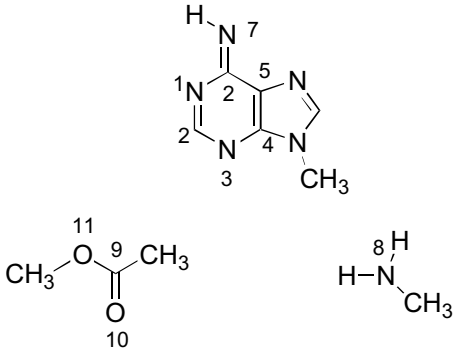
Supporting Information

Quantum Chemical Study of Ester Aminolysis Catalyzed by a Single Adenine: A Reference Reaction for Ribosomal Peptide Synthesis

Dimas Suárez,[†] and Kenneth M. Merz, Jr. [‡] *

Table S1. HF/6-31+G** and *B3LYP/6-31+G*** NPA Charges for the Structures Involved in the Ester Aminolysis Reaction between Methylamine and Methylacetate Catalyzed by a Single Adenine Anion. (Hydrogens were summed into heavy atoms).



Atom Numbering

Atom	C	TS_1	I_1	TS_2	I_2 [a]	TS_3 [a]	P
N1	-0.74	-0.69	-0.67	-0.67	-0.67	-0.68	-0.72
	-0.62	*-0.58*	*-0.52*	*-0.57*	*-0.56*	*-0.58*	*-0.60*
C2	0.55	0.63	0.66	0.64	0.63	0.62	0.56
	042	*0.50*	*0.52*	*0.52*	*0.50*	*0.50*	*043*
N3	-0.78	-0.27 [b]	-0.22	-0.20	-0.21	-0.20	-0.83
	-0.68	*-0.19* [b]	*-0.16*	*-0.13*	*-0.13*	*-0.13*	*-0.72*
C4	0.42	0.43	0.42	0.42	0.42	0.43	0.42
	0.33	*0.35*	*0.34*	*0.35*	*0.34*	*0.34*	*0.33*
C5	-0.07	-0.05	-0.04	-0.04	-0.04	-0.04	-0.06
	-0.01	*0.01*	*0.01*	*0.00*	*0.00*	*0.00*	*0.00*
C6	0.50	0.50	0.49	0.49	0.49	0.49	0.50
	0.36	*0.37*	*0.37*	*0.37*	*0.37*	*0.37*	*0.37*
N7	-0.53	-0.47	-0.44	-0.43	-0.44	-0.45	-0.50
	-0.45	*-0.40*	*-0.39*	*-0.38*	*-0.37*	*-0.38*	*-0.43*
N8	-0.16	-0.41	-0.46	-0.46	-0.45	-0.43	-0.30
	-0.15	*-0.38*	*-0.40*	*-0.42*	*-0.40*	*-0.38*	*-0.23*
C9	0.98	0.86	0.84	0.83	0.84	0.87	0.82
	0.82	*0.72*	*0.70*	*0.70*	*0.70*	*0.70*	*0.67*
O10	-0.73	-0.99	-1.00	-1.00	-1.00	-0.89	-0.78
	-0.64	*-0.86*	*-0.87*	*-0.85*	*-0.89*	*-0.77*	*-0.69*
O11	-0.66	-0.75	-0.77	-0.79	-0.79	-0.91	-0.33
	-0.56	*-0.68*	*-0.70*	*-0.73*	*-0.71*	*-0.80*	*-0.32*

[a] *B3LYP* charges were obtained from single-point B3LYP/6-31+G**//HF/6-31+G** calculations
[b] Including charge of the H atom being transferred (see Figure 2).

Cartesian Coordinates

HF/6-31+G**				B3LYP/6-31+G**		
			C			
N	.50619	-.20932	.97720	N	.50953	-.29526	.49148
C	1.45141	.28301	.15163	C	1.55127	.35240	-.09078
C	2.49015	-.39492	-.43134	C	2.87954	-.06632	-.17608
C	2.62710	-1.81104	-.14623	C	3.23191	-1.34669	.42074
N	1.64092	-2.29890	.71215	N	2.14273	-2.00823	1.02804
C	.71563	-1.50927	1.18014	C	.93781	-1.46889	1.02071
N	1.55036	1.57534	-.28288	N	1.49774	1.57657	-.73360
C	2.64782	1.60367	-1.10445	C	2.79007	1.83315	-1.16042
N	3.23018	.46621	-1.21978	N	3.63712	.87830	-.85173
C	.67208	2.66607	.05255	C	.33632	2.42930	-.87010
N	3.55169	-2.55261	-.62955	N	4.43307	-1.84919	.40572
N	-2.20472	1.08121	2.35824	N	-2.09232	.99699	1.79363
C	-1.88453	1.77562	3.58966	C	-1.69796	1.80076	2.95053
C	-2.41281	-.13225	-1.49484	C	-2.95694	-.58695	-1.30397
C	-1.25782	-.50476	-2.37748	C	-1.78398	-1.20089	-2.01465
O	-3.01385	-1.20027	-.99700	O	-3.59481	-1.48789	-.52446
C	-4.06346	-.99654	-.06567	C	-4.61021	-.96658	.35581
O	-2.77242	.98417	-1.26450	O	-3.29054	.58389	-1.37765
H	-1.13894	2.56681	3.48326	H	-.94635	2.58339	2.74336
H	-1.50365	1.06412	4.31466	H	-1.27659	1.14348	3.71862
H	-2.78335	2.21976	4.00984	H	-2.57801	2.29104	3.38633
H	-.87115	.37895	-2.86333	H	-1.59429	-.66352	-2.94560
H	-.48038	-.95502	-1.77255	H	-.91218	-1.08406	-1.35446
H	-1.57601	-1.23363	-3.11414	H	-1.93702	-2.26555	-2.20267
H	.67483	2.84453	1.12184	H	.03059	2.84095	.09905
H	-.00243	-1.98307	1.83490	H	.15686	-2.05339	1.51402
H	-1.38366	.65153	1.96678	H	-1.26887	.53454	1.38830
H	1.01897	3.55999	-.45259	H	.58117	3.25518	-1.54409
H	-.34253	2.45496	-.26216	H	-.50818	1.87104	-1.28437
H	2.95519	2.51248	-1.58519	H	3.02928	2.74236	-1.69878
H	3.41545	-3.48319	-.27592	H	4.37996	-2.74713	.89569
H	-2.55462	1.71442	1.66661	H	-2.47423	1.58674	1.05768
H	-4.86442	-.42678	-.51928	H	-5.35442	-.40014	-.21080
H	-4.41146	-1.98491	.19645	H	-5.06588	-1.84382	.81754
H	-3.69751	-.48309	.81127	H	-4.14097	-.32922	1.11149

HF/6-31+G**			B3LYP/6-31+G**		
TS_1					
N	-3.92061	-.66015	-.15884	N	.60679	.06691	-.21051
C	-2.89181	.25220	-.04778	C	1.30328	-1.06816	.11156
C	-1.69726	-.40388	-.00486	C	2.68234	-1.16855	.00053
N	-1.97967	-1.73498	-.09051	C	3.44962	-.02490	-.48017
C	-3.34881	-1.80603	-.18127	N	2.66653	1.12197	-.78320
C	-2.89568	1.70521	.01307	C	1.37621	1.11724	-.64360
N	-1.61309	2.26914	.10111	N	.84504	-2.27002	.58482
C	-.56046	1.53001	.13512	C	1.98063	-3.04978	.73529
N	-.47720	.18388	.09466	N	3.08674	-2.42891	.40122
N	-3.95023	2.41357	-.01144	C	-.53401	-2.67796	.81687
C	-1.05320	-2.83837	-.11469	N	4.73279	-.03251	-.62469
N	1.83625	-.86513	.51740	O	-1.63950	1.80729	-.61881
C	2.99953	-.29514	-.32065	C	-2.06647	2.65702	-1.65567
O	2.82972	1.11671	-.05026	C	-2.73971	1.48574	.48076
C	3.98538	1.88772	-.14504	C	-2.08902	2.00924	1.78043
C	2.08089	-.74142	1.95540	N	-2.59147	-.04592	.49406
H	1.32078	-1.29458	2.50118	C	-3.30726	-.65412	-.63632
O	4.12928	-.78816	.01419	H	-3.36755	-1.74165	-.49728
C	2.60158	-.52258	-1.78970	O	-3.90153	1.94000	.20378
H	2.01557	.30037	2.23600	H	-1.17700	-1.79067	.81820
H	3.06499	-1.11532	2.20467	H	-.87145	-3.36101	.02935
H	2.60439	-1.58810	-2.00827	H	-.61013	-3.18127	1.78546
H	1.62994	-.10293	-2.03229	H	1.90956	-4.06554	1.10193
H	3.35324	-.05988	-2.41999	H	5.00449	.89127	-.97205
H	-.51355	-2.91665	.82230	H	.79275	2.00417	-.87077
H	.39450	2.02212	.20275	H	-.41210	.19965	-.13132
H	.63955	-.35522	.25005	H	-3.08400	-.32568	1.34478
H	-1.61038	-3.75345	-.26860	H	-2.70486	1.71926	2.64203
H	-.34274	-2.72571	-.92495	H	-2.06677	3.10155	1.73400
H	-3.84591	-2.75275	-.26207	H	-1.06926	1.63600	1.92638
H	-3.68204	3.38018	.04013	H	-1.92566	2.17161	-2.63645
H	1.85745	-1.84413	.29694	H	-1.48855	3.59769	-1.65614
H	4.35666	1.93843	-1.16862	H	-3.13181	2.89010	-1.52183
H	3.72079	2.89218	.17220	H	-4.31865	-.24250	-.75635
H	4.77571	1.49649	.48276	H	-2.75012	-.45821	-1.55886

HF/6-31+G**			B3LYP/6-31+G**		
I_1					
N	-3.90951	-.77504	-.14304	N	3.95646	-.66876	.12312
C	-2.92168	.17909	-.03352	C	2.92115	.24577	.03038
C	-1.70756	-.43146	-.01638	C	1.70760	-.42487	.01440
N	-1.92252	-1.76701	-.11578	N	1.98856	-1.76660	.09836
C	-3.28783	-1.89523	-.18843	C	3.37327	-1.84140	.16243
C	-2.98708	1.63243	.05039	C	2.92381	1.70281	-.04302
N	-1.72679	2.25961	.13528	N	1.63176	2.28736	-.11465
C	-.64054	1.58769	.14471	C	.55338	1.55872	-.12248
N	-.52547	.23834	.07566	N	.48961	.19004	-.06175
N	-4.06710	2.29244	.04769	N	4.00070	2.41732	-.04243
C	-.94110	-2.82916	-.15705	C	1.04750	-2.87074	.14487
N	2.10116	-1.07247	.42983	N	-1.95414	-1.06014	-.34461
C	3.09398	-.21662	-.31141	C	-3.08427	-.24820	.35599
O	4.31808	-.38006	.03598	O	-4.27664	-.57969	.02400
C	2.32242	-1.04548	1.86995	C	-2.21273	-1.18732	-1.78827
C	2.82827	-.44903	-1.81327	C	-2.76329	-.29527	1.87204
O	2.55493	1.12181	-.01115	O	-2.65299	1.15537	-.10349
C	3.48174	2.15697	-.04653	C	-3.71577	2.07903	-.14618
H	1.67058	-1.77391	2.35172	H	-1.54271	-1.94040	-2.22382
H	2.07064	-.06475	2.25575	H	-2.01268	-.22594	-2.26913
H	3.35463	-1.25789	2.12829	H	-3.25742	-1.46142	-1.98167
H	3.11439	-1.46458	-2.07941	H	-2.94274	-1.30881	2.25380
H	1.78910	-.28336	-2.08885	H	-1.73400	.00523	2.09960
H	3.45524	.22635	-2.38562	H	-3.45222	.37840	2.39054
H	-1.46419	-3.76759	-.28537	H	1.61298	-3.80404	.19665
H	.30314	2.09550	.20904	H	-.42555	2.02863	-.17621
H	.38910	-.21147	.13336	H	-.46522	-.32275	-.12733
H	-.25936	-2.68718	-.98531	H	.40170	-2.79621	1.02524
H	-.37083	-2.86270	.76177	H	.41824	-2.88402	-.74958
H	-3.74389	-2.86137	-.27423	H	3.87223	-2.79917	.23482
H	-3.84582	3.26989	.11235	H	3.71242	3.39805	-.09944
H	2.30210	-2.00491	.11905	H	-2.05902	-1.99044	.06229
H	3.84001	2.35110	-1.05868	H	-3.94837	2.49476	.85177
H	2.97932	3.05371	.31103	H	-3.41113	2.90932	-.79697
H	4.33956	1.94285	.57815	H	-4.62393	1.60754	-.54182

TS_2

HF/6-31+G**			B3LYP/6-31+G**		
N	-.57897	-.37468	-.13855	N	.60679	.06691	-.21051
C	-1.65768	.45422	-.03805	C	1.30328	-1.06816	.11156
C	-2.93843	.00262	.03742	C	2.68234	-1.16855	.00053
C	-3.19690	-1.43093	.01685	C	3.44962	-.02490	-.48017
N	-2.03228	-2.22275	-.07664	N	2.66653	1.12197	-.78320
C	-.87204	-1.69793	-.14208	C	1.37621	1.11724	-.64360
N	-1.69940	1.80749	.00740	N	.84504	-2.27002	.58482
C	-3.03356	2.11037	.10292	C	1.98063	-3.04978	.73529
N	-3.79392	1.07755	.12759	N	3.08674	-2.42891	.40122
C	-.60141	2.74642	-.11729	C	-.53401	-2.67796	.81687
N	-4.35201	-1.94347	.07593	N	4.73279	-.03251	-.62469
O	2.25092	-.95640	-.44915	O	-1.63950	1.80729	-.61881
C	2.86149	-2.06099	-1.03258	C	-2.06647	2.65702	-1.65567
C	3.11947	-.13999	.44614	C	-2.73971	1.48574	.48076
C	2.77633	-.60290	1.87539	C	-2.08902	2.00924	1.78043
N	2.48616	1.20437	.26339	N	-2.59147	-.04592	.49406
C	2.89292	1.83489	-.98326	C	-3.30726	-.65412	-.63632
H	2.51293	2.85601	-1.01486	H	-3.36755	-1.74165	-.49728
O	4.36522	-.21254	.15396	O	-3.90153	1.94000	.20378
H	.30787	2.29601	.25337	H	-1.17700	-1.79067	.81820
H	-.45516	3.03353	-1.15294	H	-.87145	-3.36101	.02935
H	-.82887	3.62892	.46754	H	-.61013	-3.18127	1.78546
H	-3.36170	3.12935	.15694	H	1.90956	-4.06554	1.10193
H	-4.26265	-2.94323	.04498	H	5.00449	.89127	-.97205
H	-.00751	-2.33141	-.20637	H	.79275	2.00417	-.87077
H	.38702	-.09295	-.17783	H	-.41210	.19965	-.13132
H	2.85234	1.76198	1.01268	H	-3.08400	-.32568	1.34478
H	3.32530	.00352	2.59224	H	-2.70486	1.71926	2.64203
H	3.10499	-1.62989	1.99601	H	-2.06677	3.10155	1.73400
H	1.71345	-.54118	2.09715	H	-1.06926	1.63600	1.92638
H	2.18399	-2.44652	-1.79259	H	-1.92566	2.17161	-2.63645
H	3.04738	-2.85531	-.30718	H	-1.48855	3.59769	-1.65614
H	3.80690	-1.79438	-1.48603	H	-3.13181	2.89010	-1.52183
H	3.97101	1.85053	-1.10838	H	-4.31865	-.24250	-.75635
H	2.46557	1.29240	-1.81979	H	-2.75012	-.45821	-1.55886

HF/6-31+G**				HF/6-31+G**			
	I_2				TS_3		
N	.68766	-.16558	-.56150	N	3.47169	1.47414	.17747
C	1.45350	-.53705	.50340	C	2.85943	.24668	.04868
C	2.60164	-1.25692	.38915	C	1.52596	.43078	-.15216
C	3.05496	-1.67278	-.93105	N	1.29287	1.76417	-.14724
N	2.20477	-1.26473	-1.98336	C	2.52404	2.33158	.05401
C	1.14846	-.58590	-1.76150	C	3.38781	-1.10880	.10255
N	1.25214	-.29052	1.81787	N	2.40858	-2.11058	-.06555
C	2.31608	-.88203	2.44712	C	1.17881	-1.81482	-.25259
N	3.13091	-1.46377	1.64320	N	.63367	-.58310	-.31602
C	.17802	.47614	2.42400	N	4.61021	-1.39027	.28225
N	4.10941	-2.33855	-1.14488	C	.02635	2.44180	-.35264
O	-1.54522	1.53329	-.73638	O	-1.94466	-.30927	-.93822
C	-1.46379	2.41305	-1.81170	C	-2.28036	-1.10280	-2.01158
C	-2.93493	1.35908	-.16418	C	-3.29485	-.06526	.24340
C	-3.03438	2.41923	.95104	O	-3.93828	-1.11761	.31447
N	-2.78347	.03948	.50157	C	-3.94280	1.13819	-.43054
C	-2.95439	-1.08094	-.40893	N	-2.47074	.35039	1.35253
H	-2.90232	-2.00959	.15638	C	-2.10578	-.71139	2.26983
O	-3.84567	1.44873	-1.05739	H	-2.96348	-1.22508	2.69666
H	2.41304	-.84317	3.51376	H	2.63614	3.39649	.10363
H	.53320	-.29887	-2.59668	H	.47262	-2.61791	-.37750
H	-.16232	.38942	-.50039	H	-.38308	-.44882	-.50529
H	4.19608	-2.49740	-2.13262	H	4.71238	-2.38931	.27967
H	.09907	.18705	3.46426	H	.10780	3.44350	.05097
H	.38485	1.53873	2.36467	H	-.21504	2.49768	-1.40763
H	-.75625	.26542	1.92115	H	-.76006	1.90523	.15743
H	-3.52469	-.00683	1.17466	H	-2.95171	1.07981	1.84067
H	-1.65978	3.44218	-1.51010	H	-2.72929	-.52829	-2.83195
H	-.44766	2.36979	-2.20143	H	-1.39381	-1.59393	-2.42955
H	-2.16939	2.14943	-2.58899	H	-2.98867	-1.87976	-1.72560
H	-2.14990	-1.09226	-1.13485	H	-1.50064	-.29078	3.06874
H	-3.89158	-1.03868	-.95585	H	-1.50928	-1.44756	1.74802
H	-3.98982	2.31147	1.45962	H	-4.77739	1.47243	.18584
H	-2.23107	2.34518	1.67983	H	-3.24893	1.95860	-.57241
H	-3.01513	3.40628	.50243	H	-4.33965	.83386	-1.38958

HF/6-31+G**			B3LYP/6-31+G**		
		P			
N	.32288	.39639	-.52741	N	.33809	.43977	-.54579
C	1.25589	.12995	.41885	C	1.24692	.13193	.42542
C	2.50982	-.38183	.22691	C	2.50256	-.44601	.25359
C	2.92927	-.68565	-1.12961	C	2.93405	-.77009	-1.09902
N	1.95089	-.40023	-2.08964	N	1.98248	-.44320	-2.09390
C	.80207	.08688	-1.74003	C	.83285	.10440	-1.77098
N	1.12359	.32268	1.76489	N	1.10117	.33645	1.78341
C	2.31157	-.09135	2.31043	C	2.26949	-.13423	2.35709
N	3.15573	-.51080	1.44056	N	3.12677	-.60326	1.48047
C	-.03804	.81125	2.46647	C	-.06229	.87205	2.46627
N	4.07076	-1.16544	-1.43590	N	4.07778	-1.31312	-1.38566
O	-1.11713	2.94432	-.39340	O	-1.14296	2.77590	-.27888
C	-.33012	3.92140	-1.00175	C	-.54746	3.81723	-1.02725
C	-3.58849	-1.07161	-.04594	C	-3.53077	-.96081	-.07378
N	-2.28968	-1.38510	-.13469	N	-2.21132	-1.24648	-.18730
C	-1.83352	-2.75489	-.05925	C	-1.73394	-2.61968	-.17865
O	-4.45477	-1.90423	.12078	O	-4.39052	-1.84212	.06461
C	-3.93724	.39575	-.17047	C	-3.90973	.51064	-.12851
H	-2.10206	-3.20386	.89062	H	-1.93714	-3.10512	.78274
H	2.47758	-.04745	3.36938	H	2.41830	-.09380	3.42902
H	.11347	.27446	-2.55249	H	.15987	.32708	-2.60250
H	-.67466	2.09698	-.44697	H	-.61796	1.93917	-.41398
H	4.10254	-1.28101	-2.43333	H	4.10582	-1.42635	-2.40308
H	-.85136	.09506	2.42296	H	-.88634	.14929	2.46924
H	.22766	.97369	3.50403	H	.21256	1.09909	3.49984
H	-.37559	1.74659	2.03972	H	-.40433	1.78719	1.97544
H	-1.60170	-.67250	-.27739	H	-1.51133	-.50936	-.30351
H	-.83843	4.87350	-.89501	H	-1.09129	4.74332	-.80905
H	.65054	4.00102	-.53663	H	.50996	3.96973	-.76183
H	-.18806	3.72664	-2.06324	H	-.60290	3.63679	-2.11226
H	-.75713	-2.75854	-.16342	H	-.65749	-2.61118	-.35721
H	-2.26986	-3.35572	-.84942	H	-2.22784	-3.20885	-.95868
H	-4.52650	.68154	.69333	H	-4.47428	.75738	.77616
H	-3.07610	1.04512	-.25114	H	-3.05964	1.19122	-.22094
H	-4.56166	.52192	-1.04840	H	-4.58297	.66049	-.97906