297	0.0000	10	7.1200
144	0.0636	15.3785	3.6190	0.0000	7	7.7429
145	0.0230	15.5272	0.7383	0.0000	10	7.7612
146	0.0235	15.5272	1.1815	0.0000	10	7.7103
147	15.6051	15.4746	4.5605	0.0000	1	7.8054
148	0.1350	15.7128	1.5510	0.0000	10	7.7070
149	0.1355	15.7499	1.9941	0.0000	10	7.7250
150	15.6422	15.4745	4.6344	0.0000	1	7.8299
151	15.4579	15.4375	5.5575	0.0000	1	7.7359
152	15.6039	15.4746	3.5634	0.0000	3	7.8476
153	0.1373	15.6385	3.4344	0.0000	10	7.8192
154	15.6045	15.4746	4.1173	0.0000	1	7.8214
155	15.6371	15.4746	0.1658	0.0000	1	7.9151
156	15.7171	15.8459	5.5578	0.0000	1	8.2109
157	0.3992	15.4896	5.2813	0.0000	10	7.6757
158	15.7480	15.8460	0.1659	0.0000	10	8.1483
159	-0.0093	15.8243	5.1700	0.0000	7	8.2064
160	0.3194	15.8612	0.7387	0.0000	10	7.7260
161	0.6565	15.4151	3.2504	0.0000	10	7.2445
162	15.6407	15.9203	3.7111	0.0000	3	8.1499
163	0.1383	15.9356	4.5793	0.0000	7	8.0693
164	0.1016	15.8242	4.8378	0.0000	7	8.0640
165	0.2086	15.7499	1.0340	0.0000	10	7.7078
166	0.2086	16.0842	1.3295	0.0000	10	7.8901
167	0.3590	15.8240	2.9177	0.0000	10	7.6686
168	15.7884	15.8087	3.0096	0.0000	10	7.9986
169	15.6373	16.1061	0.8305	0.0000	10	8.2803
170	15.6397	16.1060	2.9725	0.0000	10	8.2891
171	-0.0092	16.0843	5.4285	0.0000	10	8.2993
172	15.6371	15.9575	0.5351	0.0000	10	8.2333
173	15.7132	16.1060	2.3817	0.0000	10	8.1728
174	0.0623	16.1586	3.1389	0.0000	10	8.1379
175	15.6794	16.1060	5.1884	0.0000	1	8.3517
176	0.2128	16.0841	4.9487	0.0000	7	8.1553
177	15.6047	16.1432	4.8190	0.0000	1	8.3169
178	0.2100	16.1213	2.5482	0.0000	10	7.9276
179	0.2236	0.1855	1.0713	0.0000	18	7.9617
180	0.2624	0.1854	2.5485	0.0000	18	7.9259
181	0.4117	0.7796	3.9152	0.0000	15	7.5843
182	0.2277	1.0026	5.3183	0.0000	18	7.7323
183	0.1502	0.8913	2.3637	0.0000	18	7.5708
184	0.3725	1.2997	2.4748	0.0000	18	7.1666
185	0.4481	1.6711	4.0629	0.0000	15	7.0573
186	0.4699	14.3009	1.2559	0.0000	10	6.6755
187	0.4003	14.6352	5.5029	0.0000	13	7.1493
188	0.3985	14.6352	3.9518	0.0000	7	7.0626
189	0.3998	14.6724	5.1705	0.0000	8	7.1775
190	0.3593	15.0068	2.4745	0.0000	10	7.1388
191	0.3575	15.1183	0.9603	0.0000	10	7.2283
192	6.2967	11.0634	1.8537	8.3414	10	0.0232
193	0.3617	15.2296	4.6904	0.0000	7	7.4865
194	0.4727	15.4524	4.6536	0.0000	7	7.5227
195	0.4347	15.4896	3.9149	0.0000	7	7.5125
196	0.3585	15.8612	2.5114	0.0000	10	7.6458
197	0.4302	15.8240	0.2587	0.0000	10	7.7017
198	0.2083	16.1214	1.1079	0.0000	10	7.9314
199	0.1877	0.0741	1.9945	0.0000	18	8.0247
200	0.3340	-0.0003	0.1481	0.0000	10	8.1128
201	0.4124	1.0767	4.7276	0.0000	15	7.4806
202	0.4079	1.2254	0.9237	0.0000	18	7.2096
203	0.4083	1.2626	1.2930	0.0000	18	7.1508
204	0.5084	14.3009	2.4747	0.0000	10	6.6463
205	0.3931	15.4897	0.0002	0.0000	10	7.5880
206	0.3571	15.8612	1.2188	0.0000	10	7.6429
207	0.3963	15.8240	3.0285	0.0000	10	7.6562

	208	0.2463	16.0842	1.8465	0.0000	10	7.8444	
	209	0.3757	0.0738	4.2106	0.0000	15	8.0725	
	210	0.5249	0.2223	5.1340	0.0000	15	7.9815	
	211	0.4871	0.2223	4.4692	0.0000	15	7.9139	
	212	0.4475	0.2224	2.2902	0.0000	18	7.7421	
	213	0.5224	0.5195	3.1767	0.0000	18	7.5992	
	214	0.4857	0.4824	3.4351	0.0000	18	7.6996	
	215	0.7054	0.8165	1.2565	0.0000	18	7.1767	
	216	0.3383	0.4453	4.2475	0.0000	15	7.8659	
	217	0.4137	0.7796	5.5771	0.0000	18	7.6458	
	218	0.3610	15.4525	4.2841	0.0000	7	7.5714	
	219	0.4090	0.4082	1.2192	0.0000	18	7.6649	
	220	0.3020	0.4825	5.0230	0.0000	15	7.9669	
	221	0.3750	0.8168	4.2475	0.0000	15	7.6098	
	222	1.3223	15.5630	1.7370	0.0000	10	6.6902	
	223	0.4323	16.1211	2.3269	0.0000	10	7.7413	
	224	0.3943	16.2697	1.6620	0.0000	10	7.8544	
	225	0.5238	0.2223	4.1369	0.0000	15	7.8590	
	226	0.6688	0.8165	1.6996	0.0000	18	7.1828	
	227	0.6550	15.4894	1.9947	0.0000	10	7.1546	
	228	0.3203	15.8612	1.5142	0.0000	10	7.6532	
	229	0.6547	15.4894	1.7362	0.0000	10	7.1540	
	230	0.7081	-0.0008	2.9184	0.0000	10	7.7316	
	231	1.0986	15.8604	0.9981	0.0000	10	7.1053	
	232	1.0764	0.4075	1.0723	0.0000	18	7.1775	
	233	0.4141	0.1481	5.4663	0.0000	18	8.0574	
	234	0.4338	15.8239	3.4348	0.0000	10	7.7010	
	235	0.5457	15.7866	3.9520	0.0000	7	7.6107	
	236	0.5097	16.0838	5.1337	0.0000	7	7.9639	
	237	0.6937	16.0094	3.8413	0.0000	7	7.6387	
	238	0.5089	16.1210	4.4320	0.0000	7	7.8880	
	239	0.3931	16.2698	0.6649	0.0000	10	7.9409	
	240	0.5417	16.1210	0.7759	0.0000	10	7.7173	
	241	0.5601	0.2594	3.4722	0.0000	18	7.7920	
	242	0.7075	1.0022	3.2507	0.0000	18	7.1769	
	243	0.7070	0.8536	2.6968	0.0000	18	7.1794	
	244	0.6561	15.4522	2.9180	0.0000	10	7.2101	
	245	0.6905	15.3780	0.5175	0.0000	10	7.1798	
	246	0.7284	15.4893	1.2931	0.0000	10	7.1165	
	247	0.3982	15.9354	4.8012	0.0000	7	7.8979	
	248	0.5827	16.0838	4.1366	0.0000	7	7.7842	
	249	0.4729	16.1582	5.4291	0.0000	10	7.9859	
	250	0.6586	15.9722	5.4663	0.0000	10	7.7230	
	251	0.5449	16.0838	3.5088	0.0000	10	7.7969	
	252	0.7100	0.1106	4.7280	0.0000	15	7.8530	
	253	0.5231	0.5195	3.7676	0.0000	15	7.6542	
	254	0.7077	1.0765	3.4723	0.0000	15	7.1672	
	255	0.6906	15.4522	0.6283	0.0000	10	7.2050	
	256	0.6534	16.1952	1.1822	0.0000	10	7.6380	
	257	0.7271	16.2694	0.8130	0.0000	10	7.6747	
	258	1.0760	0.4447	0.7029	0.0000	18	7.2020	
	259	0.7467	1.2621	5.2820	0.0000	18	7.1936	
	260	0.6581	14.8950	4.2106	0.0000	7	7.0017	
	261	0.7704	15.0806	5.2448	0.0000	10	7.1693	
	262	0.6579	15.6379	4.6538	0.0000	7	7.4916	
	263	0.6677	0.8908	0.8502	0.0000	18	7.2053	
	264	0.7469	1.3364	5.5405	0.0000	18	7.0782	
	265	0.8770	14.7834	0.8871	0.0000	10	6.6256	
	266	0.6539	15.4523	0.9607	0.0000	10	7.1853	
	267	0.7459	0.2964	3.8048	0.0000	15	7.6299	
	268	0.6349	0.6308	4.3217	0.0000	15	7.5259	
	269	0.6356	-0.0007	4.4325	0.0000	7	7.9291	
	270	0.5929	0.5938	0.0376	0.0000	18	7.5973	
	271	0.9911	16.1205	4.5064	0.0000	7	7.5412	
	272	1.0629	15.8976	2.2537	0.0000	10	7.1184	
	273	1.4000	15.4886	4.7654	0.0000	7	6.8545	
	274	1.0444	-0.0011	5.0977	0.0000	7	7.7318	
	275	1.1157	0.4446	2.9927	0.0000	18	7.1747	
	276	1.1009	15.8604	2.9924	0.0000	10	7.1466	
	277	1.0236	15.7491	0.1856	0.0000	10	7.2283	
	278	1.0611	15.8605	0.6657	0.0000	10	7.1796	
	279	0.9680	0.1104	3.3249	0.0000	18	7.5651	
	280	0.9161	16.1949	3.8785	0.0000	7	7.6011	
	281	1.0803	0.0360	4.1375	0.0000	15	7.5782	
	282	1.0657	16.0461	4.7650	0.0000	7	7.4709	
	283	1.2831	15.9717	0.2597	0.0000	10	7.1743	
	284	1.3253	16.1202	4.8392	0.0000	7	7.3506	
	285	1.4116	0.0357	1.9221	0.0000	18	7.1598	
	286	1.4476	-0.0015	0.9988	0.0000	10	7.1827	
	287	1.4496	-0.0015	2.6977	0.0000	10	7.1829	

288	1.5582	0.0356	0.4450	0.0000	18	7.1968	
289	1.8590	-0.0019	3.9538	0.0000	7	7.0455	
290	1.5615	-0.0016	3.2148	0.0000	10	7.1883	
291	1.5262	0.3699	5.1352	0.0000	15	7.1660	
292	1.8198	0.3696	2.3657	0.0000	18	6.6574	
293	1.7673	15.9341	2.0330	0.0000	10	6.6352	
294	1.8419	15.9711	2.4393	0.0000	10	6.6361	
295	1.9350	-0.0020	5.5050	0.0000	10	7.0881	
296	1.8182	0.4068	1.0362	0.0000	18	6.6597	
297	1.8189	0.3696	1.6640	0.0000	18	6.6398	
298	1.8039	15.9340	1.5898	0.0000	10	6.6123	
299	1.8422	15.9340	2.6240	0.0000	10	6.6279	
300	1.8943	0.3695	2.6612	0.0000	18	6.6372	
301	1.8773	15.9711	0.9252	0.0000	10	6.6489	
302	7.9007	4.8583	4.6255	8.3153	16	0.0151	
303	2.3048	0.0348	4.5821	0.0000	15	6.8132	
304	7.8944	11.3961	4.6254	8.2980	4	0.0180	
305	2.6336	-0.0026	0.1877	0.0000	10	6.5949	
306	7.8592	4.9698	0.8585	11.7230	21	0.0117	
307	7.8160	11.2848	0.8584	11.6422	9	0.0242	
308	9.3011	10.8375	1.8203	8.3101	6	0.0190	
309	9.3434	5.4513	1.8205	8.3051	22	0.0145	
310	9.3033	10.8004	3.6669	11.6562	3	0.0212	
311	9.3455	5.4884	3.6670	11.6622	19	0.0183	
312	13.9738	15.8476	5.4819	0.0000	6	7.1113	
313	13.9355	16.2563	4.7801	0.0000	3	7.2490	
314	13.9515	0.4319	5.4083	0.0000	19	7.0611	
315	13.9867	0.4318	3.8203	0.0000	19	6.8703	
316	13.9840	0.0233	1.0874	0.0000	22	7.1685	
317	13.9724	16.2563	4.5586	0.0000	3	7.2421	
318	13.9719	15.8477	3.8200	0.0000	3	6.8826	
319	14.0213	0.0232	1.3090	0.0000	22	7.1734	
320	13.9694	15.5134	1.3825	0.0000	6	6.6129	
321	13.9724	15.7362	4.1893	0.0000	3	6.8195	
322	14.0220	0.0232	1.8630	0.0000	22	7.1556	
323	14.0588	-0.0139	1.6415	0.0000	22	7.2100	
324	14.1908	15.9218	0.7550	0.0000	6	7.1255	
325	14.2856	0.0229	5.3718	0.0000	19	7.5651	
326	14.3953	-0.0143	4.0054	0.0000	19	7.4810	
327	14.2675	15.9588	2.9340	0.0000	3	7.2020	
328	14.2844	-0.0142	4.2638	0.0000	19	7.4223	
329	14.2852	-0.0142	5.0024	0.0000	19	7.5177	
330	14.4290	0.3943	1.3834	0.0000	22	7.1755	
331	14.2445	0.2830	2.0848	0.0000	22	7.1173	
332	14.4141	15.9216	1.3830	0.0000	6	7.2147	
333	14.3405	15.8102	1.7892	0.0000	6	7.0708	
334	14.3536	0.1344	0.0907	0.0000	22	7.4982	
335	14.3934	0.3572	2.6390	0.0000	22	7.2095	
336	14.3544	0.3944	0.9770	0.0000	22	7.1593	
337	14.3766	15.9216	1.0137	0.0000	6	7.2202	
338	14.3784	15.9216	2.6017	0.0000	6	7.2187	
339	14.3925	0.4315	1.8634	0.0000	22	7.1100	
340	14.4705	0.7657	5.4827	0.0000	20	7.1700	
341	14.4686	0.7657	3.8208	0.0000	19	6.9757	
342	14.4174	15.4758	3.8574	0.0000	3	6.9356	
343	14.4564	15.5128	5.5194	0.0000	1	7.1770	
344	14.3754	16.1445	0.1273	0.0000	6	7.5267	
345	14.3386	16.0702	0.3858	0.0000	6	7.3953	
346	14.3793	16.1073	3.4881	0.0000	3	7.3511	
347	14.3947	0.1714	3.5623	0.0000	19	7.3386	
348	14.4521	15.1043	1.4939	0.0000	6	6.6862	
349	14.4646	0.8029	0.4232	0.0000	22	7.0473	
350	14.6171	1.4713	4.5227	0.0000	20	6.6448	
351	14.6043	14.8069	4.5594	0.0000	1	6.6470	
352	14.6016	16.2557	3.4145	0.0000	3	7.6141	
353	14.6922	0.7654	4.7813	0.0000	19	7.2260	
354	14.5250	15.6986	0.8292	0.0000	6	7.1947	
355	14.6414	15.8098	5.4088	0.0000	1	7.5116	
356	14.7625	-0.0146	0.7559	0.0000	22	7.7607	
357	14.7256	0.0226	0.9775	0.0000	22	7.6813	
358	14.6561	0.4312	5.3352	0.0000	19	7.5251	
359	14.6917	0.8026	4.4120	0.0000	19	7.1540	
360	14.6781	15.4755	4.8179	0.0000	3	7.2188	
361	14.6351	15.9585	0.0907	0.0000	6	7.5848	
362	14.6739	16.2556	1.7896	0.0000	6	7.6216	
363	14.6742	16.2556	2.0850	0.0000	6	7.6264	
364	14.8385	-0.0147	2.3441	0.0000	22	7.7584	
365	14.7278	-0.0146	2.8610	0.0000	22	7.7326	
366	14.6911	-0.0146	3.1933	0.0000	19	7.6925	
367	14.7297	0.1711	4.6336	0.0000	19	7.6336	

	368	14.7148	15.4754	4.4487	0.0000	3	7.1968	
	369	14.6766	15.7727	3.7469	0.0000	3	7.3253	
	370	14.6773	16.1070	4.6333	0.0000	3	7.6182	
	371	14.8018	-0.0147	2.6764	0.0000	22	7.7619	
	372	14.7283	0.2082	3.4519	0.0000	19	7.5494	
	373	14.9140	0.4309	3.8952	0.0000	19	7.5322	
	374	14.6920	0.3197	4.2274	0.0000	19	7.4630	
	375	14.7246	0.2083	0.2389	0.0000	22	7.6687	
	376	14.7265	0.7283	2.3439	0.0000	22	7.1711	
	377	14.8226	15.5868	1.5682	0.0000	6	7.2773	
	378	14.6752	15.5498	2.3436	0.0000	6	7.1567	
	379	14.8003	-0.0147	1.3838	0.0000	22	7.7262	
	380	14.6884	0.6541	1.4206	0.0000	22	7.1841	
	381	14.7492	15.5869	2.1959	0.0000	6	7.2273	
	382	14.6723	16.1071	0.2754	0.0000	6	7.6725	
	383	14.6928	0.3940	4.9660	0.0000	19	7.5037	
	384	14.6919	0.9883	4.6705	0.0000	19	7.0658	
	385	14.9091	1.1368	0.2021	0.0000	20	7.1908	
	386	14.9498	1.1738	3.3413	0.0000	19	7.0883	
	387	14.6757	15.5870	2.8237	0.0000	6	7.2325	
	388	14.8369	0.7282	1.6054	0.0000	22	7.2389	
	389	14.8586	15.1039	0.2018	0.0000	1	7.1411	
	390	14.8238	15.5868	2.6023	0.0000	6	7.3158	
	391	14.8992	15.8467	3.8949	0.0000	3	7.5424	
	392	14.9528	0.4680	5.4095	0.0000	20	7.6818	
	393	14.8221	15.5868	1.0881	0.0000	6	7.3092	
	394	14.9875	0.4309	3.2306	0.0000	19	7.5965	
	395	14.9510	0.3566	3.6737	0.0000	19	7.6062	
	396	14.9845	1.0624	1.1624	0.0000	22	7.1693	
	397	14.9152	1.1738	5.5202	0.0000	20	7.1193	
	398	14.9365	15.0666	3.3780	0.0000	3	7.0744	
	399	14.9010	15.8096	5.3722	0.0000	1	7.6575	
	400	14.9902	0.3937	5.5942	0.0000	20	7.7842	
	401	14.9469	0.4310	0.2391	0.0000	22	7.6793	
	402	14.9473	0.5053	0.6084	0.0000	22	7.5633	
	403	14.9692	15.8467	0.2388	0.0000	6	7.7181	
	404	14.9360	15.9210	3.7103	0.0000	3	7.6163	
	405	14.9152	0.0223	4.5600	0.0000	19	7.8598	
	406	15.1013	-0.0150	5.1142	0.0000	19	8.0986	
	407	14.9893	0.7651	5.0771	0.0000	20	7.4413	
	408	15.1311	2.2881	0.7194	0.0000	23	6.4928	
	409	14.8249	15.1039	3.1562	0.0000	3	7.0217	
	410	15.0112	15.9209	4.5967	0.0000	3	7.7276	
	411	15.0474	16.1066	3.9690	0.0000	3	7.8296	
	412	15.0267	0.1336	4.8556	0.0000	19	7.9020	
	413	14.9689	15.8839	0.0173	0.0000	1	7.7899	
	414	15.0213	0.1337	0.1653	0.0000	22	7.9444	
	415	15.0634	0.1707	4.5602	0.0000	19	7.8648	
	416	15.0261	0.3937	4.5232	0.0000	19	7.6842	
	417	15.0257	0.4680	4.3016	0.0000	19	7.6135	
	418	15.0637	0.4308	5.0403	0.0000	20	7.7492	
	419	15.0964	1.1737	1.8642	0.0000	22	7.1609	
	420	14.9837	1.2110	0.5715	0.0000	22	7.1583	
	421	15.0460	15.1037	1.8639	0.0000	6	7.1445	
	422	14.9725	15.2152	2.6024	0.0000	6	7.1961	
	423	15.0064	15.5495	0.0542	0.0000	1	7.5535	
	424	15.0489	15.8466	5.0030	0.0000	1	7.7482	
	425	15.0099	15.8466	3.3780	0.0000	3	7.6269	
	426	15.0454	15.8095	1.9747	0.0000	6	7.5887	
	427	15.1003	-0.0150	4.1909	0.0000	19	7.9855	
	428	15.1235	15.1036	4.7446	0.0000	1	7.2092	
	429	15.0497	15.1408	5.1138	0.0000	1	7.2048	
	430	15.0858	15.1408	4.3014	0.0000	1	7.2191	
	431	15.0102	15.5495	3.4150	0.0000	3	7.4318	
	432	15.0114	16.1066	4.8553	0.0000	3	7.8871	
	433	15.1331	0.3936	0.8302	0.0000	22	7.7424	
	434	15.0963	0.4308	1.1256	0.0000	22	7.6582	
	435	14.9870	0.7652	3.0828	0.0000	19	7.3885	
	436	15.0993	1.1365	4.3386	0.0000	20	7.2162	
	437	15.1370	1.1365	4.8188	0.0000	20	7.2375	
	438	15.1686	1.5823	0.4609	0.0000	23	7.0222	
	439	15.0466	15.5123	2.7133	0.0000	6	7.4502	
	440	15.0851	15.8465	4.2275	0.0000	3	7.6978	
	441	15.1186	15.8466	1.1254	0.0000	6	7.6981	
	442	15.2665	15.9950	0.8301	0.0000	6	7.9376	
	443	15.0430	16.1067	0.1281	0.0000	6	7.9653	
	444	15.0468	16.1066	3.4150	0.0000	3	7.8276	
	445	15.0621	0.1708	3.4522	0.0000	19	7.8170	
	446	15.1708	0.4307	1.4212	0.0000	22	7.6933	
	447	15.0582	0.6909	0.4978	0.0000	22	7.5461	

448	15.0850	13.9521	2.5657	0.0000	6	6.5981
449	15.0851	15.5494	3.9690	0.0000	3	7.4908
450	15.1346	0.4307	2.1967	0.0000	22	7.6645
451	15.1333	-0.0150	0.6825	0.0000	22	8.0344
452	15.0617	-0.0150	2.8983	0.0000	22	7.9739
453	15.2088	0.8764	2.6030	0.0000	22	7.4709
454	15.1932	15.9951	1.6425	0.0000	6	7.8225
455	15.1935	16.0694	1.9749	0.0000	6	7.8715
456	15.2459	0.2078	1.9752	0.0000	22	7.8874
457	15.3560	-0.0152	0.8305	0.0000	22	8.1772
458	15.2320	15.3635	2.6027	0.0000	6	7.4905
459	15.2834	0.0220	2.1969	0.0000	22	8.0467
460	15.3225	0.0219	3.9696	0.0000	19	8.1116
461	15.3589	-0.0153	3.3418	0.0000	19	8.1650
462	15.2833	0.3563	2.3815	0.0000	22	7.8365
463	15.2816	0.5421	1.0889	0.0000	22	7.7308
464	15.2441	0.9136	1.0150	0.0000	22	7.4790
465	15.4543	14.6204	1.7536	0.0000	6	7.2107
466	15.2302	15.3264	0.9778	0.0000	6	7.4731
467	15.4524	15.2148	0.6087	0.0000	5	7.5937
468	15.2688	15.2892	2.3073	0.0000	6	7.4499
469	15.2670	15.6978	1.0886	0.0000	6	7.7193
470	15.2683	15.9578	2.3812	0.0000	6	7.8727
471	15.4293	0.1333	0.1658	0.0000	22	8.2411
472	15.3456	16.2549	5.3358	0.0000	1	8.2741
473	15.3556	0.2448	0.7197	0.0000	22	8.0204
474	15.3568	0.7277	2.0861	0.0000	22	7.6427
475	15.3564	0.6906	1.7168	0.0000	22	7.6615
476	15.3581	0.8020	3.3049	0.0000	19	7.6398
477	15.3916	0.8391	0.2396	0.0000	20	7.7285
478	15.3548	0.9506	0.6089	0.0000	22	7.5988
479	15.3182	1.4707	1.4213	0.0000	22	7.1829
480	15.5036	1.6934	1.6062	0.0000	23	7.2076
481	15.3776	15.4377	0.2763	0.0000	5	7.7279
482	15.5315	15.4375	5.0405	0.0000	1	7.7394
483	15.3437	15.4006	2.9722	0.0000	3	7.6267
484	15.3420	15.6606	1.7165	0.0000	6	7.7201
485	15.3046	15.6235	1.4580	0.0000	6	7.6756
486	15.3425	15.5120	2.0489	0.0000	6	7.6311
487	15.3042	15.8835	1.3102	0.0000	6	7.8484
488	15.3607	0.1704	5.0776	0.0000	20	8.1377
489	15.5071	0.1332	3.3420	0.0000	19	8.1772
490	15.3577	0.8763	3.0094	0.0000	19	7.6143
491	15.3955	0.8391	3.6373	0.0000	19	7.6380
492	15.4344	0.8390	5.1884	0.0000	20	7.6751
493	15.2818	1.4707	2.0122	0.0000	22	7.1439
494	15.3440	15.4748	3.3046	0.0000	3	7.6490
495	15.4944	15.4747	5.1144	0.0000	1	7.7471
496	15.3028	15.9207	0.1284	0.0000	1	8.0342
497	15.3455	16.0320	5.0772	0.0000	1	8.0792
498	15.3425	16.2549	2.6398	0.0000	6	8.1461
499	15.3603	0.3933	4.8560	0.0000	20	7.9528
500	15.3960	0.8019	4.0435	0.0000	19	7.6698
501	15.2829	1.6193	3.0832	0.0000	19	7.1202
502	15.3816	15.5491	3.8216	0.0000	3	7.7171
503	15.4179	16.0691	3.6001	0.0000	3	8.0750
504	15.4882	16.1063	0.2025	0.0000	6	8.2758
505	15.3074	16.0692	4.2278	0.0000	3	8.0110
506	15.3453	15.9206	4.8557	0.0000	1	7.9821
507	15.4516	16.1434	0.7195	0.0000	6	8.1871
508	15.3788	16.2549	1.9751	0.0000	6	8.1333
509	15.4677	0.2447	1.4215	0.0000	22	8.0394
510	15.5064	0.4675	2.9727	0.0000	19	7.9859
511	15.5031	1.0619	0.6091	0.0000	23	7.6231
512	15.3169	1.6564	0.4611	0.0000	23	7.0729
513	15.4529	15.1033	0.9411	0.0000	5	7.5085
514	15.3448	15.4748	4.0062	0.0000	3	7.6483
515	15.4569	15.8462	5.0404	0.0000	1	8.0015
516	15.4520	15.8091	0.7195	0.0000	6	7.9745
517	15.4545	15.8462	2.9354	0.0000	3	7.9926
518	15.5288	16.1062	3.3048	0.0000	3	8.1911
519	15.4676	-0.0153	1.0891	0.0000	22	8.2326
520	15.4712	-0.0154	4.2283	0.0000	19	8.2602
521	15.4313	0.3190	2.0493	0.0000	22	7.9568
522	15.5409	0.4675	0.7199	0.0000	22	8.0203
523	15.5440	0.5046	3.4528	0.0000	19	7.9641
524	15.4913	14.5832	1.6429	0.0000	5	7.2078
525	15.4922	15.7719	3.4525	0.0000	3	7.9440
526	15.4560	15.7719	4.2280	0.0000	3	7.9325
527	15.4541	15.9205	2.6399	0.0000	6	8.0125

	528	15.4549	16.1434	3.5632	0.0000	3	8.1521	
	529	15.4350	0.0218	5.0038	0.0000	20	8.2969	
	530	15.5031	0.5419	0.2028	0.0000	20	8.0179	
	531	15.5412	1.7305	2.0125	0.0000	22	7.2243	
	532	15.5665	15.2518	3.1202	0.0000	3	7.7049	
	533	15.4885	15.7348	0.1656	0.0000	1	8.0125	
	534	15.5430	1.0618	3.0835	0.0000	19	7.6472	
	535	15.6529	0.4674	1.3848	0.0000	22	8.0438	
	536	15.5077	0.1703	3.8959	0.0000	19	8.1496	
	537	15.6567	0.4673	4.6717	0.0000	20	8.0813	
	538	15.6027	14.8803	1.9754	0.0000	6	7.4762	
	539	15.6790	15.8460	4.6345	0.0000	1	8.1332	
	540	15.6386	15.6232	1.5691	0.0000	10	7.9333	
	541	15.6392	15.6232	2.0862	0.0000	10	7.9306	
	542	15.6396	15.7346	2.6032	0.0000	10	8.0261	
	543	15.6932	0.0958	3.8962	0.0000	19	8.3390	
	544	15.6900	0.6902	1.5695	0.0000	18	7.9082	
+-----+								
	Atomic Charge Difference							
+-----+								
	Atom # x y z Charge							
+-----+								
	Si	0	10.7049	8.1372	3.6703	-2.3310		
	C	1	10.3940	9.6639	4.6274	2.3043		
	C	2	10.7754	8.1402	1.8217	2.3628		
	Si	3	9.3143	10.7826	3.6703	-2.3438		
	C	4	7.8921	11.4138	4.6279	2.2980		
	Si	5	10.3139	9.6295	0.8630	-2.3624		
	C	6	9.3193	10.8320	1.8200	2.3101		
	Si	7	6.4207	10.9583	3.6461	-2.3274		
	C	8	5.5690	9.7106	4.7498	2.2365		
	Si	9	7.8338	11.3010	0.8610	-2.3578		
	C	10	6.2881	11.0811	1.8415	2.3414		
	Al	11	5.3250	8.1527	3.8612	-2.2372		
	C	12	5.5865	6.6051	4.7454	2.2560		
	Si	13	5.4402	9.6994	1.0217	-2.3406		
	C	14	5.2738	8.1554	1.9883	2.3677		
	Si	15	6.4491	5.3626	3.6557	-2.3092		
	C	16	7.9105	4.8471	4.6282	2.3153		
	Si	17	5.4710	6.6132	1.0090	-2.3169		
	C	18	6.3205	5.2472	1.8429	2.3311		
	Si	19	9.3302	5.4812	3.6741	-2.3378		
	C	20	10.4048	6.6092	4.6279	2.3033		
	Si	21	7.8573	4.9809	0.8551	-2.2770		
	C	22	9.3431	5.4370	1.8229	2.3051		
	Si	23	10.3219	6.6478	0.8630	-2.3490		
+-----+								
	Atomic Charge Volumes							
+-----+								
	Atom # x y z Charge							
+-----+								
	Si	0	10.7049	8.1372	3.6703	11.6690		
	C	1	10.3940	9.6639	4.6274	8.3043		
	C	2	10.7754	8.1402	1.8217	8.3628		
	Si	3	9.3143	10.7826	3.6703	11.6562		
	C	4	7.8921	11.4138	4.6279	8.2980		
	Si	5	10.3139	9.6295	0.8630	11.6376		
	C	6	9.3193	10.8320	1.8200	8.3101		
	Si	7	6.4207	10.9583	3.6461	11.6726		
	C	8	5.5690	9.7106	4.7498	8.2365		
	Si	9	7.8338	11.3010	0.8610	11.6422		
	C	10	6.2881	11.0811	1.8415	8.3414		
	Al	11	5.3250	8.1527	3.8612	10.7628		
	C	12	5.5865	6.6051	4.7454	8.2560		
	Si	13	5.4402	9.6994	1.0217	11.6594		
	C	14	5.2738	8.1554	1.9883	8.3677		
	Si	15	6.4491	5.3626	3.6557	11.6908		
	C	16	7.9105	4.8471	4.6282	8.3153		
	Si	17	5.4710	6.6132	1.0090	11.6831		
	C	18	6.3205	5.2472	1.8429	8.3311		
	Si	19	9.3302	5.4812	3.6741	11.6622		
	C	20	10.4048	6.6092	4.6279	8.3033		
	Si	21	7.8573	4.9809	0.8551	11.7230		
	C	22	9.3431	5.4370	1.8229	8.3051		
	Si	23	10.3219	6.6478	0.8630	11.6510		
+-----+								
	Total number of electrons: 238.8417							
+-----+								

Table 2. Bader Charges Analysis for Ga-doped (6,0) SWSiCNTs at Si site

```
# Item: 0
# File: G:/SiC-Al-Ga/Electron Density/Bader charge-LSDA-SiCNT-(6.0)-Ga(Si)-115-50Ha-0.001.hdf5
# Title: Bader charge-LSDA-SiCNT-(6.0)-Ga(Si)-115-50Ha-0.001.hdf5 - BaderCharges_0
# Type: BaderCharges
+-----+
| |
| Bader Charges Analysis |
| |
+-----+
+-----+
| | Bader charge analysis only makes sense on an all electron density. |
| If a pseudo-potential DFT calculation was used to generate this charge |
| density then the core electron density must be included in order to get |
| meaningful results. |
| |
| Additionally, a fine electron density grid mesh should be used in order |
| to correctly reproduce the total charge. |
+-----+
| Electron Density Grid: 436 x 432 x 152 |
| Identified 551 charge maxima |
+-----+
| Bader Charge Volumes |
+-----+
| # x y z Charge Atom Distance |
+-----+
| 0 0.1645 0.0000 5.5294 0.0000 12 8.3181 |
| 1 16.0338 15.7014 0.3064 0.0000 1 8.1942 |
| 2 16.0338 0.3341 0.3064 0.0000 20 8.1942 |
| 3 0.0768 0.1856 0.8908 0.0000 17 8.3076 |
| 4 0.0768 15.8499 0.8908 0.0000 13 8.3076 |
| 5 16.0008 15.8499 1.7163 0.0000 6 8.2314 |
| 6 16.0008 0.1856 1.7163 0.0000 22 8.2314 |
| 7 0.2658 0.1856 2.0787 0.0000 18 8.2419 |
| 8 0.2658 15.8499 2.0787 0.0000 10 8.2419 |
| 9 16.1135 0.1856 2.1619 0.0000 22 8.3200 |
| 10 15.7446 15.8499 2.9401 0.0000 6 8.0980 |
| 11 0.1933 0.0000 2.6722 0.0000 18 8.4481 |
| 12 0.0084 0.2227 2.8943 0.0000 22 8.4157 |
| 13 16.0795 0.0000 3.2379 0.0000 19 8.4901 |
| 14 16.0432 15.7385 3.5347 0.0000 1 8.2141 |
| 15 16.0432 0.2970 3.5347 0.0000 20 8.2141 |
| 16 0.1584 0.1856 3.4143 0.0000 12 8.2499 |
| 17 0.2705 0.0000 3.6743 0.0000 12 8.2835 |
| 18 16.0814 15.9984 3.9059 0.0000 1 8.3915 |
| 19 0.1602 0.0000 4.0451 0.0000 12 8.3130 |
| 20 0.0119 0.1114 4.1189 0.0000 12 8.3170 |
| 21 0.1239 0.0000 4.3418 0.0000 12 8.3164 |
| 22 16.0839 0.0000 4.7593 0.0000 1 8.3814 |
| 23 15.9994 0.1856 1.2339 0.0000 22 8.2560 |
| 24 15.7446 0.1856 2.9401 0.0000 22 8.0980 |
| 25 16.0422 0.3341 3.2007 0.0000 20 8.2408 |
| 26 16.0814 0.0371 3.9059 0.0000 20 8.3915 |
| 27 16.1186 0.1856 3.9431 0.0000 20 8.2979 |
| 28 16.1577 0.1485 4.6111 0.0000 12 8.2908 |
| 29 16.1233 0.1856 5.5387 0.0000 20 8.3032 |
| 30 0.2329 0.4083 3.5258 0.0000 12 8.0173 |
| 31 16.0444 0.3712 3.9429 0.0000 20 8.1093 |
| 32 16.0738 0.5568 1.2713 0.0000 23 8.0489 |
| 33 16.1512 0.4825 2.3847 0.0000 22 8.1765 |
| 34 16.0784 0.5568 2.8669 0.0000 22 8.1162 |
| 35 16.1570 0.4825 4.3885 0.0000 12 8.0501 |
| 36 16.0115 0.4825 5.3899 0.0000 20 7.9927 |
| 37 0.0763 0.5197 0.7052 0.0000 17 8.0602 |
| 38 0.1544 0.6310 2.0413 0.0000 17 8.0031 |
| 39 16.0462 0.4083 4.5737 0.0000 20 8.0456 |
| 40 0.3712 0.5197 0.0382 0.0000 12 7.7953 |
| 41 0.0152 0.8166 5.2321 0.0000 12 7.7849 |
| 42 16.1079 0.8166 0.2324 0.0000 20 7.8762 |
| 43 16.0420 0.7053 3.1265 0.0000 20 7.9813 |
| 44 0.0108 0.7795 3.7107 0.0000 12 7.8674 |
| 45 16.1577 0.8909 4.6111 0.0000 12 7.7457 |
| 46 0.2360 0.4454 4.6019 0.0000 12 7.8955 |
| 47 0.0121 0.8166 4.1560 0.0000 12 7.7939 |
| 48 0.1631 0.6681 5.0470 0.0000 12 7.7824 |
| 49 16.0726 0.7053 0.8631 0.0000 23 7.9317 |
| 50 0.1908 0.6681 1.8188 0.0000 17 7.9231 |
| 51 0.1959 0.7795 3.5628 0.0000 12 7.7626 |
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| 52 16.1586 0.8909 4.9451 0.0000 12 7.7445 |
| 53 16.0387 1.0393 1.9762 0.0000 23 7.7347 |
| 54 0.1179 0.7424 2.2639 0.0000 17 7.9814 |
| 55 0.3361 0.7424 0.7060 0.0000 17 7.7209 |
| 56 16.1117 0.7424 1.5682 0.0000 23 7.9555 |
| 57 15.7012 0.8166 0.7878 0.0000 23 7.6022 |
| 58 0.2234 0.7795 0.2604 0.0000 12 7.7296 |
| 59 16.1099 1.2249 0.9374 0.0000 23 7.5834 |
| 60 0.0031 1.2992 1.0761 0.0000 17 7.5540 |
| 61 16.1525 1.2621 2.8300 0.0000 20 7.7309 |
| 62 0.0105 1.0022 3.6365 0.0000 12 7.7201 |
| 63 16.0427 1.1878 3.3491 0.0000 20 7.5950 |
| 64 16.0769 1.0765 2.3474 0.0000 22 7.7688 |
| 65 15.7486 1.2249 4.3131 0.0000 20 7.2498 |
| 66 0.3492 1.2992 5.2331 0.0000 12 7.2076 |
| 67 0.3474 1.2621 4.6022 0.0000 12 7.2201 |
| 68 0.0137 1.6332 4.7126 0.0000 12 7.2055 |
| 69 0.3836 1.2621 4.3055 0.0000 12 7.2066 |
| 70 0.4602 1.2249 5.1221 0.0000 12 7.1768 |
| 71 15.7764 1.7075 1.1220 0.0000 23 7.0104 |
| 72 16.0458 1.7817 4.4252 0.0000 20 7.0674 |
| 73 5.3951 6.4216 4.7282 8.0022 12 0.0265 |
| 74 0.3765 1.2621 1.8564 0.0000 17 7.3726 |
| 75 16.0066 1.1878 3.7201 0.0000 20 7.5114 |
| 76 10.6914 6.5330 0.9588 11.6318 23 0.0264 |
| 77 16.1485 1.4476 1.4570 0.0000 23 7.4749 |
| 78 0.0059 1.7075 2.0409 0.0000 17 7.3632 |
| 79 16.1495 1.7075 1.7910 0.0000 23 7.3321 |
| 80 15.8191 1.7446 3.0516 0.0000 20 7.1197 |
| 81 0.3792 1.7446 2.7841 0.0000 12 7.1341 |
| 82 16.1223 1.7817 5.2047 0.0000 20 7.1339 |
| 83 10.7766 6.4959 4.7439 8.2991 20 0.0232 |
| 84 5.4954 6.4959 0.9065 11.7139 17 0.0132 |
| 85 16.1173 1.9673 3.4978 0.0000 20 7.1000 |
| 86 0.3378 1.7817 1.2997 0.0000 17 6.9895 |
| 87 16.1521 2.1900 2.6815 0.0000 20 7.1754 |
| 88 11.2138 8.0177 1.9250 8.3386 2 0.0208 |
| 89 4.9785 8.0177 1.8327 7.9445 14 0.0107 |
| 90 4.9471 8.0177 3.7993 29.9517 11 0.0158 |
| 91 5.3951 9.6139 4.7282 8.0024 8 0.0265 |
| 92 5.4954 9.5396 0.9065 11.7140 13 0.0132 |
| 93 10.6914 9.5025 0.9588 11.6319 5 0.0264 |
| 94 10.7766 9.5396 4.7439 8.2995 1 0.0232 |
| 95 16.1521 13.8454 2.6815 0.0000 1 7.1754 |
| 96 16.1173 14.0682 3.4978 0.0000 1 7.1000 |
| 97 16.1495 14.3280 1.7910 0.0000 5 7.3321 |
| 98 0.0059 14.3280 2.0409 0.0000 13 7.3632 |
| 99 16.0458 14.2538 4.4252 0.0000 1 7.0674 |
| 100 16.1223 14.2538 5.2047 0.0000 1 7.1339 |
| 101 0.0137 14.4022 4.7126 0.0000 8 7.2055 |
| 102 0.3378 14.2538 1.2997 0.0000 13 6.9895 |
| 103 0.3792 14.2909 2.7841 0.0000 8 7.1341 |
| 104 0.0031 14.7363 1.0761 0.0000 13 7.5540 |
| 105 16.1525 14.7734 2.8300 0.0000 1 7.7309 |
| 106 16.1485 14.5878 1.4570 0.0000 5 7.4749 |
| 107 15.7764 14.3280 1.1220 0.0000 5 7.0104 |
| 108 16.1099 14.8105 0.9374 0.0000 5 7.5834 |
| 109 15.8191 14.2909 3.0516 0.0000 1 7.1197 |
| 110 16.0427 14.8477 3.3491 0.0000 1 7.5950 |
| 111 16.0066 14.8477 3.7201 0.0000 1 7.5114 |
| 112 0.3836 14.7734 4.3055 0.0000 8 7.2066 |
| 113 0.3492 14.7363 5.2331 0.0000 8 7.2076 |
| 114 0.3765 14.7734 1.8564 0.0000 13 7.3726 |
| 115 16.0387 14.9961 1.9762 0.0000 5 7.7347 |
| 116 16.0769 14.9590 2.3474 0.0000 6 7.7688 |
| 117 0.3474 14.7734 4.6022 0.0000 8 7.2201 |
| 118 16.1079 15.2189 0.2324 0.0000 1 7.8762 |
| 119 0.0105 15.0333 3.6365 0.0000 8 7.7201 |
| 120 15.7486 14.8105 4.3131 0.0000 1 7.2498 |
| 121 0.4602 14.8105 5.1221 0.0000 8 7.1768 |
| 122 0.0121 15.2189 4.1560 0.0000 8 7.7939 |
| 123 16.1577 15.1446 4.6111 0.0000 8 7.7457 |
| 124 16.1586 15.1446 4.9451 0.0000 8 7.7445 |
| 125 0.0152 15.2189 5.2321 0.0000 8 7.7849 |
| 126 0.1179 15.2931 2.2639 0.0000 13 7.9814 |
| 127 16.1117 15.2931 1.5682 0.0000 5 7.9555 |
| 128 16.0726 15.3302 0.8631 0.0000 5 7.9317 |
| 129 16.0420 15.3302 3.1265 0.0000 1 7.9813 |
| 130 0.1959 15.2560 3.5628 0.0000 8 7.7626 |
| 131 0.0108 15.2560 3.7107 0.0000 8 7.8674 |

132	16.0784	15.4787	2.8669	0.0000	6	8.1162
133	0.2234	15.2560	0.2604	0.0000	8	7.7296
134	0.3361	15.2931	0.7060	0.0000	13	7.7209
135	16.0738	15.4787	1.2713	0.0000	5	8.0489
136	15.7012	15.2189	0.7878	0.0000	5	7.6022
137	0.0763	15.5158	0.7052	0.0000	13	8.0602
138	0.1908	15.3673	1.8188	0.0000	13	7.9231
139	0.1544	15.4045	2.0413	0.0000	13	8.0031
140	0.1631	15.3673	5.0470	0.0000	8	7.7824
141	16.1512	15.5529	2.3847	0.0000	6	8.1765
142	16.1570	15.5529	4.3885	0.0000	8	8.0501
143	16.0115	15.5529	5.3899	0.0000	1	7.9927
144	16.0444	15.6643	3.9429	0.0000	1	8.1093
145	0.2360	15.5900	4.6019	0.0000	8	7.8955
146	16.0422	15.7014	3.2007	0.0000	1	8.2408
147	16.0462	15.6272	4.5737	0.0000	1	8.0456
148	0.3712	15.5158	0.0382	0.0000	8	7.7953
149	16.1135	15.8499	2.1619	0.0000	6	8.3200
150	0.0119	15.9241	4.1189	0.0000	8	8.3170
151	16.1577	15.8870	4.6111	0.0000	8	8.2908
152	0.0084	15.8128	2.8943	0.0000	6	8.4157
153	16.1233	15.8499	5.5387	0.0000	1	8.3032
154	15.9994	15.8499	1.2339	0.0000	6	8.2560
155	16.1186	15.8499	3.9431	0.0000	1	8.2979
156	0.2329	15.6272	3.5258	0.0000	8	8.0173
157	0.1584	15.8499	3.4143	0.0000	8	8.2499
158	0.4851	15.8499	0.8920	0.0000	13	8.0473
159	0.4851	0.1856	0.8920	0.0000	17	8.0473
160	0.4596	0.5197	4.8994	0.0000	12	7.6941
161	0.2237	0.4454	0.3346	0.0000	12	7.9871
162	0.1977	0.6681	4.1936	0.0000	12	7.7726
163	0.3110	1.2992	4.8619	0.0000	12	7.2189
164	0.3827	1.2992	3.9715	0.0000	12	7.2089
165	0.3827	14.7363	3.9715	0.0000	8	7.2089
166	0.3110	14.7363	4.8619	0.0000	8	7.2189
167	0.1977	15.3673	4.1936	0.0000	8	7.7726
168	0.4596	15.5158	4.8994	0.0000	8	7.6941
169	0.2237	15.5900	0.3346	0.0000	8	7.9871
170	0.1992	0.0000	4.7131	0.0000	12	8.2590
171	0.2372	0.0000	5.0101	0.0000	12	8.2393
172	0.4572	0.5939	4.0831	0.0000	12	7.6659
173	0.3495	0.1485	5.3444	0.0000	12	8.0713
174	0.3786	0.8909	2.5615	0.0000	18	7.7435
175	0.3058	0.7795	3.0807	0.0000	12	7.7778
176	0.3058	15.2560	3.0807	0.0000	8	7.7778
177	0.3786	15.1446	2.5615	0.0000	10	7.7435
178	0.4572	15.4416	4.0831	0.0000	8	7.6659
179	0.3495	15.8870	5.3444	0.0000	8	8.0713
180	0.2607	0.0000	0.2976	0.0000	12	8.2965
181	0.4576	1.2249	4.2315	0.0000	12	7.1868
182	0.4576	14.8105	4.2315	0.0000	8	7.1868
183	0.4491	0.1485	1.3000	0.0000	17	8.1081
184	0.3778	0.0000	2.3017	0.0000	18	8.2840
185	0.2617	0.3341	0.6687	0.0000	17	8.0781
186	0.3814	0.6310	3.5262	0.0000	12	7.7549
187	0.3743	0.8909	1.0772	0.0000	17	7.5844
188	0.6045	1.1878	3.6753	0.0000	12	7.1751
189	0.6045	14.8477	3.6753	0.0000	8	7.1751
190	0.3743	15.1446	1.0772	0.0000	13	7.5844
191	0.3814	15.4045	3.5262	0.0000	8	7.7549
192	0.2617	15.7014	0.6687	0.0000	13	8.0781
193	0.3394	0.0000	1.8563	0.0000	18	8.3049
194	0.5664	0.7424	3.3412	0.0000	12	7.5844
195	0.4865	0.8166	1.3744	0.0000	17	7.5770
196	0.4865	15.2189	1.3744	0.0000	13	7.5770
197	0.5664	15.2931	3.3412	0.0000	8	7.5844
198	0.4491	15.8870	1.3000	0.0000	13	8.1081
199	0.4875	0.5939	1.7454	0.0000	17	7.7754
200	0.4579	0.4825	4.3057	0.0000	12	7.7345
201	0.4094	0.5939	0.4094	0.0000	12	7.7684
202	0.4579	15.5529	4.3057	0.0000	8	7.7345
203	0.4094	15.4416	0.4094	0.0000	8	7.7684
204	0.4875	15.4416	1.7454	0.0000	13	7.7754
205	0.5655	0.0000	3.0444	0.0000	7	8.1839
206	0.4537	0.1856	2.8585	0.0000	18	8.1500
207	0.4225	0.1485	4.8993	0.0000	12	8.0048
208	0.4571	0.1114	4.0460	0.0000	12	8.0412
209	0.5707	0.4454	4.8255	0.0000	12	7.6794
210	0.7853	1.0022	2.0432	0.0000	17	7.3148
211	0.5598	0.6681	1.0777	0.0000	17	7.6288

	212	0.6017	0.7053	2.7105	0.0000	18	7.6922	
	213	0.6028	0.6681	3.0816	0.0000	12	7.6690	
	214	0.6028	15.3673	3.0816	0.0000	8	7.6690	
	215	0.5598	15.3673	1.0777	0.0000	13	7.6288	
	216	0.6017	15.3302	2.7105	0.0000	10	7.6922	
	217	0.7853	15.0333	2.0432	0.0000	13	7.3148	
	218	0.4537	15.8499	2.8585	0.0000	10	8.1500	
	219	0.4571	15.9241	4.0460	0.0000	8	8.0412	
	220	0.4225	15.8870	4.8993	0.0000	8	8.0048	
	221	0.5707	15.5900	4.8255	0.0000	8	7.6794	
	222	0.6317	0.0000	0.2616	0.0000	12	8.0669	
	223	0.5945	0.4083	0.2244	0.0000	12	7.7641	
	224	0.4558	0.1856	3.6007	0.0000	12	8.0352	
	225	0.6049	0.0000	3.8237	0.0000	12	8.0618	
	226	0.4913	0.9280	3.0442	0.0000	12	7.5571	
	227	0.4913	15.1075	3.0442	0.0000	8	7.5571	
	228	0.5945	15.6272	0.2244	0.0000	8	7.7641	
	229	0.4558	15.8499	3.6007	0.0000	8	8.0352	
	230	1.0536	0.7795	4.9754	0.0000	12	7.1209	
	231	0.7451	1.3363	0.9669	0.0000	17	7.0039	
	232	0.7451	14.6992	0.9669	0.0000	13	7.0039	
	233	1.0536	15.2560	4.9754	0.0000	8	7.1209	
	234	1.0037	0.3341	0.5595	0.0000	17	7.6227	
	235	0.4869	0.0000	1.5228	0.0000	18	8.2039	
	236	0.4954	0.0371	4.4542	0.0000	12	8.0511	
	237	0.5705	0.0000	4.7513	0.0000	12	8.0298	
	238	0.6738	0.4083	1.9686	0.0000	18	7.7850	
	239	0.6040	0.4454	3.5269	0.0000	12	7.7541	
	240	1.0877	0.3712	3.9365	0.0000	12	7.4680	
	241	0.7572	0.9651	5.1600	0.0000	12	7.1724	
	242	0.6322	0.7424	0.4471	0.0000	12	7.5215	
	243	0.7874	1.2992	2.7482	0.0000	12	7.1727	
	244	0.7874	14.7363	2.7482	0.0000	8	7.1727	
	245	0.6322	15.2931	0.4471	0.0000	8	7.5215	
	246	0.7572	15.0704	5.1600	0.0000	8	7.1724	
	247	0.6040	15.5900	3.5269	0.0000	8	7.7541	
	248	1.0877	15.6643	3.9365	0.0000	8	7.4680	
	249	0.6738	15.6272	1.9686	0.0000	10	7.7850	
	250	0.4954	15.9984	4.4542	0.0000	8	8.0511	
	251	0.6040	0.0000	3.5269	0.0000	12	8.1015	
	252	1.0483	0.3341	3.1571	0.0000	15	7.5943	
	253	0.8183	0.4825	0.6332	0.0000	17	7.6128	
	254	0.8183	15.5529	0.6332	0.0000	13	7.6128	
	255	1.0483	15.7014	3.1571	0.0000	7	7.5943	
	256	1.0037	15.7014	0.5595	0.0000	13	7.6227	
	257	0.7090	0.0000	1.3379	0.0000	18	8.0511	
	258	0.7796	0.1856	0.0765	0.0000	12	7.8070	
	259	0.8246	0.5197	2.7854	0.0000	18	7.6459	
	260	0.8194	0.5197	1.0043	0.0000	17	7.5785	
	261	1.0121	0.4083	3.4539	0.0000	12	7.5496	
	262	0.8194	15.5158	1.0043	0.0000	13	7.5785	
	263	1.0121	15.6272	3.4539	0.0000	8	7.5496	
	264	0.8246	15.5158	2.7854	0.0000	10	7.6459	
	265	0.7796	15.8499	0.0765	0.0000	8	7.8070	
	266	0.9676	0.2970	0.9305	0.0000	17	7.6659	
	267	6.6117	5.4565	1.9117	8.2673	18	0.0199	
	268	6.6117	10.5790	1.9117	8.2673	10	0.0199	
	269	0.9676	15.7385	0.9305	0.0000	13	7.6659	
	270	0.8590	0.1856	1.8578	0.0000	18	7.7936	
	271	0.7863	0.0000	2.3771	0.0000	18	7.9853	
	272	0.7929	0.1856	4.6777	0.0000	12	7.7482	
	273	0.7896	0.2598	3.5274	0.0000	12	7.7860	
	274	0.7207	0.3341	5.3455	0.0000	12	7.6968	
	275	0.7207	15.7014	5.3455	0.0000	8	7.6968	
	276	0.7896	15.7756	3.5274	0.0000	8	7.7860	
	277	0.7929	15.8499	4.6777	0.0000	8	7.7482	
	278	0.8590	15.8499	1.8578	0.0000	10	7.7936	
	279	1.0160	0.0000	4.7897	0.0000	12	7.7696	
	280	0.9744	1.0765	3.2682	0.0000	12	7.0903	
	281	0.9744	14.9590	3.2682	0.0000	8	7.0903	
	282	1.0064	0.8537	1.4872	0.0000	17	7.2230	
	283	1.0064	15.1817	1.4872	0.0000	13	7.2230	
	284	1.0099	0.3712	2.7117	0.0000	18	7.5971	
	285	1.1556	0.6310	1.7474	0.0000	18	7.2771	
	286	1.0151	0.7424	4.4929	0.0000	12	7.1745	
	287	1.0529	0.7424	4.7156	0.0000	12	7.1470	
	288	1.0151	15.2931	4.4929	0.0000	8	7.1745	
	289	1.0529	15.2931	4.7156	0.0000	8	7.1470	
	290	1.1556	15.4045	1.7474	0.0000	10	7.2771	
	291	1.0099	15.6643	2.7117	0.0000	10	7.5971	

	292	1.0829	0.0000	2.2667	0.0000	18	7.7662	
	293	1.1282	0.0742	5.0869	0.0000	12	7.6526	
	294	1.5288	0.2970	2.4535	0.0000	18	7.2526	
	295	0.8917	0.4825	0.3366	0.0000	12	7.5429	
	296	0.8917	15.5529	0.3366	0.0000	8	7.5429	
	297	1.5288	15.7385	2.4535	0.0000	10	7.2526	
	298	1.2272	0.8909	0.8570	0.0000	17	7.0349	
	299	1.2272	15.1446	0.8570	0.0000	13	7.0349	
	300	1.1282	15.9612	5.0869	0.0000	8	7.6526	
	301	1.3105	0.1485	3.9742	0.0000	15	7.5086	
	302	0.9286	0.4825	0.2624	0.0000	12	7.5091	
	303	1.2380	0.5568	4.5677	0.0000	12	7.1880	
	304	1.1971	0.9280	3.2689	0.0000	12	7.0675	
	305	1.2334	0.8537	2.9721	0.0000	15	7.1320	
	306	1.2334	15.1817	2.9721	0.0000	7	7.1320	
	307	1.1971	15.1075	3.2689	0.0000	8	7.0675	
	308	0.9286	15.5529	0.2624	0.0000	8	7.5091	
	309	1.2380	15.4787	4.5677	0.0000	8	7.1880	
	310	6.6172	5.4565	3.8041	11.6852	15	0.0130	
	311	6.6172	10.5790	3.8041	11.6852	7	0.0130	
	312	1.3105	15.8870	3.9742	0.0000	7	7.5086	
	313	1.3370	0.0000	0.3007	0.0000	12	7.6777	
	314	1.0796	0.0000	1.1534	0.0000	18	7.7999	
	315	1.3449	0.0000	3.0467	0.0000	7	7.6248	
	316	1.3464	0.0000	3.5662	0.0000	7	7.5904	
	317	1.0820	0.0000	1.9698	0.0000	18	7.7596	
	318	1.0768	0.2227	0.1887	0.0000	12	7.6200	
	319	1.0768	15.8128	0.1887	0.0000	8	7.6200	
	320	1.1241	0.1856	3.6768	0.0000	15	7.6147	
	321	1.1241	15.8499	3.6768	0.0000	7	7.6147	
	322	1.2773	0.1485	5.3100	0.0000	12	7.5217	
	323	1.5353	0.3341	4.7170	0.0000	12	7.2042	
	324	1.5353	15.7014	4.7170	0.0000	8	7.2042	
	325	1.2773	15.8870	5.3100	0.0000	8	7.5217	
	326	1.4498	0.0000	0.8206	0.0000	18	7.5836	
	327	1.6721	0.4454	0.6728	0.0000	18	7.1387	
	328	1.4526	0.4454	1.7853	0.0000	18	7.1845	
	329	1.4534	0.4083	2.0451	0.0000	18	7.2094	
	330	1.4534	15.6272	2.0451	0.0000	10	7.2094	
	331	1.4526	15.5900	1.7853	0.0000	10	7.1845	
	332	1.6721	15.5900	0.6728	0.0000	10	7.1387	
	333	1.6473	0.2598	4.9400	0.0000	12	7.2104	
	334	1.5693	0.5568	3.6410	0.0000	15	7.0373	
	335	1.5693	15.4787	3.6410	0.0000	7	7.0373	
	336	1.6473	15.7756	4.9400	0.0000	8	7.2104	
	337	1.4137	0.0000	1.1544	0.0000	18	7.5668	
	338	1.7546	0.3712	3.5302	0.0000	15	7.0415	
	339	1.7546	15.6643	3.5302	0.0000	7	7.0415	
	340	1.5633	0.2227	1.5630	0.0000	18	7.2719	
	341	1.5650	0.2970	2.1567	0.0000	18	7.2118	
	342	2.0489	0.0000	2.6405	0.0000	18	7.1392	
	343	1.5633	15.8128	1.5630	0.0000	10	7.2719	
	344	1.5650	15.7385	2.1567	0.0000	10	7.2118	
	345	1.6834	0.2598	4.5690	0.0000	12	7.1911	
	346	1.6834	15.7756	4.5690	0.0000	8	7.1911	
	347	2.1210	0.0000	1.8986	0.0000	18	7.0577	
	348	1.8186	0.3341	0.0053	0.0000	12	7.1050	
	349	1.8186	15.7014	0.0053	0.0000	8	7.1050	
	350	1.9439	0.0000	4.8295	0.0000	7	7.2585	
	351	1.7456	0.3712	0.4504	0.0000	12	7.1805	
	352	1.7456	15.6643	0.4504	0.0000	8	7.1805	
	353	2.0843	0.0000	2.0469	0.0000	18	7.0820	
	354	1.9732	0.7053	2.1208	0.0000	18	6.6337	
	355	1.9732	15.3302	2.1208	0.0000	10	6.6337	
	356	2.0816	0.0000	1.1193	0.0000	18	7.1289	
	357	2.0454	0.0000	1.4531	0.0000	18	7.1218	
	358	2.2374	0.0000	3.6430	0.0000	7	6.9983	
	359	2.2281	0.0000	0.4518	0.0000	18	7.1445	
	360	2.3169	0.0000	5.4614	0.0000	7	7.1444	
	361	2.3873	0.0000	4.1629	0.0000	7	6.9135	
	362	8.1416	5.0111	4.7362	8.3335	16	0.0087	
	363	8.1416	11.0244	4.7362	8.3335	4	0.0087	
	364	8.1306	5.1224	0.9513	11.7154	21	0.0146	
	365	8.1306	10.9130	0.9513	11.7154	9	0.0146	
	366	9.6233	5.4936	3.7758	11.6704	19	0.0166	
	367	9.6550	10.6161	1.9205	8.2885	6	0.0121	
	368	9.6233	10.5418	3.7758	11.6704	3	0.0166	
	369	11.1077	8.0177	3.7430	11.6677	0	0.0201	
	370	9.6550	5.4194	1.9205	8.2885	22	0.0121	
	371	13.1762	0.0000	0.3352	0.0000	6	6.6532	

	372	13.4484	0.0000	4.6032	0.0000	19	6.7388	
	373	13.3263	0.0000	0.8922	0.0000	6	6.6256	
	374	13.9289	0.0000	3.9367	0.0000	19	6.9754	
	375	13.9551	0.0000	0.1519	0.0000	6	7.1402	
	376	13.8961	0.0000	5.4209	0.0000	19	7.1468	
	377	13.9929	0.0000	0.4118	0.0000	6	7.1037	
	378	14.1796	0.0000	0.7834	0.0000	6	7.1513	
	379	14.2596	0.0000	2.7874	0.0000	6	7.1664	
	380	14.2930	0.0000	1.4887	0.0000	6	7.1473	
	381	14.3791	0.3341	5.6078	0.0000	20	7.1873	
	382	14.3791	15.7014	5.6078	0.0000	1	7.1873	
	383	14.2204	0.0000	2.0822	0.0000	6	7.0896	
	384	14.3743	0.3712	3.9380	0.0000	19	6.9832	
	385	14.3743	15.6643	3.9380	0.0000	3	6.9832	
	386	14.2936	0.7053	1.7114	0.0000	22	6.6190	
	387	14.2936	15.3302	1.7114	0.0000	6	6.6190	
	388	14.4001	1.0765	0.0419	0.0000	20	6.5922	
	389	14.4012	1.1136	0.4129	0.0000	22	6.5846	
	390	14.4001	14.9590	0.0419	0.0000	1	6.5922	
	391	14.4012	14.9219	0.4129	0.0000	6	6.5846	
	392	14.4748	0.3712	0.1905	0.0000	22	7.1913	
	393	14.4748	15.6643	0.1905	0.0000	6	7.1913	
	394	14.8457	0.7424	0.1174	0.0000	20	7.1253	
	395	14.8457	15.2931	0.1174	0.0000	1	7.1253	
	396	14.5209	0.4083	3.3076	0.0000	19	7.0702	
	397	14.7101	0.4454	4.5698	0.0000	19	7.2065	
	398	14.5209	15.6272	3.3076	0.0000	3	7.0702	
	399	14.7101	15.5900	4.5698	0.0000	3	7.2065	
	400	14.8192	0.6681	3.7909	0.0000	19	7.0868	
	401	14.8192	15.3673	3.7909	0.0000	3	7.0868	
	402	14.6372	0.0000	5.0149	0.0000	19	7.5360	
	403	14.6996	0.4083	0.9333	0.0000	22	7.1802	
	404	14.7413	0.3712	2.5290	0.0000	22	7.1950	
	405	14.7753	0.3341	1.4530	0.0000	22	7.2336	
	406	14.8833	0.7795	0.3030	0.0000	20	7.1462	
	407	14.8833	15.2560	0.3030	0.0000	1	7.1462	
	408	14.7753	15.7014	1.4530	0.0000	6	7.2336	
	409	14.7413	15.6643	2.5290	0.0000	6	7.1950	
	410	14.6996	15.6272	0.9333	0.0000	6	7.1802	
	411	14.7763	0.4083	1.7870	0.0000	22	7.1687	
	412	14.7763	15.6272	1.7870	0.0000	6	7.1687	
	413	14.9299	0.0000	3.5685	0.0000	19	7.6356	
	414	14.8985	0.0000	5.5351	0.0000	1	7.7305	
	415	14.8938	0.0000	3.9024	0.0000	19	7.6091	
	416	14.8925	0.7424	3.4571	0.0000	19	7.0977	
	417	14.8925	15.2931	3.4571	0.0000	3	7.0977	
	418	14.9200	0.0000	0.1547	0.0000	6	7.7601	
	419	14.9586	15.8870	0.6743	0.0000	6	7.5818	
	420	14.9586	0.1485	0.6743	0.0000	22	7.5818	
	421	14.9587	0.8909	0.7114	0.0000	23	7.0789	
	422	14.9587	15.1446	0.7114	0.0000	5	7.0789	
	423	15.1114	0.7424	2.1590	0.0000	22	7.1939	
	424	15.1114	15.2931	2.1590	0.0000	6	7.1939	
	425	15.1566	0.8166	4.9422	0.0000	20	7.1687	
	426	15.1553	0.7795	4.4969	0.0000	20	7.1980	
	427	15.1553	15.2560	4.4969	0.0000	1	7.1980	
	428	15.1566	15.2189	4.9422	0.0000	1	7.1687	
	429	15.1215	0.1856	5.6471	0.0000	20	7.7108	
	430	15.1844	0.7795	1.7511	0.0000	22	7.2233	
	431	15.1844	15.2560	1.7511	0.0000	6	7.2233	
	432	15.1215	15.8499	5.6471	0.0000	1	7.7108	
	433	15.0714	0.0000	1.1570	0.0000	6	7.7017	
	434	15.1526	0.1856	3.5692	0.0000	19	7.6628	
	435	15.1526	15.8499	3.5692	0.0000	3	7.6628	
	436	15.1850	0.0000	1.9366	0.0000	6	7.7453	
	437	15.4156	15.8499	4.6832	0.0000	1	7.8260	
	438	15.3003	0.4083	3.3099	0.0000	19	7.6314	
	439	15.2652	0.3712	4.0148	0.0000	19	7.6203	
	440	15.2695	0.3712	5.4991	0.0000	20	7.6289	
	441	15.2695	15.6643	5.4991	0.0000	1	7.6289	
	442	15.3003	15.6272	3.3099	0.0000	3	7.6314	
	443	15.2652	15.6643	4.0148	0.0000	3	7.6203	
	444	15.4156	0.1856	4.6832	0.0000	20	7.8260	
	445	15.2615	0.5568	2.7161	0.0000	22	7.4677	
	446	15.2913	0.4083	0.1929	0.0000	20	7.6625	
	447	15.3740	0.4825	3.1246	0.0000	19	7.6510	
	448	15.4038	1.2992	0.6014	0.0000	23	7.0502	
	449	15.4038	14.7363	0.6014	0.0000	5	7.0502	
	450	15.2615	15.4787	2.7161	0.0000	6	7.4677	
	451	15.3740	15.5529	3.1246	0.0000	3	7.6510	

	452	15.2913	15.6272	0.1929	0.0000	1	7.6625	
	453	15.2939	0.2227	1.1206	0.0000	22	7.7120	
	454	15.3664	0.4454	0.5271	0.0000	23	7.6876	
	455	15.3664	15.5900	0.5271	0.0000	5	7.6876	
	456	15.2939	15.8128	1.1206	0.0000	6	7.7120	
	457	15.4421	1.3363	1.0097	0.0000	23	7.0405	
	458	15.4485	1.3363	3.2361	0.0000	20	7.1111	
	459	15.3769	1.7817	4.1264	0.0000	20	6.6060	
	460	15.1446	1.8560	0.8233	0.0000	23	6.4579	
	461	15.1446	14.1795	0.8233	0.0000	5	6.4579	
	462	15.3769	14.2538	4.1264	0.0000	1	6.6060	
	463	15.4485	14.6992	3.2361	0.0000	1	7.1111	
	464	15.4421	14.6992	1.0097	0.0000	5	7.0405	
	465	15.2252	0.0000	3.0128	0.0000	6	7.8513	
	466	15.4101	1.2992	2.7907	0.0000	22	7.1360	
	467	15.4101	14.7363	2.7907	0.0000	6	7.1360	
	468	15.5140	0.1856	0.2306	0.0000	20	7.9765	
	469	15.3793	0.0000	4.9428	0.0000	1	7.9583	
	470	15.5237	0.1485	3.5703	0.0000	19	7.9599	
	471	15.3433	0.0000	5.3509	0.0000	1	7.9591	
	472	15.3718	0.1856	2.3824	0.0000	22	7.7677	
	473	15.6727	0.7424	3.7562	0.0000	20	7.6099	
	474	15.4069	0.9651	1.6775	0.0000	22	7.2824	
	475	15.4069	15.0704	1.6775	0.0000	6	7.2824	
	476	15.6727	15.2931	3.7562	0.0000	1	7.6099	
	477	15.3718	15.8499	2.3824	0.0000	6	7.7677	
	478	15.5237	15.8870	3.5703	0.0000	3	7.9599	
	479	15.6729	0.0000	3.8305	0.0000	19	8.1679	
	480	15.5140	15.8499	0.2306	0.0000	1	7.9765	
	481	15.4791	0.0000	0.9727	0.0000	6	8.0137	
	482	15.4484	0.1856	3.1990	0.0000	19	7.8972	
	483	15.4411	0.1856	0.6757	0.0000	22	7.9025	
	484	15.7123	0.5197	4.6098	0.0000	20	7.7448	
	485	15.6296	0.7424	1.6781	0.0000	22	7.5947	
	486	15.4771	0.5939	0.3047	0.0000	20	7.6459	
	487	15.4049	0.7053	0.9725	0.0000	23	7.4957	
	488	15.6631	0.7424	0.4537	0.0000	23	7.6475	
	489	15.4049	15.3302	0.9725	0.0000	5	7.4957	
	490	15.4771	15.4416	0.3047	0.0000	1	7.6459	
	491	15.6631	15.2931	0.4537	0.0000	5	7.6475	
	492	15.6296	15.2931	1.6781	0.0000	6	7.5947	
	493	15.7123	15.5158	4.6098	0.0000	1	7.7448	
	494	15.4411	15.8499	0.6757	0.0000	6	7.9025	
	495	15.4484	15.8499	3.1990	0.0000	3	7.8972	
	496	15.5933	0.4083	1.9749	0.0000	22	7.7736	
	497	15.5933	15.6272	1.9749	0.0000	6	7.7736	
	498	15.6625	0.0000	0.2311	0.0000	1	8.2117	
	499	15.7081	0.7424	3.1626	0.0000	20	7.7307	
	500	15.7884	1.2621	5.2408	0.0000	20	7.2564	
	501	15.7884	14.7734	5.2408	0.0000	1	7.2564	
	502	15.7081	15.2931	3.1626	0.0000	1	7.7307	
	503	15.6768	0.0000	5.1663	0.0000	1	8.1423	
	504	15.7051	0.6310	2.1236	0.0000	22	7.7221	
	505	15.7517	0.5568	5.3892	0.0000	20	7.7685	
	506	15.6274	0.9280	0.9360	0.0000	23	7.4682	
	507	15.7445	0.8537	2.9030	0.0000	22	7.6787	
	508	15.6274	15.1075	0.9360	0.0000	5	7.4682	
	509	15.7445	15.1817	2.9030	0.0000	6	7.6787	
	510	15.7051	15.4045	2.1236	0.0000	6	7.7221	
	511	15.7517	15.4787	5.3892	0.0000	1	7.7685	
	512	15.6639	0.0000	0.7135	0.0000	6	8.1832	
	513	15.5954	0.2598	2.6799	0.0000	22	7.9085	
	514	15.5914	0.2227	1.3070	0.0000	22	7.9160	
	515	15.6679	1.4105	2.0864	0.0000	23	7.2318	
	516	15.7432	1.7075	2.4577	0.0000	23	7.1470	
	517	15.7432	14.3280	2.4577	0.0000	5	7.1470	
	518	15.6679	14.6249	2.0864	0.0000	5	7.2318	
	519	15.5954	15.7756	2.6799	0.0000	6	7.9085	
	520	15.5914	15.8128	1.3070	0.0000	6	7.9160	
	521	15.6712	0.0000	3.2367	0.0000	19	8.1837	
	522	15.6721	0.0000	3.5336	0.0000	19	8.1704	
	523	15.7045	0.5568	1.9010	0.0000	22	7.7649	
	524	15.7062	0.7795	2.4947	0.0000	22	7.6510	
	525	15.7062	15.2560	2.4947	0.0000	6	7.6510	
	526	15.7045	15.4787	1.9010	0.0000	6	7.7649	
	527	15.6756	0.0000	4.7581	0.0000	1	8.1299	
	528	15.7389	0.1856	0.9734	0.0000	22	8.0834	
	529	15.7477	0.4825	4.0162	0.0000	20	7.8275	
	530	15.7477	15.5529	4.0162	0.0000	1	7.8275	
	531	15.7389	15.8499	0.9734	0.0000	6	8.0834	

532	15.8893	0.1114	1.6418	0.0000	22	8.1956
533	15.7400	0.9651	1.3445	0.0000	23	7.5261
534	15.8238	1.2992	4.6472	0.0000	20	7.2365
535	15.8238	14.7363	4.6472	0.0000	1	7.2365
536	15.7400	15.0704	1.3445	0.0000	5	7.5261
537	15.8893	15.9241	1.6418	0.0000	6	8.1956
538	15.8241	0.1856	4.7586	0.0000	20	8.0739
539	15.7807	0.5568	2.6062	0.0000	22	7.8551
540	15.7807	15.4787	2.6062	0.0000	6	7.8551
541	15.8241	15.8499	4.7586	0.0000	1	8.0739
542	15.8136	0.0000	1.1592	0.0000	6	8.2412
543	15.7801	0.1856	2.3836	0.0000	22	8.0734
544	15.7801	15.8499	2.3836	0.0000	6	8.0734
545	15.8137	0.4454	1.1963	0.0000	22	7.9523
546	15.8137	15.5900	1.1963	0.0000	6	7.9523
547	15.9276	0.0000	2.0501	0.0000	6	8.2936
548	15.9376	0.4454	5.5010	0.0000	20	7.9828
549	15.9376	15.5900	5.5010	0.0000	1	7.9828
550	15.9744	0.0000	5.3898	0.0000	1	8.3389

Atomic Charge Difference						
Atom #	x	y	z	Charge		
Si 0	11.1198	8.0177	3.7590	-2.3323		
C 1	10.7933	9.5350	4.7285	2.2995		
C 2	11.2033	8.0177	1.9071	2.3386		
Si 3	9.6167	10.5553	3.7685	-2.3296		
C 4	8.1352	11.0184	4.7359	2.3335		
Si 5	10.7060	9.4903	0.9404	-2.3681		
C 6	9.6463	10.6215	1.9142	2.2885		
Si 7	6.6235	10.5843	3.7941	-2.3148		
C 8	5.4110	9.6287	4.7435	2.0024		
Si 9	8.1226	10.9241	0.9461	-2.2846		
C 10	6.6065	10.5866	1.9293	2.2673		
Ga 11	4.9628	8.0177	3.7987	-1.0483		
C 12	5.4110	6.4068	4.7435	2.0022		
Si 13	5.4951	9.5525	0.9097	-2.2860		
C 14	4.9698	8.0177	1.8264	1.9445		
Si 15	6.6235	5.4511	3.7941	-2.3148		
C 16	8.1352	5.0170	4.7359	2.3335		
Si 17	5.4951	6.4830	0.9097	-2.2861		
C 18	6.6065	5.4489	1.9293	2.2673		
Si 19	9.6167	5.4802	3.7685	-2.3296		
C 20	10.7933	6.5005	4.7285	2.2991		
Si 21	8.1226	5.1113	0.9461	-2.2846		
C 22	9.6463	5.4140	1.9142	2.2885		
Si 23	10.7060	6.5452	0.9404	-2.3682		

Atomic Charge Volumes						
Atom #	x	y	z	Charge		
Si 0	11.1198	8.0177	3.7590	11.6677		
C 1	10.7933	9.5350	4.7285	8.2995		
C 2	11.2033	8.0177	1.9071	8.3386		
Si 3	9.6167	10.5553	3.7685	11.6704		
C 4	8.1352	11.0184	4.7359	8.3335		
Si 5	10.7060	9.4903	0.9404	11.6319		
C 6	9.6463	10.6215	1.9142	8.2885		
Si 7	6.6235	10.5843	3.7941	11.6852		
C 8	5.4110	9.6287	4.7435	8.0024		
Si 9	8.1226	10.9241	0.9461	11.7154		
C 10	6.6065	10.5866	1.9293	8.2673		
Ga 11	4.9628	8.0177	3.7987	29.9517		
C 12	5.4110	6.4068	4.7435	8.0022		
Si 13	5.4951	9.5525	0.9097	11.7140		
C 14	4.9698	8.0177	1.8264	7.9445		
Si 15	6.6235	5.4511	3.7941	11.6852		
C 16	8.1352	5.0170	4.7359	8.3335		
Si 17	5.4951	6.4830	0.9097	11.7139		
C 18	6.6065	5.4489	1.9293	8.2673		
Si 19	9.6167	5.4802	3.7685	11.6704		
C 20	10.7933	6.5005	4.7285	8.2991		
Si 21	8.1226	5.1113	0.9461	11.7154		
C 22	9.6463	5.4140	1.9142	8.2885		
Si 23	10.7060	6.5452	0.9404	11.6318		

Total number of electrons: 257.1175						
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Table 3. Bader Charges Analysis for Al-doped (6,0) SWSiCNTs at C site

```
# Item: 0
# File: G:/SiC-Al-Ga/Electron Density/Bader-Charges-LSDA+U-SiCNT-(6.0)-Al(C)-115-50Ha-0.001.hdf5
# Title: Bader-Charges-LSDA+U-SiCNT-(6.0)-Al(C)-115-50Ha-0.001.hdf5 - BaderCharges_0
# Type: BaderCharges
+-----+
| |
| Bader Charges Analysis |
| |
+-----+
+-----+
| | Bader charge analysis only makes sense on an all electron density. |
| If a pseudo-potential DFT calculation was used to generate this charge |
| density then the core electron density must be included in order to get |
| meaningful results. |
| |
| Additionally, a fine electron density grid mesh should be used in order |
| to correctly reproduce the total charge. |
+-----+
| Electron Density Grid: 439 x 433 x 152 |
| Identified 505 charge maxima |
+-----+
| Bader Charge Volumes |
+-----+
| # x y z Charge Atom Distance |
+-----+
| 0 0.1069 0.0000 5.5311 0.0000 13 8.4259 |
| 1 16.1530 0.0000 0.4694 0.0000 5 8.4772 |
| 2 16.0785 0.2226 0.6922 0.0000 23 8.2494 |
| 3 0.1849 0.0000 0.9650 0.0000 13 8.3170 |
| 4 0.1846 15.8418 1.2620 0.0000 13 8.1540 |
| 5 0.1846 0.2226 1.2620 0.0000 17 8.1540 |
| 6 0.0728 0.2226 1.8189 0.0000 17 8.2696 |
| 7 16.1889 0.0000 1.8800 0.0000 6 8.3997 |
| 8 0.0728 15.8418 1.8189 0.0000 13 8.2696 |
| 9 16.2627 15.8418 2.5110 0.0000 6 8.3396 |
| 10 16.1512 0.0000 2.5483 0.0000 6 8.3973 |
| 11 16.2625 0.0000 2.7338 0.0000 6 8.4989 |
| 12 16.1506 0.0000 3.3278 0.0000 3 8.4533 |
| 13 0.1083 0.0000 3.8235 0.0000 8 8.5488 |
| 14 0.0336 0.1855 4.2690 0.0000 20 8.3748 |
| 15 16.1868 0.0000 4.5157 0.0000 1 8.4112 |
| 16 16.1494 0.0000 4.8498 0.0000 1 8.3867 |
| 17 0.0703 0.1855 4.8630 0.0000 12 8.3864 |
| 18 0.0700 0.2226 5.1971 0.0000 17 8.3295 |
| 19 16.2640 0.4823 0.8405 0.0000 17 8.1008 |
| 20 16.2627 0.2226 2.5110 0.0000 22 8.3396 |
| 21 16.0765 0.2226 3.1052 0.0000 22 8.2621 |
| 22 16.1504 0.2597 3.5506 0.0000 20 8.2670 |
| 23 16.0788 0.2226 0.2839 0.0000 20 8.2567 |
| 24 16.0044 0.1855 0.5438 0.0000 23 8.2362 |
| 25 15.9649 0.1484 3.3280 0.0000 19 8.2160 |
| 26 0.0333 0.1113 4.7145 0.0000 20 8.4188 |
| 27 0.1089 0.5936 3.0068 0.0000 17 8.1919 |
| 28 16.1859 0.2226 5.5551 0.0000 20 8.2812 |
| 29 16.1902 0.4823 0.3580 0.0000 23 8.1415 |
| 30 16.2267 0.2968 1.1375 0.0000 17 8.2660 |
| 31 0.1093 0.5936 2.5614 0.0000 17 8.0891 |
| 32 16.1506 0.4452 3.3649 0.0000 20 8.1561 |
| 33 0.0698 0.3710 5.4940 0.0000 17 8.1761 |
| 34 16.1862 0.4081 5.1839 0.0000 20 8.1110 |
| 35 0.1104 0.5565 1.1878 0.0000 17 7.9503 |
| 36 16.1890 0.3710 1.8429 0.0000 22 8.1661 |
| 37 16.0016 0.4081 3.9590 0.0000 20 8.0114 |
| 38 16.1870 0.4081 4.2559 0.0000 20 8.1097 |
| 39 16.2261 1.1130 1.8057 0.0000 17 7.7315 |
| 40 5.5663 6.4925 4.7100 8.3256 12 0.0232 |
| 41 5.4580 6.4183 0.9236 12.8590 17 0.0227 |
| 42 0.2942 0.7791 3.5264 0.0000 12 7.8850 |
| 43 15.9279 0.8904 3.2538 0.0000 20 7.7022 |
| 44 16.0004 0.4452 5.4068 0.0000 20 7.9786 |
| 45 15.9304 0.9646 0.2097 0.0000 20 7.5954 |
| 46 0.0737 0.5565 0.6681 0.0000 17 7.9740 |
| 47 16.2242 0.8533 4.1816 0.0000 20 7.8102 |
| 48 10.8764 6.5296 4.7057 8.3036 20 0.0203 |
| 49 0.0707 0.6307 4.3433 0.0000 12 8.0636 |
| 50 16.0033 0.6678 1.8802 0.0000 22 7.8378 |
| 51 16.1878 0.7420 3.2164 0.0000 20 7.9890 |
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| 52 0.1463 0.6307 2.7469 0.0000 17 8.0781 |
| 53 16.0039 0.9646 1.1377 0.0000 23 7.6436 |
| 54 15.9672 0.9275 0.5438 0.0000 23 7.6516 |
| 55 16.1884 0.7420 2.5111 0.0000 22 7.9673 |
| 56 0.0738 1.2985 0.5939 0.0000 17 7.4485 |
| 57 15.8905 1.0017 3.5508 0.0000 20 7.5455 |
| 58 0.0715 1.2985 3.3781 0.0000 12 7.6991 |
| 59 16.0416 1.7437 0.3581 0.0000 23 7.1396 |
| 60 16.0391 1.7437 3.4393 0.0000 20 7.1479 |
| 61 4.8984 8.0136 3.9681 12.8287 11 0.0283 |
| 62 3.9347 8.0136 1.8158 11.7365 14 0.0212 |
| 63 5.5663 9.5718 4.7100 8.3256 8 0.0232 |
| 64 5.4580 9.6460 0.9236 12.8590 13 0.0227 |
| 65 16.0391 14.3206 3.4393 0.0000 1 7.1479 |
| 66 16.0416 14.3206 0.3581 0.0000 5 7.1396 |
| 67 10.8764 9.5347 4.7057 8.3036 1 0.0203 |
| 68 0.0715 14.7658 3.3781 0.0000 8 7.6991 |
| 69 0.0738 14.7658 0.5939 0.0000 13 7.4485 |
| 70 16.2261 14.9513 1.8057 0.0000 13 7.7315 |
| 71 15.9672 15.1368 0.5438 0.0000 5 7.6516 |
| 72 15.9279 15.1739 3.2538 0.0000 1 7.7022 |
| 73 15.9304 15.0997 0.2097 0.0000 1 7.5954 |
| 74 16.0039 15.0997 1.1377 0.0000 5 7.6436 |
| 75 16.0033 15.3966 1.8802 0.0000 6 7.8378 |
| 76 16.1884 15.3223 2.5111 0.0000 6 7.9673 |
| 77 0.1463 15.4337 2.7469 0.0000 13 8.0781 |
| 78 15.8905 15.0626 3.5508 0.0000 1 7.5455 |
| 79 16.1878 15.3223 3.2164 0.0000 1 7.9890 |
| 80 0.2942 15.2852 3.5264 0.0000 8 7.8850 |
| 81 16.2242 15.2110 4.1816 0.0000 1 7.8102 |
| 82 0.0737 15.5079 0.6681 0.0000 13 7.9740 |
| 83 16.2640 15.5821 0.8405 0.0000 13 8.1008 |
| 84 0.1093 15.4708 2.5614 0.0000 13 8.0891 |
| 85 0.1089 15.4708 3.0068 0.0000 13 8.1919 |
| 86 0.1104 15.5079 1.1878 0.0000 13 7.9503 |
| 87 16.1862 15.6563 5.1839 0.0000 1 8.1110 |
| 88 16.1902 15.5821 0.3580 0.0000 5 8.1415 |
| 89 16.1506 15.6192 3.3649 0.0000 1 8.1561 |
| 90 16.0016 15.6563 3.9590 0.0000 1 8.0114 |
| 91 0.0707 15.4337 4.3433 0.0000 8 8.0636 |
| 92 16.1870 15.6563 4.2559 0.0000 1 8.1097 |
| 93 16.0004 15.6192 5.4068 0.0000 1 7.9786 |
| 94 0.0333 15.9531 4.7145 0.0000 1 8.4188 |
| 95 16.1890 15.6934 1.8429 0.0000 6 8.1661 |
| 96 0.0703 15.8789 4.8630 0.0000 8 8.3864 |
| 97 0.0698 15.6934 5.4940 0.0000 13 8.1761 |
| 98 16.1859 15.8418 5.5551 0.0000 1 8.2812 |
| 99 16.1504 15.8047 3.5506 0.0000 1 8.2670 |
| 100 0.0700 15.8418 5.1971 0.0000 13 8.3295 |
| 101 16.2267 15.7676 1.1375 0.0000 13 8.2660 |
| 102 0.0336 15.8789 4.2690 0.0000 1 8.3748 |
| 103 16.0788 15.8418 0.2839 0.0000 1 8.2567 |
| 104 16.0785 15.8418 0.6922 0.0000 5 8.2494 |
| 105 16.0765 15.8418 3.1052 0.0000 6 8.2621 |
| 106 16.0044 15.8789 0.5438 0.0000 5 8.2362 |
| 107 15.9649 15.9160 3.3280 0.0000 3 8.2160 |
| 108 0.1834 0.0000 2.7840 0.0000 13 8.5261 |
| 109 0.2562 0.3339 4.5658 0.0000 12 8.1528 |
| 110 0.2932 0.8533 4.6772 0.0000 12 7.7402 |
| 111 0.5565 0.9646 0.5935 0.0000 17 7.3503 |
| 112 0.5565 15.0997 0.5935 0.0000 13 7.3503 |
| 113 0.2932 15.2110 4.6772 0.0000 8 7.7402 |
| 114 0.2562 15.7305 4.5658 0.0000 8 8.1528 |
| 115 0.2966 0.0000 0.5195 0.0000 13 8.2554 |
| 116 0.2943 0.0000 3.3408 0.0000 8 8.4959 |
| 117 0.2596 0.4823 0.4453 0.0000 17 7.9148 |
| 118 0.3688 0.1855 3.0809 0.0000 18 8.3332 |
| 119 0.4823 0.2226 0.4822 0.0000 17 7.9678 |
| 120 0.2578 0.3339 2.6355 0.0000 17 8.1978 |
| 121 0.2564 0.3710 4.2689 0.0000 12 8.1357 |
| 122 0.2556 0.8533 5.2340 0.0000 17 7.7392 |
| 123 0.2565 0.8533 4.1946 0.0000 12 7.7831 |
| 124 0.5173 0.9646 3.1179 0.0000 12 7.6758 |
| 125 0.3689 1.0759 2.9695 0.0000 17 7.6711 |
| 126 0.3689 14.9884 2.9695 0.0000 13 7.6711 |
| 127 0.5173 15.0997 3.1179 0.0000 8 7.6758 |
| 128 0.2565 15.2110 4.1946 0.0000 8 7.7831 |
| 129 0.2556 15.2110 5.2340 0.0000 13 7.7392 |
| 130 0.2564 15.6934 4.2689 0.0000 8 8.1357 |
| 131 0.4823 15.8418 0.4822 0.0000 13 7.9678 |

	132	0.2578	15.7305	2.6355	0.0000	13	8.1978	
	133	0.3688	15.8789	3.0809	0.0000	10	8.3332	
	134	0.2596	15.5821	0.4453	0.0000	13	7.9148	
	135	0.2939	0.1855	3.8605	0.0000	12	8.2849	
	136	0.2554	0.1855	5.5681	0.0000	17	8.1856	
	137	0.4455	0.0000	0.1110	0.0000	13	8.1926	
	138	0.2557	0.3710	5.1598	0.0000	17	8.1052	
	139	0.2955	0.4081	1.9301	0.0000	17	7.9987	
	140	0.2557	15.6934	5.1598	0.0000	13	8.1052	
	141	0.2955	15.6563	1.9301	0.0000	13	7.9987	
	142	0.2554	15.8789	5.5681	0.0000	13	8.1856	
	143	0.2939	15.8789	3.8605	0.0000	8	8.2849	
	144	0.2955	0.0000	1.8930	0.0000	13	8.3051	
	145	0.2950	0.0000	2.4870	0.0000	13	8.3964	
	146	0.3304	0.0000	4.6771	0.0000	8	8.3603	
	147	0.3302	0.0000	4.9370	0.0000	12	8.3630	
	148	0.5183	0.5936	1.9671	0.0000	17	7.7203	
	149	0.5183	15.4708	1.9671	0.0000	13	7.7203	
	150	0.3703	0.0000	1.2247	0.0000	13	8.2060	
	151	0.5559	15.8418	1.2988	0.0000	13	7.9198	
	152	0.4042	0.2226	5.1968	0.0000	17	8.1168	
	153	6.7197	5.4537	1.8878	8.2716	18	0.0160	
	154	6.7197	10.6106	1.8878	8.2716	10	0.0160	
	155	0.4042	15.8418	5.1968	0.0000	13	8.1168	
	156	0.5559	0.2226	1.2988	0.0000	17	7.9198	
	157	0.5550	0.2226	2.4867	0.0000	17	8.0664	
	158	0.4421	0.2226	4.2687	0.0000	12	8.1296	
	159	0.5184	0.1855	1.8557	0.0000	17	8.0186	
	160	0.4804	0.1855	2.8580	0.0000	18	8.2189	
	161	0.4801	0.2226	3.2664	0.0000	12	8.2229	
	162	0.7753	0.5194	5.5306	0.0000	17	7.6076	
	163	0.7395	0.5565	3.9344	0.0000	12	7.7106	
	164	0.6291	0.7791	2.6352	0.0000	17	7.6320	
	165	0.6305	0.8533	1.0018	0.0000	17	7.3782	
	166	0.6273	0.7791	4.8254	0.0000	12	7.5725	
	167	0.6273	15.2852	4.8254	0.0000	8	7.5725	
	168	0.6291	15.2852	2.6352	0.0000	13	7.6320	
	169	0.6305	15.2110	1.0018	0.0000	13	7.3782	
	170	0.7395	15.5079	3.9344	0.0000	8	7.7106	
	171	0.7753	15.5450	5.5306	0.0000	13	7.6076	
	172	0.4804	15.8789	2.8580	0.0000	10	8.2189	
	173	0.4801	15.8418	3.2664	0.0000	8	8.2229	
	174	0.5184	15.8789	1.8557	0.0000	13	8.0186	
	175	0.4421	15.8418	4.2687	0.0000	8	8.1296	
	176	0.5550	15.8418	2.4867	0.0000	13	8.0664	
	177	0.7036	0.0742	2.4124	0.0000	17	8.0782	
	178	0.8151	15.8418	2.3009	0.0000	13	7.8754	
	179	0.8151	0.2226	2.3009	0.0000	17	7.8754	
	180	0.6682	0.0000	0.2222	0.0000	13	8.0474	
	181	0.6659	0.0000	3.0064	0.0000	10	8.2204	
	182	0.5909	0.0000	3.9345	0.0000	8	8.2368	
	183	0.5896	0.0000	5.5307	0.0000	13	8.1271	
	184	0.5911	0.2968	3.7117	0.0000	12	8.0293	
	185	0.5911	15.7676	3.7117	0.0000	8	8.0293	
	186	0.7036	15.9902	2.4124	0.0000	13	8.0782	
	187	0.6307	0.0000	0.7419	0.0000	13	8.0423	
	188	0.7783	0.0000	1.8184	0.0000	13	8.0040	
	189	0.6655	0.0000	3.5261	0.0000	7	8.2261	
	190	0.6277	0.0000	4.3799	0.0000	8	8.1839	
	191	1.2217	0.8533	4.5650	0.0000	12	7.1398	
	192	0.8909	0.5194	0.3334	0.0000	17	7.4922	
	193	0.9268	0.2226	1.8554	0.0000	17	7.7429	
	194	0.5918	0.3710	2.8951	0.0000	18	8.0205	
	195	0.8144	0.7049	3.1176	0.0000	18	7.6730	
	196	0.8144	15.3595	3.1176	0.0000	10	7.6730	
	197	0.5918	15.6934	2.8951	0.0000	10	8.0205	
	198	0.8909	15.5450	0.3334	0.0000	13	7.4922	
	199	0.9268	15.8418	1.8554	0.0000	13	7.7429	
	200	1.2217	15.2110	4.5650	0.0000	8	7.1398	
	201	0.6271	0.0000	5.0852	0.0000	13	8.1728	
	202	0.8908	0.5194	0.5190	0.0000	17	7.4803	
	203	0.7388	0.5194	4.7882	0.0000	12	7.6998	
	204	0.6287	0.3710	3.1549	0.0000	15	8.0283	
	205	0.8140	0.5194	3.6002	0.0000	12	7.7342	
	206	1.2583	0.8533	5.2332	0.0000	17	7.1023	
	207	0.8140	15.5450	3.6002	0.0000	8	7.7342	
	208	0.7388	15.5450	4.7882	0.0000	8	7.6998	
	209	1.2583	15.2110	5.2332	0.0000	13	7.1023	
	210	0.8908	15.5450	0.5190	0.0000	13	7.4803	
	211	0.6287	15.6934	3.1549	0.0000	7	8.0283	

212	0.7045	0.0000	1.3358	0.0000	13	8.0076	
213	0.6274	0.0000	4.6769	0.0000	8	8.1770	
214	0.7787	0.4823	1.3358	0.0000	17	7.5803	
215	0.8886	0.5194	3.2289	0.0000	15	7.7296	
216	0.7787	15.5821	1.3358	0.0000	13	7.5803	
217	0.8886	15.5450	3.2289	0.0000	7	7.7296	
218	0.8163	0.2226	0.7418	0.0000	17	7.7528	
219	0.7775	0.1855	2.7835	0.0000	18	7.9872	
220	0.8145	0.1855	3.0434	0.0000	18	7.9936	
221	0.8142	0.1855	3.4146	0.0000	15	7.9952	
222	0.7775	15.8789	2.7835	0.0000	10	7.9872	
223	0.8163	15.8418	0.7418	0.0000	13	7.7528	
224	0.8145	15.8789	3.0434	0.0000	10	7.9936	
225	0.8142	15.8789	3.4146	0.0000	7	7.9952	
226	0.8869	0.0000	5.3078	0.0000	13	7.9838	
227	0.8167	0.1855	0.3334	0.0000	17	7.8018	
228	1.2210	0.2226	5.3817	0.0000	17	7.6028	
229	0.9245	0.2968	4.7509	0.0000	12	7.7610	
230	0.8167	15.8789	0.3334	0.0000	13	7.8018	
231	0.9245	15.7676	4.7509	0.0000	8	7.7610	
232	1.2210	15.8418	5.3817	0.0000	13	7.6028	
233	0.9621	0.0000	4.0827	0.0000	8	8.0041	
234	0.9621	0.3710	4.1198	0.0000	12	7.7026	
235	0.9613	0.3710	5.1592	0.0000	17	7.6703	
236	0.9621	15.6934	4.1198	0.0000	8	7.7026	
237	0.9613	15.6934	5.1592	0.0000	13	7.6703	
238	6.7553	5.5279	3.7438	11.6356	15	0.0244	
239	6.7553	10.5364	3.7438	11.6356	7	0.0244	
240	1.0380	0.4081	2.1151	0.0000	17	7.5663	
241	1.2214	0.8904	4.8620	0.0000	12	7.1103	
242	1.1852	0.9275	3.7484	0.0000	12	7.1685	
243	1.1852	15.1368	3.7484	0.0000	8	7.1685	
244	1.2214	15.1739	4.8620	0.0000	8	7.1103	
245	1.0380	15.6563	2.1151	0.0000	13	7.5663	
246	1.2988	0.0000	1.0755	0.0000	13	7.6582	
247	0.9989	0.0000	4.5281	0.0000	8	7.9597	
248	1.2217	15.8789	4.6022	0.0000	8	7.6787	
249	1.2227	0.9646	3.3400	0.0000	15	7.1821	
250	1.2227	15.0997	3.3400	0.0000	7	7.1821	
251	1.0374	0.0000	2.8947	0.0000	10	7.9362	
252	1.2227	0.2226	3.3400	0.0000	15	7.6737	
253	1.2227	15.8418	3.3400	0.0000	7	7.6737	
254	1.1879	15.8418	0.4816	0.0000	13	7.5457	
255	1.0391	0.0000	0.7787	0.0000	13	7.8023	
256	1.0379	0.0000	2.2265	0.0000	10	7.8778	
257	1.1112	0.0000	3.4886	0.0000	7	7.9023	
258	1.2217	0.1855	4.6022	0.0000	12	7.6787	
259	1.4099	0.0000	1.4095	0.0000	13	7.6127	
260	1.2978	0.1484	2.3376	0.0000	18	7.5942	
261	1.1879	0.2226	0.4816	0.0000	17	7.5457	
262	1.2221	0.2226	4.0825	0.0000	15	7.6726	
263	1.2224	0.2226	3.7112	0.0000	15	7.6641	
264	1.2221	15.8418	4.0825	0.0000	7	7.6726	
265	1.2224	15.8418	3.7112	0.0000	7	7.6641	
266	1.2978	15.9160	2.3376	0.0000	10	7.5942	
267	1.3351	0.0000	2.1149	0.0000	10	7.6622	
268	1.1488	0.2597	2.9317	0.0000	18	7.6839	
269	1.2208	0.2226	5.6045	0.0000	17	7.5718	
270	1.4455	0.8162	3.3770	0.0000	15	7.1069	
271	1.4455	15.2481	3.3770	0.0000	7	7.1069	
272	1.2208	15.8418	5.6045	0.0000	13	7.5718	
273	1.1488	15.8047	2.9317	0.0000	10	7.6839	
274	1.1876	0.2226	0.8157	0.0000	17	7.5342	
275	1.4109	0.8533	0.2216	0.0000	17	6.9246	
276	1.4109	15.2110	0.2216	0.0000	13	6.9246	
277	1.1876	15.8418	0.8157	0.0000	13	7.5342	
278	1.4477	0.8533	0.5928	0.0000	17	6.8759	
279	1.4457	0.8162	3.1171	0.0000	15	7.1242	
280	1.4477	15.2110	0.5928	0.0000	13	6.8759	
281	1.4457	15.2481	3.1171	0.0000	7	7.1242	
282	1.5571	0.1855	3.0799	0.0000	18	7.4685	
283	1.5926	0.5194	5.1216	0.0000	17	7.2022	
284	1.5926	15.5450	5.1216	0.0000	13	7.2022	
285	1.3734	15.9902	0.7042	0.0000	13	7.5564	
286	1.3734	0.0742	0.7042	0.0000	17	7.5564	
287	1.5571	15.8789	3.0799	0.0000	10	7.4685	
288	1.6673	0.4452	4.6018	0.0000	12	7.2153	
289	1.6673	15.6192	4.6018	0.0000	8	7.2153	
290	1.8161	0.0000	4.2676	0.0000	7	7.4300	
291	1.7782	0.0000	5.1586	0.0000	13	7.5337	

| 292 1.5937 0.5936 3.7109 0.0000 15 7.1394 |
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| 294 1.5966 15.8789 0.1843 0.0000 13 7.3758 |
| 295 1.5966 0.1855 0.1843 0.0000 17 7.3758 |
| 296 1.4826 0.0000 3.3769 0.0000 7 7.6452 |
| 297 1.5938 0.1855 3.5996 0.0000 15 7.4275 |
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| 299 2.0021 0.4081 3.8220 0.0000 15 6.9843 |
| 300 2.0021 15.6563 3.8220 0.0000 7 6.9843 |
| 301 2.2275 0.0000 0.6664 0.0000 10 7.1632 |
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| 304 2.0784 0.0000 1.3347 0.0000 10 7.1765 |
| 305 2.0406 0.0000 2.1143 0.0000 10 7.1848 |
| 306 1.7452 0.0000 0.1842 0.0000 13 7.4578 |
| 307 2.2256 0.0000 3.0422 0.0000 10 7.1578 |
| 308 2.2624 0.0000 3.3763 0.0000 7 7.1286 |
| 309 2.4107 0.0000 3.7103 0.0000 7 7.0271 |
| 310 2.4093 0.0000 5.3808 0.0000 13 7.2057 |
| 311 2.4136 0.0000 0.1094 0.0000 13 7.1548 |
| 312 8.2399 5.0085 4.7078 8.3296 16 0.0110 |
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| 314 2.9297 0.0000 4.7864 0.0000 7 6.8007 |
| 315 2.6323 0.0000 5.1579 0.0000 7 7.0388 |
| 316 8.2430 10.9816 0.9213 11.6859 9 0.0214 |
| 317 8.2430 5.0827 0.9213 11.6859 21 0.0214 |
| 318 9.7647 5.4166 1.8853 8.2962 22 0.0166 |
| 319 10.8053 6.5667 0.9192 11.6725 23 0.0157 |
| 320 10.8053 9.4976 0.9192 11.6725 5 0.0157 |
| 321 9.7647 10.6477 1.8853 8.2962 6 0.0166 |
| 322 9.7261 5.4537 3.7414 11.6680 19 0.0188 |
| 323 9.7261 10.6106 3.7414 11.6680 3 0.0188 |
| 324 11.2872 8.0507 1.8840 8.3372 2 0.0245 |
| 325 11.1743 8.0136 3.7402 11.6858 0 0.0209 |
| 326 13.6244 0.0000 4.6292 0.0000 3 6.7804 |
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| 328 14.2220 0.0000 0.4710 0.0000 6 7.1493 |
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| 332 14.5521 0.4081 5.4080 0.0000 20 7.1651 |
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| 337 14.4801 0.0000 2.6610 0.0000 6 7.2180 |
| 338 14.6280 0.4452 3.4033 0.0000 19 7.0329 |
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| 340 14.8131 15.9902 4.1827 0.0000 3 7.4343 |
| 341 14.9605 0.0000 5.5190 0.0000 1 7.7352 |
| 342 14.8131 0.0742 4.1827 0.0000 19 7.4343 |
| 343 14.9619 0.0000 3.8856 0.0000 3 7.5786 |
| 344 14.8517 0.3339 2.3266 0.0000 22 7.2002 |
| 345 15.0763 0.8162 0.1733 0.0000 20 7.1668 |
| 346 15.0763 15.2481 0.1733 0.0000 1 7.1668 |
| 347 14.8517 15.7305 2.3266 0.0000 6 7.2002 |
| 348 15.0365 0.7791 3.4030 0.0000 19 7.0990 |
| 349 15.0365 15.2852 3.4030 0.0000 3 7.0990 |
| 350 14.9607 0.0000 5.2963 0.0000 1 7.7150 |
| 351 15.0390 0.0000 0.3218 0.0000 6 7.7149 |
| 352 15.0365 0.0000 3.4772 0.0000 3 7.6333 |
| 353 15.0388 0.8162 0.6559 0.0000 22 7.1016 |
| 354 15.0388 15.2481 0.6559 0.0000 6 7.1016 |
| 355 15.0355 0.0000 4.7023 0.0000 3 7.6893 |
| 356 15.0730 0.7420 4.2568 0.0000 20 7.1546 |
| 357 15.0722 0.7791 5.1477 0.0000 20 7.1241 |
| 358 15.0730 15.3223 4.2568 0.0000 1 7.1546 |
| 359 15.0722 15.2852 5.1477 0.0000 1 7.1241 |
| 360 15.1130 0.0000 0.6559 0.0000 6 7.7056 |
| 361 15.2236 0.1484 1.7323 0.0000 22 7.5835 |
| 362 15.3349 0.0000 1.8065 0.0000 6 7.7655 |
| 363 15.2604 0.1113 2.0664 0.0000 22 7.6365 |
| 364 15.2227 0.0000 2.7346 0.0000 6 7.7321 |
| 365 15.1482 0.0000 3.1059 0.0000 6 7.7296 |
| 366 15.2979 0.7791 1.6951 0.0000 22 7.2187 |
| 367 15.2582 0.8533 4.8134 0.0000 20 7.1638 |
| 368 15.2615 1.8550 0.7671 0.0000 23 6.4847 |
| 369 15.2615 14.2093 0.7671 0.0000 5 6.4847 |
| 370 15.2582 15.2110 4.8134 0.0000 1 7.1638 |
| 371 15.2979 15.2852 1.6951 0.0000 6 7.2187 |

	372	15.2236	15.9160	1.7323	0.0000	6	7.5835	
	373	15.2604	15.9531	2.0664	0.0000	6	7.6365	
	374	15.2612	15.9160	1.1383	0.0000	6	7.6454	
	375	15.2612	0.1484	1.1383	0.0000	22	7.6454	
	376	15.2250	0.2226	-0.0124	0.0000	20	7.7053	
	377	15.2206	0.2226	5.2961	0.0000	20	7.6725	
	378	15.2217	0.2226	4.0339	0.0000	19	7.6098	
	379	15.2604	0.7791	2.1035	0.0000	22	7.1910	
	380	15.2231	0.8162	2.2892	0.0000	22	7.1468	
	381	15.2608	0.7791	1.5467	0.0000	22	7.1958	
	382	15.2608	15.2852	1.5467	0.0000	6	7.1958	
	383	15.2231	15.2481	2.2892	0.0000	6	7.1468	
	384	15.2604	15.2852	2.1035	0.0000	6	7.1910	
	385	15.2217	15.8418	4.0339	0.0000	3	7.6098	
	386	15.2206	15.8418	5.2961	0.0000	1	7.6725	
	387	15.2250	15.8418	-0.0124	0.0000	1	7.7053	
	388	15.2619	0.9646	0.3216	0.0000	23	7.1797	
	389	15.2594	0.9646	3.2543	0.0000	19	7.1577	
	390	15.2619	15.0997	0.3216	0.0000	5	7.1797	
	391	15.2594	15.0997	3.2543	0.0000	3	7.1577	
	392	15.2597	0.1855	2.9202	0.0000	22	7.6533	
	393	15.2597	15.8789	2.9202	0.0000	6	7.6533	
	394	15.2947	0.4452	5.5187	0.0000	20	7.5551	
	395	15.7069	1.4469	0.9895	0.0000	23	7.0863	
	396	15.2993	1.0017	-0.0125	0.0000	20	7.1296	
	397	15.2957	1.5582	4.3308	0.0000	20	6.6557	
	398	15.2957	14.5061	4.3308	0.0000	1	6.6557	
	399	15.2993	15.0626	-0.0125	0.0000	1	7.1296	
	400	15.7069	14.6174	0.9895	0.0000	5	7.0863	
	401	15.2947	15.6192	5.5187	0.0000	1	7.5551	
	402	15.2986	0.2226	0.8042	0.0000	22	7.6616	
	403	15.5193	0.4452	3.3283	0.0000	19	7.6853	
	404	15.5193	15.6192	3.3283	0.0000	3	7.6853	
	405	15.2986	15.8418	0.8042	0.0000	6	7.6616	
	406	15.5587	0.4823	0.5441	0.0000	22	7.7238	
	407	15.4451	1.1501	3.2542	0.0000	19	7.1894	
	408	15.4451	14.9142	3.2542	0.0000	3	7.1894	
	409	15.5587	15.5821	0.5441	0.0000	6	7.7238	
	410	15.3352	0.0000	1.4353	0.0000	6	7.7782	
	411	15.6683	1.4469	2.7714	0.0000	22	7.1680	
	412	15.6330	1.4098	0.5441	0.0000	23	7.0715	
	413	15.6330	14.6545	0.5441	0.0000	5	7.0715	
	414	15.6683	14.6174	2.7714	0.0000	6	7.1680	
	415	15.5948	0.2226	1.8805	0.0000	22	7.8044	
	416	15.5575	1.2243	2.0662	0.0000	22	7.1509	
	417	15.5573	1.2614	2.3260	0.0000	22	7.1405	
	418	15.5575	14.8400	2.0662	0.0000	6	7.1509	
	419	15.5573	14.8029	2.3260	0.0000	6	7.1405	
	420	15.5948	15.8418	1.8805	0.0000	6	7.8044	
	421	15.6308	1.3727	3.2169	0.0000	20	7.1640	
	422	15.6308	14.6916	3.2169	0.0000	1	7.1640	
	423	15.7419	0.0000	3.5880	0.0000	3	8.1378	
	424	15.6323	0.2226	1.4350	0.0000	22	7.8453	
	425	15.6316	0.2226	2.3259	0.0000	22	7.8445	
	426	15.5580	1.2614	1.4351	0.0000	23	7.1393	
	427	15.5580	14.8029	1.4351	0.0000	5	7.1393	
	428	15.6323	15.8418	1.4350	0.0000	6	7.8453	
	429	15.6316	15.8418	2.3259	0.0000	6	7.8445	
	430	15.5554	0.2597	4.6647	0.0000	20	7.8153	
	431	15.7066	0.5194	1.3978	0.0000	22	7.7120	
	432	15.6661	0.5565	5.5184	0.0000	20	7.6921	
	433	15.6671	1.1130	4.2563	0.0000	20	7.2385	
	434	15.6671	14.9513	4.2563	0.0000	1	7.2385	
	435	15.6661	15.5079	5.5184	0.0000	1	7.6921	
	436	15.7066	15.5450	1.3978	0.0000	6	7.7120	
	437	15.5554	15.8047	4.6647	0.0000	1	7.8153	
	438	15.8190	0.0000	0.2098	0.0000	1	8.2588	
	439	15.5920	0.0000	5.2215	0.0000	1	8.0626	
	440	15.6686	0.5194	2.4002	0.0000	22	7.6850	
	441	15.6333	0.5194	0.2100	0.0000	20	7.7402	
	442	15.6674	0.5194	3.8479	0.0000	20	7.7262	
	443	15.7410	0.4823	4.7388	0.0000	20	7.7537	
	444	15.6295	0.6307	4.8874	0.0000	20	7.5704	
	445	15.7440	1.5211	0.9895	0.0000	23	7.0589	
	446	15.7440	14.5432	0.9895	0.0000	5	7.0589	
	447	15.6333	15.5450	0.2100	0.0000	1	7.7402	
	448	15.6674	15.5450	3.8479	0.0000	1	7.7262	
	449	15.7410	15.5821	4.7388	0.0000	1	7.7537	
	450	15.6295	15.4337	4.8874	0.0000	1	7.5704	
	451	15.6686	15.5450	2.4002	0.0000	6	7.6850	

	452	15.6681	0.1855	3.0312	0.0000	22	7.9672	
	453	15.6668	1.2243	4.6275	0.0000	20	7.1421	
	454	15.6320	1.2985	1.7691	0.0000	22	7.1673	
	455	15.7798	1.5953	2.6599	0.0000	22	7.1675	
	456	15.7798	14.4690	2.6599	0.0000	6	7.1675	
	457	15.6320	14.7658	1.7691	0.0000	6	7.1673	
	458	15.6668	14.8400	4.6275	0.0000	1	7.1421	
	459	15.6681	15.8789	3.0312	0.0000	6	7.9672	
	460	15.8556	0.0000	0.7666	0.0000	6	8.2233	
	461	15.6699	0.1855	0.8410	0.0000	22	7.9537	
	462	15.6683	0.1855	2.8085	0.0000	22	7.9383	
	463	15.7433	0.3710	1.8804	0.0000	22	7.8199	
	464	15.7433	15.6934	1.8804	0.0000	6	7.8199	
	465	15.6699	15.8789	0.8410	0.0000	6	7.9537	
	466	15.6683	15.8789	2.8085	0.0000	6	7.9383	
	467	15.8538	0.0000	3.0311	0.0000	6	8.2265	
	468	15.8146	0.0000	5.4812	0.0000	1	8.2156	
	469	15.8191	0.7049	0.0242	0.0000	20	7.6898	
	470	15.8191	15.3595	0.0242	0.0000	1	7.6898	
	471	15.8174	0.0000	2.1031	0.0000	6	8.1217	
	472	15.8150	0.0000	5.0357	0.0000	1	8.1857	
	473	15.8523	0.7049	4.7758	0.0000	20	7.6542	
	474	15.8523	15.3595	4.7758	0.0000	1	7.6542	
	475	15.7805	0.0000	1.7690	0.0000	6	8.0920	
	476	15.8914	0.2226	2.4742	0.0000	22	8.0505	
	477	15.8540	0.0000	2.7712	0.0000	6	8.1944	
	478	15.8155	0.0000	4.3675	0.0000	1	8.1862	
	479	15.8150	0.8533	4.9986	0.0000	20	7.5231	
	480	15.8150	15.2110	4.9986	0.0000	1	7.5231	
	481	15.8914	15.8418	2.4742	0.0000	6	8.0505	
	482	15.8530	0.0000	3.9220	0.0000	3	8.2212	
	483	15.8552	0.2226	1.2492	0.0000	22	8.0261	
	484	15.8532	0.2226	3.7364	0.0000	19	8.0728	
	485	15.8562	0.2968	0.0613	0.0000	20	8.0300	
	486	15.8517	0.7049	5.5925	0.0000	20	7.7049	
	487	15.8517	15.3595	5.5925	0.0000	1	7.7049	
	488	15.8532	15.8418	3.7364	0.0000	3	8.0728	
	489	15.8562	15.7676	0.0613	0.0000	1	8.0300	
	490	15.8552	15.8418	1.2492	0.0000	6	8.0261	
	491	15.9271	0.2968	4.2189	0.0000	20	8.0296	
	492	15.9271	15.7676	4.2189	0.0000	1	8.0296	
	493	15.8910	0.3710	2.8826	0.0000	22	7.9963	
	494	15.9298	0.3339	0.8779	0.0000	22	8.0499	
	495	15.9275	1.7066	3.7364	0.0000	20	7.0458	
	496	15.9275	14.3577	3.7364	0.0000	1	7.0458	
	497	15.8910	15.6934	2.8826	0.0000	6	7.9963	
	498	15.9298	15.7305	0.8779	0.0000	6	8.0499	
	499	15.9290	0.1855	1.8802	0.0000	22	8.0814	
	500	15.9262	0.6678	5.2584	0.0000	20	7.7501	
	501	15.9262	15.3966	5.2584	0.0000	1	7.7501	
	502	15.9290	15.8789	1.8802	0.0000	6	8.0814	
	503	16.1131	0.4823	3.7362	0.0000	20	8.0512	
	504	16.1131	15.5821	3.7362	0.0000	1	8.0512	
+-----+								
	Atomic Charge Difference							
+-----+								
	Atom # x y z Charge							
+-----+								
	Si	0	11.1830	8.0322	3.7361	-2.3142		
	C	1	10.8664	9.5523	4.7039	2.3036		
	C	2	11.2713	8.0322	1.8826	2.3372		
	Si	3	9.7179	10.5950	3.7349	-2.3320		
	C	4	8.2305	11.0542	4.7023	2.3296		
	Si	5	10.7960	9.5094	0.9143	-2.3275		
	C	6	9.7570	10.6620	1.8821	2.2962		
	Si	7	6.7666	10.5502	3.7271	-2.3644		
	C	8	5.5810	9.5587	4.7223	2.3256		
	Si	9	8.2326	10.9640	0.9151	-2.3141		
	C	10	6.7112	10.6101	1.8742	2.2716		
	Si	11	4.9121	8.0322	3.9517	-1.1713		
	C	12	5.5810	6.5056	4.7223	2.3256		
	Si	13	5.4765	9.6481	0.9107	-1.1410		
	Al	14	3.9291	8.0322	1.8071	-1.2635		
	Si	15	6.7666	5.5142	3.7271	-2.3644		
	C	16	8.2305	5.0102	4.7023	2.3296		
	Si	17	5.4765	6.4162	0.9107	-1.1410		
	C	18	6.7112	5.4543	1.8742	2.2716		
	Si	19	9.7179	5.4694	3.7349	-2.3320		
	C	20	10.8664	6.5120	4.7039	2.3036		
	Si	21	8.2326	5.1004	0.9151	-2.3141		

```

| C 22 9.7570 5.4023 1.8821 2.2962 |
| Si 23 10.7960 6.5550 0.9143 -2.3275 |
+-----+
| Atomic Charge Volumes |
+-----+
| Atom # x y z Charge |
+-----+
| Si 0 11.1830 8.0322 3.7361 11.6858 |
| C 1 10.8664 9.5523 4.7039 8.3036 |
| C 2 11.2713 8.0322 1.8826 8.3372 |
| Si 3 9.7179 10.5950 3.7349 11.6680 |
| C 4 8.2305 11.0542 4.7023 8.3296 |
| Si 5 10.7960 9.5094 0.9143 11.6725 |
| C 6 9.7570 10.6620 1.8821 8.2962 |
| Si 7 6.7666 10.5502 3.7271 11.6356 |
| C 8 5.5810 9.5587 4.7223 8.3256 |
| Si 9 8.2326 10.9640 0.9151 11.6859 |
| C 10 6.7112 10.6101 1.8742 8.2716 |
| Si 11 4.9121 8.0322 3.9517 12.8287 |
| C 12 5.5810 6.5056 4.7223 8.3256 |
| Si 13 5.4765 9.6481 0.9107 12.8590 |
| Al 14 3.9291 8.0322 1.8071 11.7365 |
| Si 15 6.7666 5.5142 3.7271 11.6356 |
| C 16 8.2305 5.0102 4.7023 8.3296 |
| Si 17 5.4765 6.4162 0.9107 12.8590 |
| C 18 6.7112 5.4543 1.8742 8.2716 |
| Si 19 9.7179 5.4694 3.7349 11.6680 |
| C 20 10.8664 6.5120 4.7039 8.3036 |
| Si 21 8.2326 5.1004 0.9151 11.6859 |
| C 22 9.7570 5.4023 1.8821 8.2962 |
| Si 23 10.7960 6.5550 0.9143 11.6725 |
+-----+
| Total number of electrons: 246.6835 |
+-----+

```

Table 4. Bader Charges Analysis for Ga-doped (6,0) SWSiCNTs at C site

```

# Item: 0
# File: G:/SiC-Al-Ga/Electron Density/Barder charge-LSDA+U-SiCNT-(6.0)-Ga(C)-115-50Ha-0.001-0.001.hdf5
# Title: Barder charge-LSDA+U-SiCNT-(6.0)-Ga(C)-115-50Ha-0.001-0.001.hdf5 - BaderCharges_0
# Type: BaderCharges

```

```

+-----+
| |
| Bader Charges Analysis |
| |
+-----+
+-----+
| | Bader charge analysis only makes sense on an all electron density. |
| If a pseudo-potential DFT calculation was used to generate this charge |
| density then the core electron density must be included in order to get |
| meaningful results. |
| |
| Additionally, a fine electron density grid mesh should be used in order |
| to correctly reproduce the total charge. |
+-----+
| Electron Density Grid: 439 x 433 x 153 |
| Identified 540 charge maxima |
+-----+
| Bader Charge Volumes |
+-----+
| # x y z Charge Atom Distance |
+-----+
| 0 0.0331 0.0000 5.5403 0.0000 13 8.4384 |
| 1 15.9983 15.9172 0.5057 0.0000 5 8.2673 |
| 2 0.1107 15.8059 0.8864 0.0000 13 8.1332 |
| 3 0.1105 15.8801 1.2557 0.0000 13 8.1971 |
| 4 0.1105 0.1855 1.2557 0.0000 17 8.1971 |
| 5 15.9231 15.8801 1.8723 0.0000 6 8.0895 |
| 6 15.9231 0.1855 1.8723 0.0000 22 8.0895 |
| 7 0.0358 0.2226 1.8468 0.0000 17 8.2651 |
| 8 0.0358 15.8430 1.8468 0.0000 13 8.2651 |
| 9 16.1458 0.0000 1.8722 0.0000 6 8.3793 |
| 10 16.1824 15.7317 2.6109 0.0000 6 8.2284 |
| 11 16.0711 0.0000 2.5001 0.0000 6 8.3452 |
| 12 16.0336 15.8801 3.1281 0.0000 6 8.2681 |
| 13 16.1448 0.0000 3.2757 0.0000 3 8.4671 |
| 14 0.0715 0.0000 3.7674 0.0000 8 8.5503 |
| 15 0.0340 0.1855 4.2845 0.0000 20 8.3754 |

```

| 16 16.1810 0.0000 4.5685 0.0000 1 8.4116 |
| 17 0.0709 0.1113 4.7277 0.0000 12 8.4119 |
| 18 16.1808 0.0000 4.8639 0.0000 1 8.4117 |
| 19 0.0334 0.2226 5.2079 0.0000 17 8.3184 |
| 20 15.9983 0.1484 0.5057 0.0000 23 8.2673 |
| 21 0.1107 0.2597 0.8864 0.0000 17 8.1332 |
| 22 16.1824 0.3339 2.6109 0.0000 22 8.2284 |
| 23 16.0336 0.1855 3.1281 0.0000 22 8.2681 |
| 24 16.0727 0.2226 0.2840 0.0000 20 8.2584 |
| 25 16.1075 0.2226 3.5343 0.0000 20 8.2759 |
| 26 16.1446 0.2226 3.6082 0.0000 20 8.2893 |
| 27 0.0721 0.2968 2.9179 0.0000 17 8.3778 |
| 28 16.1821 0.3710 3.1280 0.0000 22 8.2670 |
| 29 15.9592 0.1484 3.3128 0.0000 19 8.2279 |
| 30 0.0707 0.1855 4.8755 0.0000 12 8.3572 |
| 31 16.1469 0.4823 0.3947 0.0000 23 8.1147 |
| 32 16.1432 0.1855 5.5658 0.0000 20 8.2875 |
| 33 16.1448 0.4452 3.3496 0.0000 20 8.1608 |
| 34 16.1835 0.3339 1.0965 0.0000 17 8.2297 |
| 35 0.2967 0.8163 0.2953 0.0000 17 7.6192 |
| 36 -0.0006 0.5194 0.8495 0.0000 17 8.0153 |
| 37 0.1092 0.5936 2.9917 0.0000 17 8.1591 |
| 38 0.0734 0.5565 1.1819 0.0000 17 7.9426 |
| 39 0.0723 0.5936 2.6593 0.0000 17 8.1047 |
| 40 0.0729 0.8905 1.8837 0.0000 17 7.7591 |
| 41 16.1830 0.3710 1.8722 0.0000 22 8.1737 |
| 42 0.1086 0.3710 3.8782 0.0000 12 8.2358 |
| 43 16.1072 0.4823 4.0145 0.0000 20 8.0241 |
| 44 15.8848 1.0018 3.5345 0.0000 20 7.5501 |
| 45 15.9241 0.8905 0.5057 0.0000 23 7.6562 |
| 46 0.0738 0.5565 0.5909 0.0000 17 7.9433 |
| 47 0.2216 0.6679 1.5142 0.0000 17 7.7796 |
| 48 0.2574 0.7792 3.4718 0.0000 12 7.8905 |
| 49 0.2565 0.4081 4.6168 0.0000 12 8.0668 |
| 50 0.0707 0.5194 4.8755 0.0000 12 8.1085 |
| 51 15.9231 0.5936 1.8354 0.0000 22 7.8321 |
| 52 15.9221 0.8905 3.2390 0.0000 20 7.7073 |
| 53 10.8728 6.5301 4.7200 8.3014 20 0.0189 |
| 54 0.0705 1.0760 5.1709 0.0000 17 7.6886 |
| 55 16.1834 0.7421 1.2073 0.0000 23 7.9353 |
| 56 5.5646 6.4930 4.7238 8.3465 12 0.0103 |
| 57 0.0366 1.2986 0.7018 0.0000 17 7.4399 |
| 58 16.1825 0.7421 2.5370 0.0000 22 7.9765 |
| 59 15.9594 0.9647 2.9804 0.0000 22 7.7169 |
| 60 5.4560 6.3817 0.8826 12.4689 17 0.0205 |
| 61 0.3691 1.0389 2.9546 0.0000 17 7.6645 |
| 62 0.0349 1.2986 3.0656 0.0000 20 7.7366 |
| 63 0.0347 1.2986 3.3981 0.0000 20 7.6721 |
| 64 0.3331 1.1502 1.3294 0.0000 17 7.3413 |
| 65 16.2201 1.0760 1.8721 0.0000 17 7.7348 |
| 66 0.0723 1.4099 2.6963 0.0000 17 7.5524 |
| 67 15.9968 1.0018 2.6479 0.0000 22 7.6856 |
| 68 0.0734 1.4099 1.1450 0.0000 17 7.3387 |
| 69 4.8970 8.0514 3.9856 12.4410 11 0.0188 |
| 70 15.9963 1.7067 3.3497 0.0000 20 7.1642 |
| 71 15.9984 1.7067 0.3949 0.0000 23 7.1344 |
| 72 4.0076 8.0143 1.8439 30.2898 14 0.0280 |
| 73 11.1704 8.0514 3.7225 11.6266 0 0.0285 |
| 74 5.5646 9.5726 4.7238 8.3465 8 0.0103 |
| 75 10.8728 9.5355 4.7200 8.3014 1 0.0189 |
| 76 5.4560 9.6839 0.8826 12.4689 13 0.0205 |
| 77 15.9963 14.3589 3.3497 0.0000 1 7.1642 |
| 78 15.9984 14.3589 0.3949 0.0000 5 7.1344 |
| 79 0.0723 14.6557 2.6963 0.0000 13 7.5524 |
| 80 0.0734 14.6557 1.1450 0.0000 13 7.3387 |
| 81 0.0347 14.7670 3.3981 0.0000 1 7.6721 |
| 82 0.0366 14.7670 0.7018 0.0000 13 7.4399 |
| 83 0.0349 14.7670 3.0656 0.0000 1 7.7366 |
| 84 16.2201 14.9896 1.8721 0.0000 13 7.7348 |
| 85 0.0705 14.9896 5.1709 0.0000 13 7.6886 |
| 86 0.3331 14.9154 1.3294 0.0000 13 7.3413 |
| 87 16.1834 15.3235 1.2073 0.0000 5 7.9353 |
| 88 0.0729 15.1751 1.8837 0.0000 13 7.7591 |
| 89 15.9231 15.4720 1.8354 0.0000 6 7.8321 |
| 90 15.9968 15.0638 2.6479 0.0000 6 7.6856 |
| 91 16.1825 15.3235 2.5370 0.0000 6 7.9765 |
| 92 0.3691 15.0267 2.9546 0.0000 13 7.6645 |
| 93 15.9594 15.1009 2.9804 0.0000 6 7.7169 |
| 94 15.9221 15.1751 3.2390 0.0000 1 7.7073 |
| 95 15.9241 15.1751 0.5057 0.0000 5 7.6562 |

| 96 0.0723 15.4720 2.6593 0.0000 13 8.1047 |
| 97 15.8848 15.0638 3.5345 0.0000 1 7.5501 |
| 98 0.0738 15.5091 0.5909 0.0000 13 7.9433 |
| 99 0.1092 15.4720 2.9917 0.0000 13 8.1591 |
| 100 0.2967 15.2493 0.2953 0.0000 13 7.6192 |
| 101 -0.0006 15.5462 0.8495 0.0000 13 8.0153 |
| 102 0.0734 15.5091 1.1819 0.0000 13 7.9426 |
| 103 0.2574 15.2864 3.4718 0.0000 8 7.8905 |
| 104 16.1469 15.5833 0.3947 0.0000 5 8.1147 |
| 105 16.1448 15.6204 3.3496 0.0000 1 8.1608 |
| 106 0.2565 15.6575 4.6168 0.0000 8 8.0668 |
| 107 0.0707 15.5462 4.8755 0.0000 8 8.1085 |
| 108 0.0334 15.8430 5.2079 0.0000 13 8.3184 |
| 109 0.2216 15.3978 1.5142 0.0000 13 7.7796 |
| 110 0.0340 15.8801 4.2845 0.0000 1 8.3754 |
| 111 16.1072 15.5833 4.0145 0.0000 1 8.0241 |
| 112 0.0707 15.8801 4.8755 0.0000 8 8.3572 |
| 113 16.1830 15.6946 1.8722 0.0000 6 8.1737 |
| 114 16.1821 15.6946 3.1280 0.0000 6 8.2670 |
| 115 16.1446 15.8430 3.6082 0.0000 1 8.2893 |
| 116 0.1086 15.6946 3.8782 0.0000 8 8.2358 |
| 117 0.0709 15.9543 4.7277 0.0000 8 8.4119 |
| 118 16.1432 15.8801 5.5658 0.0000 1 8.2875 |
| 119 16.1075 15.8430 3.5343 0.0000 1 8.2759 |
| 120 16.1835 15.7317 1.0965 0.0000 13 8.2297 |
| 121 0.0721 15.7688 2.9179 0.0000 13 8.3778 |
| 122 16.0727 15.8430 0.2840 0.0000 1 8.2584 |
| 123 15.9592 15.9172 3.3128 0.0000 3 8.2279 |
| 124 0.2595 0.4823 0.4061 0.0000 17 7.8831 |
| 125 0.2565 0.8163 4.6907 0.0000 12 7.7633 |
| 126 0.5193 0.9276 0.4798 0.0000 17 7.3746 |
| 127 0.2965 0.8163 0.5908 0.0000 17 7.6017 |
| 128 0.2581 0.7421 2.4745 0.0000 17 7.8361 |
| 129 0.2202 1.0389 3.5087 0.0000 12 7.7245 |
| 130 0.2202 15.0267 3.5087 0.0000 8 7.7245 |
| 131 0.2581 15.3235 2.4745 0.0000 13 7.8361 |
| 132 0.5193 15.1380 0.4798 0.0000 13 7.3746 |
| 133 0.2965 15.2493 0.5908 0.0000 13 7.6017 |
| 134 0.2565 15.2493 4.6907 0.0000 8 7.7633 |
| 135 0.2595 15.5833 0.4061 0.0000 13 7.8831 |
| 136 0.2221 0.0000 0.9232 0.0000 13 8.2592 |
| 137 0.1836 0.0000 2.7331 0.0000 13 8.4843 |
| 138 0.2575 0.0000 3.3240 0.0000 8 8.4942 |
| 139 0.4079 0.1855 0.6276 0.0000 17 8.0025 |
| 140 0.3319 0.1855 3.1024 0.0000 17 8.3425 |
| 141 0.2201 0.2226 3.6565 0.0000 12 8.2998 |
| 142 0.2558 0.1855 5.5771 0.0000 17 8.1506 |
| 143 0.2575 0.4452 3.3240 0.0000 12 8.1593 |
| 144 0.2568 0.3710 4.2844 0.0000 12 8.1060 |
| 145 0.2561 0.8534 5.2447 0.0000 17 7.7046 |
| 146 0.2197 0.8534 4.1736 0.0000 12 7.7812 |
| 147 0.2585 1.1131 1.8466 0.0000 17 7.4679 |
| 148 0.4430 1.7067 3.3978 0.0000 12 7.1269 |
| 149 0.4430 14.3589 3.3978 0.0000 8 7.1269 |
| 150 0.2585 14.9525 1.8466 0.0000 13 7.4679 |
| 151 0.2197 15.2122 4.1736 0.0000 8 7.7812 |
| 152 0.2575 15.6204 3.3240 0.0000 8 8.1593 |
| 153 0.2561 15.2122 5.2447 0.0000 13 7.7046 |
| 154 0.2568 15.6946 4.2844 0.0000 8 8.1060 |
| 155 0.3319 15.8801 3.1024 0.0000 13 8.3425 |
| 156 0.2201 15.8430 3.6565 0.0000 8 8.2998 |
| 157 0.2558 15.8801 5.5771 0.0000 13 8.1506 |
| 158 0.4079 15.8801 0.6276 0.0000 13 8.0025 |
| 159 0.2585 0.0000 1.9205 0.0000 13 8.2992 |
| 160 0.3678 0.0000 4.6906 0.0000 8 8.3079 |
| 161 0.2580 0.3339 2.6223 0.0000 17 8.1646 |
| 162 0.2562 0.3710 5.1339 0.0000 17 8.0761 |
| 163 0.2585 0.4081 1.8835 0.0000 17 7.9851 |
| 164 0.2562 15.6946 5.1339 0.0000 13 8.0761 |
| 165 0.2585 15.6575 1.8835 0.0000 13 7.9851 |
| 166 0.2580 15.7317 2.6223 0.0000 13 8.1646 |
| 167 0.3703 0.0000 1.2555 0.0000 13 8.1736 |
| 168 0.5550 15.8430 2.5112 0.0000 13 8.0400 |
| 169 0.3695 0.0000 2.4375 0.0000 13 8.3100 |
| 170 0.5550 0.2226 2.5112 0.0000 17 8.0400 |
| 171 0.4454 0.0000 0.1105 0.0000 13 8.1573 |
| 172 0.4057 0.0000 3.6933 0.0000 8 8.3486 |
| 173 0.6291 0.0000 2.7697 0.0000 18 8.2006 |
| 174 0.7384 0.5194 5.5768 0.0000 17 7.5904 |
| 175 0.4812 0.5936 1.8464 0.0000 17 7.6967 |

	176	0.4812	15.4720	1.8464	0.0000	13	7.6967	
	177	0.7384	15.5462	5.5768	0.0000	13	7.5904	
	178	0.4812	0.1855	1.8834	0.0000	17	8.0124	
	179	0.7025	0.5565	3.9147	0.0000	12	7.7078	
	180	0.5905	0.7421	4.8382	0.0000	12	7.5957	
	181	0.7019	1.1873	4.7273	0.0000	12	7.1883	
	182	0.7019	14.8783	4.7273	0.0000	8	7.1883	
	183	0.5905	15.3235	4.8382	0.0000	8	7.5957	
	184	0.4812	15.8801	1.8834	0.0000	13	8.0124	
	185	0.7025	15.5091	3.9147	0.0000	8	7.7078	
	186	0.5559	0.2226	1.2924	0.0000	17	7.8859	
	187	6.7174	5.4541	1.8789	8.2941	18	0.0224	
	188	0.5173	0.9276	3.2500	0.0000	12	7.6489	
	189	0.5173	15.1380	3.2500	0.0000	8	7.6489	
	190	6.7174	10.6115	1.8789	8.2941	10	0.0224	
	191	0.5559	15.8430	1.2924	0.0000	13	7.8859	
	192	0.7036	15.9914	2.4003	0.0000	13	8.0441	
	193	0.6309	0.0000	0.2581	0.0000	13	8.0313	
	194	0.8521	0.2226	2.3633	0.0000	17	7.8329	
	195	0.5929	0.7050	1.4770	0.0000	17	7.5032	
	196	0.5918	0.7421	2.9914	0.0000	17	7.7417	
	197	0.5918	15.3235	2.9914	0.0000	13	7.7417	
	198	0.5929	15.3606	1.4770	0.0000	13	7.5032	
	199	0.8521	15.8430	2.3633	0.0000	13	7.8329	
	200	0.6303	0.0000	1.0707	0.0000	13	8.0079	
	201	0.6289	0.0000	3.0283	0.0000	18	8.2328	
	202	0.6654	15.9914	3.8778	0.0000	8	8.1108	
	203	0.6682	15.8801	-0.0005	0.0000	13	7.8872	
	204	0.6654	0.0742	3.8778	0.0000	12	8.1108	
	205	0.6682	0.1855	-0.0005	0.0000	17	7.8872	
	206	0.8165	0.5194	0.1841	0.0000	17	7.5155	
	207	0.5912	0.2597	3.7301	0.0000	12	8.0278	
	208	0.8140	0.5194	3.6561	0.0000	12	7.6986	
	209	0.8146	0.5936	2.8435	0.0000	17	7.6752	
	210	0.8146	15.4720	2.8435	0.0000	13	7.6752	
	211	0.8165	15.5462	0.1841	0.0000	13	7.5155	
	212	0.8140	15.5462	3.6561	0.0000	8	7.6986	
	213	0.5912	15.8059	3.7301	0.0000	8	8.0278	
	214	0.6305	0.0000	0.7383	0.0000	13	8.0075	
	215	0.7040	0.0000	1.8093	0.0000	13	8.0136	
	216	0.7027	0.0000	3.5823	0.0000	8	8.1834	
	217	0.6274	0.0000	5.0228	0.0000	13	8.1497	
	218	0.7036	0.0742	2.4003	0.0000	17	8.0441	
	219	0.6280	0.4452	4.2841	0.0000	12	7.8107	
	220	0.7019	0.4823	4.7273	0.0000	12	7.7226	
	221	0.6286	0.7421	3.3607	0.0000	12	7.6926	
	222	0.6298	0.7050	1.6986	0.0000	17	7.4996	
	223	0.6298	15.3606	1.6986	0.0000	13	7.4996	
	224	0.6286	15.3235	3.3607	0.0000	8	7.6926	
	225	0.7019	15.5833	4.7273	0.0000	8	7.7226	
	226	0.6280	15.6204	4.2841	0.0000	8	7.8107	
	227	0.6279	0.0000	4.3949	0.0000	8	8.1546	
	228	0.8156	0.1855	1.5138	0.0000	17	7.7707	
	229	0.5917	0.3710	3.1391	0.0000	12	8.0372	
	230	0.7039	0.3339	1.9202	0.0000	17	7.7643	
	231	0.8905	0.4823	0.5534	0.0000	17	7.4730	
	232	0.5917	15.6946	3.1391	0.0000	8	8.0372	
	233	0.8905	15.5833	0.5534	0.0000	13	7.4730	
	234	0.8156	15.8801	1.5138	0.0000	13	7.7707	
	235	0.7039	15.7317	1.9202	0.0000	13	7.7643	
	236	0.8531	0.5565	0.9228	0.0000	17	7.4297	
	237	0.7785	0.4823	1.3661	0.0000	17	7.5486	
	238	0.8531	15.5091	0.9228	0.0000	13	7.4297	
	239	0.7785	15.5833	1.3661	0.0000	13	7.5486	
	240	0.8896	0.1855	1.8461	0.0000	17	7.7602	
	241	0.8896	15.8801	1.8461	0.0000	13	7.7602	
	242	0.8886	0.5194	3.2128	0.0000	15	7.7176	
	243	0.8886	15.5462	3.2128	0.0000	7	7.7176	
	244	0.8161	0.2226	0.7751	0.0000	17	7.7174	
	245	0.7773	0.1484	3.0282	0.0000	18	8.0253	
	246	0.9248	0.4081	4.5055	0.0000	12	7.6465	
	247	1.2619	0.9647	0.2576	0.0000	17	6.8861	
	248	0.9252	1.1131	3.9145	0.0000	12	7.1419	
	249	0.9252	14.9525	3.9145	0.0000	8	7.1419	
	250	1.2619	15.1009	0.2576	0.0000	13	6.8861	
	251	0.9248	15.6575	4.5055	0.0000	8	7.6465	
	252	0.8161	15.8430	0.7751	0.0000	13	7.7174	
	253	0.7773	15.9172	3.0282	0.0000	10	8.0253	
	254	0.8500	0.1855	5.2443	0.0000	17	7.8329	
	255	0.9251	0.0000	4.0253	0.0000	8	8.0023	

	256	0.8142	0.1855	3.3975	0.0000	15	7.9827	
	257	0.8146	0.1855	2.8435	0.0000	18	7.9489	
	258	0.9246	0.2968	4.7271	0.0000	12	7.7321	
	259	0.9630	0.4452	2.9172	0.0000	18	7.6776	
	260	1.2224	0.9276	3.5080	0.0000	12	7.1550	
	261	1.1844	0.8905	4.7269	0.0000	12	7.1027	
	262	0.9645	1.2244	0.8488	0.0000	17	6.8451	
	263	0.9645	14.8412	0.8488	0.0000	13	6.8451	
	264	1.2224	15.1380	3.5080	0.0000	8	7.1550	
	265	1.1844	15.1751	4.7269	0.0000	8	7.1027	
	266	0.9630	15.6204	2.9172	0.0000	10	7.6776	
	267	0.8146	15.8801	2.8435	0.0000	10	7.9489	
	268	0.8142	15.8801	3.3975	0.0000	7	7.9827	
	269	0.9246	15.7688	4.7271	0.0000	8	7.7321	
	270	0.8500	15.8801	5.2443	0.0000	13	7.8329	
	271	1.4083	0.8163	3.1016	0.0000	18	7.1332	
	272	1.2220	0.1855	4.0621	0.0000	12	7.6779	
	273	1.1840	0.2226	5.3918	0.0000	17	7.5869	
	274	1.1121	0.8163	2.0676	0.0000	17	7.1614	
	275	1.1121	15.2493	2.0676	0.0000	13	7.1614	
	276	1.4083	15.2493	3.1016	0.0000	10	7.1332	
	277	1.1840	15.8430	5.3918	0.0000	13	7.5869	
	278	1.2220	15.8801	4.0621	0.0000	8	7.6779	
	279	0.9997	0.4081	3.5451	0.0000	12	7.6896	
	280	0.9997	15.6575	3.5451	0.0000	8	7.6896	
	281	1.2250	0.2226	-0.0009	0.0000	17	7.5309	
	282	1.2250	15.8430	-0.0009	0.0000	13	7.5309	
	283	1.1846	0.1855	4.5792	0.0000	12	7.6717	
	284	1.0391	0.0000	0.3686	0.0000	13	7.7839	
	285	1.0388	0.0000	0.8118	0.0000	13	7.7665	
	286	1.3353	15.8801	1.4026	0.0000	13	7.4628	
	287	1.0377	0.0000	2.2893	0.0000	18	7.8630	
	288	1.0373	0.0000	2.9172	0.0000	18	7.9209	
	289	1.1846	15.8801	4.5792	0.0000	8	7.6717	
	290	1.0378	0.4081	2.1415	0.0000	17	7.5382	
	291	1.2246	0.9647	0.5532	0.0000	17	6.8879	
	292	1.2246	15.1009	0.5532	0.0000	13	6.8879	
	293	1.0378	15.6575	2.1415	0.0000	13	7.5382	
	294	1.1855	15.8430	3.3234	0.0000	7	7.6885	
	295	1.0741	0.3339	3.2496	0.0000	15	7.6985	
	296	1.2227	0.9647	3.2125	0.0000	15	7.1771	
	297	1.2227	15.1009	3.2125	0.0000	7	7.1771	
	298	1.0741	15.7317	3.2496	0.0000	7	7.6985	
	299	1.3346	15.9172	2.3629	0.0000	10	7.5515	
	300	1.3346	0.1484	2.3629	0.0000	18	7.5515	
	301	1.1855	0.2226	3.3234	0.0000	15	7.6885	
	302	1.0751	0.0000	1.8830	0.0000	13	7.8076	
	303	1.1875	0.2226	0.5163	0.0000	17	7.5081	
	304	1.3353	0.1855	1.4026	0.0000	17	7.4628	
	305	1.1857	0.2226	2.9171	0.0000	18	7.6622	
	306	1.1875	15.8430	0.5163	0.0000	13	7.5081	
	307	1.1857	15.8430	2.9171	0.0000	10	7.6622	
	308	1.3729	0.0742	0.7008	0.0000	17	7.5207	
	309	1.2608	0.1855	1.7351	0.0000	17	7.5339	
	310	1.2606	0.1484	2.0675	0.0000	18	7.5912	
	311	1.1873	0.2226	0.8117	0.0000	17	7.4990	
	312	1.2215	0.2226	4.8377	0.0000	12	7.6195	
	313	1.3326	0.7792	5.1331	0.0000	17	7.1017	
	314	1.4101	0.8163	0.6269	0.0000	17	6.8910	
	315	6.7532	5.4912	3.7257	11.6431	15	0.0179	
	316	6.7532	10.5744	3.7257	11.6431	7	0.0179	
	317	1.4101	15.2493	0.6269	0.0000	13	6.8910	
	318	1.3326	15.2864	5.1331	0.0000	13	7.1017	
	319	1.1873	15.8430	0.8117	0.0000	13	7.4990	
	320	1.2606	15.9172	2.0675	0.0000	10	7.5912	
	321	1.2215	15.8430	4.8377	0.0000	8	7.6195	
	322	1.2608	15.8801	1.7351	0.0000	13	7.5339	
	323	1.3729	15.9914	0.7008	0.0000	13	7.5207	
	324	1.5925	0.5194	5.1699	0.0000	17	7.1574	
	325	1.5925	15.5462	5.1699	0.0000	13	7.1574	
	326	1.6675	15.9543	4.0248	0.0000	7	7.4216	
	327	1.5929	0.4823	4.5420	0.0000	12	7.1978	
	328	1.5929	15.5833	4.5420	0.0000	8	7.1978	
	329	1.7409	0.0000	5.2067	0.0000	13	7.5072	
	330	1.5184	0.5194	4.9483	0.0000	12	7.2094	
	331	1.5184	15.5462	4.9483	0.0000	8	7.2094	
	332	1.6331	15.8801	0.1835	0.0000	13	7.3197	
	333	1.3348	0.0000	2.1044	0.0000	18	7.6440	
	334	1.3701	0.0000	4.6160	0.0000	8	7.7218	
	335	1.6331	0.1855	0.1835	0.0000	17	7.3197	

	336	1.4466	0.0000	1.4764	0.0000	13	7.5629	
	337	1.4452	0.0000	3.4340	0.0000	7	7.6557	
	338	1.6675	0.1113	4.0248	0.0000	15	7.4216	
	339	1.5935	0.5936	3.6924	0.0000	15	7.1262	
	340	1.5935	15.4720	3.6924	0.0000	7	7.1262	
	341	1.5936	0.1855	3.5816	0.0000	15	7.4149	
	342	1.5936	15.8801	3.5816	0.0000	7	7.4149	
	343	1.8535	0.4452	3.5076	0.0000	15	7.0496	
	344	1.8535	15.6204	3.5076	0.0000	7	7.0496	
	345	2.0026	0.0000	2.5841	0.0000	18	7.2216	
	346	2.0036	0.0000	1.1805	0.0000	18	7.2204	
	347	2.0777	0.0000	1.3651	0.0000	18	7.1567	
	348	1.7787	0.0000	4.2833	0.0000	7	7.4425	
	349	2.1145	0.0000	1.8822	0.0000	18	7.1144	
	350	2.1879	0.0000	2.9902	0.0000	18	7.1541	
	351	1.7406	0.0000	5.5760	0.0000	13	7.4501	
	352	2.1896	0.0000	0.7002	0.0000	18	7.1639	
	353	1.7445	0.0000	0.1834	0.0000	13	7.4208	
	354	2.0017	15.6575	3.8768	0.0000	7	6.9722	
	355	2.0017	0.4081	3.8768	0.0000	15	6.9722	
	356	2.4498	0.0000	0.1091	0.0000	13	7.1010	
	357	2.4102	0.0000	3.6549	0.0000	7	7.0150	
	358	2.6324	0.0000	4.2827	0.0000	7	6.9009	
	359	8.2372	5.0089	4.7219	8.3306	16	0.0241	
	360	2.4089	0.0000	5.3909	0.0000	13	7.1672	
	361	8.2372	11.0567	4.7219	8.3306	4	0.0241	
	362	2.8919	0.0000	4.7996	0.0000	7	6.8106	
	363	8.2400	10.9454	0.9175	11.7029	9	0.0165	
	364	8.2400	5.1202	0.9175	11.7029	21	0.0165	
	365	9.7612	5.4170	1.8767	8.3162	22	0.0138	
	366	9.7612	10.6486	1.8767	8.3162	6	0.0138	
	367	10.8012	6.5672	0.9157	11.7268	23	0.0107	
	368	9.7228	5.4912	3.7236	11.6359	19	0.0217	
	369	10.8012	9.4984	0.9157	11.7268	5	0.0107	
	370	9.7228	10.5744	3.7236	11.6359	3	0.0217	
	371	11.2831	8.0514	1.8757	8.3518	2	0.0227	
	372	13.6197	0.0000	4.6442	0.0000	3	6.7951	
	373	14.2535	0.0000	0.7285	0.0000	6	7.1362	
	374	14.2519	0.0000	3.0185	0.0000	6	7.1317	
	375	14.4357	0.3710	5.5300	0.0000	20	7.1550	
	376	14.4357	15.6946	5.5300	0.0000	1	7.1550	
	377	14.5110	0.4081	3.9787	0.0000	19	6.9905	
	378	14.5110	15.6575	3.9787	0.0000	3	6.9905	
	379	14.4760	0.0000	1.1347	0.0000	6	7.2253	
	380	14.4749	0.0000	2.6490	0.0000	6	7.2261	
	381	14.4362	0.8905	4.7544	0.0000	20	6.6644	
	382	14.4362	15.1751	4.7544	0.0000	1	6.6644	
	383	14.7702	0.4823	4.8650	0.0000	20	7.1898	
	384	14.7702	15.5833	4.8650	0.0000	1	7.1898	
	385	14.8108	0.1484	0.1372	0.0000	22	7.5091	
	386	14.8822	15.9543	4.0892	0.0000	3	7.4656	
	387	14.7698	0.1113	5.4559	0.0000	20	7.5390	
	388	14.7698	15.9543	5.4559	0.0000	1	7.5390	
	389	14.9926	0.0000	5.3080	0.0000	1	7.7374	
	390	14.8822	0.1113	4.0892	0.0000	19	7.4656	
	391	14.8467	0.3710	1.7623	0.0000	22	7.1707	
	392	14.8467	15.6946	1.7623	0.0000	6	7.1707	
	393	14.8108	15.9172	0.1372	0.0000	6	7.5091	
	394	14.9939	0.0000	3.4982	0.0000	3	7.6189	
	395	14.9222	0.7050	0.0263	0.0000	20	7.1515	
	396	14.9222	15.3606	0.0263	0.0000	1	7.1515	
	397	14.9962	0.0000	0.3217	0.0000	6	7.6989	
	398	15.0332	0.8163	0.5802	0.0000	22	7.1238	
	399	14.9940	0.8163	3.3874	0.0000	19	7.0589	
	400	15.0332	15.2493	0.5802	0.0000	6	7.1238	
	401	14.9940	15.2493	3.3874	0.0000	3	7.0589	
	402	15.0302	0.0000	4.6432	0.0000	3	7.6937	
	403	15.0692	1.4841	2.0207	0.0000	22	6.6146	
	404	15.0692	14.5815	2.0207	0.0000	6	6.6146	
	405	15.1074	0.0000	0.6171	0.0000	6	7.7211	
	406	15.1807	15.8430	1.8359	0.0000	6	7.5128	
	407	15.2157	0.8534	4.8277	0.0000	20	7.1430	
	408	15.2157	15.2122	4.8277	0.0000	1	7.1430	
	409	15.1056	0.0371	3.1287	0.0000	22	7.6901	
	410	15.1807	0.2226	1.8359	0.0000	22	7.5128	
	411	15.2171	15.8801	2.9070	0.0000	6	7.6333	
	412	15.2154	0.2226	5.3079	0.0000	20	7.6749	
	413	15.2154	15.8430	5.3079	0.0000	1	7.6749	
	414	15.2171	0.1855	2.9070	0.0000	22	7.6333	
	415	15.2922	0.7792	1.7250	0.0000	22	7.2263	

	416	15.2175	0.8163	2.3530	0.0000	22	7.1588	
	417	15.2928	1.9294	0.8755	0.0000	23	6.4556	
	418	15.2928	14.1362	0.8755	0.0000	5	6.4556	
	419	15.2922	15.2864	1.7250	0.0000	6	7.2263	
	420	15.2175	15.2493	2.3530	0.0000	6	7.1588	
	421	15.1056	16.0285	3.1287	0.0000	6	7.6901	
	422	15.2534	0.2226	4.0890	0.0000	19	7.6505	
	423	15.2188	0.9647	0.4693	0.0000	23	7.1466	
	424	15.2188	15.1009	0.4693	0.0000	5	7.1466	
	425	15.2534	15.8430	4.0890	0.0000	3	7.6505	
	426	15.5158	0.4452	0.5060	0.0000	22	7.7349	
	427	15.5158	15.6204	0.5060	0.0000	6	7.7349	
	428	15.3663	0.0000	1.8727	0.0000	6	7.8007	
	429	15.2557	0.1855	0.8386	0.0000	22	7.6642	
	430	15.5138	0.4452	3.2762	0.0000	19	7.6996	
	431	15.3266	0.4452	5.5294	0.0000	20	7.5792	
	432	15.3266	15.6204	5.5294	0.0000	1	7.5792	
	433	15.5138	15.6204	3.2762	0.0000	3	7.6996	
	434	15.2557	15.8801	0.8386	0.0000	6	7.6642	
	435	15.2157	0.1855	4.7908	0.0000	20	7.6828	
	436	15.2919	0.8163	2.0575	0.0000	22	7.2026	
	437	15.6268	1.3728	0.9492	0.0000	23	7.0890	
	438	15.6268	14.6928	0.9492	0.0000	5	7.0890	
	439	15.2919	15.2493	2.0575	0.0000	6	7.2026	
	440	15.2157	15.8801	4.7908	0.0000	1	7.6828	
	441	15.3295	0.0000	1.4295	0.0000	6	7.7875	
	442	15.5499	0.2597	4.6797	0.0000	20	7.8170	
	443	15.6626	1.4099	2.7959	0.0000	22	7.1985	
	444	15.5900	1.3728	0.5798	0.0000	23	7.0717	
	445	15.4395	1.1502	3.3132	0.0000	20	7.1892	
	446	15.5900	14.6928	0.5798	0.0000	5	7.0717	
	447	15.4395	14.9154	3.3132	0.0000	1	7.1892	
	448	15.6626	14.6557	2.7959	0.0000	6	7.1985	
	449	15.5499	15.8059	4.6797	0.0000	1	7.8170	
	450	15.5519	0.1855	1.8726	0.0000	22	7.8099	
	451	15.5151	1.2615	1.5033	0.0000	22	7.1148	
	452	15.5519	1.0389	1.9095	0.0000	22	7.2664	
	453	15.5516	1.2244	2.3158	0.0000	22	7.1689	
	454	15.5519	15.0267	1.9095	0.0000	6	7.2664	
	455	15.5516	14.8412	2.3158	0.0000	6	7.1689	
	456	15.5151	14.8041	1.5033	0.0000	6	7.1148	
	457	15.5519	15.8801	1.8726	0.0000	6	7.8099	
	458	15.5881	1.3728	3.1653	0.0000	20	7.1528	
	459	15.5881	14.6928	3.1653	0.0000	1	7.1528	
	460	15.4045	0.0000	0.3953	0.0000	6	7.9686	
	461	15.6991	0.0000	3.6085	0.0000	3	8.1214	
	462	15.6265	0.2226	1.4293	0.0000	22	7.8541	
	463	15.5497	0.3339	4.9383	0.0000	20	7.7609	
	464	15.6244	1.1131	4.2734	0.0000	20	7.2145	
	465	15.6244	14.9525	4.2734	0.0000	1	7.2145	
	466	15.6265	15.8430	1.4293	0.0000	6	7.8541	
	467	15.5497	15.7317	4.9383	0.0000	1	7.7609	
	468	15.7349	0.0000	5.5291	0.0000	1	8.1768	
	469	15.7758	0.0000	0.2103	0.0000	1	8.2386	
	470	15.5887	0.2226	2.3527	0.0000	22	7.8266	
	471	15.5887	15.8430	2.3527	0.0000	6	7.8266	
	472	15.5866	0.0000	5.2337	0.0000	1	8.0648	
	473	15.6629	0.5194	2.3896	0.0000	22	7.6922	
	474	15.6636	0.5194	1.3924	0.0000	22	7.6919	
	475	15.7355	0.4823	4.6796	0.0000	20	7.7552	
	476	15.6240	0.5936	4.8643	0.0000	20	7.6001	
	477	15.7752	1.5954	1.0968	0.0000	23	7.0344	
	478	15.7752	14.4702	1.0968	0.0000	5	7.0344	
	479	15.7355	15.5833	4.6796	0.0000	1	7.7552	
	480	15.6240	15.4720	4.8643	0.0000	1	7.6001	
	481	15.6636	15.5462	1.3924	0.0000	6	7.6919	
	482	15.6629	15.5462	2.3896	0.0000	6	7.6922	
	483	15.6253	0.1855	3.0176	0.0000	22	7.9458	
	484	15.5519	0.5936	1.8357	0.0000	22	7.5430	
	485	15.6612	1.1873	4.7166	0.0000	20	7.1703	
	486	15.6612	14.8783	4.7166	0.0000	1	7.1703	
	487	15.5519	15.4720	1.8357	0.0000	6	7.5430	
	488	15.6253	15.8801	3.0176	0.0000	6	7.9458	
	489	15.6640	0.2226	0.8753	0.0000	22	7.9335	
	490	15.6989	0.5194	3.9409	0.0000	20	7.7416	
	491	16.0352	1.0018	0.8381	0.0000	23	7.6393	
	492	16.0352	15.0638	0.8381	0.0000	5	7.6393	
	493	15.6989	15.5462	3.9409	0.0000	1	7.7416	
	494	15.6640	15.8430	0.8753	0.0000	6	7.9335	
	495	15.7374	0.0000	2.0202	0.0000	6	8.0731	

	496	15.8497	0.0000	0.7643	0.0000	6	8.2321	
	497	15.7376	0.0000	1.7617	0.0000	6	8.0730	
	498	15.8096	0.7421	4.8273	0.0000	20	7.6037	
	499	15.8096	15.3235	4.8273	0.0000	1	7.6037	
	500	15.8481	0.0000	3.0174	0.0000	6	8.2326	
	501	15.8099	0.0000	4.4210	0.0000	1	8.1860	
	502	15.8095	0.0000	5.0120	0.0000	1	8.1862	
	503	15.8469	0.7421	4.6056	0.0000	20	7.6279	
	504	15.8469	15.3235	4.6056	0.0000	1	7.6279	
	505	15.8864	15.8430	1.2814	0.0000	6	8.0601	
	506	15.8864	0.2226	1.2814	0.0000	22	8.0601	
	507	15.8483	0.0000	2.7219	0.0000	6	8.1974	
	508	15.9979	0.9647	1.1705	0.0000	23	7.6448	
	509	15.9979	15.1009	1.1705	0.0000	5	7.6448	
	510	15.8849	0.0000	3.3867	0.0000	3	8.2658	
	511	15.8856	0.2226	2.4633	0.0000	22	8.0577	
	512	15.8856	15.8430	2.4633	0.0000	6	8.0577	
	513	15.8501	0.3710	0.1733	0.0000	20	7.9892	
	514	15.8836	0.2968	5.2335	0.0000	20	8.0096	
	515	15.9596	0.2226	2.7957	0.0000	22	8.1446	
	516	15.8856	0.7421	2.3525	0.0000	22	7.7258	
	517	15.8856	15.3235	2.3525	0.0000	6	7.7258	
	518	15.9596	15.8430	2.7957	0.0000	6	8.1446	
	519	15.8501	15.6946	0.1733	0.0000	1	7.9892	
	520	15.8836	15.7688	5.2335	0.0000	1	8.0096	
	521	15.8843	0.2968	4.1993	0.0000	20	8.0093	
	522	15.9609	0.2226	0.9120	0.0000	22	8.1527	
	523	15.9215	0.6679	4.0885	0.0000	20	7.7571	
	524	15.8845	0.7050	4.0146	0.0000	20	7.7112	
	525	15.8845	15.3606	4.0146	0.0000	1	7.7112	
	526	15.9215	15.3978	4.0885	0.0000	1	7.7571	
	527	15.9609	15.8430	0.9120	0.0000	6	8.1527	
	528	15.8843	15.7688	4.1993	0.0000	1	8.0093	
	529	15.9948	0.4452	5.4181	0.0000	20	7.9803	
	530	15.9207	0.6679	5.2335	0.0000	20	7.7492	
	531	15.9207	15.3978	5.2335	0.0000	1	7.7492	
	532	15.9948	15.6204	5.4181	0.0000	1	7.9803	
	533	15.9961	0.0000	3.6821	0.0000	3	8.3419	
	534	15.9216	0.3710	3.9407	0.0000	20	7.9962	
	535	15.9216	15.6946	3.9407	0.0000	1	7.9962	
	536	16.0358	0.5194	0.0255	0.0000	20	7.9752	
	537	16.1074	0.5194	3.7190	0.0000	20	8.0275	
	538	16.0358	15.5462	0.0255	0.0000	1	7.9752	
	539	16.1074	15.5462	3.7190	0.0000	1	8.0275	
-----+								
	Atomic Charge Difference							
-----+								
	Atom # x y z Charge							
-----+								
	Si	0	11.1853	8.0328	3.7383	-2.3734		
	C	1	10.8639	9.5493	4.7106	2.3014		
	C	2	11.2735	8.0328	1.8845	2.3518		
	Si	3	9.7094	10.5826	3.7385	-2.3641		
	C	4	8.2251	11.0390	4.7110	2.3306		
	Si	5	10.7943	9.5062	0.9133	-2.2732		
	C	6	9.7503	10.6517	1.8846	2.3162		
	Si	7	6.7550	10.5587	3.7342	-2.3569		
	C	8	5.5607	9.5807	4.7288	2.3465		
	Si	9	8.2280	10.9567	0.9168	-2.2971		
	C	10	6.7042	10.6297	1.8793	2.2941		
	Si	11	4.8974	8.0328	3.9886	-1.5590		
	C	12	5.5607	6.4849	4.7288	2.3465		
	Si	13	5.4684	9.6868	0.8986	-1.5311		
	Ga	14	4.0244	8.0328	1.8313	-0.7102		
	Si	15	6.7550	5.5069	3.7342	-2.3569		
	C	16	8.2251	5.0266	4.7110	2.3306		
	Si	17	5.4684	6.3788	0.8986	-1.5311		
	C	18	6.7042	5.4360	1.8793	2.2941		
	Si	19	9.7094	5.4830	3.7385	-2.3641		
	C	20	10.8639	6.5164	4.7106	2.3014		
	Si	21	8.2280	5.1089	0.9168	-2.2971		
	C	22	9.7503	5.4139	1.8846	2.3162		
	Si	23	10.7943	6.5594	0.9133	-2.2732		
-----+								
	Atomic Charge Volumes							
-----+								
	Atom # x y z Charge							
-----+								
	Si	0	11.1853	8.0328	3.7383	11.6266		
	C	1	10.8639	9.5493	4.7106	8.3014		

	C	2	11.2735	8.0328	1.8845	8.3518	
	Si	3	9.7094	10.5826	3.7385	11.6359	
	C	4	8.2251	11.0390	4.7110	8.3306	
	Si	5	10.7943	9.5062	0.9133	11.7268	
	C	6	9.7503	10.6517	1.8846	8.3162	
	Si	7	6.7550	10.5587	3.7342	11.6431	
	C	8	5.5607	9.5807	4.7288	8.3465	
	Si	9	8.2280	10.9567	0.9168	11.7029	
	C	10	6.7042	10.6297	1.8793	8.2941	
	Si	11	4.8974	8.0328	3.9886	12.4410	
	C	12	5.5607	6.4849	4.7288	8.3465	
	Si	13	5.4684	9.6868	0.8986	12.4689	
	Ga	14	4.0244	8.0328	1.8313	30.2898	
	Si	15	6.7550	5.5069	3.7342	11.6431	
	C	16	8.2251	5.0266	4.7110	8.3306	
	Si	17	5.4684	6.3788	0.8986	12.4689	
	C	18	6.7042	5.4360	1.8793	8.2941	
	Si	19	9.7094	5.4830	3.7385	11.6359	
	C	20	10.8639	6.5164	4.7106	8.3014	
	Si	21	8.2280	5.1089	0.9168	11.7029	
	C	22	9.7503	5.4139	1.8846	8.3162	
	Si	23	10.7943	6.5594	0.9133	11.7268	
+-----+							
	Total number of electrons: 264.2423						
+-----+							