

QM/MM studies reveal pathways leading to the quenching of the formation of thymine dimer  
photoproduct by flanking bases

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### **Supplementary information**

Table S1. Vertical excitation energies and oscillator strengths of all frames

ATTA								
#1	Energy (eV)	Character	#2	Energy (eV)	Character	#3	Energy (eV)	Character
S1	4.949 (0.0009)		S1	4.893 (0.0004)		S1	4.910 (0.0002)	
S2	4.970 (0.0003)		S2	4.901 (0.0003)		S2	4.956 (0.0007)	
S3	4.999 (0.1403)		S3	5.027 (0.0754)	DP (11%)	S3	5.017 (0.0372)	DP (17%)
S4	5.086 (0.0056)	DP (94%)	S4	5.060 (0.0773)	DP (87%)	S4	5.038 (0.1039)	DP (15%)
S5	5.287 (0.1167)		S5	5.154 (0.0479)	CT (89%)	S5	5.193 (0.0297)	CT, DP (98%)
S6	5.307 (0.1594)	CT (58%)	S6	5.324 (0.1000)		S6	5.309 (0.1142)	
S7	5.433 (0.0950)	CT (83%)	S7	5.384 (0.2328)		S7	5.399 (0.2499)	
S8	5.548 (0.0001)		S8	5.578 (0.0002)		S8	5.562 (0.0017)	
S9	6.023 (0.0092)		S9	5.985 (0.0246)		S9	6.037 (0.0056)	
#4	Energy (eV)	Character	#5	Energy (eV)	Character			
S1	4.954 (0.0005)		S1	4.887 (0.0014)				
S2	5.031 (0.0003)		S2	4.949 (0.0006)				
S3	5.059 (0.1189)		S3	4.974 (0.0493)	CT (81%)			
S4	5.192 (0.0231)	DP (93%)	S4	5.126 (0.0389)	DP (18%)			
S5	5.230 (0.1453)	CT (91%)	S5	5.284 (0.1634)	DP (20%)			
S6	5.363 (0.1967)		S6	5.335 (0.1048)	CT (91%)			
S7	5.468 (0.0758)	CT (89%)	S7	5.477 (0.1267)				
S8	5.655 (0.0001)		S8	5.561 (0.0001)				
S9	6.093 (0.0136)		S9	5.952 (0.0122)				
CTTA								
#1	Energy (eV)	Character	#2	Energy (eV)	Character	#3	Energy (eV)	Character
S1	4.866 (0.0003)		S1	4.827 (0.0653)		S1	4.954 (0.0008)	
S2	4.934 (0.0593)		S2	4.911 (0.0002)		S2	4.964 (0.0010)	
S3	5.091 (0.0006)		S3	4.970 (0.0007)		S3	4.994 (0.0500)	
S4	5.176 (0.0330)	DP (96%)	S4	5.190 (0.0218)	DP (95%)	S4	5.175 (0.0174)	DP (96%)
S5	5.405 (0.2045)		S5	5.355 (0.1757)		S5	5.360 (0.1779)	
S6	5.673 (0.2521)		S6	5.544 (0.1132)		S6	5.503 (0.2807)	
S7	5.707 (0.0067)		S7	5.730 (0.1226)		S7	5.762 (0.0032)	
S8	5.924 (0.0012)		S8	5.809 (0.0050)		S8	5.856 (0.0449)	
S9	5.990 (0.0342)		S9	5.910 (0.0490)		S9	6.020 (0.0072)	CT (97%)
#4	Energy (eV)	Character	#5	Energy (eV)	Character			
S1	4.951 (0.0005)		S1	4.911 (0.0002)				
S2	5.018 (0.0045)		S2	5.036 (0.0009)				
S3	5.035 (0.0362)		S3	5.090 (0.0504)				
S4	5.157 (0.0220)	DP (96%)	S4	5.230 (0.0203)	DP (94%)			
S5	5.390 (0.1876)		S5	5.410 (0.1655)				
S6	5.497 (0.2885)		S6	5.511 (0.3012)				
S7	5.736 (0.0042)		S7	5.856 (0.0025)				
S8	6.023 (0.0035)	CT (96%)	S8	6.028 (0.0386)				
S9	6.069 (0.0059)		S9	6.140 (0.0036)	CT (98%)			
GTTA								

#1	<b>Energy (eV)</b>	<b>Character</b>	#2	<b>Energy (eV)</b>	<b>Character</b>	#3	<b>Energy (eV)</b>	<b>Character</b>
S1	4.871 (0.0755)	CT (92%)	S1	4.905 (0.0375)	CT (88%)	S1	4.827 (0.0007)	
S2	4.980 (0.0166)		S2	4.957 (0.0003)		S2	4.908 (0.0002)	
S3	4.998 (0.0008)		S3	5.007 (0.0005)		S3	5.062 (0.0647)	
S4	5.072 (0.0133)		S4	5.098 (0.0289)	DP (85%)	S4	5.139 (0.0828)	CT (88%)
S5	5.226 (0.0344)	DP (90%)	S5	5.173 (0.1541)	CT (63%)	S5	5.323 (0.0464)	CT (23%)
S6	5.400 (0.2399)		S6	5.378 (0.1623)	CT (84%)	S6	5.442 (0.1948)	CT (74%)
S7	5.542 (0.2746)		S7	5.527 (0.0474)		S7	5.564 (0.2354)	
S8	5.572 (0.0009)		S8	5.564 (0.2138)		S8	5.714 (0.0008)	
S9	5.757 (0.0048)		S9	5.624 (0.0025)		S9	5.863 (0.0328)	
#4	<b>Energy (eV)</b>	<b>Character</b>	#5	<b>Energy (eV)</b>	<b>Character</b>			
S1	4.871 (0.0001)		S1	4.865 (0.0032)				
S2	4.972 (0.0009)		S2	4.918 (0.0194)	CT (97%)			
S3	4.991 (0.0579)	CT (95%)	S3	5.060 (0.0966)				
S4	5.068 (0.0393)	CT (90%)	S4	5.111 (0.0004)				
S5	5.227 (0.0507)	DP (92%)	S5	5.172 (0.0180)	DP (94%)			
S6	5.393 (0.2104)		S6	5.369 (0.2282)				
S7	5.532 (0.2773)		S7	5.575 (0.2586)				
S8	5.596 (0.0161)		S8	5.635 (0.0145)				
S9	5.818 (0.0046)		S9	5.669 (0.0045)				

The states marked as CT in character columns are the CT between a flanking base and an adjacent thymine.

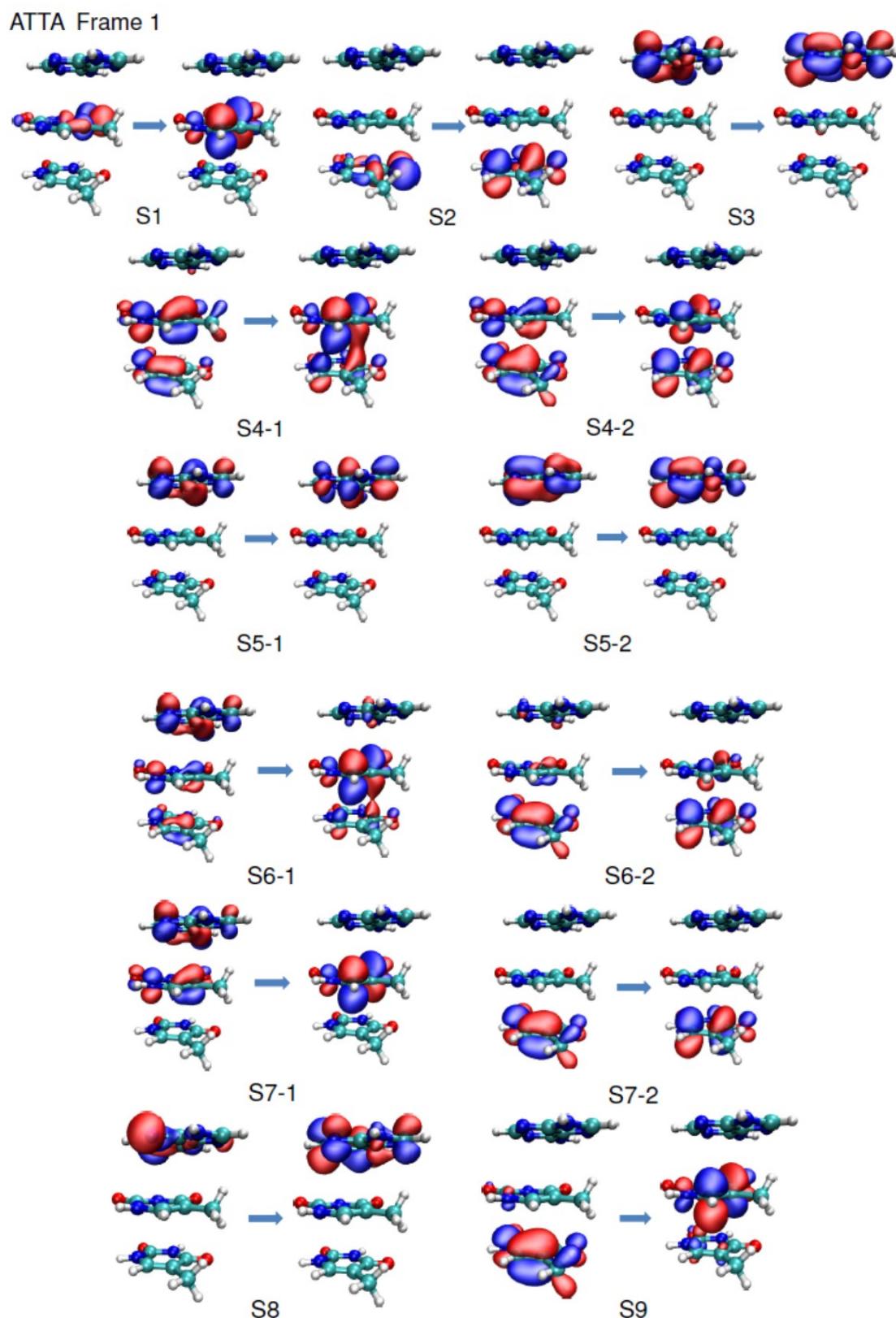
Table S2. Vertical excitation energies of a thymine monomer

Frame		1	2	3	4	5	Average
ATTA	nπ*	5.10108	5.08622	5.03823	5.10435	5.02534	5.071044
	ππ*	5.39422	5.4097	5.41395	5.41306	5.484	5.422986
CTTA	nπ*	5.2056	5.06997	5.06314	5.10823	5.10781	5.11095
	ππ*	5.37852	5.42716	5.44038	5.41149	5.47611	5.426732
GTAA	nπ*	5.1761	5.159	5.09189	5.06296	5.03528	5.105046
	ππ*	5.37172	5.31215	5.38089	5.36876	5.36436	5.359576

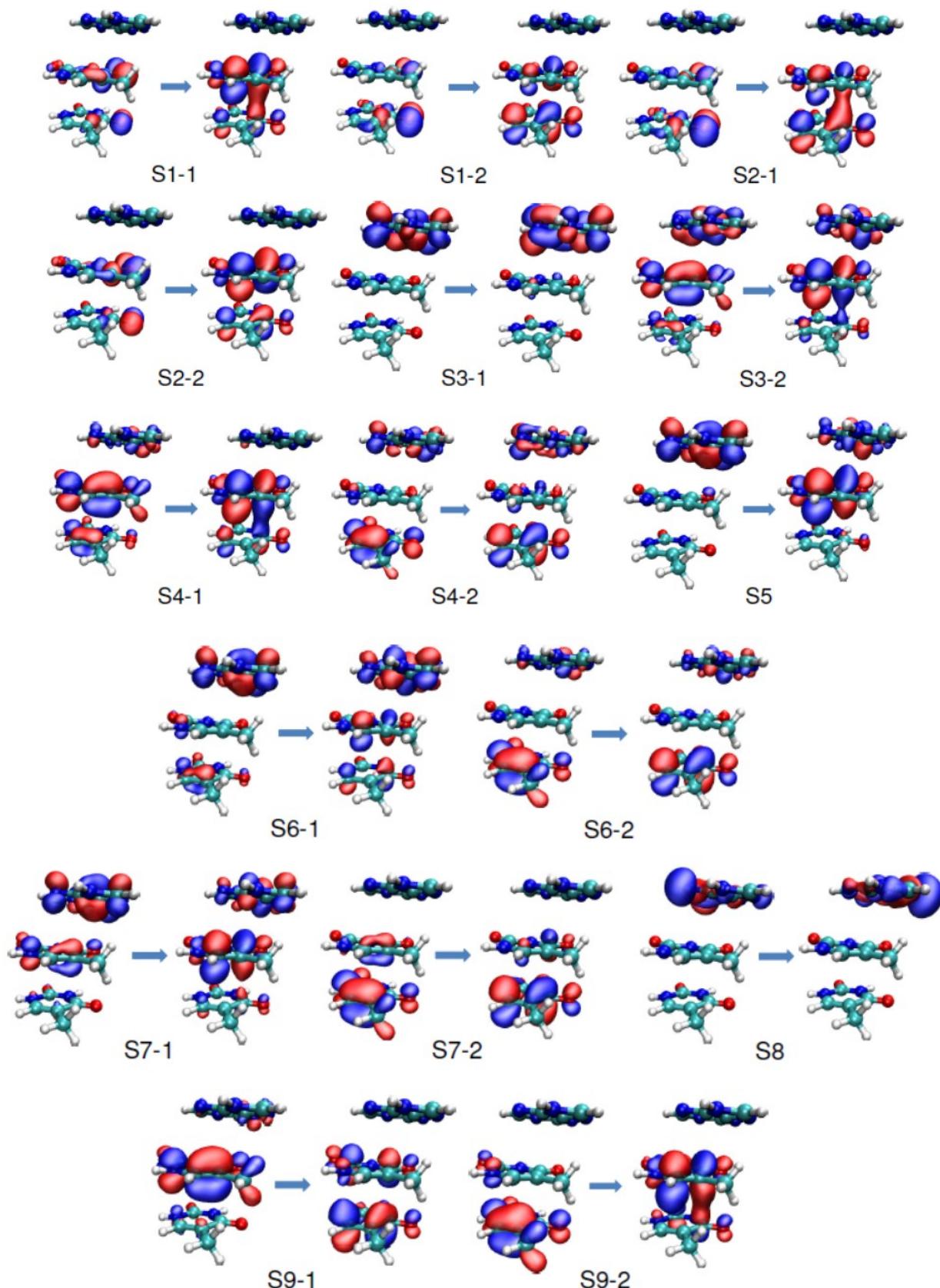
Table S3. Vertical excitation energies of flanking bases in selected frames

	Guanine (Frame 1)	Cytosine (Frame 4)	Adenine (Frame 4)
ππ <sub>1</sub> *	5.01164	5.02857	5.13917
ππ <sub>2</sub> *	5.61813	5.55651	5.35501
nπ*	5.63811	5.74521	5.69671

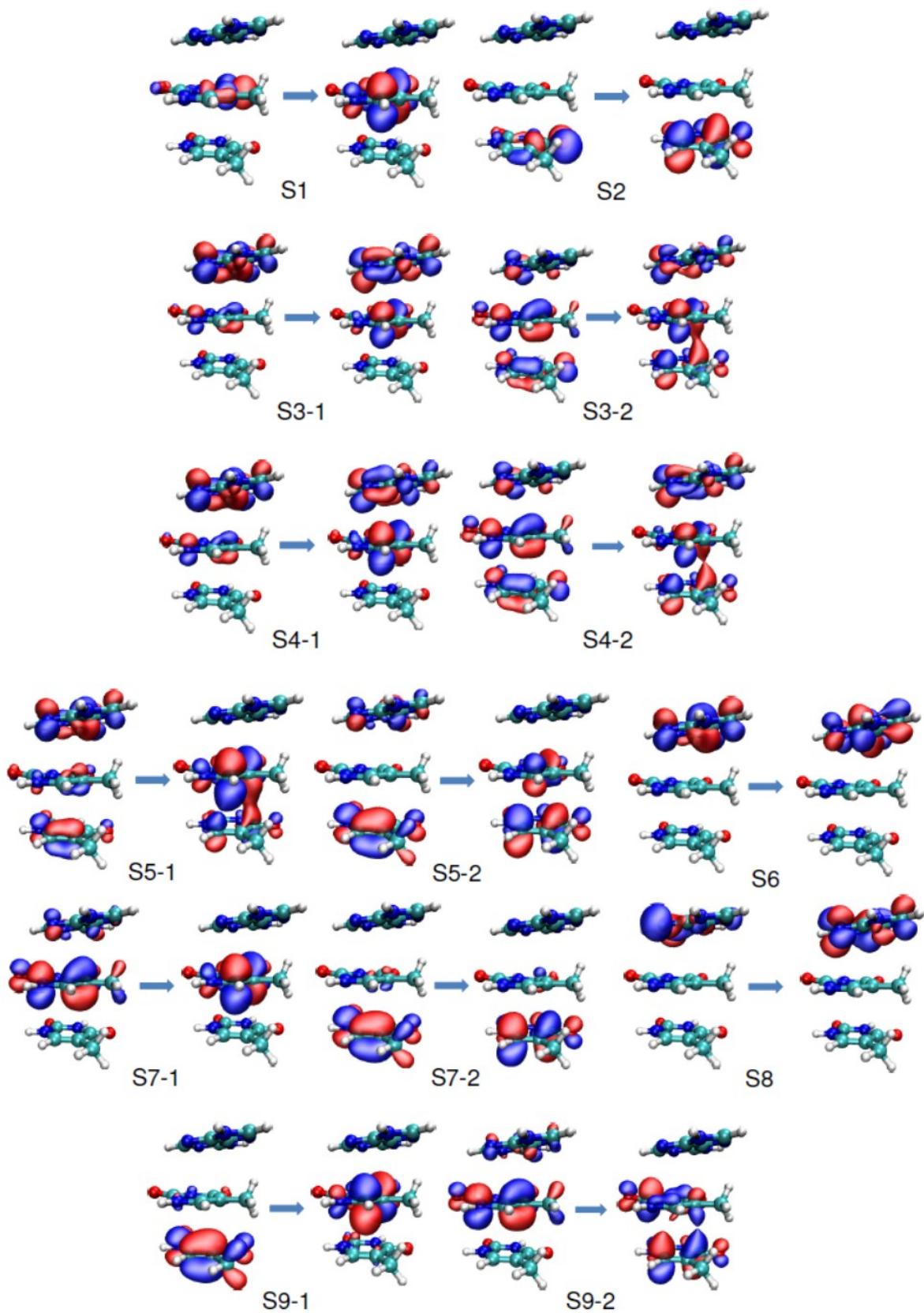
Figure S1. Corresponding NTOs of excited states listed in Table S1.



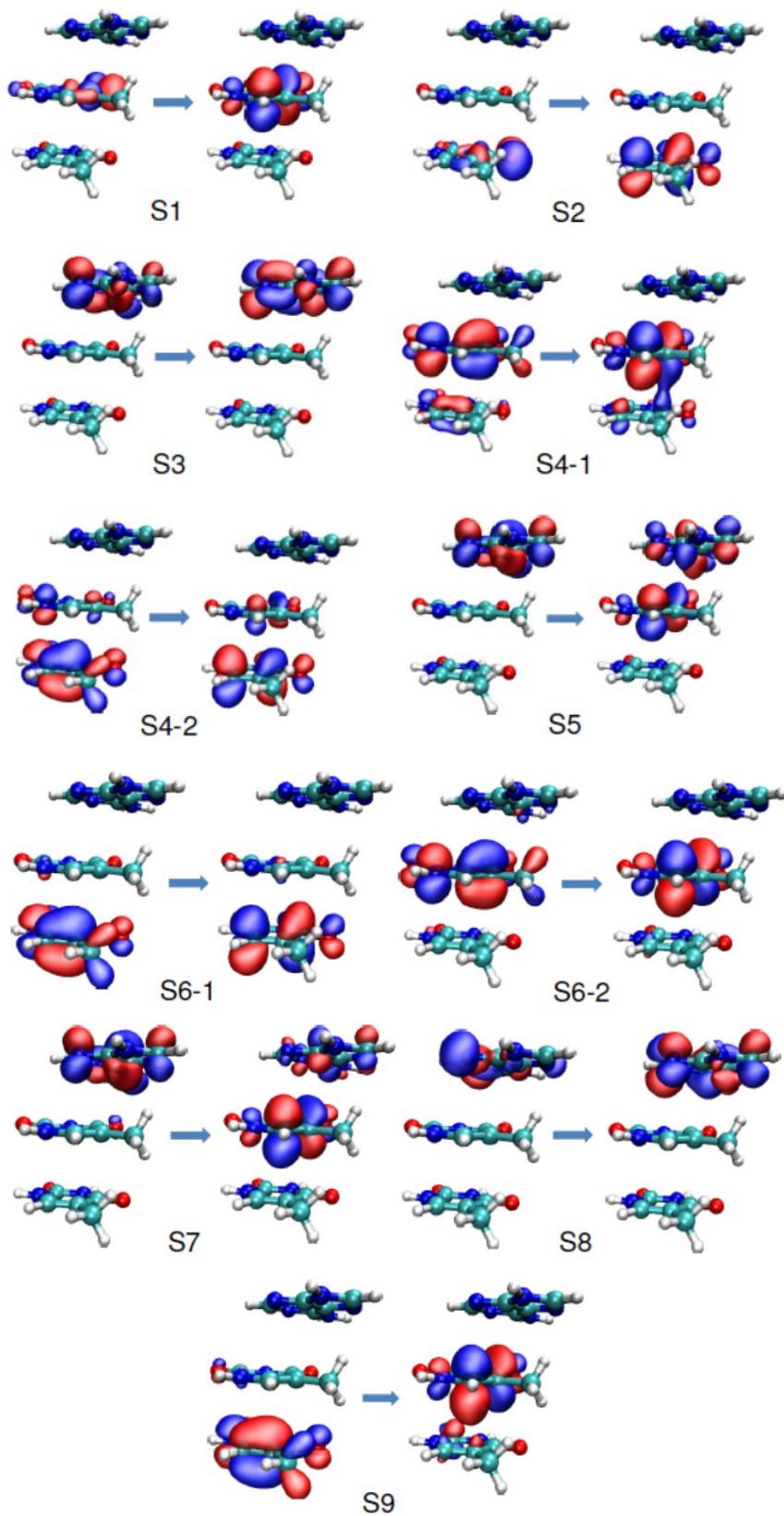
ATTA Frame 2



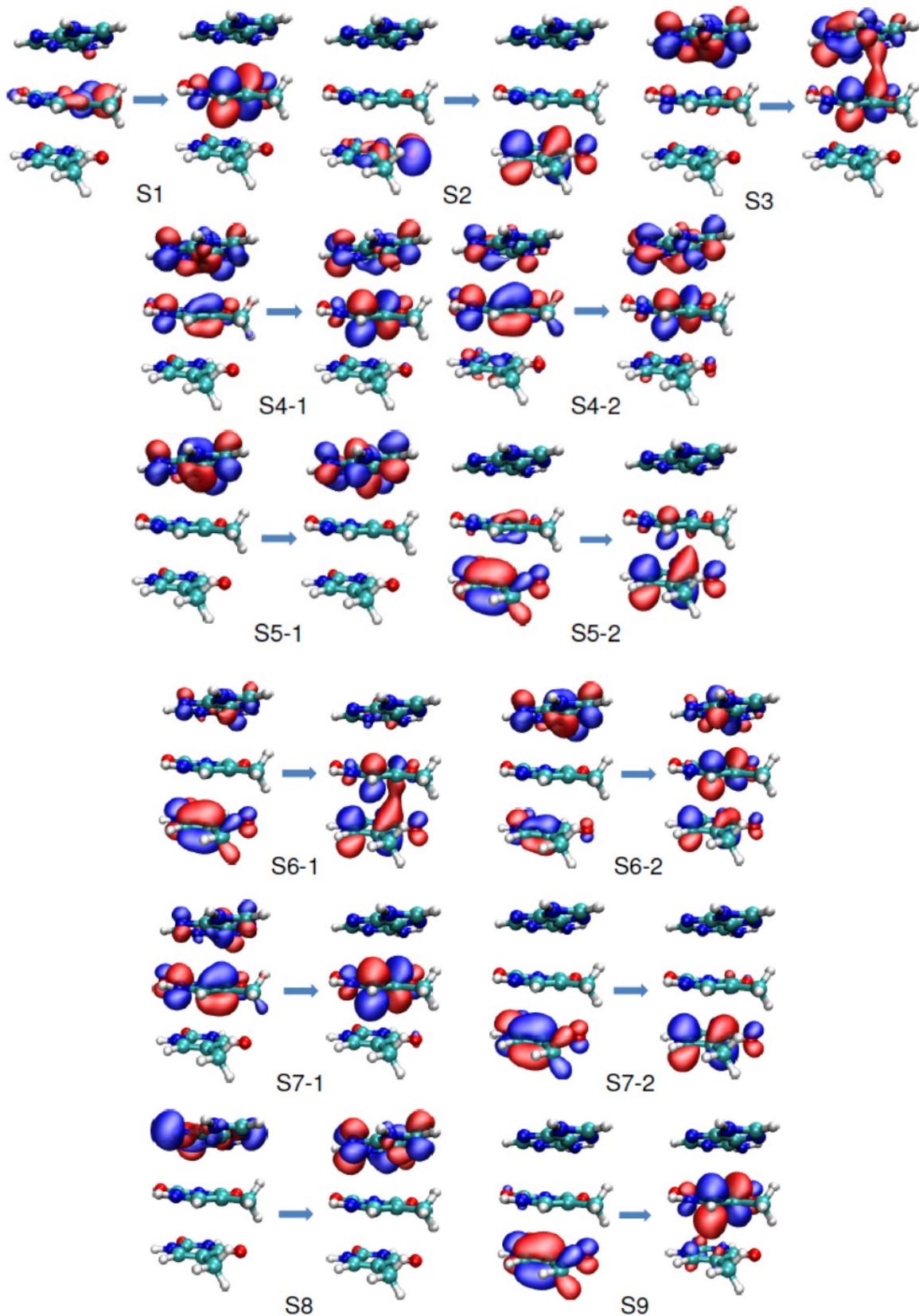
ATTA Frame 3



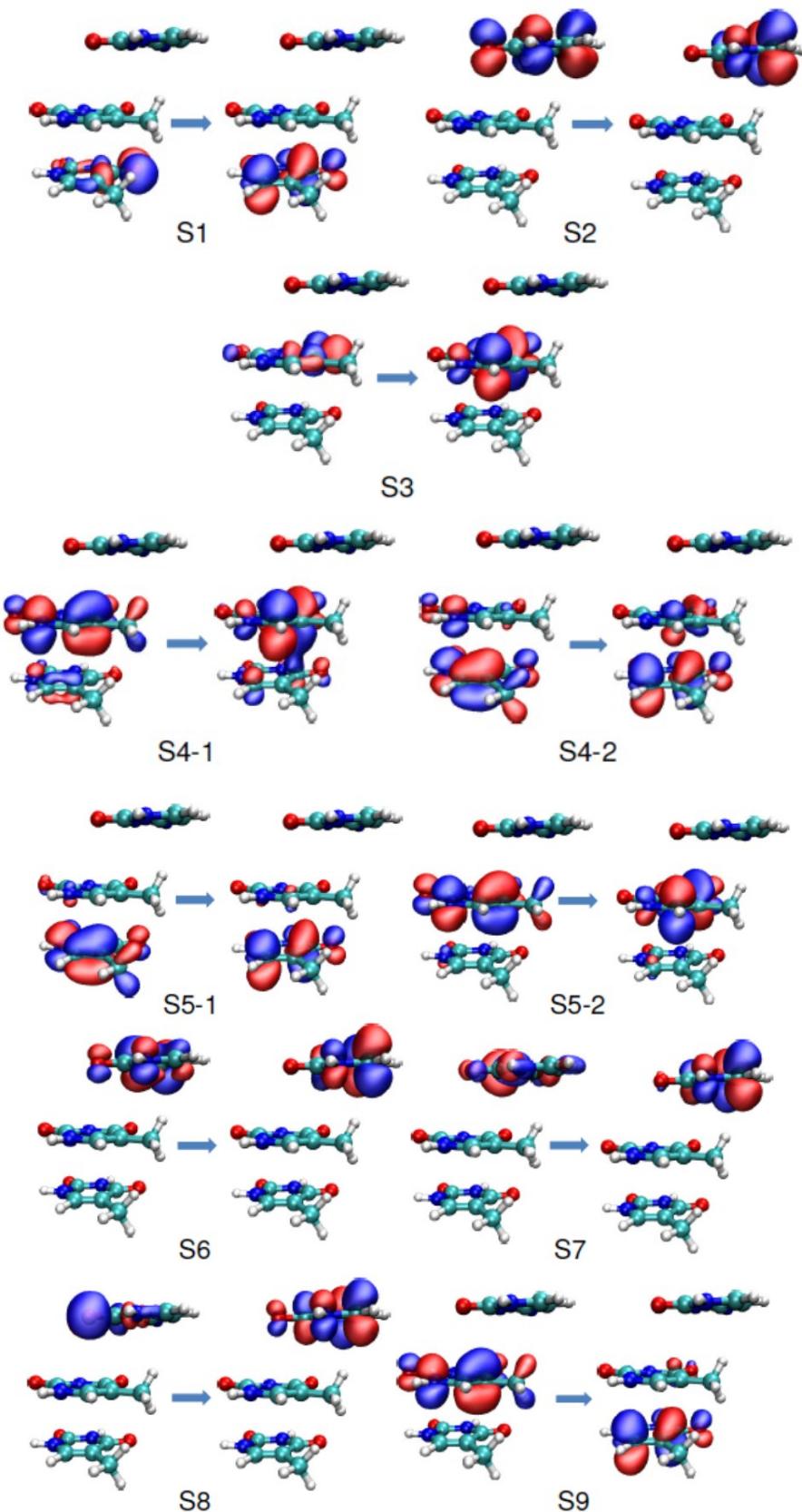
ATTA Frame 4



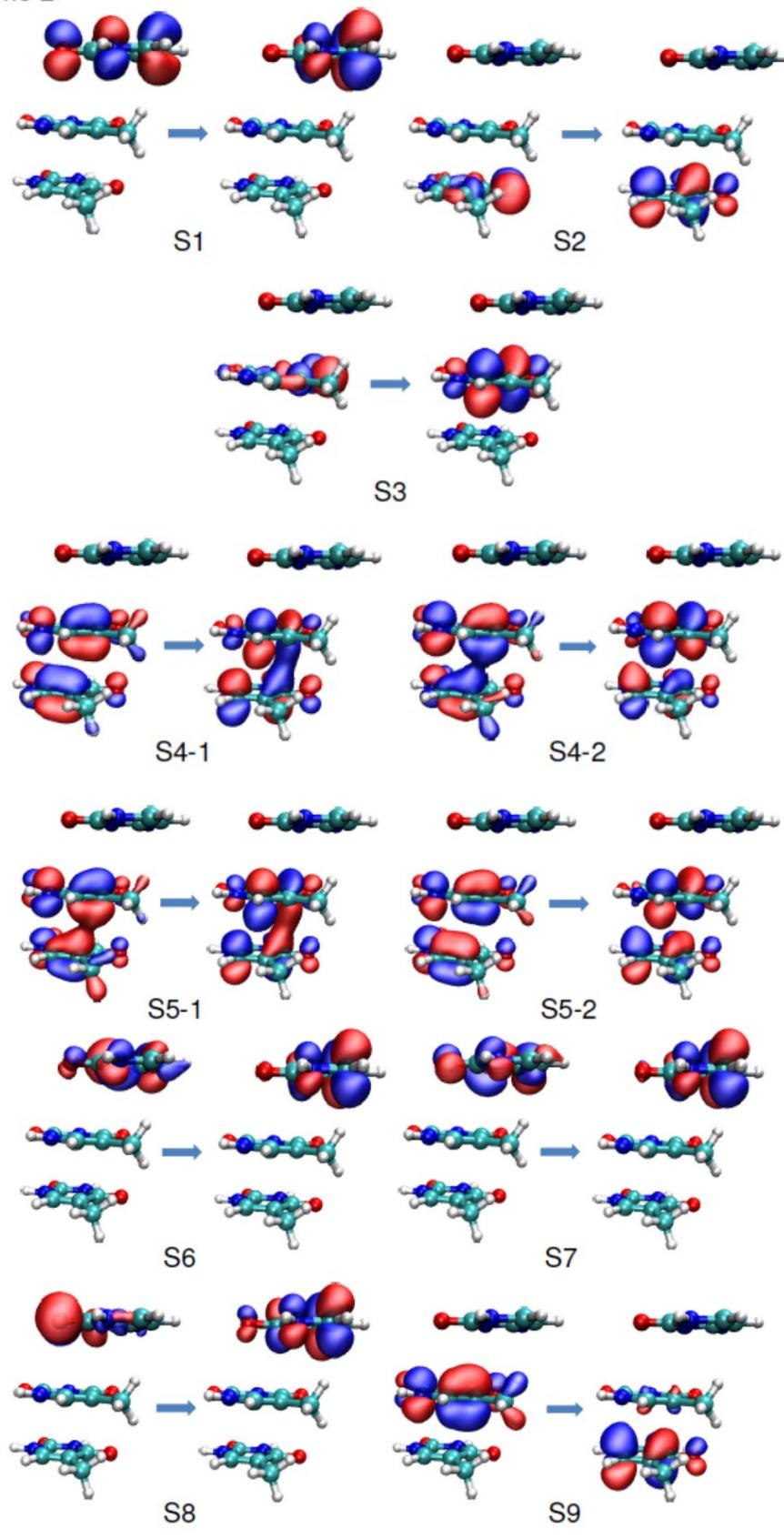
ATTA Frame 5



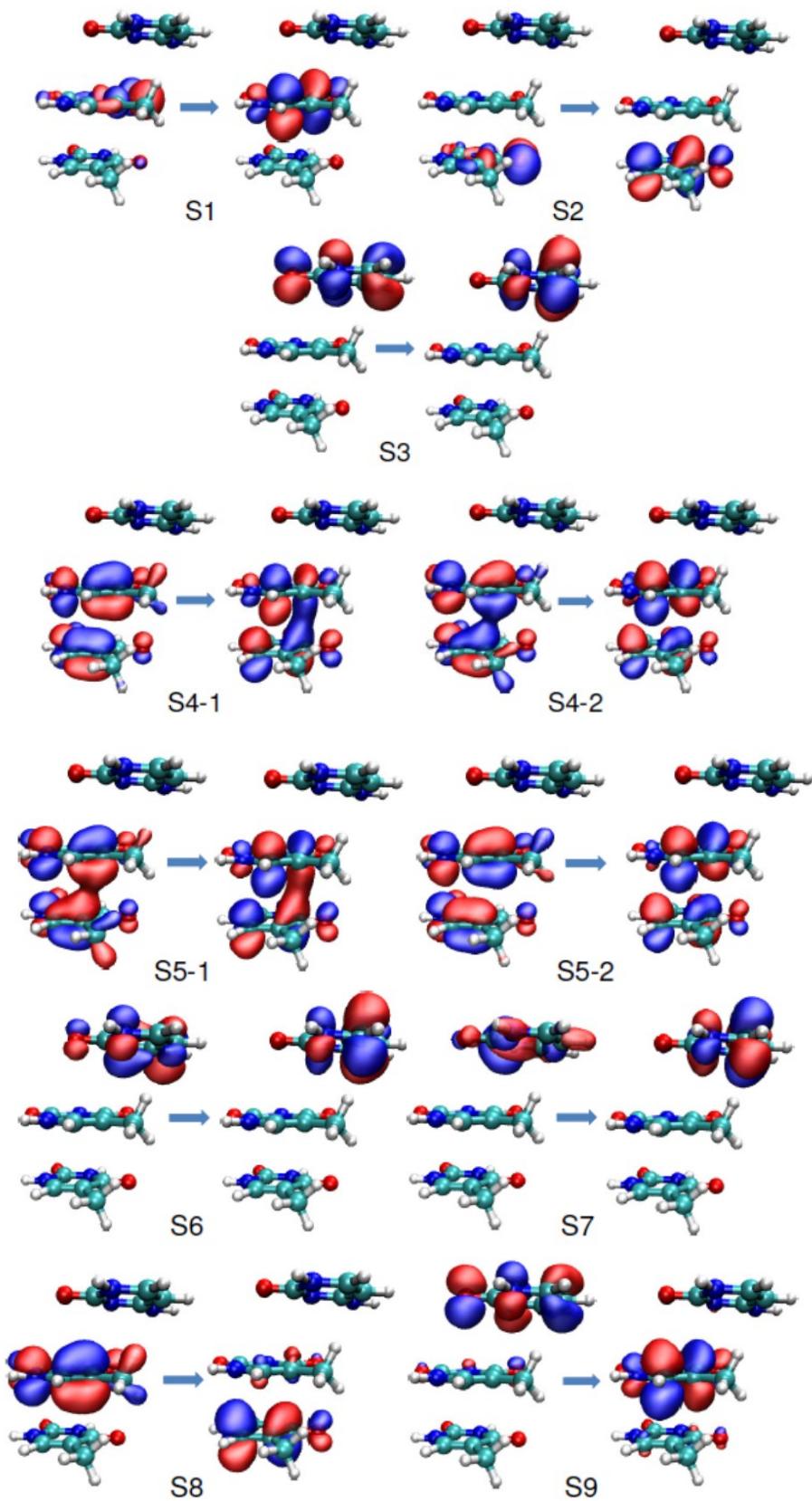
CTTA Frame 1



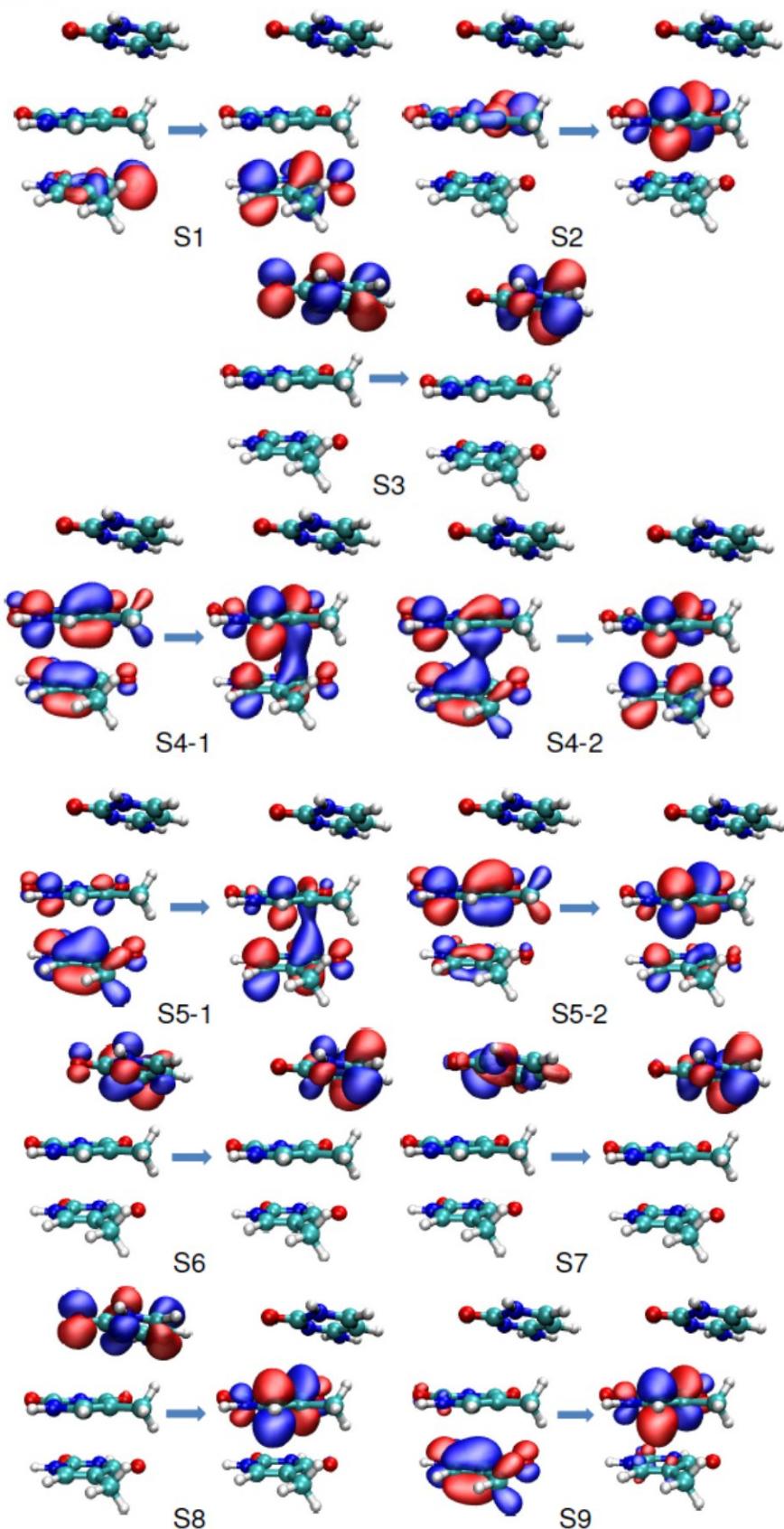
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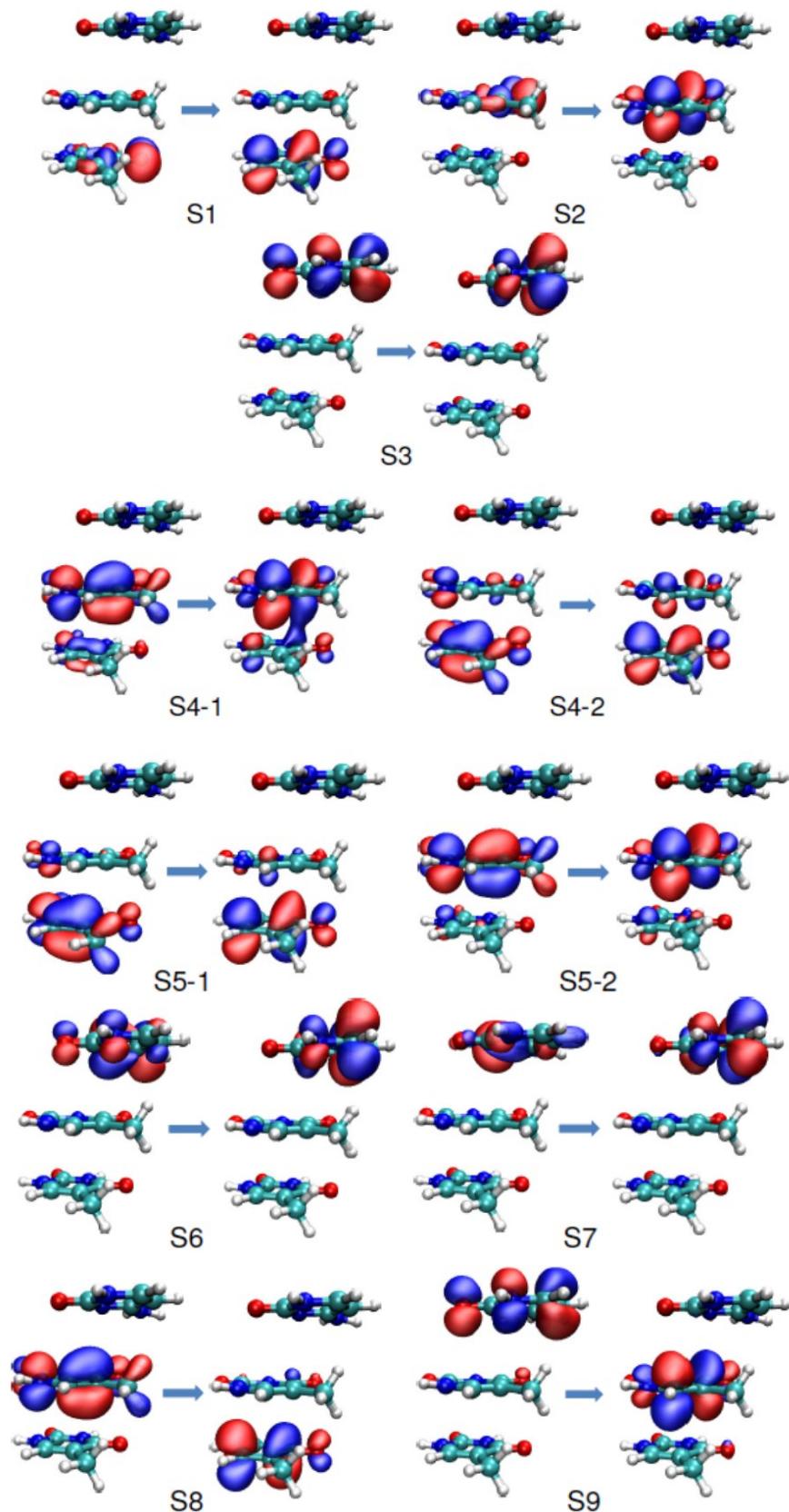
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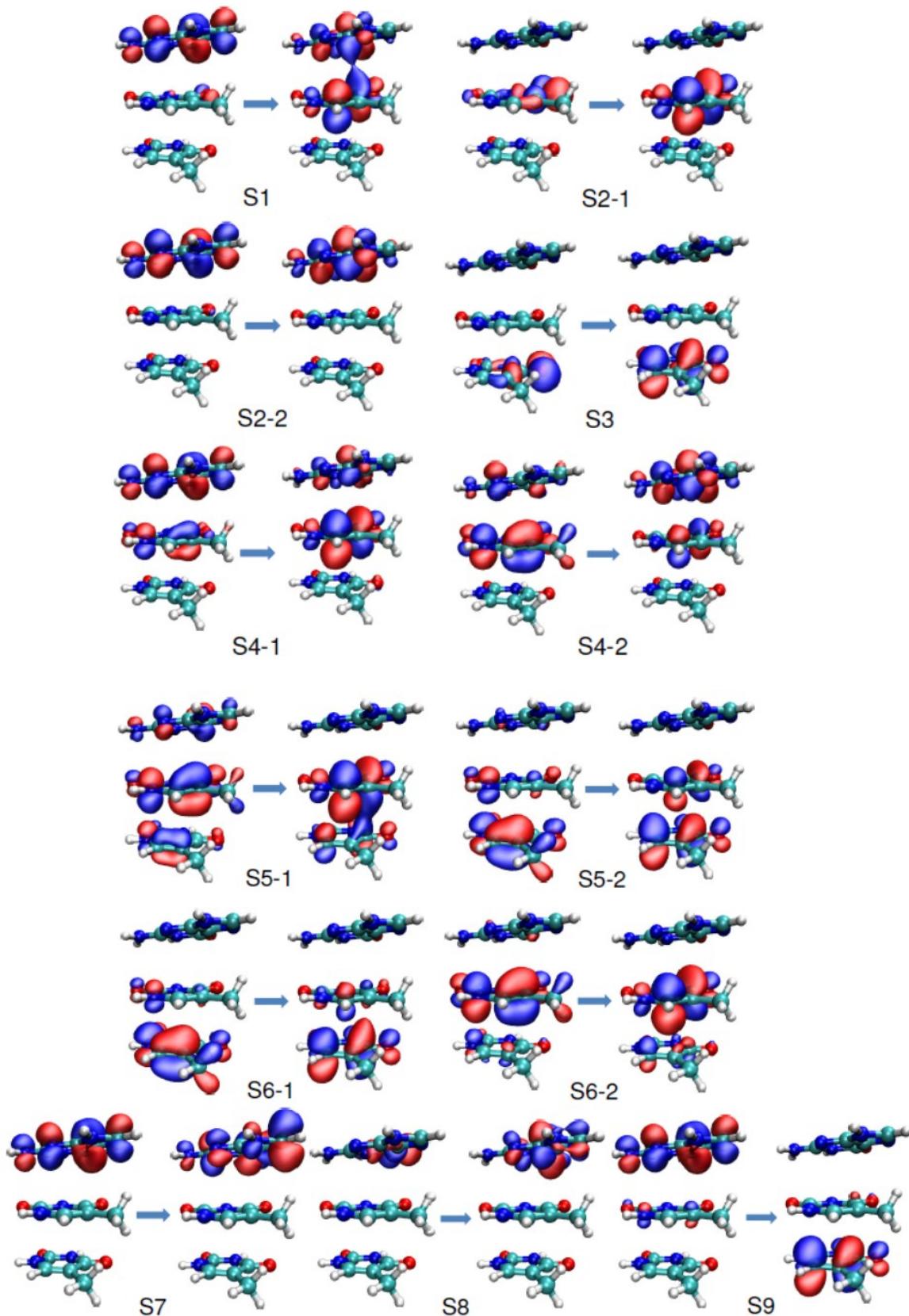
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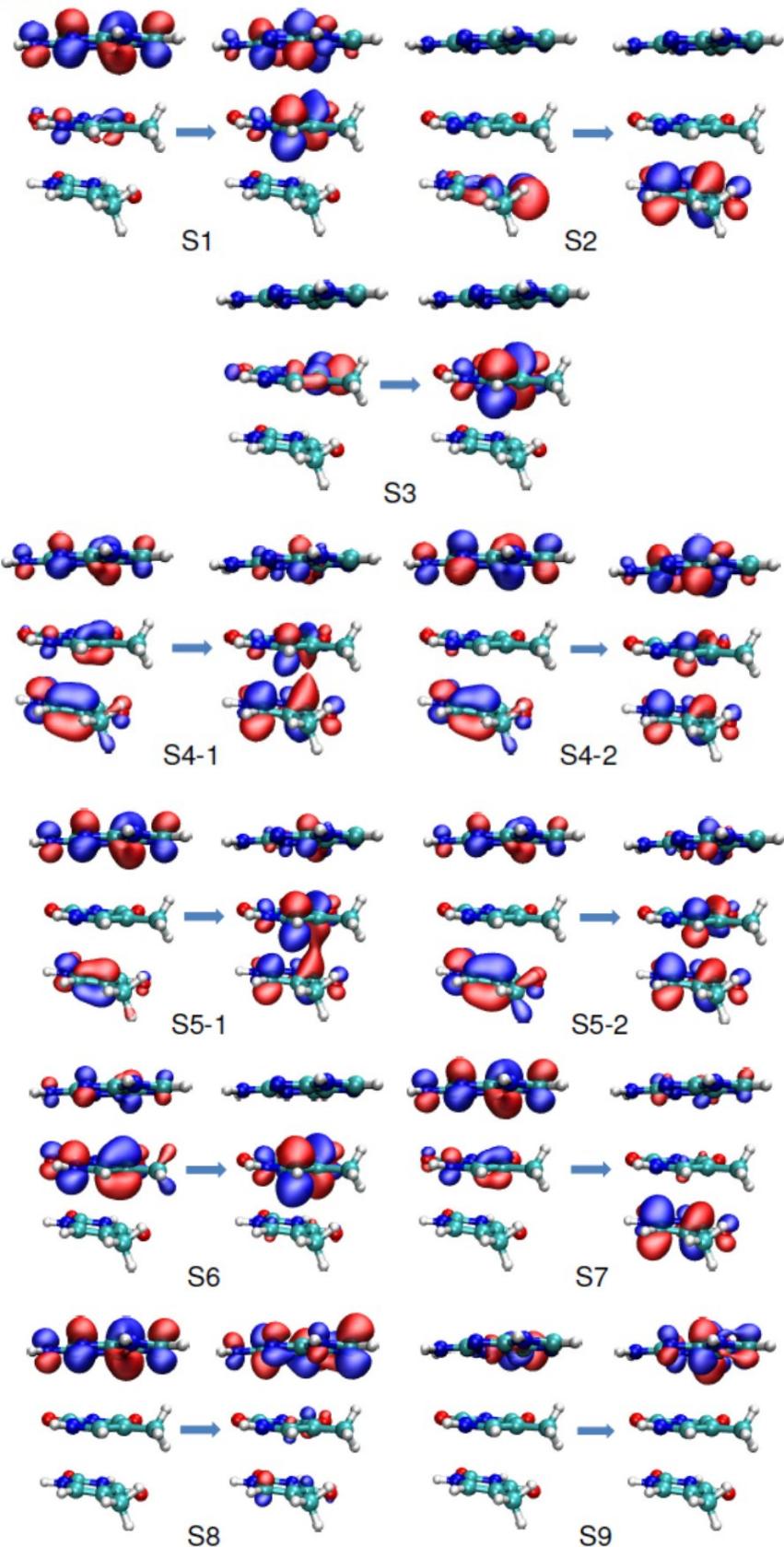
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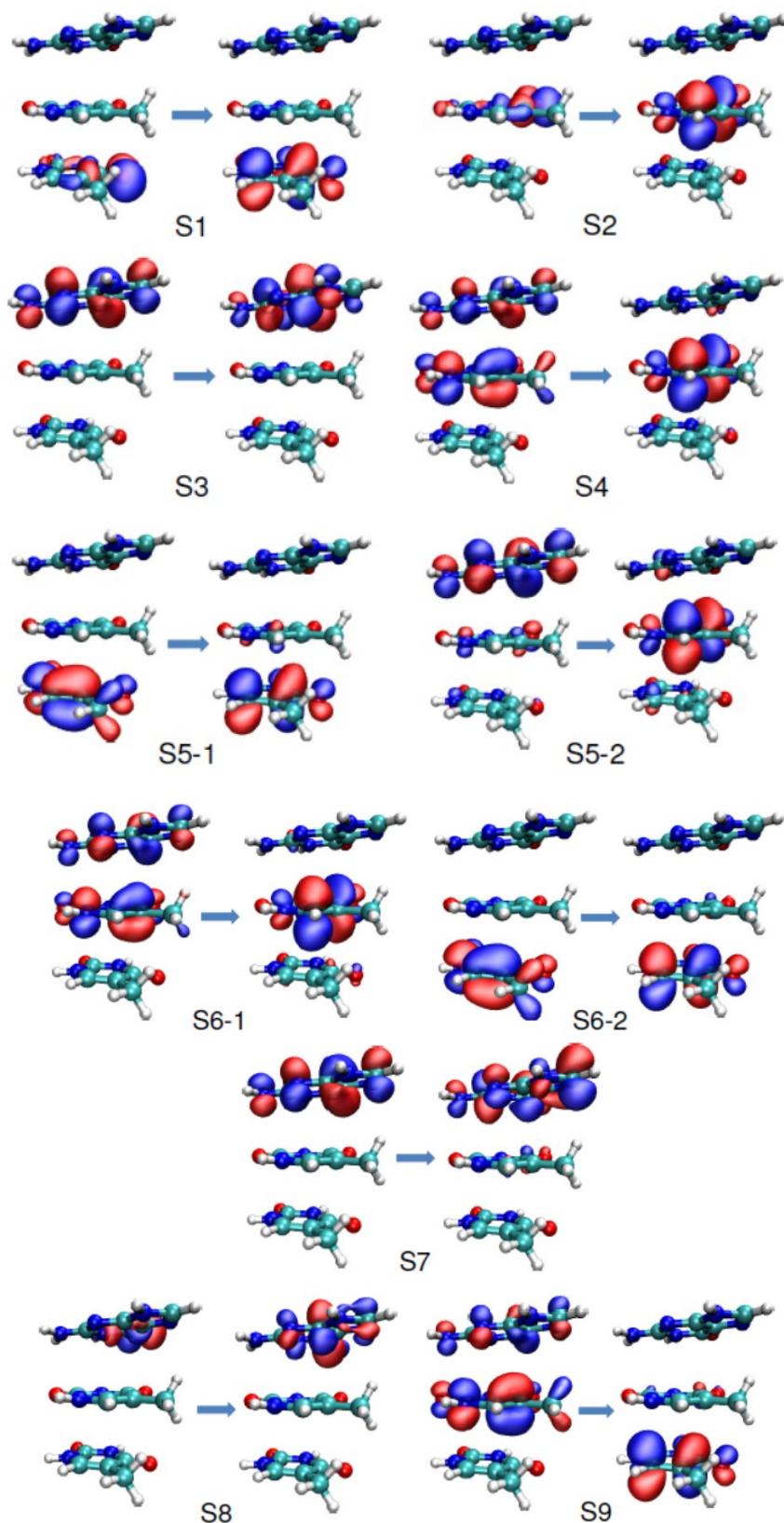
GTAA Frame 1



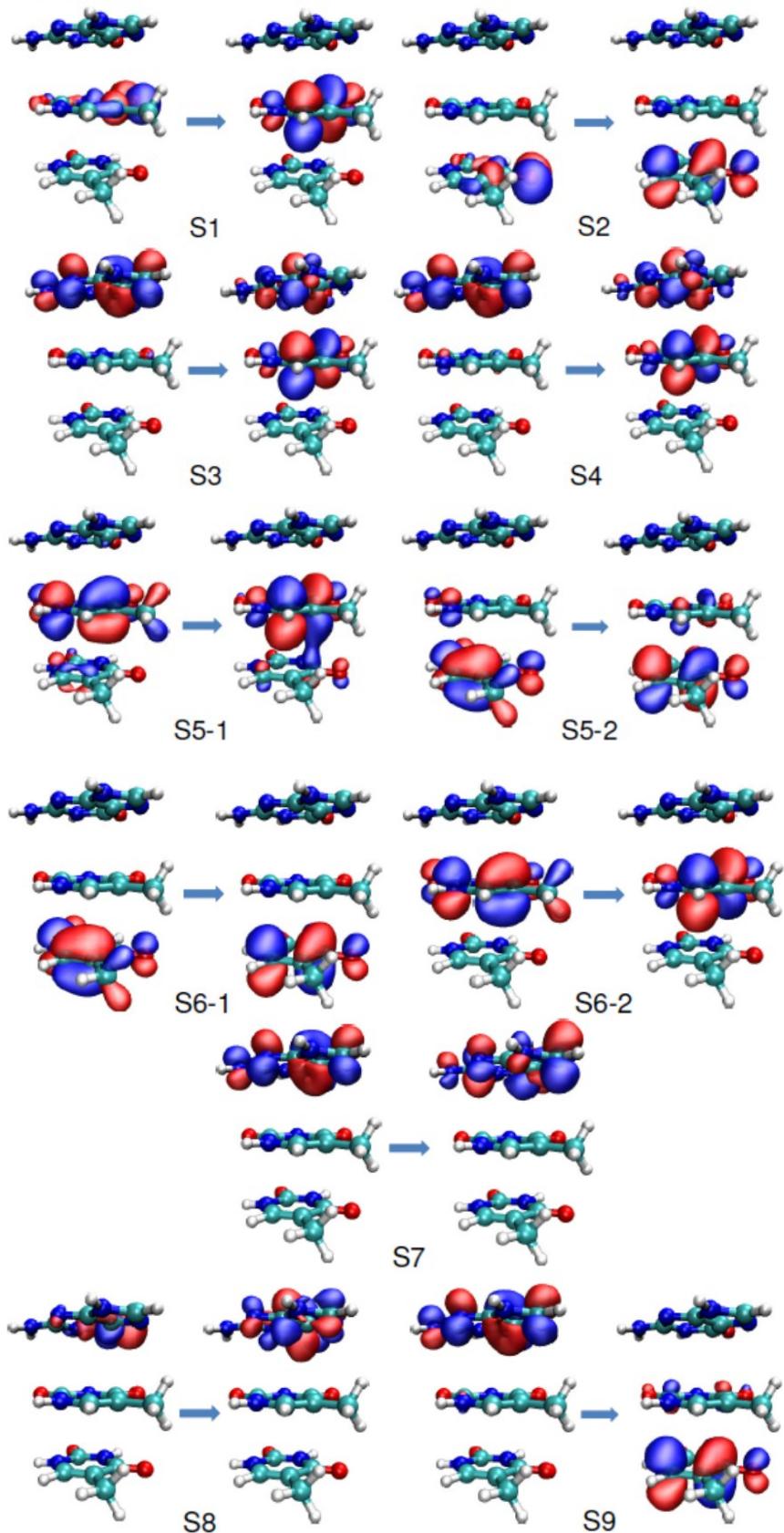
GTAA Frame 2



GTAA Frame 3



GTAA Frame 4



GTAA Frame 5

