1:

**Organic &
Biomolecular Chemistry**

Carbones (−C^{2-}−), carbenes (−C:−) and carbodications (−C^{2+}−) on the magnetic criterion

Erich Kleinpeter* and Andreas Koch

Universität Potsdam, Institut für Chemie, Karl-Liebknecht-Str. 24-25, D-14476 Potsdam(Golm), Germany

Corresponding author: Erich Kleinpeter, E-mail: ekleinp@uni-potsdam.de,

ORCID-ID: https://orcid.org/0000-0001-8993-0033.

Author: Andreas Koch, E-mail: Andreas.Koch@uni-potsdam.de,

ORCID-ID: https://orcid.org/0009-0002-4375-6767.

Electronically Supplementary Information

Table S1. Coordinates and absolute energies of the Compounds 1−11 studied at the MP2/6-311G(d,p) level of theory.

1

MP2= -116,6080181 eV

1	6	1.346200	0.000059	0.000004
2	6	-0.000001	-0.000023	0.000059
3	6	-1.346200	-0.000005	-0.000007
4	1	1.726108	-0.821840	0.676473
5	1	1.726694	0.996606	0.373357

2:

6	1	1.726394	-0.175355	-1.049794
7	1	-1.725796	0.825336	-0.672458
8	1	-1.726770	0.169752	1.050549
9	1	-1.726625	-0.994682	-0.378460

2

MP2= -117,1376369 eV

1	6	-1.142178	0.132494	0.000000
2	6	0.000004	-0.767084	0.000003
3	6	1.142173	0.132489	-0.000014
4	1	-1.190950	0.924242	0.905267
5	1	-2.155017	-0.342229	-0.000003
6	1	-1.190910	0.924273	-0.905260
7	1	1.190900	0.924285	-0.905239
8	1	2.155012	-0.342225	-0.000007
9	1	1.190968	0.924260	0.905309

3

MP2= -117,4255018 eV

1	6	-1.225221	0.162129	-0.016812
2	6	-0.000060	-0.669566	-0.055230
3	6	1.225126	0.162221	-0.016730
4	1	-1.416867	0.170172	1.073632
5	1	-2.093153	-0.340031	-0.449822
6	1	-1.147833	1.205982	-0.356990
7	1	1.147087	1.206956	-0.354045
8	1	2.091924	-0.338887	-0.453286
9	1	1.419771	0.167109	1.073142

4

MP2= -305,6649538 eV

1	6	-2.499399	0.985707	-0.277444
2	7	-1.345046	0.009714	-0.141651
3	6	-0.166471	0.377114	-0.300923
4	7	1.012078	0.744350	-0.460414
5	6	1.843021	1.252499	0.703824
6	6	1.672677	0.699982	-1.826373
7	6	-1.681491	-1.431422	0.195530
8	1	-3.132921	0.594727	-1.075538
9	1	-2.106875	1.972717	-0.519859
10	1	-3.014401	0.980031	0.684802
11	1	2.706953	0.588919	0.770265
12	1	1.241404	1.224877	1.611735
13	1	2.136588	2.270895	0.443373
14	1	0.958412	0.321727	-2.557033
15	1	2.535140	0.039066	-1.723294
16	1	1.974817	1.724921	-2.048698
17	1	-2.325055	-1.787793	-0.610711

3:

18	1	-2.210137	-1.402591	1.149924
19	1	-0.759458	-2.008079	0.261586

5

MP2= -306,0029615 eV

2	7	1.092151	-0.107592	0.614004
3	6	0.017468	0.553963	-0.116431
4	7	-1.234267	0.041240	0.426869
5	6	-2.327705	0.759466	-0.182626
6	6	-1.428952	-1.370566	0.062035
7	6	2.352207	0.276144	0.024665
8	1	1.947579	-0.171240	2.597637
9	1	0.171308	0.133390	2.463026
10	1	1.276795	1.476496	2.048843
11	1	-2.275914	0.672023	-1.304210
12	1	-2.211415	1.821808	0.071918
13	1	-3.294174	0.369252	0.170701
14	1	-0.575426	-1.931318	0.458411
15	1	-1.411201	-1.494426	-1.061017
16	1	-2.376551	-1.791731	0.503393
17	1	3.192500	-0.169111	0.578602
18	1	2.457657	1.397345	0.022684
19	1	2.345650	-0.057143	-1.022110

6

MP2= -306,3115994 eV

1	6	1.487791	-0.869646	0.805567
2	7	1.252167	0.161594	-0.208128
3	6	0.105282	0.422699	-0.879403
4	7	-1.043406	0.062910	-0.258741
5	6	-2.267180	0.225259	-1.032464
6	6	-1.282599	-0.084020	1.179232
7	6	2.477870	0.662797	-0.815672
8	1	2.394879	-1.417386	0.528601
9	1	0.658312	-1.576433	0.813337
10	1	1.632265	-0.466500	1.814593
11	1	-2.871842	-0.688074	-0.988777
12	1	-1.982519	0.426241	-2.063421
13	1	-2.869259	1.058341	-0.645011
14	1	-0.453813	0.350227	1.737945
15	1	-1.429351	-1.123572	1.494411
16	1	-2.189453	0.475782	1.431794
17	1	3.080021	-0.161001	-1.222379
18	1	3.081399	1.198993	-0.074095
19	1	2.195703	1.342156	-1.617649

7

MP2= -116,3051214 eV

4:

1	1	1.869873	-0.658643	0.658868
2	1	-1.869873	-0.659133	-0.658378
3	6	-1.312868	-0.000054	-0.000036
4	6	-0.000000	0.000154	-0.000000
5	6	1.312868	-0.000054	0.000036
6	1	-1.869698	0.658998	0.658592
7	1	1.869698	0.658507	-0.659082

8

MP2= -960,3109898 eV

1	6	4.120055	-0.876856	1.047508
2	6	4.696919	0.127129	0.023400
3	7	3.436150	0.712111	-0.562869
4	6	2.376092	0.039569	-0.227037
5	6	2.641959	-1.136349	0.670724
6	6	3.457454	1.880346	-1.449472
7	6	5.507061	1.234986	0.687774
8	6	5.485004	-0.545005	-1.102015
9	7	1.152075	0.398119	-0.721147
10	6	0.000058	0.000426	-0.597748
11	7	-1.151949	-0.397121	-0.721583
12	6	-2.376039	-0.039166	-0.227254
13	7	-3.435857	-0.712131	-0.562983
14	6	-4.696801	-0.127707	0.023460
15	6	-4.120252	0.876572	1.047457
16	6	-2.642291	1.136653	0.670529
17	6	-3.456770	-1.880382	-1.449580
18	6	-5.506341	-1.235925	0.687955
19	6	-5.485347	0.544058	-1.101856
20	6	-1.720250	1.115828	1.895775
21	6	-2.434857	2.435703	-0.130194
22	6	2.433941	-2.435347	-0.129918
23	6	1.720032	-1.115093	1.896060
24	1	4.166933	-0.436768	2.048926
25	1	4.699945	-1.803414	1.056234
26	1	2.474294	2.001700	-1.902324
27	1	4.210950	1.716230	-2.220719
28	1	3.716948	2.761217	-0.859216
29	1	5.924824	1.931683	-0.044291
30	1	6.343515	0.773668	1.220839
31	1	4.902389	1.785897	1.414767
32	1	6.366499	-1.021997	-0.664322
33	1	5.836700	0.180746	-1.840225
34	1	4.894509	-1.312510	-1.608833
35	1	-4.166854	0.436527	2.048906
36	1	-4.700512	1.802898	1.056182
37	1	-2.473700	-2.001131	-1.902794
38	1	-4.210652	-1.716724	-2.220543
39	1	-3.715507	-2.761412	-0.859228
40	1	-5.923878	-1.932826	-0.044048
41	1	-6.342943	-0.774994	1.221122
42	1	-4.901318	-1.786549	1.414873

5:

43	1	-5.836829	-0.181851	-1.840014
44	1	-4.895268	1.311822	-1.608761
45	1	-6.366993	1.020661	-0.664041
46	1	-2.035268	1.902681	2.587906
47	1	-0.679751	1.319651	1.620271
48	1	-1.773583	0.157019	2.421328
49	1	-2.677626	3.286047	0.514117
50	1	-3.076076	2.479504	-1.014087
51	1	-1.391992	2.543081	-0.448334
52	1	2.676407	-3.285756	0.514421
53	1	3.075088	-2.479453	-1.013849
54	1	1.391012	-2.542327	-0.447988
55	1	0.679444	-1.318593	1.620659
56	1	2.034852	-1.901974	2.588248
57	1	1.773728	-0.156239	2.421493

9

MP2= -381,6820875 eV

1	6	3.235383	0.950262	0.874121
2	6	2.520894	0.000035	0.000060
3	7	1.209863	-0.000141	-0.000307
4	6	-0.000002	-0.000153	-0.000390
5	7	-1.209869	-0.000021	-0.001033
6	6	-2.520906	-0.000040	-0.000068
7	6	-3.235177	-0.950142	0.874312
8	6	-3.236328	0.949943	-0.873568
9	6	3.236103	-0.949901	-0.873689
10	1	4.138465	0.474528	1.271266
11	1	2.611196	1.368378	1.663045
12	1	3.582828	1.764853	0.213368
13	1	-4.138123	-0.474297	1.271638
14	1	-2.610793	-1.368143	1.663144
15	1	-3.582826	-1.764802	0.213762
16	1	-3.583419	1.764404	-0.212422
17	1	-4.139694	0.474064	-1.269895
18	1	-2.612934	1.368252	-1.663003
19	1	2.612278	-1.368815	-1.662462
20	1	3.584516	-1.763867	-0.212686
21	1	4.138745	-0.473445	-1.271038

10

MP2= -349,0410175 eV

1	6	-3.401973	0.858482	-0.957199
2	6	-2.609756	0.000360	0.000291
3	6	-3.402683	-0.858134	0.956887
4	6	-1.283489	-0.000920	-0.000288
5	6	0.000024	0.000010	0.000277
6	1	-4.051520	0.228996	-1.577893
7	6	1.283534	-0.001172	-0.000305
8	6	2.609809	-0.000039	0.000023

6:

9	6	3.403074	-0.956912	-0.857892
10	6	3.401512	0.957693	0.858253
11	1	-2.746901	1.439972	-1.608682
12	1	-4.048764	1.546665	-0.399097
13	1	-4.047195	-1.547953	0.398131
14	1	-4.054556	-0.229032	1.575493
15	1	-2.748102	-1.437979	1.610329
16	1	2.748685	-1.607416	-1.441246
17	1	4.051222	-1.578649	-0.228002
18	1	4.051353	-0.398353	-1.544309
19	1	4.049381	0.399906	1.545687
20	1	2.746110	1.608120	1.440558
21	1	4.049969	1.579506	0.228754

11

MP2= -492,2279820 eV

1	6	-3.731726	1.039377	0.948139
2	7	-3.507641	-0.049985	-0.021933
3	6	-2.333040	-0.458680	-0.380532
4	7	-1.208693	0.113669	0.136247
5	6	-0.000010	-0.014239	-0.000419
6	7	1.208712	0.113702	-0.136546
7	6	2.332953	-0.458741	0.380337
8	7	3.507627	-0.049973	0.022064
9	6	3.731934	1.039432	-0.947866
10	6	4.720234	-0.675184	0.594403
11	6	-4.720356	-0.675075	-0.594111
12	1	-2.777933	1.409965	1.316350
13	1	-4.333545	0.636231	1.764805
14	1	-4.283354	1.830460	0.436233
15	1	-2.253474	-1.267191	-1.105165
16	1	2.253223	-1.267351	1.104843
17	1	4.332682	0.635978	-1.765180
18	1	4.284756	1.829832	-0.436202
19	1	2.778194	1.411058	-1.315168
20	1	5.302881	-1.093496	-0.228133
21	1	4.435902	-1.456887	1.297595
22	1	5.292981	0.104075	1.100095
23	1	-5.293350	0.104325	-1.099310
24	1	-5.302724	-1.093775	0.228427
25	1	-4.436199	-1.456463	-1.297725