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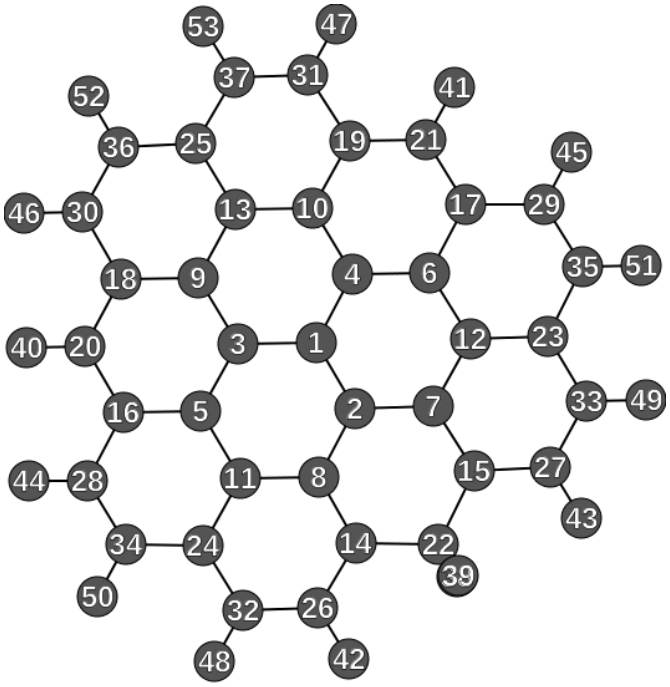

Figure 1 Type I structure as a reference to data in the tables 1.

Table 1 Partial charges for C-flake of type I system with the total charge -1e for 6-31+G(2df, p) basis set

Index	Atom	Distance	RESP	MBIS
1	C	0	-0.005659	-0.02664
2	C	1.41	-0.007322	-0.08248
3	C	1.425	-0.03109	-0.002956
4	C	1.425	-0.0227	-0.005166
5	C	2.463	-0.03727	-0.01254
6	C	2.463	-0.04991	-0.01484
7	C	2.467	-0.1015	0.01214
8	C	2.467	-0.09952	0.008184
9	C	2.468	-0.03258	-0.01359
10	C	2.468	-0.04708	-0.004081
11	C	2.846	0.06367	0.01119
12	C	2.846	0.07197	0.009711
13	C	2.856	0.02688	-0.008475
14	C	3.758	0.1177	0.03482
15	C	3.758	0.118	0.03527
16	C	3.76	0.1869	0.09588
17	C	3.76	0.2013	0.101
18	C	3.772	0.2046	0.1347
19	C	3.772	0.225	0.1276
20	C	4.245	-0.4235	-0.3552
21	C	4.245	-0.4396	-0.3523
22	C	4.35	-0.08859	-0.248
23	C	4.265	0.07891	0.08825
24	C	4.265	0.08679	0.08917
25	C	4.279	0.07832	0.03395
26	C	4.889	-0.2314	-0.2201
27	C	4.889	-0.2368	-0.2214
28	C	4.912	-0.2253	-0.2125
29	C	4.912	-0.2323	-0.2146
30	C	4.926	-0.2558	-0.2637
31	C	4.926	-0.2621	-0.2616
32	C	5.104	-0.2319	-0.2541
33	C	5.104	-0.2244	-0.2506
34	C	5.106	-0.2195	-0.2291
35	C	5.106	-0.2149	-0.2304
36	C	5.114	-0.2072	-0.188
37	C	5.114	-0.2074	-0.1964
38	H	5.097	0.0218	0.107
39	H	5.097	0.0218	0.1061
40	H	5.332	0.1324	0.1379
41	H	5.332	0.1374	0.1364
42	H	5.852	0.1111	0.1298
43	H	5.852	0.1126	0.1302
44	H	5.873	0.1164	0.1312
45	H	5.873	0.1168	0.1325
46	H	5.888	0.1179	0.1323
47	H	5.888	0.1177	0.1327
48	H	6.164	0.1145	0.1313
49	H	6.164	0.1134	0.1299
50	H	6.164	0.1099	0.1325
51	H	6.164	0.1093	0.1329
52	H	6.173	0.1119	0.1264
53	H	6.173	0.1105	0.1292

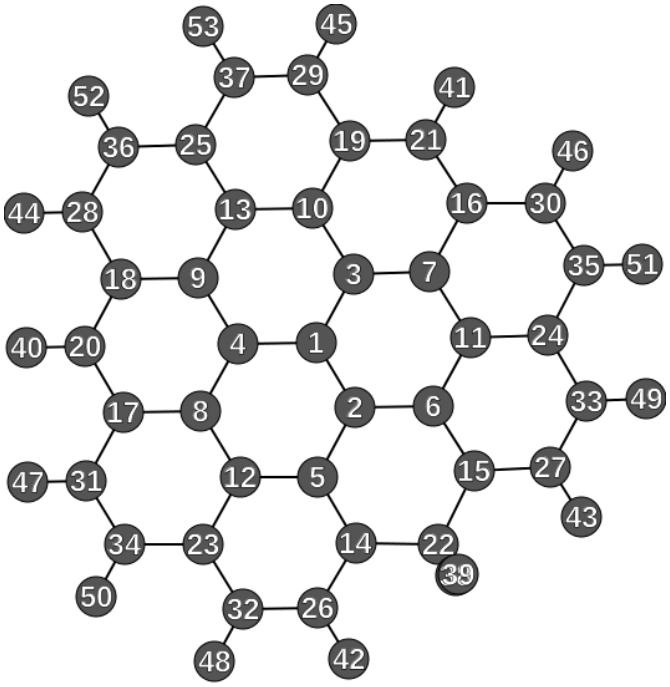

Figure 2 Type I structure as a reference to data in the tables 2.

Table 2 Partial charges for C-flake of type I system with the total charge 0e for 6-31+G(2df, p) basis set

Index	Atom	Distance	RESP	MBIS
1	C	0	-0.007898	-0.01317
2	C	1.387	0.0899	0.002553
3	C	1.438	0.002424	0.007957
4	C	1.438	-0.00221	5.739e-05
5	C	2.452	-0.1488	-0.01545
6	C	2.452	-0.1561	-0.02231
7	C	2.462	-0.06853	-0.01008
8	C	2.462	-0.06494	0.001812
9	C	2.474	-0.02799	-0.003169
10	C	2.474	-0.03915	-0.005532
11	C	2.835	0.09512	0.01852
12	C	2.835	0.08859	0.006437
13	C	2.86	0.02047	0.007775
14	C	3.737	0.1877	0.07927
15	C	3.737	0.1962	0.08385
16	C	3.769	0.2253	0.09798
17	C	3.769	0.2235	0.08372
18	C	3.77	0.1891	0.08587
19	C	3.77	0.205	0.09558
20	C	4.249	-0.3725	-0.2524
21	C	4.249	-0.3803	-0.263
22	C	4.316	-0.1466	-0.288
23	C	4.253	0.08338	0.07718
24	C	4.253	0.078	0.071
25	C	4.262	0.1428	0.07452
26	C	4.864	-0.2395	-0.2119
27	C	4.864	-0.2485	-0.2168
28	C	4.923	-0.1985	-0.1884
29	C	4.923	-0.2053	-0.1895
30	C	4.929	-0.2199	-0.1937
31	C	4.929	-0.2199	-0.1883
32	C	5.076	-0.1788	-0.1846
33	C	5.076	-0.1714	-0.178
34	C	5.11	-0.1764	-0.1888
35	C	5.11	-0.1763	-0.19
36	C	5.111	-0.2149	-0.1886
37	C	5.111	-0.2135	-0.1935
38	H	5.058	0.05968	0.1437
39	H	5.058	0.05968	0.1436
40	H	5.335	0.154	0.1492
41	H	5.335	0.1565	0.151
42	H	5.828	0.137	0.1481
43	H	5.828	0.1386	0.1484
44	H	5.884	0.1365	0.1471
45	H	5.884	0.1369	0.1472
46	H	5.889	0.1372	0.1493
47	H	5.889	0.1375	0.1482
48	H	6.137	0.1356	0.1458
49	H	6.137	0.1339	0.1442
50	H	6.165	0.1261	0.1478
51	H	6.165	0.127	0.1491
52	H	6.167	0.1379	0.1472
53	H	6.167	0.1364	0.1486

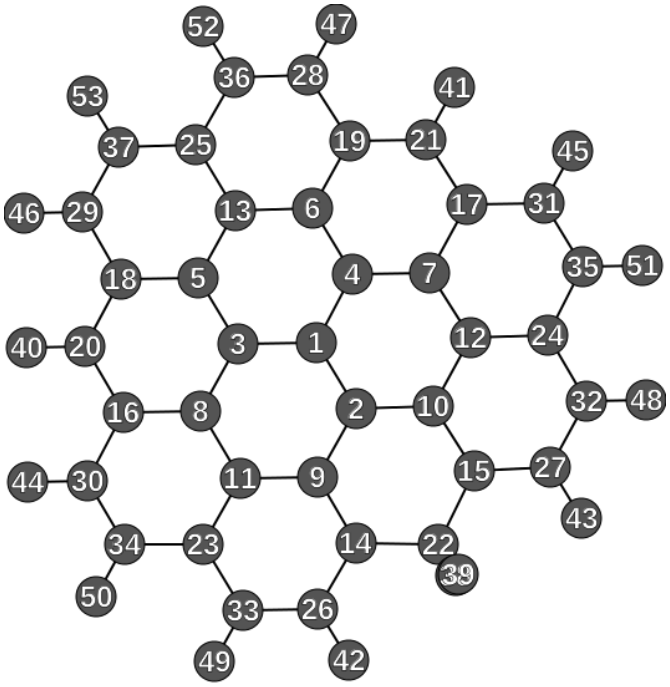

Figure 3 Type I structure as a reference to data in the tables 3.

Table 3 Partial charges for C-flake of type I system with the total charge +1e for 6-31+G(2df, p) basis set

Index	Atom	Distance	RESP	MBIS
1	C	0	0.002145	-0.002238
2	C	1.414	0.1748	0.09644
3	C	1.424	-0.0041	0.007802
4	C	1.424	0.004048	0.009364
5	C	2.459	-0.008786	0.01506
6	C	2.459	-0.02163	0.01688
7	C	2.459	-0.05252	0.005274
8	C	2.459	-0.04492	0.01138
9	C	2.463	-0.1824	-0.0601
10	C	2.463	-0.1847	-0.05529
11	C	2.839	0.08589	0.02
12	C	2.839	0.08747	0.01627
13	C	2.839	0.0178	-0.0001265
14	C	3.748	0.276	0.1514
15	C	3.748	0.2791	0.1515
16	C	3.755	0.2148	0.06923
17	C	3.755	0.2226	0.07332
18	C	3.758	0.1614	0.03646
19	C	3.758	0.1783	0.03681
20	C	4.234	-0.2872	-0.1503
21	C	4.234	-0.299	-0.1524
22	C	4.318	-0.2801	-0.3541
23	C	4.251	0.08431	0.06223
24	C	4.251	0.0872	0.06699
25	C	4.259	0.195	0.1442
26	C	4.885	-0.2491	-0.222
27	C	4.885	-0.2526	-0.2194
28	C	4.914	-0.1487	-0.1158
29	C	4.914	-0.1419	-0.1147
30	C	4.914	-0.1969	-0.1618
31	C	4.914	-0.1979	-0.1605
32	C	5.084	-0.1128	-0.1116
33	C	5.084	-0.1129	-0.1077
34	C	5.103	-0.1488	-0.1533
35	C	5.103	-0.1519	-0.1595
36	C	5.106	-0.2124	-0.2027
37	C	5.106	-0.2146	-0.2035
38	H	5.065	0.1188	0.1854
39	H	5.065	0.1188	0.1854
40	H	5.32	0.1632	0.161
41	H	5.32	0.1665	0.1621
42	H	5.848	0.1621	0.1717
43	H	5.848	0.163	0.1709
44	H	5.874	0.1595	0.1643
45	H	5.874	0.1594	0.1642
46	H	5.874	0.1545	0.1614
47	H	5.874	0.1547	0.1624
48	H	6.143	0.1492	0.1613
49	H	6.143	0.1492	0.1607
50	H	6.158	0.148	0.1641
51	H	6.158	0.1491	0.1666
52	H	6.162	0.1589	0.1704
53	H	6.162	0.1603	0.1708

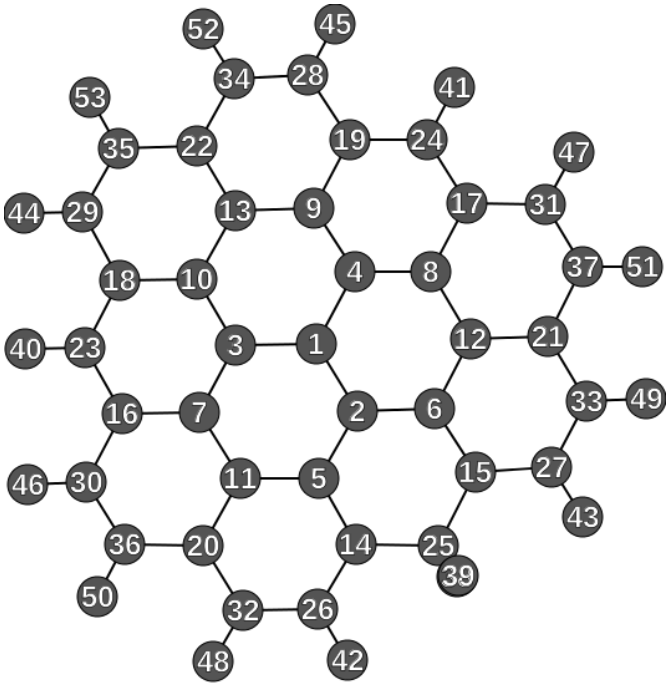

Figure 4 Type I structure as a reference to data in the tables 4.

Table 4 Partial charges for B-doped type I system with the total charge -1e for 6-31+G(2df, p) basis set

Index	Atom	Distance	RESP	MBIS
1	B	0	0.05931	0.2663
2	C	1.463	-0.1817	-0.3754
3	C	1.503	-0.1383	-0.2395
4	C	1.503	-0.1327	-0.2444
5	C	2.488	-0.01481	0.0998
6	C	2.488	-0.01909	0.09611
7	C	2.502	0.008491	0.06045
8	C	2.502	0.002717	0.06047
9	C	2.51	0.01692	0.05874
10	C	2.51	0.02488	0.05165
11	C	2.852	-0.02041	-0.04462
12	C	2.852	-0.01818	-0.04053
13	C	2.868	-0.04149	-0.004974
14	C	3.783	0.1167	0.03888
15	C	3.783	0.1244	0.04007
16	C	3.81	0.2013	0.0904
17	C	3.81	0.2072	0.09158
18	C	3.812	0.1764	0.08708
19	C	3.812	0.186	0.08372
20	C	4.27	0.1181	0.08892
21	C	4.27	0.1192	0.08653
22	C	4.272	0.1571	0.05975
23	C	4.283	-0.4029	-0.2979
24	C	4.283	-0.4103	-0.2995
25	C	4.353	-0.05887	-0.2446
26	C	4.907	-0.2376	-0.2261
27	C	4.907	-0.2467	-0.2236
28	C	4.958	-0.2167	-0.2129
29	C	4.958	-0.215	-0.2215
30	C	4.963	-0.2253	-0.2148
31	C	4.963	-0.2272	-0.2152
32	C	5.106	-0.2419	-0.2502
33	C	5.107	-0.2379	-0.2534
34	C	5.126	-0.2436	-0.2127
35	C	5.126	-0.2419	-0.203
36	C	5.127	-0.2	-0.203
37	C	5.127	-0.2019	-0.2003
38	H	5.096	0.02156	0.1134
39	H	5.096	0.02156	0.1134
40	H	5.372	0.1322	0.1307
41	H	5.372	0.1352	0.13
42	H	5.877	0.1087	0.1268
43	H	5.877	0.1108	0.1267
44	H	5.927	0.1146	0.1324
45	H	5.927	0.1138	0.1299
46	H	5.932	0.1131	0.1301
47	H	5.932	0.1129	0.1307
48	H	6.167	0.1164	0.1278
49	H	6.167	0.1159	0.1282
50	H	6.182	0.1035	0.1301
51	H	6.182	0.1044	0.1289
52	H	6.182	0.1155	0.1292
53	H	6.182	0.1157	0.1262

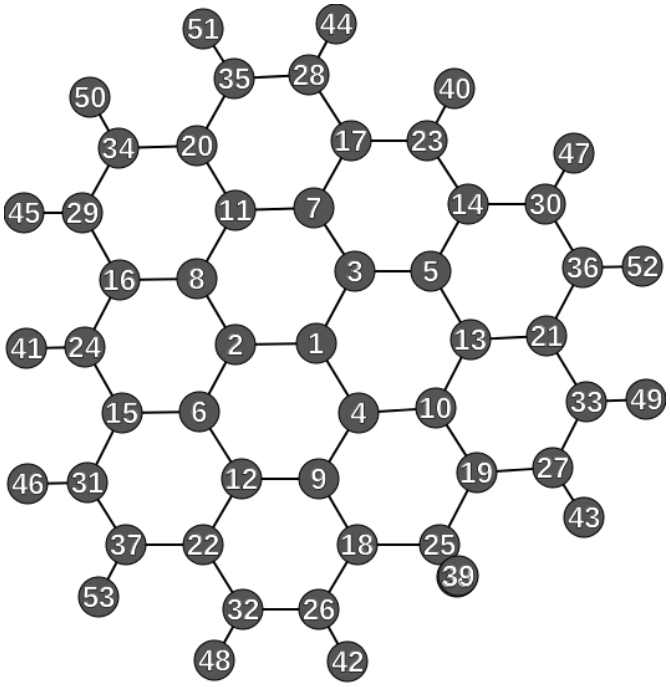

Figure 5 Type I structure as a reference to data in the tables 5.

Table 5 Partial charges for B-doped type I system with the total charge 0e for 6-31+G(2df, p) basis set

Index	Atom	Distance	RESP	MBIS
1	B	0	0.2052	0.4245
2	C	1.499	-0.2236	-0.3228
3	C	1.499	-0.2197	-0.3153
4	C	1.5	-0.02612	-0.2155
5	C	2.496	0.03476	0.08837
6	C	2.496	0.04392	0.09729
7	C	2.498	0.08036	0.09671
8	C	2.498	0.08622	0.09621
9	C	2.513	-0.09952	0.02018
10	C	2.513	-0.09871	0.02371
11	C	2.855	-0.1048	-0.05066
12	C	2.856	-0.01322	-0.01795
13	C	2.856	-0.007125	-0.01912
14	C	3.799	0.2	0.06088
15	C	3.799	0.1893	0.05014
16	C	3.8	0.1538	0.04952
17	C	3.8	0.1629	0.0519
18	C	3.802	0.2268	0.1076
19	C	3.802	0.2224	0.1095
20	C	4.254	0.2217	0.1104
21	C	4.262	0.1351	0.07898
22	C	4.262	0.1409	0.07352
23	C	4.267	-0.3334	-0.2044
24	C	4.267	-0.3245	-0.1966
25	C	4.368	-0.2096	-0.3066
26	C	4.931	-0.2579	-0.2291
27	C	4.931	-0.2579	-0.2326
28	C	4.948	-0.1819	-0.1744
29	C	4.948	-0.1801	-0.1711
30	C	4.953	-0.2101	-0.1774
31	C	4.954	-0.2043	-0.1754
32	C	5.108	-0.1716	-0.1554
33	C	5.108	-0.1682	-0.156
34	C	5.113	-0.2412	-0.2046
35	C	5.113	-0.2428	-0.2023
36	C	5.122	-0.2026	-0.1991
37	C	5.122	-0.2061	-0.1967
38	H	5.113	0.08233	0.1536
39	H	5.113	0.08232	0.1529
40	H	5.355	0.1477	0.1437
41	H	5.355	0.145	0.1411
42	H	5.903	0.1393	0.1505
43	H	5.903	0.1399	0.1514
44	H	5.917	0.1343	0.1466
45	H	5.917	0.1347	0.1461
46	H	5.92	0.1366	0.1471
47	H	5.92	0.1372	0.1465
48	H	6.165	0.1336	0.1421
49	H	6.165	0.1333	0.1425
50	H	6.167	0.1381	0.1467
51	H	6.167	0.1381	0.1467
52	H	6.176	0.1293	0.1471
53	H	6.176	0.1299	0.147

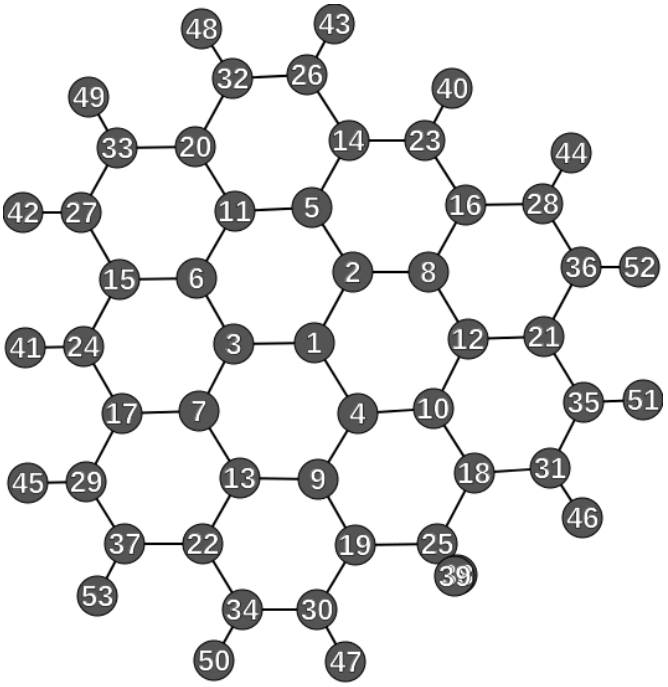

Figure 6 Type I structure as a reference to data in the tables 6.

Table 6 Partial charges for B-doped type I system with the total charge +1e for 6-31+G(2df, p) basis set

Index	Atom	Distance	RESP	MBIS
1	B	0	0.2261	0.4441
2	C	1.486	-0.2527	-0.3547
3	C	1.486	-0.2482	-0.3566
4	C	1.536	0.1215	-0.04159
5	C	2.481	0.1316	0.1358
6	C	2.481	0.1248	0.1421
7	C	2.492	0.03995	0.1033
8	C	2.492	0.04863	0.1083
9	C	2.526	-0.1585	-0.0415
10	C	2.526	-0.1595	-0.03821
11	C	2.837	-0.152	-0.09074
12	C	2.857	0.007496	-0.004253
13	C	2.857	0.01192	0.006443
14	C	3.786	0.133	0.01688
15	C	3.786	0.1434	0.01454
16	C	3.787	0.193	0.03418
17	C	3.787	0.2032	0.03797
18	C	3.818	0.3359	0.2058
19	C	3.818	0.3313	0.2052
20	C	4.239	0.2921	0.173
21	C	4.256	0.1219	0.0557
22	C	4.256	0.1194	0.05044
23	C	4.253	-0.2581	-0.1149
24	C	4.253	-0.2674	-0.1194
25	C	4.365	-0.3536	-0.3805
26	C	4.937	-0.1324	-0.1163
27	C	4.937	-0.136	-0.1211
28	C	4.942	-0.1825	-0.137
29	C	4.942	-0.1871	-0.1435
30	C	4.952	-0.2843	-0.2645
31	C	4.952	-0.2863	-0.2647
32	C	5.103	-0.2473	-0.2134
33	C	5.103	-0.2472	-0.2045
34	C	5.108	-0.07353	-0.04368
35	C	5.108	-0.07401	-0.04573
36	C	5.118	-0.1858	-0.1831
37	C	5.118	-0.1842	-0.178
38	H	5.118	0.1478	0.2046
39	H	5.118	0.1478	0.2044
40	H	5.34	0.1572	0.1533
41	H	5.34	0.1597	0.1546
42	H	5.906	0.1525	0.161
43	H	5.906	0.1524	0.16
44	H	5.908	0.1577	0.1611
45	H	5.908	0.1583	0.1625
46	H	5.926	0.1685	0.1783
47	H	5.926	0.1686	0.1783
48	H	6.156	0.1604	0.1679
49	H	6.156	0.1601	0.1661
50	H	6.163	0.1471	0.1578
51	H	6.163	0.147	0.1587
52	H	6.172	0.1501	0.1636
53	H	6.172	0.1501	0.1629

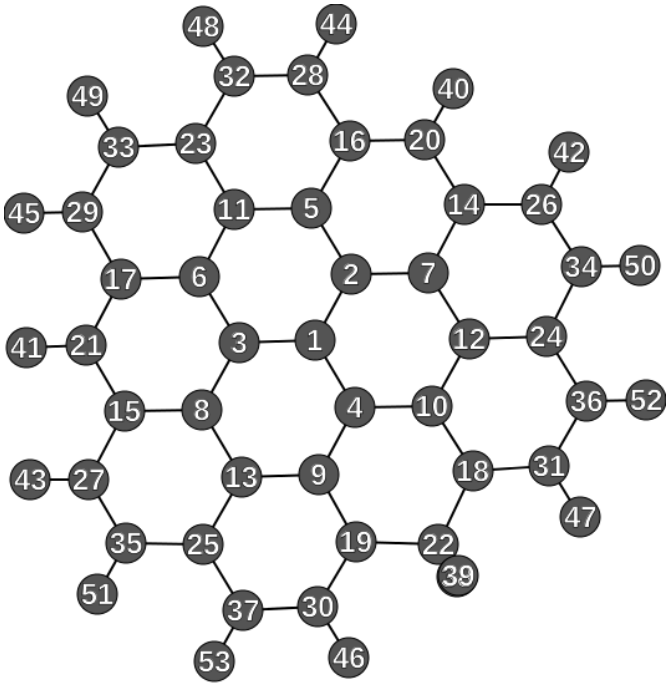

Figure 7 Type I structure as a reference to data in the tables 7.

Table 7 Partial charges for N-doped type I system with the total charge -1e for 6-31+G(2df, p) basis set

Index	Atom	Distance	RESP	MBIS
1	N	0	0.1403	-0.09866
2	C	1.385	0.02683	0.1983
3	C	1.385	0.02759	0.1919
4	C	1.438	-0.123	-0.09038
5	C	2.43	-0.1016	-0.1034
6	C	2.43	-0.103	-0.1041
7	C	2.436	-0.06359	-0.09681
8	C	2.436	-0.06763	-0.09012
9	C	2.477	-0.0643	-0.001328
10	C	2.477	-0.06507	-0.00445
11	C	2.833	0.09953	0.0711
12	C	2.861	0.05727	0.02262
13	C	2.861	0.05937	0.01827
14	C	3.72	0.197	0.1368
15	C	3.72	0.2025	0.1336
16	C	3.739	0.2406	0.1595
17	C	3.739	0.242	0.1669
18	C	3.779	0.05077	0.001997
19	C	3.779	0.05115	-0.008817
20	C	4.218	-0.4515	-0.3847
21	C	4.218	-0.454	-0.3873
22	C	4.393	-0.02297	-0.2198
23	C	4.241	0.0362	-0.01021
24	C	4.267	0.108	0.09883
25	C	4.267	0.1052	0.107
26	C	4.882	-0.2304	-0.2347
27	C	4.882	-0.2344	-0.2315
28	C	4.894	-0.2815	-0.2722
29	C	4.894	-0.2784	-0.2778
30	C	4.905	-0.1987	-0.1753
31	C	4.905	-0.1931	-0.1786
32	C	5.08	-0.1853	-0.1751
33	C	5.08	-0.1898	-0.17
34	C	5.09	-0.2092	-0.1916
35	C	5.09	-0.2077	-0.1997
36	C	5.132	-0.2927	-0.3394
37	C	5.132	-0.2871	-0.3429
38	H	5.142	-0.00296	0.08466
39	H	5.143	-0.002961	0.08455
40	H	5.304	0.1403	0.1438
41	H	5.304	0.142	0.1442
42	H	5.835	0.1183	0.134
43	H	5.835	0.1185	0.1342
44	H	5.853	0.1239	0.139
45	H	5.853	0.1225	0.1399
46	H	5.866	0.1085	0.1266
47	H	5.866	0.107	0.1259
48	H	6.139	0.1121	0.1294
49	H	6.139	0.1125	0.1279
50	H	6.151	0.112	0.1303
51	H	6.151	0.1119	0.1318
52	H	6.189	0.1188	0.1371
53	H	6.189	0.1183	0.1371

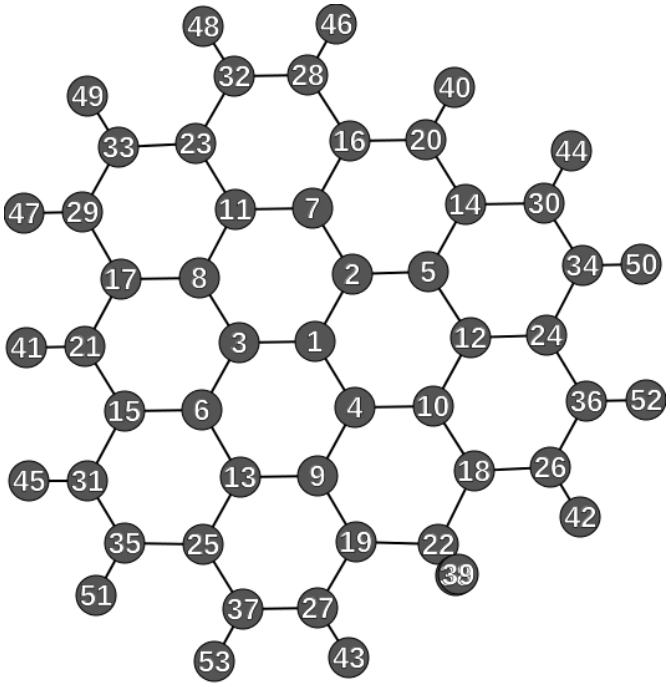

Figure 8 Type I structure as a reference to data in the tables 8.

Table 8 Partial charges for N-doped type I system with the total charge 0e for 6-31+G(2df, p) basis set

Index	Atom	Distance	RESP	MBIS
1	N	0	0.1053	-0.1364
2	C	1.403	0.02977	0.1858
3	C	1.403	0.03181	0.1923
4	C	1.41	0.06998	0.1149
5	C	2.438	-0.08569	-0.09432
6	C	2.438	-0.09103	-0.09196
7	C	2.439	-0.07204	-0.08136
8	C	2.439	-0.07558	-0.08486
9	C	2.461	-0.1598	-0.06543
10	C	2.461	-0.1596	-0.07052
11	C	2.841	0.07115	0.05793
12	C	2.847	0.1047	0.04439
13	C	2.847	0.1085	0.04048
14	C	3.735	0.2224	0.1233
15	C	3.735	0.229	0.1245
16	C	3.741	0.2189	0.1263
17	C	3.741	0.2237	0.1281
18	C	3.75	0.1675	0.07691
19	C	3.75	0.1672	0.07779
20	C	4.226	-0.3979	-0.3017
21	C	4.226	-0.4026	-0.3044
22	C	4.345	-0.1384	-0.2905
23	C	4.239	0.0941	0.03061
24	C	4.253	0.07905	0.06634
25	C	4.253	0.07501	0.06479
26	C	4.882	-0.2287	-0.203
27	C	4.882	-0.232	-0.2069
28	C	4.895	-0.2268	-0.2171
29	C	4.895	-0.2262	-0.2167
30	C	4.898	-0.2219	-0.2009
31	C	4.898	-0.2266	-0.2033
32	C	5.085	-0.1883	-0.1653
33	C	5.085	-0.1912	-0.164
34	C	5.096	-0.1762	-0.1796
35	C	5.096	-0.1734	-0.1736
36	C	5.096	-0.1934	-0.2049
37	C	5.096	-0.1893	-0.2
38	H	5.089	0.05407	0.137
39	H	5.089	0.05407	0.1383
40	H	5.311	0.1573	0.1558
41	H	5.311	0.159	0.1565
42	H	5.842	0.1366	0.1486
43	H	5.842	0.1376	0.1489
44	H	5.852	0.1396	0.1502
45	H	5.852	0.14	0.1501
46	H	5.853	0.1413	0.1519
47	H	5.853	0.1407	0.152
48	H	6.142	0.1353	0.1456
49	H	6.142	0.1355	0.1454
50	H	6.153	0.1293	0.1484
51	H	6.153	0.129	0.1468
52	H	6.155	0.1349	0.1474
53	H	6.155	0.1346	0.1463

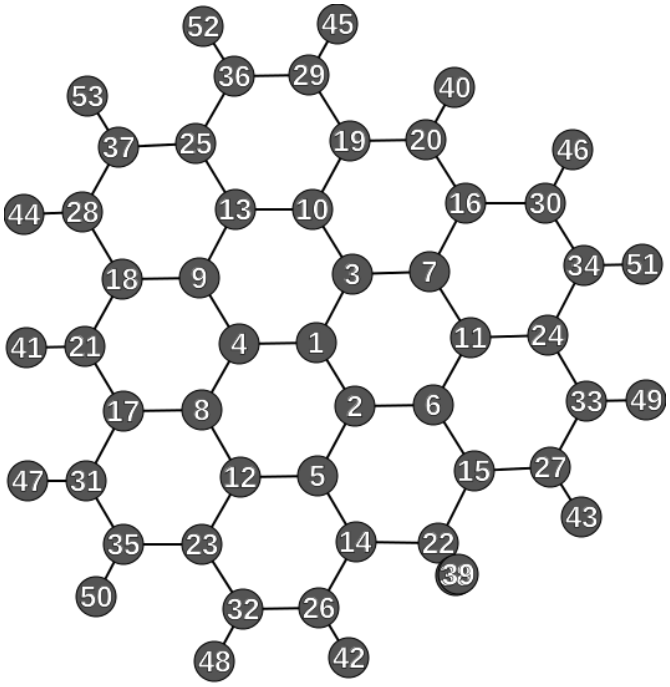

Figure 9 Type I structure as a reference to data in the tables 9.

Table 9 Partial charges for N-doped type I system with the total charge +1e for 6-31+G(2df, p) basis set

Index	Atom	Distance	RESP	MBIS
1	N	0	0.1143	-0.09297
2	C	1.36	0.2403	0.2861
3	C	1.421	0.01927	0.1543
4	C	1.421	0.02801	0.1509
5	C	2.427	-0.2254	-0.1197
6	C	2.427	-0.2235	-0.1278
7	C	2.441	-0.08435	-0.05709
8	C	2.441	-0.09285	-0.04696
9	C	2.457	-0.05227	-0.05054
10	C	2.457	-0.03849	-0.05301
11	C	2.825	0.1418	0.07342
12	C	2.825	0.1435	0.06318
13	C	2.864	0.04017	0.02317
14	C	3.711	0.2447	0.1314
15	C	3.711	0.242	0.1352
16	C	3.75	0.2336	0.09473
17	C	3.75	0.243	0.08799
18	C	3.751	0.2178	0.09853
19	C	3.751	0.1996	0.1065
20	C	4.233	-0.3363	-0.2152
21	C	4.233	-0.3495	-0.2111
22	C	4.296	-0.2303	-0.3374
23	C	4.238	0.07682	0.0583
24	C	4.238	0.07472	0.05098
25	C	4.262	0.1427	0.07654
26	C	4.838	-0.2389	-0.2047
27	C	4.838	-0.2354	-0.2088
28	C	4.91	-0.1917	-0.1746
29	C	4.91	-0.1842	-0.18
30	C	4.911	-0.2091	-0.1721
31	C	4.911	-0.2111	-0.169
32	C	5.053	-0.1196	-0.1167
33	C	5.053	-0.1206	-0.1155
34	C	5.1	-0.164	-0.1676
35	C	5.1	-0.1664	-0.1722
36	C	5.108	-0.1867	-0.1563
37	C	5.108	-0.1842	-0.1588
38	H	5.037	0.1015	0.1758
39	H	5.038	0.1015	0.1769
40	H	5.319	0.1734	0.1691
41	H	5.319	0.177	0.1687
42	H	5.8	0.1636	0.1701
43	H	5.8	0.1628	0.1711
44	H	5.865	0.1591	0.1659
45	H	5.865	0.1586	0.1678
46	H	5.867	0.1614	0.1674
47	H	5.867	0.1614	0.1681
48	H	6.115	0.1528	0.1634
49	H	6.115	0.153	0.1637
50	H	6.153	0.1516	0.1671
51	H	6.153	0.1505	0.1669
52	H	6.165	0.1581	0.1656
53	H	6.165	0.1565	0.1647

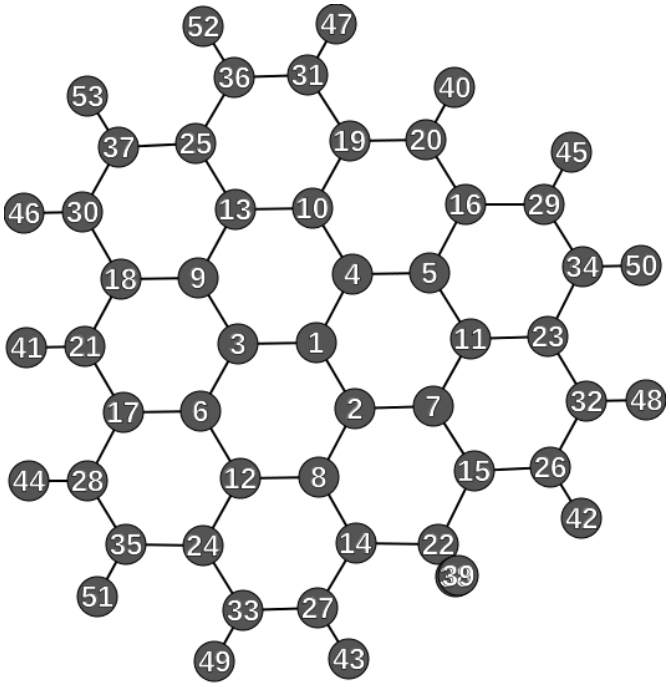

Figure 10 Type I structure as a reference to data in the tables 10.

Table 10 Partial charges for C-flake of type I system with the total charge -1e for Def2TZVP basis set

Index	Atom	Distance	RESP	MBIS
1	C	0	-0.00676	-0.02972
2	C	1.407	-0.002496	-0.07969
3	C	1.422	-0.02018	-0.009882
4	C	1.422	-0.02885	-0.003938
5	C	2.458	-0.04249	-0.01884
6	C	2.458	-0.04998	-0.008957
7	C	2.462	-0.1059	0.002368
8	C	2.462	-0.109	0.002941
9	C	2.463	-0.04606	-0.005933
10	C	2.463	-0.0318	-0.008893
11	C	2.84	0.06951	0.01773
12	C	2.84	0.0705	0.01631
13	C	2.85	0.01771	-0.002523
14	C	3.749	0.129	0.03559
15	C	3.749	0.1221	0.02972
16	C	3.751	0.1901	0.08553
17	C	3.751	0.1986	0.0836
18	C	3.764	0.2263	0.1195
19	C	3.764	0.2083	0.1184
20	C	4.234	-0.4262	-0.3315
21	C	4.234	-0.4392	-0.3347
22	C	4.339	-0.09409	-0.2373
23	C	4.255	0.08494	0.06886
24	C	4.255	0.08715	0.06677
25	C	4.269	0.09359	0.01442
26	C	4.877	-0.2319	-0.2117
27	C	4.877	-0.2412	-0.2159
28	C	4.9	-0.2269	-0.2025
29	C	4.9	-0.2254	-0.2051
30	C	4.915	-0.26	-0.2553
31	C	4.915	-0.2547	-0.2549
32	C	5.091	-0.2306	-0.2369
33	C	5.091	-0.2259	-0.2333
34	C	5.093	-0.2181	-0.2122
35	C	5.093	-0.2212	-0.2125
36	C	5.101	-0.2145	-0.1772
37	C	5.101	-0.2143	-0.1787
38	H	5.084	0.02223	0.1025
39	H	5.084	0.02223	0.1031
40	H	5.32	0.1323	0.1299
41	H	5.32	0.1369	0.1318
42	H	5.838	0.1105	0.1252
43	H	5.838	0.1125	0.1252
44	H	5.859	0.1154	0.1256
45	H	5.859	0.1158	0.1275
46	H	5.874	0.1163	0.128
47	H	5.874	0.1169	0.1272
48	H	6.149	0.1136	0.1248
49	H	6.149	0.1128	0.1236
50	H	6.15	0.109	0.1253
51	H	6.15	0.1102	0.1252
52	H	6.158	0.1126	0.1212
53	H	6.158	0.111	0.1219

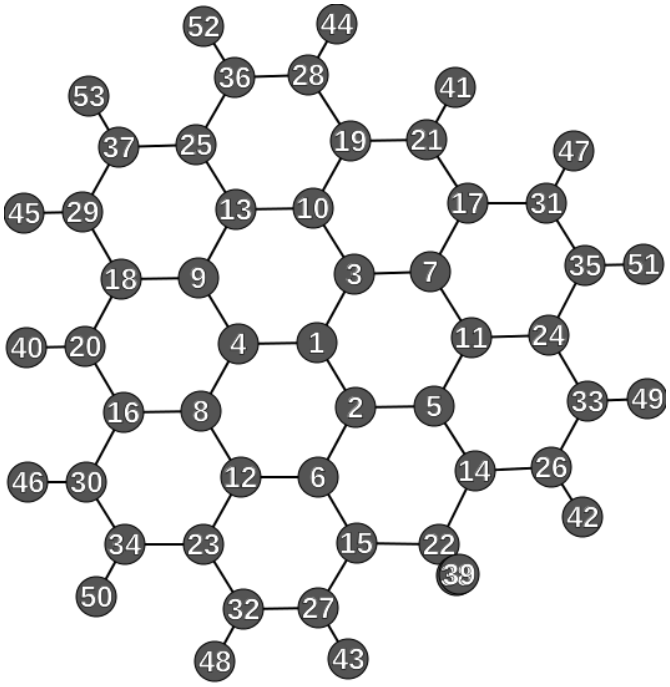

Figure 11 Type I structure as a reference to data in the tables 11.

Table 11 Partial charges for C-flake of type I system with the total charge 0e for Def2TZVP basis set

Index	Atom	Distance	RESP	MBIS	ACKS2
1	C	0	-0.007508	-0.01444	-0.009806
2	C	1.384	0.09081	0.0007256	-0.01008
3	C	1.435	0.0018	0.006882	-0.00861
4	C	1.435	-0.002775	0.002206	-0.00861
5	C	2.446	-0.1581	-0.01675	-0.01201
6	C	2.446	-0.1509	-0.01238	-0.01201
7	C	2.456	-0.06867	-0.005948	-0.009596
8	C	2.456	-0.06522	-0.002417	-0.009596
9	C	2.468	-0.02749	-0.002957	-0.009169
10	C	2.468	-0.03873	-0.008133	-0.009169
11	C	2.828	0.09688	0.01053	-0.007992
12	C	2.828	0.09044	0.009191	-0.007992
13	C	2.854	0.02037	0.007523	-0.007093
14	C	3.728	0.1981	0.08623	0.004944
15	C	3.728	0.1898	0.07856	0.004944
16	C	3.761	0.2241	0.08247	0.009535
17	C	3.761	0.2258	0.08499	0.009535
18	C	3.761	0.1895	0.08404	0.009385
19	C	3.761	0.2055	0.0841	0.009385
20	C	4.239	-0.372	-0.2455	-0.1877
21	C	4.239	-0.3799	-0.2461	-0.1877
22	C	4.305	-0.1451	-0.2923	-0.3345
23	C	4.242	0.08231	0.07182	0.002946
24	C	4.242	0.07691	0.06827	0.002946
25	C	4.252	0.1431	0.06628	0.002737
26	C	4.851	-0.2486	-0.2093	-0.1681
27	C	4.851	-0.2398	-0.2039	-0.1681
28	C	4.912	-0.2047	-0.1873	-0.1559
29	C	4.912	-0.1979	-0.1881	-0.1559
30	C	4.917	-0.2196	-0.1824	-0.1558
31	C	4.917	-0.2196	-0.1857	-0.1558
32	C	5.062	-0.1772	-0.1775	-0.157
33	C	5.062	-0.1698	-0.1768	-0.157
34	C	5.098	-0.1751	-0.1839	-0.1542
35	C	5.098	-0.1749	-0.1812	-0.1542
36	C	5.099	-0.2129	-0.1779	-0.1539
37	C	5.099	-0.2142	-0.1774	-0.1539
38	H	5.045	0.05871	0.143	0.1982
39	H	5.045	0.05871	0.1433	0.1982
40	H	5.323	0.153	0.1463	0.1787
41	H	5.323	0.1555	0.1461	0.1787
42	H	5.814	0.1377	0.1446	0.1609
43	H	5.814	0.1362	0.1442	0.1609
44	H	5.871	0.1361	0.1447	0.16
45	H	5.871	0.1358	0.1447	0.16
46	H	5.876	0.1367	0.1448	0.1595
47	H	5.876	0.1365	0.1461	0.1595
48	H	6.121	0.1345	0.1414	0.1585
49	H	6.121	0.1328	0.1421	0.1585
50	H	6.151	0.1251	0.1444	0.158
51	H	6.151	0.126	0.1453	0.158
52	H	6.153	0.1355	0.1423	0.1587
53	H	6.153	0.137	0.1424	0.1587

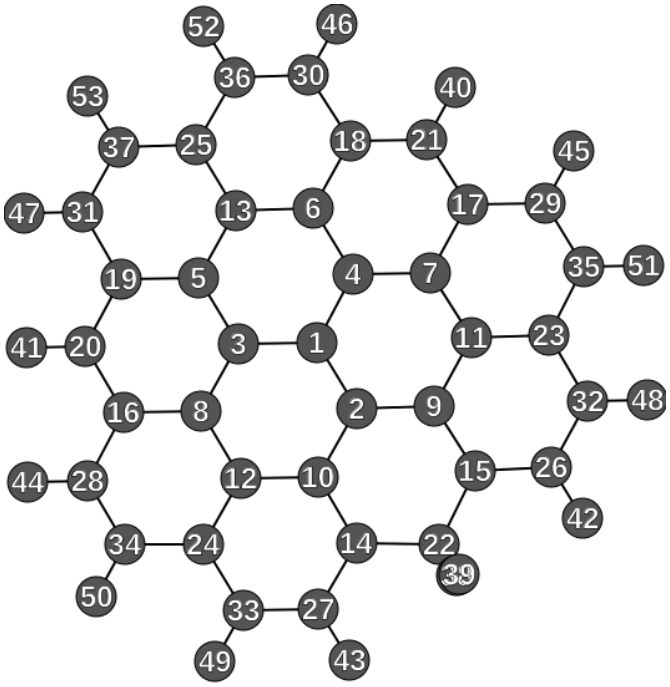

Figure 12 Type I structure as a reference to data in the tables 12.

Table 12 Partial charges for C-flake type I system with the total charge +1e for Def2TZVP basis set

Index	Atom	Distance	RESP	MBIS
1	C	0	0.001933	-0.004219
2	C	1.411	0.1769	0.1018
3	C	1.42	0.005943	0.008899
4	C	1.42	-0.001548	0.005409
5	C	2.453	-0.02161	0.01357
6	C	2.453	-0.009694	0.01675
7	C	2.453	-0.04535	0.009273
8	C	2.453	-0.0566	0.005974
9	C	2.457	-0.1871	-0.05669
10	C	2.457	-0.1876	-0.06111
11	C	2.832	0.08459	0.01652
12	C	2.832	0.09119	0.0185
13	C	2.833	0.01151	-0.002872
14	C	3.74	0.2808	0.1546
15	C	3.74	0.2836	0.1492
16	C	3.746	0.2254	0.07285
17	C	3.746	0.2138	0.06675
18	C	3.749	0.1647	0.03571
19	C	3.749	0.1819	0.04102
20	C	4.223	-0.3015	-0.1474
21	C	4.223	-0.2884	-0.1422
22	C	4.306	-0.2824	-0.3507
23	C	4.24	0.09073	0.05928
24	C	4.24	0.08662	0.0625
25	C	4.249	0.2066	0.1407
26	C	4.872	-0.2519	-0.2126
27	C	4.872	-0.2522	-0.2167
28	C	4.902	-0.1978	-0.1597
29	C	4.902	-0.1937	-0.1605
30	C	4.902	-0.1415	-0.1119
31	C	4.902	-0.1483	-0.1135
32	C	5.071	-0.1143	-0.1047
33	C	5.071	-0.1121	-0.1065
34	C	5.09	-0.1512	-0.1478
35	C	5.09	-0.1528	-0.1462
36	C	5.093	-0.2193	-0.1968
37	C	5.093	-0.2177	-0.1972
38	H	5.052	0.1188	0.1832
39	H	5.052	0.1188	0.1831
40	H	5.307	0.1629	0.1588
41	H	5.307	0.1664	0.1593
42	H	5.834	0.1616	0.1672
43	H	5.834	0.1622	0.1678
44	H	5.86	0.1586	0.1615
45	H	5.86	0.1582	0.1618
46	H	5.86	0.1537	0.1589
47	H	5.86	0.1539	0.1587
48	H	6.128	0.1484	0.1577
49	H	6.128	0.1484	0.1591
50	H	6.143	0.1483	0.161
51	H	6.143	0.1484	0.1608
52	H	6.147	0.1605	0.1669
53	H	6.147	0.1592	0.1677

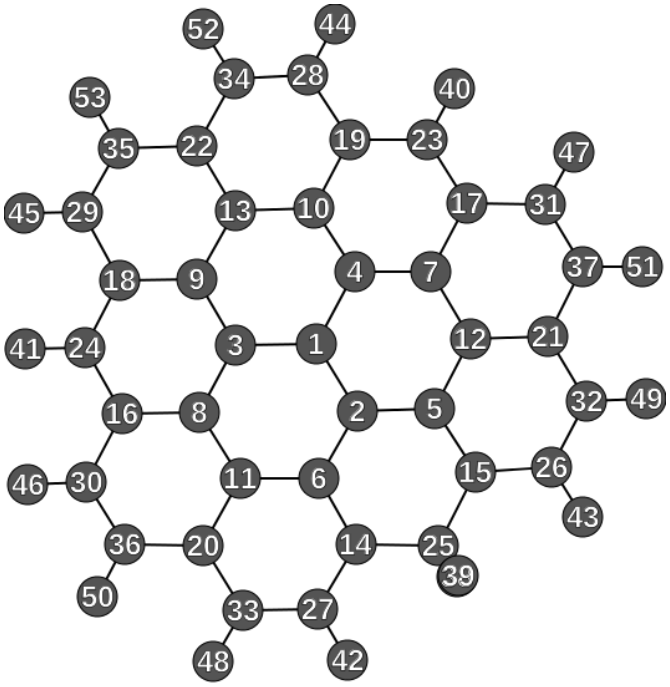

Figure 13 Type I structure as a reference to data in the tables 13.

Table 13 Partial charges for B-doped type I system with the total charge -1e for Def2TZVP basis set

Index	Atom	Distance	RESP	MBIS	ACKS2
1	B	0	0.05827	0.2684	0.2509
2	C	1.46	-0.1797	-0.3739	-0.4627
3	C	1.501	-0.1391	-0.2512	-0.4378
4	C	1.501	-0.1348	-0.2435	-0.4378
5	C	2.483	-0.02055	0.08884	0.03223
6	C	2.483	-0.01843	0.09587	0.03222
7	C	2.496	0.003713	0.06085	0.0343
8	C	2.496	0.01382	0.06609	0.0343
9	C	2.505	0.02516	0.06093	0.0336
10	C	2.505	0.01874	0.05902	0.0336
11	C	2.845	-0.02641	-0.04385	-0.06103
12	C	2.845	-0.01756	-0.03086	-0.06103
13	C	2.862	-0.04154	-0.01397	-0.05961
14	C	3.775	0.1254	0.03648	-0.001834
15	C	3.775	0.1253	0.0389	-0.001834
16	C	3.801	0.197	0.07823	0.003575
17	C	3.801	0.2076	0.07349	0.003575
18	C	3.803	0.1762	0.07585	0.003393
19	C	3.803	0.1859	0.07298	0.003394
20	C	4.259	0.1286	0.07988	0.007094
21	C	4.259	0.1199	0.0698	0.007094
22	C	4.261	0.1574	0.05907	0.00677
23	C	4.273	-0.4095	-0.2793	-0.1803
24	C	4.273	-0.4005	-0.2858	-0.1803
25	C	4.342	-0.06232	-0.2347	-0.3232
26	C	4.894	-0.2451	-0.222	-0.1677
27	C	4.894	-0.2402	-0.2185	-0.1677
28	C	4.946	-0.216	-0.2043	-0.1565
29	C	4.946	-0.2145	-0.2042	-0.1565
30	C	4.951	-0.2209	-0.2026	-0.1566
31	C	4.951	-0.2267	-0.1992	-0.1566
32	C	5.093	-0.2377	-0.2311	-0.1595
33	C	5.093	-0.245	-0.2391	-0.1595
34	C	5.114	-0.2433	-0.2019	-0.1563
35	C	5.114	-0.2408	-0.2035	-0.1563
36	C	5.114	-0.2061	-0.1925	-0.1565
37	C	5.114	-0.2016	-0.1909	-0.1565
38	H	5.084	0.0218	0.1098	0.1939
39	H	5.084	0.0218	0.1098	0.1939
40	H	5.359	0.1341	0.1239	0.1753
41	H	5.359	0.1309	0.1265	0.1753
42	H	5.863	0.108	0.1221	0.1583
43	H	5.863	0.1095	0.1232	0.1583
44	H	5.914	0.1131	0.1252	0.1576
45	H	5.914	0.1138	0.1252	0.1576
46	H	5.918	0.1118	0.1253	0.1571
47	H	5.918	0.1122	0.124	0.1571
48	H	6.151	0.1158	0.1215	0.157
49	H	6.151	0.1151	0.1208	0.157
50	H	6.167	0.1045	0.1241	0.157
51	H	6.167	0.1037	0.1231	0.157
52	H	6.167	0.1147	0.1228	0.1576
53	H	6.167	0.1147	0.1241	0.1576

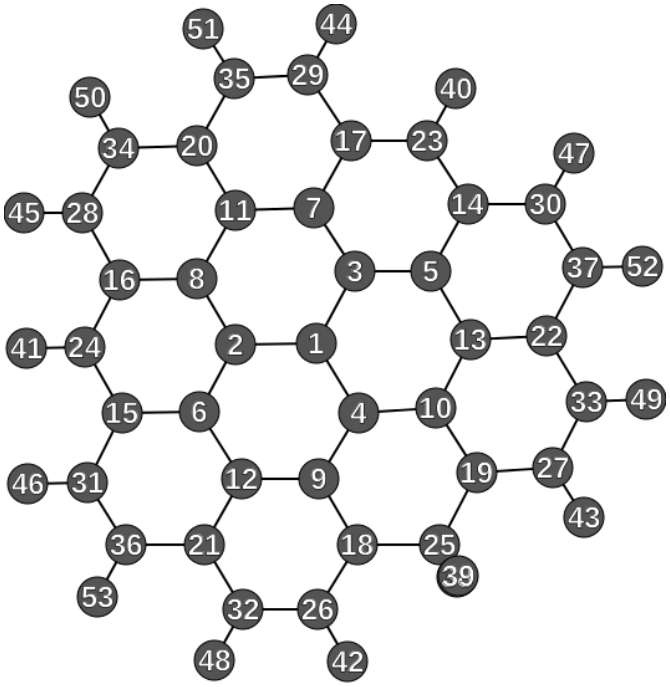

Figure 14 Type I structure as a reference to data in the tables 14.

Table 14 Partial charges for B-doped type I system with the total charge 0e for Def2TZVP basis set

Index	Atom	Distance	RESP	MBIS
1	B	0	0.2055	0.4259
2	C	1.497	-0.2255	-0.32
3	C	1.497	-0.2216	-0.3265
4	C	1.498	-0.02722	-0.2147
5	C	2.49	0.0361	0.1017
6	C	2.49	0.04532	0.09346
7	C	2.492	0.08229	0.1003
8	C	2.492	0.08811	0.09968
9	C	2.508	-0.09911	0.02133
10	C	2.508	-0.09835	0.02351
11	C	2.849	-0.1061	-0.05335
12	C	2.849	-0.01365	-0.0195
13	C	2.849	-0.007451	-0.02463
14	C	3.79	0.2002	0.04592
15	C	3.79	0.1894	0.04805
16	C	3.791	0.1539	0.043
17	C	3.791	0.1629	0.04705
18	C	3.794	0.2275	0.1028
19	C	3.794	0.2231	0.1016
20	C	4.243	0.2226	0.113
21	C	4.251	0.1416	0.07138
22	C	4.251	0.1357	0.07557
23	C	4.257	-0.3328	-0.1894
24	C	4.257	-0.3239	-0.192
25	C	4.356	-0.2071	-0.2926
26	C	4.918	-0.2575	-0.2252
27	C	4.918	-0.2576	-0.2247
28	C	4.936	-0.1796	-0.1588
29	C	4.936	-0.1814	-0.1669
30	C	4.941	-0.2095	-0.1718
31	C	4.941	-0.2036	-0.1712
32	C	5.095	-0.1711	-0.1513
33	C	5.095	-0.1674	-0.1541
34	C	5.101	-0.2407	-0.2055
35	C	5.101	-0.2424	-0.1992
36	C	5.109	-0.2058	-0.1884
37	C	5.109	-0.2021	-0.189
38	H	5.1	0.08129	0.1496
39	H	5.1	0.08129	0.1485
40	H	5.342	0.1467	0.1384
41	H	5.342	0.144	0.1392
42	H	5.889	0.1383	0.1475
43	H	5.889	0.1389	0.1482
44	H	5.903	0.1335	0.142
45	H	5.903	0.1339	0.1411
46	H	5.907	0.1358	0.1429
47	H	5.907	0.1364	0.1427
48	H	6.149	0.1328	0.1396
49	H	6.149	0.1325	0.1395
50	H	6.153	0.1373	0.1451
51	H	6.153	0.1372	0.1433
52	H	6.161	0.1285	0.1425
53	H	6.161	0.129	0.1426

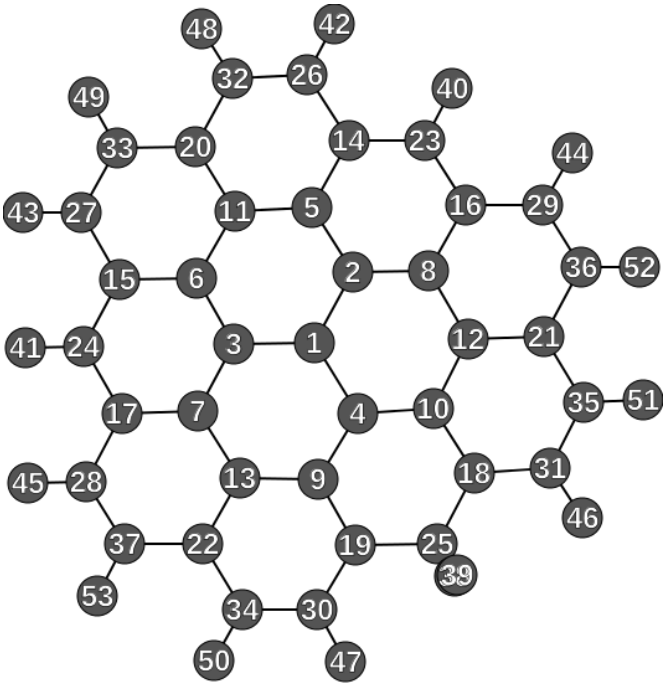

Figure 15 Type I structure as a reference to data in the tables 15.

Table 15 Partial charges for B-doped type I system with the total charge +1e for Def2TZVP basis set

Index	Atom	Distance	RESP	MBIS
1	B	0	0.227	0.4396
2	C	1.484	-0.2553	-0.3508
3	C	1.484	-0.2506	-0.3592
4	C	1.534	0.122	-0.03704
5	C	2.476	0.1338	0.1348
6	C	2.476	0.127	0.1424
7	C	2.487	0.04108	0.108
8	C	2.487	0.04996	0.1011
9	C	2.521	-0.1594	-0.04772
10	C	2.521	-0.1605	-0.04169
11	C	2.831	-0.1537	-0.0878
12	C	2.851	0.007464	0.0004086
13	C	2.851	0.01189	0.0001246
14	C	3.778	0.133	0.01522
15	C	3.778	0.1434	0.009959
16	C	3.778	0.1933	0.03648
17	C	3.778	0.2037	0.03688
18	C	3.81	0.3382	0.2067
19	C	3.81	0.3335	0.2082
20	C	4.229	0.2932	0.1711
21	C	4.246	0.1223	0.05214
22	C	4.246	0.1198	0.0513
23	C	4.243	-0.2576	-0.117
24	C	4.243	-0.2671	-0.1142
25	C	4.354	-0.3541	-0.381
26	C	4.926	-0.132	-0.1127
27	C	4.926	-0.1356	-0.1072
28	C	4.931	-0.1867	-0.1402
29	C	4.931	-0.182	-0.1357
30	C	4.94	-0.2845	-0.2574
31	C	4.94	-0.2866	-0.2605
32	C	5.09	-0.2468	-0.2039
33	C	5.09	-0.2469	-0.2077
34	C	5.096	-0.07245	-0.04375
35	C	5.096	-0.07293	-0.04199
36	C	5.106	-0.1855	-0.177
37	C	5.106	-0.1839	-0.1746
38	H	5.106	0.1476	0.2039
39	H	5.106	0.1476	0.2037
40	H	5.328	0.1562	0.1535
41	H	5.328	0.1588	0.1525
42	H	5.893	0.1517	0.1559
43	H	5.893	0.1517	0.1551
44	H	5.895	0.1569	0.1585
45	H	5.895	0.1575	0.1594
46	H	5.912	0.1677	0.1761
47	H	5.912	0.1678	0.1746
48	H	6.141	0.1595	0.1643
49	H	6.141	0.1592	0.1646
50	H	6.148	0.1462	0.1563
51	H	6.148	0.1462	0.1552
52	H	6.157	0.1493	0.1601
53	H	6.157	0.1493	0.1598

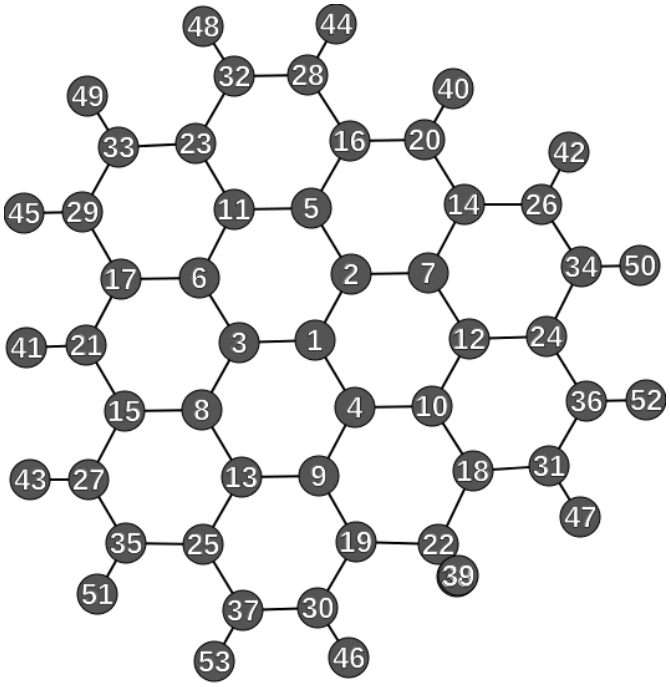

Figure 16 Type I structure as a reference to data in the tables 16.

Table 16 Partial charges for N-doped type I system with the total charge -1e for Def2TZVP basis set

Index	Atom	Distance	RESP	MBIS
1	N	0	0.1416	-0.09959
2	C	1.382	0.0256	0.193
3	C	1.382	0.02909	0.1948
4	C	1.437	-0.1223	-0.08992
5	C	2.425	-0.0979	-0.09709
6	C	2.425	-0.1042	-0.1002
7	C	2.431	-0.06761	-0.09141
8	C	2.431	-0.06688	-0.08962
9	C	2.472	-0.06921	-0.006643
10	C	2.472	-0.0674	-0.0123
11	C	2.826	0.09478	0.06952
12	C	2.854	0.06126	0.02604
13	C	2.854	0.06059	0.01878
14	C	3.711	0.2023	0.1264
15	C	3.711	0.1996	0.1235
16	C	3.731	0.2378	0.1457
17	C	3.731	0.2469	0.1478
18	C	3.771	0.05493	-0.009848
19	C	3.771	0.05512	-0.01243
20	C	4.208	-0.4512	-0.3712
21	C	4.208	-0.4551	-0.3681
22	C	4.383	-0.02389	-0.2045
23	C	4.23	0.04306	-0.02281
24	C	4.257	0.1041	0.0846
25	C	4.257	0.1066	0.08624
26	C	4.87	-0.2343	-0.223
27	C	4.87	-0.2299	-0.2241
28	C	4.882	-0.2743	-0.2604
29	C	4.882	-0.2826	-0.2604
30	C	4.894	-0.1943	-0.1663
31	C	4.894	-0.1996	-0.1712
32	C	5.067	-0.194	-0.1623
33	C	5.067	-0.1867	-0.1623
34	C	5.078	-0.2059	-0.1895
35	C	5.078	-0.2079	-0.1834
36	C	5.119	-0.2857	-0.3102
37	C	5.119	-0.291	-0.3165
38	H	5.13	-0.003617	0.07987
39	H	5.13	-0.00362	0.08019
40	H	5.292	0.1404	0.1388
41	H	5.292	0.1402	0.1376
42	H	5.822	0.118	0.1287
43	H	5.822	0.1175	0.1285
44	H	5.84	0.1212	0.133
45	H	5.84	0.123	0.1335
46	H	5.853	0.1065	0.1194
47	H	5.853	0.108	0.1207
48	H	6.124	0.1129	0.1228
49	H	6.124	0.1112	0.1226
50	H	6.137	0.1108	0.1268
51	H	6.137	0.111	0.1251
52	H	6.175	0.1173	0.1261
53	H	6.175	0.1178	0.1274

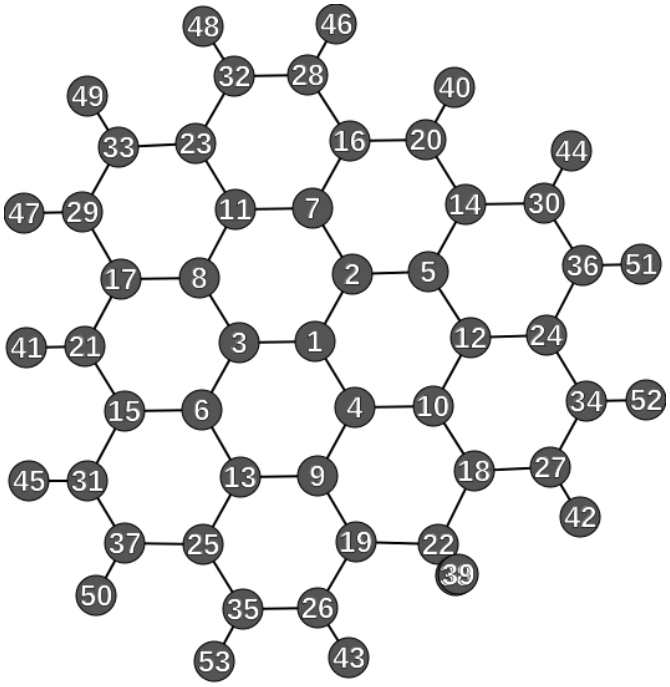

Figure 17 Type I structure as a reference to data in the tables 17.

Table 17 Partial charges for N-doped type I system with the total charge 0e for Def2TZVP basis set

Index	Atom	Distance	RESP	MBIS
1	N	0	0.1072	-0.1364
2	C	1.4	0.02802	0.1898
3	C	1.4	0.03025	0.1873
4	C	1.408	0.06987	0.1193
5	C	2.433	-0.08518	-0.09578
6	C	2.433	-0.09063	-0.09259
7	C	2.434	-0.07093	-0.08566
8	C	2.434	-0.07479	-0.07639
9	C	2.456	-0.1619	-0.07741
10	C	2.456	-0.1616	-0.07727
11	C	2.835	0.07046	0.05253
12	C	2.841	0.1057	0.04722
13	C	2.841	0.1095	0.05006
14	C	3.726	0.2229	0.1202
15	C	3.726	0.2297	0.1167
16	C	3.732	0.2192	0.1295
17	C	3.732	0.2243	0.115
18	C	3.742	0.1703	0.08125
19	C	3.742	0.17	0.07952
20	C	4.216	-0.3975	-0.2961
21	C	4.216	-0.4024	-0.2907
22	C	4.335	-0.1385	-0.2837
23	C	4.229	0.09485	0.03104
24	C	4.243	0.07882	0.05486
25	C	4.243	0.07463	0.05681
26	C	4.87	-0.2323	-0.2025
27	C	4.87	-0.229	-0.2023
28	C	4.884	-0.2262	-0.2115
29	C	4.884	-0.2256	-0.2049
30	C	4.886	-0.2214	-0.1997
31	C	4.886	-0.2262	-0.196
32	C	5.073	-0.1878	-0.1622
33	C	5.073	-0.1905	-0.1606
34	C	5.084	-0.1924	-0.1904
35	C	5.084	-0.1881	-0.1904
36	C	5.084	-0.1752	-0.1666
37	C	5.084	-0.1723	-0.1712
38	H	5.076	0.05337	0.1342
39	H	5.076	0.05337	0.1344
40	H	5.299	0.1562	0.152
41	H	5.299	0.158	0.1521
42	H	5.829	0.1358	0.1459
43	H	5.829	0.1368	0.1458
44	H	5.839	0.1388	0.1478
45	H	5.839	0.1392	0.1473
46	H	5.84	0.1406	0.1481
47	H	5.84	0.1399	0.1471
48	H	6.128	0.1344	0.1424
49	H	6.128	0.1344	0.1417
50	H	6.139	0.128	0.1443
51	H	6.139	0.1284	0.1428
52	H	6.14	0.1339	0.1422
53	H	6.14	0.1335	0.1416

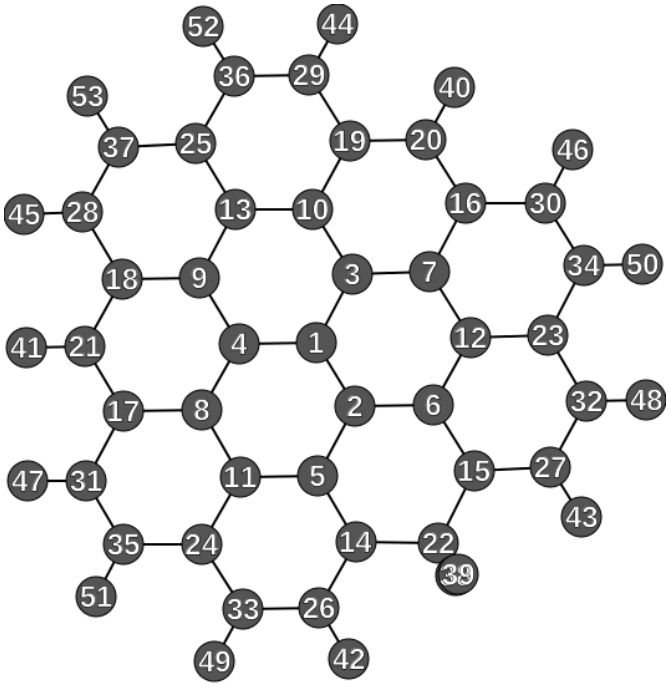

Figure 18 Type I structure as a reference to data in the tables 18.

Table 18 Partial charges for N-doped type I system with the total charge +1e for Def2TZVP basis set

Index	Atom	Distance	RESP	MBIS	ACKS2
1	N	0	0.1163	-0.09289	-0.07418
2	C	1.358	0.2409	0.289	0.4146
3	C	1.419	0.02075	0.1568	0.3794
4	C	1.419	0.02508	0.1528	0.3794
5	C	2.422	-0.2283	-0.1266	-0.06596
6	C	2.422	-0.2227	-0.1283	-0.06596
7	C	2.436	-0.08727	-0.06047	-0.06089
8	C	2.436	-0.09063	-0.05921	-0.06089
9	C	2.453	-0.05102	-0.05121	-0.05935
10	C	2.453	-0.04043	-0.05374	-0.05935
11	C	2.819	0.1445	0.07036	0.03631
12	C	2.819	0.1392	0.07461	0.03631
13	C	2.858	0.04049	0.02333	0.0359
14	C	3.702	0.2479	0.1352	0.01212
15	C	3.702	0.2421	0.1344	0.01212
16	C	3.742	0.2398	0.09066	0.01608
17	C	3.742	0.2414	0.09181	0.01608
18	C	3.743	0.217	0.09129	0.01585
19	C	3.743	0.2019	0.09364	0.01585
20	C	4.224	-0.3398	-0.2052	-0.194
21	C	4.224	-0.3472	-0.206	-0.194
22	C	4.285	-0.2301	-0.3394	-0.343
23	C	4.228	0.08009	0.0516	-0.001214
24	C	4.228	0.07648	0.04907	-0.001214
25	C	4.252	0.1435	0.07968	-0.001329
26	C	4.826	-0.2395	-0.2032	-0.1683
27	C	4.826	-0.2335	-0.2013	-0.1683
28	C	4.899	-0.1906	-0.1654	-0.1556
29	C	4.899	-0.1835	-0.1674	-0.1556
30	C	4.9	-0.2106	-0.1676	-0.1553
31	C	4.9	-0.21	-0.1687	-0.1553
32	C	5.04	-0.1232	-0.1128	-0.1548
33	C	5.04	-0.1181	-0.1106	-0.1548
34	C	5.088	-0.1648	-0.1661	-0.1523
35	C	5.088	-0.1658	-0.1606	-0.1523
36	C	5.096	-0.1865	-0.1586	-0.1518
37	C	5.096	-0.1844	-0.1618	-0.1518
38	H	5.025	0.1009	0.1754	0.2007
39	H	5.025	0.1009	0.1748	0.2007
40	H	5.307	0.1734	0.1659	0.1809
41	H	5.307	0.1756	0.1662	0.1809
42	H	5.786	0.1628	0.1682	0.1623
43	H	5.786	0.1618	0.1673	0.1623
44	H	5.852	0.1577	0.1627	0.1615
45	H	5.852	0.1582	0.1621	0.1615
46	H	5.854	0.1607	0.1644	0.1609
47	H	5.854	0.1605	0.165	0.1609
48	H	6.1	0.153	0.1605	0.1595
49	H	6.1	0.1517	0.1598	0.1595
50	H	6.139	0.1495	0.1645	0.1587
51	H	6.139	0.1506	0.163	0.1587
52	H	6.151	0.1573	0.1624	0.1594
53	H	6.151	0.1558	0.1637	0.1594

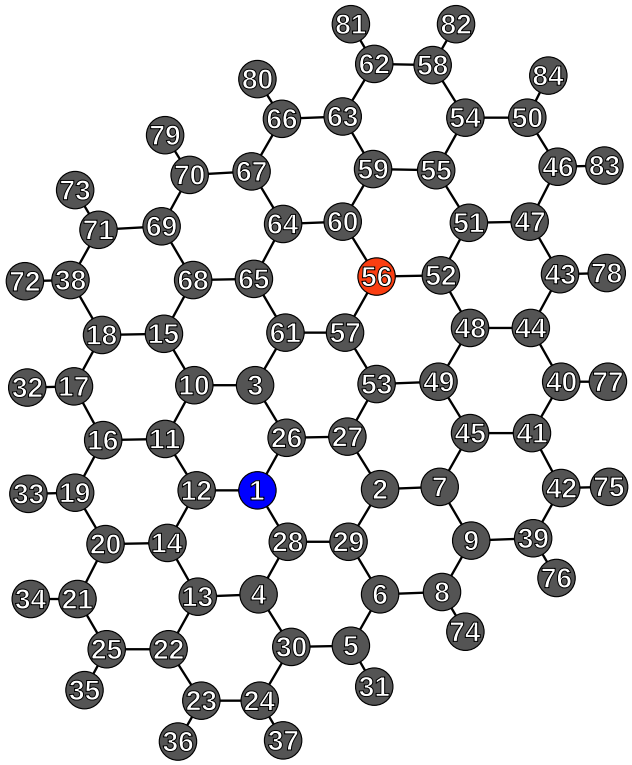

Figure 19 Type II structure as a reference to data in the tables 19-20.

Table 19 Partial charges of type II system for Def2TZVP basis set – MBIS, ACKS2; RESP-A1 model on the B3LYP – RESP fitting

Total charge:		**-1e**		**0e**			**+1e**	
Index	Atom	RESP	MBIS	RESP	MBIS	ACKS2	RESP	MBIS
1	N	0.1627	-0.1274	0.1634	-0.1353	-0.0768	0.1721	-0.0903
2	C	0.0159	0.0601	0.0297	0.0641	0.0391	0.0305	0.0561
3	C	-0.0454	-0.1192	-0.0607	-0.124	-0.0682	-0.0416	-0.0894
4	C	-0.0685	-0.0605	-0.0584	-0.081	-0.0603	-0.0564	-0.0648
5	C	-0.4071	-0.3199	-0.3759	-0.2876	-0.1937	-0.3065	-0.1821
6	C	0.2479	0.1144	0.2603	0.1256	0.0228	0.2497	0.0873
7	C	-0.0609	-0.0572	-0.0665	-0.0567	-0.0162	-0.0426	-0.014
8	C	-0.4061	-0.273	-0.3944	-0.2747	-0.1874	-0.3599	-0.2186
9	C	0.2075	0.0748	0.2147	0.1078	0.0139	0.2275	0.1068
10	C	0.0159	0.0361	0.0297	0.0682	0.0391	0.0305	0.0468
11	C	-0.0528	-0.0547	-0.0595	-0.0883	-0.0625	-0.0632	-0.0662
12	C	-0.0003	0.1079	0.0019	0.1864	0.3925	0.0256	0.1899
13	C	0.0586	-0.0125	0.0531	0.0564	0.0383	0.0559	0.0463
14	C	-0.0685	-0.044	-0.0584	-0.0825	-0.0603	-0.0564	-0.0618
15	C	-0.0609	-0.0372	-0.0665	-0.0512	-0.0162	-0.0426	-0.0068
16	C	0.2479	0.111	0.2603	0.1336	0.0228	0.2497	0.0812
17	C	-0.4061	-0.2834	-0.3944	-0.2733	-0.1874	-0.3599	-0.2175
18	C	0.2075	0.0549	0.2147	0.102	0.0139	0.2275	0.1055
19	C	-0.4071	-0.3322	-0.3759	-0.2922	-0.1937	-0.3065	-0.1766
20	C	0.1954	0.1354	0.1887	0.1182	0.0171	0.1726	0.0637
21	C	-0.2297	-0.267	-0.203	-0.2058	-0.1542	-0.1621	-0.1436
22	C	0.1063	0.0016	0.1301	0.0209	-0.0014	0.1718	0.0926
23	C	-0.2164	-0.1532	-0.2101	-0.1554	-0.1502	-0.2081	-0.175
24	C	-0.2297	-0.2804	-0.203	-0.2071	-0.1542	-0.1621	-0.1445
25	C	-0.2164	-0.174	-0.2101	-0.1589	-0.1502	-0.2081	-0.173
26	C	0.0033	0.2399	0.0519	0.23	0.4131	0.0458	0.2046
27	C	-0.0454	-0.1285	-0.0607	-0.1151	-0.0682	-0.0416	-0.0969
28	C	-0.0003	0.1469	0.0019	0.1788	0.3925	0.0256	0.1953

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Table 19 – continued from previous page

Index	Atom	RESP	MBIS	RESP	MBIS	RESP	MBIS	
29	C	-0.0528	-0.0763	-0.0595	-0.0787	-0.0625	-0.0632	-0.0759
30	C	0.1954	0.1435	0.1887	0.1186	0.0171	0.1726	0.0691
31	H	0.1489	0.1421	0.1611	0.1534	0.1827	0.1695	0.1624
32	H	0.1522	0.1363	0.1653	0.1506	0.1821	0.1787	0.1611
33	H	0.1489	0.1389	0.1611	0.1549	0.1827	0.1695	0.1619
34	H	0.1258	0.1303	0.138	0.1493	0.1619	0.1526	0.1604
35	H	0.1261	0.1259	0.141	0.1436	0.1599	0.1589	0.1637
36	H	0.1261	0.1249	0.141	0.143	0.1599	0.1589	0.1643
37	H	0.1258	0.1324	0.138	0.1486	0.1619	0.1526	0.161
38	C	-0.2489	-0.1736	-0.2223	-0.1891	-0.154	-0.2279	-0.2004
39	C	-0.2489	-0.1812	-0.2223	-0.1914	-0.154	-0.2279	-0.2021
40	C	-0.3555	-0.2419	-0.3322	-0.205	-0.1873	-0.3091	-0.1702
41	C	0.1195	0.071	0.1456	0.0532	0.0082	0.1386	0.04
42	C	-0.1617	-0.2054	-0.1757	-0.1686	-0.1534	-0.1501	-0.1328
43	C	-0.3569	-0.224	-0.2912	-0.1796	-0.1797	-0.26	-0.1323
44	C	0.1907	0.0566	0.187	0.0385	0.0104	0.195	0.0213
45	C	0.046	0.0457	0.0695	0.0526	0.0025	0.0646	0.0426
46	C	-0.2056	-0.1799	-0.1674	-0.1618	-0.1553	-0.1457	-0.1348
47	C	0.1463	0.0509	0.1282	0.0435	0.0052	0.1261	0.0237
48	C	0.0834	0.0911	0.0841	0.1054	0.0398	0.077	0.1095
49	C	-0.1338	-0.0761	-0.1424	-0.0782	-0.0629	-0.1174	-0.0578
50	C	-0.2432	-0.211	-0.2445	-0.1967	-0.155	-0.242	-0.1929
51	C	0.0744	0.0801	0.0865	0.0985	0.0381	0.1116	0.1227
52	C	-0.2312	-0.3077	-0.2476	-0.328	-0.4479	-0.2628	-0.3449
53	C	0.1148	0.1448	0.1435	0.1412	0.0537	0.1233	0.1211
54	C	0.1728	0.0865	0.2244	0.1071	0.0079	0.2641	0.1389
55	C	-0.0896	-0.0326	-0.1001	-0.0451	-0.0612	-0.1303	-0.0693
56	B	0.1815	0.4211	0.2849	0.4587	0.2704	0.3151	0.4852
57	C	-0.2237	-0.4045	-0.2727	-0.3765	-0.4689	-0.2288	-0.3215
58	C	-0.2432	-0.2118	-0.2445	-0.2001	-0.155	-0.242	-0.1962
59	C	0.0744	0.0791	0.0865	0.1014	0.0381	0.1116	0.1217
60	C	-0.2312	-0.3126	-0.2476	-0.3248	-0.4479	-0.2628	-0.3405
61	C	0.1148	0.1418	0.1435	0.1425	0.0537	0.1233	0.1174
62	C	-0.2056	-0.1796	-0.1674	-0.1595	-0.1553	-0.1457	-0.136
63	C	0.1463	0.0519	0.1282	0.0382	0.0052	0.1261	0.0302
64	C	0.0834	0.0944	0.0841	0.1006	0.0398	0.077	0.1007
65	C	-0.1338	-0.0763	-0.1424	-0.0724	-0.0629	-0.1174	-0.0542
66	C	-0.3569	-0.2343	-0.2912	-0.1802	-0.1797	-0.26	-0.143
67	C	0.1907	0.062	0.187	0.0376	0.0104	0.195	0.0321
68	C	0.046	0.0404	0.0695	0.0466	0.0025	0.0646	0.0425
69	C	0.1195	0.0871	0.1456	0.0526	0.0082	0.1386	0.0407
70	C	-0.3555	-0.2605	-0.3322	-0.2017	-0.1873	-0.3091	-0.172
71	C	-0.1617	-0.232	-0.1757	-0.1671	-0.1534	-0.1501	-0.1351
72	H	0.1231	0.1323	0.1379	0.1478	0.1609	0.1539	0.1606
73	H	0.1121	0.1351	0.1303	0.1444	0.1608	0.1451	0.1566
74	H	0.1522	0.1373	0.1653	0.1513	0.1821	0.1787	0.1614
75	H	0.1121	0.1344	0.1303	0.145	0.1608	0.1451	0.1557
76	H	0.1231	0.1341	0.1379	0.1475	0.1609	0.1539	0.1605
77	H	0.1433	0.1343	0.1583	0.1451	0.1797	0.17	0.1538
78	H	0.1311	0.1294	0.1433	0.1383	0.1786	0.1542	0.1467
79	H	0.1433	0.1357	0.1583	0.1435	0.1797	0.17	0.1544
80	H	0.1311	0.1317	0.1433	0.1392	0.1786	0.1542	0.1485
81	H	0.1148	0.132	0.1309	0.1415	0.1588	0.1443	0.1523
82	H	0.1191	0.1321	0.1384	0.1446	0.1589	0.1533	0.1569
83	H	0.1148	0.1312	0.1309	0.1418	0.1588	0.1443	0.1529
84	H	0.1191	0.1325	0.1384	0.1436	0.1589	0.1533	0.1562

Table 20 Partial charges of type II system for 6-31+G(2df, p) basis set – MBIS, ACKS2; RESP-A1 model on the B3LYP – RESP fitting

Total charge:		**-1e**		**0e**		**+1e**	
Index	Atom	RESP	MBIS	RESP	MBIS	RESP	MBIS
1	N	0.1755	-0.1428	0.1742	-0.1428	0.1867	-0.0919
2	C	0.0116	0.0453	0.0262	0.0555	0.0272	0.0491
3	C	-0.0418	-0.1034	-0.0599	-0.1213	-0.0389	-0.0891
4	C	-0.0681	-0.0973	-0.058	-0.0785	-0.0562	-0.0571
5	C	-0.4038	-0.3487	-0.3733	-0.295	-0.3055	-0.1824
6	C	0.2465	0.145	0.2597	0.128	0.2507	0.0866
7	C	-0.058	-0.0383	-0.0649	-0.0445	-0.041	-0.0123
8	C	-0.4032	-0.3101	-0.3929	-0.2776	-0.3602	-0.2294
9	C	0.2075	0.1208	0.2151	0.103	0.2287	0.1141
10	C	0.0116	0.0492	0.0262	0.0698	0.0272	0.0449
11	C	-0.0518	-0.0928	-0.0582	-0.0928	-0.0623	-0.0632
12	C	-0.0046	0.1963	-0.0026	0.1925	0.0213	0.1877
13	C	0.0564	0.0679	0.051	0.0539	0.0557	0.0449
14	C	-0.0681	-0.1002	-0.058	-0.085	-0.0562	-0.0605
15	C	-0.058	-0.0478	-0.0649	-0.0581	-0.041	-0.0065
16	C	0.2465	0.1473	0.2597	0.1394	0.2507	0.0871
17	C	-0.4032	-0.317	-0.3929	-0.2799	-0.3602	-0.2255
18	C	0.2075	0.1328	0.2151	0.1085	0.2287	0.1048
19	C	-0.4038	-0.3448	-0.3733	-0.3061	-0.3056	-0.1886
20	C	0.195	0.1403	0.1884	0.1306	0.1736	0.0712
21	C	-0.2279	-0.2405	-0.2015	-0.2159	-0.1615	-0.1483
22	C	0.1086	0.0061	0.1324	0.0306	0.1735	0.0965
23	C	-0.2158	-0.1716	-0.2097	-0.1605	-0.2077	-0.1821
24	C	-0.2279	-0.2436	-0.2015	-0.2151	-0.1615	-0.1467
25	C	-0.2158	-0.1724	-0.2097	-0.1646	-0.2077	-0.1824
26	C	-0.0051	0.1736	0.0485	0.2325	0.0387	0.2031
27	C	-0.0418	-0.1014	-0.0599	-0.118	-0.0389	-0.0901
28	C	-0.0046	0.1898	-0.0026	0.1763	0.0213	0.1895
29	C	-0.0518	-0.0877	-0.0582	-0.0723	-0.0623	-0.0676
30	C	0.195	0.144	0.1884	0.1218	0.1736	0.0677
31	H	0.1475	0.15	0.1597	0.1573	0.1683	0.1638
32	H	0.1506	0.1464	0.1638	0.154	0.1775	0.1648
33	H	0.1475	0.1506	0.1597	0.16	0.1683	0.166
34	H	0.1247	0.1429	0.1368	0.1532	0.1516	0.1639
35	H	0.1246	0.1356	0.1395	0.1482	0.1579	0.1678
36	H	0.1246	0.1357	0.1395	0.1464	0.1579	0.1688
37	H	0.1247	0.1433	0.1368	0.1525	0.1516	0.163
38	C	-0.2478	-0.2384	-0.2213	-0.1963	-0.2276	-0.2039
39	C	-0.2478	-0.2348	-0.2213	-0.1952	-0.2276	-0.2076
40	C	-0.3554	-0.2487	-0.3327	-0.2068	-0.3097	-0.1742
41	C	0.1201	0.0535	0.1469	0.0553	0.1394	0.0412
42	C	-0.1598	-0.1646	-0.1752	-0.1743	-0.1499	-0.1387
43	C	-0.3573	-0.2843	-0.2902	-0.1938	-0.2597	-0.143
44	C	0.191	0.07	0.1869	0.0431	0.1949	0.0272
45	C	0.0443	0.007	0.0706	0.0488	0.0657	0.0436
46	C	-0.2055	-0.2179	-0.1674	-0.1679	-0.147	-0.138
47	C	0.1468	0.0872	0.1281	0.0494	0.127	0.0255
48	C	0.0843	0.0878	0.0862	0.0993	0.0796	0.1114
49	C	-0.1327	-0.0601	-0.1439	-0.072	-0.1192	-0.0587
50	C	-0.2424	-0.2117	-0.2438	-0.2063	-0.2411	-0.2026
51	C	0.076	0.081	0.0896	0.1034	0.1155	0.1305
52	C	-0.2327	-0.295	-0.2508	-0.324	-0.2677	-0.3485
53	C	0.1131	0.1137	0.1452	0.1419	0.1243	0.1161
54	C	0.1735	0.0778	0.2262	0.1199	0.2663	0.1439
55	C	-0.0901	-0.0507	-0.1028	-0.06	-0.1343	-0.0746
56	B	0.1784	0.3174	0.2895	0.4598	0.3206	0.4865
57	C	-0.2198	-0.3208	-0.2751	-0.379	-0.2293	-0.3136

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Table 20 – continued from previous page

Index	Atom	RESP	MBIS	RESP	MBIS	RESP	MBIS
58	C	-0.2424	-0.2085	-0.2438	-0.2102	-0.2411	-0.2015
59	C	0.076	0.0854	0.0896	0.1113	0.1155	0.1234
60	C	-0.2327	-0.2988	-0.2508	-0.3303	-0.2677	-0.3482
61	C	0.1131	0.1182	0.1452	0.1436	0.1243	0.1192
62	C	-0.2055	-0.2184	-0.1674	-0.1622	-0.147	-0.1414
63	C	0.1468	0.0817	0.1281	0.0409	0.127	0.0358
64	C	0.0844	0.088	0.0862	0.1084	0.0796	0.1104
65	C	-0.1327	-0.0605	-0.1439	-0.079	-0.1192	-0.0582
66	C	-0.3573	-0.2776	-0.2902	-0.1855	-0.2597	-0.1457
67	C	0.191	0.0658	0.1869	0.0357	0.1949	0.0276
68	C	0.0443	0.0148	0.0706	0.0571	0.0657	0.042
69	C	0.1201	0.0491	0.1469	0.0507	0.1393	0.0428
70	C	-0.3554	-0.2521	-0.3327	-0.2006	-0.3097	-0.1754
71	C	-0.1598	-0.1599	-0.1752	-0.1718	-0.1499	-0.1405
72	H	0.1219	0.1401	0.1367	0.1509	0.1528	0.1643
73	H	0.1106	0.1339	0.1292	0.1481	0.1441	0.1596
74	H	0.1506	0.1448	0.1638	0.1535	0.1775	0.1657
75	H	0.1106	0.1344	0.1292	0.1489	0.1441	0.1594
76	H	0.1219	0.1401	0.1367	0.1508	0.1528	0.1639
77	H	0.1421	0.1328	0.157	0.1466	0.1686	0.1554
78	H	0.1301	0.1318	0.1416	0.1432	0.1522	0.1515
79	H	0.1421	0.135	0.157	0.1451	0.1686	0.1564
80	H	0.1301	0.1309	0.1416	0.1417	0.1522	0.1507
81	H	0.1137	0.1319	0.1299	0.1447	0.1435	0.156
82	H	0.1176	0.1311	0.1372	0.1488	0.152	0.16
83	H	0.1137	0.1316	0.1299	0.1458	0.1435	0.1562
84	H	0.1176	0.1314	0.1372	0.1483	0.152	0.1605