

Synthesis, characterisation and theoretical calculations of 2,6-diaminopurine etheno derivatives

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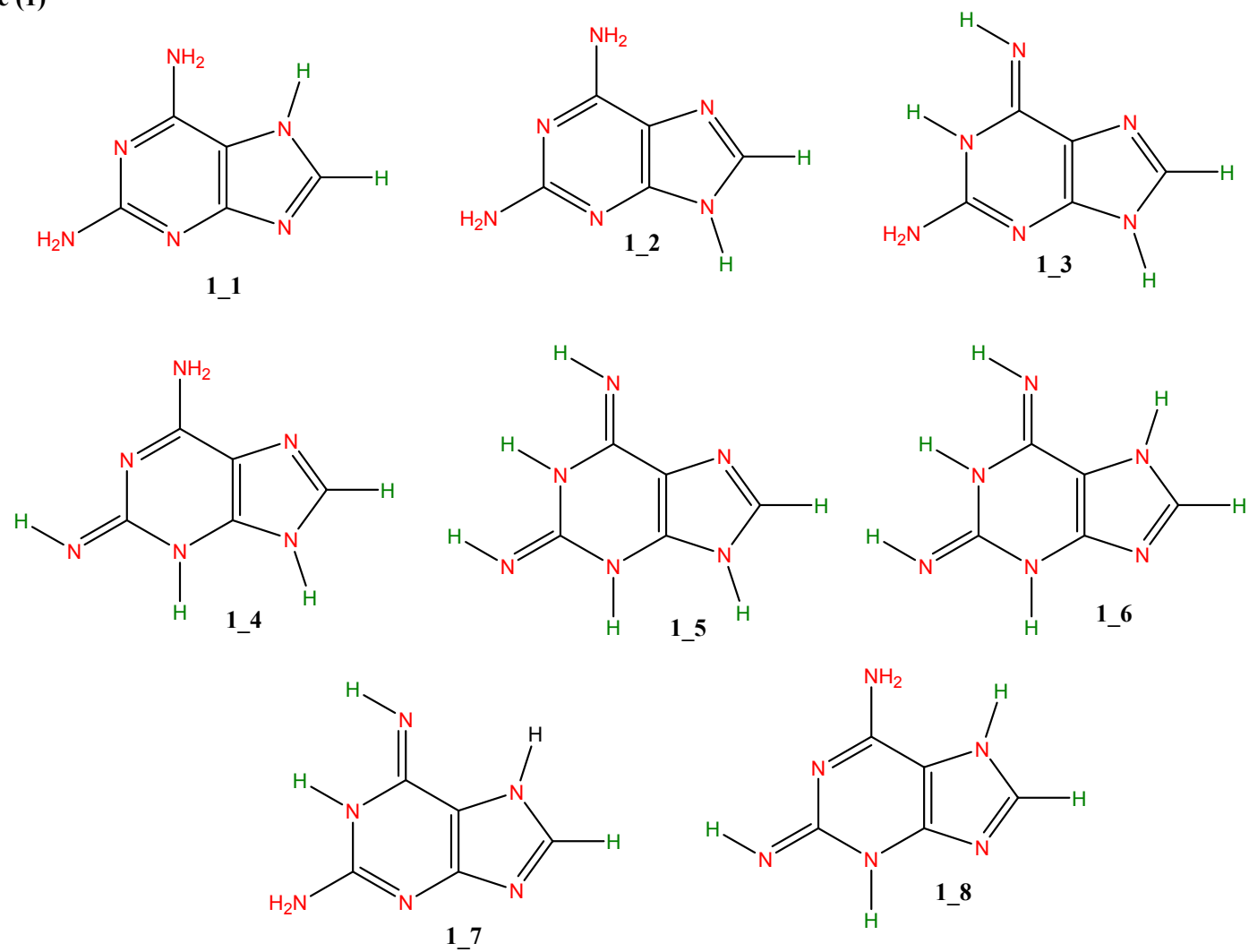
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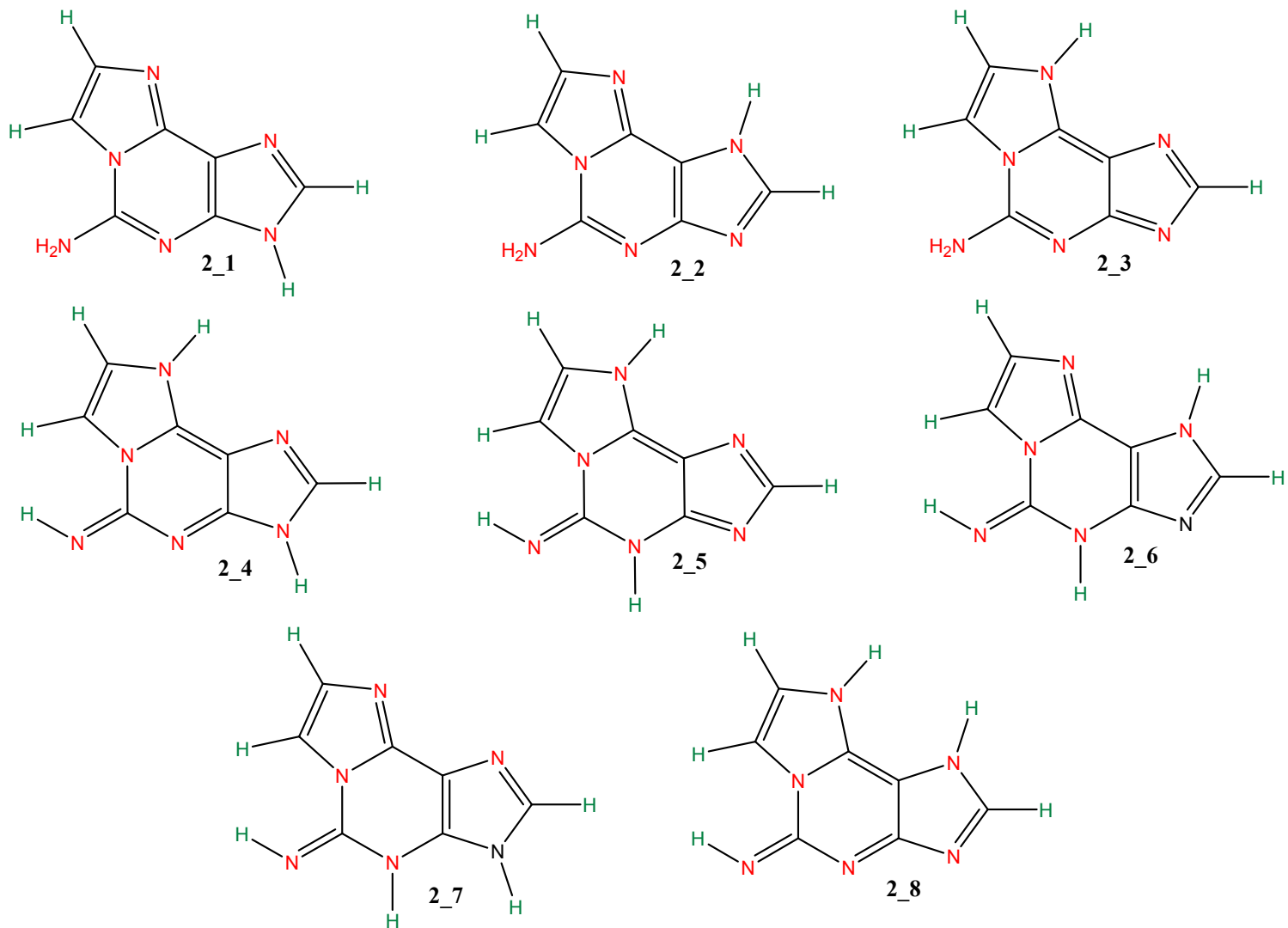
Modelling

All tautomers for compounds 1–5

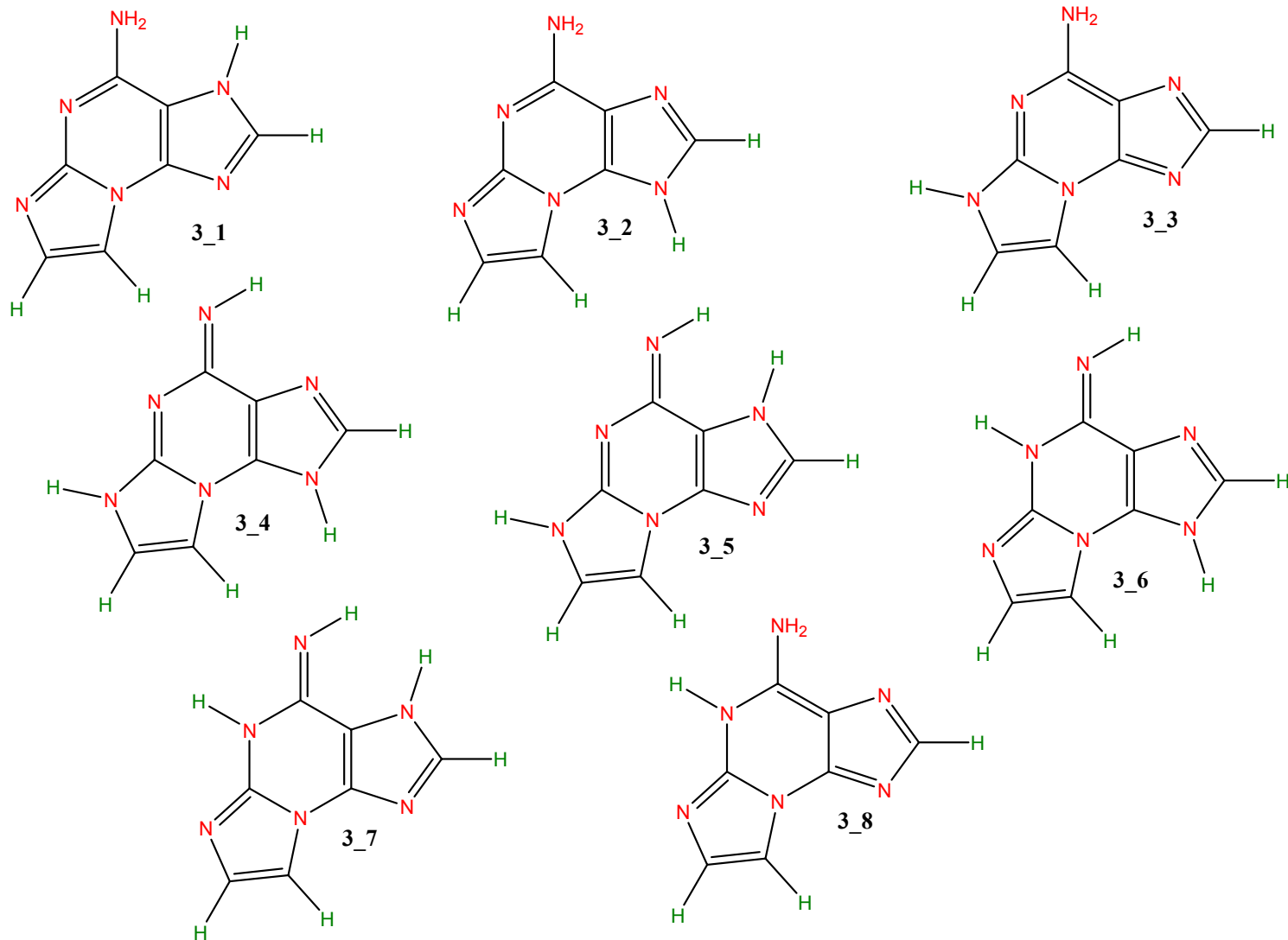
2,6-Diaminopurine (1)



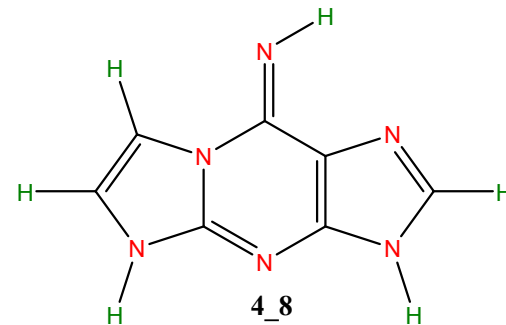
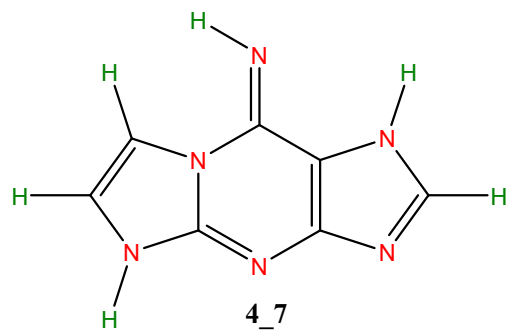
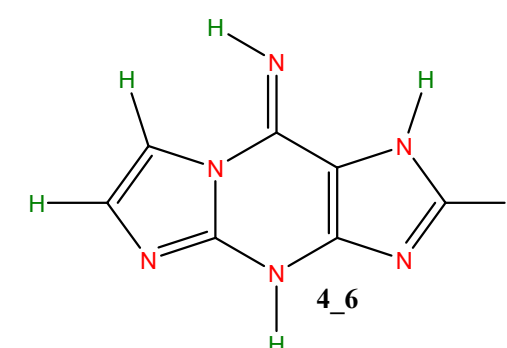
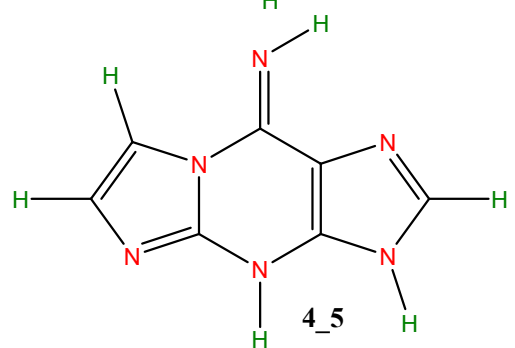
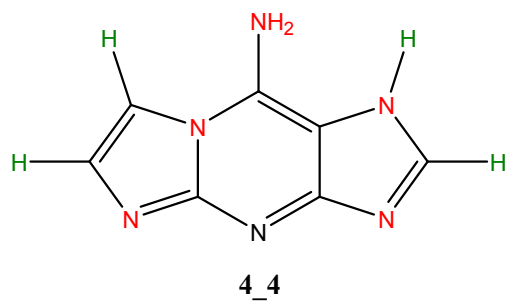
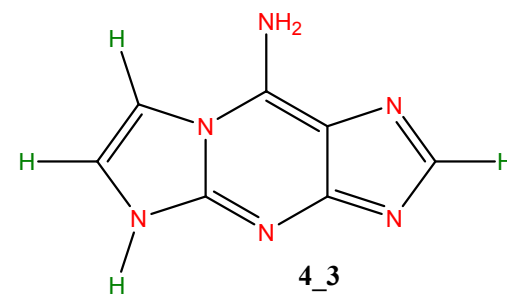
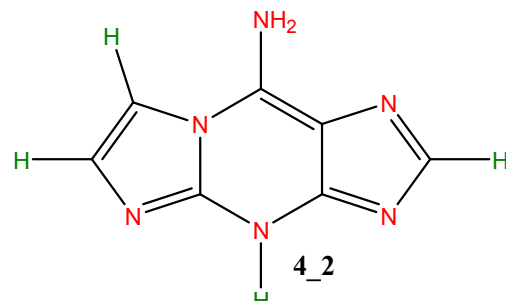
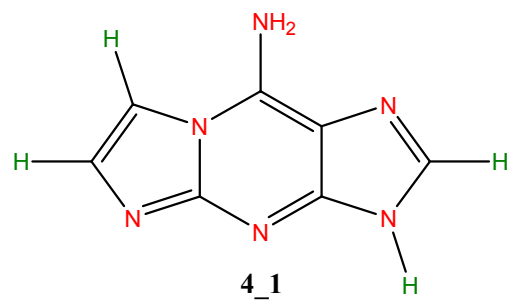
5-Aminoimidazo[2,1-*i*]purine (2)



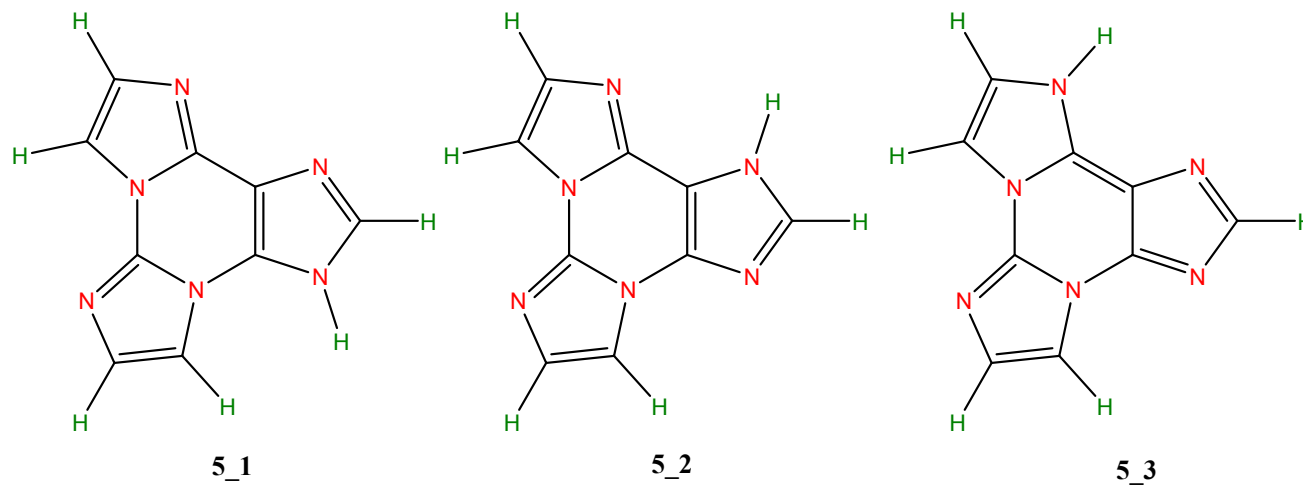
9-Aminoimidazo[2,1-*b*]purine (3)



9-Aminoimidazo[1,2-*a*]purine (4)



Diimidazo[2,1-*b*:2',1'-*i*]purine (5)



Calculated energies for all tautomers:

3 4a, 3 4b *etc.* refer to different configurations of the =N-H group in the same tautomeric form.

	HF/TZP	kcal/mol	MP2	kcal/mol	B3LYP	kcal/mol	HF/SCI	kcal/mol	B3/SCI	kcal/mol	MP2/SCI	kcal/mol
4 1	-595.397	2.12	-597.161	0.00	-599.017	0.00	-595.421	0.00	-599.037	0.00		
4 2	-595.393	4.59	-597.153	5.09	-599.009	4.73	-595.413	4.84	-599.027	6.16		
4 3	-595.384	10.36	-597.146	9.29	-599.002	9.46						
4 4	-595.375	15.60	-597.143	11.44	-598.998	11.82						
4 5a	-595.389	7.08	-597.15	7.01	-599.004	8.18						
4 5b	-595.378	13.54										
4 6a	-595.393	4.74										
4 6b	-595.395	3.28	-597.156	3.24	-599.012	3.16	-595.412	5.22	-599.026	6.67		
4 7a	-595.389	6.87	-597.149	7.32	-599.007	5.87						
4 7b	-595.387	8.31										
4 8a	-595.4	0.00	-597.159	1.40	-599.016	0.56	-595.419	0.77	-599.033	2.57		
4 8b	-595.385	9.26										
3 1	-595.396	6.56	-597.164	1.98	-599.016	4.20	-595.422	3.70	-599.038	2.20	-597.186	1.04
3 2	-595.397	6.08	-597.161	4.02	-599.015	4.58	-595.422	3.79	-599.037	2.98	-597.184	2.37
3 3	-595.406	0.00	-597.167	0.00	-599.023	0.00	-595.428	0.00	-599.042	0.00	-597.188	0.00
3 4a	-595.363	27.56	-597.123	28.06	-598.981	26.14	-595.397	19.44	-599.011	19.14		
3 4b	-595.362	28.00										
3 5	-595.388	11.68	-597.149	11.62	-599.006	10.45	-595.409	11.94				
3 6a	-595.386	12.90	-597.146	13.23	-599.002	13.04	-595.408	12.48				

3_6b	-595.377	18.54											
3_7a	-595.394	7.63	-597.156	6.79	-599.01	7.58	-595.413	9.33					
3_7b	-595.391	9.99											
3_8	-595.395	7.32	-597.157	6.70	-599.011	7.39	-595.417	6.74					
1_1	-519.68	10.27	-521.196	8.32	-522.814	8.95							
1_2	-519.696	0.00	-521.209	0.00	-522.829	0.00							
1_3	-519.671	15.92	-521.186	14.16	-522.806	14.44							
1_4	-519.657	24.53	-521.171	23.83	-522.794	21.59							
1_5	-519.649	29.94	-521.163	28.75	-522.785	27.56							
1_6	-519.653	27.22	-521.168	25.51	-522.79	24.18							
1_7	-519.66	22.72	-521.179	19.02	-522.797	19.96							
1_8	-519.654	26.81	-521.169	24.81	-522.792	23.00							
2_1	-595.405	0.00	-597.171	0.83	-599.022	0.34	-595.428	0.00	-599.042	0.00	-597.191	0.00	
2_2	-595.405	0.44	-597.172	0.00	-599.023	0.00	-595.426	1.55	-599.041	0.78	-597.191	0.50	
2_3	-595.379	16.29	-597.145	16.67	-598.998	15.21							
2_4	-595.385	12.87	-597.143	17.91	-599.004	11.85							
2_5	-595.374	19.62	-597.132	25.14	-598.992	19.10							
2_6	-595.395	6.82	-597.158	9.03	-599.013	6.22							
2_7	-595.382	14.53	-597.144	17.46	-598.999	14.74							
2_8	-595.361	28.09	-597.12	32.62	-598.982	25.37							
5_1	-671.124	9.3	-673.135	10.32					-673.157	4.92			
5_2	-671.139	0.00	-673.151	0.00					-673.164	0.00			
5_3	-671.122	10.17	-673.131	12.42					-673.152	7.93			

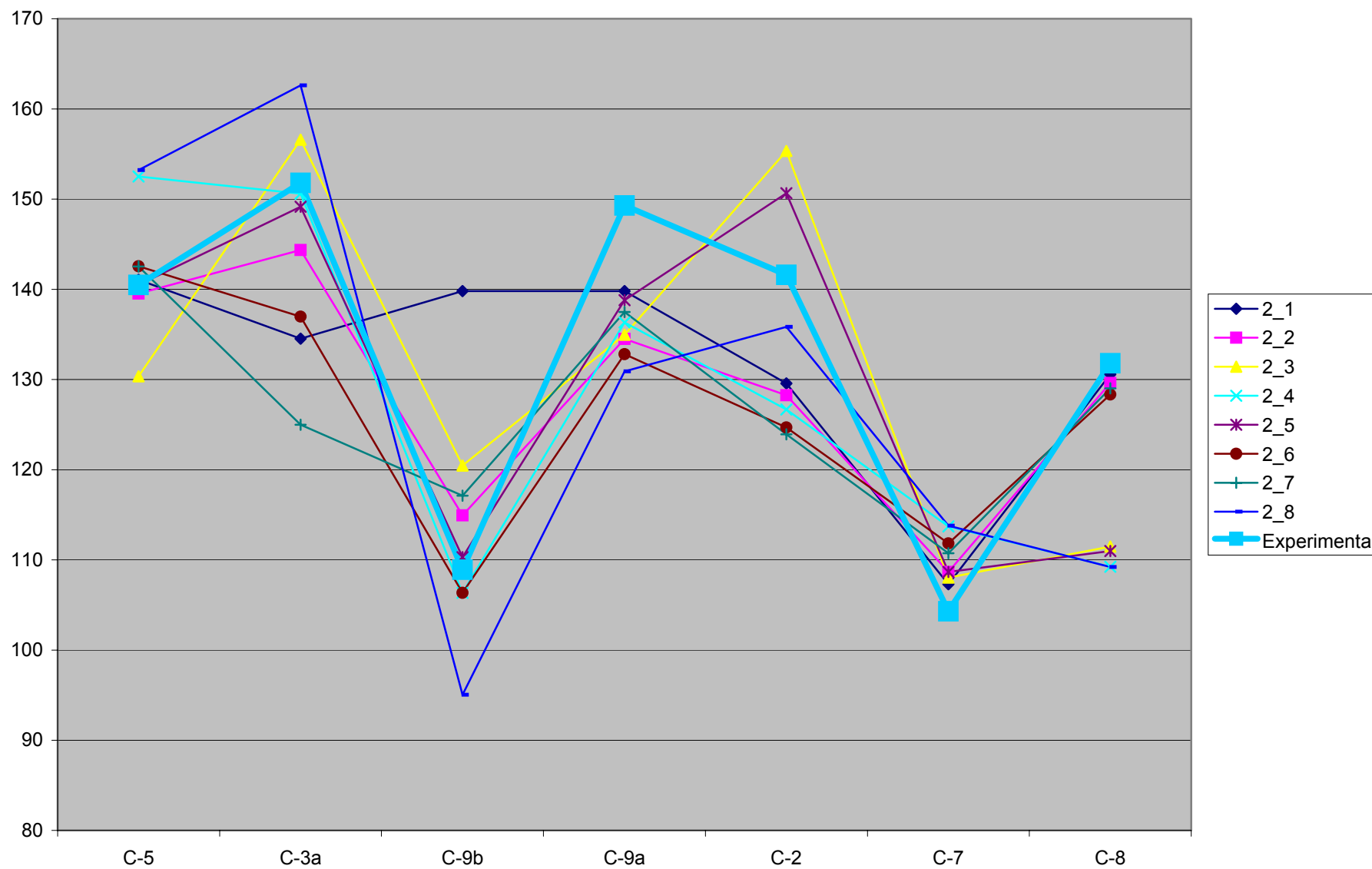
Calculated chemical shifts at the MP2/6-31G** level

The chemical shifts were calibrated against the well known chemical shifts of 2,6-diaminopurine.

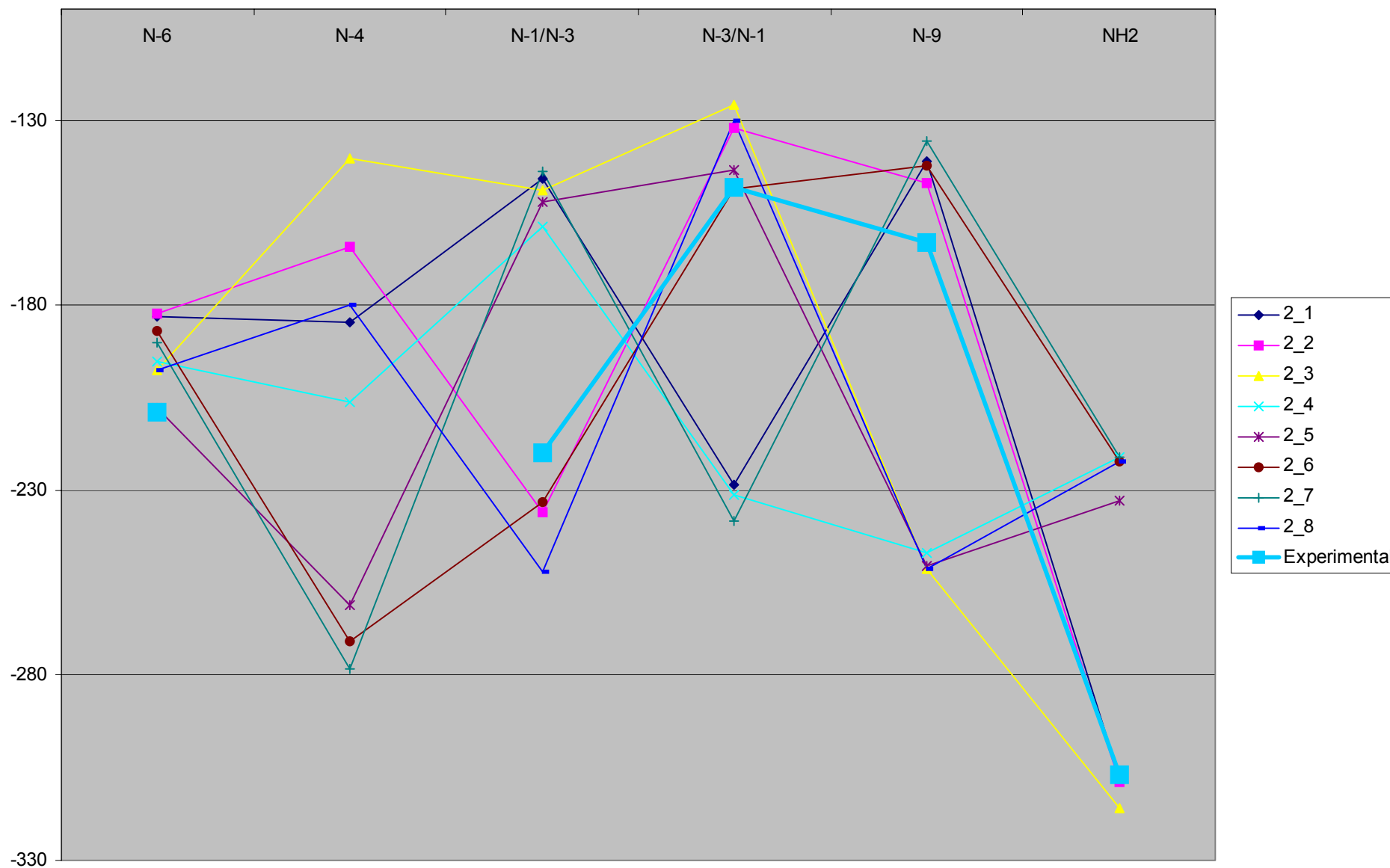
Compound 2

Atom	2_1	2_2	2_3	2_4	2_5	2_6	2_7	2_8
N-6	-183,0849739	-182,346	-197,503	-195,375	-207,819	-187,07	-190,052	-197,686
N-4	-184,5132439	-164,37	-140,354	-206,313	-260,847	-270,645	-278,241	-180,075
N-1/N-3	-145,9408838	-235,86	-149,097	-158,881	-152,107	-233,204	-143,785	-251,917
N-3/N-1	-228,4597834	-132,13	-125,71	-231,216	-143,672	-148,595	-238,351	-129,993
N-9	-141,1023174	-146,997	-251,217	-247,013	-250,444	-142,234	-135,686	-251,362
NH ₂	-307,858013	-308,916	-315,743	-221,018	-232,805	-222,435	-221,155	-222,059
C-5	141,051932	139,55	130,3472	152,5131	140,4785	142,5707	142,541	153,2199
C-3a	134,5244339	144,3548	156,6063	150,6093	149,1433	136,9749	124,9904	162,6285
C-9b	139,8209371	114,9409	120,4715	106,3479	110,2876	106,3461	117,102	95,05143
C-9a	139,8209371	134,5009	134,9582	136,313	138,7949	132,8026	137,506	130,9024
C-2	129,5733986	128,2428	155,3275	126,6679	150,6434	124,6758	123,9242	135,831
C-7	107,298037	108,664	108,0408	113,6977	108,656	111,8277	110,7228	113,801
C-8	130,5626932	129,6284	111,4621	109,2427	110,972	128,3277	129,0211	109,2199

MP2/6-31G** Carbon Calibrated



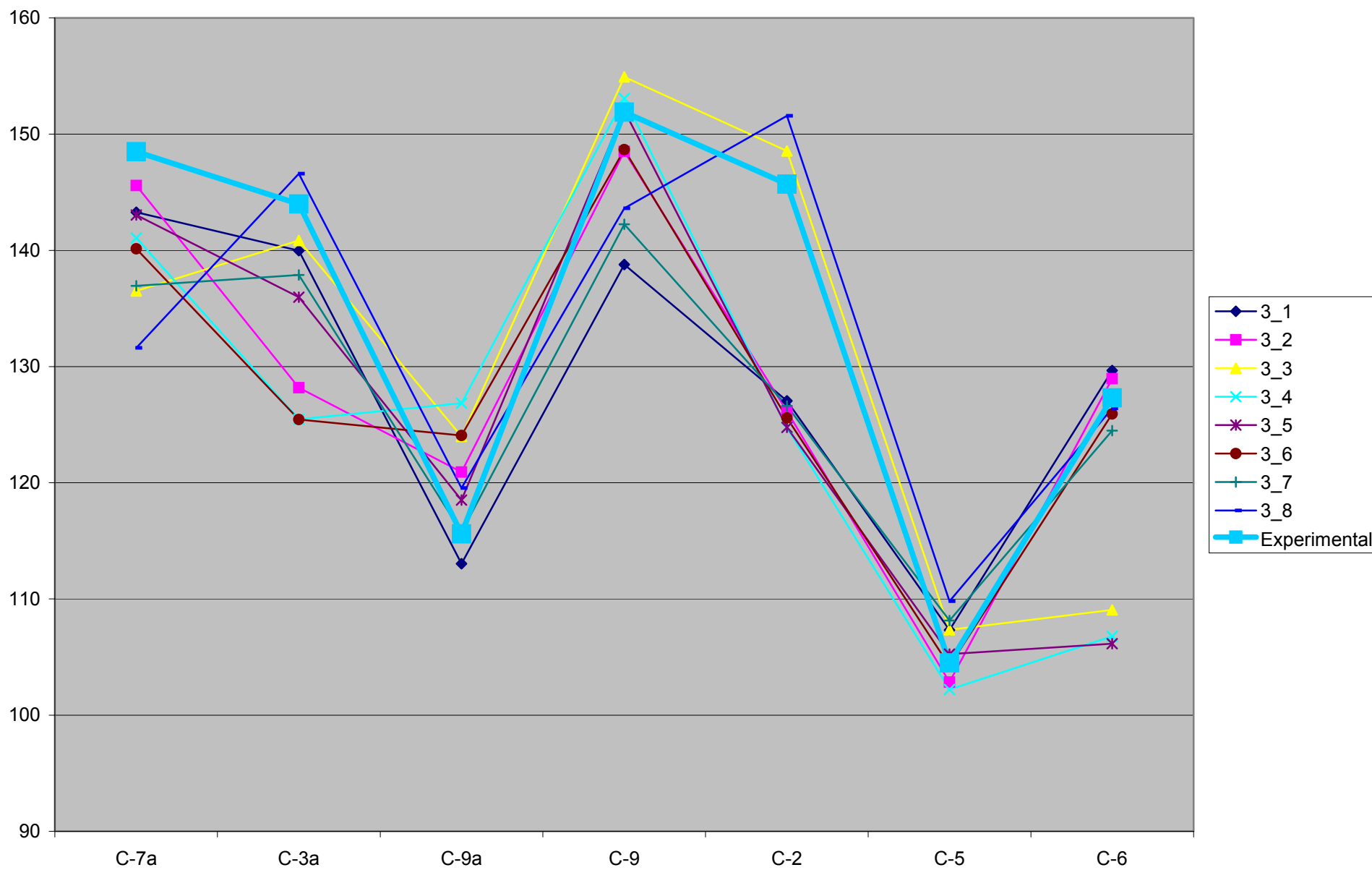
MP2/6-31G** Nitrogen



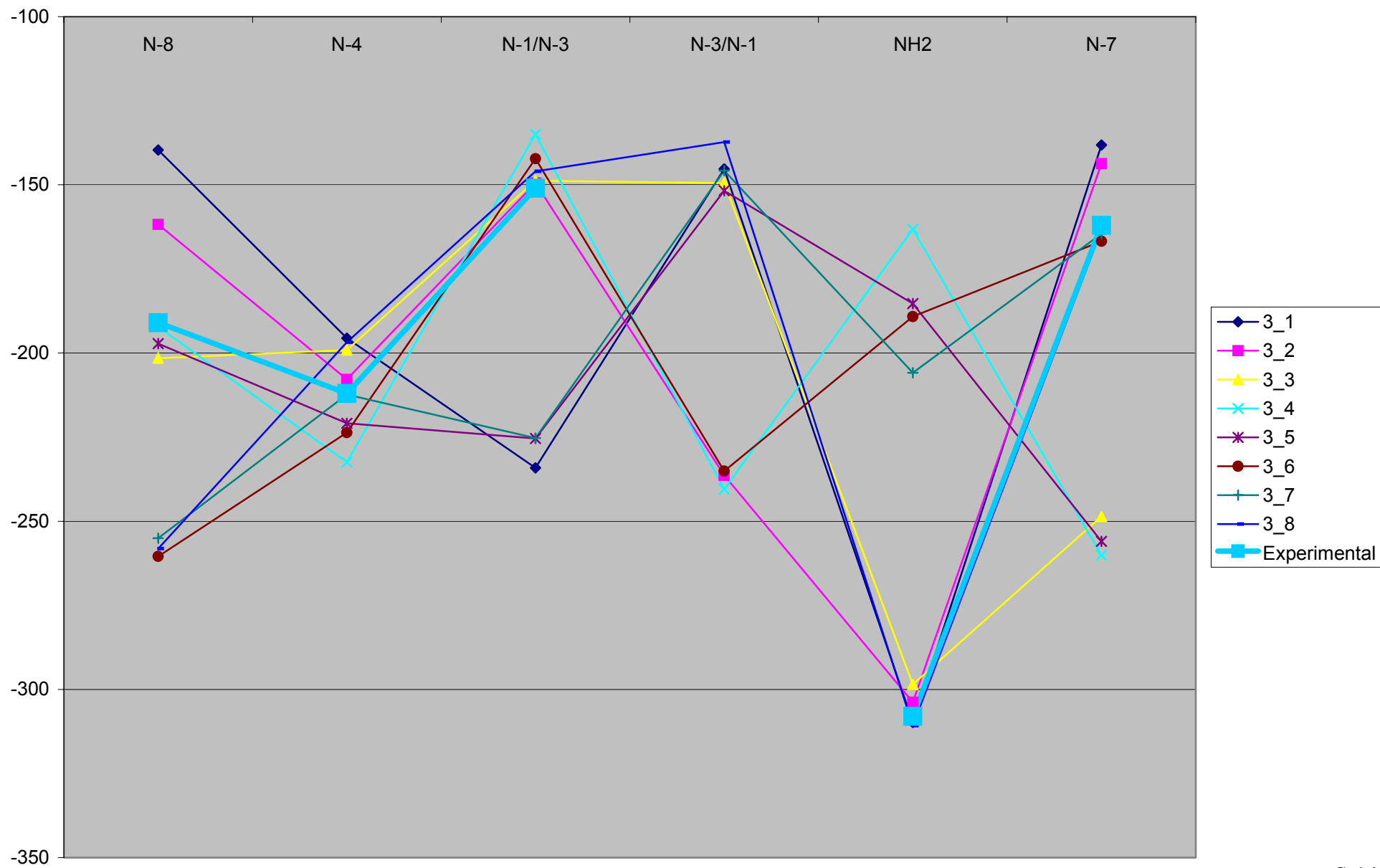
Compound 3

Atom	3_1	3_2	3_3	3_4	3_5	3_6	3_7	3_8
N-8	-139,623	-161,757	-201,528	-192,205	-197,182	-260,452	-255,036	-258,114
N-4	-195,577	-207,793	-199,061	-232,453	-220,845	-223,654	-212,345	-196,771
N-1/N-3	-234,109	-149,44	-148,761	-134,988	-225,427	-142,202	-225,27	-146,02
N-3/N-1	-145,255	-236,379	-149,454	-240,504	-151,715	-235,056	-145,794	-137,268
NH ₂	-309,834	-303,8	-298,501	-163,188	-185,305	-189,17	-205,863	-310,761
N-7	-138,161	-143,719	-248,574	-260,128	-255,959	-166,785	-164,54	-163,345
C-7a	143,2676	145,5901	136,5016	141,0724	143,0421	140,1295	136,9496	131,6089
C-3a	139,9752	128,1784	140,8572	125,4574	135,9763	125,4326	137,8728	146,5972
C-9a	113,0331	120,9279	123,9908	126,8457	118,5108	124,0708	115,7519	119,5394
C-9	138,7857	148,5123	154,915	153,0719	152,0372	148,6659	142,2334	143,6051
C-2	127,0553	126,1457	148,5488	124,7351	124,7685	125,5869	126,6059	151,5749
C-5	107,3253	102,8467	107,3379	102,2132	105,2562	104,2301	108,1438	109,8121
C-6	129,6574	128,9672	109,0559	106,7833	106,1532	125,9095	124,491	126,3988

MP2/6-31G** Carbon



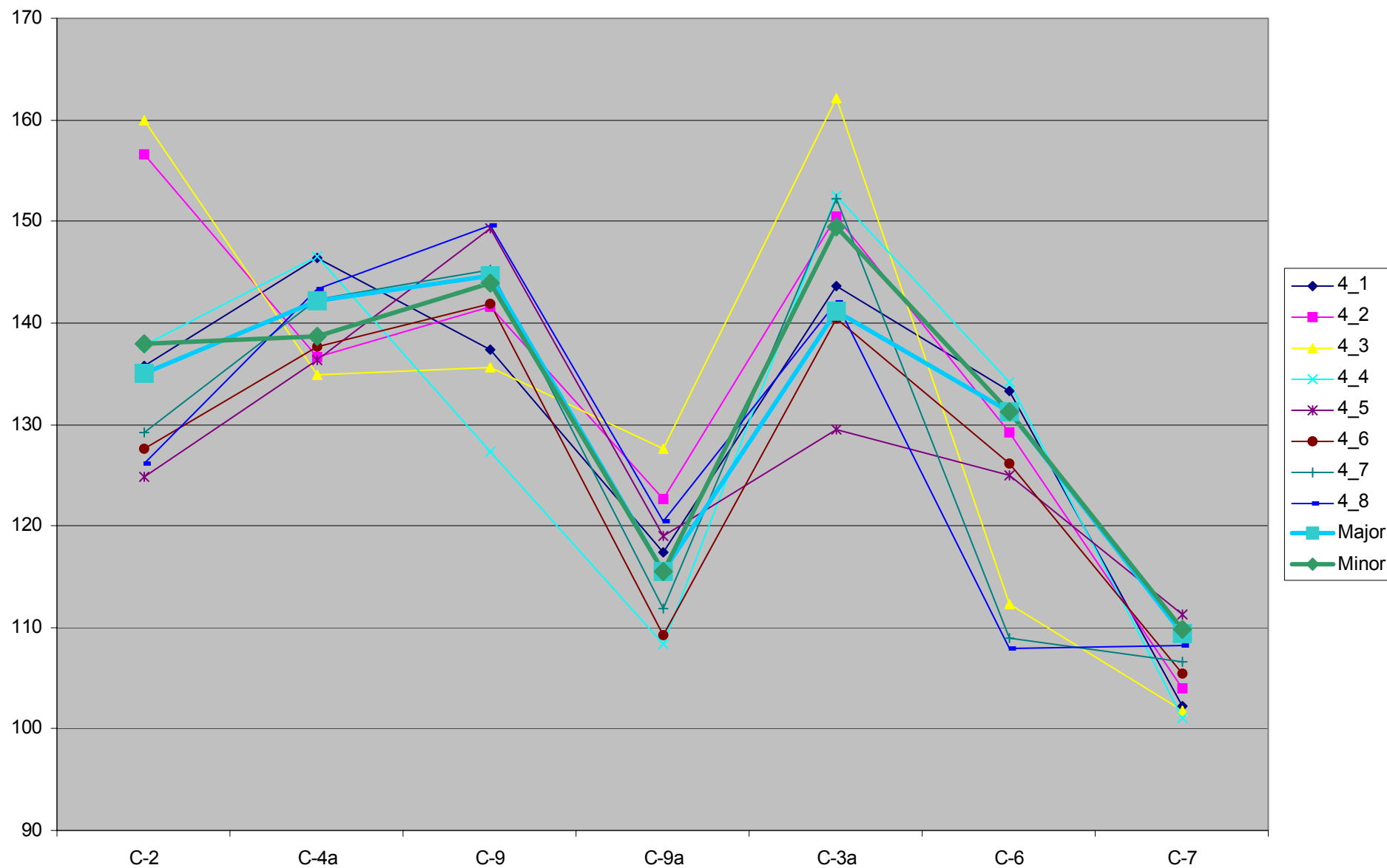
MP2/6-31G** Nitrogen

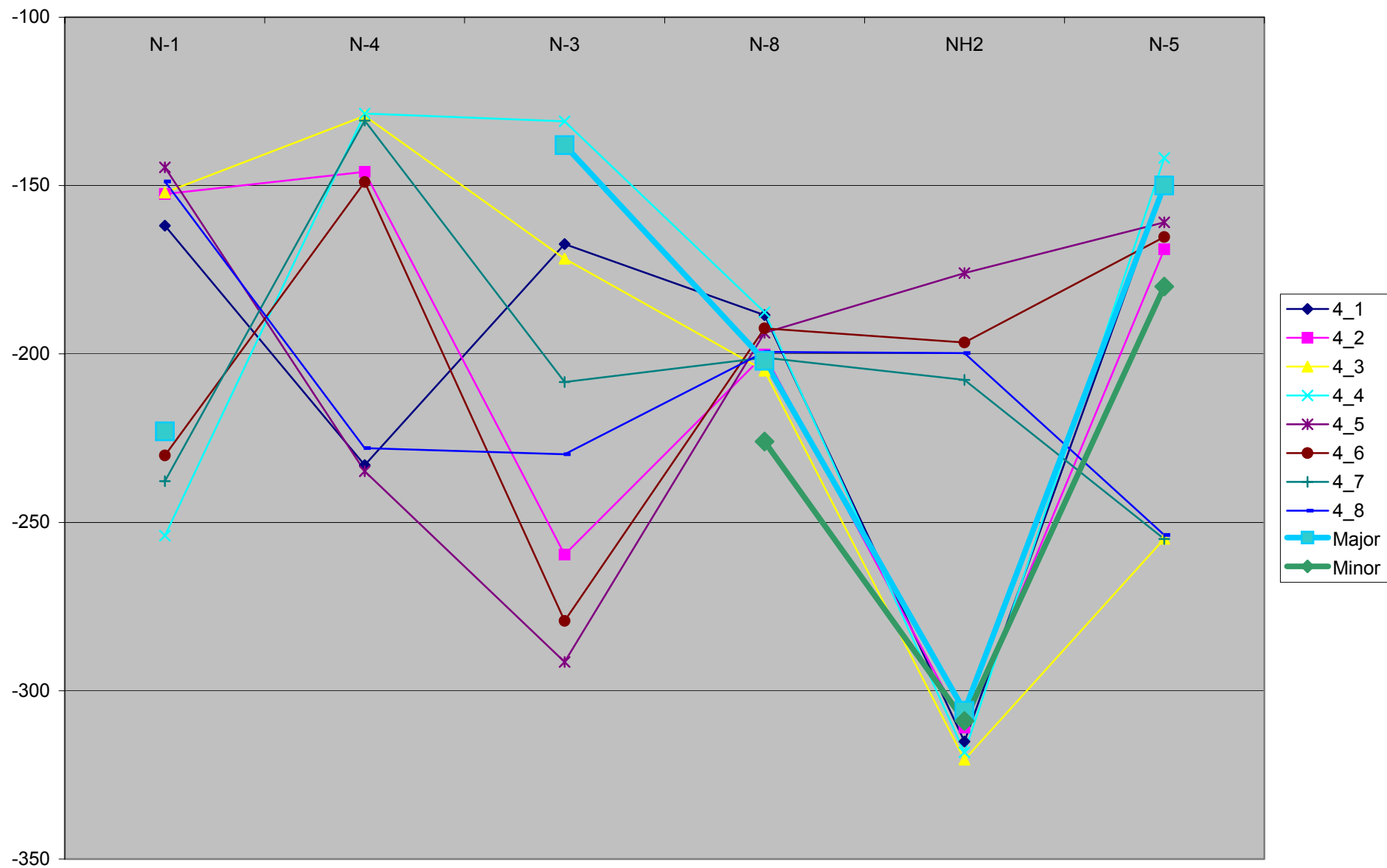


Compound 4

Atom	4_1	4_2	4_3	4_4	4_5	4_6	4_7	4_8
N-1	-161,894	-152,544	-152,117	-253,973	-144,616	-230,139	-237,794	-148,788
N-4	-233,017	-145,937	-129,284	-128,609	-234,782	-148,933	-130,673	-227,953
N-3	-167,348	-259,582	-171,737	-130,902	-291,464	-279,234	-208,326	-229,75
N-8	-188,488	-200,201	-204,926	-187,629	-193,741	-192,371	-201,112	-199,386
NH ₂	-315,075	-310,952	-320,489	-318,292	-175,982	-196,613	-207,685	-199,733
N-5	-150,053	-168,893	-254,895	-141,778	-160,934	-165,285	-254,945	-253,738
C-2	135,7181	156,6059	159,9274	137,815	124,7938	127,594	129,1988	126,1369
C-4a	146,4032	136,6522	134,882	146,5907	136,3729	137,6496	142,313	143,2889
C-9	137,3034	141,6221	135,5713	127,3189	149,3156	141,8376	145,2561	149,5563
C-9a	117,3823	122,686	127,5239	108,3198	118,9714	109,1825	111,8023	120,4025
C-3a	143,601	150,4196	162,1175	152,5529	129,5336	140,413	152,2441	142,0704
C-6	133,2433	129,1852	112,3245	134,1789	124,9947	126,127	108,9749	107,856
C-7	102,2265	104,0118	101,7868	101,1368	111,3361	105,4415	106,6709	108,2421

MP2/6-31G** Carbon

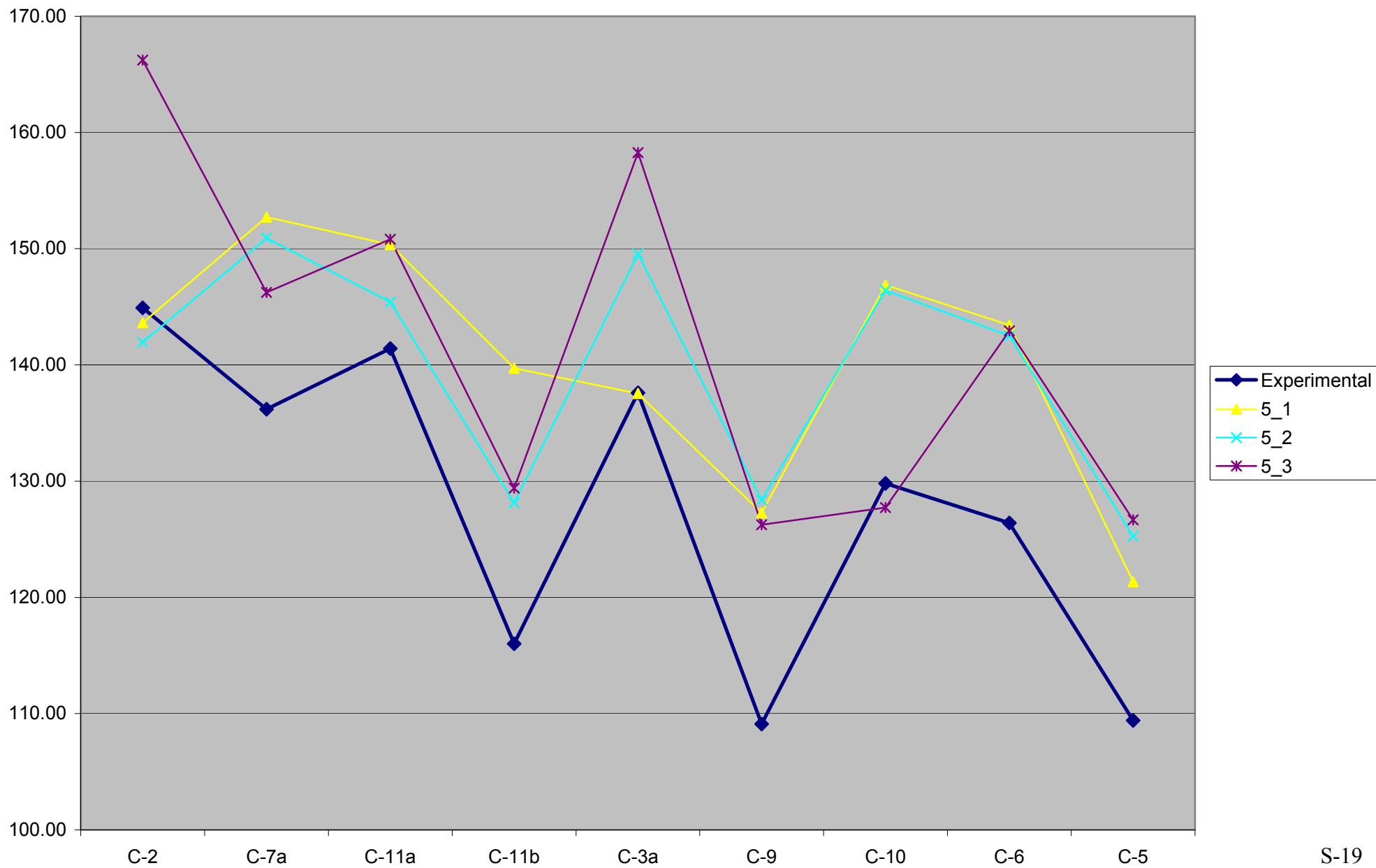




Compound 5

Atom	5_1	5_2	5_3
N-1	-107,488843	-209,47975	-116,598755
N-3	-217,422657	-116,244099	-110,371644
N-4	-190,579739	-180,835475	-169,215754
N-8	-169,470621	-167,302099	-184,052305
N-11	-104,130685	-112,570341	-227,869835
N-7	-127,071334	-126,481959	-130,80869
C-2	143,624692	141,9494484	166,226105
C-7a	152,7263295	150,9200499	146,2454102
C-11a	150,3638635	145,4035973	150,8215873
C-11b	139,7163206	128,1278657	129,3959962
C-3a	137,5390025	149,5522897	158,2579546
C-9	127,265469	128,3620327	126,2388266
C-10	146,8766107	146,4082767	127,7209647
C-6	143,4340268	142,4958734	142,9340745
C-5	121,329171	125,2394523	126,6613245

MP2/6-31G** Carbon Calibrated



MP2/6-31G** Nitrogen

