Supporting Information

Theoretical studies of chemical reactivity of metabolically activated forms of aromatic amines towards DNA

Igor Shamovsky, Lena Ripa, Niklas Blomberg, Leif A. Eriksson, Peter Hansen, Christine Mee, Christian Tyrchan, Mike O'Donovan, and Peter Sjö

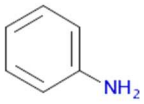
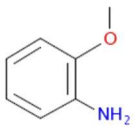
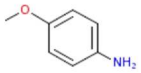
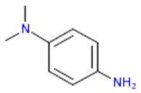
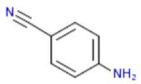
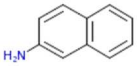
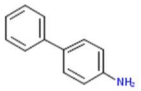
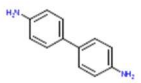
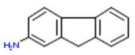
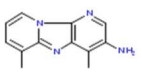
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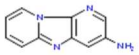
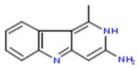
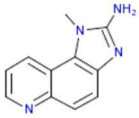
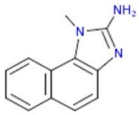
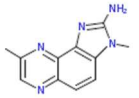
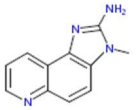
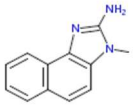
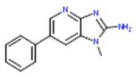
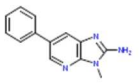
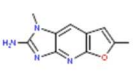
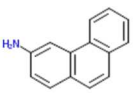
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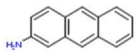
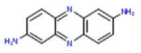
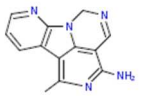
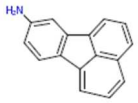
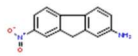
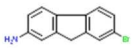
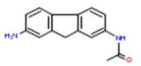
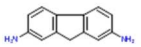
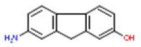
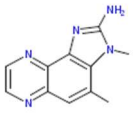
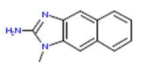
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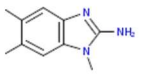
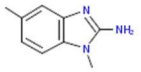
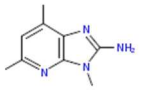
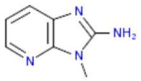
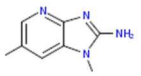
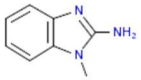
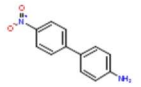
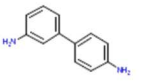
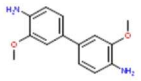
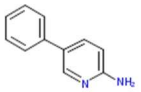
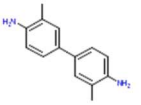
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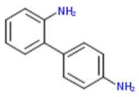
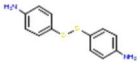
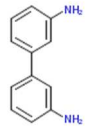
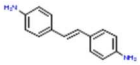
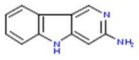
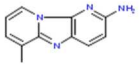
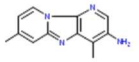
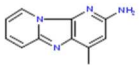
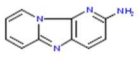
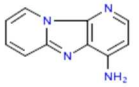
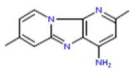
Table 1S. Structures, mutagenic potencies, absolute and relative energies of $ArNH_2$, $ArNH^+$ and $ArNH^-$ for Figure 10

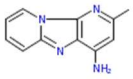
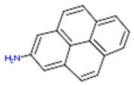
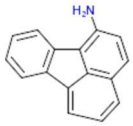
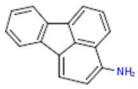
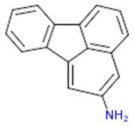
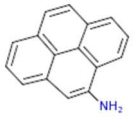
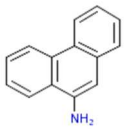
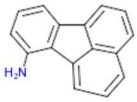
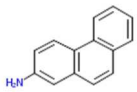
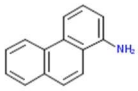
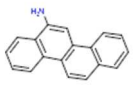
Molecule	SMILES	No.	ArNH2, M06-2X/ 6-31+G(d), hartree	$ArNH^+$, M062X/ 6-31+G(d), hartree	$ArNH^-$, M062X/ 6-31+G(d), hartree	Relative $ArNH^+$ stability, kcal/mol	Relative $ArNH^-$ stability, kcal/mol	Class	LogMP[a]
	Nc1ccccc1	**1**	-287.479976	-286.532094	-286.885485	0.0	0.0	Monocyclic	-3.39
	Nc1c(OC)cccc1	**2**	-401.961702	-401.043533	-401.364496	-18.6	1.7	Monocyclic	-1.672
	Nc1ccc(cc1)OC	**3**	-401.957706	-401.049402	-401.359153	-24.8	2.5	Monocyclic	-2.305
	Nc1ccc(cc1)N(C)C	**4**	-421.384196	-420.510113	-420.777921	-46.3	7.4	Monocyclic	ROS
	Nc1ccc(C#N)cc1	**5**	-379.700105	-378.726829	-379.136772	15.9	-19.6	Monocyclic	Mutagenic
	c1cc(N)cc(c12)cccc2	**6**	-441.065174	-440.137522	-440.483016	-12.7	-7.7	Fused	-0.67
	Nc1ccc(cc1)-c2ccccc2	**7**	-518.447376	-517.526903	-517.86491	-17.2	-7.5	Amino-biphenyls	-0.14
	Nc1ccc(cc1)-c(cc2)ccc2N	**10**	-573.781963	-572.890444	-573.191345	-35.4	-2.4	Amino-biphenyls	-0.39
	c1cc(N)cc(c1-2)Cc3c2cccc3	**11**	-556.551993	-555.644299	-555.970461	-25.2	-8.1	2-AF	1.93
	Cc1cccn(c12)c3c(n2)c(C)c(cn3)N	**12**	-683.270075	-682.352	-682.689423	-18.7	-8.7	Amino-carbolines	4.83

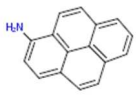
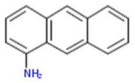
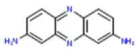
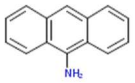
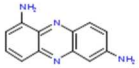
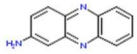
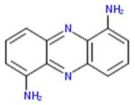
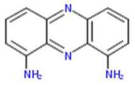
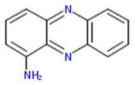
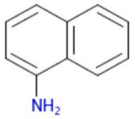
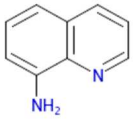
Molecule	SMILES	No.	ArNH2, M06-2X/ 6-31+G(d), hartree	$ArNH^+$, M062X/ 6-31+G(d), hartree	$ArNH^-$, M062X/ 6-31+G(d), hartree	Relative $ArNH^+$ stability, kcal/mol	Relative $ArNH^-$ stability, kcal/mol	Class	LogMP[a]
	c1cccn(c12)c3c(n2)cc(cn3)N	**13**	-604.668652	-603.740369	-604.088838	-12.3	-9.2	Amino-carbolines	2.26
	c1cccc(c12)c3c([nH]2)cc(N)nc(C)3	**14**	-627.949671	-627.031615	-627.369689	-18.7	-9.1	Amino-carbolines	4.09
	n1c(N)n(C)c(c12)c3c(cc2)nccc3	**15**	-643.977201	-643.075383	-643.42047	-28.9	-23.7	AIA	5.8
	n1c(N)n(C)c(c12)c3c(cc2)cccc3	**16**	-627.939926	-627.046948	-627.378662	-34.5	-20.9	AIA	2.29
	Cn1c(N)nc(c12)c3c(cc2)ncc(n3)C	**17**	-699.311946	-698.407546	-698.753484	-27.3	-22.6	AIA	4.33
	Cn1c(N)nc(c12)c3c(cc2)nccc3	**18**	-643.981674	-643.081335	-643.424525	-29.8	-23.4	AIA	4.5
	Cn1c(N)nc(c12)c3c(cc2)cccc3	**19**	-627.94334	-627.052607	-627.382817	-35.9	-21.3	AIA	0.59
	Cn1c(N)nc(c12)ncc(c2)-c3ccccc3	**20**	-721.359098	-720.445108	-720.809999	-21.3	-28.5	AIA	2.75
	Cn1c(N)nc(c12)cc(cn2)-c3ccccc3	**21**	-721.36659	-720.447248	-720.812587	-17.9	-25.4	AIA	0.65
	Cn1c(N)nc(c12)nc3c(c2)cc(o3)C	**22**	-681.078291	-680.170002	-680.524192	-24.8	-25.3	AIA	3.31
	c1cc(N)cc(c12)c3c(cc2)cccc3	**23**	-594.653945	-593.737883	-594.077138	-20.0	-11.1	Fused	3.77

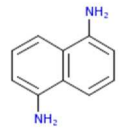
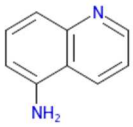
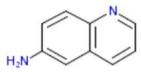
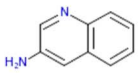
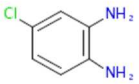
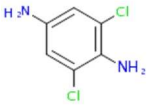
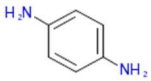
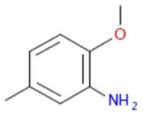
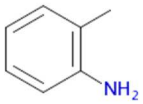
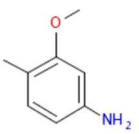
Molecule	SMILES	No.	ArNH2, M06-2X/ 6-31+G(d), hartree	$ArNH^+$, M062X/ 6-31+G(d), hartree	$ArNH^-$, M062X/ 6-31+G(d), hartree	Relative $ArNH^+$ stability, kcal/mol	Relative $ArNH^-$ stability, kcal/mol	Class	LogMP[a]
	c1cc(N)cc(c12)cc3c(c2)cccc3	**24**	-594.643638	-593.73216	-594.070573	-22.8	-13.4	Fused	2.62
	c1cc(N)cc(c12)nc3c(n2)cc(N)cc3	**25**	-682.058177	-681.152808	-681.492987	-26.7	-18.4	Fused	3.97
	n1cccc(c12)c3c4c(C=NCn24)c(N)nc3C	**26**	-775.496811	-774.569228	-774.939609	-12.7	-23.4	Amino-carbolines	4.17
	c1ccc(c2c13)-c4c(-c2ccc3)cc(N)cc4	**27**	-670.838871	-669.931394	-670.263635	-25.4	-12.1	Fused	3.8
	ON(O)c(cc1)cc(c1-2)Cc3c2ccc(c3)N		-760.989473	-760.058622	-760.431307	-10.7	-22.8	2-AF	3
	c1cc(N)cc(c1-2)Cc3c2ccc(Br)c3		-3127.760424	-3126.848439	-3127.185748	-22.5	-12.4	2-AF	2.62
	c1cc(N)cc(c1-2)Cc3c2ccc(NC(=O)C)c3		-764.491744	-763.597624	-763.912295	-33.7	-9.4	2-AF	1.18
	c1cc(N)cc(c1-2)Cc3c2ccc(N)c3		-611.886036	-611.005978	-611.299754	-42.6	-5.2	2-AF	0.48
	c1cc(N)cc(c1-2)Cc3c2ccc(c3)O		-631.747767	-630.852228	-631.164456	-32.8	-7.0	2-AF	0.41
	Cn1c(N)nc(c12)c3c(cc2C)nccn3		-699.306938	-698.402029	-698.749787	-27.0	-23.4	AIA	5.23
	Cn1c(N)nc(c12)cc3c(c2)cccc3		-627.939075	-627.020246	-627.387891	-18.2	-27.2	AIA	2.59

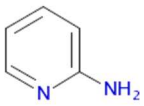
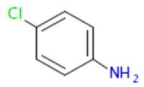
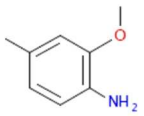
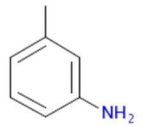
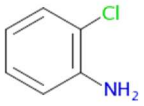
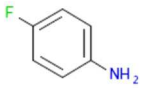
Molecule	SMILES	No.	ArNH2, M06-2X/ 6-31+G(d), hartree	$ArNH^+$, M062X/ 6-31+G(d), hartree	$ArNH^-$, M062X/ 6-31+G(d), hartree	Relative $ArNH^+$ stability, kcal/mol	Relative $ArNH^-$ stability, kcal/mol	Class	LogMP[a]
	Cn1c(N)nc(c12)cc(C)c(c2)C		-552.948771	-552.047698	-552.38117	-29.4	-16.9	AIA	2.54
	Cn1c(N)nc(c12)cc(C)cc2		-513.651849	-512.742505	-513.08783	-24.2	-19.1	AIA	2.31
	Cn1c(N)nc(c12)c(C)cc(n2)C		-568.999402	-568.090103	-568.43709	-24.2	-20.2	AIA	1.65
	Cn1c(N)nc(c12)cccn2		-490.399895	-489.470719	-489.840777	-11.7	-22.2	AIA	0.37
	Cn1c(N)nc(c12)ncc(c2)C		-529.688688	-528.769836	-529.132499	-18.2	-24.0	AIA	0.11
	Cn1c(N)nc(c12)cccc2		-474.355736	-473.438925	-473.792125	-19.5	-19.4	AIA	-0.43
	Nc1ccc(cc1)-c(cc2)ccc2N(O)O		-722.883451	-721.940824	-722.324917	-3.3	-22.6	Amino-biphenyls	1.04
	Nc1ccc(cc1)-c2cccc(c2)N		-573.782571	-572.868342	-573.199945	-21.1	-7.4	Amino-biphenyls	0.2
	Nc1c(OC)cc(cc1)-c(cc2)cc(c2N)OC		-802.746252	-801.872353	-802.158187	-46.4	-4.0	Amino-biphenyls	0.15
	Nc1ccc(cn1)-c2ccccc2		-534.492747	-533.552582	-533.917119	-4.8	-11.8	Amino-biphenyls	0.054
	Nc1ccc(cc1C)-c(cc2C)ccc2N		-652.37846	-651.496061	-651.788995	-41.1	-3.2	Amino-biphenyls	0.01

Molecule	SMILES	No.	ArNH2, M06-2X/ 6-31+G(d), hartree	$ArNH^+$, M062X/ 6-31+G(d), hartree	$ArNH^-$, M062X/ 6-31+G(d), hartree	Relative $ArNH^+$ stability, kcal/mol	Relative $ArNH^-$ stability, kcal/mol	Class	LogMP[a]
	Nc1ccc(cc1)-c2ccccc2N		-573.783193	-572.874551	-573.200773	-24.6	-7.6	Amino-biphenyls	-0.92
	Nc1ccc(cc1)SSc(cc2)ccc2N		-1370.09273	-1369.183105	-1369.522236	-24.0	-15.1	Amino-biphenyls	-1.03
	c1c(N)cccc1-c2cccc(c2)N		-573.782674	-572.844972	-573.193057	-6.4	-3.1	Amino-biphenyls	-1.3
	Nc1ccc(cc1)/C=C/c(cc2)ccc2N		-651.149969	-650.270755	-650.572983	-43.1	-11.0	Amino-biphenyls	-2.15
	c1cccc(c12)c3c([nH]2)cc(N)nc3		-588.646537	-587.723434	-588.067097	-15.5	-9.4	Amino-carbolines	4.26
	Cc1cccn(c12)c3c(n2)ccc(n3)N		-643.977642	-643.072904	-643.404011	-27.1	-13.1	Amino-carbolines	4
	c1c(C)ccn(c12)c3c(n2)c(C)c(cn3)N		-683.268455	-682.351616	-682.684594	-19.5	-6.7	Amino-carbolines	3.73
	c1cccn(c12)c3c(n2)c(C)cc(n3)N		-643.979821	-643.074174	-643.405447	-26.5	-12.6	Amino-carbolines	3.4
	c1cccn(c12)c3c(n2)ccc(n3)N		-604.679058	-603.769532	-604.106266	-24.1	-13.6	Amino-carbolines	2.56
	c1cccn(c12)c3c(n2)c(N)ccn3		-604.679578	-603.754545	-604.109533	-14.3	-15.3	Amino-carbolines	-0.44
	c1c(C)ccn(c12)c3c(n2)c(N)cc(n3)C		-683.275802	-682.360358	-682.70235	-20.4	-13.2	Amino-carbolines	-0.47

Molecule	SMILES	No.	ArNH2, M06-2X/ 6-31+G(d), hartree	$ArNH^+$, M062X/ 6-31+G(d), hartree	$ArNH^-$, M062X/ 6-31+G(d), hartree	Relative $ArNH^+$ stability, kcal/mol	Relative $ArNH^-$ stability, kcal/mol	Class	LogMP[a]
	c1cccn(c12)c3c(n2)c(N)cc(n3)C		-643.978766	-643.056083	-643.407491	-15.8	-14.6	Amino-carbolines	-0.5
	c1c(N)cc(c2c13)ccc4c2c(cc3)ccc4		-670.862787	-669.941675	-670.28529	-16.8	-10.7	Fused	3.5
	c1ccc(c2c13)-c4c(-c2c(N)cc3)cccc4		-670.842001	-669.927029	-670.280104	-20.7	-20.5	Fused	3.35
	Nc1ccc(c2c13)-c4c(-c2ccc3)cccc4		-670.840421	-669.93498	-670.280458	-26.6	-21.7	Fused	3.31
	c1c(N)cc(c2c13)-c4c(-c2ccc3)cccc4		-670.838438	-669.91899	-670.260532	-17.8	-10.4	Fused	3.23
	c1ccc(c2c13)cc(N)c4c2c(cc3)ccc4		-670.86267	-669.955137	-670.291972	-25.3	-14.9	Fused	3.16
	c1cccc2c1c(N)cc(c23)cccc3		-594.652972	-593.74144	-594.079985	-22.8	-13.5	Fused	2.98
	c1ccc(c2c13)-c4c(-c2ccc3)cccc4N		-670.839805	-669.927643	-670.265385	-22.4	-12.6	Fused	2.88
	c1cc(N)cc(c12)ccc3c2cccc3		-594.653953	-593.733936	-594.076318	-17.5	-10.6	Fused	2.46
	c1cccc(c12)c3c(cc2)c(N)ccc3		-594.652334	-593.741641	-594.077352	-23.3	-12.2	Fused	2.38
	c1cccc2c1c(N)cc(c23)c4c(cc3)cccc4		-748.240362	-747.341712	-747.673765	-30.9	-17.5	Fused	1.83

Molecule	SMILES	No.	ArNH2, M06-2X/ 6-31+G(d), hartree	$ArNH^+$, M062X/ 6-31+G(d), hartree	$ArNH^-$, M062X/ 6-31+G(d), hartree	Relative $ArNH^+$ stability, kcal/mol	Relative $ArNH^-$ stability, kcal/mol	Class	LogMP[a]
	Nc1ccc(c2c13)ccc4c2c(cc3)ccc4		-670.862178	-669.974806	-670.29789	-38.0	-19.0	Fused	1.43
	c1ccc(N)c(c12)cc3c(c2)cccc3		-594.642882	-593.743215	-594.072697	-30.3	-15.3	Fused	1.18
	c1cc(N)cc(c12)nc3c(n2)ccc(c3)N		-682.059195	-681.128965	-681.496061	-11.1	-19.7	Fused	1.12
	c1cccc(c12)c(N)c3c(c2)cccc3		-594.640728	-593.75749	-594.078778	-40.6	-20.4	Fused	0.87
	Nc1cccc(c12)nc3c(n2)ccc(c3)N		-682.061925	-681.130746	-681.501142	-10.5	-21.2	Fused	0.75
	c1cc(N)cc(c12)nc3c(n2)cccc3		-626.721003	-625.782007	-626.162498	-5.6	-22.6	Fused	0.55
	c1ccc(N)c(c12)nc3c(n2)c(N)ccc3		-682.065207	-681.154655	-681.497694	-23.4	-16.9	Fused	0.2
	c1ccc(N)c(c12)nc3c(n2)cccc3N		-682.063256	-681.141739	-681.497585	-16.5	-18.1	Fused	0.04
	c1ccc(N)c(c12)nc3c(n2)cccc3		-626.723746	-625.797741	-626.157927	-13.7	-18.0	Fused	-0.01
	c1ccc(N)c(c12)cccc2		-441.064277	-440.147432	-440.48594	-19.5	-10.1	Fused	-0.6
	c1ccc(N)c(c12)nccc2		-457.108448	-456.1789	-456.524489	-11.5	-6.6	Fused	-1.14

Molecule	SMILES	No.	ArNH2, M06-2X/ 6-31+G(d), hartree	$ArNH^+$, M062X/ 6-31+G(d), hartree	$ArNH^-$, M062X/ 6-31+G(d), hartree	Relative $ArNH^+$ stability, kcal/mol	Relative $ArNH^-$ stability, kcal/mol	Class	LogMP[a]
	c1ccc(N)c(c12)cccc2N		-496.3994	-495.502611	-495.818552	-32.1	-8.6	Fused	-1.35
	c1ccc(N)c(c12)cccn2		-457.101693	-456.172396	-456.529826	-11.7	-14.2	Fused	-2
	c1cc(N)cc(c12)cccn2		-457.103207	-456.164309	-456.526178	-5.6	-11.0	Fused	-2.67
	n1cc(N)cc(c12)cccc2		-457.102187	-456.163223	-456.528577	-5.6	-13.1	Fused	-3.14
	Nc1c(N)cc(Cl)cc1		-802.38215	-801.492584	-801.806429	-36.6	-11.8	Monocyclic	-0.49
	Nc1c(Cl)cc(N)cc1Cl		-1261.954376	-1261.048839	-1261.373536	-26.6	-8.6	Monocyclic	-0.69
	Nc1cc(C(F)(F)F)ccc1		-624.43769	-623.470809	-623.860274	11.9	-10.7	Monocyclic	-0.8
	Nc1ccc(N)cc1		-342.811269	-341.924785	-342.211951	-38.5	3.0	Monocyclic	-0.983
	Nc1c(OC)ccc(c1)C		-441.257981	-440.344008	-440.660964	-21.3	1.6	Monocyclic	-1.66
	Nc1c(C)cccc1		-326.777997	-325.842527	-326.18564	-7.8	-1.3	Monocyclic	-1.8
	Nc1cc(OC)c(C)cc1		-441.25835	-440.331546	-440.662091	-13.2	1.1	Monocyclic	-1.96

Molecule	SMILES	No.	ArNH2, M06-2X/ 6-31+G(d), hartree	$ArNH^+$, M062X/ 6-31+G(d), hartree	$ArNH^-$, M062X/ 6-31+G(d), hartree	Relative $ArNH^+$ stability, kcal/mol	Relative $ArNH^-$ stability, kcal/mol	Class	LogMP[a]
	Nc1ccccn1		-303.526041	-302.551281	-302.939712	16.9	-5.1	Monocyclic	-2.41
	Nc1ccc(Cl)cc1		-747.049767	-746.104718	-746.466157	-1.8	-6.8	Monocyclic	-2.52
	Nc1c(OC)cc(C)cc1		-441.257877	-440.352849	-440.658249	-26.9	3.2	Monocyclic	-2.58
	Nc1cc(C)ccc1		-326.776889	-325.834094	-326.181945	-3.2	0.3	Monocyclic	-2.92
	Nc1c(Cl)cccc1		-747.051931	-746.099569	-746.466201	2.8	-5.5	Monocyclic	-3
	Nc1ccc(F)cc1		-386.690861	-385.747685	-386.100283	-3.0	-2.5	Monocyclic	-3.32

[a]ROS indicates that the compound causes DNA mutations through the oxidative damage of DNA; Mutagenic indicates that the compound is mutagenic in Ames strains TA98 and TA100 but the actual mutagenic potency was not determined.

3. **Table 2S.** Absolute energies of the key structures of the focused compounds[a]

Compound	Structure	E_g, F1/B1	G_w, F1/B1	G_w,F1/B2//F1/B1	G_w,F2/B2//F1/B1
9MG	9MG	-581.658272	-581.572631	-581.771141	-581.800231
H3O+	H3O+	-76.654307	-76.762911	-76.80778	-76.823391
1	ArNH+	-286.532094	-286.538426	-286.629203	-286.65837
	ArNHOH	-362.617151	-362.534435	-362.660556	-362.688405
	ArNHOAc	-515.223301	-515.105779	-515.286213	-515.324192
	TS-(1a)	-439.333553	-439.289586	-439.456927	-439.506464
	TS-(1b)	-591.952207	-591.868291	-592.085764	-592.146153
	σ-TS-(2)	-868.227606	-868.096392	-868.384194	-868.440726
	π-TS-(2)	-868.248242	-868.11851	-868.408657	-868.46221
2	ArNH+	-401.043533	-401.014389	-401.148444	-401.184812
	ArNHOH	-477.098828	-476.987015	-477.155499	-477.190456
	ArNHOAc	-629.70511	-629.564316	-629.781773	-629.82596
	TS-(1a)	-553.828774	-553.752346	-553.961819	-554.016024
	TS-(1b)	-706.449160	-706.331451	-706.591	-706.658401
	σ-TS-(2)	-982.723814	-982.566419	-982.894462	-982.958615
	π-TS-(2)	-982.741341	-982.579344	-982.911876	-982.973543
3	ArNH+	-401.049402	-401.021266	-401.156195	-401.192131
	ArNHOH	-477.095837	-476.985771	-477.154294	-477.189592
	ArNHOAc	-629.703704	-629.560577	-629.779194	-629.824899
	TS-(1a)	-553.826268	-553.753657	-553.964475	-554.017283
	TS-(1b)	-706.448775	-706.331343	-706.593141	-706.65899
	σ-TS-(2)	-982.729182	-982.564665	-982.897537	-982.960814
	π-TS-(2)	-982.745907	-982.584178	-982.917446	-982.979199
4	ArNH+	-420.510113	-420.44013	-420.577612	-420.624557
	ArNHOH	-496.522734	-496.372534	-496.545153	-496.59254

	ArNHOAc	-649.13129	-648.947761	-649.171169	-649.229641
	TS-(1a)	-573.263728	-573.151523	-573.363617	-573.427286
	TS-(1b)	-725.889349	-725.733869	-725.996358	-726.071465
	σ-TS-(2)	-1002.174380	-1001.968798	-1002.304035	-1002.37596
	π-TS-(2)	-1002.188823	-1001.984859	-1002.320353	-1002.39315
5	ArNH+	-378.726829	-378.745073	-378.86394	-378.884635
	ArNHOH	-454.836217	-454.763688	-454.917892	-454.937594
	ArNHOAc	-607.441385	-607.335249	-607.542062	-607.57204
	TS-(1a)	-531.533255	-531.504994	-531.699615	-531.741774
	TS-(1b)	-684.151254	-684.081775	-684.326609	-684.379238
	σ-TS-(2)	-960.428941	-960.308118	-960.623908	-960.671624
	π-TS-(2)	-960.456475	-960.334778	-960.653081	-960.673991
6	ArNH+	-440.137522	-440.092842	-440.227348	-440.261969
	ArNHOH	-516.202962	-516.078506	-516.248136	-516.281530
	ArNHOAc	-668.808983	-668.650883	-668.87296	-668.917166
	TS-(1a)	-592.925759	-592.83686	-593.047482	-593.100414
	TS-(1b)	-745.546181	-745.41393	-745.674935	-745.739961
	σ-TS-(2)	-1021.824120	-1021.645794	-1021.977825	-1022.039012
	π-TS-(2)	-1021.849417	-1021.673454	-1022.005524	-1022.065741
7	ArNH+	-517.526903	-517.446018	-517.604429	-517.645466
	ArNHOH	-593.584178	-593.429498	-593.622585	-593.663574
	ArNHOAc	-746.19017	-746.000086	-746.247843	-746.298882
	TS-(1a)	-670.308641	-670.18749	-670.421916	-670.482657
	TS-(1b)	-822.929046	-822.76463	-823.050149	-823.123369
	σ-TS-(2)	-1099.208069	-1098.997885	-1099.353308	-1099.421293
	π-TS-(2)	-1099.229436	-1099.020966	-1099.376893	-1099.444313
8	ArNH+	-596.117619	-595.982881	-596.166537	-596.224889

	ArNHOH	-672.176073	-671.968498	-672.18765	-672.247161
	ArNHOAc	-824.782567	-824.543828	-824.812965	-824.882421
	TS-(1a)	-748.902121	-748.72599	-748.986693	-749.066923
	TS-(1b)	-901.522137	-901.307627	-901.615129	-901.706249
	σ-TS-(2)	-1177.799418	-1177.536874	-1177.916786	-1178.003447
	π-TS-(2)	-1177.811982	-1177.547767	-1177.930188	-1178.019853
9	ArNH+	-632.02333	-631.910155	-632.112945	-632.161223
	ArNHOH	-708.064833	-707.881146	-708.118687	-708.16677
	ArNHOAc	-860.671222	-860.457319	-860.743429	-860.802881
	TS-(1a)	-784.794036	-784.642857	-784.920403	-784.987111
	TS-(1b)	-937.414517	-937.223318	-937.549854	-937.628895
	σ-TS-(2)	-1213.696171	-1213.454324	-1213.853466	-1213.92768
	π-TS-(2)	-1213.715349	-1213.476393	-1213.876239	-1213.950262
10	ArNH+	-572.890444	-572.796844	-572.978545	-573.023877
	ArNHOH	-648.919469	-683.096499	-648.971215	-649.016462
	ArNHOAc	-801.525572	-801.325178	-801.596415	-801.65143
	TS-(1a)	-725.652563	-725.519127	-725.77774	-725.839466
	TS-(1b)	-878.273058	-878.099461	-878.405551	-878.480709
	σ-TS-(2)	-1154.556991	-1154.333026	-1154.712289	-1154.782288
	π-TS-(2)	-1154.575240	-1154.351885	-1154.730955	-1154.801046
11	ArNH+	-555.644299	-555.556591	-555.723709	-555.766576
	ArNHOH	-631.689693	-631.527998	-631.730159	-631.772688
	ArNHOAc	-784.295877	-784.100634	-784.355316	-784.407795
	TS-(1a)	-708.418924	-708.292346	-708.534011	-708.594925
	TS-(1b)	-861.039467	-860.871677	-861.163357	-861.236491
	σ-TS-(2)	-1137.319800	-1137.101592	-1137.467264	-1137.535759
	π-TS-(2)	-1137.339980	-1137.125105	-1137.490097	-1137.559485

	N7-σ-TS-(2)	-1137.328337	-1137.105232	-1137.467777	-1137.539593
	N2-σ-TS-(2)	-1137.297938	-1137.098326	-1137.456335	-1137.526046
12	ArNH+	-682.352000	-682.247136	-682.461724	-682.507068
	ArNHOH	-758.406714	-758.229992	-758.477042	-758.520819
	ArNHOAc	-911.013856	-910.804739	-911.100338	-911.154664
	TS-(1a)	-835.134917	-834.991133	-835.27906	-835.341728
	TS-(1b)	-987.755812	-987.570991	-987.910130	-987.985385
	σ-TS-(2)	-1264.033839	-1263.803451	-1264.21178	-1264.283411
	π-TS-(2)	-1264.048649	-1263.818224	-1264.227542	-1264.297593

[a]Absolute energies are given in hartrees, E_g – optimized energy in gas phase, G_w – single-point Gibbs energy in water, F1 and F2 - Density Functionals M06-2X and ωB97X-D, respectively, B1 and B2 – basis sets 6-31+G(d) and 6-311++G(3df,3p), respectively.

4. Atomic Cartesian coordinates (in Å) of the key structures optimized at the M06-2X/6-31+G* level of theory

9MG

Atom	X	Y	Z
C	-4.20770	0.19530	0.70020
N	-4.89890	0.83460	-0.40150
C	-6.25560	0.88820	-0.64360
N	-6.56300	1.53890	-1.73170
C	-5.35080	1.93800	-2.24070
C	-5.03400	2.70140	-3.42030
O	-5.74720	3.19100	-4.27030
N	-3.61710	2.86740	-3.51560
C	-2.67840	2.38130	-2.64650
N	-2.96760	1.68480	-1.58270
C	-4.30850	1.51000	-1.42830
H	-3.32920	3.46400	-4.28440
H	-1.09530	2.76100	-3.88680
H	-0.71330	2.20140	-2.33620
H	-3.12940	0.33090	0.59380
H	-6.96060	0.42220	0.03300
H	-4.54280	0.65360	1.63180
H	-4.43290	-0.87350	0.71730
N	-1.36890	2.71380	-2.91340

H3O+

Atom	X	Y	Z
H	0.49450	-0.18750	0.81940
H	0.49450	-0.18750	-0.81940
O	-0.03280	-0.03030	-0.00000

H	-0.46770	0.85580	0.00000

Compound 1

ArNH+

Atom	X	Y	Z
C	-0.01740	-0.99430	0.00000
C	1.25110	-0.26450	0.00000
C	1.25360	1.10400	0.00000
C	0.01660	1.78180	0.00000
C	-1.24080	1.11950	0.00000
C	-1.27440	-0.24290	0.00000
H	2.16020	-0.85990	0.00000
H	2.17980	1.66770	0.00000
H	0.02260	2.86960	0.00000
H	-2.15340	1.70540	0.00000
H	-2.21360	-0.79140	0.00000
N	0.07120	-2.27880	0.00000
H	-0.85000	-2.73800	0.00000

ArNHOH

Atom	X	Y	Z
C	2.61280	0.41910	0.10230
C	1.90970	1.62360	0.12030
C	0.51770	1.60700	0.04190
C	-0.17990	0.40610	-0.05260
C	0.53140	-0.79470	-0.06680
C	1.91880	-0.79300	0.00920
H	2.45190	2.55720	0.21050

H	-0.02370	2.54860	0.06010
H	-1.26360	0.40230	-0.11140
H	0.00270	-1.74080	-0.13700
H	2.47070	-1.73000	-0.01360
N	4.02850	0.37620	0.10050
H	4.37080	-0.37820	0.69080
O	4.60110	1.55620	0.61500
H	5.14640	1.88490	-0.11420

ArNHOAc

Atom	X	Y	Z
C	2.71550	0.32090	-0.22220
C	2.05940	1.54700	-0.32610
C	0.73140	1.65040	0.08620
C	0.05260	0.54540	0.59200
C	0.71610	-0.67860	0.68570
C	2.04070	-0.79540	0.28240
H	2.58240	2.40670	-0.72910
H	0.22590	2.60820	0.00560
H	-0.98130	0.63410	0.90970
H	0.20120	-1.54940	1.08040
H	2.55500	-1.75070	0.35320
N	4.03930	0.12850	-0.70310
H	4.56660	-0.48140	-0.07570
O	4.74980	1.34890	-0.74900
C	5.65170	1.51320	0.25230
O	5.84670	0.67860	1.10020
C	6.38730	2.81410	0.10500

H	5.81600	3.53110	-0.48500
H	6.59950	3.21030	1.09860
H	7.33890	2.61940	-0.39880

TS-(1a)

Atom	X	Y	Z
H	3.70740	3.00810	2.16070
H	3.50340	2.01040	3.32810
O	3.67300	2.06300	2.37450
H	4.77410	0.95690	1.76840
C	2.93890	-0.22760	0.28030
C	2.42620	0.87430	-0.45330
C	0.77870	-0.58500	1.30730
C	2.10280	-0.94830	1.17700
H	3.09280	1.39470	-1.13530
H	0.11910	-1.13190	1.97230
H	2.51420	-1.78230	1.74140
N	4.22560	-0.56710	0.03840
H	4.45190	-1.47770	0.45310
O	5.28740	0.16750	1.43440
C	1.09790	1.22840	-0.31310
C	0.28370	0.50040	0.56430
H	0.68230	2.05280	-0.88220
H	-0.76150	0.77740	0.66980
H	6.05990	0.49270	0.93950

TS-(1b)

Atom	X	Y	Z

H	5.61120	-0.92210	-3.15020
H	6.61840	-1.71950	-2.28840
O	5.86330	-1.11330	-2.23370
H	6.16210	0.31720	-1.23010
C	2.49040	0.26080	-0.41340
C	1.88870	1.54300	-0.61610
C	0.60290	1.77170	-0.17740
C	-0.08910	0.73940	0.47610
C	0.48590	-0.52630	0.70350
C	1.76960	-0.76860	0.27550
H	2.47050	2.30150	-1.13160
H	0.12440	2.73230	-0.33190
H	-0.08260	-1.29310	1.21790
H	2.25280	-1.72690	0.44930
N	3.71100	0.09100	-0.90780
H	4.03670	-0.87970	-0.82540
O	4.88010	0.42230	0.76080
C	5.95930	0.99110	0.55430
O	6.59140	0.94110	-0.59020
C	6.65090	1.79550	1.61060
H	6.05790	1.80950	2.52300
H	7.63680	1.36360	1.80180
H	6.80170	2.81290	1.23740
H	-1.10290	0.92290	0.82180

σ-TS-(2)

Atom	X	Y	Z
C	-3.70710	2.00670	2.73460

C	-2.90650	1.55500	3.84160
C	-3.49110	1.33380	5.06570
C	-4.87620	1.53480	5.21160
C	-5.69190	1.95230	4.14140
C	-5.12850	2.17600	2.90950
H	-1.84030	1.43120	3.67590
H	-2.89930	1.01160	5.91540
H	-6.75850	2.07700	4.29260
H	-5.73480	2.45060	2.04850
N	-3.07810	2.26630	1.60380
H	-3.72830	2.68630	0.93050
C	-1.26980	0.67200	-1.64050
N	-2.64990	0.80920	-1.19250
C	-3.18950	0.40280	-0.00030
N	-4.48420	0.70280	0.10980
C	-4.77980	1.34990	-1.03780
C	-5.99550	2.01950	-1.44310
O	-7.02700	2.17720	-0.83070
N	-5.83610	2.55950	-2.74980
C	-4.68900	2.53380	-3.50100
N	-3.55400	1.99060	-3.08780
C	-3.65410	1.42910	-1.87890
H	-6.66430	3.03120	-3.10250
H	-5.55520	3.51420	-5.11370
H	-3.87940	3.08230	-5.27080
H	-0.71160	1.58450	-1.42090
H	-2.62780	-0.20030	0.69950
H	-0.81520	-0.17520	-1.12640

H	-1.26940	0.49270	-2.71590
N	-4.72280	3.10710	-4.71340
H	-5.33400	1.35490	6.18070

π-TS-(2)

Atom	X	Y	Z
C	-3.71730	3.52910	0.50960
C	-4.87140	4.00950	-0.21270
C	-4.71060	4.84540	-1.31290
C	-3.42860	5.14420	-1.76540
C	-2.27390	4.68210	-1.08460
C	-2.40930	3.89930	0.02740
H	-5.86250	3.77890	0.17410
H	-5.58150	5.24770	-1.82120
H	-1.29120	4.96770	-1.44480
H	-1.55420	3.56470	0.60690
N	-3.78610	2.70790	1.53470
H	-4.75960	2.55560	1.82130
C	-1.58830	0.65270	-0.77840
N	-3.01580	0.93860	-0.70980
C	-3.86710	0.63440	0.32660
N	-5.14210	0.93640	0.05510
C	-5.09950	1.54190	-1.13360
C	-6.18440	2.01820	-1.98770
O	-7.35920	2.11210	-1.74760
N	-5.66630	2.42790	-3.25030
C	-4.34900	2.44480	-3.61620
N	-3.35590	2.02930	-2.83090

C	-3.76740	1.56280	-1.65660
H	-6.37950	2.75340	-3.89810
H	-4.73980	3.12070	-5.53390
H	-3.07840	2.81980	-5.13730
H	-1.42430	-0.40370	-0.56310
H	-3.53390	0.06400	1.18340
H	-1.25410	0.88140	-1.79030
H	-1.03610	1.26100	-0.06020
N	-4.04170	2.90120	-4.83690
H	-3.30550	5.77860	-2.63920

Compound 2

ArNH+

Atom	X	Y	Z
C	-0.89660	0.69840	0.00000
C	-0.22520	2.00160	0.00000
C	1.12420	2.07480	0.00000
C	1.89570	0.86260	0.00000
C	1.35290	-0.40900	0.00000
C	-0.04200	-0.53230	0.00000
H	-0.87300	2.87300	0.00000
H	1.64060	3.02780	0.00000
H	2.97950	0.95070	0.00000
H	1.99740	-1.27960	0.00000
N	-2.17310	0.66680	0.00000
H	-2.53960	-0.29370	0.00000
O	-0.70590	-1.63950	0.00000
C	-0.02900	-2.92030	0.00000

H	-0.82590	-3.65900	0.00000
H	0.57730	-3.00520	-0.90350
H	0.57730	-3.00520	0.90350

ArNHOH

Atom	X	Y	Z
C	2.58320	0.42490	0.07060
C	1.93750	1.65330	0.11540
C	0.54260	1.71560	0.05770
C	-0.20530	0.55130	-0.04090
C	0.43410	-0.69320	-0.07510
C	1.82030	-0.75630	-0.01760
H	2.53380	2.55350	0.20920
H	0.04900	2.68160	0.09500
H	-1.28880	0.59430	-0.08680
H	-0.15620	-1.60010	-0.14200
N	3.98740	0.29360	0.04180
H	4.28380	-0.55090	0.52600
O	4.62630	1.38050	0.67370
H	5.20680	1.73660	-0.01410
O	2.55730	-1.90710	-0.02590
C	1.85610	-3.13120	-0.08190
H	2.61380	-3.91440	-0.06910
H	1.19380	-3.24520	0.78450
H	1.26930	-3.20420	-1.00510

ArNHOAc

Atom	X	Y	Z

C	2.73430	0.33390	-0.3442
C	2.14330	1.58310	-0.4772
C	0.84950	1.80140	0.0032
C	0.14890	0.76660	0.6070
C	0.73340	-0.49710	0.7411
C	2.02210	-0.71390	0.2676
H	2.69940	2.37970	-0.9602
H	0.39630	2.78180	-0.1024
H	-0.85720	0.92870	0.9803
H	0.18180	-1.29770	1.2206
N	4.01480	0.03190	-0.8738
H	4.46220	-0.69170	-0.3089
O	4.85350	1.16810	-0.8469
C	5.48580	1.37780	0.3434
O	5.41150	0.61240	1.2683
C	6.26570	2.66080	0.2974
H	5.56700	3.50290	0.3021
H	6.91240	2.71690	1.1719
H	6.85360	2.71710	-0.6213
O	2.70170	-1.89270	0.3440
C	2.07630	-2.96840	1.0129
H	2.78740	-3.79350	0.9870
H	1.85410	-2.70560	2.0536
H	1.15330	-3.26380	0.5005

TS-(1a)

Atom	X	Y	Z
H	3.07880	2.56080	1.42810

H	3.87690	2.77780	2.75630
O	3.68170	2.13440	2.05740
H	4.67530	0.95260	1.63350
C	2.92220	-0.32820	0.40260
C	2.44500	0.56060	-0.58490
C	0.75050	-0.29560	1.50220
C	2.07410	-0.74520	1.46870
H	3.12050	0.84090	-1.38890
H	0.07440	-0.60800	2.28910
N	4.20830	-0.79490	0.29210
H	4.33010	-1.62210	0.88700
O	5.21000	0.13310	1.37280
C	1.14280	1.01400	-0.53290
C	0.30860	0.57390	0.51070
H	0.75420	1.67700	-1.29770
H	5.93210	0.40530	0.77690
H	-0.72090	0.91870	0.54580
O	2.64450	-1.54700	2.36530
C	1.84980	-2.07500	3.43290
H	2.51880	-2.71410	4.00480
H	1.47870	-1.26200	4.06270
H	1.02100	-2.66330	3.03020

TS-(1b)

Atom	X	Y	Z
H	5.10600	-0.70910	-3.07490
H	6.57580	-1.17630	-2.89920
O	5.79180	-0.87940	-2.41230

H	6.01350	0.32520	-1.23770
C	2.63190	0.18180	-0.06470
C	2.05710	1.40310	-0.50710
C	0.77320	1.73310	-0.14950
C	0.04490	0.84860	0.67220
C	0.57320	-0.34780	1.14260
C	1.88190	-0.69170	0.79300
H	2.66200	2.04400	-1.14190
H	0.31740	2.65520	-0.49090
H	-0.02490	-0.99090	1.77670
N	3.87850	-0.12660	-0.46990
H	4.09910	-1.10090	-0.23330
O	4.94920	0.41300	0.94770
C	6.00640	0.97870	0.59470
O	6.49690	0.92870	-0.60130
C	6.79470	1.78150	1.57930
H	6.31010	1.77140	2.55360
H	7.80430	1.36800	1.64800
H	6.87900	2.80640	1.20540
H	-0.97150	1.10890	0.95370
O	2.51970	-1.78680	1.18290
C	1.84590	-2.72580	2.02850
H	2.56390	-3.52270	2.20760
H	1.57110	-2.24890	2.97300
H	0.96200	-3.12210	1.52160

σ-TS-(2)

Atom	X	Y	Z

C	4.44540	-2.24340	-1.63460
C	5.35670	-3.35950	-1.39750
C	5.69790	-1.65440	-3.64190
C	4.69210	-1.38030	-2.76580
H	5.87950	-1.02000	-4.50190
H	4.04920	-0.51180	-2.88750
N	3.42970	-2.10490	-0.81560
H	2.83910	-1.32900	-1.13410
C	2.33820	-1.90650	2.69470
N	2.71780	-0.85620	1.76170
C	3.87980	-0.78670	1.02880
N	3.90370	0.26060	0.20240
C	2.70590	0.85470	0.37570
C	2.11600	1.98790	-0.30810
O	2.55600	2.65900	-1.21130
N	0.82280	2.25320	0.22580
C	0.18380	1.53090	1.20020
N	0.70430	0.46520	1.78320
C	1.93840	0.17890	1.34770
H	0.35550	3.04300	-0.21060
H	-1.47150	2.78250	1.23330
H	-1.50210	1.42240	2.31040
H	2.18140	-2.84060	2.14990
H	4.72630	-1.41800	1.26120
H	3.12090	-2.03430	3.44430
H	1.41150	-1.60280	3.18210
N	-1.05060	1.92450	1.55780
C	6.37950	-3.62180	-2.31980

C	6.53060	-2.78390	-3.41150
H	7.05420	-4.45780	-2.18340
H	7.33180	-2.99290	-4.11490
O	5.14060	-4.04450	-0.30100
C	5.94440	-5.19790	-0.01790
H	5.55170	-5.60000	0.91300
H	5.83880	-5.93340	-0.81950
H	6.99020	-4.90550	0.10760

π-TS-(2)

Atom	X	Y	Z
C	1.91760	-1.20990	-1.41860
C	1.46610	-0.18990	-2.34090
C	-0.42280	-1.43410	-0.64410
C	0.92550	-1.81290	-0.53440
H	2.22170	0.31030	-2.94240
H	-1.17600	-1.87950	-0.00580
N	3.16670	-1.60440	-1.31760
H	3.73190	-1.14550	-2.04010
C	3.56330	-1.83080	2.13730
N	3.29230	-0.67650	1.29320
C	4.08820	-0.22850	0.24860
N	3.60530	0.86530	-0.33330
C	2.41170	1.04780	0.24620
C	1.37160	2.03110	-0.01680
O	1.30540	2.87370	-0.87630
N	0.30580	1.86740	0.91260
C	0.22520	0.92630	1.90750

N	1.14070	0.00220	2.12150
C	2.19430	0.10200	1.29070
H	-0.43930	2.54930	0.79850
H	-1.50900	1.72500	2.69660
H	-0.86740	0.34120	3.49530
H	3.70030	-2.70900	1.50280
H	5.08720	-0.61860	0.10650
H	4.45680	-1.64740	2.73710
H	2.70590	-1.97260	2.79620
N	-0.88720	0.92840	2.67120
C	0.14680	0.13970	-2.44780
C	-0.79040	-0.49380	-1.59170
H	-0.18280	0.89780	-3.14890
H	-1.84020	-0.22410	-1.67210
O	1.37480	-2.71290	0.30820
C	0.46310	-3.37410	1.19340
H	1.07250	-4.07430	1.76140
H	-0.00020	-2.64330	1.86230
H	-0.29010	-3.92040	0.61940

Compound 3

ArNH+

Atom	X	Y	Z
C	0.01700	-1.02830	0.14520
C	1.24630	-0.25010	-0.05530
C	1.20070	1.08520	-0.24270
C	-0.07550	1.75030	-0.24570
C	-1.31360	1.02940	-0.05220

C	-1.26570	-0.30710	0.13590
H	2.18010	-0.80480	-0.04420
H	2.08530	1.69470	-0.39450
H	-2.25820	1.56040	-0.05840
H	-2.17890	-0.87870	0.28500
N	0.14470	-2.29120	0.31610
H	-0.75760	-2.76350	0.44920
O	-0.02700	3.02220	-0.43160
C	-1.21090	3.85680	-0.46780
H	-1.72260	3.80180	0.49450
H	-0.83340	4.86050	-0.64340
H	-1.85380	3.53890	-1.29040

ArNHOH

Atom	X	Y	Z
C	2.66250	0.41430	0.15180
C	1.93380	1.60630	0.14440
C	0.56220	1.58020	-0.06800
C	-0.10600	0.37140	-0.27560
C	0.61810	-0.82190	-0.26660
C	1.99640	-0.79180	-0.05420
H	2.44350	2.54610	0.32090
H	-0.01740	2.49810	-0.07130
H	0.13040	-1.77750	-0.42180
H	2.55600	-1.72450	-0.06050
N	4.07920	0.39320	0.28570
H	4.36400	-0.36900	0.89710
O	4.56220	1.56640	0.90460

H	5.17930	1.93030	0.25380
O	-1.45370	0.45760	-0.47350
C	-2.16000	-0.74460	-0.67990
H	-2.07160	-1.41150	0.18710
H	-3.20440	-0.46240	-0.81460
H	-1.80440	-1.26540	-1.57810

ArNHOAc

Atom	X	Y	Z
C	2.90400	0.51990	-0.59510
C	2.13070	1.60970	-1.01240
C	0.76910	1.63020	-0.77050
C	0.15220	0.54550	-0.12990
C	0.91510	-0.54830	0.27930
C	2.29540	-0.54490	0.05820
H	2.61710	2.42960	-1.53250
H	0.14980	2.46460	-1.08430
H	0.46190	-1.39520	0.78110
H	2.89910	-1.37750	0.40990
N	4.30410	0.52350	-0.90440
H	4.69770	-0.39100	-0.67490
O	4.97430	1.43440	-0.01750
O	-1.19140	0.65360	0.04430
C	-1.86280	-0.41800	0.67190
H	-1.49440	-0.57200	1.69340
H	-2.91520	-0.13630	0.70400
H	-1.74940	-1.34550	0.09740
C	5.35790	0.89420	1.16400

O	5.23110	-0.27750	1.42560
C	5.95020	1.94450	2.06080
H	5.13790	2.54580	2.48040
H	6.49690	1.45910	2.86870
H	6.60500	2.60940	1.49430

TS-(1a)

Atom	X	Y	Z
H	3.01990	2.42710	1.59760
H	4.03890	2.80840	2.73550
O	3.82220	2.14380	2.06370
H	4.65840	0.92930	1.64280
C	2.91090	-0.32780	0.44150
C	2.47600	0.55820	-0.55690
C	0.72930	-0.26330	1.47240
C	2.02380	-0.72650	1.46630
H	3.16700	0.83780	-1.34780
H	0.01690	-0.56440	2.23310
N	4.21820	-0.80190	0.34600
H	4.33460	-1.66090	0.89080
O	5.17730	0.08670	1.36680
C	1.17630	1.03870	-0.55470
C	0.29110	0.61900	0.45870
H	0.84450	1.70050	-1.34580
H	5.92230	0.34510	0.79060
H	2.36230	-1.40580	2.24560
O	-0.97920	0.99770	0.54360
C	-1.52950	1.84470	-0.46420

H	-2.57110	1.98780	-0.18530
H	-1.01360	2.80970	-0.47920
H	-1.46930	1.36140	-1.44380

TS-(1b)

Atom	X	Y	Z
H	4.91320	-0.58910	-3.04700
H	6.43640	-0.89310	-3.12380
O	5.70940	-0.71070	-2.50900
H	5.95100	0.37440	-1.27330
C	2.66760	0.11380	0.03300
C	2.09240	1.31330	-0.46090
C	0.79980	1.64100	-0.14550
C	0.03990	0.77980	0.68300
C	0.60230	-0.41230	1.19510
C	1.90630	-0.72510	0.88070
H	2.69140	1.95410	-1.10170
H	0.32560	2.54340	-0.51570
H	0.02400	-1.07100	1.83120
N	3.94370	-0.18170	-0.34670
H	4.18090	-1.15150	-0.11620
O	4.97220	0.41710	0.97230
C	6.01020	1.00610	0.57580
O	6.44750	0.97410	-0.63450
C	6.81680	1.80650	1.54450
H	6.35970	1.78660	2.53190
H	7.83020	1.39790	1.58190
H	6.88530	2.83400	1.17450

H	2.35740	-1.63000	1.28200
O	-1.19970	1.17470	0.92510
C	-2.05410	0.38020	1.75040
H	-2.99850	0.91850	1.78930
H	-2.20550	-0.60670	1.30360
H	-1.63490	0.28960	2.75650

σ-TS-(2)

Atom	X	Y	Z
C	4.43500	-2.28080	-1.57080
C	5.29500	-3.40400	-1.31720
C	5.75890	-1.72210	-3.54620
C	4.72240	-1.44020	-2.69870
H	5.07310	-4.03120	-0.45870
H	5.95990	-1.08130	-4.39600
H	4.10810	-0.55730	-2.86040
N	3.41170	-2.07710	-0.74860
H	2.81160	-1.33190	-1.11780
C	2.35190	-1.92320	2.56030
N	2.72080	-0.83510	1.66820
C	3.87220	-0.75690	0.90660
N	3.88240	0.32990	0.11840
C	2.69110	0.90740	0.32060
C	2.08550	2.05610	-0.33030
O	2.51840	2.75350	-1.21510
N	0.79510	2.29740	0.21870
C	0.16830	1.54390	1.17810
N	0.70100	0.46770	1.73300

C	1.93390	0.20000	1.28860
H	0.31850	3.09480	-0.19330
H	-1.50250	2.77250	1.24340
H	-1.51140	1.38770	2.29030
H	2.21240	-2.83710	1.97710
H	4.75090	-1.32820	1.17030
H	3.13380	-2.06870	3.30760
H	1.41860	-1.65150	3.05370
N	-1.06520	1.91710	1.55310
C	6.33530	-3.68610	-2.15050
C	6.57870	-2.85260	-3.27940
H	6.99180	-4.53560	-1.99600
O	7.59960	-3.20540	-4.02650
C	7.94570	-2.44850	-5.19370
H	8.80580	-2.95930	-5.62000
H	7.11510	-2.45290	-5.90430
H	8.21550	-1.42720	-4.91320

π-TS-(2)

Atom	X	Y	Z
C	1.96180	-1.16870	-1.35790
C	1.25760	-0.03200	-1.89500
C	-0.16660	-2.06040	-0.53970
C	1.18940	-2.16830	-0.67680
H	1.82250	0.73260	-2.42540
H	-0.72790	-2.83850	-0.03650
H	1.71850	-3.03950	-0.30120
N	3.28010	-1.33110	-1.39760

H	3.71660	-0.64010	-2.01640
C	3.05200	-1.93490	2.06580
N	3.05570	-0.70970	1.27970
C	4.01450	-0.33310	0.35680
N	3.75800	0.88100	-0.17240
C	2.54970	1.19100	0.27730
C	1.70240	2.34230	-0.02040
O	1.89120	3.25020	-0.78740
N	0.49860	2.26530	0.73270
C	0.13200	1.24480	1.56860
N	0.88660	0.18440	1.82340
C	2.06000	0.20200	1.18730
H	-0.13490	3.04430	0.57300
H	-1.61960	2.17530	2.14870
H	-1.27160	0.65240	2.88520
H	3.42260	-2.75540	1.44730
H	4.98450	-0.80970	0.33140
H	3.68860	-1.81930	2.94550
H	2.02680	-2.13510	2.38090
N	-1.07670	1.32270	2.15220
C	-0.10450	0.07800	-1.76590
C	-0.82800	-0.91810	-1.07200
H	-0.65190	0.91890	-2.17990
O	-2.13100	-0.71410	-0.97390
C	-2.96720	-1.69970	-0.36130
H	-3.97860	-1.30640	-0.43650
H	-2.89650	-2.64720	-0.90250
H	-2.69260	-1.83350	0.68900

Compound 4

ArNH+

Atom	X	Y	Z
C	0.00180	-1.05480	0.14630
C	1.24120	-0.29340	-0.05010
C	1.23520	1.03960	-0.23580
C	-0.02240	1.77230	-0.24820
C	-1.26980	1.03720	-0.05620
C	-1.25680	-0.29460	0.13070
H	2.16490	-0.86400	-0.03860
H	2.16800	1.56890	-0.37970
H	-2.21160	1.57080	-0.06100
H	-2.18750	-0.83750	0.27560
N	0.10600	-2.31870	0.31590
H	-0.80730	-2.76850	0.44490
N	-0.03910	3.07400	-0.42890
C	-1.30600	3.82940	-0.45980
H	-1.81650	3.74960	0.50280
H	-1.08340	4.87540	-0.65260
H	-1.94870	3.45500	-1.25940
C	1.21250	3.83400	-0.60900
H	0.96960	4.88870	-0.70700
H	1.86090	3.70190	0.25980
H	1.72630	3.50390	-1.51500

ArNHOH

Atom	X	Y	Z

C	2.66700	0.41760	0.13660
C	1.95720	1.61320	0.10410
C	0.57470	1.61080	-0.06420
C	-0.15050	0.41370	-0.19400
C	0.58750	-0.78600	-0.17610
C	1.96620	-0.77990	-0.01010
H	2.48540	2.55230	0.22140
H	0.06530	2.56680	-0.08230
H	0.09050	-1.74210	-0.28790
H	2.50480	-1.72520	-0.00970
N	4.08840	0.37090	0.22420
H	4.37470	-0.37560	0.85400
O	4.61070	1.55320	0.79590
H	5.21310	1.88730	0.11640
N	-1.54410	0.41220	-0.31410
C	-2.16990	-0.79850	-0.80690
H	-2.00890	-1.62650	-0.11040
H	-3.24680	-0.63620	-0.87550
H	-1.79450	-1.10010	-1.79900
C	-2.17920	1.65850	-0.69370
H	-3.25420	1.49400	-0.78350
H	-2.02850	2.41880	0.07810
H	-1.80130	2.05510	-1.65080

ArNHOAc

Atom	X	Y	Z
C	2.89840	0.54690	-0.60410
C	2.11840	1.59420	-1.09300

C	0.75360	1.63980	-0.85140
C	0.11280	0.61670	-0.11730
C	0.90940	-0.44920	0.34910
C	2.28180	-0.46830	0.12480
H	2.59750	2.37390	-1.67850
H	0.18300	2.46930	-1.25130
H	0.46580	-1.26740	0.90320
H	2.88000	-1.28390	0.52370
N	4.29920	0.53650	-0.91190
H	4.68040	-0.38510	-0.68980
O	4.98000	1.42500	-0.00290
N	-1.24840	0.66280	0.13890
C	-1.89660	-0.52580	0.65440
H	-1.49270	-0.79290	1.63640
H	-2.96090	-0.32280	0.78060
H	-1.78150	-1.39250	-0.01540
C	-2.05970	1.61790	-0.58820
H	-3.10090	1.50160	-0.28450
H	-1.75910	2.64360	-0.35040
H	-1.99560	1.48150	-1.67910
C	5.38640	0.85400	1.15270
O	5.27010	-0.32560	1.38640
C	5.99090	1.88070	2.06960
H	5.18310	2.45930	2.52790
H	6.56140	1.37510	2.84820
H	6.62550	2.57070	1.51020

TS-(1a)

Atom	X	Y	Z
H	3.98030	2.45640	2.68730
H	2.96530	1.26540	2.52360
O	3.90940	1.48960	2.63160
H	4.69800	0.77120	1.70650
C	2.97790	-0.16380	0.26020
C	2.41700	0.87610	-0.49750
C	0.92110	-0.33390	1.53050
C	2.20900	-0.76140	1.27480
H	3.00820	1.32660	-1.29040
H	0.34640	-0.83590	2.29890
H	2.62610	-1.57470	1.86680
N	4.30500	-0.54130	-0.01520
H	4.48390	-1.50490	0.27520
O	5.25480	0.13430	1.04470
C	1.13020	1.31290	-0.25860
C	0.33200	0.71280	0.75860
H	0.72510	2.10800	-0.87150
H	5.88990	0.64460	0.50710
N	-0.94120	1.10850	0.97900
C	-1.71410	0.52690	2.06890
H	-1.91470	-0.53610	1.89270
H	-1.19410	0.64090	3.02630
H	-2.66830	1.04580	2.14040
C	-1.54440	2.14080	0.14540
H	-2.59280	2.24700	0.41840
H	-1.04920	3.10920	0.28450
H	-1.49740	1.86370	-0.91270

TS-(1b)

Atom	X	Y	Z
H	4.56590	-0.55340	-2.54320
H	5.36670	0.46890	-3.41920
O	4.93320	0.34300	-2.56120
H	5.58550	0.82260	-1.20750
C	3.01000	-0.21580	0.35330
C	2.38510	0.73180	-0.47280
C	1.04850	1.03070	-0.31470
C	0.27170	0.38710	0.69020
C	0.92300	-0.56760	1.52370
C	2.26100	-0.84780	1.35980
H	2.96080	1.21900	-1.25630
H	0.59280	1.75730	-0.97530
H	0.37120	-1.08360	2.29890
H	2.73920	-1.57160	2.01700
N	4.37360	-0.49130	0.14730
H	4.61420	-1.40430	0.53910
O	5.19280	0.33950	1.20650
C	5.95850	1.22350	0.69280
O	6.11220	1.41050	-0.55460
C	6.70770	2.10700	1.62630
H	6.59950	1.76380	2.65360
H	7.75870	2.12950	1.32820
H	6.30850	3.12170	1.52670
N	-1.04330	0.66910	0.84700
C	-1.81850	-0.00050	1.88180

H	-1.41610	0.21280	2.87860
H	-2.84490	0.36060	1.84450
H	-1.83120	-1.08550	1.72720
C	-1.69030	1.64430	-0.01840
H	-2.73870	1.72710	0.26340
H	-1.22850	2.63310	0.08400
H	-1.64110	1.33530	-1.06890

σ-TS-(2)

Atom	X	Y	Z
C	4.17000	-1.87060	-2.17170
C	4.94160	-3.04480	-1.92140
C	5.38140	-1.56090	-4.26340
C	4.44730	-1.13430	-3.36350
H	4.74060	-3.60590	-1.01230
H	5.55130	-0.98310	-5.16250
H	3.89750	-0.21460	-3.55000
N	3.22730	-1.51380	-1.28130
H	2.68060	-0.73780	-1.66610
C	2.94700	-2.07700	1.91000
N	3.03000	-0.78090	1.26350
C	3.91380	-0.45900	0.22960
N	3.65090	0.77860	-0.26600
C	2.52320	1.15200	0.32860
C	1.69880	2.33420	0.11470
O	1.84980	3.24080	-0.66470
N	0.58120	2.31100	0.99580
C	0.27800	1.32070	1.89330

N	1.01000	0.23140	2.06860
C	2.09810	0.19150	1.29440
H	-0.04330	3.10510	0.88490
H	-1.36820	2.32360	2.65050
H	-1.02650	0.76580	3.32760
H	2.73120	-2.83450	1.14980
H	4.91270	-0.87490	0.23510
H	3.88950	-2.30180	2.41260
H	2.13970	-2.04190	2.64160
N	-0.84500	1.46060	2.61510
C	5.88970	-3.47740	-2.80320
C	6.14150	-2.75280	-4.01710
H	6.44570	-4.38040	-2.58530
N	7.06430	-3.17800	-4.89230
C	7.82620	-4.39820	-4.63480
H	8.42940	-4.29650	-3.72700
H	7.15770	-5.25860	-4.53200
H	8.49410	-4.58010	-5.47420
C	7.32560	-2.43000	-6.12110
H	8.11260	-2.93260	-6.67920
H	6.42890	-2.38560	-6.74750
H	7.65910	-1.41290	-5.89320

π-TS-(2)

Atom	X	Y	Z
C	1.89080	-1.17290	-1.29760
C	1.27080	-0.15240	-2.09140
C	-0.33260	-1.89160	-0.58690

C	1.02680	-2.00950	-0.52580
H	1.90720	0.54040	-2.63940
H	-0.94760	-2.57020	-0.00960
H	1.47810	-2.78840	0.08230
N	3.21820	-1.38640	-1.24810
H	3.68990	-0.86600	-1.99310
C	3.27460	-1.89400	2.06640
N	3.17210	-0.67850	1.27630
C	3.99840	-0.34340	0.19930
N	3.66960	0.87540	-0.30830
C	2.50490	1.15660	0.24700
C	1.56770	2.24170	-0.03010
O	1.61890	3.09850	-0.87470
N	0.46140	2.16560	0.85940
C	0.25750	1.20960	1.82210
N	1.07590	0.19740	2.04860
C	2.15450	0.19910	1.25790
H	-0.22490	2.90250	0.72290
H	-1.40450	2.16040	2.59770
H	-0.94300	0.67540	3.34590
H	3.46260	-2.73750	1.39630
H	5.00300	-0.74270	0.15500
H	4.09240	-1.80650	2.78470
H	2.33360	-2.03680	2.59920
N	-0.86580	1.30630	2.55800
C	-0.08970	-0.03580	-2.18110
C	-0.94530	-0.91230	-1.43910
H	-0.51030	0.73930	-2.80950

N	-2.28160	-0.82260	-1.53890
C	-2.89280	0.12300	-2.47060
H	-2.65910	1.15600	-2.19240
H	-2.54640	-0.05940	-3.49270
H	-3.97330	-0.00460	-2.44550
C	-3.14470	-1.72450	-0.78020
H	-4.18360	-1.46180	-0.96980
H	-2.98840	-2.76520	-1.08340
H	-2.95680	-1.63020	0.29370

Compound 5

ArNH+

Atom	X	Y	Z
C	-0.02400	1.82200	0.00000
C	1.24290	1.09240	0.00000
C	1.25330	-0.27470	0.00000
C	0.01100	-0.95670	0.00000
C	-1.25220	-0.29150	0.00000
C	-1.27900	1.06970	0.00000
H	2.15410	1.68470	0.00000
H	2.17730	-0.84290	0.00000
H	-2.16170	-0.88310	0.00000
H	-2.22070	1.61380	0.00000
N	0.06540	3.10740	0.00000
H	-0.85430	3.56970	0.00000
N	0.02480	-3.54310	0.00000
C	0.01890	-2.38460	0.00000

ArNHOH

Atom	X	Y	Z
C	2.61660	0.41880	0.10970
C	1.91250	1.62600	0.12880
C	0.52580	1.61450	0.05050
C	-0.16940	0.40520	-0.04590
C	0.54070	-0.80340	-0.06000
C	1.92260	-0.79640	0.01720
H	2.45350	2.55940	0.21990
H	-0.02630	2.54860	0.06820
H	0.00160	-1.74250	-0.13070
H	2.47310	-1.73330	-0.00440
N	4.02150	0.38120	0.10770
H	4.38550	-0.38570	0.66770
O	4.60160	1.55810	0.60680
H	5.15100	1.87820	-0.12400
N	-2.75990	0.39250	-0.19140
C	-1.60380	0.39880	-0.12620

ArNHOAc

Atom	X	Y	Z
C	2.79030	0.34550	-0.29990
C	2.18930	1.57980	-0.04100
C	0.81710	1.64610	0.16580
C	0.03680	0.48800	0.11040
C	0.64410	-0.74700	-0.15540
C	2.01170	-0.81760	-0.35870
H	2.79200	2.47950	-0.01000

H	0.34430	2.60130	0.36990
H	0.03810	-1.64610	-0.19660
H	2.48260	-1.77410	-0.56820
N	4.16500	0.23500	-0.59900
H	4.56870	-0.61020	-0.19360
O	4.90430	1.32210	-0.09950
N	-2.52570	0.62040	0.49730
C	-1.38230	0.56150	0.32490
C	5.46630	1.09890	1.12560
O	5.37430	0.04330	1.69560
C	6.21690	2.30790	1.60230
H	6.08010	3.15610	0.93200
H	5.86840	2.55690	2.60700
H	7.27860	2.05620	1.66740

TS-(1a)

Atom	X	Y	Z
H	3.65060	3.00150	2.12440
H	3.37220	1.98770	3.25520
O	3.57920	2.05210	2.30940
H	4.80900	0.95540	1.79290
C	2.94580	-0.25070	0.24360
C	2.42710	0.86320	-0.47920
C	0.79820	-0.59740	1.31100
C	2.11170	-0.96950	1.15370
H	3.08990	1.38300	-1.16500
H	0.13540	-1.12970	1.98470
H	2.52340	-1.80810	1.71040

N	4.21660	-0.58300	-0.01170
H	4.46980	-1.47470	0.42860
O	5.32040	0.15870	1.49700
C	1.10880	1.23210	-0.32250
C	0.30520	0.50380	0.57440
H	0.68220	2.06250	-0.87430
H	6.12120	0.46690	1.03960
N	-2.16710	1.21080	0.90360
C	-1.06500	0.89310	0.75320

TS-(1b)

Atom	X	Y	Z
H	5.80640	-1.11130	-3.07510
H	6.49040	-1.92620	-1.95370
O	5.84960	-1.21510	-2.11160
H	6.28950	0.29780	-1.21100
C	2.44590	0.34310	-0.56470
C	1.79980	1.62110	-0.67620
C	0.54900	1.81100	-0.13880
C	-0.06710	0.73420	0.53230
C	0.54880	-0.53340	0.67700
C	1.79570	-0.72780	0.14300
H	2.32670	2.40980	-1.20500
H	0.03210	2.76100	-0.21710
H	0.02870	-1.32050	1.21210
H	2.31010	-1.67940	0.24970
N	3.62690	0.23040	-1.13440
H	4.01350	-0.72120	-1.08920

O	4.87830	0.43430	0.65580
C	5.97490	0.98440	0.54020
O	6.69570	0.91710	-0.55740
C	6.60600	1.78730	1.63580
H	5.96230	1.79780	2.51330
H	7.58070	1.35820	1.88210
H	6.77610	2.80630	1.27540
N	-2.42160	1.08330	1.55600
C	-1.37000	0.92850	1.09820

σ-TS-(2)

Atom	X	Y	Z
C	4.28940	-2.46070	-1.66400
C	5.21370	-3.56180	-1.69990
C	5.46570	-1.39910	-3.51270
C	4.45780	-1.36190	-2.58360
H	5.61530	-0.58580	-4.21450
H	3.80430	-0.49420	-2.50440
N	3.31280	-2.52850	-0.77870
H	2.65360	-1.75630	-0.92570
C	2.09220	-1.71900	3.15940
N	2.58260	-0.97010	2.00610
C	3.74790	-1.17100	1.31730
N	3.91430	-0.30700	0.31530
C	2.80570	0.46230	0.34620
C	2.34260	1.45210	-0.59670
O	2.83540	1.79120	-1.65090
N	1.11100	2.00420	-0.15470

C	0.39500	1.59600	0.94210
N	0.77390	0.60700	1.73950
C	1.95340	0.08310	1.39970
H	0.73560	2.72260	-0.76810
H	-1.08180	3.03080	0.68970
H	-1.27630	1.93780	2.02460
H	2.05760	-2.78230	2.91710
H	4.47650	-1.90500	1.63390
H	2.74040	-1.54790	4.02060
H	1.08700	-1.36120	3.38250
N	-0.76450	2.21820	1.19820
C	6.22020	-3.58920	-2.63290
C	6.34050	-2.51050	-3.53690
H	6.91790	-4.41730	-2.69230
H	5.06580	-4.37130	-0.99150
N	8.24480	-2.56200	-5.29210
C	7.39420	-2.53800	-4.50750

π-TS-(2)

Atom	X	Y	Z
C	-3.74050	3.60090	0.56970
C	-4.88460	4.05570	-0.18560
C	-4.71320	4.82120	-1.33200
C	-3.42100	5.04040	-1.81440
C	-2.26780	4.63980	-1.08000
C	-2.42580	3.94660	0.08320
H	-5.88200	3.86100	0.20400
H	-5.57140	5.19690	-1.88090

H	-1.28370	4.88210	-1.46730
H	-1.57640	3.63280	0.68240
N	-3.82030	2.80270	1.60820
H	-4.79640	2.64250	1.88110
C	-1.56700	0.74350	-0.76880
N	-2.99730	1.02220	-0.68210
C	-3.84470	0.69910	0.34550
N	-5.12650	0.98940	0.08360
C	-5.09450	1.60030	-1.09900
C	-6.19060	2.04430	-1.96250
O	-7.36600	2.10530	-1.72370
N	-5.68040	2.46170	-3.22660
C	-4.36300	2.52060	-3.58820
N	-3.35920	2.10820	-2.79820
C	-3.76190	1.63070	-1.63330
H	-6.40190	2.74330	-3.88680
H	-4.72790	3.41530	-5.41700
H	-3.07310	3.06030	-5.04120
H	-0.98840	1.56380	-0.34030
H	-3.50360	0.14000	1.20670
H	-1.35610	-0.17890	-0.22740
H	-1.30570	0.62070	-1.82030
N	-4.05300	2.99660	-4.79030
N	-3.15730	6.06050	-4.18110
C	-3.26000	5.65210	-3.10240

Compound 6

ArNH+

Atom	X	Y	Z
C	1.14140	-1.36160	-1.27600
C	0.03710	-0.47900	-1.66530
C	-0.33820	-2.52490	0.27660
C	0.88710	-2.39670	-0.27130
H	0.22900	0.29060	-2.41210
H	-0.54020	-3.28660	1.02310
H	1.72410	-3.03330	-0.00380
N	2.32300	-1.26910	-1.77410
H	2.39870	-0.51500	-2.46750
C	-1.20640	-0.61370	-1.10480
C	-1.42210	-1.65040	-0.11090
C	-2.69390	-1.77060	0.44890
C	-3.71480	-0.91220	0.05410
C	-3.52000	0.10530	-0.91470
C	-2.28900	0.25560	-1.48720
H	-2.88540	-2.53600	1.19420
H	-4.69750	-1.02390	0.50400
H	-4.34600	0.75100	-1.19070
H	-2.10390	1.02380	-2.23280

ArNHOH

Atom	X	Y	Z
C	2.62080	0.43620	0.11660
C	1.93360	1.62410	0.13670
C	0.55550	-0.81150	-0.07080
C	1.92040	-0.79850	0.00920
H	2.47130	2.56080	0.23440

H	0.02210	-1.75540	-0.15030
H	2.48490	-1.72750	-0.02010
N	4.03350	0.36060	0.12670
H	4.35620	-0.36350	0.76510
O	4.62900	1.55680	0.56750
H	5.17590	1.83250	-0.18230
C	0.51470	1.62980	0.04850
C	-0.19120	0.39970	-0.05560
C	-1.60740	0.41420	-0.13940
C	-2.29950	1.60040	-0.12060
C	-1.59910	2.82680	-0.01590
C	-0.22810	2.84080	0.06690
H	-2.13620	-0.53290	-0.21880
H	-3.38340	1.60330	-0.18520
H	-2.15320	3.76090	-0.00090
H	0.31060	3.78150	0.14840

ArNHOAc

Atom	X	Y	Z
C	2.76370	0.33440	-0.32820
C	2.16150	1.54010	-0.07070
C	0.64340	-0.81610	-0.17340
C	1.99290	-0.85980	-0.38710
H	2.74780	2.45260	-0.04160
H	0.05590	-1.72970	-0.21340
H	2.48870	-1.80120	-0.60980
N	4.14440	0.19840	-0.62930
H	4.55080	-0.58110	-0.10810

O	4.86780	1.34590	-0.24820
C	5.52300	1.23000	0.93720
O	5.52440	0.21430	1.58570
C	6.25800	2.49510	1.27540
H	6.01090	3.30060	0.58430
H	6.00440	2.77970	2.29870
H	7.33190	2.29490	1.23730
C	-0.01680	0.41380	0.10280
C	0.75860	1.60450	0.15090
C	0.10270	2.83470	0.42260
C	-1.25360	2.87590	0.63630
C	-2.02390	1.68870	0.58880
C	-1.41560	0.48540	0.32710
H	0.69430	3.74600	0.45830
H	-1.74160	3.82390	0.84300
H	-3.09510	1.73450	0.75950
H	-1.99870	-0.43150	0.28810

TS-(1a)

Atom	X	Y	Z
H	3.14390	2.59560	2.10040
H	3.77700	2.14100	3.45350
O	3.66390	1.89510	2.52250
H	4.65830	0.88010	1.77840
C	2.95230	-0.20890	0.27140
C	2.44560	0.85630	-0.47360
C	0.81590	-0.55470	1.33720
C	2.12200	-0.91920	1.19540

H	3.10120	1.36280	-1.17910
H	0.16670	-1.08850	2.02530
H	2.54060	-1.74220	1.76950
N	4.26960	-0.53100	0.03910
H	4.48180	-1.47030	0.39100
O	5.22600	0.16180	1.34830
H	5.95060	0.58930	0.85550
C	0.27000	0.53150	0.58440
C	1.10080	1.24400	-0.33910
C	0.55230	2.31510	-1.10080
C	-0.76350	2.66740	-0.94370
C	-1.58340	1.96420	-0.02580
C	-1.08200	0.92100	0.72020
H	1.18870	2.83980	-1.80830
H	-1.18570	3.48090	-1.52440
H	-2.62430	2.25230	0.08460
H	-1.72090	0.38410	1.41540

TS-(1b)

Atom	X	Y	Z
H	5.19570	-0.54450	-3.15180
H	6.59860	-1.13880	-2.85890
O	5.80930	-0.76740	-2.43560
H	6.05440	0.43740	-1.24380
C	2.62240	0.21410	-0.09680
C	2.04710	1.45570	-0.41530
C	0.61230	-0.46910	1.05930
C	1.88440	-0.75140	0.67030

H	2.63620	2.16960	-0.98650
H	0.03660	-1.18960	1.63300
H	2.35700	-1.69540	0.92830
N	3.87450	0.00060	-0.56170
H	4.14050	-0.98590	-0.46660
O	4.95770	0.38970	0.91200
C	6.02360	0.97130	0.62010
O	6.53290	1.00030	-0.57070
C	6.80120	1.69720	1.67040
H	6.30650	1.61220	2.63610
H	7.81130	1.28220	1.71740
H	6.88560	2.74800	1.37670
C	0.73730	1.75870	-0.02380
C	0.00210	0.78470	0.72790
C	-1.31450	1.09240	1.12680
C	-1.87530	2.30830	0.79580
C	-1.15220	3.27280	0.05150
C	0.12980	3.00520	-0.35280
H	-1.88120	0.36240	1.69700
H	-2.89010	2.53320	1.10960
H	-1.61950	4.22020	-0.19530
H	0.69780	3.73350	-0.92510

σ-TS-(2)

Atom	X	Y	Z
C	4.36970	-2.41480	-1.61100
C	5.23690	-3.55930	-1.42380
C	4.62480	-1.51770	-2.69550

H	5.02510	-4.22120	-0.58990
H	4.00930	-0.62420	-2.79190
N	3.36520	-2.23590	-0.76980
H	2.78290	-1.45220	-1.08430
C	2.34290	-1.85650	2.70760
N	2.73730	-0.85560	1.72630
C	3.89530	-0.84610	0.98120
N	3.93590	0.16780	0.11240
C	2.75610	0.79450	0.26810
C	2.17750	1.89360	-0.47840
O	2.62220	2.49710	-1.42680
N	0.89520	2.21250	0.04770
C	0.24870	1.55190	1.06140
N	0.75250	0.50750	1.69610
C	1.97930	0.17750	1.27490
H	0.43650	2.98300	-0.43050
H	-1.38760	2.82810	1.03190
H	-1.43500	1.52630	2.17910
H	2.19610	-2.81740	2.20870
H	4.73580	-1.47460	1.24090
H	3.11240	-1.94400	3.47620
H	1.40730	-1.52930	3.16140
N	-0.97530	1.98540	1.40410
C	6.24850	-3.79450	-2.29430
H	6.89480	-4.65890	-2.17550
C	5.65620	-1.75600	-3.59430
C	6.49100	-2.91240	-3.40460
C	7.53520	-3.14030	-4.31370

C	7.75040	-2.26350	-5.36330
C	6.93780	-1.11910	-5.55220
C	5.90870	-0.86580	-4.68460
H	8.17440	-4.00860	-4.18600
H	8.56330	-2.45450	-6.05760
H	7.13660	-0.45010	-6.38240
H	5.27330	0.00700	-4.80640

π-TS-(2)

Atom	X	Y	Z
C	1.14350	-1.36710	-1.29470
C	0.07740	-0.46370	-1.63790
C	-0.35180	-2.52090	0.25150
C	0.87300	-2.40110	-0.30760
H	0.24620	0.27160	-2.42440
H	-0.55350	-3.30070	0.98130
H	1.68680	-3.07910	-0.06750
N	2.37070	-1.23230	-1.74230
H	2.42110	-0.51590	-2.47400
C	-1.21770	-0.62810	-1.10290
C	-1.43260	-1.63410	-0.11180
C	-2.70930	-1.75330	0.46400
C	-3.73400	-0.90760	0.07630
C	-3.52850	0.08060	-0.91320
C	-2.29040	0.21690	-1.49860
H	-2.88580	-2.52330	1.21010
H	-4.71860	-1.01900	0.52170
H	-4.35390	0.71430	-1.22230

H	-2.11270	0.97110	-2.26260
C	2.97840	-1.03860	1.87830
N	2.48390	-0.06480	0.91290
C	3.13540	0.37700	-0.22290
N	2.44700	1.30160	-0.89220
C	1.26880	1.35690	-0.26160
C	0.11260	2.21930	-0.49270
O	-0.12410	2.94210	-1.42730
N	-0.82280	2.07320	0.56310
C	-0.75490	1.15890	1.58110
N	0.29320	0.36710	1.80080
C	1.26570	0.52520	0.90900
H	-1.66230	2.63370	0.44250
H	-2.61820	1.65780	2.33240
H	-1.72800	0.43850	3.19520
H	3.63310	-0.55100	2.60360
H	4.16850	0.11760	-0.41210
H	2.12010	-1.47440	2.39170
H	3.52630	-1.81760	1.34470
N	-1.79920	1.07160	2.40910

Compound 7

ArNH+

Atom	X	Y	Z
C	-0.02990	3.17040	0.00000
C	1.22260	2.41650	0.00000
C	1.22850	1.06200	0.00000
C	0.00050	0.30880	0.00000

C	-1.24670	1.04490	0.00000
C	-1.27260	2.39650	0.00000
H	2.14080	2.99640	0.00000
H	2.18020	0.54960	0.00000
H	-2.18720	0.51200	0.00000
H	-2.21820	2.93320	0.00000
N	0.05250	4.45160	0.00000
H	-0.87300	4.89710	0.00000
C	0.02810	-3.94360	0.00000
C	-1.19040	-3.25720	0.00000
C	-1.20400	-1.87540	0.00000
C	0.00760	-1.13100	0.00000
C	1.22990	-1.85760	0.00000
C	1.23640	-3.23930	0.00000
H	0.03620	-5.02940	0.00000
H	-2.12530	-3.80670	0.00000
H	-2.16590	-1.37980	0.00000
H	2.18390	-1.34670	0.00000
H	2.17940	-3.77480	0.00000

ArNHOH

Atom	X	Y	Z
C	2.63250	0.42930	0.07180
C	1.91510	1.60360	0.29740
C	0.52430	1.58450	0.23270
C	-0.18100	0.41150	-0.05220
C	0.55820	-0.75920	-0.27200
C	1.94440	-0.75530	-0.21380

H	2.44530	2.51520	0.54540
H	-0.02500	2.49980	0.43760
H	0.03950	-1.68230	-0.51720
H	2.50040	-1.66920	-0.41000
N	4.04740	0.40300	0.04670
H	4.40590	-0.43140	0.50490
O	4.61530	1.49380	0.73360
H	5.14830	1.93940	0.05940
C	-4.47170	0.38500	-0.23890
C	-3.78810	-0.67610	0.35230
C	-2.39720	-0.66610	0.41400
C	-1.66280	0.40230	-0.11680
C	-2.36120	1.46190	-0.71030
C	-3.75220	1.45460	-0.76920
H	-5.55650	0.37840	-0.28600
H	-4.33970	-1.51010	0.77660
H	-1.87280	-1.48360	0.90170
H	-1.80590	2.28590	-1.15060
H	-4.27530	2.28210	-1.23990

ArNHOAc

Atom	X	Y	Z
C	2.75330	0.35950	-0.52910
C	2.08860	1.57990	-0.41850
C	0.70720	1.59730	-0.24340
C	-0.03770	0.41600	-0.18150
C	0.65000	-0.79940	-0.30080
C	2.02620	-0.83330	-0.47280

H	2.64870	2.50680	-0.46420
H	0.20210	2.55310	-0.13110
H	0.09540	-1.73340	-0.27890
H	2.54000	-1.78570	-0.57770
N	4.14590	0.27320	-0.79560
H	4.56900	-0.49300	-0.26850
O	4.81840	1.44600	-0.38600
C	-4.29810	0.49080	0.35200
C	-3.52420	-0.46070	1.01420
C	-2.14270	-0.48280	0.84240
C	-1.50940	0.44340	0.00380
C	-2.29780	1.39380	-0.65730
C	-3.67910	1.41860	-0.48390
H	-5.37550	0.50870	0.48610
H	-3.99610	-1.18260	1.67440
H	-1.54340	-1.21040	1.38330
H	-1.82560	2.10190	-1.33310
H	-4.27450	2.15790	-1.01160
C	5.52760	1.31390	0.76410
O	5.59930	0.27520	1.37220
C	6.22820	2.59410	1.11760
H	5.86100	3.42970	0.52200
H	6.08300	2.78770	2.18200
H	7.29950	2.46440	0.93990

TS-(1a)

Atom	X	Y	Z
H	2.90630	2.41690	1.57380

H	4.05710	3.07840	2.40040
O	3.86700	2.42390	1.71050
H	4.74240	1.09530	1.52280
C	2.94090	-0.34510	0.46350
C	2.41050	0.58510	-0.45970
C	0.80090	-0.46470	1.58140
C	2.12010	-0.85550	1.49720
H	3.05070	0.95020	-1.25820
H	0.17780	-0.84650	2.38310
H	2.53560	-1.55130	2.22300
N	4.24270	-0.73540	0.27950
H	4.45660	-1.56410	0.84340
O	5.26570	0.24480	1.35690
C	1.09160	0.97840	-0.35930
C	0.25670	0.45810	0.65720
H	0.67390	1.65120	-1.10070
H	6.00860	0.46400	0.76390
C	-3.84360	1.62650	0.91260
C	-2.88690	2.53560	0.46040
C	-1.55360	2.15510	0.36970
C	-1.15520	0.86280	0.74840
C	-2.12630	-0.04170	1.20820
C	-3.46170	0.33690	1.28140
H	-4.88610	1.92260	0.97510
H	-3.18080	3.54210	0.18060
H	-0.81540	2.87830	0.03470
H	-1.84550	-1.05800	1.46880
H	-4.20630	-0.37630	1.61960

TS-(1b)

Atom	X	Y	Z
H	5.10280	-0.65860	-3.09590
H	6.57920	-1.11310	-2.93700
O	5.80080	-0.81470	-2.44230
H	6.02330	0.39750	-1.27530
C	2.66280	0.14390	-0.03260
C	2.05340	1.35940	-0.43530
C	0.75920	1.63880	-0.06160
C	0.02380	0.72660	0.73130
C	0.64080	-0.48040	1.14210
C	1.93710	-0.76350	0.78400
H	2.62070	2.04090	-1.06270
H	0.28110	2.54830	-0.40870
H	0.09560	-1.16660	1.78140
H	2.41910	-1.67600	1.12770
N	3.92190	-0.10110	-0.46820
H	4.19710	-1.06950	-0.27270
O	4.99760	0.46450	0.92350
C	6.03880	1.05150	0.55440
O	6.50870	1.01070	-0.64950
C	6.82740	1.86520	1.52900
H	6.36150	1.83880	2.51220
H	7.84690	1.47340	1.57570
H	6.88200	2.89390	1.15990
C	-3.99230	1.59220	1.88810
C	-3.60420	0.27330	1.65190

C	-2.29510	-0.01100	1.28330
C	-1.35920	1.02490	1.12720
C	-1.76430	2.34990	1.35830
C	-3.06930	2.62840	1.74500
H	-5.01330	1.81250	2.18370
H	-4.32390	-0.53280	1.75110
H	-2.01050	-1.03840	1.07590
H	-1.04680	3.16120	1.27590
H	-3.36680	3.65360	1.94010

σ-TS-(2)

Atom	X	Y	Z
C	4.42080	-2.27340	-1.55360
C	5.22960	-3.44320	-1.35740
C	5.79030	-1.67900	-3.47600
C	4.75810	-1.38250	-2.63090
H	4.96110	-4.11500	-0.54700
H	6.05240	-0.98550	-4.26730
H	4.19630	-0.45730	-2.73860
N	3.39460	-2.08310	-0.73860
H	2.83980	-1.28380	-1.06430
C	2.23150	-1.93900	2.59470
N	2.66330	-0.85380	1.72680
C	3.85460	-0.78140	1.03600
N	3.92230	0.29820	0.24830
C	2.72640	0.89360	0.38740
C	2.17020	2.04590	-0.29670
O	2.65530	2.73590	-1.16070

N	0.85390	2.30160	0.18110
C	0.16790	1.55650	1.10550
N	0.65780	0.47530	1.68790
C	1.91000	0.19430	1.30800
H	0.40880	3.10270	-0.25780
H	-1.49050	2.80400	1.08040
H	-1.57170	1.42000	2.12530
H	2.10360	-2.84830	2.00190
H	4.69760	-1.40130	1.30650
H	2.97230	-2.10110	3.37930
H	1.27990	-1.65210	3.04250
N	-1.08060	1.94380	1.41320
C	6.27000	-3.71900	-2.20130
C	6.57440	-2.85310	-3.28880
H	6.84010	-4.63230	-2.07370
C	9.78520	-3.74070	-5.94330
C	9.84070	-4.17050	-4.61610
C	8.79120	-3.89360	-3.75210
C	7.67550	-3.15780	-4.19680
C	7.63920	-2.72100	-5.53560
C	8.68030	-3.02160	-6.40200
H	10.60340	-3.96640	-6.62020
H	10.70580	-4.71800	-4.25680
H	8.85870	-4.20950	-2.71580
H	6.77310	-2.18530	-5.91140
H	8.63130	-2.69930	-7.43690

π-TS-(2)

Atom	X	Y	Z
C	-3.43380	3.30270	0.61810
C	-4.51250	3.97850	-0.06110
C	-1.86430	4.38260	-0.90960
C	-2.09230	3.57230	0.16200
H	-5.53080	3.82440	0.29240
H	-0.84610	4.58720	-1.22390
H	-1.27700	3.11330	0.71480
N	-3.59700	2.38450	1.54760
H	-4.58130	2.30760	1.82570
C	-4.25760	4.82430	-1.12170
C	-2.94900	4.98800	-1.61740
H	-5.09280	5.29990	-1.62640
C	-2.25770	7.15410	-5.24010
C	-3.34860	7.47830	-4.43240
C	-3.57160	6.78600	-3.24710
C	-2.69910	5.76090	-2.84230
C	-1.59710	5.45220	-3.66080
C	-1.38180	6.13900	-4.85050
H	-2.08420	7.69830	-6.16340
H	-4.01840	8.28290	-4.71940
H	-4.40290	7.07800	-2.61230
H	-0.92120	4.64840	-3.38100
H	-0.52810	5.88750	-5.47250
C	-1.50820	0.51090	-0.85690
N	-2.93310	0.80770	-0.79040
C	-3.79330	0.48820	0.23190
N	-5.06130	0.84310	-0.02790

C	-4.99040	1.50810	-1.17930
C	-6.04140	2.15320	-1.95930
O	-7.20870	2.29210	-1.70200
N	-5.49770	2.67430	-3.16760
C	-4.17780	2.66780	-3.53060
N	-3.21430	2.09140	-2.81210
C	-3.65910	1.51700	-1.69690
H	-6.19090	3.09390	-3.78150
H	-4.48630	3.82990	-5.21300
H	-2.86340	3.30410	-4.92270
H	-1.08640	0.57530	0.14790
H	-3.48990	-0.15590	1.04570
H	-1.35010	-0.49050	-1.26300
H	-1.03470	1.24800	-1.50730
N	-3.84630	3.25060	-4.68750

Compound 8

ArNH+

Atom	X	Y	Z
C	-0.03140	3.14270	0.04890
C	1.22110	2.40140	0.10240
C	1.25990	1.03940	0.04640
C	0.00070	0.32700	0.00280
C	-1.27930	1.02430	-0.02700
C	-1.27310	2.38430	-0.03590
H	2.12520	2.99500	0.21180
H	-2.20460	2.93920	-0.12950
N	0.05070	4.42600	0.08280

H	-0.87490	4.87030	0.03940
C	0.02540	-3.92260	-0.05790
C	-0.72910	-3.24650	0.90390
C	-0.76790	-1.86030	0.90600
C	0.00880	-1.12900	-0.01630
C	0.79580	-1.82330	-0.95830
C	0.77300	-3.20950	-0.99780
H	0.03160	-5.00800	-0.07420
H	-1.29380	-3.80280	1.64450
H	1.34560	-3.73680	-1.75340
H	1.37290	-1.27260	-1.69410
H	-1.34840	-1.33910	1.66040
C	2.59040	0.33320	0.14710
H	2.52570	-0.56680	0.76220
H	2.96760	0.04100	-0.83670
H	3.32840	1.00340	0.59210
C	-2.59010	0.28810	-0.16100
H	-3.34770	0.95810	-0.57230
H	-2.50080	-0.57840	-0.81940
H	-2.95660	-0.06390	0.80710

ArNHOH

Atom	X	Y	Z
C	2.62290	0.42200	0.11670
C	1.91640	1.61710	0.20820
C	0.52190	1.61920	0.11970
C	-0.16780	0.41070	-0.05850
C	0.54610	-0.79910	-0.14550

C	1.93480	-0.78110	-0.05790
H	2.45550	2.54470	0.36460
H	2.49160	-1.71290	-0.13940
N	4.03930	0.38310	0.12050
H	4.37790	-0.41290	0.65590
O	4.60570	1.52170	0.72840
H	5.15460	1.90630	0.03000
C	-0.17860	-2.11030	-0.33050
H	0.53020	-2.92630	-0.49300
H	-0.78540	-2.35660	0.54730
H	-0.86110	-2.06830	-1.18550
C	-0.22890	2.92480	0.22640
H	-1.01570	2.86900	0.98580
H	0.44840	3.74140	0.48850
H	-0.71930	3.17910	-0.71960
C	-4.46120	0.38980	-0.32780
C	-3.83290	0.06280	0.87290
C	-2.44170	0.07020	0.95850
C	-1.65860	0.40450	-0.15160
C	-2.30000	0.73180	-1.35100
C	-3.69100	0.72440	-1.44030
H	-5.54510	0.38360	-0.39610
H	-4.42670	-0.19760	1.74440
H	-1.95060	-0.18240	1.89540
H	-1.69800	0.98980	-2.21920
H	-4.17360	0.97870	-2.37970

ArNHOAc

Atom	X	Y	Z
C	2.79560	0.50140	-0.74330
C	2.12580	1.70150	-0.52120
C	0.75250	1.70500	-0.27310
C	0.04530	0.49070	-0.26460
C	0.72030	-0.72040	-0.49860
C	2.09470	-0.70260	-0.72810
H	2.67710	2.63640	-0.55330
H	2.62660	-1.63900	-0.88410
N	4.17900	0.48690	-1.07930
H	4.59110	-0.40670	-0.80760
O	4.88600	1.47660	-0.35380
C	-4.18450	0.45810	0.51060
C	-3.28140	0.64100	1.55660
C	-1.91100	0.65370	1.30270
C	-1.42390	0.48280	0.00250
C	-2.33900	0.29980	-1.03960
C	-3.71000	0.28810	-0.78890
H	-5.25250	0.44780	0.70730
H	-3.64410	0.77110	2.57220
H	-1.20520	0.78960	2.11910
H	-1.96850	0.17150	-2.05400
H	-4.40810	0.14720	-1.60910
C	5.28750	1.08290	0.88730
O	5.14870	-0.04240	1.29220
C	5.91820	2.23050	1.62210
H	5.13860	2.94600	1.90000
H	6.40740	1.85480	2.51980

H	6.63520	2.74600	0.97940
C	-0.01830	-2.03650	-0.47340
H	0.68280	-2.87430	-0.49950
H	-0.63570	-2.12800	0.42600
H	-0.69140	-2.13190	-1.33220
C	0.04030	3.01470	-0.03520
H	-0.28150	3.11040	1.00760
H	0.69490	3.85940	-0.26520
H	-0.85920	3.09440	-0.65340

TS-(1a)

Atom	X	Y	Z
H	2.85450	2.40180	1.48270
H	3.94760	3.12320	2.33590
O	3.80770	2.44760	1.65510
H	4.76570	1.12080	1.51530
C	2.93060	-0.35920	0.46840
C	2.39980	0.54450	-0.48090
C	0.79370	-0.46050	1.62120
C	2.12110	-0.83990	1.52450
H	3.04460	0.87800	-1.29040
H	2.55260	-1.51260	2.26390
N	4.21890	-0.75750	0.28350
H	4.44470	-1.55200	0.89140
O	5.29160	0.27660	1.38000
C	1.07940	0.95640	-0.39970
C	0.27530	0.44730	0.65620
H	6.02330	0.48120	0.77020

C	-3.82410	1.64810	0.92630
C	-2.81010	2.57280	1.17160
C	-1.47620	2.18710	1.07160
C	-1.14770	0.86580	0.74830
C	-2.16940	-0.06100	0.51230
C	-3.50250	0.33370	0.59060
H	-4.86370	1.95190	0.99630
H	-3.05750	3.59570	1.43780
H	-0.68800	2.91150	1.26360
H	-1.92090	-1.08600	0.24810
H	-4.28980	-0.38660	0.39230
C	0.50300	1.87360	-1.44940
H	-0.44810	1.48480	-1.82470
H	0.30300	2.87210	-1.04980
H	1.19400	1.97680	-2.28860
C	-0.06440	-0.98330	2.74510
H	-0.65360	-0.18140	3.19790
H	-0.77130	-1.73680	2.38530
H	0.55390	-1.44540	3.51780

TS-(1b)

Atom	X	Y	Z
H	5.23320	-0.79900	-3.08410
H	6.63310	-1.38150	-2.75800
O	5.84020	-0.99590	-2.35500
H	6.08070	0.27640	-1.22020
C	2.64380	0.17200	-0.11450
C	2.10890	1.43250	-0.47720

C	0.81760	1.77860	-0.12640
C	0.05190	0.84930	0.62770
C	0.57560	-0.41500	1.02120
C	1.86610	-0.73490	0.65090
H	2.73860	2.11320	-1.04470
N	3.88870	-0.11640	-0.54630
H	4.12090	-1.10140	-0.37640
O	4.98850	0.33570	0.93080
C	6.05370	0.90020	0.61270
O	6.56420	0.87000	-0.57930
C	6.83760	1.67520	1.62330
H	6.33200	1.66260	2.58690
H	7.83670	1.23980	1.70890
H	6.95170	2.70260	1.26460
H	2.29660	-1.69420	0.93240
C	-3.95090	1.86130	1.74900
C	-2.95430	1.78110	2.72040
C	-1.65290	1.44190	2.35970
C	-1.33690	1.20370	1.01750
C	-2.33770	1.29720	0.04390
C	-3.64280	1.61370	0.41210
H	-3.19010	1.97940	3.76120
H	-0.87610	1.38170	3.11800
H	-2.09870	1.10110	-0.99860
H	-4.41790	1.66920	-0.34570
C	-0.26300	-1.39850	1.79770
H	0.21590	-2.37990	1.81600
H	-0.40510	-1.07230	2.83220

H	-1.25720	-1.50200	1.35400
C	0.25540	3.12280	-0.51380
H	-0.49350	3.02880	-1.30560
H	-0.23580	3.60260	0.33710
H	1.04900	3.77970	-0.87650
H	-4.96680	2.11640	2.03370

σ-TS-(2)

Atom	X	Y	Z
C	4.40330	-2.31660	-1.52930
C	5.19960	-3.49540	-1.36790
C	5.76530	-1.64600	-3.44640
C	4.73640	-1.39160	-2.57270
H	4.91290	-4.19090	-0.58310
H	4.17800	-0.45880	-2.63330
N	3.38090	-2.14550	-0.70570
H	2.83060	-1.33270	-1.00620
C	2.15330	-1.93380	2.63230
N	2.63600	-0.87350	1.76050
C	3.84760	-0.83830	1.10510
N	3.96180	0.22170	0.30010
C	2.77530	0.84830	0.39520
C	2.26300	1.99440	-0.33050
O	2.78420	2.65020	-1.20110
N	0.94160	2.29090	0.10710
C	0.21350	1.58020	1.02700
N	0.66230	0.50060	1.64320
C	1.91880	0.18520	1.30320

H	0.52460	3.08880	-0.36410
H	-1.40940	2.87060	0.94020
H	-1.55460	1.50630	2.00270
H	1.94330	-2.82740	2.03890
H	4.66260	-1.48570	1.39630
H	2.90590	-2.15460	3.39050
H	1.23930	-1.58520	3.11300
N	-1.03520	2.00090	1.28990
C	6.25290	-3.76460	-2.20930
C	6.53450	-2.83990	-3.26370
C	9.76110	-3.65120	-5.94330
C	10.01460	-3.46770	-4.58420
C	8.96430	-3.22170	-3.70570
C	7.65200	-3.12040	-4.18840
C	7.40620	-3.28700	-5.55870
C	8.45550	-3.56970	-6.42720
H	10.58030	-3.85690	-6.62500
H	11.03100	-3.52010	-4.20710
H	9.16500	-3.07240	-2.64810
H	6.38920	-3.22720	-5.93710
H	8.25470	-3.72110	-7.48300
C	6.10840	-0.64030	-4.51670
H	7.18880	-0.49320	-4.59040
H	5.75580	-0.96490	-5.49990
H	5.63940	0.32010	-4.29310
C	7.03460	-5.04530	-2.05480
H	7.20300	-5.52500	-3.02240
H	8.01540	-4.86810	-1.60480

H	6.49250	-5.74060	-1.41090

π-TS-(2)

Atom	X	Y	Z
C	-3.44710	3.34510	0.49070
C	-4.52400	4.04230	-0.14400
C	-1.89020	4.33900	-1.11790
C	-2.13140	3.52990	-0.03460
H	-5.52420	3.94980	0.27840
H	-1.31880	3.00370	0.46090
N	-3.61020	2.47110	1.48710
H	-4.57560	2.48380	1.83190
C	-4.30920	4.87430	-1.23820
C	-2.99700	4.99200	-1.75530
C	-2.25520	7.70670	-4.99590
C	-2.98680	6.54360	-5.22780
C	-3.22930	5.65190	-4.18560
C	-2.73260	5.90910	-2.90180
C	-2.01370	7.08960	-2.67330
C	-1.77500	7.98100	-3.71640
H	-2.06800	8.40300	-5.80720
H	-3.37360	6.33700	-6.22110
H	-3.80260	4.74740	-4.35740
H	-1.64390	7.30830	-1.67440
H	-1.21920	8.89500	-3.53020
C	-1.51340	0.42220	-0.66990
N	-2.92610	0.77170	-0.61260
C	-3.77980	0.61240	0.45860

N	-5.05260	0.95720	0.15430
C	-4.97360	1.47700	-1.05960
C	-6.01120	2.06650	-1.90130
O	-7.16350	2.29680	-1.64590
N	-5.46880	2.40160	-3.17460
C	-4.16210	2.27000	-3.55430
N	-3.20020	1.78540	-2.77080
C	-3.64220	1.38670	-1.58350
H	-6.15900	2.74990	-3.83520
H	-4.46380	3.14210	-5.40710
H	-2.84900	2.60100	-5.04840
H	-1.09460	0.48560	0.33610
H	-3.49330	0.03620	1.32700
H	-1.39150	-0.59050	-1.06010
H	-1.00790	1.13140	-1.32820
N	-3.81790	2.69470	-4.77280
C	-0.49160	4.45800	-1.67080
H	-0.18880	5.49310	-1.83860
H	0.22780	3.98490	-0.99810
H	-0.43230	3.94670	-2.63870
C	-5.47220	5.64050	-1.82220
H	-5.46010	5.65400	-2.91430
H	-6.42140	5.22110	-1.47850
H	-5.43410	6.68510	-1.49260

Compound 9

ArNH+

Atom	X	Y	Z

C	0.22400	4.03060	0.00000
C	-1.04710	3.30660	0.00000
C	-1.09040	1.95630	0.00000
C	0.11800	1.16050	0.00000
C	1.38490	1.87100	0.00000
C	1.44440	3.21930	0.00000
H	-1.94990	3.90990	0.00000
H	-2.05750	1.47320	0.00000
H	2.31260	1.31560	0.00000
H	2.40390	3.73040	0.00000
N	0.17880	5.31280	0.00000
H	1.11750	5.72790	0.00000
C	-0.03240	-3.08790	0.00000
C	1.21850	-2.42030	0.00000
C	1.26590	-1.05550	0.00000
C	0.07400	-0.25950	0.00000
C	-1.16750	-0.96640	0.00000
C	-1.23210	-2.33720	0.00000
H	2.12010	-3.02310	0.00000
H	2.24280	-0.59000	0.00000
H	-2.10690	-0.42910	0.00000
H	-2.19630	-2.83060	0.00000
O	0.02070	-4.40070	0.00000
C	-1.18550	-5.17530	0.00000
H	-0.85940	-6.21250	0.00000
H	-1.76780	-4.96470	0.90070
H	-1.76780	-4.96470	-0.90070

ArNHOH

Atom	X	Y	Z
C	2.65710	0.38280	0.10360
C	1.96200	1.57280	0.31440
C	0.57170	1.58280	0.23300
C	-0.15630	0.42540	-0.05860
C	0.56180	-0.76110	-0.26540
C	1.94700	-0.78740	-0.18660
H	2.50820	2.47390	0.56600
H	0.04020	2.51000	0.43090
H	0.02760	-1.67400	-0.51560
H	2.48530	-1.71430	-0.37120
N	4.07250	0.32510	0.09850
H	4.40370	-0.51380	0.56920
O	4.65320	1.40700	0.79000
H	5.20700	1.83680	0.12250
C	-4.44960	0.47950	-0.29480
C	-3.78750	-0.59720	0.30590
C	-2.40440	-0.60820	0.37940
C	-1.63650	0.44610	-0.14190
C	-2.31510	1.50950	-0.73880
C	-3.70850	1.53930	-0.81950
H	-4.38280	-1.40630	0.71740
H	-1.90630	-1.43840	0.87310
H	-1.74770	2.32750	-1.17510
H	-4.19440	2.38110	-1.29930
O	-5.80800	0.40260	-0.31820
C	-6.51660	1.47130	-0.90690

H	-7.57290	1.21860	-0.81670
H	-6.31960	2.41380	-0.38140
H	-6.25640	1.58270	-1.96670

ArNHOAc

Atom	X	Y	Z
C	2.81150	0.34010	-0.59200
C	2.16100	1.57350	-0.56920
C	0.78270	1.62160	-0.38160
C	0.02310	0.45660	-0.22850
C	0.69650	-0.77170	-0.25920
C	2.07270	-0.83430	-0.43190
H	2.73290	2.48650	-0.69490
H	0.28940	2.58880	-0.33630
H	0.13180	-1.69490	-0.16000
H	2.57550	-1.79820	-0.45420
N	4.20070	0.23420	-0.87640
H	4.59930	-0.57190	-0.39300
O	4.90900	1.36270	-0.40230
C	-4.23950	0.60790	0.30910
C	-3.46560	-0.29710	1.04460
C	-2.09240	-0.33930	0.86910
C	-1.44680	0.51400	-0.04070
C	-2.23510	1.40950	-0.76450
C	-3.62010	1.46690	-0.59980
H	-3.96570	-0.94890	1.75400
H	-1.50210	-1.03040	1.46520
H	-1.76680	2.06350	-1.49560

H	-4.19610	2.17020	-1.19020
C	5.40890	1.22610	0.85760
O	5.31820	0.20430	1.48820
C	6.08670	2.49380	1.29080
H	5.34160	3.28870	1.38650
H	6.57590	2.32700	2.24940
H	6.81560	2.80520	0.53890
O	-5.57820	0.57470	0.54860
C	-6.39650	1.47210	-0.17020
H	-7.41570	1.28780	0.16870
H	-6.12300	2.51300	0.04150
H	-6.33120	1.28890	-1.24970

TS-(1a)

Atom	X	Y	Z
H	2.95830	2.32270	1.51120
H	3.92130	2.81210	2.65100
O	3.86740	2.26770	1.85040
H	4.66270	0.95180	1.65110
C	2.96040	-0.32490	0.37900
C	2.53100	0.68520	-0.50560
C	0.75130	-0.41930	1.35070
C	2.05640	-0.86620	1.31700
H	3.23930	1.08940	-1.22420
H	0.04840	-0.88070	2.03610
N	4.27510	-0.74590	0.26810
H	4.40910	-1.63790	0.75390
O	5.18460	0.09450	1.44290

C	1.22890	1.14130	-0.44960
C	0.30420	0.59720	0.47390
H	0.91200	1.93220	-1.12150
H	5.98420	0.34370	0.94060
H	2.38500	-1.65060	1.99570
C	-3.74730	1.96900	0.56930
C	-3.01740	1.99350	-0.63150
C	-1.70920	1.55850	-0.65540
C	-1.08310	1.06890	0.50970
C	-1.82900	1.04290	1.69650
C	-3.14260	1.49280	1.74080
H	-3.51300	2.34920	-1.52880
H	-1.17820	1.55630	-1.60280
H	-1.37190	0.69910	2.62020
H	-3.68140	1.47490	2.68060
O	-5.00830	2.41730	0.49310
C	-5.81210	2.40100	1.66410
H	-6.78110	2.79390	1.36160
H	-5.92880	1.37890	2.03980
H	-5.38020	3.04190	2.44020

TS-(1b)

Atom	X	Y	Z
H	4.96420	-0.49460	-3.05420
H	6.48860	-0.78930	-3.16690
O	5.76670	-0.65110	-2.53480
H	6.01050	0.36690	-1.24380
C	2.68390	0.11830	-0.02820

C	2.14940	1.35540	-0.45680
C	0.85640	1.69900	-0.13310
C	0.04520	0.83270	0.63820
C	0.59430	-0.39930	1.07300
C	1.88740	-0.74750	0.75990
H	2.77810	2.02140	-1.04150
H	0.46360	2.66050	-0.44510
H	-0.02400	-1.09050	1.63530
N	3.95840	-0.19090	-0.41030
H	4.15910	-1.18110	-0.23760
O	4.97230	0.27990	0.97150
C	6.03790	0.86090	0.64620
O	6.50780	0.90350	-0.55170
C	6.84150	1.56050	1.69280
H	6.35880	1.47790	2.66470
H	7.84190	1.12040	1.72220
H	6.94710	2.61100	1.40580
H	2.30020	-1.69510	1.09930
C	-3.97520	1.88740	1.64220
C	-3.21860	1.07550	2.50500
C	-1.92560	0.73130	2.17350
C	-1.32930	1.19770	0.98280
C	-2.09640	2.01420	0.13880
C	-3.40670	2.35420	0.44900
H	-3.67590	0.73950	3.42970
H	-1.35250	0.12520	2.86890
H	-1.68300	2.36250	-0.80330
H	-3.97580	2.96810	-0.23880

O	-5.22480	2.15900	2.04610
C	-6.04630	2.97540	1.22440
H	-6.99710	3.05810	1.74800
H	-5.60480	3.97020	1.10090
H	-6.20310	2.50820	0.24630

σ-TS-(2)

Atom	X	Y	Z
C	4.42340	-2.22080	-1.61910
C	5.25230	-3.36520	-1.38740
C	5.78890	-1.66320	-3.55470
C	4.74950	-1.36160	-2.72000
H	4.99660	-4.02040	-0.55930
H	6.03420	-0.98310	-4.36260
H	4.17190	-0.45100	-2.86110
N	3.38770	-2.01800	-0.80700
H	2.81640	-1.24590	-1.16680
C	2.27300	-2.09220	2.40900
N	2.67690	-0.93270	1.63060
C	3.84370	-0.81360	0.89430
N	3.88350	0.33560	0.19790
C	2.69400	0.90700	0.41830
C	2.11420	2.11070	-0.15260
O	2.57450	2.87560	-0.96440
N	0.81040	2.31800	0.38000
C	0.15400	1.49690	1.26030
N	0.66520	0.37750	1.74450
C	1.90740	0.13370	1.31140

H	0.35050	3.14970	0.02040
H	-1.51460	2.72610	1.37040
H	-1.55730	1.26670	2.31040
H	2.14450	-2.94700	1.73940
H	4.71520	-1.40270	1.14250
H	3.03130	-2.31390	3.16200
H	1.32750	-1.85730	2.89810
N	-1.08700	1.84990	1.63120
C	6.30110	-3.64740	-2.21800
C	6.60100	-2.81430	-3.33530
H	6.88180	-4.54770	-2.05340
C	9.84950	-3.73490	-5.94370
C	9.85410	-4.19970	-4.61390
C	8.80110	-3.90940	-3.77890
C	7.70730	-3.12480	-4.22010
C	7.72950	-2.66180	-5.55110
C	8.77130	-2.96470	-6.41110
H	10.70640	-4.77840	-4.27400
H	8.84420	-4.25600	-2.75180
H	6.89370	-2.09030	-5.94180
H	8.73920	-2.61200	-7.43490
O	10.90900	-4.07620	-6.68000
C	10.98300	-3.63830	-8.03190
H	11.92420	-4.02840	-8.41460
H	10.14960	-4.04380	-8.61450
H	10.98660	-2.54480	-8.08300

π-TS-(2)

Atom	X	Y	Z
C	2.12400	-1.08580	-1.50730
C	1.39200	0.06450	-1.96010
C	0.00720	-2.11370	-0.86710
C	1.36400	-2.18680	-0.98550
H	1.94120	0.89760	-2.39550
H	-0.54440	-2.97200	-0.49930
H	1.90750	-3.08690	-0.71210
N	3.44940	-1.15810	-1.44590
H	3.88540	-0.36690	-1.93040
C	2.73210	-2.07100	1.93240
N	2.83110	-0.79090	1.24620
C	3.90090	-0.33850	0.49990
N	3.70620	0.92030	0.04690
C	2.44580	1.19070	0.35090
C	1.63680	2.36840	0.04580
O	1.92700	3.34900	-0.58830
N	0.33610	2.21930	0.60000
C	-0.14510	1.11250	1.24820
N	0.59050	0.04030	1.53390
C	1.84350	0.12610	1.09610
H	-0.27550	3.01270	0.42730
H	-2.05750	1.88830	1.43950
H	-1.78810	0.30740	2.10510
H	3.27890	-2.82300	1.36030
H	4.86950	-0.81340	0.56750
H	3.15110	-1.99270	2.93770
H	1.67800	-2.34580	1.99490

N	-1.42960	1.11730	1.61670
C	0.01680	0.11380	-1.85460
C	-0.70640	-0.93700	-1.25010
H	-0.49990	1.01010	-2.18190
C	-4.91910	-0.61340	-0.55130
C	-4.31020	0.13570	-1.57460
C	-2.95420	0.02880	-1.80030
C	-2.14690	-0.83240	-1.02420
C	-2.77420	-1.57160	-0.00720
C	-4.13760	-1.46840	0.24070
H	-4.93820	0.77230	-2.18950
H	-2.52260	0.58460	-2.62710
H	-2.18590	-2.22770	0.62850
H	-4.58270	-2.05590	1.03530
O	-6.24020	-0.44560	-0.41520
C	-6.93850	-1.22330	0.54880
H	-7.98510	-0.94110	0.45170
H	-6.82230	-2.29190	0.34050
H	-6.58800	-0.99440	1.56090

Compound 10

ArNH+

Atom	X	Y	Z
C	-0.01640	-1.04230	-0.06740
C	1.23480	-0.28310	-0.05620
C	1.24360	1.06640	-0.02960
C	0.01440	1.83460	-0.01060
C	-1.23330	1.08700	-0.02220

C	-1.25670	-0.26100	-0.04880
H	2.15310	-0.86230	-0.07020
H	2.19850	1.57410	-0.02220
H	-2.17660	1.61570	-0.00940
H	-2.20260	-0.79690	-0.05700
N	0.06010	-2.32260	-0.09230
H	-0.86890	-2.75820	-0.09810
C	0.04850	6.09420	0.07700
C	-1.18500	5.37870	0.06660
C	-1.18830	4.01600	0.03840
C	0.02340	3.24620	0.01800
C	1.24840	3.99510	0.02900
C	1.26930	5.35750	0.05710
H	-2.12000	5.93020	0.08160
H	-2.15190	3.52340	0.03180
H	2.20230	3.48430	0.01480
H	2.21390	5.89250	0.06470
N	0.06020	7.42650	0.10430
H	0.92730	7.94860	0.11360
H	-0.79740	7.96390	0.12030

ArNHOH

Atom	X	Y	Z
C	2.64220	0.42360	0.09120
C	1.92500	1.59820	0.31310
C	0.53410	1.58160	0.23980
C	-0.17350	0.41210	-0.05590
C	0.56760	-0.75820	-0.27520

C	1.95340	-0.75810	-0.20310
H	2.45500	2.50830	0.56760
H	-0.01420	2.49720	0.44620
H	0.04990	-1.67940	-0.52970
H	2.50890	-1.67310	-0.39690
N	4.05890	0.39340	0.07790
H	4.40820	-0.44230	0.54100
O	4.62230	1.48060	0.77580
H	5.16180	1.92810	0.10820
C	-4.48370	0.38880	-0.28130
C	-3.79000	-0.67810	0.30330
C	-2.40260	-0.66470	0.37370
C	-1.65380	0.40530	-0.13190
C	-2.35720	1.46810	-0.71210
C	-3.74470	1.46600	-0.78600
H	-4.34610	-1.51420	0.72070
H	-1.89060	-1.49420	0.85480
H	-1.80650	2.30380	-1.13630
H	-4.26420	2.30450	-1.24410
N	-5.88160	0.40750	-0.30110
H	-6.28820	0.99190	-1.02070
H	-6.31890	-0.50510	-0.27690

ArNHOAc

Atom	X	Y	Z
C	2.77990	0.33160	-0.42690
C	2.12280	1.54840	-0.25470
C	0.73420	1.57190	-0.14670

C	-0.02850	0.40190	-0.21920
C	0.65440	-0.80960	-0.39930
C	2.03780	-0.85050	-0.49940
H	2.69380	2.46820	-0.19850
H	0.23590	2.52340	0.01860
H	0.09050	-1.73470	-0.48310
H	2.54590	-1.79960	-0.65200
N	4.18520	0.24300	-0.63090
H	4.56940	-0.56120	-0.13150
O	4.84840	1.37720	-0.11020
C	-4.33340	0.49150	0.07770
C	-3.59300	-0.52930	0.68730
C	-2.20740	-0.55150	0.59050
C	-1.50660	0.43640	-0.11260
C	-2.25580	1.45450	-0.71500
C	-3.64170	1.48720	-0.62350
H	-4.10920	-1.30020	1.25440
H	-1.65650	-1.34220	1.09320
H	-1.74680	2.22340	-1.29040
H	-4.19770	2.28840	-1.10490
N	-5.72240	0.55010	0.22030
H	-6.20300	1.07000	-0.50300
H	-6.17040	-0.34080	0.39450
C	5.50030	1.15850	1.05970
O	5.53110	0.08150	1.60100
C	6.19460	2.40340	1.53430
H	5.92260	3.27000	0.93220
H	5.93390	2.56930	2.58170

H	7.27450	2.24140	1.47730

TS-(1a)

Atom	X	Y	Z
H	2.79660	1.98370	1.95290
H	3.67170	2.16960	3.24820
O	3.70300	1.94200	2.30570
H	4.56020	0.83340	1.77960
C	2.97990	-0.23130	0.26400
C	2.48560	0.90980	-0.39200
C	0.79780	-0.63080	1.21660
C	2.12330	-0.99470	1.07840
H	3.15660	1.48880	-1.02150
H	0.13520	-1.26050	1.80030
H	2.50020	-1.88360	1.58050
N	4.33040	-0.54330	0.08340
H	4.51440	-1.51210	0.35860
O	5.16010	0.09710	1.35170
C	1.16460	1.28260	-0.22610
C	0.28070	0.52000	0.57560
H	0.80280	2.17990	-0.71700
H	5.91910	0.53160	0.91580
C	-3.84210	1.65180	1.02500
C	-3.12120	1.99020	-0.13940
C	-1.79520	1.63050	-0.27230
C	-1.12170	0.90620	0.73010
C	-1.85380	0.56420	1.88300
C	-3.17550	0.93130	2.03820

H	-3.62120	2.52540	-0.94160
H	-1.28560	1.88140	-1.19810
H	-1.37080	0.02960	2.69600
H	-3.70890	0.66890	2.94740
N	-5.15090	1.99540	1.15900
H	-5.65270	1.81290	2.01470
H	-5.60910	2.57770	0.47460

TS-(1b)

Atom	X	Y	Z
H	4.73680	-0.46970	-2.94490
H	6.24730	-0.52260	-3.32800
O	5.63330	-0.48660	-2.57910
H	5.92000	0.48930	-1.28630
C	2.76590	0.05560	0.16850
C	2.15510	1.22550	-0.33200
C	0.85360	1.52440	0.00430
C	0.10500	0.67670	0.85780
C	0.73640	-0.48660	1.36420
C	2.04000	-0.78670	1.04050
H	2.71930	1.86490	-1.00590
H	0.38090	2.40000	-0.42690
H	0.19910	-1.12990	2.05240
H	2.52060	-1.66790	1.46040
N	4.05220	-0.22120	-0.22940
H	4.30040	-1.18680	0.00640
O	5.06760	0.40730	1.01940
C	6.06630	1.04440	0.58640

O	6.43700	1.07120	-0.64210
C	6.89210	1.83190	1.54820
H	6.48620	1.75340	2.55500
H	7.91930	1.45850	1.51780
H	6.90620	2.87580	1.22100
C	-3.96110	1.59740	1.88860
C	-3.50610	0.26300	1.86690
C	-2.19560	-0.02460	1.54320
C	-1.27740	0.99000	1.20710
C	-1.74620	2.31840	1.22270
C	-3.04880	2.62230	1.56280
H	-4.19690	-0.54160	2.10250
H	-1.89040	-1.06640	1.50930
H	-1.06620	3.13690	1.00540
H	-3.37510	3.65800	1.59390
N	-5.24220	1.89250	2.24910
H	-5.60700	2.82250	2.10490
H	-5.92670	1.15530	2.33200

σ-TS-(2)

Atom	X	Y	Z
C	4.42190	-2.20630	-1.61670
C	5.27810	-3.30950	-1.31030
C	5.75700	-1.77010	-3.60300
C	4.71970	-1.42890	-2.78060
H	5.04700	-3.90750	-0.43290
H	5.97280	-1.14590	-4.46220
H	4.12080	-0.54470	-2.98640

N	3.38700	-1.95830	-0.80600
H	2.79300	-1.23320	-1.22180
C	2.35600	-2.01480	2.35290
N	2.71760	-0.84530	1.57040
C	3.84850	-0.72620	0.77060
N	3.84650	0.43190	0.07750
C	2.66480	0.98880	0.34920
C	2.05010	2.19010	-0.19240
O	2.46960	2.96250	-1.01860
N	0.76920	2.38570	0.39720
C	0.15950	1.55860	1.30470
N	0.70090	0.44370	1.76640
C	1.92500	0.20920	1.28070
H	0.28810	3.21510	0.06090
H	-1.51690	2.76940	1.48240
H	-1.50310	1.31180	2.42700
H	2.20560	-2.86260	1.67830
H	4.75030	-1.26670	1.02280
H	3.14920	-2.24000	3.06800
H	1.43210	-1.79290	2.88720
N	-1.06600	1.90150	1.73150
C	6.32580	-3.63170	-2.12770
C	6.60090	-2.88310	-3.31140
H	6.92450	-4.50500	-1.89680
C	9.85430	-3.92210	-5.89710
C	9.84250	-4.34060	-4.54520
C	8.78980	-4.01230	-3.72450
C	7.69840	-3.23390	-4.18240

C	7.73150	-2.81540	-5.53560
C	8.76640	-3.15360	-6.37510
H	10.67720	-4.91720	-4.15730
H	8.83310	-4.32980	-2.68810
H	6.90320	-2.25000	-5.94950
H	8.75020	-2.83930	-7.41460
N	10.88130	-4.24900	-6.71280
H	10.89800	-3.95820	-7.67930
H	11.65710	-4.80490	-6.38420

π-TS-(2)

Atom	X	Y	Z
C	1.95310	-1.24060	-1.41710
C	1.25680	-0.10070	-1.94050
C	-0.16880	-2.05850	-0.53650
C	1.16970	-2.23330	-0.74080
H	1.82010	0.65120	-2.49110
H	-0.73720	-2.84130	-0.04560
H	1.67580	-3.13850	-0.41660
N	3.27980	-1.38480	-1.43040
H	3.71850	-0.68960	-2.04220
C	2.85590	-1.97290	2.00790
N	2.93440	-0.75470	1.21500
C	3.93450	-0.42990	0.31360
N	3.75070	0.80660	-0.21490
C	2.54340	1.16110	0.18800
C	1.74870	2.34160	-0.14940
O	2.01510	3.25180	-0.89020

N	0.50120	2.29610	0.52810
C	0.04450	1.27100	1.31450
N	0.76680	0.20090	1.63560
C	1.97550	0.19060	1.07990
H	-0.08790	3.10700	0.35980
H	-1.86310	2.04590	1.45750
H	-1.55910	0.57940	2.31650
H	3.30260	-2.79250	1.44090
H	4.89390	-0.92740	0.35090
H	3.38970	-1.84190	2.95180
H	1.80500	-2.18740	2.20810
N	-1.19330	1.37730	1.81270
C	-0.09980	0.05310	-1.74400
C	-0.83860	-0.87510	-0.97670
H	-0.57880	0.95040	-2.12290
C	-4.92910	-0.10790	0.10810
C	-4.35180	0.51340	-1.02100
C	-3.04130	0.25810	-1.37110
C	-2.23390	-0.63220	-0.63120
C	-2.82430	-1.24830	0.49320
C	-4.12920	-0.99170	0.86530
H	-4.95540	1.18050	-1.63020
H	-2.65300	0.72520	-2.27120
H	-2.23810	-1.92280	1.11170
H	-4.55080	-1.47670	1.74150
N	-6.21150	0.16170	0.47340
H	-6.67060	-0.40790	1.16980
H	-6.82140	0.66350	-0.15610

Compound 11

ArNH+

Atom	X	Y	Z
C	-3.41470	3.27750	0.61300
C	-4.52900	3.98250	-0.04420
C	-2.05400	3.46680	0.09290
H	-5.53010	3.83080	0.35240
H	-1.25630	2.93160	0.60130
N	-3.54560	2.49740	1.62380
H	-4.52350	2.41790	1.92690
C	-4.31440	4.79210	-1.10680
H	-5.13300	5.31240	-1.59300
C	-2.97160	4.95190	-1.58510
C	-1.85390	4.27810	-0.96890
C	-0.58570	4.64740	-1.69730
H	0.13670	5.13840	-1.03490
H	-0.09080	3.76790	-2.12570
C	-1.09010	5.58090	-2.76460
C	-2.50150	5.73620	-2.66810
C	-3.21520	6.56500	-3.56230
C	-2.50150	7.22650	-4.53950
C	-1.10230	7.06930	-4.62930
C	-0.38710	6.25260	-3.75180
H	-4.29190	6.67960	-3.48440
H	-3.01120	7.87250	-5.24590
H	-0.56580	7.60270	-5.40860

H	0.68950	6.15170	-3.84630

ArNHOH

Atom	X	Y	Z
C	2.66990	0.42880	0.07370
C	1.95330	1.60750	0.30060
C	0.56060	1.60220	0.23800
C	1.99960	-0.76850	-0.21620
H	2.49320	2.51530	0.54100
H	0.01240	2.52200	0.42390
H	2.56650	-1.67920	-0.40230
N	4.08690	0.41040	0.05120
H	4.44620	-0.42400	0.50910
O	4.65000	1.50010	0.74440
H	5.18360	1.94940	0.07320
C	-0.11060	0.41860	-0.05010
C	0.61710	-0.76330	-0.27600
C	-0.32790	-1.90960	-0.56520
H	-0.14980	-2.34160	-1.55780
H	-0.21980	-2.72000	0.16600
C	-1.68740	-1.24930	-0.47620
C	-1.54390	0.11640	-0.17480
C	-2.66470	0.93400	-0.04360
C	-3.92930	0.37140	-0.21600
C	-4.07170	-0.98560	-0.51460
C	-2.94770	-1.80520	-0.64690
H	-2.56010	1.99060	0.18870
H	-4.81350	0.99450	-0.11690

H	-5.06430	-1.40690	-0.64490
H	-3.06250	-2.86120	-0.87950

ArNHOAc

Atom	X	Y	Z
C	2.82980	0.40740	-0.73260
C	2.14850	1.62890	-0.70380
C	0.77550	1.65930	-0.47470
C	2.14590	-0.79720	-0.53980
H	2.70240	2.54710	-0.86760
H	0.25430	2.61240	-0.44890
H	2.68780	-1.74090	-0.54670
N	4.21610	0.36520	-1.05430
H	4.63520	-0.48530	-0.67570
O	4.90890	1.44120	-0.44610
C	5.32560	1.19060	0.82720
O	5.20620	0.11370	1.35220
C	5.93820	2.42120	1.43030
H	5.13590	3.11290	1.70470
H	6.49780	2.14250	2.32220
H	6.58470	2.92280	0.70750
C	0.08620	0.46270	-0.29300
C	0.77630	-0.76040	-0.33050
C	-0.18140	-1.90710	-0.09290
H	-0.19850	-2.60370	-0.93990
H	0.09200	-2.48580	0.79780
C	-1.50830	-1.20030	0.08100
C	-1.33650	0.18970	-0.03930

C	-2.42430	1.05170	0.08460
C	-3.68510	0.50880	0.32980
C	-3.85590	-0.87250	0.44980
C	-2.76510	-1.73650	0.32580
H	-2.29760	2.12710	-0.00790
H	-4.54420	1.16580	0.42860
H	-4.84510	-1.27760	0.64100
H	-2.90230	-2.81100	0.42010

TS-(1a)

Atom	X	Y	Z
H	2.88480	2.35920	1.44670
H	3.90800	2.97130	2.46900
O	3.82110	2.38010	1.70530
H	4.68760	1.10810	1.49780
C	2.96020	-0.34210	0.45060
C	2.41410	0.57980	-0.47000
C	2.17650	-0.87380	1.50270
H	3.05050	0.94880	-1.26980
H	2.61630	-1.57720	2.20810
N	4.28450	-0.69810	0.25850
H	4.50990	-1.54490	0.78920
O	5.23920	0.26800	1.30070
C	1.09250	0.97750	-0.35920
H	0.66460	1.67140	-1.07610
H	5.97930	0.52380	0.71720
C	0.85790	-0.49030	1.60070
C	0.31180	0.43690	0.67550

C	-0.20160	-0.91690	2.58890
H	0.08300	-0.67990	3.62110
H	-0.37990	-1.99780	2.54150
C	-1.08860	0.65740	1.01080
C	-1.40720	-0.12770	2.13450
C	-2.69150	-0.10460	2.66230
C	-3.64660	0.70920	2.05250
C	-3.32950	1.48950	0.93230
C	-2.04690	1.47140	0.39940
H	-2.95270	-0.70700	3.52760
H	-4.65620	0.73750	2.45060
H	-4.09520	2.10980	0.47810
H	-1.80300	2.07270	-0.47170

TS-(1b)

Atom	X	Y	Z
H	4.94060	-0.48920	-3.10050
H	6.47670	-0.69940	-3.22690
O	5.75740	-0.58080	-2.58820
H	5.96550	0.47400	-1.31070
C	2.71560	0.05110	0.01820
C	2.11380	1.24780	-0.44520
C	0.81150	1.55280	-0.10850
C	1.99970	-0.83950	0.86280
H	2.70050	1.90460	-1.08130
H	0.34400	2.46210	-0.47200
H	2.48590	-1.74120	1.23110
N	3.99320	-0.19870	-0.39300

H	4.25850	-1.16760	-0.18990
O	5.02340	0.38230	0.94260
C	6.02820	1.03130	0.55810
O	6.44920	1.06810	-0.65850
C	6.81280	1.82730	1.54840
H	6.37700	1.73790	2.54160
H	7.84680	1.47210	1.54860
H	6.81920	2.87310	1.22660
C	0.10260	0.65700	0.70890
C	0.70140	-0.53820	1.19010
C	-0.28500	-1.30130	2.04210
H	-0.48640	-2.29830	1.63280
H	0.08380	-1.43710	3.06560
C	-1.50760	-0.41550	1.99550
C	-1.26140	0.72520	1.20790
C	-2.24740	1.69820	1.01250
C	-3.48300	1.51180	1.61800
C	-3.72760	0.37650	2.40320
C	-2.74530	-0.59440	2.59900
H	-2.05770	2.57780	0.40390
H	-4.26790	2.24890	1.48430
H	-4.70120	0.25160	2.86700
H	-2.94930	-1.46910	3.20980

σ-TS-(2)

Atom	X	Y	Z
C	-3.90590	-0.19320	0.48530
N	-4.79510	0.37550	-0.51560

N	-6.68290	0.84810	-1.66710
C	-5.69650	1.66100	-2.05980
C	-5.70730	2.75510	-3.01400
O	-6.61720	3.18730	-3.67790
N	-4.41040	3.33560	-3.09550
C	-3.31320	2.97840	-2.35540
N	-3.31540	2.01130	-1.45330
C	-4.49580	1.39390	-1.35290
H	-4.34270	4.08680	-3.77650
H	-2.10290	4.45370	-3.17190
H	-1.36940	3.40690	-2.00270
H	-3.61850	0.57900	1.20190
H	-4.43720	-0.99150	1.00320
H	-3.01490	-0.59370	-0.00050
N	-2.17140	3.64580	-2.57080
C	-6.13980	0.10080	-0.69040
H	-6.56400	-0.82500	-0.32970
N	-7.06590	1.23180	0.87490
H	-6.89510	2.07970	0.32320
C	-10.14390	-0.25930	2.08750
C	-8.81140	-0.01550	1.87790
C	-8.37910	1.01980	0.97940
C	-9.35860	1.78350	0.25550
H	-10.46730	-1.02910	2.78020
H	-8.04250	-0.57360	2.40420
H	-9.02050	2.52740	-0.46330
C	-10.68370	1.54110	0.47290
C	-11.08960	0.52230	1.38740

C	-12.53110	0.47610	1.41840
C	-13.03350	1.45170	0.52960
C	-14.40310	1.61350	0.37490
C	-15.25680	0.79540	1.11580
C	-14.75900	-0.17650	1.99850
C	-13.39310	-0.34660	2.15870
H	-14.80620	2.35930	-0.30350
H	-16.33100	0.91050	1.00770
H	-15.45230	-0.79580	2.55760
H	-13.00450	-1.09590	2.84180
C	-11.90120	2.19340	-0.13640
H	-11.93440	3.26810	0.07650
H	-11.91840	2.07600	-1.22620

π-TS-(2)

Atom	X	Y	Z
C	-3.40740	3.25270	0.63470
C	-4.51110	3.97700	0.04370
C	-2.07780	3.49080	0.12790
H	-5.51050	3.80080	0.43770
H	-1.25340	2.96730	0.60470
N	-3.56210	2.29980	1.53810
H	-4.53130	2.26180	1.87050
C	-4.31050	4.87990	-0.97960
H	-5.14930	5.42520	-1.40250
C	-1.53840	0.32020	-0.67090
N	-2.94010	0.71040	-0.69840
C	-3.87320	0.46940	0.28710

N	-5.10380	0.88290	-0.06060
C	-4.92470	1.53240	-1.20690
C	-5.88280	2.24170	-2.05040
O	-7.05410	2.45090	-1.86760
N	-5.23200	2.73410	-3.21620
C	-3.89140	2.65590	-3.48980
N	-3.01820	2.00850	-2.72590
C	-3.56410	1.45810	-1.64250
H	-5.85550	3.20820	-3.86400
H	-4.01390	3.86180	-5.16940
H	-2.44930	3.22410	-4.78390
H	-1.08270	0.65750	0.26260
H	-1.45140	-0.76440	-0.75760
H	-1.04150	0.79550	-1.51780
N	-3.44480	3.24800	-4.60410
C	-3.01570	5.02040	-1.50020
C	-1.89830	4.33830	-0.92270
C	-0.64330	4.67800	-1.69220
H	0.09730	5.18470	-1.06230
H	-0.16710	3.77710	-2.09800
C	-1.16350	5.58510	-2.78290
C	-2.55030	5.79030	-2.63680
C	-3.26140	6.60940	-3.52290
C	-2.56540	7.21690	-4.56050
C	-1.18620	7.00780	-4.70960
C	-0.47550	6.19390	-3.82540
H	-4.32630	6.78480	-3.39350
H	-3.08560	7.86910	-5.25460

H	-0.66030	7.49860	-5.52280
H	0.59460	6.05270	-3.94770
H	-3.66350	-0.20540	1.10540

N7-σ-TS-(2)

Atom	X	Y	Z
C	-4.01860	0.74460	0.65560
N	-4.86150	1.27300	-0.41230
C	-6.19870	1.56270	-0.34750
C	-5.57850	2.03620	-2.34310
C	-5.50170	2.39230	-3.72440
O	-6.39850	2.78600	-4.45650
N	-4.18760	2.21720	-4.19740
C	-3.12070	1.75580	-3.45350
N	-3.20850	1.42020	-2.18710
C	-4.45230	1.56720	-1.68770
H	-4.06720	2.42160	-5.18530
H	-1.77800	1.98490	-5.02440
H	-1.14120	1.33990	-3.54690
H	-3.03120	0.56110	0.23160
H	-3.93820	1.47120	1.46580
H	-4.43530	-0.19220	1.02870
N	-1.93890	1.63660	-4.09160
N	-6.64620	2.02890	-1.48540
N	-8.57610	2.39670	-2.09700
H	-8.18220	2.23930	-3.03440
C	-9.59510	4.05160	-0.75450
C	-8.86380	3.69310	-1.93090

C	-8.51770	4.69350	-2.89740
C	-8.92150	5.99490	-2.72600
H	-9.84110	3.26620	-0.04450
H	-7.93600	4.38830	-3.76470
H	-8.68040	6.75320	-3.46380
C	-9.65520	6.32730	-1.56850
C	-9.98580	5.35180	-0.58540
C	-10.77960	5.99510	0.52690
H	-11.77450	5.54520	0.62470
H	-10.27910	5.89390	1.49690
C	-10.19310	7.60590	-1.15210
C	-10.85670	7.43490	0.07980
C	-11.46460	8.51800	0.70060
C	-11.40060	9.76370	0.07630
C	-10.74120	9.93410	-1.15040
C	-10.13120	8.85770	-1.77740
H	-11.98090	8.40280	1.64900
H	-11.87190	10.62070	0.54740
H	-10.71170	10.91680	-1.60930
H	-9.62180	8.98690	-2.72790
H	-6.78780	1.40750	0.54630

N2-σ-TS-(2)

Atom	X	Y	Z
N	-6.51610	-7.23040	0.84220
H	-7.06910	-7.58890	1.62890
C	-7.54570	-9.97230	-1.39710
C	-7.54000	-9.12710	-0.31230

C	-6.60630	-8.05000	-0.23210
C	-5.68890	-7.81980	-1.29980
H	-8.24040	-10.80470	-1.44630
H	-8.23640	-9.28260	0.50930
H	-4.97420	-7.00520	-1.20620
C	-5.70410	-8.65710	-2.38460
C	-6.62710	-9.73800	-2.44110
C	-6.41610	-10.46610	-3.67500
C	-5.36590	-9.84880	-4.38530
C	-4.95920	-10.35640	-5.61160
C	-5.61260	-11.48230	-6.11350
C	-6.65750	-12.09760	-5.40730
C	-7.06990	-11.59690	-4.18130
H	-4.15100	-9.89350	-6.17010
H	-5.30620	-11.89360	-7.07040
H	-7.14310	-12.97260	-5.82650
H	-7.87720	-12.07330	-3.63290
C	-4.83460	-8.66150	-3.61900
H	-4.92950	-7.72950	-4.18850
H	-3.77510	-8.78090	-3.36370
C	-10.88630	-3.98960	4.50720
N	-9.47400	-3.64270	4.53720
C	-8.81380	-2.87670	5.46550
N	-7.53600	-2.72970	5.21030
C	-7.34040	-3.42850	4.05810
C	-6.12680	-3.63730	3.29490
O	-4.99490	-3.27350	3.48290
N	-6.43050	-4.44200	2.13780

C	-7.65960	-4.92090	1.81890
N	-8.74320	-4.76600	2.50940
C	-8.53090	-4.00610	3.62290
H	-5.61660	-4.72720	1.59860
H	-7.28200	-5.29760	-0.17190
H	-8.69260	-5.98150	0.45180
H	-11.00590	-5.07400	4.54400
H	-9.33560	-2.45210	6.31360
H	-11.36810	-3.54240	5.37690
H	-11.34650	-3.60050	3.59700
N	-7.72660	-5.70930	0.64800

Compound 12

ArNH+

Atom	X	Y	Z
C	-4.40830	2.95650	0.01380
C	-5.01690	1.73710	0.01470
C	-4.28210	0.49790	0.00830
C	-2.93170	0.48250	0.00090
H	-6.10220	1.68880	0.02040
H	-4.81770	-0.44430	0.00940
H	-2.29350	-0.39230	-0.00440
C	-2.97130	2.96710	0.00680
C	-0.89100	3.42320	-0.00200
C	-0.97680	1.99340	-0.00560
C	1.20420	1.58690	-0.01850
C	1.47900	3.05630	-0.01490
C	0.34460	4.01800	-0.00670

H	2.06250	0.91470	-0.02490
N	2.66570	3.52990	-0.01760
H	3.38220	2.79380	-0.02380
C	0.55930	5.48290	-0.00620
H	1.61790	5.73510	0.02070
H	0.09250	5.91490	-0.89990
H	0.03990	5.92490	0.85200
C	-5.14460	4.26650	0.02010
H	-4.44920	5.10660	0.01400
H	-5.79120	4.34330	-0.85860
H	-5.77490	4.34320	0.91040
N	0.02620	1.06750	-0.01360
N	-2.28450	1.71100	0.00030
N	-2.14690	3.98370	0.00560

ArNHOH

Atom	X	Y	Z
C	-4.41010	2.95220	0.01460
C	-5.05930	1.74790	0.00080
C	-4.35430	0.50310	-0.02600
C	-2.99580	0.49560	-0.03900
H	-6.14600	1.73350	0.00980
H	-4.89490	-0.43550	-0.03610
H	-2.36430	-0.38500	-0.05940
C	-2.97980	2.93610	0.00180
C	-0.89290	3.37830	-0.00930
C	-0.97860	1.97230	-0.03300
C	1.22410	1.65080	-0.06200

C	1.44620	3.04600	-0.03540
C	0.38420	3.95330	-0.00500
H	2.07070	0.97580	-0.09570
N	2.76220	3.57270	0.04300
H	2.87090	4.36960	-0.58190
C	0.58980	5.43870	0.03760
H	1.27290	5.71540	0.84860
H	1.02060	5.81020	-0.90190
H	-0.36660	5.94270	0.18800
C	-5.09490	4.28500	0.04190
H	-4.81160	4.87840	-0.83340
H	-6.18070	4.16420	0.05620
H	-4.78620	4.85590	0.92350
N	0.01170	1.09900	-0.05820
N	-2.33920	1.69580	-0.02550
N	-2.13830	3.95790	0.01240
O	3.73430	2.63650	-0.36480
H	4.31240	2.55380	0.40740

ArNHOAc

Atom	X	Y	Z
C	-4.14010	2.87350	-0.53410
C	-4.76730	1.65790	-0.54110
C	-4.06890	0.43870	-0.26840
C	-2.73960	0.46700	0.00810
H	-5.83080	1.61340	-0.76040
H	-4.59250	-0.50950	-0.28100
H	-2.11630	-0.39180	0.22760

C	-2.73990	2.89650	-0.24060
C	-0.70090	3.39170	0.14100
C	-0.77620	1.99140	0.26450
C	1.37240	1.73060	0.75580
C	1.58680	3.12380	0.64190
C	0.55140	4.00200	0.32630
H	2.20920	1.08890	1.01630
N	2.88930	3.61870	0.95450
H	2.97200	4.58840	0.64640
C	0.73030	5.48580	0.18320
H	1.00360	5.95020	1.13800
H	1.51530	5.71150	-0.54820
H	-0.20460	5.93590	-0.15580
C	-4.82030	4.17960	-0.81200
H	-4.35270	4.68070	-1.66560
H	-5.88120	4.02740	-1.02370
H	-4.71930	4.85380	0.04450
N	0.19890	1.14340	0.55610
N	-2.10400	1.68000	0.01720
N	-1.92210	3.93490	-0.17260
O	3.87430	2.90180	0.21570
C	4.09090	3.37870	-1.03850
O	3.55010	4.36880	-1.46370
C	5.09830	2.54070	-1.77320
H	5.37880	1.65660	-1.20130
H	4.66910	2.24960	-2.73450
H	5.98340	3.15100	-1.97030

TS-(1a)

Atom	X	Y	Z
H	2.70280	2.53170	1.73070
H	3.81390	3.17540	2.62380
O	3.65960	2.55420	1.89490
H	4.57730	1.28460	1.65970
N	4.29250	-0.52110	0.36190
H	4.56040	-1.36280	0.88130
O	5.17640	0.48860	1.44970
H	5.90840	0.80440	0.88610
C	-2.32690	2.07580	-0.42270
C	-3.38510	1.61760	0.31110
C	-3.24650	0.59440	1.30660
C	-2.03740	0.03810	1.55630
H	-4.37080	2.03830	0.13510
H	-4.11210	0.25670	1.86380
H	-1.82570	-0.74050	2.27910
C	-1.04770	1.48980	-0.15910
C	1.00070	0.91310	-0.11560
C	0.35530	0.11190	0.86650
C	2.18590	-0.96700	1.50110
C	2.95330	-0.25200	0.52840
C	2.36870	0.72530	-0.31800
H	2.68050	-1.70290	2.13460
C	3.13930	1.50940	-1.33020
H	3.91180	0.89410	-1.79670
H	2.46050	1.90170	-2.08970
H	3.63160	2.36630	-0.85210

C	-2.41600	3.13510	-1.47900
H	-2.08480	2.74170	-2.44510
H	-3.44100	3.49760	-1.57670
H	-1.76260	3.97870	-1.23500
N	0.89080	-0.80820	1.67050
N	-0.95950	0.49300	0.82430
N	0.11820	1.75630	-0.72890

TS-(1b)

Atom	X	Y	Z
H	4.87030	-0.79080	-3.09150
H	6.35510	-1.23080	-2.98640
O	5.60400	-0.90230	-2.46840
H	5.89790	0.36450	-1.38300
N	3.88130	-0.09230	-0.39490
H	4.13440	-1.07010	-0.21640
O	5.03180	0.47700	0.88340
C	6.04000	1.06430	0.42480
O	6.41770	1.00070	-0.80840
C	6.89050	1.89850	1.32600
H	6.45840	1.94350	2.32390
H	7.89320	1.46360	1.36480
H	6.97950	2.90110	0.89780
C	-2.37070	3.05470	1.00370
C	-3.35060	2.43780	1.72820
C	-3.19080	1.11990	2.27450
C	-2.04110	0.43140	2.08490
H	-4.28800	2.95890	1.90000

H	-3.99320	0.66650	2.84410
H	-1.81970	-0.56330	2.45200
C	-1.15080	2.33050	0.80240
C	0.78800	1.64030	0.26430
C	0.20000	0.58540	1.01420
C	1.94630	-0.77250	0.89830
C	2.65290	0.19200	0.09970
C	2.07980	1.45780	-0.21720
H	2.43520	-1.71650	1.13790
C	2.80850	2.51930	-0.97000
H	3.43940	3.09130	-0.27700
H	3.45790	2.08990	-1.73640
H	2.09890	3.21590	-1.42010
C	-2.48280	4.42630	0.41090
H	-1.70250	5.08190	0.81010
H	-2.34550	4.38770	-0.67420
H	-3.45920	4.86270	0.62990
N	0.72600	-0.60000	1.34460
N	-1.04110	1.04190	1.35400
N	-0.06490	2.70360	0.14850

σ-TS-(2)

Atom	X	Y	Z
C	4.48540	-2.37220	-1.47450
C	5.29890	-3.53330	-1.18660
N	5.76230	-1.74160	-3.46010
C	4.79670	-1.51540	-2.61550
H	4.19040	-0.62250	-2.76650

N	3.45810	-2.11480	-0.68450
H	2.91000	-1.33650	-1.06730
C	2.31930	-1.85370	2.61060
N	2.73800	-0.79340	1.70740
C	3.92270	-0.74420	1.00070
N	3.97730	0.30610	0.17200
C	2.78090	0.89960	0.29890
C	2.21540	2.02800	-0.41930
O	2.69440	2.69310	-1.30470
N	0.90030	2.29240	0.05750
C	0.22360	1.57580	1.01090
N	0.72360	0.51880	1.62950
C	1.97530	0.23170	1.25350
H	0.44930	3.07750	-0.40400
H	-1.44810	2.80390	0.93990
H	-1.51190	1.46250	2.04090
H	2.17510	-2.77710	2.04290
H	4.77910	-1.32990	1.30440
H	3.07620	-2.00010	3.38290
H	1.37870	-1.55240	3.07180
N	-1.02450	1.96690	1.31250
C	5.02870	-4.41930	-0.02130
H	5.71250	-5.26880	-0.02430
H	5.15340	-3.86450	0.91630
H	3.99250	-4.77080	-0.04490
N	7.27430	-4.74730	-2.13840
C	6.32570	-3.75460	-2.08510
C	6.48220	-2.84220	-3.16960

C	7.99100	-4.46650	-3.20500
N	7.54370	-3.30400	-3.87460
C	8.13330	-2.80210	-5.02100
C	9.19760	-3.47030	-5.51980
C	9.68960	-4.65810	-4.87470
C	9.12120	-5.16770	-3.74420
H	7.68750	-1.90260	-5.42750
H	9.68120	-3.10130	-6.41640
H	10.54700	-5.16360	-5.30940
C	9.59060	-6.39850	-3.03110
H	9.87110	-6.16120	-2.00020
H	8.78980	-7.14310	-2.98320
H	10.45110	-6.83450	-3.54180

π-TS-(2)

Atom	X	Y	Z
C	-3.24190	1.12170	-1.89590
C	-4.29680	0.53970	-1.24580
C	-4.15550	-0.65700	-0.47030
C	-2.94740	-1.26190	-0.35420
H	-5.28170	0.99150	-1.32770
H	-5.01820	-1.09520	0.01760
H	-2.73720	-2.17370	0.19240
C	-1.96540	0.48330	-1.77520
C	0.08370	-0.10030	-1.84030
C	-0.56120	-1.05750	-1.02640
C	1.25830	-2.22630	-0.54890
C	2.09170	-1.29660	-1.30850

C	1.47160	-0.19810	-2.02070
H	1.75000	-3.07260	-0.06780
N	3.41460	-1.38270	-1.29660
H	3.70670	-2.24270	-0.81600
C	2.22550	0.66280	-2.96910
H	3.30130	0.55120	-2.83810
H	1.95760	0.34810	-3.98710
H	1.93000	1.71220	-2.87770
C	-3.36080	2.33780	-2.77020
H	-2.38930	2.81580	-2.91120
H	-3.72230	2.04810	-3.76290
H	-4.06990	3.05610	-2.35190
N	-0.03150	-2.13100	-0.40780
N	-1.87560	-0.68450	-0.99920
N	-0.80070	0.83990	-2.29420
C	3.00030	-1.63940	2.23230
N	2.97780	-0.51270	1.30950
C	3.97440	-0.13230	0.42020
N	3.68180	1.02300	-0.20510
C	2.42370	1.26400	0.12190
C	1.53490	2.35160	-0.28970
O	1.75100	3.25740	-1.05050
N	0.26620	2.20590	0.32970
C	-0.11000	1.19410	1.16810
N	0.70670	0.23520	1.59490
C	1.92610	0.30400	1.06730
H	-0.42020	2.88520	0.01080
H	-2.02830	1.92820	1.41170

H	-1.64040	0.47040	2.26200
H	3.36770	-2.53430	1.72380
H	4.97610	-0.53550	0.49440
H	3.64560	-1.41280	3.08320
H	1.98000	-1.81130	2.57860
N	-1.39270	1.15600	1.55950
