Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information for:

Triangulenes and theirs ions: reaching the limits of Clar's rule

*Eduardo Martín Rico-Sotomayor and José Enrique Barquera-Lozada**

Instituto de Química, Universidad Nacional Autónoma de México, Circuito exterior, Ciudad Universitaria, Coyoacán, México, D.F., Mexico.

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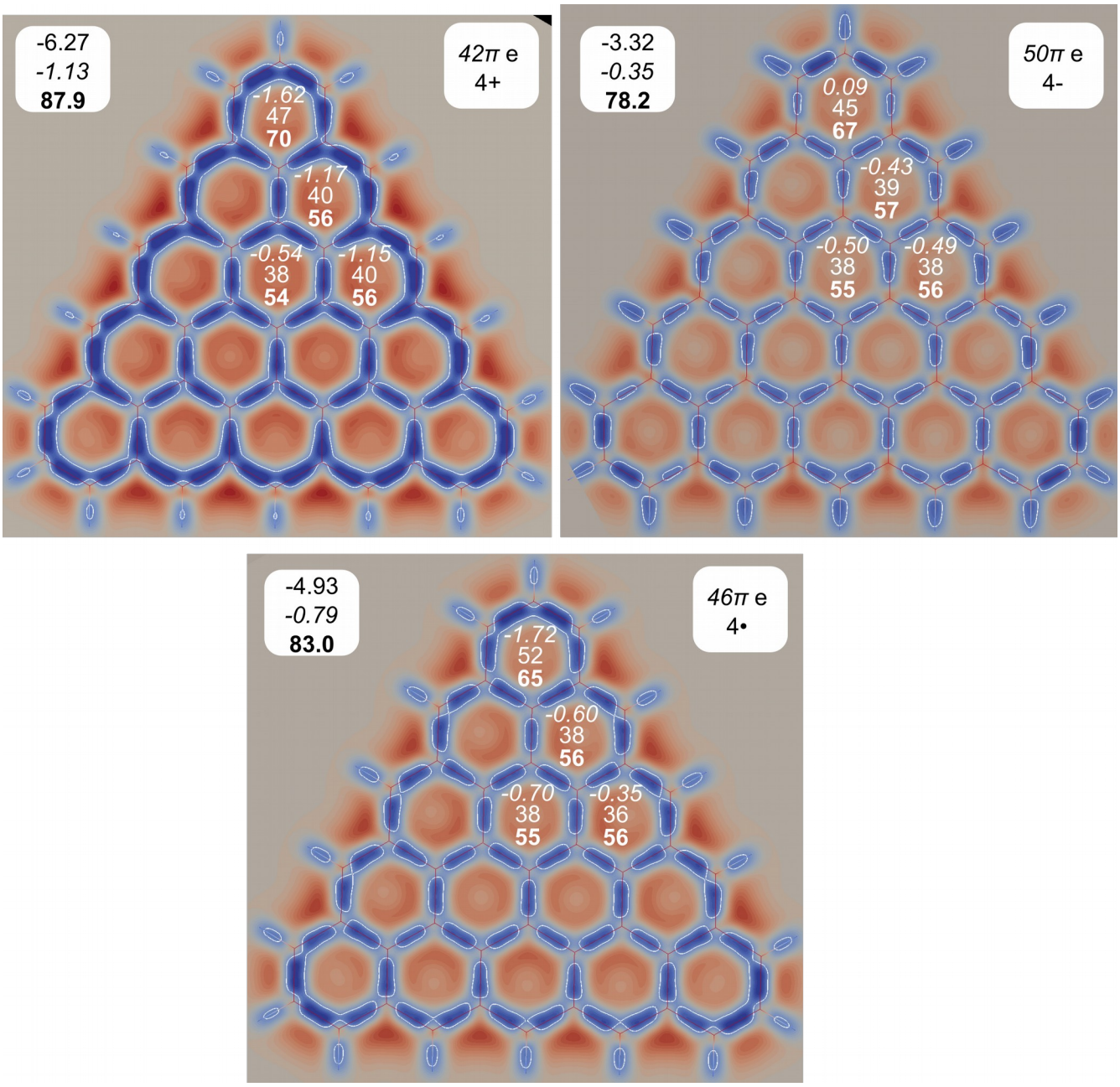

*Figure 1S: tp**J**(**r**) maps of 5-triangulene and its close shell ions. A contour line (white) is drawn at−5.0×10−4a.u. Color code:≤−1.0×10−3a.u. (dark blue), 0.0 a.u. (white) and≥1.0×10−3a.u. (red). The plane is parallel to the molecule at 1.0 Bohr from it. White square: tp**J**(**r**) (normal),C of whole molecule (italic) and 2BDI (bold). White letters:C(italic), PDI (normal) and MDI (bold) of each 6-MR.*

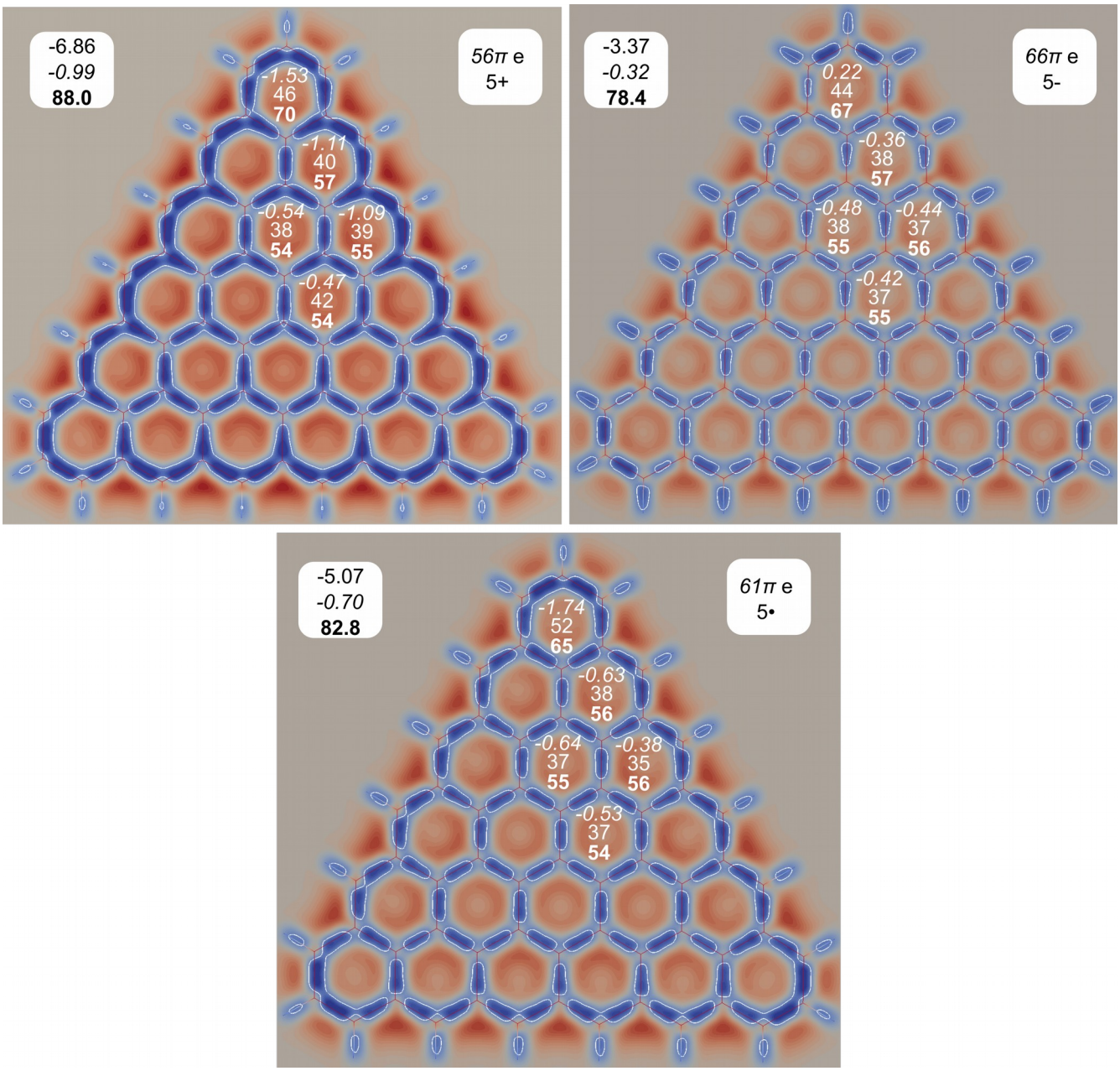

*Figure 2S: tp**J**(**r**) maps of 6-triangulene and its close shell ions. A contour line (white) is drawn at−5.0×10−4a.u. Color code:≤−1.0×10−3a.u. (dark blue), 0.0 a.u. (white) and≥1.0×10−3a.u. (red). The plane is parallel to the molecule at 1.0 Bohr from it. White square: tp**J**(**r**) (normal),C of whole molecule (italic) and 2BDI (bold). White letters:C(italic), PDI (normal) and MDI (bold) of each 6-MR.*

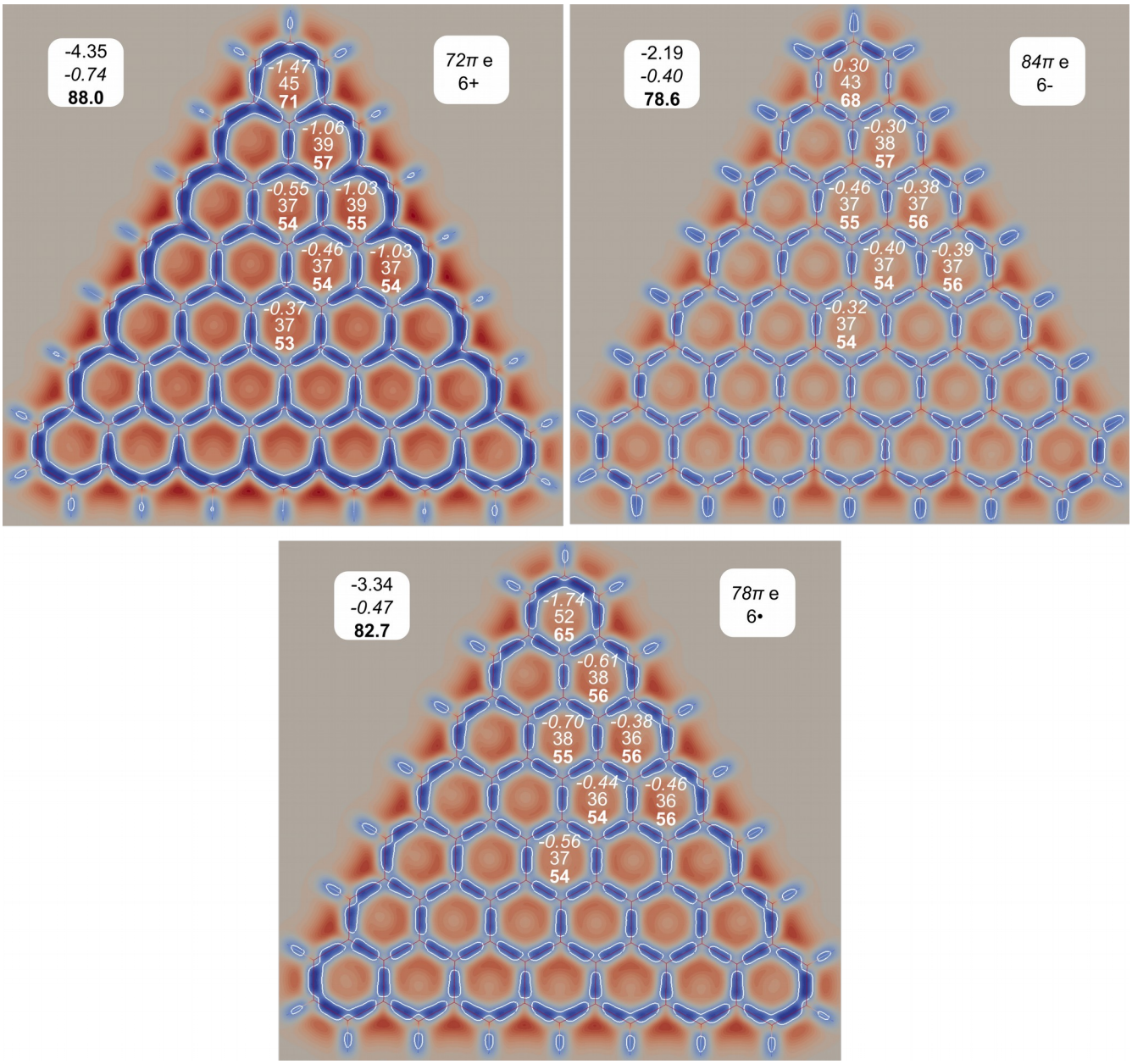

*Figure 3S: tp**J**(**r**) maps of 7-triangulene and its close shell ions. A contour line (white) is drawn at−5.0×10−4a.u. Color code:≤−1.0×10−3a.u. (dark blue), 0.0 a.u. (white) and≥1.0×10−3a.u. (red). The plane is parallel to the molecule at 1.0 Bohr from it. White square: tp**J**(**r**) (normal),C of whole molecule (italic) and 2BDI (bold). White letters:C(italic), PDI (normal) and MDI (bold) of each 6-MR.*

# bonds	cation	DI_{AB} neutral	anion	cation	DI_{BA} neutral	anion
			2-Triangulene			
3	20.2	20.5	22.1	20.2	20.5	22.1
			Pyrene			
3		17.8			37.5	
			Naphtalene			
3		29.5			29.5	
			3-Triangulene			
3	61.4	17.0	18.8	22.7	22.6	24.2
5	3.2	1.3	1.6	1.4	1.3	1.6
			Bisanthene			
3		20.8			34.2	
5		3.4			3.4	
			Anthracene			
3		21.8			40.6	
5		4.6			4.6	
			4-triangulene			
3	16.6	17.4	17.8	23.4	22.3	24.6
5	1.3	1.1	1.5	1.8	1.5	2.0
7	0.1	0.1	0.2	0.1	0.1	0.2
			HBC			
3		32.4			14.3	
5		9.6			1.0	
7		0.2			0.2	
			Tetracene			
3		19.3			46.3	
5		3.3			7.4	
7		1.2			1.2	
			5-Triangulene			
3	15.8	17.7	17.0	23.6	22.3	24.8
5	1.2	1.2	1.4	1.9	1.5	2.1
7	0.1	0.1	0.2	0.2	0.1	0.2
			6-Triangulene			
3	15.3	17.8	16.5	23.8	22.3	25.0
5	1.2	1.2	1.3	1.9	1.5	2.2
7	0.1	0.1	0.2	0.2	0.1	0.2
			7-Triangulene			
3	15.0	17.8	16.2	23.8	22.3	25.1
5	1.1	1.2	1.3	1.9	1.5	2.2
7	0.1	0.1	0.2	0.2	0.1	0.2

Table 1S: DIs at three, five and seven bonds of distance. All DIs in10^{-3}a.u

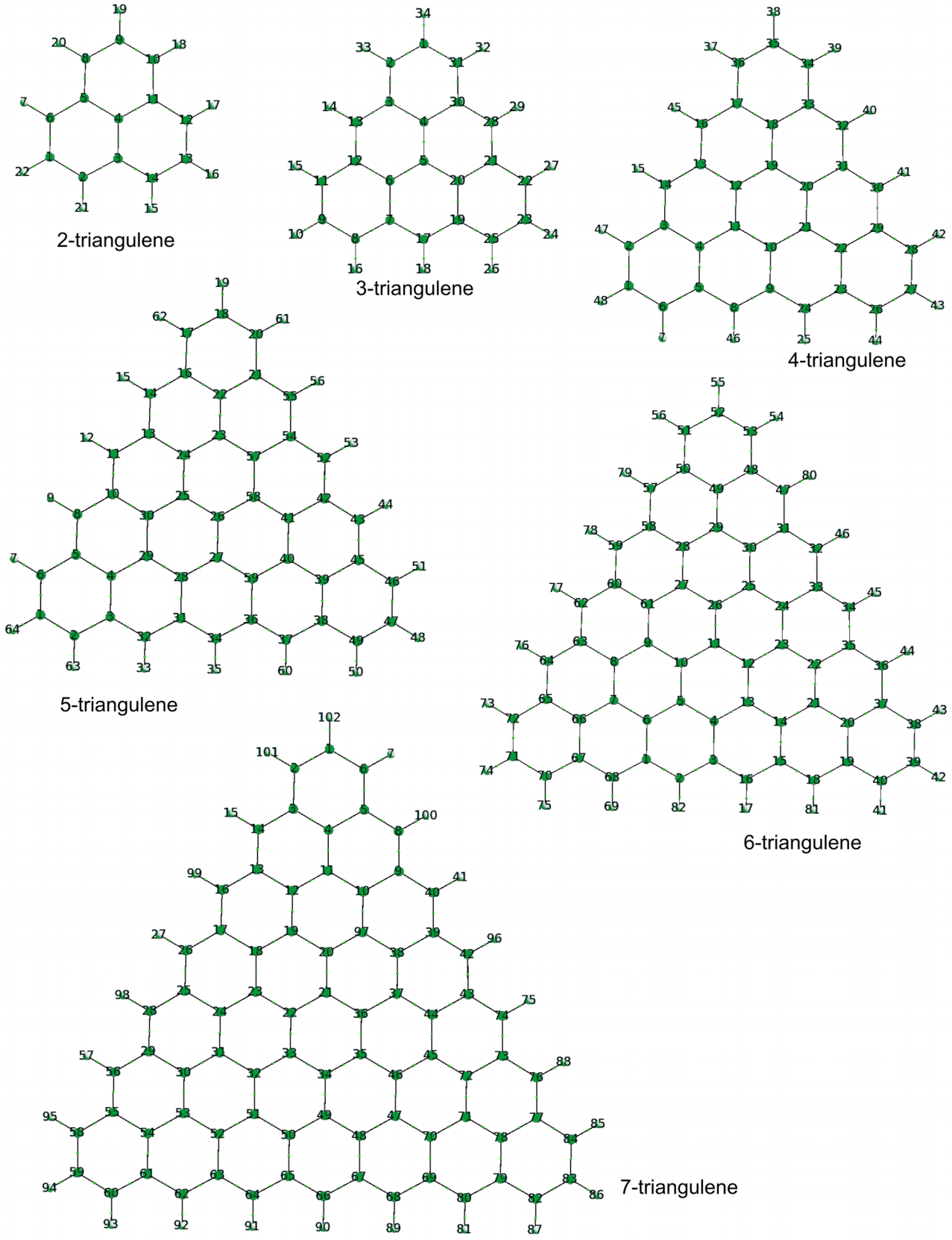

Figure 4S: Atom numbering for tables 2S, 3S, 4S, 5S, 6S, 7S.

Energy	-500.35001	-500.58282		-500.62913
	$q(\Omega_A)$ cation	$q(\Omega_A)$ neutral	spin (Ω_A)	$q(\Omega_A)$ anion
C1	0.0303	-0.0041	-0.0813	-0.0344
C2	0.0178	-0.0160	0.2379	-0.0618
C3	0.0253	0.0036	-0.0702	-0.0136
C4	0.0071	-0.0109	0.0387	-0.0278
C5	0.0254	0.0036	-0.0702	-0.0136
C6	0.0178	-0.0160	0.2379	-0.0621
H7	0.0800	0.0108	-0.0016	-0.0525
C8	0.0178	-0.0159	0.2379	-0.0618
C9	0.0304	-0.0041	-0.0813	-0.0344
C10	0.0178	-0.0158	0.2379	-0.0619
C11	0.0251	0.0033	-0.0702	-0.0138
C12	0.0179	-0.0160	0.2379	-0.0618
C13	0.0304	-0.0041	-0.0813	-0.0344
C14	0.0180	-0.0157	0.2379	-0.0620
H15	0.0800	0.0108	-0.0016	-0.0525
H16	0.0795	0.0142	-0.0005	-0.0473
H17	0.0800	0.0108	-0.0016	-0.0525
H18	0.0800	0.0108	-0.0016	-0.0525
H19	0.0795	0.0142	-0.0005	-0.0473
H20	0.0800	0.0108	-0.0016	-0.0525
H21	0.0800	0.0108	-0.0016	-0.0525
H22	0.0795	0.0142	-0.0005	-0.0473
Total	**0.9995**	**-0.0005**	**1.0000**	**-1.0004**

Table 2S: Atoms in Molecules (AIM) atomic charges ($q(\Omega_A)$) and atomic spin for 2-triangulene and its closed-shell anion and cation. Total energy in a.u.

Energy	-844.65672	-845.23533		-845.22560
	$q(\Omega_A)$ cation	$q(\Omega_A)$ neutral	spin (Ω_A)	$q(\Omega_A)$ anion
C1	0.0475	-0.0030	-0.0965	-0.0473
C2	0.0290	-0.0153	0.2674	-0.0827
C3	0.0372	0.0064	-0.0825	-0.0160
C4	0.0149	-0.0098	0.1212	-0.0342
C5	0.0275	-0.0014	-0.0860	-0.0246
C6	0.0149	-0.0098	0.1212	-0.0342
C7	0.0372	0.0067	-0.0825	-0.0162
C8	0.0290	-0.0152	0.2674	-0.0826
C9	0.0475	-0.0030	-0.0965	-0.0473
H10	0.1128	0.0151	-0.0006	-0.0760
C11	0.0289	-0.0154	0.2674	-0.0830
C12	0.0370	0.0066	-0.0825	-0.0166

C13	0.0277	-0.0166	0.3085	-0.0747
H14	0.1047	0.0087	-0.0033	-0.0770
H15	0.1088	0.0116	-0.0018	-0.0757
H16	0.1088	0.0116	-0.0018	-0.0757
C17	0.0278	-0.0164	0.3085	-0.0746
H18	0.1047	0.0087	-0.0033	-0.0770
C19	0.0372	0.0067	-0.0825	-0.0165
C20	0.0149	-0.0098	0.1212	-0.0341
C21	0.0370	0.0066	-0.0825	-0.0163
C22	0.0290	-0.0154	0.2674	-0.0827
C23	0.0474	-0.0030	-0.0965	-0.0473
H24	0.1128	0.0151	-0.0006	-0.0760
C25	0.0290	-0.0154	0.2674	-0.0829
H26	0.1088	0.0116	-0.0018	-0.0757
H27	0.1088	0.0116	-0.0018	-0.0757
C28	0.0278	-0.0166	0.3085	-0.0747
H29	0.1047	0.0087	-0.0033	-0.0770
C30	0.0371	0.0068	-0.0825	-0.0167
C31	0.0289	-0.0154	0.2674	-0.0828
H32	0.1088	0.0116	-0.0018	-0.0757
H33	0.1088	0.0116	-0.0018	-0.0757
H34	0.1128	0.0151	-0.0006	-0.0760
Total	**1.9996**	**-0.0013**	**2.0000**	**-2.0014**

Table 3S: Atoms in Molecules (AIM) atomic charges ($q(\Omega_A)$) and atomic spin for 3-triangulene and its closed-shell anion and cation. Total energy in a.u.

Energy	-1,265.10950	-1,266.09395		-1,265.97157
	$q(\Omega_A)$ cation	$q(\Omega_A)$ neutral	spin (Ω_A)	$q(\Omega_A)$ anion
C1	0.0569	-0.0026	-0.0975	-0.0548
C2	0.0341	-0.0150	0.2633	-0.0936
C3	0.0414	0.0071	-0.0855	-0.0187
C4	0.0173	-0.0098	0.1468	-0.0383
C5	0.0421	0.0074	-0.0855	-0.0189
C6	0.0342	-0.0151	0.2633	-0.0938
H7	0.1242	0.0120	-0.0018	-0.0877
C8	0.0334	-0.0161	0.3259	-0.0827
C9	0.0423	0.0091	-0.0883	-0.0167
C10	0.0200	-0.0069	0.1292	-0.0336
C11	0.0305	-0.0007	-0.0865	-0.0258
C12	0.0200	-0.0069	0.1292	-0.0336
C13	0.0420	0.0090	-0.0883	-0.0170
C14	0.0333	-0.0160	0.3260	-0.0826
H15	0.1170	0.0093	-0.0036	-0.0870

C16	0.0332	-0.0160	0.3260	-0.0826
C17	0.0418	0.0073	-0.0855	-0.0189
C18	0.0174	-0.0098	0.1468	-0.0384
C19	0.0305	-0.0007	-0.0865	-0.0258
C20	0.0201	-0.0069	0.1292	-0.0335
C21	0.0305	-0.0007	-0.0865	-0.0258
C22	0.0174	-0.0098	0.1468	-0.0383
C23	0.0416	0.0073	-0.0855	-0.0185
C24	0.0334	-0.0161	0.3259	-0.0827
H25	0.1169	0.0095	-0.0035	-0.0869
C26	0.0342	-0.0149	0.2633	-0.0935
C27	0.0571	-0.0026	-0.0975	-0.0547
C28	0.0338	-0.0150	0.2633	-0.0938
C29	0.0420	0.0071	-0.0855	-0.0189
C30	0.0329	-0.0160	0.3260	-0.0826
C31	0.0424	0.0088	-0.0883	-0.0167
C32	0.0327	-0.0160	0.3260	-0.0826
C33	0.0417	0.0070	-0.0855	-0.0182
C34	0.0336	-0.0148	0.2634	-0.0936
C35	0.0572	-0.0028	-0.0976	-0.0547
C36	0.0341	-0.0149	0.2634	-0.0936
H37	0.1242	0.0118	-0.0018	-0.0878
H38	0.1317	0.0156	-0.0006	-0.0921
H39	0.1245	0.0118	-0.0018	-0.0878
H40	0.1172	0.0093	-0.0036	-0.0870
H41	0.1172	0.0093	-0.0036	-0.0870
H42	0.1245	0.0119	-0.0018	-0.0877
H43	0.1317	0.0154	-0.0006	-0.0921
H44	0.1242	0.0120	-0.0018	-0.0877
H45	0.1169	0.0093	-0.0036	-0.0870
H46	0.1170	0.0095	-0.0035	-0.0869
H47	0.1242	0.0119	-0.0018	-0.0877
H48	0.1320	0.0154	-0.0006	-0.0921
Total	**2.9982**	**-0.0019**	**3.0000**	**-3.0018**

Table 4S: Atoms in Molecules (AIM) atomic charges ($q(\Omega_A)$) and atomic spin for 4-triangulene and its closed-shell anion and cation. Total energy in a.u.

Energy	-1,761.72918	-1,763.15750		-1,762.88717
	$q(\Omega_A)$ cation	$q(\Omega_A)$ neutral	spin (Ω_A)	$q(\Omega_A)$ anion
C1	0.0626	-0.0026	-0.0969	-0.0589
C2	0.0369	-0.0148	0.2604	-0.1004
C3	0.0445	0.0071	-0.0853	-0.0202
C4	0.0187	-0.0096	0.1461	-0.0408

C5	0.0447	0.0075	-0.0853	-0.0198
C6	0.0364	-0.0149	0.2604	-0.1004
H7	0.1340	0.0123	-0.0018	-0.0950
C8	0.0352	-0.0158	0.3231	-0.0869
H9	0.1243	0.0097	-0.0035	-0.0926
C10	0.0439	0.0094	-0.0897	-0.0178
C11	0.0353	-0.0152	0.3336	-0.0849
H12	0.1223	0.0101	-0.0038	-0.0903
C13	0.0442	0.0094	-0.0897	-0.0180
C14	0.0354	-0.0157	0.3231	-0.0870
H15	0.1243	0.0097	-0.0035	-0.0926
C16	0.0447	0.0074	-0.0853	-0.0200
C17	0.0365	-0.0147	0.2604	-0.1005
C18	0.0626	-0.0025	-0.0969	-0.0590
H19	0.1435	0.0157	-0.0006	-0.1022
C20	0.0370	-0.0146	0.2604	-0.1005
C21	0.0443	0.0073	-0.0853	-0.0201
C22	0.0187	-0.0095	0.1461	-0.0407
C23	0.0316	-0.0005	-0.0869	-0.0262
C24	0.0211	-0.0068	0.1428	-0.0346
C25	0.0305	-0.0003	-0.0844	-0.0258
C26	0.0244	-0.0028	0.1012	-0.0304
C27	0.0305	-0.0003	-0.0844	-0.0258
C28	0.0211	-0.0068	0.1428	-0.0345
C29	0.0317	-0.0006	-0.0869	-0.0262
C30	0.0210	-0.0068	0.1428	-0.0346
C31	0.0440	0.0094	-0.0896	-0.0178
C32	0.0357	-0.0157	0.3232	-0.0867
H33	0.1239	0.0095	-0.0035	-0.0926
C34	0.0359	-0.0151	0.3337	-0.0848
H35	0.1219	0.0100	-0.0039	-0.0903
C36	0.0437	0.0094	-0.0897	-0.0177
C37	0.0357	-0.0156	0.3233	-0.0868
C38	0.0442	0.0076	-0.0853	-0.0197
C39	0.0187	-0.0096	0.1462	-0.0408
C40	0.0316	-0.0005	-0.0869	-0.0262
C41	0.0210	-0.0068	0.1428	-0.0345
C42	0.0442	0.0091	-0.0897	-0.0179
C43	0.0358	-0.0156	0.3233	-0.0870
H44	0.1240	0.0095	-0.0035	-0.0926
C45	0.0447	0.0071	-0.0853	-0.0203
C46	0.0369	-0.0145	0.2605	-0.1005
C47	0.0623	-0.0026	-0.0969	-0.0592
H48	0.1438	0.0159	-0.0006	-0.1021
C49	0.0369	-0.0146	0.2605	-0.1003
H50	0.1336	0.0121	-0.0018	-0.0951
H51	0.1336	0.0121	-0.0018	-0.0951

C52	0.0359	-0.0151	0.3337	-0.0850
H53	0.1219	0.0100	-0.0039	-0.0903
C54	0.0438	0.0091	-0.0896	-0.0180
C55	0.0357	-0.0156	0.3232	-0.0869
H56	0.1239	0.0095	-0.0035	-0.0926
C57	0.0210	-0.0068	0.1428	-0.0345
C58	0.0305	-0.0004	-0.0844	-0.0258
C59	0.0210	-0.0068	0.1428	-0.0345
H60	0.1240	0.0095	-0.0035	-0.0926
H61	0.1337	0.0121	-0.0018	-0.0950
H62	0.1340	0.0123	-0.0018	-0.0950
H63	0.1337	0.0121	-0.0018	-0.0950
H64	0.1435	0.0157	-0.0006	-0.1022
Total	**3.9967**	**-0.0025**	**4.0000**	**-4.0024**

Table 5S: Atoms in Molecules (AIM) atomic charges ($q(\Omega_A)$) and atomic spin for 5-triangulene and its closed-shell anion and cation. Total energy in a.u.

Energy	-2,334.52804	-2,336.42573		-2,335.98330
	$q(\Omega_A)$ cation	$q(\Omega_A)$ neutral	spin (Ω_A)	$q(\Omega_A)$ anion
C1	0.0452	0.0092	-0.0890	-0.0185
C2	0.0369	-0.0147	0.3298	-0.0864
C3	0.0444	0.0094	-0.0909	-0.0183
C4	0.0210	-0.0066	0.1470	-0.0339
C5	0.0301	-0.0002	-0.0826	-0.0255
C6	0.0216	-0.0067	0.1431	-0.0352
C7	0.0324	-0.0003	-0.0861	-0.0266
C8	0.0215	-0.0067	0.1431	-0.0352
C9	0.0301	-0.0002	-0.0826	-0.0255
C10	0.0245	-0.0025	0.1030	-0.0297
C11	0.0288	-0.0003	-0.0784	-0.0254
C12	0.0245	-0.0025	0.1030	-0.0297
C13	0.0301	-0.0002	-0.0826	-0.0255
C14	0.0216	-0.0067	0.1431	-0.0352
C15	0.0447	0.0092	-0.0890	-0.0185
C16	0.0368	-0.0147	0.3298	-0.0863
H17	0.1249	0.0102	-0.0038	-0.0926
C18	0.0371	-0.0154	0.3202	-0.0895
C19	0.0460	0.0072	-0.0847	-0.0209
C20	0.0196	-0.0095	0.1431	-0.0422
C21	0.0324	-0.0003	-0.0861	-0.0266
C22	0.0216	-0.0067	0.1431	-0.0352
C23	0.0302	-0.0002	-0.0826	-0.0255
C24	0.0210	-0.0065	0.1470	-0.0339
C25	0.0301	-0.0002	-0.0826	-0.0255
C26	0.0245	-0.0025	0.1030	-0.0297

C27	0.0301	-0.0002	-0.0826	-0.0255
C28	0.0216	-0.0067	0.1431	-0.0352
C29	0.0325	-0.0003	-0.0861	-0.0266
C30	0.0215	-0.0066	0.1431	-0.0352
C31	0.0450	0.0095	-0.0890	-0.0183
C32	0.0362	-0.0148	0.3297	-0.0863
C33	0.0445	0.0097	-0.0910	-0.0181
C34	0.0363	-0.0148	0.3297	-0.0863
C35	0.0452	0.0095	-0.0890	-0.0186
C36	0.0367	-0.0155	0.3201	-0.0896
C37	0.0463	0.0074	-0.0847	-0.0207
C38	0.0382	-0.0145	0.2591	-0.1049
C39	0.0661	-0.0025	-0.0963	-0.0619
C40	0.0385	-0.0145	0.2592	-0.1049
H41	0.1397	0.0123	-0.0018	-0.0997
H42	0.1513	0.0160	-0.0006	-0.1088
H43	0.1401	0.0125	-0.0017	-0.0997
H44	0.1288	0.0099	-0.0035	-0.0962
H45	0.1252	0.0104	-0.0038	-0.0925
H46	0.1252	0.0104	-0.0038	-0.0925
C47	0.0366	-0.0155	0.3201	-0.0895
C48	0.0464	0.0075	-0.0847	-0.0206
C49	0.0195	-0.0095	0.1431	-0.0423
C50	0.0462	0.0072	-0.0847	-0.0210
C51	0.0385	-0.0145	0.2592	-0.1048
C52	0.0661	-0.0025	-0.0963	-0.0618
C53	0.0380	-0.0147	0.2591	-0.1048
H54	0.1401	0.0125	-0.0017	-0.0997
H55	0.1513	0.0160	-0.0006	-0.1088
H56	0.1397	0.0123	-0.0018	-0.0997
C57	0.0371	-0.0154	0.3202	-0.0893
C58	0.0450	0.0094	-0.0890	-0.0185
C59	0.0368	-0.0148	0.3298	-0.0861
C60	0.0441	0.0096	-0.0909	-0.0179
C61	0.0210	-0.0065	0.1470	-0.0338
C62	0.0368	-0.0148	0.3298	-0.0862
C63	0.0447	0.0094	-0.0890	-0.0182
C64	0.0370	-0.0154	0.3203	-0.0895
C65	0.0460	0.0075	-0.0847	-0.0205
C66	0.0196	-0.0095	0.1431	-0.0423
C67	0.0464	0.0071	-0.0847	-0.0211
C68	0.0371	-0.0154	0.3203	-0.0897
H69	0.1285	0.0097	-0.0035	-0.0962
C70	0.0385	-0.0143	0.2593	-0.1049
C71	0.0658	-0.0027	-0.0963	-0.0621
C72	0.0385	-0.0144	0.2593	-0.1048
H73	0.1397	0.0123	-0.0018	-0.0998

H74	0.1517	0.0161	-0.0006	-0.1088
H75	0.1397	0.0123	-0.0018	-0.0998
H76	0.1285	0.0097	-0.0035	-0.0962
H77	0.1249	0.0102	-0.0038	-0.0926
H78	0.1249	0.0102	-0.0038	-0.0926
H79	0.1284	0.0097	-0.0035	-0.0962
H80	0.1288	0.0099	-0.0035	-0.0962
H81	0.1284	0.0097	-0.0035	-0.0962
H82	0.1249	0.0102	-0.0038	-0.0926
Total	**4.9956**	**-0.0035**	**5.0000**	**-5.0039**

Table 6S: Atoms in Molecules (AIM) atomic charges ($q(\Omega_A)$) and atomic spin for 6-triangulene and its closed-shell anion and cation. Total energy in a.u.

Energy	-2,983.51239	-2,985.89859		-2,985.26302
	$q(\Omega_A)$ cation	$q(\Omega_A)$ neutral	spin (Ω_A)	$q(\Omega_A)$ anion
C1	0.0682	-0.0025	-0.0960	-0.0641
C2	0.0390	-0.0142	0.2591	-0.1081
C3	0.0470	0.0071	-0.0842	-0.0214
C4	0.0204	-0.0094	0.1421	-0.0429
C5	0.0479	0.0076	-0.0842	-0.0211
C6	0.0392	-0.0142	0.2591	-0.1079
H7	0.1440	0.0124	-0.0018	-0.1029
C8	0.0378	-0.0153	0.3194	-0.0918
C9	0.0463	0.0094	-0.0883	-0.0185
C10	0.0222	-0.0066	0.1399	-0.0354
C11	0.0331	-0.0003	-0.0850	-0.0267
C12	0.0221	-0.0066	0.1399	-0.0354
C13	0.0458	0.0091	-0.0883	-0.0186
C14	0.0374	-0.0151	0.3194	-0.0913
H15	0.1316	0.0099	-0.0035	-0.0986
C16	0.0370	-0.0144	0.3271	-0.0873
C17	0.0447	0.0092	-0.0900	-0.0179
C18	0.0210	-0.0064	0.1449	-0.0334
C19	0.0302	-0.0002	-0.0810	-0.0251
C20	0.0246	-0.0024	0.1030	-0.0292
C21	0.0279	-0.0004	-0.0742	-0.0245
C22	0.0240	-0.0022	0.0963	-0.0279
C23	0.0293	-0.0001	-0.0800	-0.0246
C24	0.0211	-0.0064	0.1449	-0.0334
C25	0.0447	0.0092	-0.0900	-0.0178
C26	0.0368	-0.0140	0.3230	-0.0861
H27	0.1255	0.0104	-0.0038	-0.0927
C28	0.0373	-0.0144	0.3271	-0.0873
C29	0.0460	0.0091	-0.0883	-0.0184
C30	0.0222	-0.0066	0.1399	-0.0354

C31	0.0303	-0.0002	-0.0810	-0.0251
C32	0.0246	-0.0024	0.1030	-0.0292
C33	0.0279	-0.0004	-0.0742	-0.0245
C34	0.0240	-0.0022	0.0963	-0.0279
C35	0.0279	-0.0004	-0.0742	-0.0245
C36	0.0240	-0.0022	0.0963	-0.0279
C37	0.0293	-0.0001	-0.0800	-0.0245
C38	0.0210	-0.0064	0.1449	-0.0334
C39	0.0452	0.0095	-0.0900	-0.0180
C40	0.0373	-0.0145	0.3271	-0.0877
H41	0.1269	0.0103	-0.0038	-0.0941
C42	0.0368	-0.0141	0.3230	-0.0864
C43	0.0451	0.0095	-0.0900	-0.0182
C44	0.0210	-0.0064	0.1449	-0.0334
C45	0.0303	-0.0002	-0.0810	-0.0251
C46	0.0246	-0.0024	0.1030	-0.0292
C47	0.0303	-0.0002	-0.0810	-0.0252
C48	0.0210	-0.0064	0.1449	-0.0333
C49	0.0293	-0.0001	-0.0800	-0.0246
C50	0.0210	-0.0064	0.1449	-0.0334
C51	0.0303	-0.0002	-0.0810	-0.0252
C52	0.0221	-0.0066	0.1399	-0.0354
C53	0.0331	-0.0003	-0.0850	-0.0267
C54	0.0204	-0.0094	0.1421	-0.0430
C55	0.0477	0.0073	-0.0842	-0.0212
C56	0.0379	-0.0151	0.3194	-0.0915
H57	0.1317	0.0099	-0.0035	-0.0986
C58	0.0392	-0.0144	0.2590	-0.1079
C59	0.0685	-0.0022	-0.0959	-0.0642
C60	0.0392	-0.0145	0.2590	-0.1080
C61	0.0475	0.0073	-0.0842	-0.0215
C62	0.0379	-0.0154	0.3193	-0.0914
C63	0.0458	0.0093	-0.0883	-0.0184
C64	0.0373	-0.0147	0.3269	-0.0872
C65	0.0446	0.0095	-0.0900	-0.0178
C66	0.0369	-0.0143	0.3229	-0.0859
C67	0.0446	0.0095	-0.0900	-0.0177
C68	0.0374	-0.0147	0.3269	-0.0871
C69	0.0459	0.0093	-0.0883	-0.0183
C70	0.0221	-0.0066	0.1399	-0.0354
C71	0.0331	-0.0003	-0.0850	-0.0267
C72	0.0221	-0.0066	0.1399	-0.0354
C73	0.0460	0.0093	-0.0883	-0.0186
C74	0.0373	-0.0144	0.3271	-0.0875
H75	0.1269	0.0103	-0.0038	-0.0941
C76	0.0377	-0.0152	0.3194	-0.0916
C77	0.0474	0.0071	-0.0842	-0.0216

C78	0.0204	-0.0094	0.1421	-0.0429
C79	0.0476	0.0075	-0.0842	-0.0210
C80	0.0379	-0.0155	0.3193	-0.0912
H81	0.1316	0.0101	-0.0034	-0.0985
C82	0.0394	-0.0147	0.2590	-0.1078
C83	0.0681	-0.0023	-0.0959	-0.0640
C84	0.0393	-0.0144	0.2590	-0.1083
H85	0.1439	0.0125	-0.0018	-0.1029
H86	0.1569	0.0161	-0.0006	-0.1133
H87	0.1440	0.0126	-0.0018	-0.1028
H88	0.1315	0.0099	-0.0035	-0.0986
H89	0.1269	0.0105	-0.0038	-0.0939
H90	0.1254	0.0106	-0.0038	-0.0926
H91	0.1269	0.0105	-0.0038	-0.0939
H92	0.1316	0.0101	-0.0034	-0.0984
H93	0.1440	0.0126	-0.0018	-0.1028
H94	0.1568	0.0161	-0.0006	-0.1134
H95	0.1441	0.0125	-0.0018	-0.1029
H96	0.1254	0.0104	-0.0038	-0.0927
C97	0.0303	-0.0002	-0.0810	-0.0251
H98	0.1270	0.0103	-0.0038	-0.0940
H99	0.1270	0.0103	-0.0038	-0.0940
H100	0.1316	0.0099	-0.0035	-0.0986
H101	0.1440	0.0124	-0.0018	-0.1029
H102	0.1569	0.0163	-0.0006	-0.1132
Total	**6.0107**	**-0.0046**	**6.0000**	**-5.9992**

Table 7S: Atoms in Molecules (AIM) atomic charges ($q(\Omega_A)$) and atomic spin for 7-triangulene and its closed-shell anion and cation. Total energy in a.u.