Supporting Information

Examination of Pyridazine as a Possible Scaffold for Nucleophilic Catalysis

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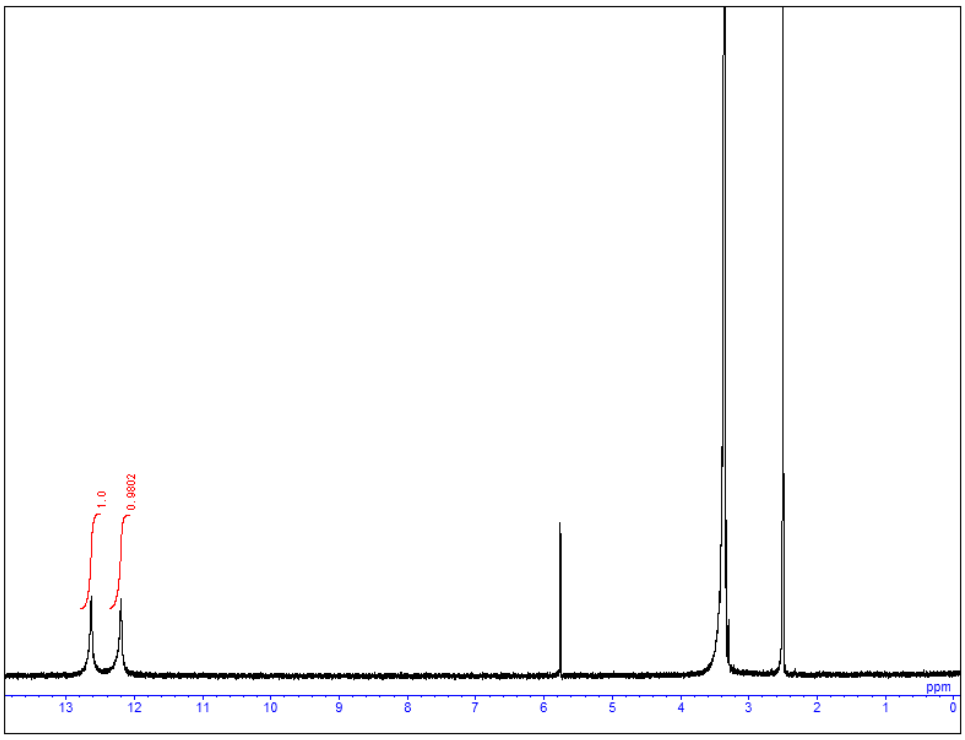
Contents

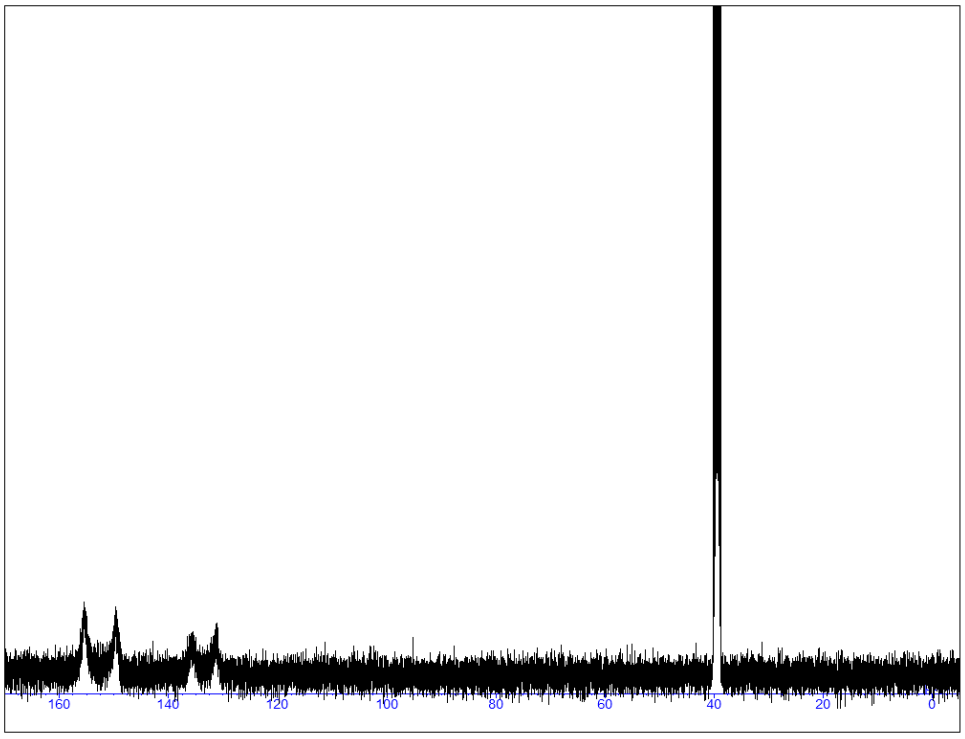
1. ^{1}H NMR and ^{13}C NMR Spectra.

1-1. 4,5-Dichloro-6-hydroxypyridazin-3(2*H*)-one (**13**).

^{1}H NMR (DMSO-d_6)

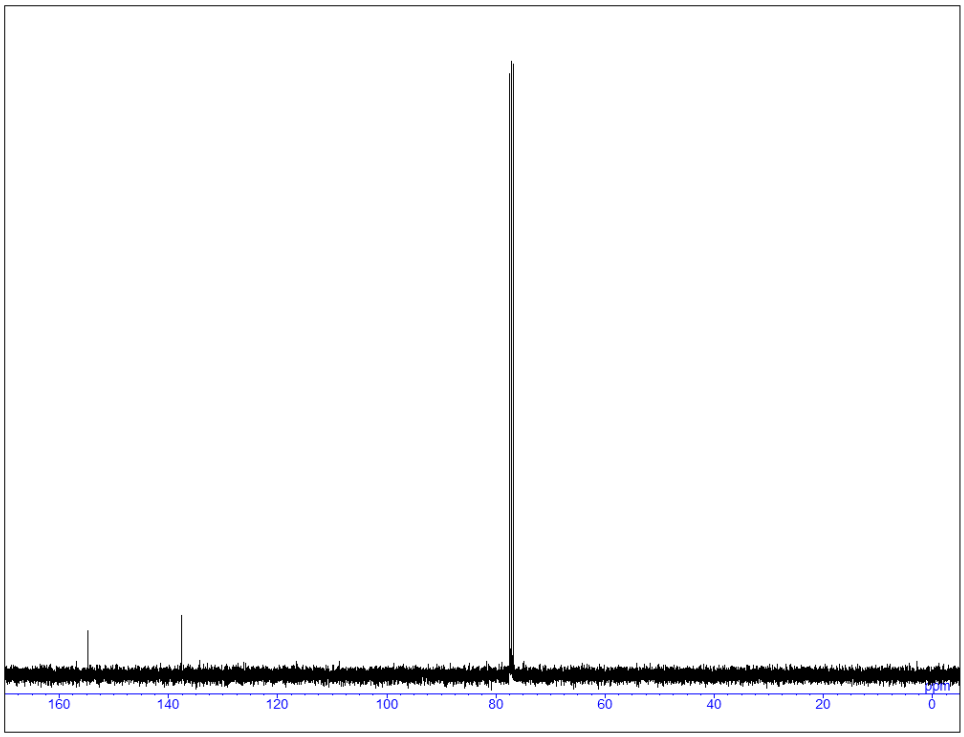


^{13}C NMR (DMSO-d_6)



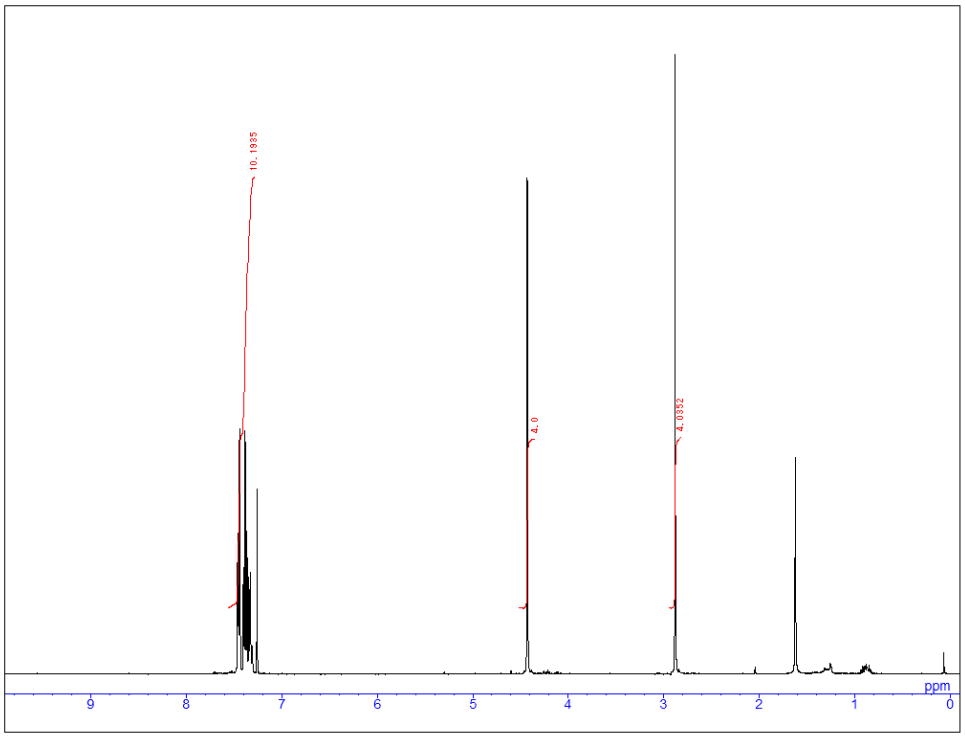
1-2. Tetrachloropyridazine (**14**).

^{13}C NMR ($CDCl_3$)

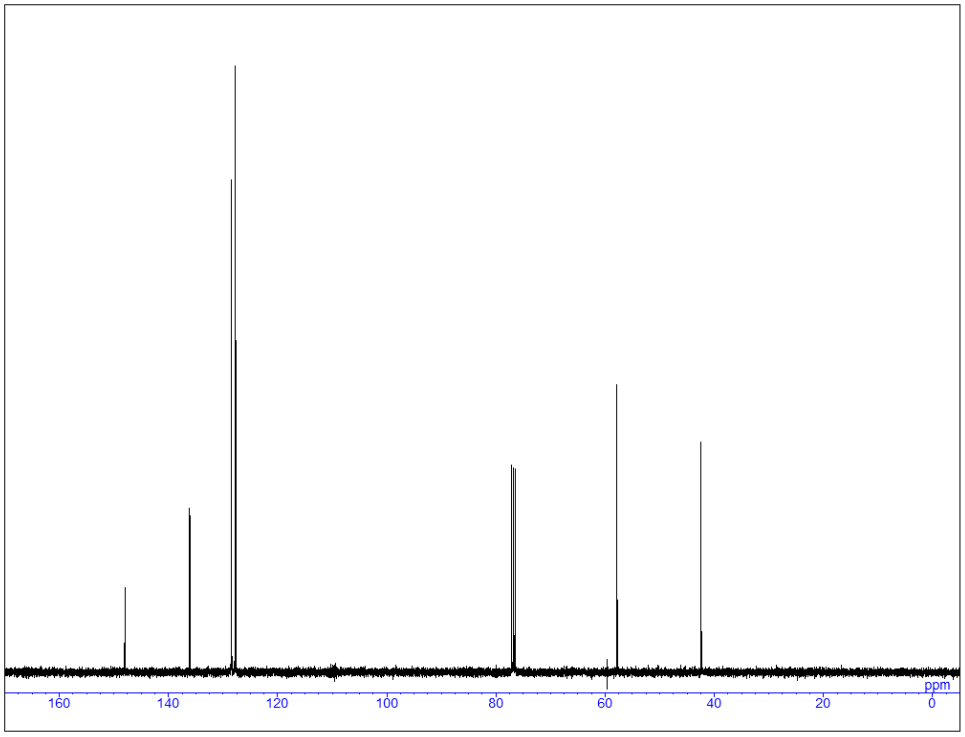


1-3. 1,4-Bis(phenylmethyl)-5,8-dichloro-1,2,3,4-tetrahydropyrazino[2,3-d]pyridazine (**15b**).

^{1}H NMR ($CDCl_3$)

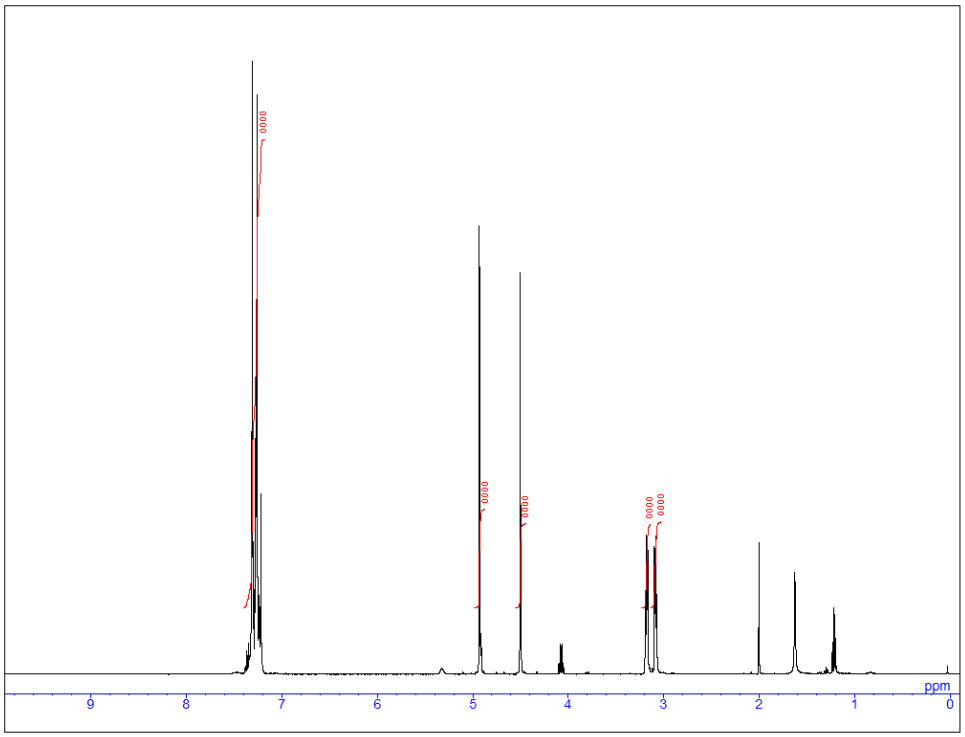


^{13}C NMR ($CDCl_3$)

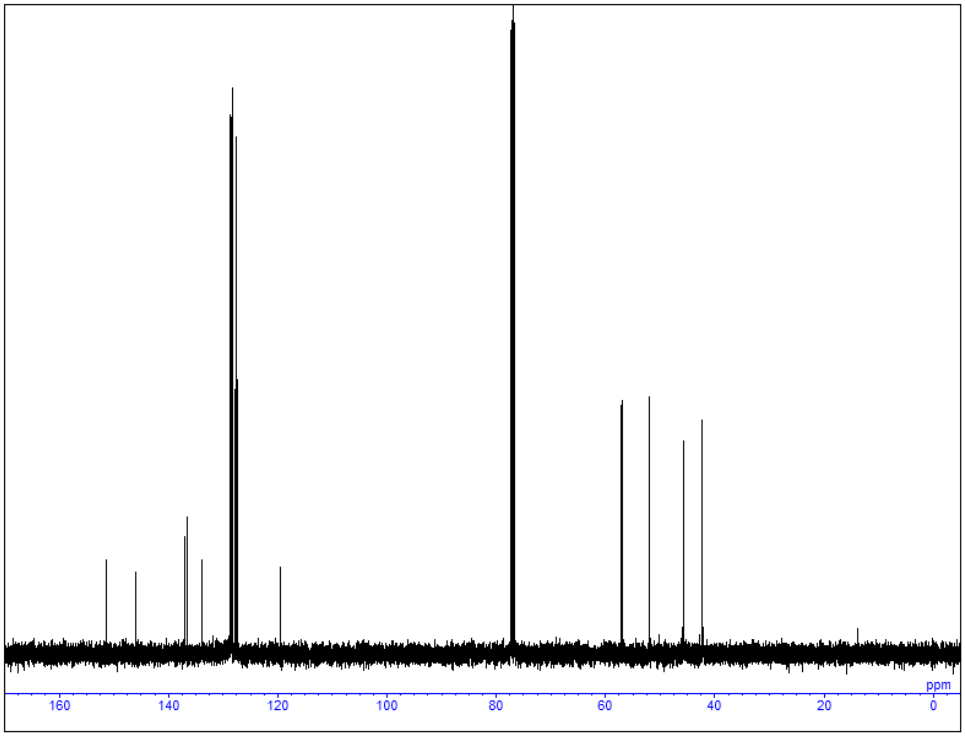


1-4. 5,8-Bis(phenylmethyl)-3,4-dichloro-5,6,7,8-tetrahydropyrazino[2,3-c]pyridazine (**15b′**).

^{1}H NMR ($CDCl_3$)

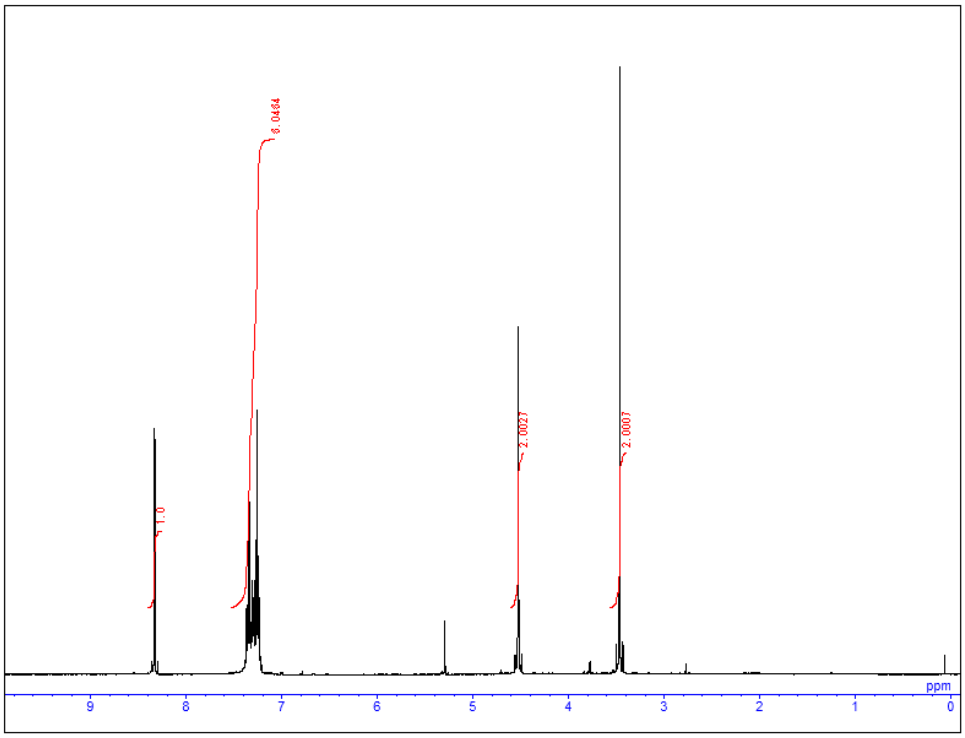


^{13}C NMR ($CDCl_3$)

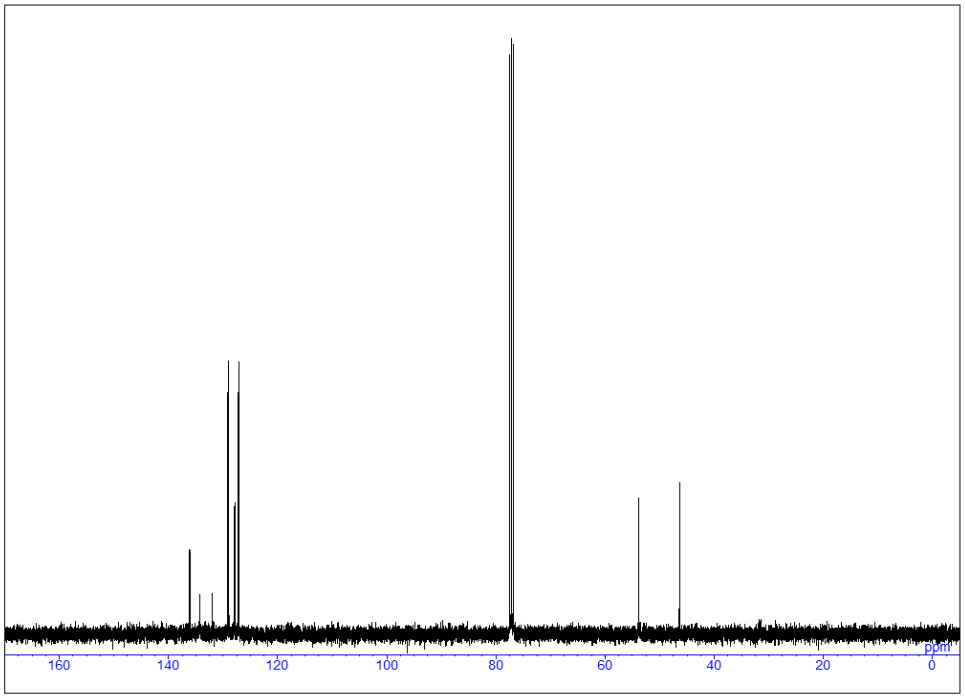


1-5. 1,4-Bis(phenylmethyl)-1,2,3,4-tetrahydropyrazino[2,3-d]pyridazine (**11b**).

^{1}H NMR ($CDCl_3$)

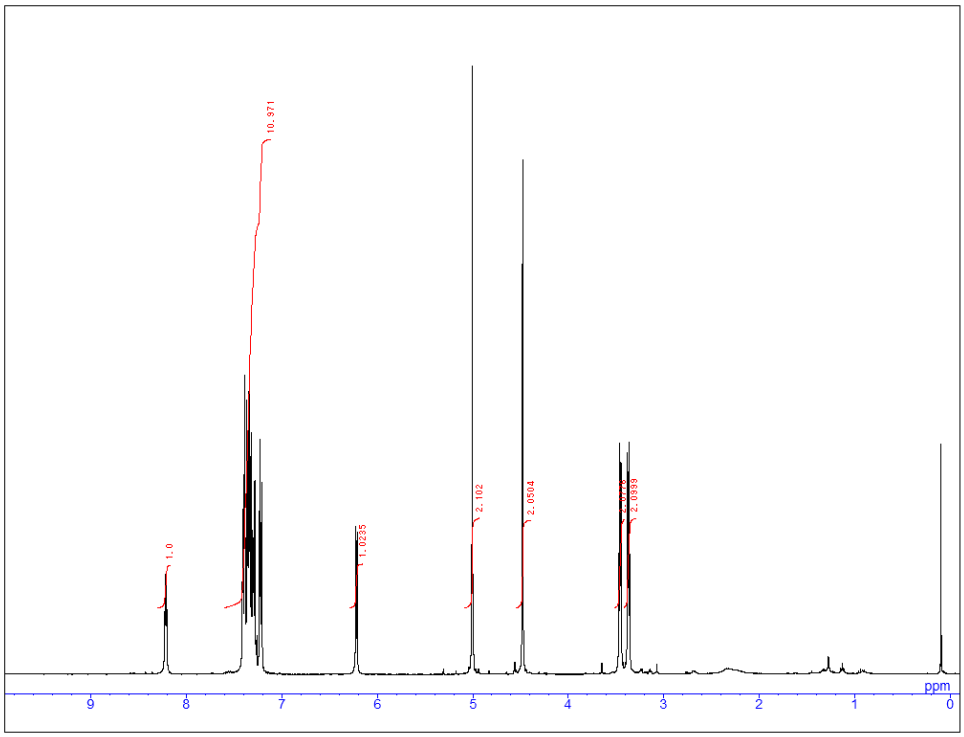


^{13}C NMR ($CDCl_3$)

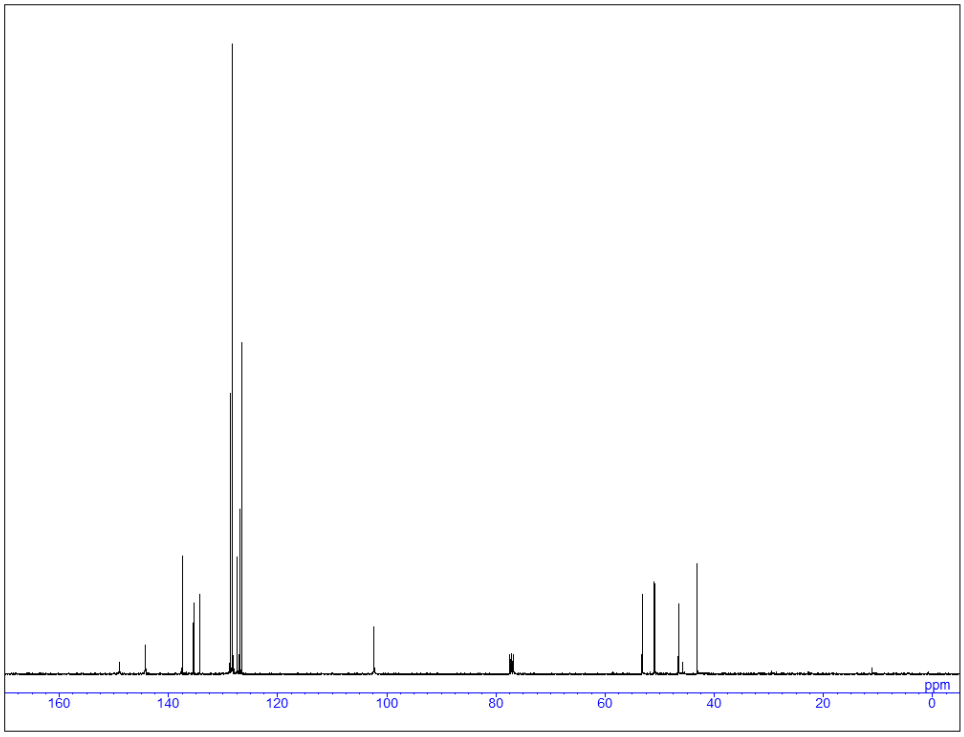


1-6. 5,8-Bis(phenylmethyl)-5,6,7,8-tetrahydropyrazino[2,3-c]pyridazine (**11b′**).

^{1}H NMR ($CDCl_3$)

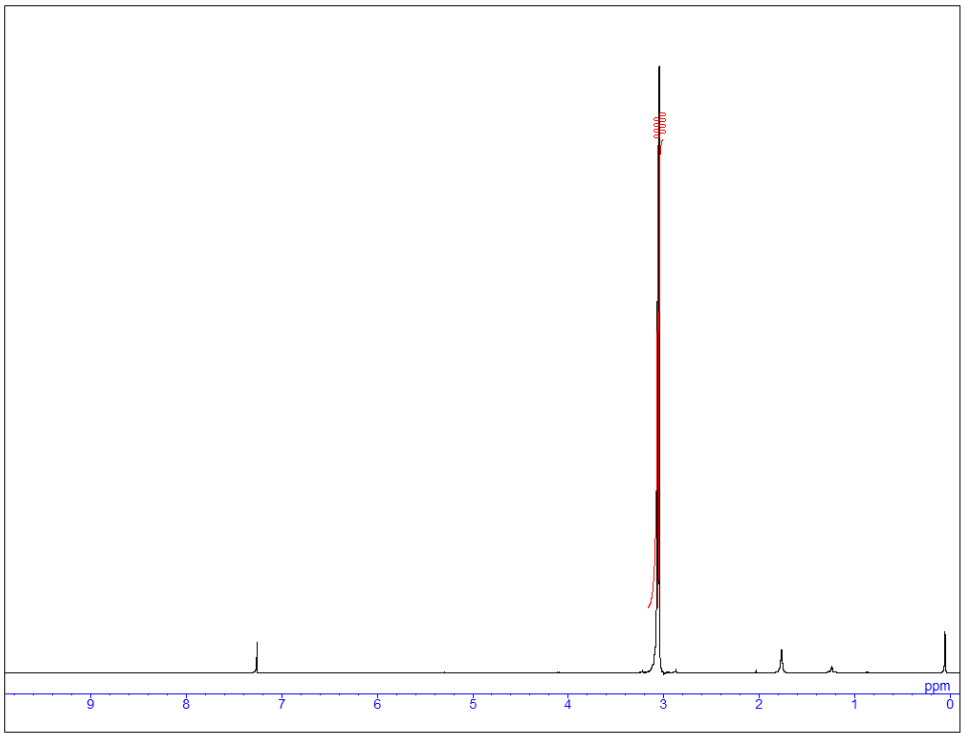


^{13}C NMR ($CDCl_3$)

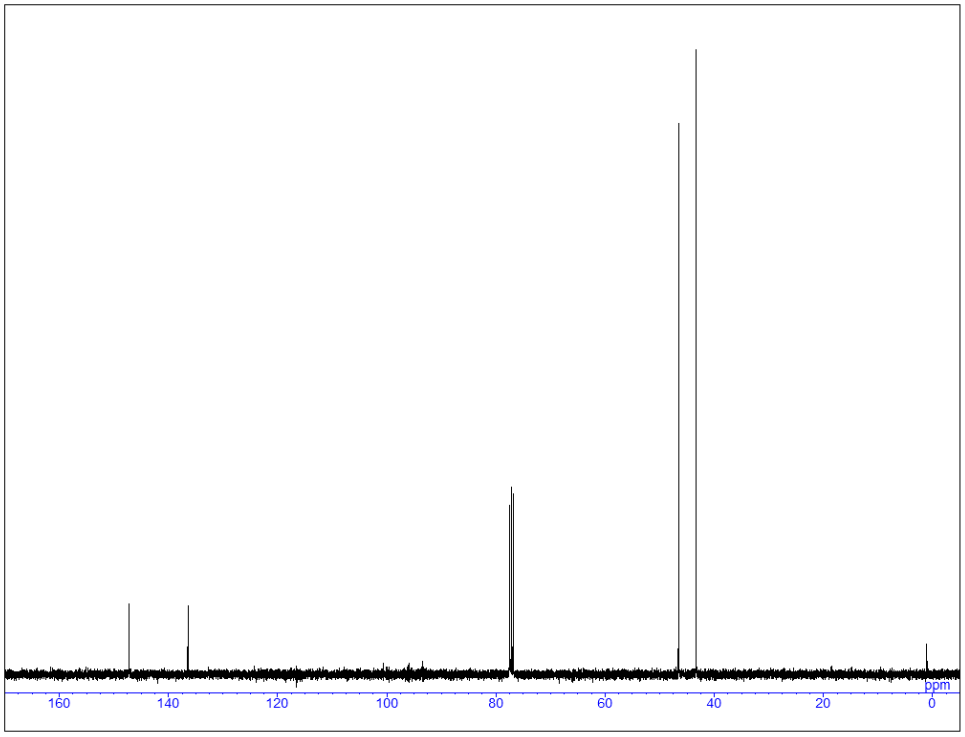


1-7. 5,8-Dichloro-1,4-dimethyl-1,2,3,4-tetrahydropyrazino[2,3-d]pyridazine (**15a**).

^{1}H NMR ($CDCl_3$)

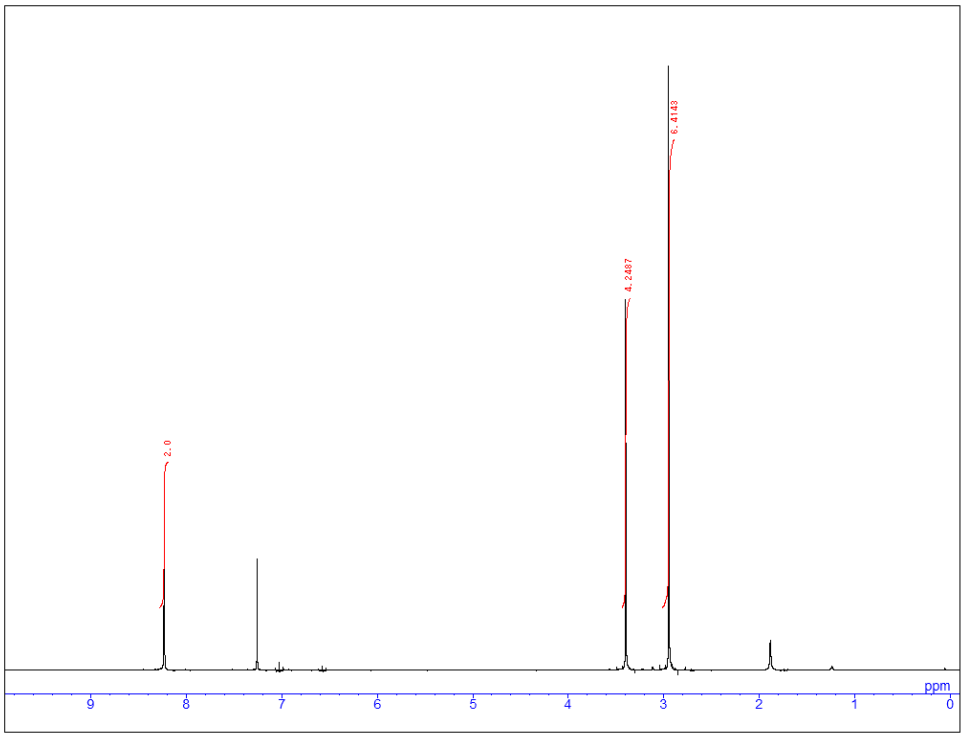


^{13}C NMR ($CDCl_3$)

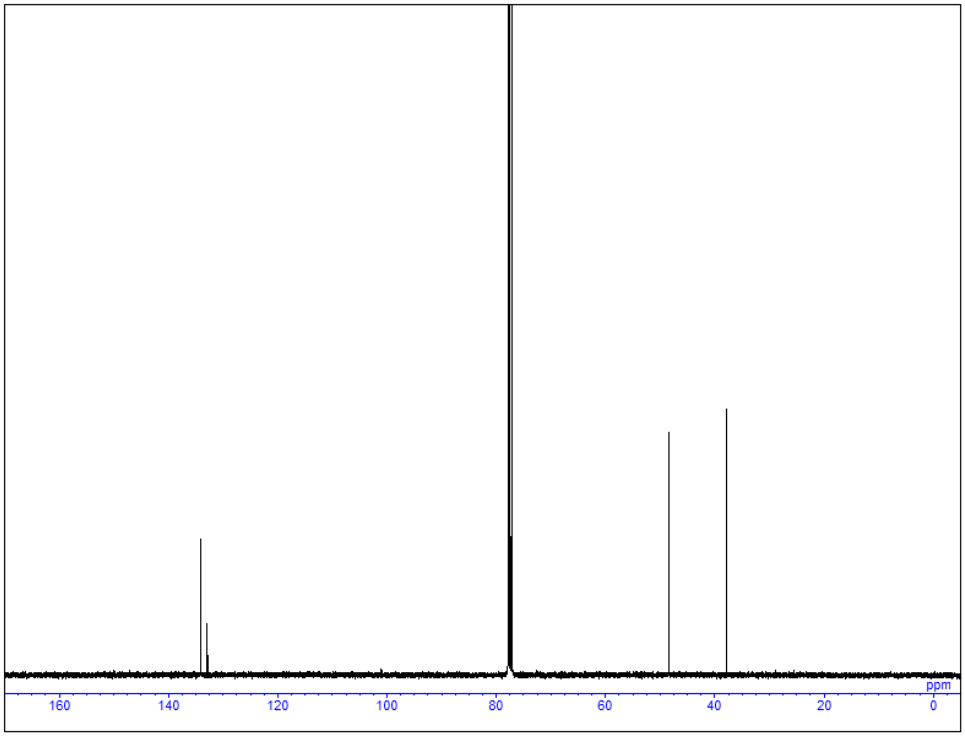


1-8. 1,4-Dimethyl-1,2,3,4-tetrahydropyrazino[2,3-d]pyridazine (**11a**).

^{1}H NMR ($CDCl_3$)

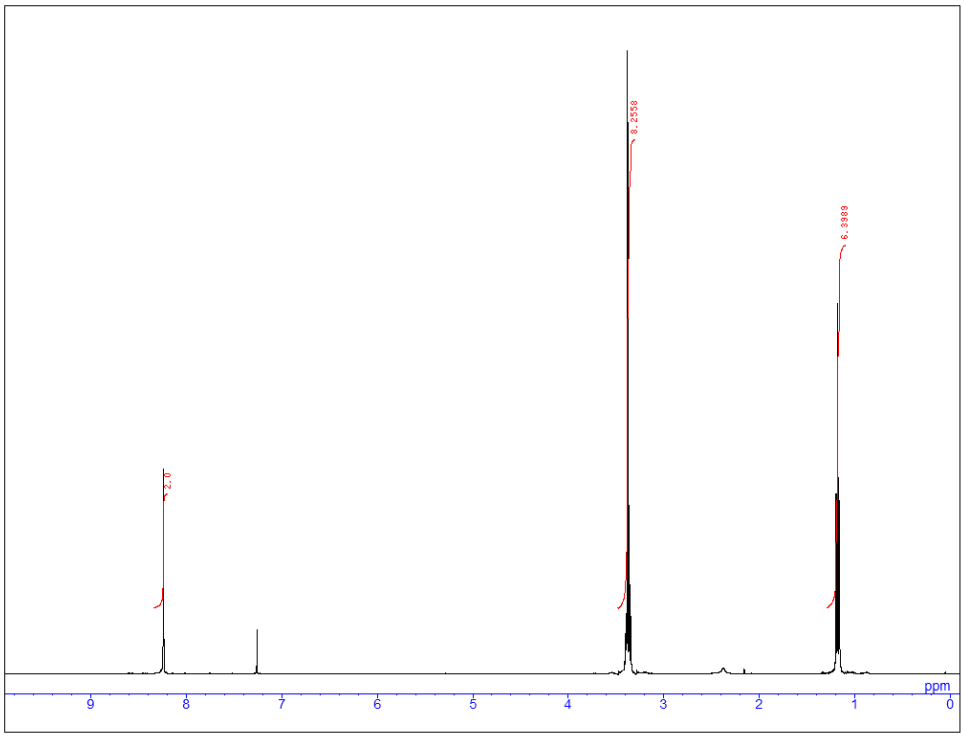


^{13}C NMR ($CDCl_3$)

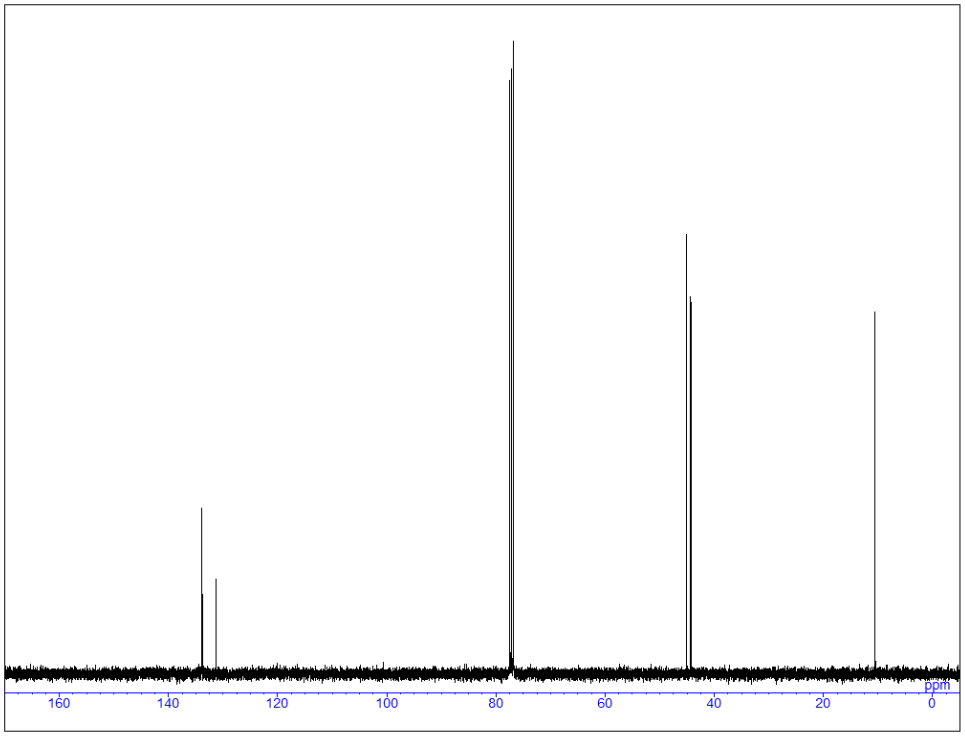


1-9. 1,4-Diethyl-1,2,3,4-tetrahydropyrazino[2,3-d]pyridazine (**11c**).

^{1}H NMR ($CDCl_3$)

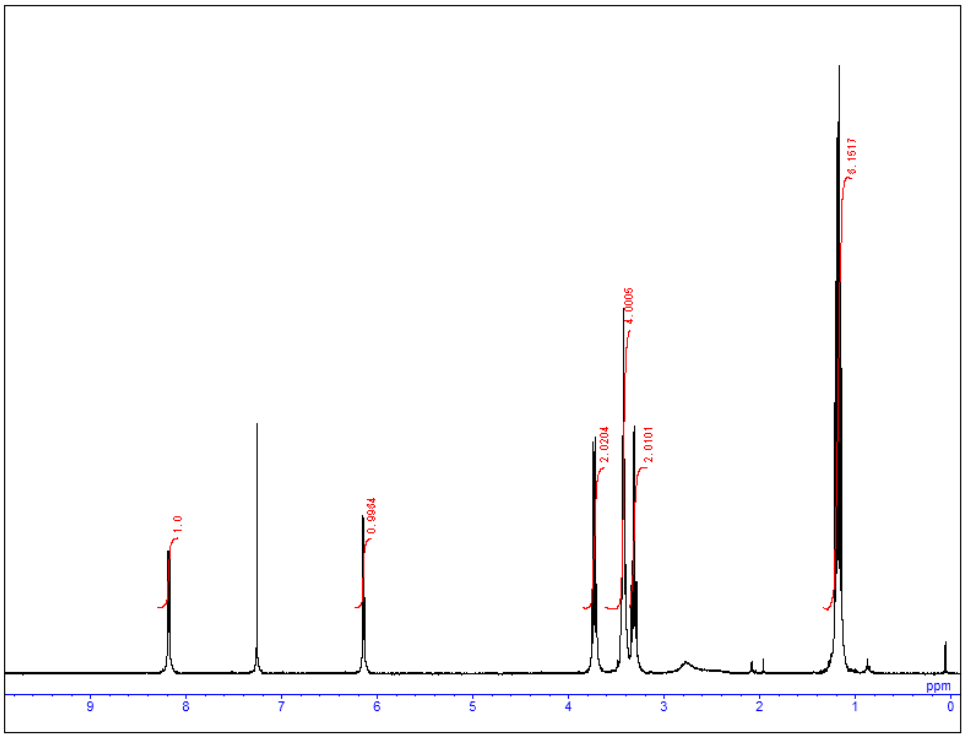


^{13}C NMR ($CDCl_3$)

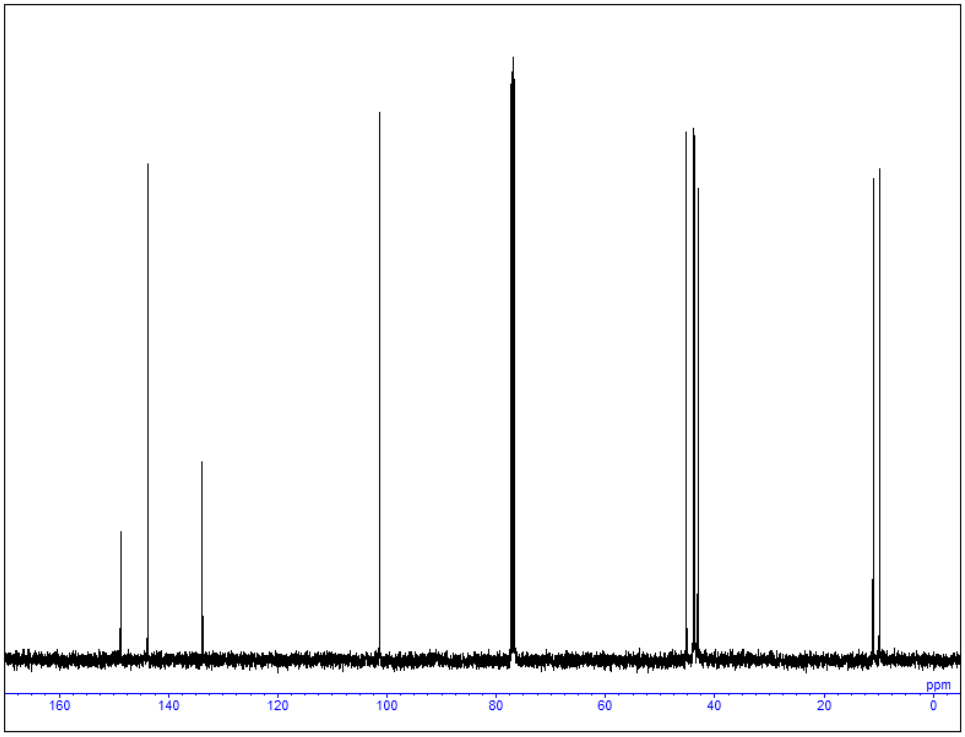


1-10. 5,8-Diethyl-5,6,7,8-tetrahydropyrazino[2,3-c]pyridazine (**11c′**).

^{1}H NMR ($CDCl_3$)

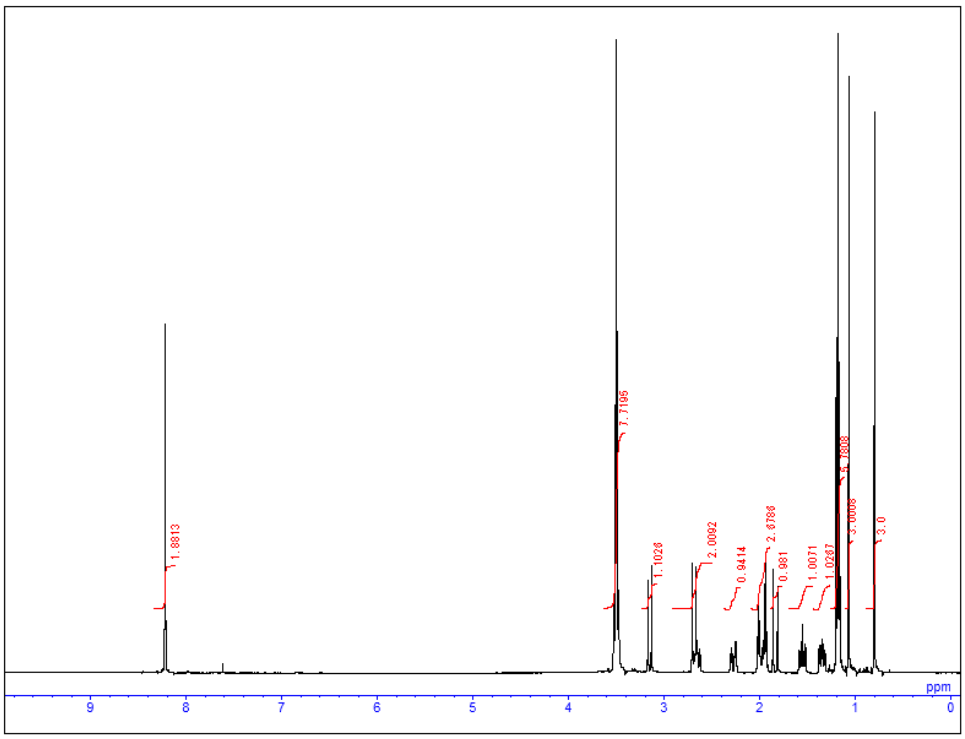


^{13}C NMR ($CDCl_3$)

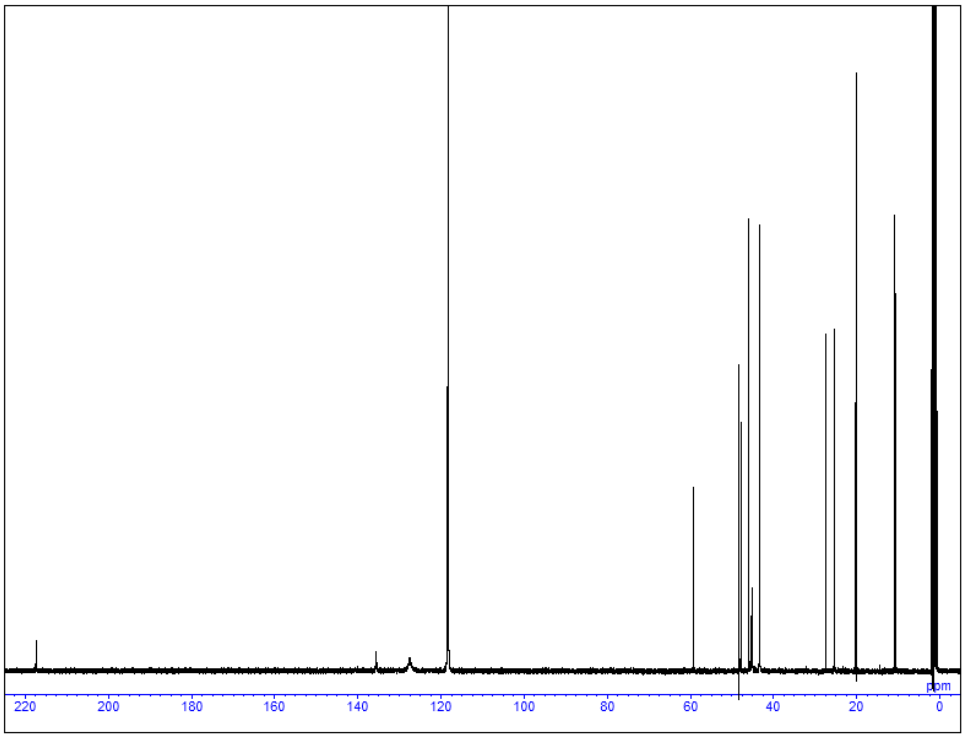


1-11. 1,4-Diethyl-1,2,3,4-tetrahydropyrazino[2,3-d]pyridazin-6-ium ((1R,4R)-7,7-dimethyl-2-oxobicyclo[2.2.1]heptan-1-yl)methanesulfonate (**11c-CSA**).

^{1}H NMR (CD_3CN)

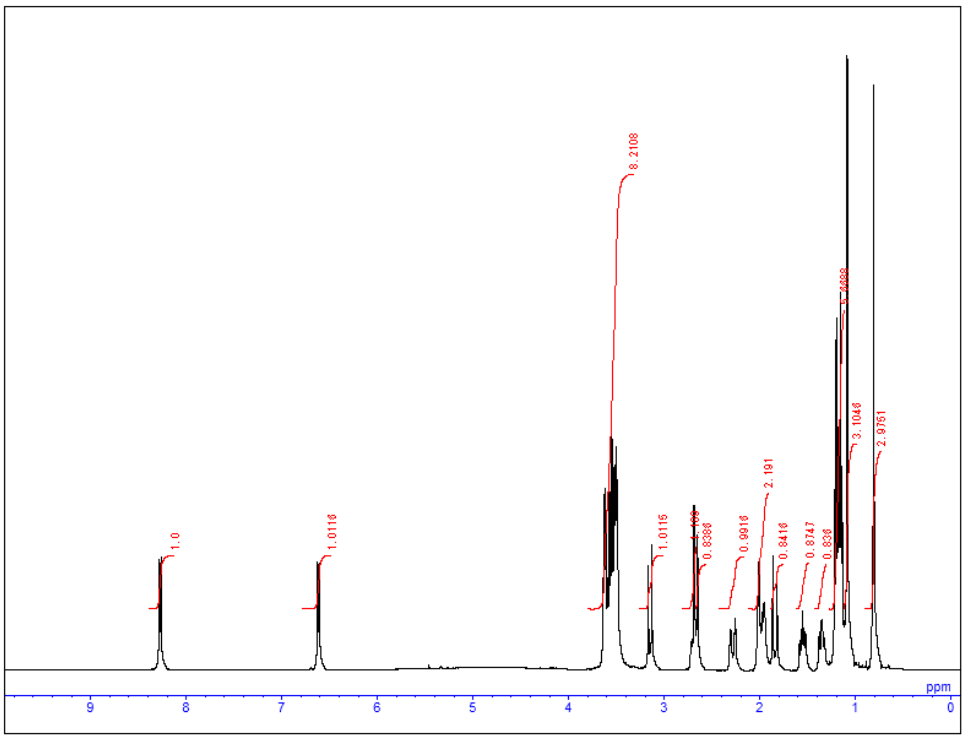


^{13}C NMR (CD_3CN)

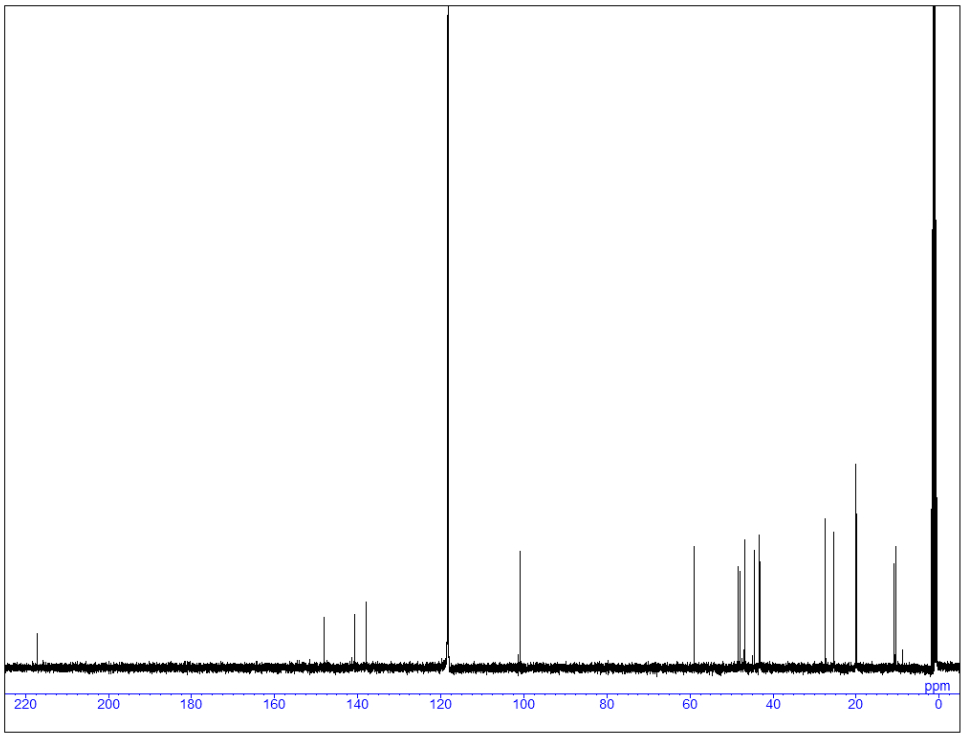


1-12. 5,8-Diethyl-5,6,7,8-tetrahydropyrazino[2,3-c]pyridazin-1-ium ((1R,4R)-7,7-dimethyl-2-oxobicyclo[2.2.1]heptan-1-yl)methanesulfonate (**11c′-CSA**)

^{1}H NMR (CD_3CN)

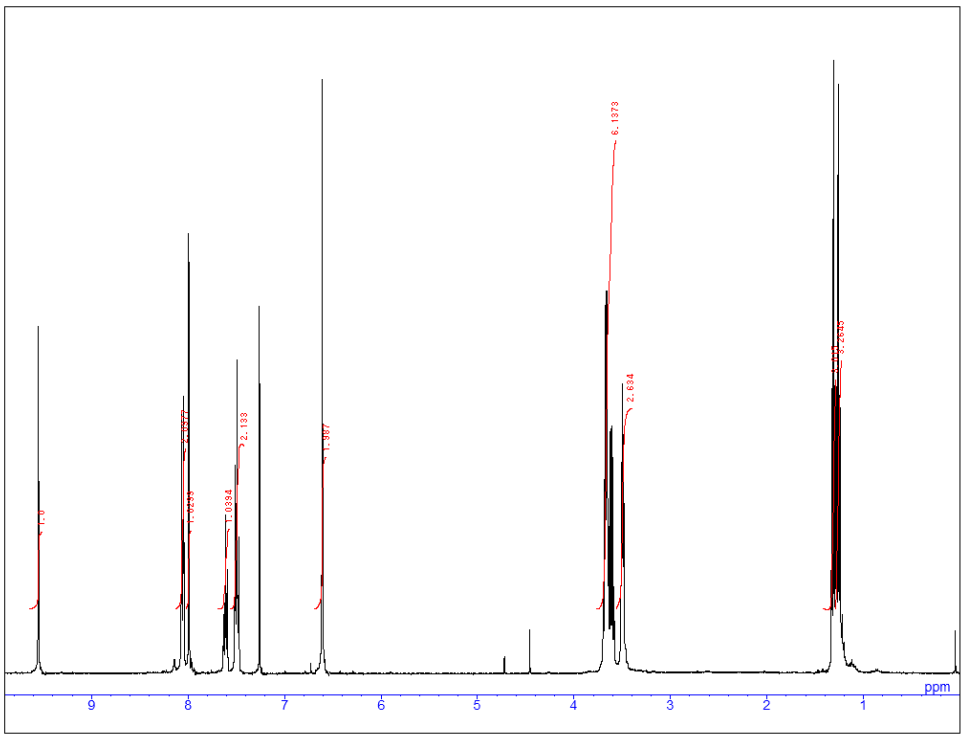


^{13}C NMR (CD_3CN)

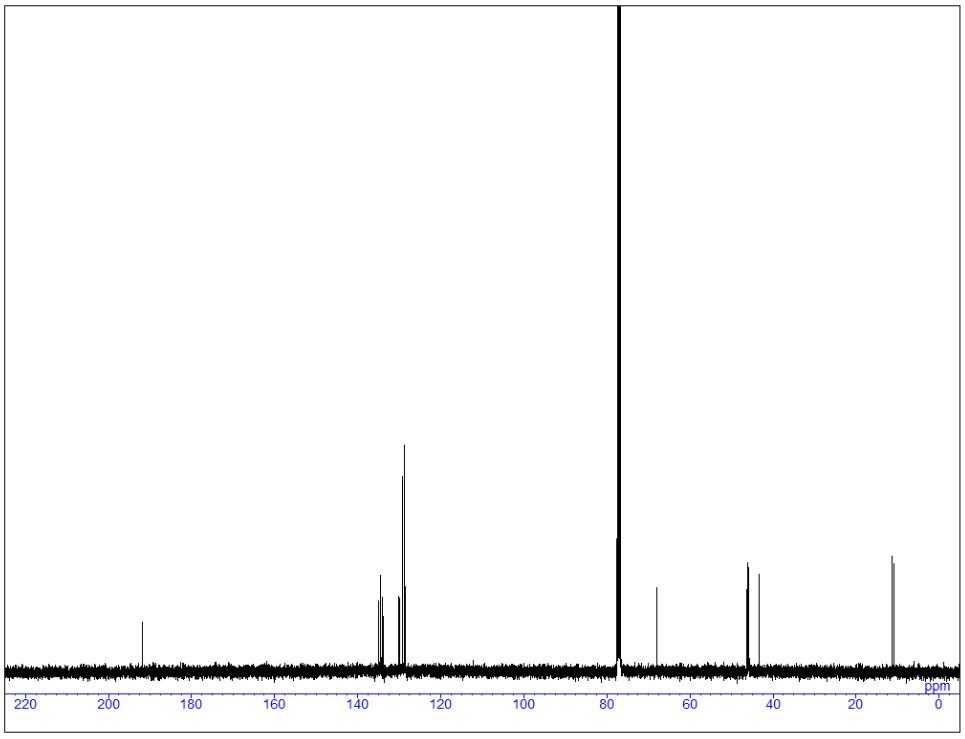


1-13. 1,4-Diethyl-6-(2-oxo-2-phenylethyl)-1,2,3,4-tetrahydropyrazino[2,3-d]pyridazin-6-ium bromide (**11c-phen**$^{+}$).

^{1}H NMR ($CDCl_3$)

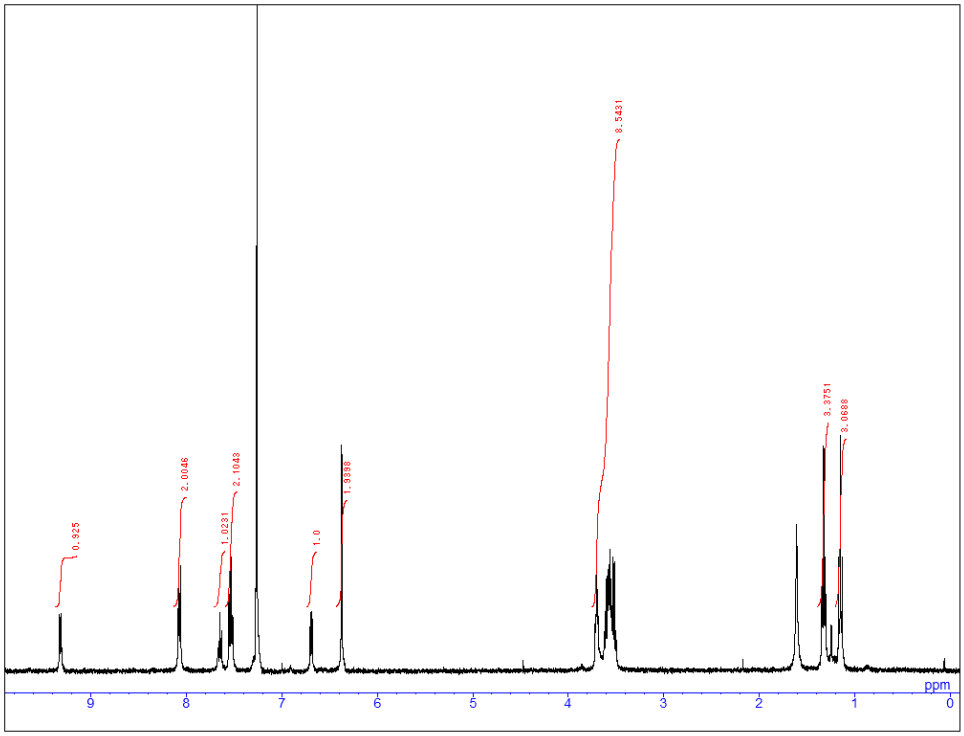


^{13}C NMR ($CDCl_3$)

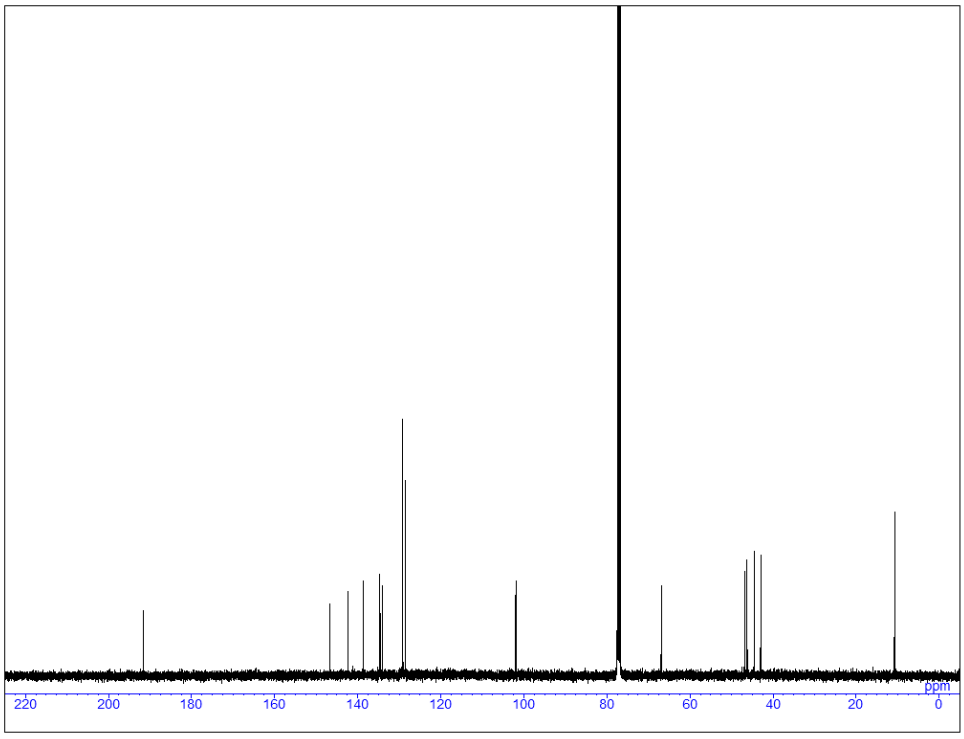


1-14. 5,8-Diethyl-2-(2-oxo-2-phenylethyl)-5,6,7,8-tetrahydropyrazino[2,3-c]pyridazin-2-ium bromide (**11c′-phen**$^{+}$).

^{1}H NMR ($CDCl_3$)

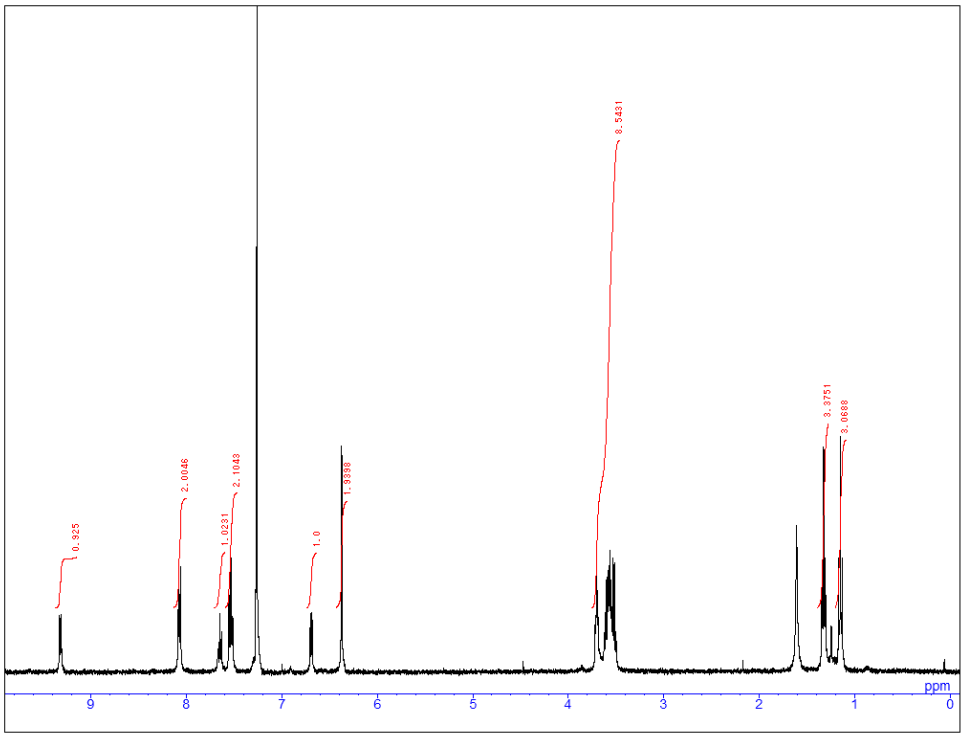


^{13}C NMR ($CDCl_3$)

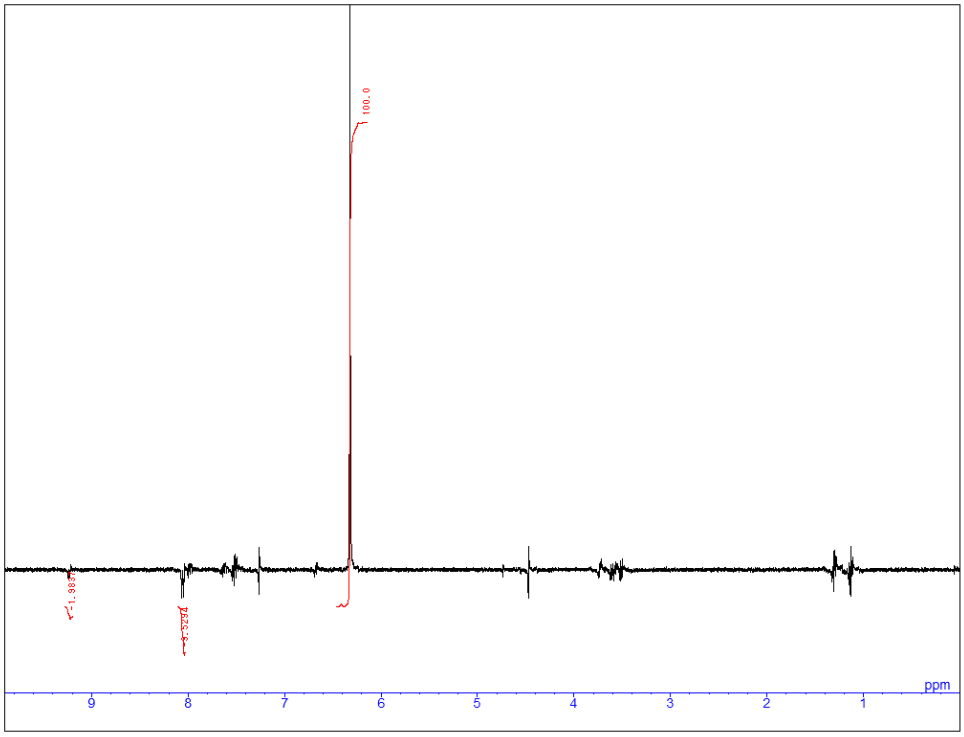


1-15. ^{1}H NMR and DIFNOE spectra of **11c′-phen**$^+$.

^{1}H NMR ($CDCl_3$)

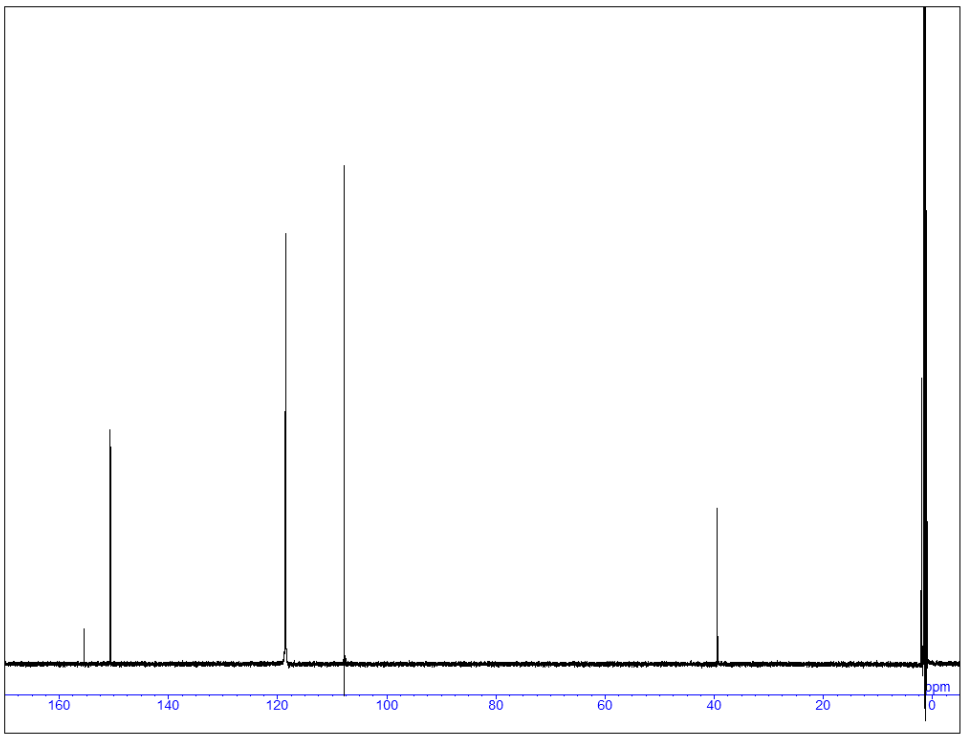


DIFNOE ($CDCl_3$)

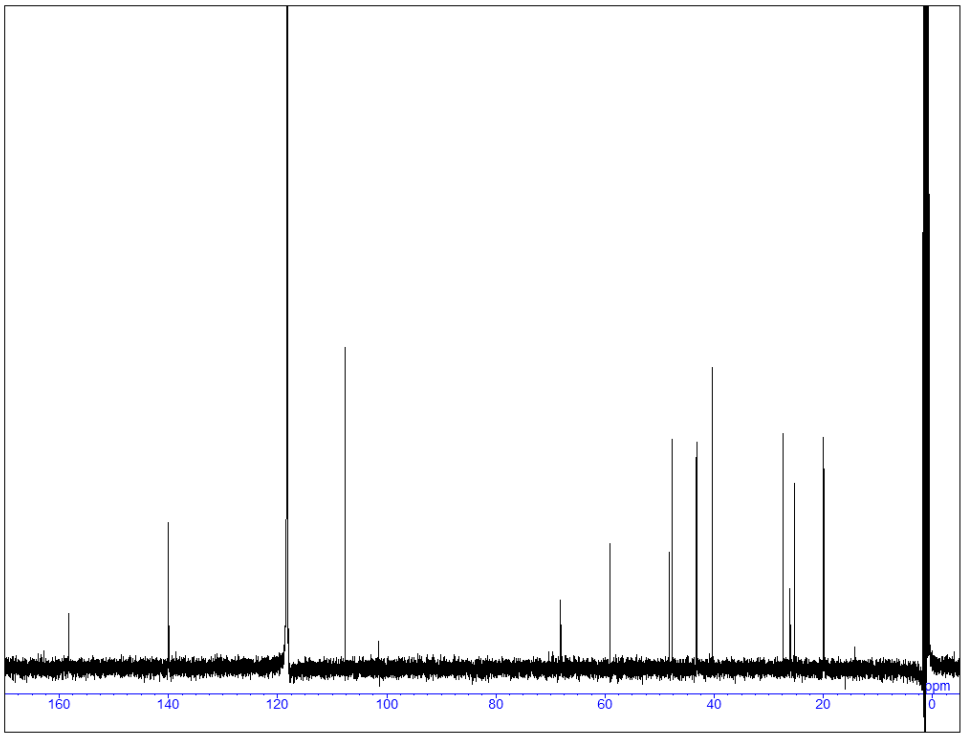


1-16. DMAP (**2**) (upper spectrum) and its CSA salt (**2-CSA**) (lower spectrum) for basicity determination by interpolation.

DMAP. ^{13}C NMR ($CDCl_3$)



DMAP-CSA: ^{13}C NMR ($CDCl_3$)



2. X-Ray Crystallography Measurement Details.

Crystals suitable for X-ray structure determination were mounted on a CCD diffractometer and irradiated with graphite monochromated Mo-Kα radiation (λ = 0.71073 Å) at 173 K for data collection. The structures were solved by a direct method using the the SHELX-97 program.[1] Refinement on F^2 was carried out using full-matrix least-squares with the SHELX-97 program.[1] All non-hydrogen atoms were refined using anisotropic thermal parameters. All hydrogen atoms were placed at calculated positions, and refined applying riding models. Selected crystallographic parameters are summarized in Table S1.

Crystallographic data have been deposited with the Cambridge Crystallographic Data Centre: Deposit number is CCDC-1468108 for **11c-phen**$^+$. Copies of the data can be obtained free of charge via http://www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge, CB2 1EZ, UK; Fax: +44 1223 336033; e-mail: deposit@ccdc.cam.ac.uk).

Table S1. Crystal data and structure refinement for **11c-phen**$^+$.

Empirical formula	C18 H23 Br N4 O	
Formula weight	391.31	
Color	Colorless	
Habit	Plates	
Method for obtaining crystals	Recrystallization from hexane-CH_2Cl_2	
Measurement temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 14.289(3) Å	α= 61.452(2)°.
	b = 15.287(3) Å	β= 88.618(3)°.
	c = 15.562(3) Å	γ = 80.588(3)°.
Volume	2940.2(11) Å^3	
Z	6	
Density (calculated)	1.326 Mg/m^3	
Absorption coefficient	2.108 mm^{-1}	
F(000)	1212	
Crystal size	0.100 x 0.071 x 0.010 mm^3	
Theta range for data collection	1.447 to 25.413°.	
Index ranges	-17<=h<=16, -18<=k<=18, -18<=l<=16	
Reflections collected	14280	
Independent reflections	10554 [R(int) = 0.0303]	
Completeness to theta = 25.242°	97.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.979 and 0.863	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10554 / 0 / 665	
Goodness-of-fit on F^2	1.040	
Final R indices [I>2sigma(I)]	R1 = 0.0709, wR2 = 0.1692	
R indices (all data)	R1 = 0.1343, wR2 = 0.2018	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.540 and -1.049 e.Å^{-3}	

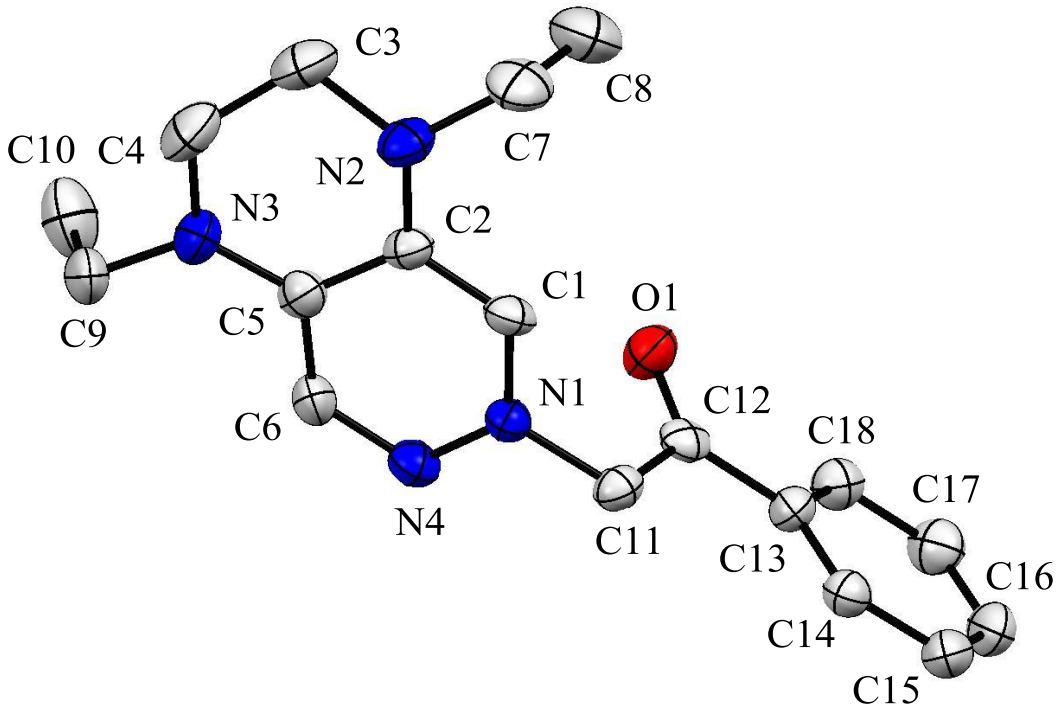


Figure S1. ORTEP drawing of one of three independent molecules of **11c-phen**$^{+}$ shown with thermal ellipsoids at the 50% probability level. Hydrogen atoms and the bromide (counteranion) have been omitted for clarity. Differences in structural parameters of all three molecules were practically within margin of error. Selected bond distances [Å] and angles [°] for the depicted molecule: N(1)-N(4) 1.332(7), N(1)-C(1) 1.346(8), N(1)-C(11) 1.462(8), C(1)-C(2) 1.368(9), N(2)-C(2) 1.363(8), C(2)-C(5) 1.425(9), N(3)-C(5) 1.348(8), N(4)-C(6) 1.329(8), C(5)-C(6) 1.413(9), N(4)-N(1)-C(1) 124.6(5), N(4)-N(1)-C(11) 114.6(5), C(1)-N(1)-C(11) 120.3(5), N(1)-C(1)-C(2) 120.9(6), C(2)-N(2)-C(3) 116.8(6), C(2)-N(2)-C(7) 119.1(6), C(3)-N(2)-C(7) 117.3(6), N(2)-C(2)-C(1) 122.8(6), N(2)-C(2)-C(5) 120.1(6), C(1)-C(2)-C(5) 117.1(6), C(5)-N(3)-C(9) 123.1(6), C(5)-N(3)-C(4) 119.6(6), C(9)-N(3)-C(4) 117.2(6), N(2)-C(3)-C(4) 111.8(6), C(6)-N(4)-N(1) 116.1(5), N(3)-C(4)-C(3) 111.0(6), N(3)-C(5)-C(6) 122.8(6), N(3)-C(5)-C(2) 120.7(6), C(6)-C(5)-C(2) 116.5(6), N(4)-C(6)-C(5) 124.4(6).

3. Resonance Structures.

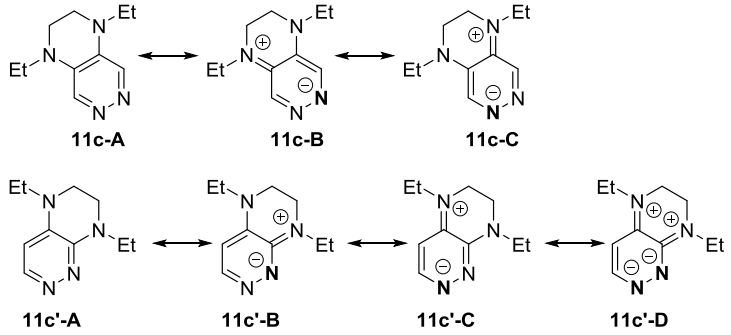


Figure S2. Resonance structures that put negative charge on aromatic ring nitrogen atoms. The upper set is for symmetric **11c** and the lower set is for unsymmetric **11c′**. The extra resonance structure **11c′-D** of the lower set suggests that unsymmetric **11c′** should be more basic and nucleophilic than symmetric **11c**.

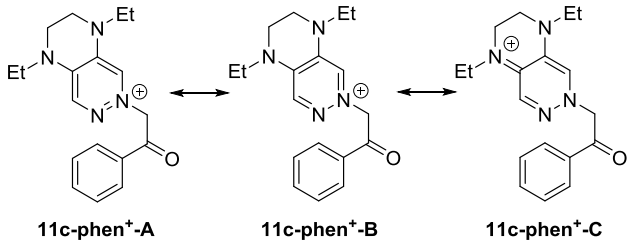


Figure S3. Important resonance structures for **11c-phen**$^{+}$.

4. Structural Optimization and Molecular Orbitals.

Table S2. Calibrated total electronic energies of structurally optimized species (kJ/mol)[a]

method	B3LYP-6-31G(d)	B3LYP-6-31G(d)	B3LYP-6-31G(d)	B3LYP-cc-pVTZ
solvent		PhH	CHCl3	
9	-693691.1298	-693701.3386	-693707.6053	-693933.8982
10a	-1045251.048	-1045260.888	-1045269.863	-1045619.448
11a'	-1393732.782	-1393747.231	-1393756.4	-1394212.865
11a	-1393710.671	-1393728.168	-1393738.8	-1394190.08
6a	-1351648.715	-1351659.403	-1351666.051	-1352116.588
2	-1003199.195	-1003208.373	-1003214.071	-1003556.347
1	-651643.7464	-651649.1382	-651652.4494	-651874.5366
1-Ac$^+$	-1053253.644	-1053372.454	-1053417.106	
2-Ac+	-1404891.869	-1404995.376	-1405039.213	
6a-Ac+ (s-trans)	-1753364.401	-1753463.29	-1753505.165	
6a-Ac+ (s-cis)	-1753367.661	-1753465.302	-1753506.558	
11a-Ac+v(s-trans)	-1795440.824	-1795539.534	-1795581.51	
11a-Ac+ (s-cis)	-1795405.927	-1795510.502	-1795556.728	
11a'-Ac+ (s-trans)	-1795464.328	-1795563.851	-1795606.347	
11a'-Ac+ (s-cis)	-1795439.196	-1795541.243	-1795586.047	
10a-Ac+ (s-trans)	-1446952.458	-1447057.552	-1447102.265	
10a-Ac+ (s-cis)	-1446922.213	-1447033.033	-1447081.457	
9-Ac+ (s-trans)	-1095305.055	-1095420.952	-1095470.086	
9-Ac+ (s-cis)	-1095274.961	-1095395.778	-1095448.338	
method	MP2-6-31G(d)	MP2-6-31G(d)	MP2-6-31G(d)	
solvent		PhH	CHCl3	
9	-691557.8908	-691569.0488	-691575.8601	
10a	-1041909.474	-1041925.637	-1041934.206	
11a'	-1389291.089	-1389306.184	-1389322.584	
11a	-1389275.099	-1389293.332	-1389304.28	
6a	-1347242.724	-1347253.899	-1347260.807	
2	-999885.7504	-999895.1016	-999900.8382	
1	-649538.9482	-649544.7953	-649548.367	
1-Ac$^+$	-1049969.518	-1050083.409	-1050131.382	
2-Ac+	-1400395.966	-1400499.21	-1400542.541	
6a-Ac+ (s-trans)	-1747773.075	-1747871.183	-1747912.681	
6a-Ac+ (s-cis)	-1747776.567	-1747873.187	-1747913.86	
11a-Ac+v(s-trans)	-1789823.437	-1789920.823	-1789961.966	
11a-Ac+ (s-cis)	-1789787.585	-1789891.747	-1789937.007	
11a'-Ac+ (s-trans)	-1789843.454	-1789941.309	-1789982.66	
11a'-Ac+ (s-cis)	-1789818.631	-1789918.46	-1789961.866	
10a-Ac+ (s-trans)	-1442427.195	-1442531.679	-1442575.894	
10a-Ac+ (s-cis)	-1442396.772	-1442506.617	-1442554.225	
9-Ac+ (s-trans)	-1091993.69	-1092109.877	-1092158.452	
9-Ac+ (s-cis)	-1091965.025	-1092084.799	-1092136.5	

[a]Scaled zero-point energies are included.

Table S3. MO orbital energies in atomic units[a]

9	method	B3LYP-6-31G(d)	B3LYP-6-31G(d)	B3LYP-6-31G(d)	B3LYP-cc-pVTZ	MP2-6-31G(d)	MP2-6-31G(d)	MP2-6-31G(d)
	solvent		C6H6	CHCl3			C6H6	CHCl3
	LUMO+1	−0. 029	−0. 029	−0. 029	−0. 041	0. 120	0. 121	0. 121
	LUMO	−0. 051	−0. 052	−0. 052	−0. 062	0. 091	0. 091	0. 090
	HOMO	−0. 234	−0. 238	−0. 241	−0. 242	−0. 380	−0. 381	−0. 381
	HOMO-1	−0. 295	−0. 295	−0. 295	−0. 304	−0. 399	−0. 399	−0. 399
	HOMO-2	−0. 309	−0. 308	−0. 308	−0. 318	−0. 405	−0. 409	−0. 412
	HOMO-3	−0. 310	−0. 313	−0. 315	−0. 319	−0. 475	−0. 477	−0. 478
	HOMO-4	−0. 416	−0. 414	−0. 413	−0. 422	−0. 568	−0. 570	−0. 572
10a	method	B3LYP-6-31G(d)	B3LYP-6-31G(d)	B3LYP-6-31G(d)	B3LYP-cc-pVTZ	MP2-6-31G(d)	MP2-6-31G(d)	MP2-6-31G(d)
	solvent		C6H6	CHCl3			C6H6	CHCl3
	LUMO+1	−0. 005	−0. 007	−0. 009	−0. 017	0. 136	0. 134	0. 133
	LUMO	−0. 024	−0. 027	−0. 029	−0. 035	0. 112	0. 108	0. 106
	HOMO	−0. 217	−0. 218	−0. 217	−0. 225	−0. 321	−0. 320	−0. 319
	HOMO-1	−0. 220	−0. 225	−0. 229	−0. 228	−0. 376	−0. 379	−0. 381
	HOMO-2	−0. 280	−0. 283	−0. 285	−0. 289	−0. 394	−0. 401	−0. 405
	HOMO-3	−0. 290	−0. 295	−0. 299	−0. 299	−0. 451	−0. 451	−0. 451
	HOMO-4	−0. 324	−0. 324	−0. 325	−0. 333	−0. 459	−0. 463	−0. 465
11a'	method	B3LYP-6-31G(d)	B3LYP-6-31G(d)	B3LYP-6-31G(d)	B3LYP-cc-pVTZ	MP2-6-31G(d)	MP2-6-31G(d)	MP2-6-31G(d)
	solvent		C6H6	CHCl3			C6H6	CHCl3
	LUMO+1	0. 011	0. 008	0. 006	−0. 002	0. 152	0. 149	0. 147
	LUMO	−0. 013	−0. 015	−0. 018	−0. 023	0. 118	0. 114	0. 112
	HOMO	−0. 191	−0. 192	−0. 193	−0. 200	−0. 287	−0. 289	−0. 290
	HOMO-1	−0. 209	−0. 217	−0. 222	−0. 217	−0. 346	−0. 348	−0. 349
	HOMO-2	−0. 235	−0. 235	−0. 236	−0. 243	−0. 382	−0. 389	−0. 394
	HOMO-3	−0. 287	−0. 292	−0. 295	−0. 296	−0. 422	−0. 424	−0. 426
	HOMO-4	−0. 299	−0. 301	−0. 303	−0. 308	−0. 448	−0. 450	−0. 452
						−0. 461	−0. 466	−0. 468
11a	method	B3LYP-6-31G(d)	B3LYP-6-31G(d)	B3LYP-6-31G(d)	B3LYP-cc-pVTZ	MP2-6-31G(d)	MP2-6-31G(d)	MP2-6-31G(d)
	solvent		C6H6	CHCl3			C6H6	CHCl3
	LUMO+1	0. 004	0. 002	0. 000	−0. 007	0. 142	0. 139	0. 137
	LUMO	−0. 009	−0. 013	−0. 015	−0. 020	0. 123	0. 118	0. 115
	HOMO	−0. 193	−0. 193	−0. 192	−0. 202	−0. 292	−0. 290	−0. 289
	HOMO-1	−0. 208	−0. 216	−0. 222	−0. 216	−0. 343	−0. 346	−0. 348
	HOMO-2	−0. 237	−0. 238	−0. 239	−0. 245	−0. 387	−0. 395	−0. 400
	HOMO-3	−0. 283	−0. 289	−0. 293	−0. 292	−0. 426	−0. 425	−0. 425
	HOMO-4	−0. 296	−0. 297	−0. 298	−0. 304	−0. 451	−0. 455	−0. 458
6a	method	B3LYP-6-31G(d)	B3LYP-6-31G(d)	B3LYP-6-31G(d)	B3LYP-cc-pVTZ	MP2-6-31G(d)	MP2-6-31G(d)	MP2-6-31G(d)
	solvent		C6H6	CHCl3			C6H6	CHCl3
	LUMO+1	0. 020	0. 017	0. 014	0. 005	0. 158	0. 154	0. 152
	LUMO	0. 011	0. 007	0. 005	−0. 003	0. 144	0. 140	0. 137
	HOMO	−0. 179	−0. 180	−0. 181	−0. 188	−0. 275	-0.276	−0. 278
	HOMO-1	−0. 218	−0. 220	−0. 221	−0. 227	−0. 320	−0. 323	−0. 325
	HOMO-2	−0. 232	−0. 239	−0. 244	−0. 240	−0. 398	−0. 404	−0. 408
	HOMO-3	−0. 279	−0. 280	−0. 281	−0. 288	−0. 411	−0. 412	−0. 412
	HOMO-4	−0. 307	−0. 310	−0. 312	−0. 317	−0. 437	−0. 440	−0. 442
2	method	B3LYP-6-31G(d)	B3LYP-6-31G(d)	B3LYP-6-31G(d)	B3LYP-cc-pVTZ	MP2-6-31G(d)	MP2-6-31G(d)	MP2-6-31G(d)
	solvent		C6H6	CHCl3			C6H6	CHCl3
	LUMO+1	0. 008	0. 005	0. 003	−0. 004	0. 147	0. 144	0. 142
	LUMO	0. 005	0. 003	0. 001	−0. 009	0. 145	0. 141	0. 139
	HOMO	−0. 207	−0. 206	−0. 207	−0. 216	−0. 311	−0. 312	−0. 312
	HOMO-1	−0. 239	−0. 245	−0. 249	−0. 248	−0. 338	−0. 341	−0. 343
	HOMO-2	−0. 248	−0. 251	−0. 253	−0. 258	−0. 404	−0. 410	−0. 414
	HOMO-3	−0. 306	−0. 308	−0. 309	−0. 316	−0. 433	−0. 435	−0. 436
	HOMO-4	−0. 344	−0. 345	−0. 346	−0. 350	−0. 492	−0. 493	−0. 493
1	method	B3LYP-6-31G(d)	B3LYP-6-31G(d)	B3LYP-6-31G(d)	B3LYP-cc-pVTZ	MP2-6-31G(d)	MP2-6-31G(d)	MP2-6-31G(d)
	solvent		C6H6	CHCl3			C6H6	CHCl3
	LUMO+1	−0. 009	−0. 010	−0. 011	−0. 023	0. 138	0. 137	0. 137
	LUMO	−0. 022	−0. 024	−0. 024	−0. 036	0. 121	0. 119	0. 118
	HOMO	−0. 253	−0. 256	−0. 258	−0. 262	−0. 343	−0. 344	−0. 344
	HOMO-1	−0. 261	−0. 262	−0. 263	−0. 272	−0. 377	−0. 378	−0. 379
	HOMO-2	−0. 286	−0. 287	−0. 287	−0. 297	−0. 413	−0. 417	−0. 419
	HOMO-3	−0. 364	−0. 364	−0. 363	−0. 371	−0. 515	−0. 515	−0. 515
	HOMO-4	−0. 394	−0. 396	−0. 397	−0. 406	−0. 533	−0. 535	−0. 537

[a]Values with a purple background correspond to those of MOs of essentially $N_{lonepair}$ character. Values with a blue background correspond to those of MOs of essentially $N_{lonepair}$-$N_{lonepair}$ bonding character, whereas those with a red background correspond to those of MOs of essentially $N_{lonepair}$-$N_{lonepair}$ anti-bonding character,

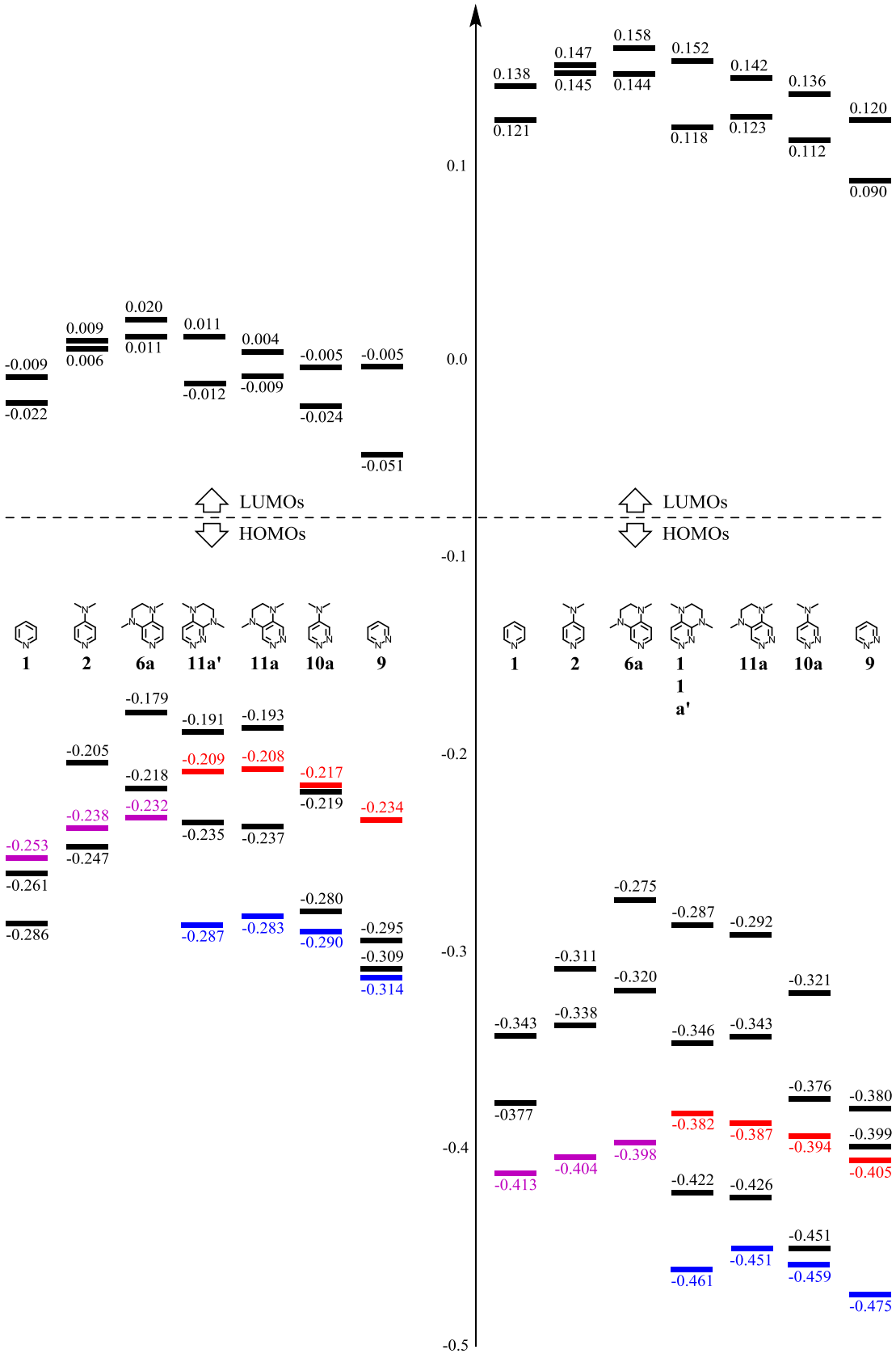


Figure S4. Energy levels of the molecular orbitals of pyridine and pyridazine derivatives calculated at the RB3LYP/6-31G(d) (left) and RMP2/6-31G(d) (right) level of theory. The levels correspond to LUMO+1 down to HOMO-2, HOMO-3 or HOMO-4 from top to bottom. As for the colors of the levels and values, black, purple, blue, and red denote π-type orbitals, nitrogen lone pair orbitals, nitrogen lone pair bonding combination orbitals, and nitrogen lone pair anti-bonding combination orbitals, respectively.

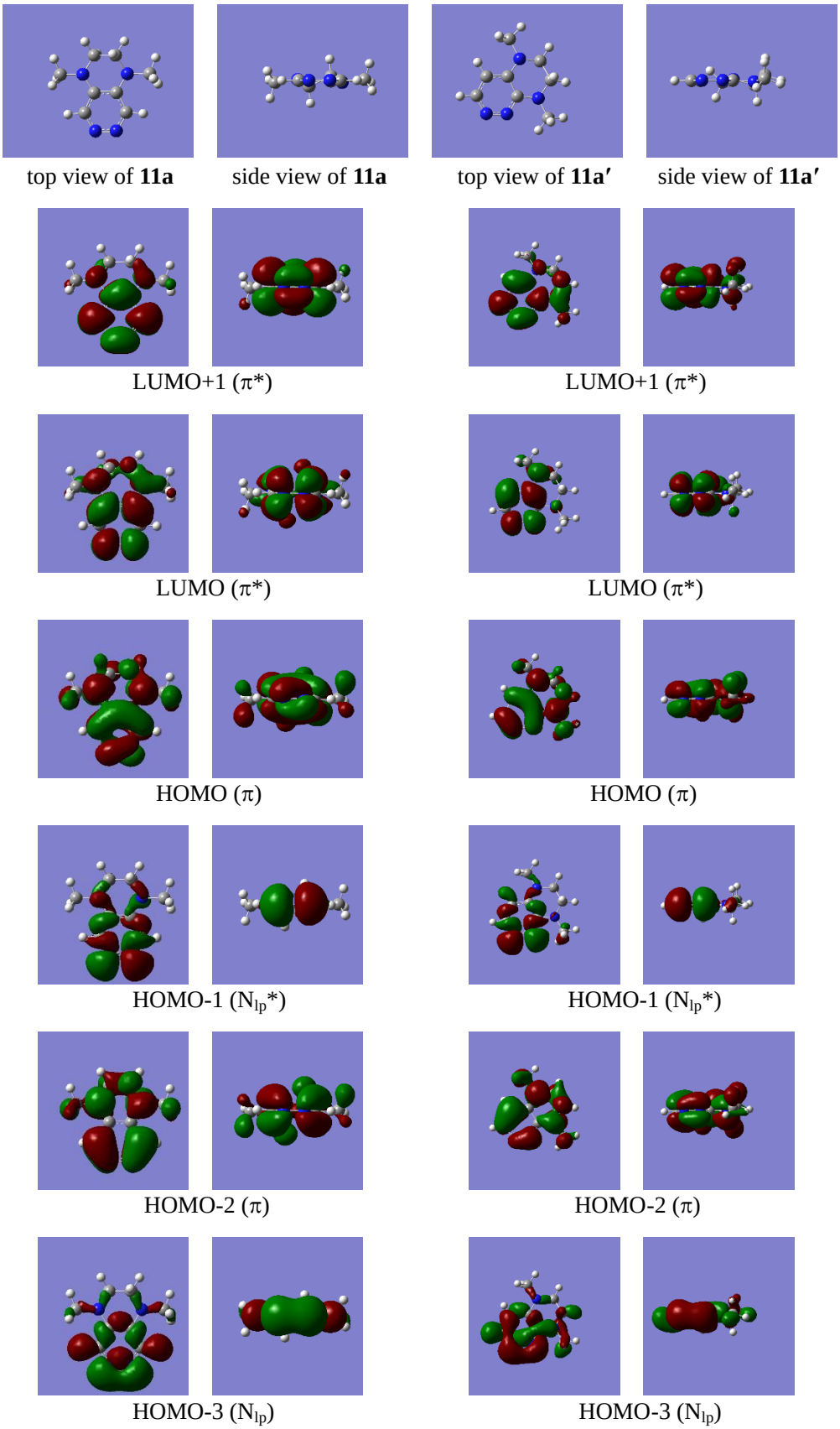


Figure S5. Molecular orbital diagrams of symmetric **11a** (left) and unsymmetric **11a′** (right) from RB3LYP/6-31G(d) calculations. Although the order of energy levels (π-type and N_{lp}-type) differ with the method used for the calculations, the orbital profiles according to type are essentially the same.

5. Experimental and TD-DFT generated UV spectra.

The weak long wavelength absorption for pyridazine **2** identified as n to π* excitation (340 nm in both C_6H_{12} (ε = 315)[S1] and C_6H_{14} (ε = ca. 400)[S2]) was speculated to no longer be observable explicitly for the newly prepared pyridazines **11c** and **11c′**, judging from the energy levels in the MO diagram in Figure 4. To assure dissolution of the substrates, CH_2Cl_2 (solvent cut-off: 230 nm) was used as the organic solvent. In fact, for symmetric **11c** (Figure S5, dotted line), an intense absorption was observed at 316 nm (CH_2Cl_2, extinction coefficient ε = 7180, log ε = 3.86) with a shoulder around 360 nm (CH_2Cl_2, ε = 710, log ε = 2.9). For unsymmetric **11c′** (Figure S5, normal line), strong absorptions were observed at 284 nm (CH_2Cl_2, ε = 5090, log ε = 3.71) and 321 nm (CH_2Cl_2, ε = 4700, log ε = 3.67) (Δ = 37 nm). The strong intensities already suggested that the transitions were of π-π* type. Analogous absorptions, but in H_2O, were observed at 281 nm (log ε = 3.94) for symmetric 4,5-diaminopyridazine, and 254 nm (log ε = 3.72) and 291 nm (log ε = 3.77) (Δ = 37 nm) for unsymmetric 3,4-diaminopyridazine.[S3] The relative relationship of the absorptions both in terms of wavelength and intensity is in good agreement between the two groups of compounds with a coincidentally same wavelength difference between the two absorptions for the unsymmetric species. The hypsochromic shift of wavelengths for the reported group of compounds is due to hydrogen-bonding by the aqueous solvent, a phenomenon also encountered with pyridine derivatives.[S4] The corresponding π-π* absorbance is observed at 260 nm ($CHCl_3$) for DMAP,[S3] and is in good accordance with the energy differences depicted in the MO diagram.

To add support for the tentatively assigned transitions, TD-DFT calculations at the RB3LYP/6-31G(d) level of theory were carried out for analogous **11a** and **11a′**. The use of the DFT based method instead of HF based methods was assumed sufficient for qualitative purposes. For symmetric **11a**, the long wavelength transition was calculated to be 269 nm (observed at 316 nm) with the oscillator strength of f = 0.1332, and identified as a mixture of the transitions of HOMO-1 to LUMO (26%) and HOMO to LUMO (65%). Thus, there is a contribution from the nitrogen lone pair. This contribution may actually be an artifact judging from the RMP2 energy level of this MO. On the other hand, for unsymmetric **11a′**, the two long wavelength transitions were calculated to be 284 nm (observed at 321 nm) with the oscillator strength of f = 0.0803 and 252 nm (observed at 284 nm) with the oscillator strength of f = 0.1159. The former was identified as a mixture of the transitions of HOMO–2 to LUMO (11%), HOMO–2 to LUMO+1 (17%) and HOMO to LUMO (67%). The latter was identified as a mixture of the transitions of HOMO–2 to LUMO (16%) and HOMO to LUMO+1 (68%). Thus, as opposed to **11a**, there is essentially no contribution from the nitrogen lone pairs regardless of the use of TD-DFT. The calculated difference of 32 nm is in good agreement with the observed difference of 37 nm. Thus, these results reproduce the experimental spectra in a relative manner and confirm that the HOMOs of pyridazines **11a** and **11a′** are indeed of π-type, even though they are based upon TD-DFT.

References

(S1) Mason, S. F. *J. Chem. Soc.* **1959**, 1247.

(S2) Halverson, F.; Hirt, R. C. *J. Phys. Chem.* **1949**, *17*, 1165.

(S3) Barlin, G. B. *J. Chem. Soc., Perkin Trans. 1* **1976**, 1424.

(S4) Baba, H.; Goodman, L.; Valenti, P. C. *J. Am. Chem. Soc.* **1966**, *88*, 5410.

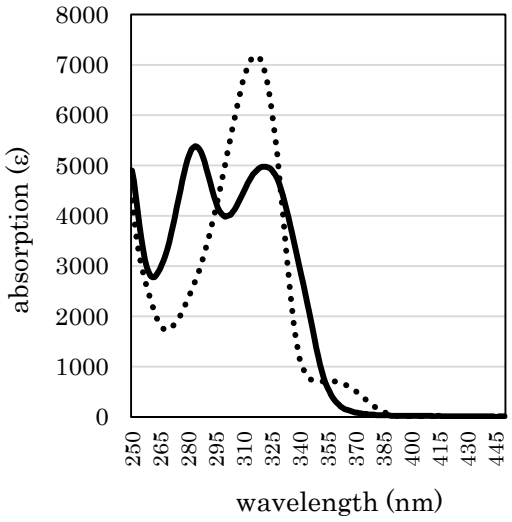
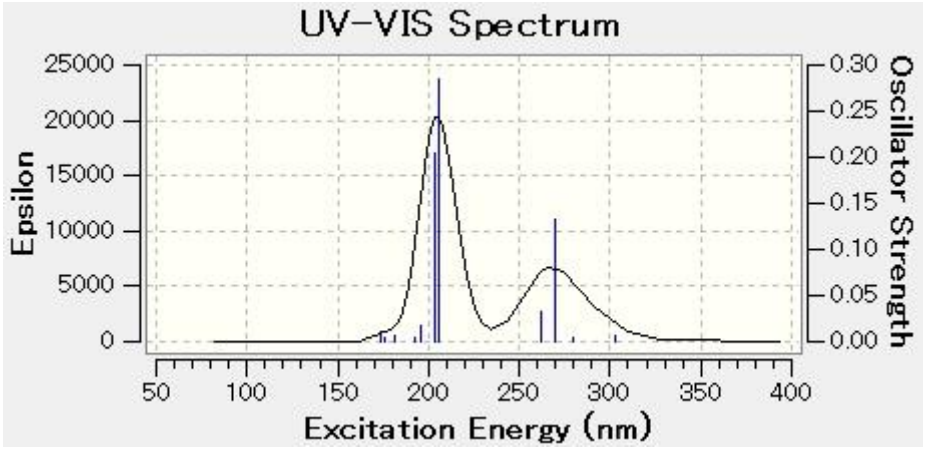
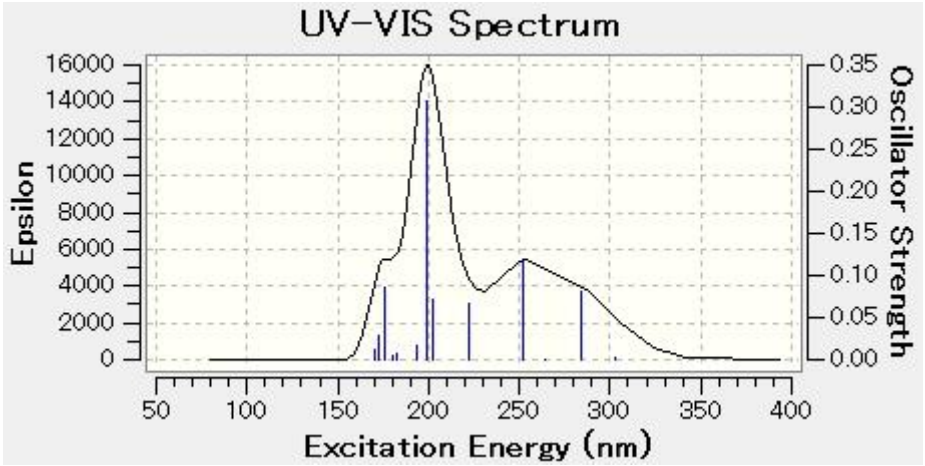


Figure S6. UV spectra of **11c** (dotted line) and **11c′** (normal line) in CH_2Cl_2.



11a



11a′

Figure S7. TD-DFT generated UV spectra of **11a** (upper diagram) and **11a′** (lower diagram).

6. Atomic Coordinates for Structurally Optimized Species.

6-1. Pyridine (**1**)

rb3lyp/6-31g(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.198670	0.673035	0.000005
2	6	0	-1.142124	-0.722100	-0.000064
3	7	0	-0.000050	-1.420841	0.000007
4	6	0	1.142137	-0.722092	0.000053
5	6	0	1.198709	0.672963	-0.000031
6	6	0	0.000002	1.385664	0.000016
7	1	0	2.157693	1.182859	-0.000052
8	1	0	2.059790	-1.308685	-0.000045
9	1	0	0.000056	2.472513	0.000015
10	1	0	-2.059868	-1.308565	0.000092
11	1	0	-2.157644	1.182950	0.000067

rb3lyp/6-31g(d) scrf=(iefpcm,solvent=benzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.199150	-0.672928	0.000026
2	6	0	1.143241	0.722042	0.000090
3	7	0	-0.000092	1.421230	-0.000001
4	6	0	-1.143369	0.721855	-0.000082
5	6	0	-1.199056	-0.673084	-0.000021
6	6	0	0.000113	-1.385504	-0.000008
7	1	0	-2.157998	-1.182679	-0.000007
8	1	0	-2.061869	1.307027	-0.000048
9	1	0	0.000171	-2.472181	-0.000014
10	1	0	2.061690	1.307303	0.000031
11	1	0	2.158180	-1.182358	0.000008

rb3lyp/6-31g(d) scrf=(iefpcm,solvent=chloroform)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.199466	-0.672914	0.000026
2	6	0	1.143972	0.722007	0.000090
3	7	0	-0.000088	1.421369	-0.000001
4	6	0	-1.144096	0.721827	-0.000082
5	6	0	-1.199376	-0.673063	-0.000020
6	6	0	0.000109	-1.385400	-0.000008
7	1	0	-2.158182	-1.182608	-0.000007
8	1	0	-2.063117	1.306127	-0.000049
9	1	0	0.000164	-2.471938	-0.000014
10	1	0	2.062945	1.306391	0.000032
11	1	0	2.158356	-1.182299	0.000008

rmp2/6-31g(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.197727	0.673629	-0.000006
2	6	0	-1.145405	-0.721095	0.000038
3	7	0	0.000125	-1.426570	-0.000002
4	6	0	1.145546	-0.720887	-0.000027
5	6	0	1.197603	0.673836	0.000008
6	6	0	-0.000128	1.387858	0.000003
7	1	0	2.156771	1.184201	0.000030
8	1	0	2.062126	-1.308373	0.000016
9	1	0	-0.000213	2.475048	-0.000008
10	1	0	-2.061890	-1.308734	-0.000058
11	1	0	-2.156998	1.183799	-0.000061

rmp2/6-31g(d) scrf=(iefpcm,solvent=benzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.198058	0.673648	0.000020
2	6	0	1.146582	-0.721047	0.000048
3	7	0	-0.000036	-1.426648	0.000000
4	6	0	-1.146624	-0.720986	-0.000042
5	6	0	-1.198022	0.673708	-0.000019
6	6	0	0.000038	1.387708	-0.000001
7	1	0	-2.157039	1.183912	-0.000021
8	1	0	-2.064125	-1.306996	-0.000028
9	1	0	0.000061	2.474742	-0.000006
10	1	0	2.064058	-1.307099	0.000012
11	1	0	2.157106	1.183793	0.000006

rmp2/6-31g(d) scrf=(iefpcm,solvent=chloroform)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.198110	-0.673699	-0.000011
2	6	0	1.147022	0.721020	0.000006
3	7	0	-0.000013	1.426996	-0.000001
4	6	0	-1.147038	0.720996	-0.000005
5	6	0	-1.198097	-0.673721	0.000013
6	6	0	0.000014	-1.387787	0.000001
7	1	0	-2.157073	-1.183810	0.000033
8	1	0	-2.064990	1.306218	0.000025
9	1	0	0.000023	-2.474730	-0.000001
10	1	0	2.064965	1.306256	-0.000034
11	1	0	2.157099	-1.183765	-0.000037

rb3lyp/cc-pvtz

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.193032	0.669700	0.000022
2	6	0	-1.138573	-0.719169	0.000090
3	7	0	0.000079	-1.413358	0.000000
4	6	0	1.138692	-0.718998	-0.000081
5	6	0	1.192951	0.669834	-0.000018
6	6	0	-0.000103	1.378933	-0.000008
7	1	0	2.147498	1.177771	-0.000004
8	1	0	2.052836	-1.302064	-0.000048
9	1	0	-0.000151	2.460810	-0.000016
10	1	0	-2.052681	-1.302303	0.000036
11	1	0	-2.147658	1.177488	0.000007

6-2. Acetylated pyridine (**1-Ac**$^{+}$)

rb3lyp/6-31g(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.797053	1.278232	-0.000084
2	6	0	0.418169	1.176780	-0.000144
3	7	0	-0.182983	-0.041373	-0.000057
4	6	0	0.549671	-1.185197	0.000068
5	6	0	1.931158	-1.132694	0.000119
6	6	0	2.568206	0.111510	0.000036
7	6	0	-1.707638	-0.208891	-0.000018
8	8	0	-2.111331	-1.329763	-0.000206
9	6	0	-2.518878	1.050297	0.000224
10	1	0	2.255639	2.260647	-0.000138
11	1	0	-0.226128	2.045009	-0.000292
12	1	0	-0.025789	-2.103011	0.000130
13	1	0	2.495707	-2.058350	0.000224
14	1	0	3.652111	0.172684	0.000127
15	1	0	-3.569471	0.757364	0.000468
16	1	0	-2.318717	1.656561	-0.890368
17	1	0	-2.318263	1.656585	0.890689

rb3lyp/6-31g(d) scrf=(iefpcm,solvent=benzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.790575	1.278441	-0.001278
2	6	0	0.412674	1.173903	-0.001127
3	7	0	-0.185410	-0.045440	0.000326
4	6	0	0.550140	-1.187623	0.001229
5	6	0	1.930249	-1.131237	0.001208
6	6	0	2.564093	0.114435	0.000015
7	6	0	-1.699175	-0.208081	0.000355
8	8	0	-2.113144	-1.328049	-0.002960
9	6	0	-2.509205	1.051415	0.002054
10	1	0	2.245659	2.261813	-0.002315
11	1	0	-0.231631	2.041180	-0.001998
12	1	0	-0.020937	-2.106979	0.001771
13	1	0	2.497251	-2.054589	0.002148
14	1	0	3.647302	0.177782	0.000078
15	1	0	-3.559999	0.760800	0.004037
16	1	0	-2.307300	1.657280	-0.887991
17	1	0	-2.303429	1.657668	0.890927

rb3lyp/6-31g(d) scrf=(iefpcm,solvent=chloroform)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.787050	1.278653	-0.001860
2	6	0	0.409491	1.173271	-0.002512
3	7	0	-0.186832	-0.047252	-0.000558
4	6	0	0.550214	-1.188925	0.001390
5	6	0	1.929602	-1.130598	0.002174
6	6	0	2.561678	0.115831	0.000776
7	6	0	-1.694146	-0.207614	-0.000554
8	8	0	-2.113087	-1.327526	-0.003969
9	6	0	-2.504258	1.051677	0.004074
10	1	0	2.240195	2.262575	-0.003310
11	1	0	-0.235488	2.039623	-0.004574
12	1	0	-0.019101	-2.108803	0.002233
13	1	0	2.497330	-2.053207	0.003982
14	1	0	3.644550	0.180376	0.001606
15	1	0	-3.554914	0.761656	0.008252
16	1	0	-2.302931	1.657696	-0.885742
17	1	0	-2.294906	1.657294	0.892278

rmp2/6-31g(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.800104	1.271614	-0.004473
2	6	0	0.415745	1.178247	-0.004661
3	7	0	-0.180226	-0.040265	-0.000209
4	6	0	0.543522	-1.187544	0.004254
5	6	0	1.928439	-1.131901	0.005032
6	6	0	2.570373	0.108039	0.000611
7	6	0	-1.710917	-0.204708	-0.001424
8	8	0	-2.120088	-1.333560	-0.009960
9	6	0	-2.507885	1.059587	0.008739
10	1	0	2.260180	2.254476	-0.008416
11	1	0	-0.225548	2.049910	-0.008557
12	1	0	-0.031822	-2.106873	0.006591
13	1	0	2.491285	-2.059744	0.009089
14	1	0	3.655180	0.166571	0.001017
15	1	0	-3.558805	0.769624	0.014107
16	1	0	-2.308191	1.661316	-0.882186
17	1	0	-2.296281	1.655050	0.901020

rmp2/6-31g(d) scrf=(iefpcm,solvent=benzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.793330	1.271979	-0.001326
2	6	0	0.409808	1.175450	-0.002116
3	7	0	-0.182477	-0.044456	-0.000725
4	6	0	0.543980	-1.189830	0.000857
5	6	0	1.928056	-1.129866	0.001635
6	6	0	2.566382	0.111231	0.000827
7	6	0	-1.702848	-0.204131	-0.000441
8	8	0	-2.120393	-1.331982	-0.002798
9	6	0	-2.499102	1.060121	0.003195
10	1	0	2.248894	2.256232	-0.002316
11	1	0	-0.231973	2.045865	-0.004034
12	1	0	-0.026896	-2.110742	0.001469
13	1	0	2.492549	-2.055850	0.003015
14	1	0	3.650457	0.172465	0.001755
15	1	0	-3.549895	0.771996	0.006612
16	1	0	-2.293366	1.658916	-0.887962
17	1	0	-2.286925	1.658446	0.893130

rmp2/6-31g(d) scrf=(iefpcm,solvent= chloroform)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.789911	1.272191	-0.002983
2	6	0	0.406850	1.174701	-0.004510
3	7	0	-0.183498	-0.046048	-0.001416
4	6	0	0.543840	-1.190818	0.002067
5	6	0	1.927313	-1.129232	0.003620
6	6	0	2.563919	0.112435	0.001590
7	6	0	-1.698465	-0.203800	-0.000959
8	8	0	-2.119900	-1.331220	-0.006352
9	6	0	-2.494483	1.060155	0.006941
10	1	0	2.243956	2.256804	-0.005180
11	1	0	-0.235510	2.044286	-0.008359
12	1	0	-0.025241	-2.112327	0.003562
13	1	0	2.492546	-2.054462	0.006767
14	1	0	3.647707	0.174813	0.003375
15	1	0	-3.545237	0.772637	0.013330
16	1	0	-2.290225	1.659555	-0.883917
17	1	0	-2.277625	1.657002	0.896545

6-3. 4-Dimethylaminopyridine (**2**)

rb3lyp/6-31g(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.558163	0.000000	-0.092370
2	6	0	-0.180374	0.000000	-0.042025
3	6	0	0.570591	1.197597	-0.017332
4	6	0	0.570591	-1.197597	-0.017329
5	1	0	0.088918	2.167951	-0.017892
6	1	0	0.088918	-2.167951	-0.017886
7	7	0	2.676346	0.000000	0.023663
8	6	0	1.958665	-1.131804	0.010716
9	6	0	1.958665	1.131804	0.010713
10	1	0	2.531602	-2.058633	0.027068
11	1	0	2.531603	2.058633	0.027063
12	6	0	-2.284029	1.253100	0.035383
13	6	0	-2.284030	-1.253100	0.035378
14	1	0	-3.353020	1.059087	-0.069546
15	1	0	-3.353020	-1.059087	-0.069557
16	1	0	-2.116549	-1.741568	1.007586
17	1	0	-1.994829	-1.958229	-0.753254
18	1	0	-1.994833	1.958231	-0.753250
19	1	0	-2.116543	1.741567	1.007591

rb3lyp/6-31g(d) scrf=(iefpcm,solvent=benzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.555945	-0.000001	-0.072008
2	6	0	-0.182361	-0.000002	-0.032647
3	6	0	0.570570	1.198433	-0.013011
4	6	0	0.570572	-1.198436	-0.013011
5	1	0	0.088877	2.168636	-0.012479
6	1	0	0.088882	-2.168639	-0.012480
7	7	0	2.677729	0.000001	0.017881
8	6	0	1.957957	-1.132768	0.008245
9	6	0	1.957955	1.132768	0.008246
10	1	0	2.529646	-2.060435	0.021109
11	1	0	2.529642	2.060437	0.021109
12	6	0	-2.284152	1.256182	0.027377
13	6	0	-2.284157	-1.256180	0.027378
14	1	0	-3.353148	1.057036	-0.060413
15	1	0	-3.353153	-1.057029	-0.060405
16	1	0	-2.107062	-1.767305	0.985138
17	1	0	-2.003717	-1.941639	-0.781646
18	1	0	-2.003702	1.941641	-0.781643
19	1	0	-2.107060	1.767304	0.985140

rb3lyp/6-31g(d) scrf=(iefpcm,solvent=chloroform)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.554633	0.000000	-0.058055
2	6	0	-0.183569	0.000001	-0.026162
3	6	0	0.570497	1.199029	-0.010232
4	6	0	0.570495	-1.199027	-0.010235
5	1	0	0.088834	2.169174	-0.009466
6	1	0	0.088830	-2.169171	-0.009471
7	7	0	2.678411	-0.000001	0.014122
8	6	0	1.957434	-1.133435	0.006602
9	6	0	1.957436	1.133435	0.006604
10	1	0	2.528329	-2.061641	0.016928
11	1	0	2.528332	2.061640	0.016932
12	6	0	-2.284089	1.258009	0.021942
13	6	0	-2.284084	-1.258011	0.021946
14	1	0	-3.353221	1.055734	-0.051489
15	1	0	-3.353217	-1.055740	-0.051481
16	1	0	-2.098355	-1.785637	0.968416
17	1	0	-2.011164	-1.928695	-0.802023
18	1	0	-2.011169	1.928694	-0.802026
19	1	0	-2.098367	1.785636	0.968413

rmp2/6-31g(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.565600	0.000000	-0.227439
2	6	0	-0.182556	0.000000	-0.100153
3	6	0	0.564679	1.193870	-0.052708
4	6	0	0.564679	-1.193870	-0.052709
5	1	0	0.087503	2.166647	-0.069345
6	1	0	0.087503	-2.166647	-0.069346
7	7	0	2.673326	0.000000	0.068020
8	6	0	1.952305	-1.134470	0.027280
9	6	0	1.952305	1.134470	0.027281
10	1	0	2.524453	-2.060745	0.065444
11	1	0	2.524452	2.060745	0.065444
12	6	0	-2.271920	1.232635	0.089792
13	6	0	-2.271920	-1.232635	0.089793
14	1	0	-3.338974	1.070971	-0.069872
15	1	0	-3.338974	-1.070971	-0.069870
16	1	0	-2.115361	-1.561216	1.128074
17	1	0	-1.957378	-2.034281	-0.582060
18	1	0	-1.957377	2.034281	-0.582060
19	1	0	-2.115361	1.561217	1.128074

rmp2/6-31g(d) scrf=(iefpcm,solvent=benzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.563316	0.000000	-0.220614
2	6	0	-0.183756	0.000000	-0.096320
3	6	0	0.565003	1.194317	-0.049890
4	6	0	0.565003	-1.194317	-0.049890
5	1	0	0.088153	2.167247	-0.063744
6	1	0	0.088152	-2.167246	-0.063744
7	7	0	2.674962	0.000000	0.064549
8	6	0	1.952323	-1.135262	0.026210
9	6	0	1.952323	1.135262	0.026210
10	1	0	2.523048	-2.062522	0.063163
11	1	0	2.523048	2.062522	0.063164
12	6	0	-2.273146	1.234893	0.086427
13	6	0	-2.273144	-1.234893	0.086427
14	1	0	-3.338772	1.070454	-0.077303
15	1	0	-3.338770	-1.070456	-0.077303
16	1	0	-2.121295	-1.566428	1.123829
17	1	0	-1.955710	-2.033689	-0.587238
18	1	0	-1.955713	2.033688	-0.587239
19	1	0	-2.121297	1.566428	1.123829

rmp2/6-31g(d) scrf=(iefpcm,solvent= chloroform)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.561895	0.000001	-0.215682
2	6	0	-0.184442	0.000002	-0.093559
3	6	0	0.565072	1.194799	-0.048029
4	6	0	0.565069	-1.194796	-0.048030
5	1	0	0.088400	2.167789	-0.060361
6	1	0	0.088394	-2.167785	-0.060363
7	7	0	2.675696	-0.000001	0.062228
8	6	0	1.952228	-1.135844	0.025459
9	6	0	1.952231	1.135844	0.025460
10	1	0	2.521984	-2.063786	0.061589
11	1	0	2.521990	2.063784	0.061591
12	6	0	-2.273638	1.236547	0.084044
13	6	0	-2.273629	-1.236550	0.084045
14	1	0	-3.338738	1.069801	-0.079214
15	1	0	-3.338730	-1.069813	-0.079215
16	1	0	-2.122438	-1.572167	1.119841
17	1	0	-1.956177	-2.032501	-0.592930
18	1	0	-1.956195	2.032499	-0.592935
19	1	0	-2.122447	1.572168	1.119838

rb3lyp/cc-pvtz

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.549942	-0.000005	-0.084569
2	6	0	-0.178774	-0.000015	-0.037703
3	6	0	0.570667	1.192815	-0.014449
4	6	0	0.570688	-1.192836	-0.014439
5	1	0	0.092284	2.159575	-0.013181
6	1	0	0.092327	-2.159605	-0.013158
7	7	0	2.665313	0.000008	0.019994
8	6	0	1.953062	-1.128786	0.009659
9	6	0	1.953042	1.128789	0.009653
10	1	0	2.522910	-2.052091	0.024507
11	1	0	2.522873	2.052105	0.024488
12	6	0	-2.278974	1.249150	0.031596
13	6	0	-2.279028	-1.249132	0.031581
14	1	0	-3.341278	1.053030	-0.085123
15	1	0	-3.341323	-1.052960	-0.085125
16	1	0	-2.125841	-1.736245	1.001536
17	1	0	-1.983988	-1.952694	-0.749449
18	1	0	-1.983890	1.952712	-0.749419
19	1	0	-2.125773	1.736239	1.001560

6-4. Acetylated 4-dimethylaminopyridine (**2-Ac**$^{+}$)

rb3lyp/6-31g(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.642178	-1.224148	-0.000596
2	6	0	0.720203	-1.221599	-0.000597
3	7	0	1.443644	-0.056150	-0.000264
4	6	0	0.774138	1.138833	-0.000109
5	6	0	-0.588020	1.203591	-0.000036
6	6	0	-1.377040	0.006472	0.000012
7	7	0	-2.715041	0.037146	0.000478
8	6	0	-3.491666	-1.212629	0.000077
9	6	0	-3.434925	1.319848	0.000186
10	6	0	2.922240	-0.168141	0.000208
11	6	0	3.703215	1.116675	-0.000300
12	8	0	3.392830	-1.271625	0.000997
13	1	0	-4.505521	1.123617	0.001660
14	1	0	-3.193589	1.903296	-0.894529
15	1	0	-3.191489	1.904760	0.893350
16	1	0	-4.552341	-0.968505	0.002716
17	1	0	-3.273086	-1.808034	0.892544
18	1	0	-3.276744	-1.805363	-0.895095
19	1	0	4.761018	0.852672	-0.000841
20	1	0	3.488012	1.719157	0.889288
21	1	0	3.487020	1.719400	-0.889448
22	1	0	-1.049194	2.181636	-0.000065
23	1	0	1.378107	2.035424	-0.000064
24	1	0	1.316545	-2.125148	-0.000865
25	1	0	-1.147409	-2.180300	-0.001187

rb3lyp/6-31g(d) scrf=(iefpcm,solvent=benzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.642367	-1.227017	-0.000059
2	6	0	0.718952	-1.226073	0.000867
3	7	0	1.444345	-0.060783	-0.006598
4	6	0	0.775655	1.135939	-0.020457
5	6	0	-0.585317	1.201518	-0.021373
6	6	0	-1.374611	0.005124	-0.006053
7	7	0	-2.711325	0.037883	0.002990
8	6	0	-3.489851	-1.209605	-0.006451
9	6	0	-3.426687	1.321991	0.024005
10	6	0	2.913171	-0.166538	0.003362
11	6	0	3.690044	1.120608	0.012962
12	8	0	3.395348	-1.268463	0.005656
13	1	0	-4.495604	1.128860	0.088567
14	1	0	-3.231322	1.893011	-0.889560
15	1	0	-3.130363	1.916187	0.894008
16	1	0	-4.549297	-0.963305	-0.038871
17	1	0	-3.296816	-1.796391	0.897465
18	1	0	-3.248325	-1.811009	-0.888283
19	1	0	4.748868	0.862706	0.033154
20	1	0	3.452105	1.725338	0.894717
21	1	0	3.485803	1.718509	-0.881906
22	1	0	-1.045480	2.179593	-0.036887
23	1	0	1.379531	2.031662	-0.032347
24	1	0	1.311977	-2.130762	0.009621
25	1	0	-1.148934	-2.182080	0.009509

rb3lyp/6-31g(d) scrf=(iefpcm,solvent=chloroform)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.642355	-1.228449	-0.000536
2	6	0	0.718341	-1.228279	0.000180
3	7	0	1.444842	-0.062969	-0.007518
4	6	0	0.776463	1.134893	-0.022108
5	6	0	-0.583843	1.200565	-0.022867
6	6	0	-1.373400	0.004573	-0.006554
7	7	0	-2.709488	0.038235	0.003296
8	6	0	-3.488635	-1.208386	-0.003840
9	6	0	-3.423476	1.322807	0.023279
10	6	0	2.908174	-0.165524	0.003289
11	6	0	3.683582	1.122312	0.016688
12	8	0	3.397110	-1.266647	0.003736
13	1	0	-4.492442	1.130138	0.086569
14	1	0	-3.225571	1.893132	-0.889991
15	1	0	-3.126776	1.916687	0.893195
16	1	0	-4.547743	-0.960889	-0.035115
17	1	0	-3.294080	-1.794113	0.900292
18	1	0	-3.247907	-1.810715	-0.885105
19	1	0	4.742604	0.866096	0.039515
20	1	0	3.441195	1.725515	0.898076
21	1	0	3.480122	1.720821	-0.877747
22	1	0	-1.043225	2.178791	-0.038785
23	1	0	1.380047	2.030369	-0.034785
24	1	0	1.309765	-2.133508	0.009075
25	1	0	-1.149447	-2.183088	0.009292

rmp2/6-31g(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.645297	-1.220335	0.000266
2	6	0	-0.721631	-1.220107	0.000424
3	7	0	-1.438541	-0.054532	0.000256
4	6	0	-0.774582	1.139859	-0.000001
5	6	0	0.593278	1.200680	-0.000169
6	6	0	1.376292	0.006762	-0.000163
7	7	0	2.712995	0.035916	-0.000554
8	6	0	3.481498	-1.215954	-0.000227
9	6	0	3.427606	1.318843	-0.000280
10	6	0	-2.920230	-0.164884	0.000362
11	6	0	-3.689908	1.121633	0.000160
12	8	0	-3.395882	-1.276258	-0.000002
13	1	0	4.496814	1.119476	-0.001111
14	1	0	3.182366	1.896673	0.895012
15	1	0	3.181232	1.897605	-0.894645
16	1	0	4.541231	-0.971249	-0.001904
17	1	0	3.258748	-1.804960	-0.894014
18	1	0	3.261037	-1.803237	0.895286
19	1	0	-4.747353	0.858355	0.000190
20	1	0	-3.470281	1.717128	-0.890175
21	1	0	-3.470280	1.717446	0.890273
22	1	0	1.051616	2.181574	-0.000289
23	1	0	-1.375727	2.039826	-0.000063
24	1	0	-1.315432	-2.127035	0.000721
25	1	0	1.146184	-2.180206	0.000593

rmp2/6-31g(d) scrf=(iefpcm,solvent=benzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.645673	-1.223426	0.000142
2	6	0	-0.720340	-1.224424	0.000328
3	7	0	-1.439076	-0.059105	0.000200
4	6	0	-0.775859	1.136891	-0.000109
5	6	0	0.590726	1.198709	-0.000295
6	6	0	1.374237	0.005143	-0.000225
7	7	0	2.709547	0.036562	-0.000488
8	6	0	3.480028	-1.213300	-0.000240
9	6	0	3.418470	1.321866	-0.000281
10	6	0	-2.911430	-0.163431	0.000456
11	6	0	-3.677362	1.124952	0.000210
12	8	0	-3.397829	-1.272728	0.000338
13	1	0	4.488127	1.127477	-0.000679
14	1	0	3.167713	1.898135	0.893994
15	1	0	3.167184	1.898680	-0.894047
16	1	0	4.539150	-0.967066	-0.001334
17	1	0	3.256584	-1.802106	-0.893597
18	1	0	3.258071	-1.800939	0.894272
19	1	0	-4.735928	0.867713	0.000387
20	1	0	-3.452331	1.719067	-0.889365
21	1	0	-3.452106	1.719495	0.889441
22	1	0	1.047485	2.179963	-0.000491
23	1	0	-1.376463	2.036336	-0.000191
24	1	0	-1.310630	-2.132642	0.000614
25	1	0	1.147618	-2.182365	0.000383

rmp2/6-31g(d) scrf=(iefpcm,solvent= chloroform)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.645711	-1.224882	0.000174
2	6	0	-0.719721	-1.226576	0.000291
3	7	0	-1.439339	-0.061155	0.000071
4	6	0	-0.776576	1.135929	-0.000251
5	6	0	0.589270	1.197898	-0.000375
6	6	0	1.373077	0.004553	-0.000205
7	7	0	2.707548	0.036987	-0.000400
8	6	0	3.478809	-1.212093	-0.000074
9	6	0	3.415167	1.322818	-0.000239
10	6	0	-2.906691	-0.162539	0.000244
11	6	0	-3.671595	1.126247	0.000459
12	8	0	-3.398649	-1.270812	0.000164
13	1	0	4.484766	1.128644	-0.000501
14	1	0	3.162956	1.898621	0.893767
15	1	0	3.162619	1.899006	-0.893896
16	1	0	4.537538	-0.964510	-0.001169
17	1	0	3.255046	-1.800850	-0.893235
18	1	0	3.256513	-1.799580	0.894304
19	1	0	-4.730246	0.869976	0.000683
20	1	0	-3.445197	1.720292	-0.888692
21	1	0	-3.444802	1.720247	0.889537
22	1	0	1.045397	2.179307	-0.000603
23	1	0	-1.377083	2.035166	-0.000419
24	1	0	-1.308639	-2.135301	0.000592
25	1	0	1.148155	-2.183472	0.000472

6-5. 1,4-Dimethyl-1,2,3,4-tetrahydropyrido[3,4-b]pyridine (**6a**)

rb3lyp/6-31g(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.333471	-0.692500	-0.056047
2	6	0	-1.602152	-1.283719	-0.047638
3	7	0	-2.766948	-0.617123	-0.010124
4	6	0	-2.691563	0.712273	0.033677
5	6	0	-1.490612	1.421670	0.052952
6	6	0	-0.271386	0.731609	0.028845
7	7	0	0.957596	1.376379	0.107515
8	6	0	2.144345	0.618954	-0.256257
9	6	0	2.053795	-0.789060	0.323574
10	7	0	0.851174	-1.438033	-0.171006
11	6	0	1.024607	2.819500	-0.019403
12	6	0	0.788672	-2.878728	-0.011479
13	1	0	1.787864	-3.292270	-0.175742
14	1	0	0.119687	-3.317855	-0.758514
15	1	0	0.440920	-3.193442	0.987594
16	1	0	2.056614	3.138737	0.148965
17	1	0	0.398491	3.303810	0.737517
18	1	0	0.707452	3.181638	-1.011218
19	1	0	2.081578	-0.734151	1.426239
20	1	0	2.923196	-1.370119	-0.003111
21	1	0	3.021773	1.127755	0.158921
22	1	0	2.278295	0.555997	-1.349015
23	1	0	-3.636784	1.252916	0.055847
24	1	0	-1.514928	2.504485	0.087470
25	1	0	-1.690316	-2.366056	-0.078986

rb3lyp/6-31g(d) scrf=(iefpcm,solvent=benzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.332017	-0.694215	-0.056664
2	6	0	-1.599907	-1.286569	-0.045123
3	7	0	-2.767790	-0.620720	-0.007478
4	6	0	-2.692529	0.710021	0.034369
5	6	0	-1.492285	1.420378	0.050697
6	6	0	-0.270804	0.732221	0.025804
7	7	0	0.953824	1.377328	0.099475
8	6	0	2.146923	0.621141	-0.252076
9	6	0	2.054593	-0.786847	0.326029
10	7	0	0.851688	-1.436956	-0.171721
11	6	0	1.020435	2.822834	-0.017660
12	6	0	0.791622	-2.879258	-0.014479
13	1	0	1.791654	-3.290019	-0.177828
14	1	0	0.124219	-3.318995	-0.762552
15	1	0	0.443767	-3.194291	0.984042
16	1	0	2.053011	3.140081	0.147603
17	1	0	0.397509	3.302419	0.744736
18	1	0	0.699134	3.188833	-1.005981
19	1	0	2.077976	-0.735084	1.428361
20	1	0	2.924236	-1.367322	0.001003
21	1	0	3.018617	1.131657	0.171427
22	1	0	2.289894	0.561399	-1.343200
23	1	0	-3.637388	1.251483	0.057045
24	1	0	-1.517869	2.503090	0.082916
25	1	0	-1.684992	-2.369055	-0.074889

rb3lyp/6-31g(d) scrf=(iefpcm,solvent=chloroform)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.330194	-0.695849	-0.057042
2	6	0	-1.596815	-1.290605	-0.043259
3	7	0	-2.767462	-0.626623	-0.005669
4	6	0	-2.694114	0.705084	0.034584
5	6	0	-1.495263	1.417646	0.048926
6	6	0	-0.271449	0.732210	0.023569
7	7	0	0.949518	1.379128	0.093799
8	6	0	2.147669	0.625416	-0.249806
9	6	0	2.056284	-0.782585	0.327354
10	7	0	0.854014	-1.435204	-0.172093
11	6	0	1.013885	2.826253	-0.015675
12	6	0	0.797533	-2.878528	-0.016158
13	1	0	1.798680	-3.286169	-0.178678
14	1	0	0.131723	-3.319636	-0.764847
15	1	0	0.449965	-3.194205	0.982012
16	1	0	2.046366	3.143526	0.147936
17	1	0	0.392122	3.301118	0.750531
18	1	0	0.689480	3.195274	-1.001396
19	1	0	2.076978	-0.732671	1.429464
20	1	0	2.926891	-1.361495	0.003417
21	1	0	3.014986	1.138295	0.178785
22	1	0	2.296458	0.567900	-1.339871
23	1	0	-3.639501	1.245759	0.057427
24	1	0	-1.523113	2.500274	0.079460
25	1	0	-1.678741	-2.373324	-0.071465

rmp2/6-31g(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.339903	-0.681480	-0.069776
2	6	0	-1.621662	-1.251000	-0.093013
3	7	0	-2.776190	-0.560352	-0.038757
4	6	0	-2.667855	0.772463	0.049531
5	6	0	-1.450665	1.449506	0.099969
6	6	0	-0.247769	0.733948	0.055415
7	7	0	0.995737	1.352519	0.184684
8	6	0	2.141392	0.573132	-0.254505
9	6	0	2.027250	-0.829949	0.308239
10	7	0	0.823468	-1.450574	-0.220438
11	6	0	1.079466	2.780346	-0.070049
12	6	0	0.719244	-2.878581	0.034472
13	1	0	1.708883	-3.320023	-0.103387
14	1	0	0.043462	-3.343439	-0.686462
15	1	0	0.364611	-3.109798	1.051012
16	1	0	2.116138	3.091508	0.076195
17	1	0	0.463122	3.331347	0.644029
18	1	0	0.768030	3.052161	-1.090065
19	1	0	2.033606	-0.785555	1.410266
20	1	0	2.888692	-1.425403	-0.013678
21	1	0	3.048207	1.053043	0.130780
22	1	0	2.220268	0.521620	-1.352376
23	1	0	-3.602360	1.330373	0.083948
24	1	0	-1.453856	2.531309	0.175222
25	1	0	-1.736892	-2.328602	-0.165593

rmp2/6-31g(d) scrf=(iefpcm,solvent=benzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.340507	0.682063	-0.069420
2	6	0	1.623031	1.250254	-0.087811
3	7	0	2.778155	0.557161	-0.034736
4	6	0	2.667235	-0.776841	0.048260
5	6	0	1.448962	-1.451992	0.094618
6	6	0	0.245892	-0.735150	0.052345
7	7	0	-0.995295	-1.350893	0.178535
8	6	0	-2.145159	-0.570138	-0.251176
9	6	0	-2.026639	0.833108	0.309048
10	7	0	-0.820021	1.451343	-0.220424
11	6	0	-1.083053	-2.781558	-0.066251
12	6	0	-0.714984	2.881257	0.030442
13	1	0	-1.704456	3.322031	-0.107938
14	1	0	-0.038943	3.344392	-0.691422
15	1	0	-0.360566	3.113408	1.046457
16	1	0	-2.120015	-3.088459	0.083945
17	1	0	-0.466021	-3.329511	0.649442
18	1	0	-0.774869	-3.058531	-1.085307
19	1	0	-2.031480	0.792907	1.410783
20	1	0	-2.886226	1.430026	-0.013444
21	1	0	-3.048616	-1.049173	0.141711
22	1	0	-2.231920	-0.522427	-1.348105
23	1	0	3.599941	-1.338052	0.081339
24	1	0	1.450899	-2.534096	0.164740
25	1	0	1.737646	2.328191	-0.156163

rmp2/6-31g(d) scrf=(iefpcm,solvent= chloroform)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.339225	0.683471	-0.069033
2	6	0	1.620829	1.254040	-0.083683
3	7	0	2.777989	0.562068	-0.031648
4	6	0	2.668843	-0.772977	0.047156
5	6	0	1.451575	-1.450066	0.090504
6	6	0	0.246654	-0.735209	0.049835
7	7	0	-0.991484	-1.352290	0.173690
8	6	0	-2.146194	-0.573627	-0.249096
9	6	0	-2.028269	0.829870	0.309994
10	7	0	-0.821733	1.449775	-0.220459
11	6	0	-1.077986	-2.785120	-0.063046
12	6	0	-0.720059	2.881200	0.027306
13	1	0	-1.710509	3.318992	-0.111901
14	1	0	-0.044684	3.344670	-0.694997
15	1	0	-0.366822	3.115397	1.043041
16	1	0	-2.114519	-3.091729	0.088941
17	1	0	-0.459669	-3.328749	0.654795
18	1	0	-0.770233	-3.065970	-1.080816
19	1	0	-2.031411	0.791853	1.411529
20	1	0	-2.888457	1.425569	-0.012041
21	1	0	-3.046091	-1.054550	0.148732
22	1	0	-2.238666	-0.528037	-1.345330
23	1	0	3.601856	-1.333921	0.079075
24	1	0	1.455455	-2.532381	0.156702
25	1	0	1.732624	2.332493	-0.148431

rb3lyp/cc-pvtz

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.326470	0.694293	-0.053390
2	6	0	1.583110	1.297962	-0.041431
3	7	0	2.750059	0.644325	-0.006797
4	6	0	2.692870	-0.679867	0.031088
5	6	0	1.503374	-1.398291	0.048950
6	6	0	0.280443	-0.725912	0.027840
7	7	0	-0.935379	-1.382676	0.101663
8	6	0	-2.133102	-0.642527	-0.248393
9	6	0	-2.057629	0.764403	0.320474
10	7	0	-0.862255	1.423318	-0.168133
11	6	0	-0.990308	-2.823709	-0.018414
12	6	0	-0.821783	2.862529	-0.017993
13	1	0	-1.819497	3.259986	-0.197614
14	1	0	-0.150514	3.307379	-0.752143
15	1	0	-0.495696	3.185309	0.981065
16	1	0	-2.012084	-3.151192	0.164264
17	1	0	-0.351272	-3.300204	0.725324
18	1	0	-0.686319	-3.183415	-1.010272
19	1	0	-2.087967	0.716415	1.419344
20	1	0	-2.927873	1.332884	-0.009555
21	1	0	-2.995690	-1.159251	0.175374
22	1	0	-2.278531	-0.587657	-1.335839
23	1	0	3.639417	-1.208826	0.050440
24	1	0	1.540869	-2.476175	0.079029
25	1	0	1.657508	2.376697	-0.068944

6-6. Acetylated 1,4-dimethyl-1,2,3,4-tetrahydropyrido[3,4-b]pyridiine (**6a-Ac**$^+$)

s-trans conformer

rb3lyp/6-31g(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.430073	0.559951	0.042566
2	6	0	0.941818	0.713431	0.011558
3	7	0	1.803745	-0.360124	-0.011697
4	6	0	1.310323	-1.626196	-0.047708
5	6	0	-0.038827	-1.857308	-0.047126
6	6	0	-0.969197	-0.787920	0.003695
7	7	0	-2.296603	-0.993727	0.027538
8	6	0	-3.224377	0.133958	0.189611
9	6	0	-2.638295	1.404213	-0.410016
10	7	0	-1.298459	1.628085	0.127387
11	6	0	-0.772919	2.985993	0.085880
12	6	0	-2.853665	-2.350011	0.058067
13	6	0	3.274334	-0.206608	-0.008954
14	8	0	3.941540	-1.204056	-0.058588
15	6	0	3.817575	1.194772	0.058898
16	1	0	1.398049	1.688974	0.011077
17	1	0	2.053110	-2.412365	-0.070535
18	1	0	-0.378608	-2.883647	-0.067877
19	1	0	-4.157381	-0.115490	-0.322816
20	1	0	-3.445941	0.278425	1.254368
21	1	0	-2.629719	1.338071	-1.508829
22	1	0	-3.270802	2.250065	-0.130553
23	1	0	-1.595256	3.685137	0.246938
24	1	0	-0.048245	3.133880	0.893422
25	1	0	-0.293137	3.227671	-0.875311
26	1	0	-2.550044	-2.914471	-0.829464
27	1	0	-2.535252	-2.889018	0.957289
28	1	0	-3.941126	-2.279453	0.065009
29	1	0	3.483303	1.712626	0.964474
30	1	0	4.905146	1.120719	0.071885
31	1	0	3.512619	1.786031	-0.811810

rb3lyp/6-31g(d) scrf=(iefpcm,solvent=benzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.428274	0.559644	0.049190
2	6	0	0.942360	0.712750	0.015609
3	7	0	1.804429	-0.362178	-0.009300
4	6	0	1.308433	-1.628882	-0.045495
5	6	0	-0.039358	-1.858741	-0.044597
6	6	0	-0.968907	-0.787520	0.007475
7	7	0	-2.294457	-0.992222	0.029612
8	6	0	-3.222687	0.135464	0.187569
9	6	0	-2.633380	1.405142	-0.407905
10	7	0	-1.296196	1.628421	0.137179
11	6	0	-0.767410	2.984272	0.079706
12	6	0	-2.853072	-2.347483	0.049540
13	6	0	3.265575	-0.206779	-0.009347
14	8	0	3.941259	-1.202515	-0.058298
15	6	0	3.807761	1.194750	0.052833
16	1	0	1.397842	1.688161	0.016024
17	1	0	2.048850	-2.416252	-0.069149
18	1	0	-0.380410	-2.884366	-0.065820
19	1	0	-4.152470	-0.113992	-0.329713
20	1	0	-3.448423	0.277621	1.251352
21	1	0	-2.617134	1.338267	-1.506341
22	1	0	-3.266933	2.250884	-0.131574
23	1	0	-1.589142	3.685757	0.232468
24	1	0	-0.041060	3.139975	0.883978
25	1	0	-0.287494	3.211863	-0.884695
26	1	0	-2.554488	-2.902262	-0.845528
27	1	0	-2.528931	-2.895014	0.940944
28	1	0	-3.939948	-2.274169	0.063693
29	1	0	3.472264	1.715868	0.955751
30	1	0	4.895138	1.122984	0.064891
31	1	0	3.499599	1.780948	-0.819803

rb3lyp/6-31g(d) scrf=(iefpcm,solvent=chloroform)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.427031	0.559052	0.052508
2	6	0	0.942797	0.711796	0.016896
3	7	0	1.804870	-0.363963	-0.008622
4	6	0	1.307094	-1.631057	-0.044050
5	6	0	-0.040002	-1.859921	-0.042695
6	6	0	-0.969040	-0.787415	0.009382
7	7	0	-2.293606	-0.991054	0.030406
8	6	0	-3.222418	0.137189	0.181144
9	6	0	-2.628821	1.406457	-0.409988
10	7	0	-1.294638	1.628274	0.143558
11	6	0	-0.763792	2.983091	0.081918
12	6	0	-2.853762	-2.345515	0.048784
13	6	0	3.260596	-0.206958	-0.010361
14	8	0	3.941578	-1.201586	-0.057645
15	6	0	3.801850	1.194884	0.048040
16	1	0	1.398110	1.686994	0.016200
17	1	0	2.045697	-2.419642	-0.067865
18	1	0	-0.381785	-2.885196	-0.064419
19	1	0	-4.148328	-0.112474	-0.342520
20	1	0	-3.455149	0.278555	1.243332
21	1	0	-2.605319	1.340160	-1.508182
22	1	0	-3.263273	2.252310	-0.136658
23	1	0	-1.584336	3.685346	0.237559
24	1	0	-0.032699	3.138076	0.881891
25	1	0	-0.287659	3.208153	-0.884875
26	1	0	-2.554213	-2.899724	-0.846127
27	1	0	-2.530688	-2.893227	0.940216
28	1	0	-3.940353	-2.270010	0.061750
29	1	0	3.468261	1.716261	0.951347
30	1	0	4.889348	1.125021	0.056181
31	1	0	3.488554	1.779666	-0.823530

rmp2/6-31g(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.434349	0.554568	-0.055971
2	6	0	-0.945593	0.716500	-0.019668
3	7	0	-1.795485	-0.358428	0.010757
4	6	0	-1.304972	-1.625000	0.049424
5	6	0	0.047752	-1.851418	0.049338
6	6	0	0.972868	-0.781124	-0.008980
7	7	0	2.301294	-0.982412	-0.023998
8	6	0	3.222590	0.147071	-0.170762
9	6	0	2.610917	1.393115	0.434663
10	7	0	1.302054	1.617655	-0.172960
11	6	0	0.763880	2.969069	-0.078280
12	6	0	2.853978	-2.337679	-0.073819
13	6	0	-3.271718	-0.205308	0.012967
14	8	0	-3.941798	-1.210452	0.075043
15	6	0	-3.805014	1.194286	-0.066087
16	1	0	-1.400975	1.694364	-0.024719
17	1	0	-2.045881	-2.415088	0.076922
18	1	0	0.385282	-2.880221	0.072136
19	1	0	4.150206	-0.102556	0.352748
20	1	0	3.451278	0.309421	-1.230531
21	1	0	2.544472	1.296421	1.528645
22	1	0	3.248067	2.251223	0.206325
23	1	0	1.580017	3.673286	-0.242256
24	1	0	0.023714	3.126447	-0.866865
25	1	0	0.306595	3.175432	0.900220
26	1	0	2.544083	-2.910545	0.804346
27	1	0	2.537530	-2.856528	-0.983899
28	1	0	3.940516	-2.262505	-0.073019
29	1	0	-3.472239	1.695894	-0.978683
30	1	0	-4.892182	1.119530	-0.074416
31	1	0	-3.495366	1.786844	0.799160

rmp2/6-31g(d) scrf=(iefpcm,solvent=benzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.432498	0.553991	-0.065366
2	6	0	-0.945811	0.715089	-0.026162
3	7	0	-1.795590	-0.361079	0.007269
4	6	0	-1.302379	-1.627814	0.046483
5	6	0	0.049129	-1.853079	0.044133
6	6	0	0.973115	-0.780648	-0.014906
7	7	0	2.299608	-0.980184	-0.028703
8	6	0	3.221468	0.150192	-0.165364
9	6	0	2.603471	1.395220	0.433765
10	7	0	1.299477	1.619058	-0.186015
11	6	0	0.755727	2.966653	-0.067639
12	6	0	2.854795	-2.334486	-0.065165
13	6	0	-3.263030	-0.206214	0.015170
14	8	0	-3.939665	-1.209195	0.084121
15	6	0	-3.795903	1.192741	-0.065840
16	1	0	-1.400144	1.692904	-0.035419
17	1	0	-2.040636	-2.419381	0.076283
18	1	0	0.387970	-2.881186	0.067638
19	1	0	4.143457	-0.099639	0.367045
20	1	0	3.459710	0.310961	-1.222844
21	1	0	2.525814	1.298126	1.526759
22	1	0	3.241940	2.253505	0.211159
23	1	0	1.568696	3.675520	-0.226270
24	1	0	0.007962	3.132445	-0.846893
25	1	0	0.304038	3.154217	0.917113
26	1	0	2.551973	-2.895596	0.822797
27	1	0	2.531077	-2.864658	-0.965452
28	1	0	3.940694	-2.255656	-0.074076
29	1	0	-3.463954	1.691877	-0.979884
30	1	0	-4.882816	1.119725	-0.070386
31	1	0	-3.481406	1.785963	0.796942

rmp2/6-31g(d) scrf=(iefpcm,solvent= chloroform)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.431051	0.553266	-0.070668
2	6	0	-0.946153	0.713998	-0.028914
3	7	0	-1.795759	-0.363028	0.006101
4	6	0	-1.300713	-1.629897	0.045534
5	6	0	0.050190	-1.854318	0.042253
6	6	0	0.973404	-0.780425	-0.017128
7	7	0	2.298799	-0.978647	-0.030732
8	6	0	3.221968	0.152470	-0.153260
9	6	0	2.596403	1.396901	0.438179
10	7	0	1.298339	1.618840	-0.195732
11	6	0	0.751814	2.965201	-0.073314
12	6	0	2.856117	-2.332107	-0.065927
13	6	0	-3.258242	-0.206733	0.016389
14	8	0	-3.939082	-1.208781	0.081092
15	6	0	-3.790490	1.192564	-0.056428
16	1	0	-1.400500	1.691580	-0.038806
17	1	0	-2.037081	-2.422751	0.076279
18	1	0	0.389841	-2.882023	0.068606
19	1	0	4.136417	-0.097939	0.391407
20	1	0	3.474193	0.312817	-1.207347
21	1	0	2.506500	1.300743	1.530189
22	1	0	3.236340	2.255395	0.221423
23	1	0	1.563496	3.675248	-0.233284
24	1	0	0.000301	3.130228	-0.849003
25	1	0	0.302781	3.149599	0.913159
26	1	0	2.560808	-2.890188	0.826361
27	1	0	2.525332	-2.865299	-0.961498
28	1	0	3.941563	-2.250493	-0.084537
29	1	0	-3.462655	1.694114	-0.970516
30	1	0	-4.877434	1.121229	-0.054937
31	1	0	-3.468997	1.782311	0.806014

s-cis conformer
rb3lyp/6-31g(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.722150	1.292569	0.404651
2	7	0	-1.395874	1.589077	-0.128490
3	6	0	-0.470605	0.572169	-0.045181
4	6	0	-0.931129	-0.803802	-0.002744
5	7	0	-2.244916	-1.085914	-0.018622
6	6	0	-3.234400	-0.012562	-0.188624
7	6	0	0.889166	0.804068	-0.018465
8	7	0	1.811419	-0.216501	0.002419
9	6	0	1.394594	-1.509552	0.038434
10	6	0	0.059572	-1.818400	0.042285
11	6	0	-0.944252	2.975336	-0.091423
12	6	0	-2.723991	-2.471079	-0.042542
13	6	0	3.236473	0.169875	-0.002297
14	6	0	4.251061	-0.941594	0.038698
15	8	0	3.498387	1.342000	-0.036778
16	1	0	5.237601	-0.477693	0.033289
17	1	0	4.164170	-1.600369	-0.832297
18	1	0	4.148854	-1.548649	0.944785
19	1	0	-3.813630	-2.463806	-0.022840
20	1	0	-2.367768	-3.019857	0.835194
21	1	0	-2.397125	-2.988817	-0.951513
22	1	0	-0.486563	3.246170	0.871887
23	1	0	-1.802670	3.626648	-0.264794
24	1	0	-0.219694	3.155675	-0.891488
25	1	0	-3.461384	0.113094	-1.254587
26	1	0	-4.152845	-0.311239	0.323613
27	1	0	-3.400895	2.099422	0.118163
28	1	0	-2.714633	1.233836	1.503969
29	1	0	2.153833	-2.277455	0.058139
30	1	0	-0.220396	-2.862636	0.062187
31	1	0	1.325609	1.790870	-0.023385

rb3lyp/6-31g(d) scrf=(iefpcm,solvent=benzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.716713	1.287382	0.419079
2	7	0	-1.400764	1.587895	-0.138655
3	6	0	-0.470287	0.574307	-0.053121
4	6	0	-0.929054	-0.802346	-0.009657
5	7	0	-2.239943	-1.086966	-0.023962
6	6	0	-3.236575	-0.016706	-0.167303
7	6	0	0.887458	0.809384	-0.025607
8	7	0	1.812557	-0.210573	-0.002811
9	6	0	1.396342	-1.505549	0.032454
10	6	0	0.063419	-1.816253	0.034605
11	6	0	-0.951630	2.973542	-0.090309
12	6	0	-2.715207	-2.473029	-0.051683
13	6	0	3.230072	0.169514	-0.003909
14	6	0	4.241552	-0.942446	0.069120
15	8	0	3.502274	1.341715	-0.056852
16	1	0	5.228774	-0.481105	0.084862
17	1	0	4.173568	-1.605678	-0.799612
18	1	0	4.113197	-1.544116	0.974697
19	1	0	-3.804695	-2.466806	-0.052289
20	1	0	-2.371279	-3.017656	0.833331
21	1	0	-2.369444	-2.990461	-0.953049
22	1	0	-0.492443	3.236527	0.874642
23	1	0	-1.812029	3.623911	-0.256831
24	1	0	-0.227778	3.161326	-0.888986
25	1	0	-3.486732	0.110032	-1.227544
26	1	0	-4.141588	-0.321432	0.364365
27	1	0	-3.402053	2.093301	0.147318
28	1	0	-2.686410	1.225685	1.517648
29	1	0	2.155406	-2.273052	0.050777
30	1	0	-0.214240	-2.860767	0.053702
31	1	0	1.320336	1.797289	-0.032237

rb3lyp/6-31g(d) scrf=(iefpcm,solvent=chloroform)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.715483	1.285776	0.419762
2	7	0	-1.402703	1.587650	-0.145796
3	6	0	-0.470069	0.575185	-0.056710
4	6	0	-0.928038	-0.801859	-0.011444
5	7	0	-2.237432	-1.087640	-0.026064
6	6	0	-3.236487	-0.018942	-0.162957
7	6	0	0.886473	0.811766	-0.027352
8	7	0	1.813301	-0.207792	-0.002882
9	6	0	1.397244	-1.503867	0.033496
10	6	0	0.065419	-1.815251	0.035014
11	6	0	-0.954124	2.972725	-0.089133
12	6	0	-2.711674	-2.474090	-0.051093
13	6	0	3.226250	0.169091	-0.002663
14	6	0	4.237262	-0.943254	0.067137
15	8	0	3.503624	1.342200	-0.052673
16	1	0	5.225088	-0.483273	0.080882
17	1	0	4.165449	-1.606025	-0.801355
18	1	0	4.109536	-1.545195	0.972377
19	1	0	-3.800987	-2.467574	-0.057729
20	1	0	-2.371422	-3.014823	0.837550
21	1	0	-2.360107	-2.993661	-0.948636
22	1	0	-0.497676	3.230692	0.878564
23	1	0	-1.814592	3.623268	-0.254694
24	1	0	-0.227484	3.164592	-0.884308
25	1	0	-3.492874	0.106376	-1.221712
26	1	0	-4.137421	-0.325311	0.374226
27	1	0	-3.403305	2.090370	0.150849
28	1	0	-2.678375	1.224853	1.518009
29	1	0	2.155964	-2.271319	0.053970
30	1	0	-0.211080	-2.859922	0.056274
31	1	0	1.317495	1.800147	-0.034038

rmp2/6-31g(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.693833	1.286863	0.426581
2	7	0	-1.395015	1.579666	-0.171185
3	6	0	-0.472995	0.567244	-0.057623
4	6	0	-0.936031	-0.797631	-0.006581
5	7	0	-2.251904	-1.072179	-0.012745
6	6	0	-3.232000	0.004899	-0.174522
7	6	0	0.894156	0.805494	-0.026307
8	7	0	1.803262	-0.218892	0.001095
9	6	0	1.387904	-1.511627	0.040153
10	6	0	0.047284	-1.813745	0.045272
11	6	0	-0.929520	2.960044	-0.085060
12	6	0	-2.729885	-2.455173	-0.054433
13	6	0	3.235497	0.162961	-0.000303
14	6	0	4.234828	-0.955273	0.046176
15	8	0	3.502241	1.342992	-0.037445
16	1	0	5.222950	-0.495873	0.041673
17	1	0	4.141337	-1.609821	-0.824371
18	1	0	4.122497	-1.553132	0.954390
19	1	0	-3.818584	-2.440535	-0.025898
20	1	0	-2.367767	-3.011508	0.814251
21	1	0	-2.408396	-2.954899	-0.973708
22	1	0	-0.490188	3.196315	0.894048
23	1	0	-1.781942	3.616904	-0.260526
24	1	0	-0.191850	3.148768	-0.868299
25	1	0	-3.460814	0.147715	-1.237068
26	1	0	-4.148722	-0.291553	0.343592
27	1	0	-3.375297	2.107275	0.187776
28	1	0	-2.631599	1.201041	1.521677
29	1	0	2.144922	-2.283728	0.062387
30	1	0	-0.231963	-2.859939	0.066445
31	1	0	1.330667	1.794528	-0.037074

rmp2/6-31g(d) scrf=(iefpcm,solvent=benzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.686563	1.282910	0.439375
2	7	0	-1.400279	1.578576	-0.185560
3	6	0	-0.472423	0.568881	-0.066474
4	6	0	-0.934037	-0.796126	-0.013547
5	7	0	-2.246878	-1.073057	-0.018750
6	6	0	-3.234391	0.001261	-0.151202
7	6	0	0.892388	0.810230	-0.031219
8	7	0	1.804171	-0.213557	-0.002594
9	6	0	1.389376	-1.507805	0.033747
10	6	0	0.050989	-1.812049	0.035794
11	6	0	-0.936138	2.957788	-0.085389
12	6	0	-2.722348	-2.456741	-0.060852
13	6	0	3.229298	0.162666	-0.000080
14	6	0	4.225912	-0.955663	0.071753
15	8	0	3.504943	1.342134	-0.051646
16	1	0	5.214463	-0.498400	0.086201
17	1	0	4.148368	-1.612588	-0.798120
18	1	0	4.090917	-1.550300	0.978363
19	1	0	-3.810985	-2.441814	-0.046166
20	1	0	-2.367754	-3.009193	0.813189
21	1	0	-2.387921	-2.956901	-0.974538
22	1	0	-0.499501	3.184740	0.897251
23	1	0	-1.789336	3.614481	-0.257329
24	1	0	-0.195502	3.153752	-0.863633
25	1	0	-3.489979	0.143989	-1.207279
26	1	0	-4.135779	-0.301037	0.389347
27	1	0	-3.374321	2.101903	0.215701
28	1	0	-2.599737	1.196673	1.532570
29	1	0	2.146012	-2.279868	0.053145
30	1	0	-0.225880	-2.858556	0.055020
31	1	0	1.325914	1.800200	-0.043654

rmp2/6-31g(d) scrf=(iefpcm,solvent= chloroform)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.682710	1.281426	0.442861
2	7	0	-1.402608	1.578522	-0.195554
3	6	0	-0.472028	0.569542	-0.072259
4	6	0	-0.933278	-0.795398	-0.016868
5	7	0	-2.244490	-1.073301	-0.022971
6	6	0	-3.234967	-0.000106	-0.142588
7	6	0	0.891333	0.812247	-0.034346
8	7	0	1.804611	-0.211188	-0.003139
9	6	0	1.389790	-1.506255	0.034092
10	6	0	0.052585	-1.811283	0.034444
11	6	0	-0.938050	2.956708	-0.085077
12	6	0	-2.719347	-2.457443	-0.060516
13	6	0	3.225535	0.162143	0.001845
14	6	0	4.221582	-0.956324	0.072267
15	8	0	3.505579	1.341972	-0.047323
16	1	0	5.210619	-0.500344	0.086511
17	1	0	4.141771	-1.612649	-0.797659
18	1	0	4.085586	-1.551417	0.978244
19	1	0	-3.807889	-2.441641	-0.056933
20	1	0	-2.372261	-3.004035	0.820093
21	1	0	-2.375186	-2.962091	-0.967702
22	1	0	-0.503325	3.176510	0.900100
23	1	0	-1.791083	3.614379	-0.254108
24	1	0	-0.195094	3.157531	-0.859843
25	1	0	-3.502133	0.142265	-1.195631
26	1	0	-4.129515	-0.304682	0.407536
27	1	0	-3.373589	2.099516	0.226308
28	1	0	-2.583810	1.194864	1.534903
29	1	0	2.145990	-2.278423	0.056281
30	1	0	-0.223204	-2.857926	0.056471
31	1	0	1.323249	1.802606	-0.047466

6-7. 1,4-Dimethyl-1,2,3,4-tetrahydropyrazino[2,3-d]pyridazine (**11a**)

rb3lyp/6-31g(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.301682	0.707389	0.043126
2	6	0	-1.565712	1.315670	0.048320
3	7	0	-2.734180	0.663936	0.020453
4	7	0	-2.734173	-0.663962	-0.020447
5	6	0	-1.565700	-1.315684	-0.048324
6	6	0	-0.301676	-0.707392	-0.043135
7	7	0	0.892770	-1.411057	-0.133975
8	6	0	2.095235	-0.707886	0.287204
9	6	0	2.095232	0.707905	-0.287199
10	7	0	0.892757	1.411066	0.133966
11	6	0	0.888971	2.856742	-0.000838
12	6	0	0.889000	-2.856733	0.000842
13	1	0	1.897282	-3.229015	-0.200035
14	1	0	0.214461	-3.307898	-0.733433
15	1	0	0.585641	-3.197154	1.004416
16	1	0	1.897250	3.229032	0.200038
17	1	0	0.214430	3.307893	0.733444
18	1	0	0.585604	3.197170	-1.004407
19	1	0	2.182993	0.658457	-1.385352
20	1	0	2.967074	1.251465	0.093016
21	1	0	2.967085	-1.251438	-0.093002
22	1	0	2.182981	-0.658437	1.385358
23	1	0	-1.658501	-2.396814	-0.077769
24	1	0	-1.658525	2.396798	0.077771

rb3lyp/6-31g(d) scrf=(iefpcm,solvent=benzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.300571	0.708853	0.040250
2	6	0	-1.565197	1.317238	0.043561
3	7	0	-2.734497	0.665060	0.018602
4	7	0	-2.734630	-0.664518	-0.018597
5	6	0	-1.565460	-1.316925	-0.043558
6	6	0	-0.300715	-0.708791	-0.040250
7	7	0	0.889683	-1.410873	-0.125144
8	6	0	2.096916	-0.707458	0.287973
9	6	0	2.097066	0.707037	-0.287957
10	7	0	0.889970	1.410698	0.125142
11	6	0	0.888801	2.859003	0.004574
12	6	0	0.888216	-2.859179	-0.004593
13	1	0	1.897753	-3.226509	-0.205505
14	1	0	0.216712	-3.304797	-0.744927
15	1	0	0.583159	-3.207057	0.995171
16	1	0	1.898423	3.226123	0.205441
17	1	0	0.217422	3.304772	0.744930
18	1	0	0.583773	3.206929	-0.995181
19	1	0	2.188325	0.659113	-1.385059
20	1	0	2.965274	1.252315	0.095973
21	1	0	2.965020	-1.252912	-0.095942
22	1	0	2.188166	-0.659550	1.385076
23	1	0	-1.656257	-2.398128	-0.068935
24	1	0	-1.655785	2.398458	0.068932

rb3lyp/6-31g(d) scrf=(iefpcm,solvent=chloroform)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.300162	0.709722	0.038193
2	6	0	-1.565347	1.317732	0.040333
3	7	0	-2.734946	0.664574	0.017423
4	7	0	-2.734632	-0.665858	-0.017397
5	6	0	-1.564730	-1.318470	-0.040320
6	6	0	-0.299826	-0.709866	-0.038186
7	7	0	0.888438	-1.410463	-0.119104
8	6	0	2.098436	-0.706263	0.288542
9	6	0	2.098121	0.707253	-0.288446
10	7	0	0.887762	1.410886	0.119118
11	6	0	0.887275	2.860797	0.008236
12	6	0	0.888667	-2.860382	-0.008363
13	1	0	1.899298	-3.224362	-0.208067
14	1	0	0.219922	-3.302124	-0.753489
15	1	0	0.581416	-3.213385	0.988457
16	1	0	1.897724	3.225294	0.207909
17	1	0	0.218308	3.302288	0.753313
18	1	0	0.579862	3.213552	-0.988622
19	1	0	2.191697	0.660169	-1.384881
20	1	0	2.963908	1.253941	0.097711
21	1	0	2.964503	-1.252549	-0.097553
22	1	0	2.191919	-0.659138	1.384983
23	1	0	-1.654193	-2.399742	-0.063066
24	1	0	-1.655316	2.398962	0.063098

rmp2/6-31g(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.293650	0.705375	0.061254
2	6	0	-1.556127	1.316529	0.087964
3	7	0	-2.733886	0.669469	0.039960
4	7	0	-2.733330	-0.671735	-0.039954
5	6	0	-1.555038	-1.317825	-0.087967
6	6	0	-0.293058	-0.705633	-0.061260
7	7	0	0.900011	-1.405990	-0.191967
8	6	0	2.083662	-0.704345	0.280962
9	6	0	2.083066	0.706092	-0.280955
10	7	0	0.898817	1.406735	0.191967
11	6	0	0.882818	2.842033	-0.042645
12	6	0	0.885269	-2.841303	0.042639
13	1	0	1.893703	-3.223136	-0.130340
14	1	0	0.215652	-3.332845	-0.666081
15	1	0	0.575924	-3.104258	1.065166
16	1	0	1.890905	3.224758	0.130381
17	1	0	0.212723	3.332980	0.666041
18	1	0	0.573289	3.104709	-1.065186
19	1	0	2.133312	0.663851	-1.380713
20	1	0	2.965719	1.245049	0.080401
21	1	0	2.966773	-1.242557	-0.080391
22	1	0	2.133863	-0.662063	1.380720
23	1	0	-1.651415	-2.397346	-0.152687
24	1	0	-1.653382	2.395974	0.152702

rmp2/6-31g(d) scrf=(iefpcm,solvent=benzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.292808	0.707235	-0.057146
2	6	0	1.555150	1.319772	-0.077948
3	7	0	2.733874	0.672331	-0.034983
4	7	0	2.734303	-0.670579	0.034992
5	6	0	1.555992	-1.318770	0.077947
6	6	0	0.293265	-0.707037	0.057144
7	7	0	-0.895645	-1.405873	0.182290
8	6	0	-2.085266	-0.705364	-0.281661
9	6	0	-2.085720	0.704016	0.281682
10	7	0	-0.896564	1.405297	-0.182289
11	6	0	-0.885092	2.844702	0.033858
12	6	0	-0.883199	-2.845267	-0.033883
13	1	0	-1.892557	-3.221927	0.142406
14	1	0	-0.214852	-3.329164	0.681305
15	1	0	-0.574046	-3.119140	-1.052957
16	1	0	-1.894718	3.220655	-0.142407
17	1	0	-0.217108	3.329049	-0.681362
18	1	0	-0.576099	3.118807	1.052920
19	1	0	-2.141123	0.663718	1.380550
20	1	0	-2.964762	1.244280	-0.084631
21	1	0	-2.963956	-1.246192	0.084662
22	1	0	-2.140712	-0.665097	-1.380528
23	1	0	1.651025	-2.398855	0.133623
24	1	0	1.649504	2.399914	-0.133609

rmp2/6-31g(d) scrf=(iefpcm,solvent= chloroform)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.292410	0.708359	-0.054571
2	6	0	1.554859	1.321422	-0.071644
3	7	0	2.734013	0.673413	-0.031899
4	7	0	2.734718	-0.670539	0.031912
5	6	0	1.556242	-1.319779	0.071645
6	6	0	0.293160	-0.708034	0.054570
7	7	0	-0.893360	-1.405565	0.176083
8	6	0	-2.086574	-0.705467	-0.282079
9	6	0	-2.087316	0.703255	0.282115
10	7	0	-0.894865	1.404621	-0.176081
11	6	0	-0.885601	2.846412	0.028290
12	6	0	-0.882496	-2.847340	-0.028332
13	1	0	-1.892269	-3.220884	0.150459
14	1	0	-0.214395	-3.326212	0.690484
15	1	0	-0.573879	-3.128139	-1.045300
16	1	0	-1.895810	3.218798	-0.150465
17	1	0	-0.218090	3.326020	-0.690581
18	1	0	-0.577254	3.127595	1.045234
19	1	0	-2.146000	0.664140	1.380409
20	1	0	-2.964045	1.244438	-0.087269
21	1	0	-2.962726	-1.247571	0.087321
22	1	0	-2.145325	-0.666406	-1.380372
23	1	0	1.650320	-2.400214	0.121634
24	1	0	1.647822	2.401951	-0.121610

rb3lyp/cc-pvtz

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.302977	-0.704959	0.042119
2	6	0	1.561615	-1.311152	0.046562
3	7	0	2.724338	-0.659577	0.019492
4	7	0	2.724334	0.659592	-0.019491
5	6	0	1.561608	1.311161	-0.046562
6	6	0	0.302974	0.704961	-0.042119
7	7	0	-0.886836	1.406410	-0.130749
8	6	0	-2.090339	0.706855	0.281630
9	6	0	-2.090336	-0.706866	-0.281628
10	7	0	-0.886828	-1.406415	0.130748
11	6	0	-0.887572	-2.849283	0.000495
12	6	0	-0.887589	2.849278	-0.000496
13	1	0	-1.889472	3.218215	-0.212755
14	1	0	-0.207635	3.301299	-0.721731
15	1	0	-0.599504	3.189873	1.002721
16	1	0	-1.889454	-3.218225	0.212753
17	1	0	-0.207617	-3.301300	0.721731
18	1	0	-0.599485	-3.189877	-1.002722
19	1	0	-2.184825	-0.664314	-1.375369
20	1	0	-2.955354	-1.247743	0.104057
21	1	0	-2.955361	1.247727	-0.104053
22	1	0	-2.184825	0.664302	1.375371
23	1	0	1.654215	2.387668	-0.075124
24	1	0	1.654228	-2.387658	0.075124

6-8. Acetylated 1,4-dimethyl-1,2,3,4-tetrahydropyrazino[2,3-d]pyridazine (**11a-Ac**$^+$)

s-trans conformer

rb3lyp/6-31g(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.784195	1.224303	-0.354111
2	7	0	-1.437325	1.581669	0.087163
3	6	0	-0.489132	0.601946	0.032237
4	6	0	-0.879275	-0.785598	-0.007078
5	7	0	-2.176157	-1.138884	0.003892
6	6	0	-3.200077	-0.113874	0.248482
7	6	0	-2.586243	-2.546868	0.004215
8	6	0	-1.045516	2.988409	0.057596
9	6	0	0.875369	0.857444	0.017089
10	7	0	1.779075	-0.157067	-0.001045
11	7	0	1.460527	-1.442745	-0.037380
12	6	0	0.176272	-1.738944	-0.043097
13	6	0	3.232156	0.179433	0.007260
14	6	0	4.167402	-0.989737	-0.023575
15	8	0	3.518035	1.344100	0.037126
16	1	0	5.184818	-0.598031	-0.011431
17	1	0	4.006372	-1.595072	-0.920608
18	1	0	4.003751	-1.643296	0.838493
19	1	0	-0.318519	3.193700	0.849141
20	1	0	-1.928713	3.600411	0.247291
21	1	0	-0.615892	3.281860	-0.910517
22	1	0	-3.670947	-2.592850	-0.092952
23	1	0	-2.297691	-3.047715	0.935859
24	1	0	-2.144083	-3.076374	-0.844908
25	1	0	-4.133245	-0.444798	-0.214040
26	1	0	-3.371118	-0.011972	1.327462
27	1	0	-2.843610	1.181074	-1.451205
28	1	0	-3.477600	1.995921	-0.011191
29	1	0	-0.033663	-2.801112	-0.062126
30	1	0	1.312459	1.845555	0.021210

rb3lyp/6-31g(d) scrf=(iefpcm,solvent=benzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.786622	1.220507	-0.348192
2	7	0	-1.439890	1.580731	0.091300
3	6	0	-0.489727	0.604126	0.033663
4	6	0	-0.877249	-0.784341	-0.007560
5	7	0	-2.170284	-1.140830	0.007763
6	6	0	-3.197981	-0.119254	0.251628
7	6	0	-2.576078	-2.549736	0.002572
8	6	0	-1.050319	2.986810	0.050408
9	6	0	0.873052	0.862562	0.016530
10	7	0	1.780261	-0.150755	-0.003203
11	7	0	1.463111	-1.439125	-0.043741
12	6	0	0.180621	-1.736568	-0.049991
13	6	0	3.222598	0.179784	0.008255
14	6	0	4.157319	-0.990636	-0.016527
15	8	0	3.521927	1.344165	0.036918
16	1	0	5.175086	-0.600847	0.001758
17	1	0	4.000215	-1.594634	-0.914709
18	1	0	3.986256	-1.642667	0.844811
19	1	0	-0.324227	3.199941	0.840571
20	1	0	-1.935418	3.598004	0.232213
21	1	0	-0.619116	3.271048	-0.919664
22	1	0	-3.661023	-2.597386	-0.085866
23	1	0	-2.276510	-3.053358	0.928720
24	1	0	-2.138100	-3.071332	-0.853066
25	1	0	-4.129162	-0.452518	-0.211869
26	1	0	-3.368075	-0.021532	1.330653
27	1	0	-2.846847	1.180061	-1.444972
28	1	0	-3.481088	1.988669	-0.000658
29	1	0	-0.029018	-2.798374	-0.074895
30	1	0	1.305542	1.851937	0.022079

rb3lyp/6-31g(d) scrf=(iefpcm,solvent=chloroform)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.786622	1.220507	-0.348192
2	7	0	-1.439890	1.580731	0.091300
3	6	0	-0.489727	0.604126	0.033663
4	6	0	-0.877249	-0.784341	-0.007560
5	7	0	-2.170284	-1.140830	0.007763
6	6	0	-3.197981	-0.119254	0.251628
7	6	0	-2.576078	-2.549736	0.002572
8	6	0	-1.050319	2.986810	0.050408
9	6	0	0.873052	0.862562	0.016530
10	7	0	1.780261	-0.150755	-0.003203
11	7	0	1.463111	-1.439125	-0.043741
12	6	0	0.180621	-1.736568	-0.049991
13	6	0	3.222598	0.179784	0.008255
14	6	0	4.157319	-0.990636	-0.016527
15	8	0	3.521927	1.344165	0.036918
16	1	0	5.175086	-0.600847	0.001758
17	1	0	4.000215	-1.594634	-0.914709
18	1	0	3.986256	-1.642667	0.844811
19	1	0	-0.324227	3.199941	0.840571
20	1	0	-1.935418	3.598004	0.232213
21	1	0	-0.619116	3.271048	-0.919664
22	1	0	-3.661023	-2.597386	-0.085866
23	1	0	-2.276510	-3.053358	0.928720
24	1	0	-2.138100	-3.071332	-0.853066
25	1	0	-4.129162	-0.452518	-0.211869
26	1	0	-3.368075	-0.021532	1.330653
27	1	0	-2.846847	1.180061	-1.444972
28	1	0	-3.481088	1.988669	-0.000658
29	1	0	-0.029018	-2.798374	-0.074895
30	1	0	1.305542	1.851937	0.022079

rmp2/6-31g(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.777023	1.220623	0.346417
2	7	0	1.429423	1.573662	-0.092749
3	6	0	0.491276	0.599572	-0.028487
4	6	0	0.883795	-0.786539	0.011151
5	7	0	2.187727	-1.125722	0.022529
6	6	0	3.185302	-0.099455	-0.282147
7	6	0	2.601174	-2.529850	0.004982
8	6	0	1.030038	2.978220	-0.034806
9	6	0	-0.881041	0.862202	-0.021054
10	7	0	-1.772657	-0.156463	-0.001551
11	7	0	-1.465800	-1.450465	0.035513
12	6	0	-0.160533	-1.736596	0.044740
13	6	0	-3.234659	0.172930	-0.010514
14	6	0	-4.150503	-1.005908	0.023083
15	8	0	-3.526939	1.344832	-0.042930
16	1	0	-5.170191	-0.621392	0.010059
17	1	0	-3.979842	-1.601272	0.922234
18	1	0	-3.976782	-1.653668	-0.838470
19	1	0	0.291060	3.185145	-0.812085
20	1	0	1.910268	3.589494	-0.234103
21	1	0	0.619690	3.250098	0.945517
22	1	0	3.678850	-2.567877	0.161110
23	1	0	2.363018	-3.006224	-0.952284
24	1	0	2.117943	-3.074244	0.819209
25	1	0	4.143219	-0.422276	0.134423
26	1	0	3.298840	0.013409	-1.367213
27	1	0	2.834790	1.156136	1.441210
28	1	0	3.460854	2.005439	0.012928
29	1	0	0.041760	-2.801677	0.057750
30	1	0	-1.320032	1.851976	-0.023223

rmp2/6-31g(d) scrf=(iefpcm,solvent=benzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.775580	1.218827	0.345624
2	7	0	1.431222	1.572750	-0.103154
3	6	0	0.491530	0.601180	-0.032768
4	6	0	0.882601	-0.785129	0.011100
5	7	0	2.183161	-1.127104	0.016846
6	6	0	3.186869	-0.102814	-0.275438
7	6	0	2.592296	-2.532339	0.001593
8	6	0	1.032362	2.976248	-0.033024
9	6	0	-0.879351	0.865989	-0.021525
10	7	0	-1.773419	-0.151964	0.000669
11	7	0	-1.467335	-1.447246	0.042603
12	6	0	-0.163168	-1.734520	0.052146
13	6	0	-3.225830	0.172477	-0.009870
14	6	0	-4.142562	-1.006147	0.015232
15	8	0	-3.529181	1.343596	-0.038434
16	1	0	-5.161886	-0.621721	-0.002954
17	1	0	-3.977009	-1.602493	0.914323
18	1	0	-3.962866	-1.650509	-0.847313
19	1	0	0.295329	3.191006	-0.809818
20	1	0	1.914276	3.587756	-0.222360
21	1	0	0.618599	3.236982	0.948766
22	1	0	3.672871	-2.571720	0.132206
23	1	0	2.329294	-3.012598	-0.946618
24	1	0	2.124885	-3.068725	0.829913
25	1	0	4.138153	-0.426798	0.154096
26	1	0	3.312264	0.005593	-1.359096
27	1	0	2.825414	1.158806	1.440837
28	1	0	3.462515	2.000548	0.012318
29	1	0	0.038713	-2.799365	0.072602
30	1	0	-1.314486	1.856782	-0.026605

rmp2/6-31g(d) scrf=(iefpcm,solvent= chloroform)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.773474	1.217243	0.349054
2	7	0	1.432449	1.572199	-0.109413
3	6	0	0.491471	0.602032	-0.036339
4	6	0	0.881986	-0.784322	0.008999
5	7	0	2.180633	-1.127764	0.013897
6	6	0	3.187903	-0.104111	-0.269323
7	6	0	2.588968	-2.533236	0.002480
8	6	0	1.034501	2.975306	-0.034515
9	6	0	-0.878496	0.867963	-0.021773
10	7	0	-1.774122	-0.149632	0.000024
11	7	0	-1.468101	-1.445658	0.040605
12	6	0	-0.164677	-1.733534	0.049532
13	6	0	-3.221241	0.172084	-0.008374
14	6	0	-4.138924	-1.006222	0.017100
15	8	0	-3.530586	1.342789	-0.035835
16	1	0	-5.158205	-0.621661	0.001582
17	1	0	-3.971716	-1.603413	0.915220
18	1	0	-3.961412	-1.648681	-0.847212
19	1	0	0.295246	3.192057	-0.808524
20	1	0	1.916715	3.586123	-0.224286
21	1	0	0.623197	3.233041	0.949052
22	1	0	3.669358	-2.571984	0.133271
23	1	0	2.325373	-3.014324	-0.944836
24	1	0	2.120382	-3.067113	0.831585
25	1	0	4.135163	-0.429712	0.167173
26	1	0	3.320436	0.003714	-1.351906
27	1	0	2.814789	1.157101	1.444470
28	1	0	3.463281	1.998068	0.020313
29	1	0	0.037511	-2.798226	0.069336
30	1	0	-1.311234	1.859468	-0.025383

s-cis conformer
rb3lyp/6-31g(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.444553	0.580266	-0.028649
2	6	0	-0.936440	0.730321	-0.006435
3	7	0	-1.771693	-0.345709	0.009834
4	7	0	-1.345518	-1.598629	0.039915
5	6	0	-0.045397	-1.797602	0.039894
6	6	0	0.939674	-0.771744	0.002624
7	7	0	2.257949	-1.028538	-0.016384
8	6	0	3.203484	0.071240	-0.248415
9	6	0	2.686702	1.368583	0.365008
10	7	0	1.318907	1.629854	-0.082758
11	6	0	0.826308	3.002249	-0.040060
12	6	0	2.769752	-2.403567	-0.027367
13	6	0	-3.277507	-0.220973	0.007673
14	8	0	-3.913772	-1.224469	0.087223
15	6	0	-3.823459	1.177560	-0.100009
16	1	0	-1.404540	1.701418	0.000107
17	1	0	0.240470	-2.842385	0.053671
18	1	0	4.157305	-0.193073	0.214917
19	1	0	3.369905	0.195582	-1.325762
20	1	0	2.742682	1.317964	1.462004
21	1	0	3.322838	2.192937	0.034109
22	1	0	1.663704	3.680086	-0.212643
23	1	0	0.095604	3.166364	-0.838698
24	1	0	0.367611	3.254182	0.927199
25	1	0	2.375846	-2.967448	0.823256
26	1	0	2.508284	-2.919768	-0.958389
27	1	0	3.855863	-2.370059	0.058168
28	1	0	-3.478316	1.678061	-1.011158
29	1	0	-4.910457	1.096979	-0.129263
30	1	0	-3.540157	1.788068	0.764870

rb3lyp/6-31g(d) scrf=(iefpcm,solvent=benzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.442353	0.579870	-0.030508
2	6	0	-0.937763	0.728797	-0.007068
3	7	0	-1.773333	-0.348456	0.007261
4	7	0	-1.345445	-1.603982	0.033315
5	6	0	-0.045787	-1.800139	0.032457
6	6	0	0.938865	-0.772045	0.000421
7	7	0	2.254967	-1.027091	-0.015678
8	6	0	3.199512	0.072885	-0.251737
9	6	0	2.683905	1.370399	0.360026
10	7	0	1.314352	1.629641	-0.083131
11	6	0	0.819904	3.000859	-0.034723
12	6	0	2.770503	-2.399955	-0.016052
13	6	0	-3.264573	-0.219922	0.008510
14	8	0	-3.912036	-1.221095	0.091747
15	6	0	-3.811802	1.177462	-0.098592
16	1	0	-1.405411	1.699645	0.000070
17	1	0	0.243027	-2.843870	0.039745
18	1	0	4.153831	-0.190700	0.209470
19	1	0	3.361249	0.193032	-1.329844
20	1	0	2.742423	1.322115	1.456578
21	1	0	3.317769	2.193960	0.024135
22	1	0	1.658547	3.679213	-0.197381
23	1	0	0.093102	3.168949	-0.835565
24	1	0	0.355816	3.244476	0.931657
25	1	0	2.349120	-2.967193	0.818307
26	1	0	2.540484	-2.911014	-0.957787
27	1	0	3.852627	-2.362341	0.106157
28	1	0	-3.457394	1.683162	-1.002726
29	1	0	-4.898040	1.096356	-0.137310
30	1	0	-3.535352	1.782926	0.771751

rb3lyp/6-31g(d) scrf=(iefpcm,solvent=chloroform)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.440845	0.579459	-0.031783
2	6	0	-0.938627	0.727427	-0.006778
3	7	0	-1.774298	-0.350651	0.008220
4	7	0	-1.344839	-1.607669	0.035275
5	6	0	-0.045333	-1.801520	0.035252
6	6	0	0.938761	-0.771913	0.001546
7	7	0	2.253499	-1.026068	-0.014931
8	6	0	3.198343	0.074296	-0.249480
9	6	0	2.680646	1.372479	0.357886
10	7	0	1.311467	1.629266	-0.087840
11	6	0	0.815615	2.999993	-0.041613
12	6	0	2.770907	-2.398043	-0.011782
13	6	0	-3.257279	-0.219645	0.006099
14	8	0	-3.911981	-1.220802	0.070053
15	6	0	-3.804221	1.179011	-0.078889
16	1	0	-1.406126	1.697944	0.000602
17	1	0	0.246575	-2.844239	0.044395
18	1	0	4.150913	-0.188407	0.215214
19	1	0	3.362355	0.191100	-1.327335
20	1	0	2.736794	1.327099	1.454459
21	1	0	3.314063	2.195391	0.020263
22	1	0	1.653939	3.677848	-0.207408
23	1	0	0.086409	3.164853	-0.840742
24	1	0	0.353136	3.244291	0.925163
25	1	0	2.350673	-2.963196	0.824373
26	1	0	2.540359	-2.910825	-0.952193
27	1	0	3.852859	-2.357499	0.109220
28	1	0	-3.459206	1.693373	-0.981694
29	1	0	-4.890899	1.100339	-0.106082
30	1	0	-3.514736	1.774924	0.793524

rmp2/6-31g(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.448715	0.577744	0.020008
2	6	0	0.941369	0.737737	-0.006456
3	7	0	1.765910	-0.339028	-0.006053
4	7	0	1.354600	-1.604582	-0.008965
5	6	0	0.035263	-1.792766	-0.002937
6	6	0	-0.942144	-0.771330	0.009457
7	7	0	-2.266045	-1.018581	0.009740
8	6	0	-3.190927	0.084462	0.270646
9	6	0	-2.678723	1.353184	-0.386790
10	7	0	-1.316260	1.621114	0.069042
11	6	0	-0.818158	2.989342	-0.030646
12	6	0	-2.776851	-2.389907	0.060704
13	6	0	3.277668	-0.214197	-0.032401
14	8	0	3.907376	-1.200497	-0.299457
15	6	0	3.814987	1.147949	0.293566
16	1	0	1.410049	1.710400	-0.044729
17	1	0	-0.241485	-2.841164	0.017416
18	1	0	-4.163888	-0.179851	-0.152541
19	1	0	-3.311190	0.235589	1.350297
20	1	0	-2.723289	1.261123	-1.480441
21	1	0	-3.309712	2.193979	-0.087421
22	1	0	-1.651848	3.668922	0.146870
23	1	0	-0.069173	3.167973	0.744773
24	1	0	-0.387913	3.204643	-1.017361
25	1	0	-2.337342	-2.985452	-0.742441
26	1	0	-2.566864	-2.859513	1.027678
27	1	0	-3.855424	-2.355362	-0.089704
28	1	0	3.405430	1.527292	1.232828
29	1	0	4.897105	1.049333	0.380799
30	1	0	3.596490	1.860289	-0.507612

rmp2/6-31g(d) scrf=(iefpcm,solvent=benzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.446928	0.577888	0.025089
2	6	0	0.942255	0.736926	-0.001629
3	7	0	1.766884	-0.341388	-0.008427
4	7	0	1.353446	-1.607615	-0.021050
5	6	0	0.034141	-1.794016	-0.015036
6	6	0	-0.941900	-0.771014	0.007931
7	7	0	-2.263404	-1.017407	0.012871
8	6	0	-3.188700	0.085027	0.276265
9	6	0	-2.676045	1.355778	-0.375028
10	7	0	-1.312523	1.621146	0.079791
11	6	0	-0.812464	2.987565	-0.035016
12	6	0	-2.774881	-2.388507	0.047453
13	6	0	3.266365	-0.214220	-0.025691
14	8	0	3.906750	-1.206991	-0.254372
15	6	0	3.805085	1.155344	0.259994
16	1	0	1.410225	1.709805	-0.029484
17	1	0	-0.245231	-2.841602	-0.003551
18	1	0	-4.160407	-0.177803	-0.149309
19	1	0	-3.308517	0.229602	1.356414
20	1	0	-2.720616	1.269519	-1.468825
21	1	0	-3.305546	2.194977	-0.069557
22	1	0	-1.645269	3.668697	0.139120
23	1	0	-0.058934	3.172282	0.733781
24	1	0	-0.386461	3.189801	-1.026011
25	1	0	-2.341010	-2.971928	-0.767317
26	1	0	-2.555881	-2.870279	1.005865
27	1	0	-3.854196	-2.349613	-0.093001
28	1	0	3.408907	1.552480	1.197550
29	1	0	4.888411	1.062447	0.331947
30	1	0	3.568135	1.849768	-0.550934

rmp2/6-31g(d) scrf=(iefpcm,solvent= chloroform)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.445395	0.576714	0.036902
2	6	0	0.943152	0.733643	0.013980
3	7	0	1.767490	-0.345885	-0.001171
4	7	0	1.350673	-1.611960	-0.023285
5	6	0	0.031189	-1.795612	-0.022348
6	6	0	-0.943414	-0.770843	0.004567
7	7	0	-2.263763	-1.015005	0.003017
8	6	0	-3.191088	0.087508	0.261197
9	6	0	-2.667784	1.362299	-0.372292
10	7	0	-1.309121	1.620348	0.101391
11	6	0	-0.804735	2.986414	0.002290
12	6	0	-2.778972	-2.384915	0.023081
13	6	0	3.260240	-0.217645	-0.015735
14	8	0	3.908166	-1.224447	-0.153597
15	6	0	3.799887	1.170979	0.147531
16	1	0	1.410720	1.706513	0.002485
17	1	0	-0.251631	-2.842229	-0.021091
18	1	0	-4.156657	-0.170928	-0.180181
19	1	0	-3.324754	0.222218	1.340667
20	1	0	-2.698359	1.285690	-1.467136
21	1	0	-3.299153	2.199795	-0.066866
22	1	0	-1.637406	3.667213	0.177597
23	1	0	-0.054783	3.161144	0.776698
24	1	0	-0.372100	3.195806	-0.984134
25	1	0	-2.342436	-2.962378	-0.794341
26	1	0	-2.565160	-2.874055	0.978646
27	1	0	-3.857310	-2.340842	-0.121864
28	1	0	3.431127	1.637278	1.063933
29	1	0	4.884976	1.086385	0.195394
30	1	0	3.532159	1.800227	-0.705728

6-9. 5,8-Dimethyl-5,6,7,8-tetrahydropyrazino[2,3-c]pyridazine (**11a′**)

rb3lyp/6-31g(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.807400	1.892908	0.046993
2	6	0	-2.189384	1.654293	0.018141
3	7	0	-2.736370	0.447460	-0.022392
4	7	0	-1.920970	-0.619926	-0.043497
5	6	0	-0.598145	-0.479379	-0.038310
6	6	0	0.050167	0.801493	0.037999
7	7	0	0.169701	-1.632874	-0.141559
8	6	0	1.551436	-1.544684	0.294798
9	6	0	2.197626	-0.286848	-0.278857
10	7	0	1.429652	0.885793	0.117445
11	6	0	-0.488157	-2.924424	-0.007437
12	6	0	2.072169	2.181764	0.001707
13	1	0	-0.435741	2.910705	0.074885
14	1	0	-2.891063	2.485208	0.028901
15	1	0	2.088688	-2.425285	-0.074238
16	1	0	1.641935	-1.536853	1.394844
17	1	0	3.213428	-0.185527	0.118342
18	1	0	2.271662	-0.377036	-1.374933
19	1	0	0.193756	-3.700284	-0.370129
20	1	0	-0.764003	-3.150756	1.034510
21	1	0	-1.401623	-2.929121	-0.601591
22	1	0	1.678142	2.871875	0.755243
23	1	0	3.143033	2.062132	0.185267
24	1	0	1.937819	2.641032	-0.991273

rb3lyp/6-31g(d) scrf=(iefpcm,solvent=benzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.832493	1.882238	0.044515
2	6	0	-2.211233	1.626132	0.019514
3	7	0	-2.743898	0.412841	-0.019305
4	7	0	-1.913404	-0.647396	-0.040324
5	6	0	-0.592215	-0.490314	-0.038988
6	6	0	0.040301	0.801963	0.033218
7	7	0	0.191251	-1.630465	-0.140043
8	6	0	1.573182	-1.522397	0.299938
9	6	0	2.204058	-0.258879	-0.275950
10	7	0	1.413863	0.905697	0.105008
11	6	0	-0.446502	-2.932998	-0.011558
12	6	0	2.041062	2.212280	0.004964
13	1	0	-0.474270	2.904576	0.069654
14	1	0	-2.921709	2.449640	0.031248
15	1	0	2.122125	-2.396535	-0.065025
16	1	0	1.657161	-1.510890	1.399606
17	1	0	3.213985	-0.139084	0.129136
18	1	0	2.288274	-0.351769	-1.370263
19	1	0	0.262470	-3.698753	-0.340399
20	1	0	-0.752573	-3.151805	1.023137
21	1	0	-1.338129	-2.967559	-0.637758
22	1	0	1.639230	2.888448	0.766722
23	1	0	3.112894	2.102258	0.185307
24	1	0	1.898899	2.678582	-0.982640

rb3lyp/6-31g(d) scrf=(iefpcm,solvent=chloroform)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.852919	1.873280	0.043702
2	6	0	-2.228792	1.602666	0.020990
3	7	0	-2.749483	0.384067	-0.017306
4	7	0	-1.906814	-0.669556	-0.038498
5	6	0	-0.587109	-0.498715	-0.039331
6	6	0	0.032207	0.802286	0.030424
7	7	0	0.209062	-1.628182	-0.139199
8	6	0	1.590203	-1.504207	0.304418
9	6	0	2.209064	-0.235879	-0.272325
10	7	0	1.401417	0.921636	0.096435
11	6	0	-0.412654	-2.939059	-0.015673
12	6	0	2.015199	2.236415	0.005191
13	1	0	-0.505792	2.899247	0.067438
14	1	0	-2.946825	2.419674	0.033543
15	1	0	2.149014	-2.372835	-0.057264
16	1	0	1.668790	-1.490211	1.403927
17	1	0	3.213882	-0.101820	0.139747
18	1	0	2.302228	-0.330552	-1.365268
19	1	0	0.313683	-3.696111	-0.324825
20	1	0	-0.736234	-3.156095	1.013895
21	1	0	-1.290181	-2.992605	-0.660730
22	1	0	1.608884	2.902342	0.773456
23	1	0	3.088462	2.135440	0.180039
24	1	0	1.863623	2.707049	-0.978351

rmp2/6-31g(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.762982	1.908165	0.063628
2	6	0	-2.145168	1.699245	0.022601
3	7	0	-2.729196	0.496903	-0.026698
4	7	0	-1.931520	-0.593747	-0.058896
5	6	0	-0.595338	-0.465612	-0.047645
6	6	0	0.073086	0.794577	0.050842
7	7	0	0.145082	-1.630628	-0.191719
8	6	0	1.511544	-1.569171	0.294578
9	6	0	2.183323	-0.329673	-0.267274
10	7	0	1.450924	0.849272	0.172056
11	6	0	-0.551549	-2.894388	0.009693
12	6	0	2.106841	2.129049	-0.032451
13	1	0	-0.371441	2.918876	0.106168
14	1	0	-2.833586	2.541272	0.034093
15	1	0	2.039825	-2.461992	-0.057438
16	1	0	1.567346	-1.553614	1.395512
17	1	0	3.206485	-0.256637	0.117449
18	1	0	2.233025	-0.402352	-1.364924
19	1	0	0.120051	-3.699500	-0.299237
20	1	0	-0.845186	-3.047002	1.057848
21	1	0	-1.452476	-2.908660	-0.600705
22	1	0	1.732402	2.861746	0.686490
23	1	0	3.175915	1.998382	0.146931
24	1	0	1.962070	2.523735	-1.049227

rmp2/6-31g(d) scrf=(iefpcm,solvent=benzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.791634	-1.897005	0.059610
2	6	0	2.170344	-1.668949	0.023180
3	7	0	2.737686	-0.458152	-0.023039
4	7	0	1.924100	0.623479	-0.054656
5	6	0	0.588982	0.476822	-0.047696
6	6	0	-0.061675	-0.795203	0.046069
7	7	0	-0.168820	1.628120	-0.190159
8	6	0	-1.536008	1.545816	0.298224
9	6	0	-2.191075	0.298769	-0.264723
10	7	0	-1.434196	-0.871222	0.159951
11	6	0	0.505764	2.905040	0.005710
12	6	0	-2.073880	-2.163362	-0.027634
13	1	0	0.414746	-2.913275	0.097340
14	1	0	2.869124	-2.502514	0.034860
15	1	0	-2.076990	2.431248	-0.051343
16	1	0	-1.586406	1.528699	1.398696
17	1	0	-3.208729	0.206124	0.128807
18	1	0	-2.252005	0.373798	-1.360992
19	1	0	-0.189692	3.697368	-0.280963
20	1	0	0.818995	3.055823	1.048137
21	1	0	1.391467	2.947018	-0.625802
22	1	0	-1.687859	-2.882741	0.698425
23	1	0	-3.143683	-2.043659	0.151972
24	1	0	-1.924876	-2.565030	-1.040249

rmp2/6-31g(d) scrf=(iefpcm,solvent= chloroform)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.811186	-1.889052	0.057595
2	6	0	2.187271	-1.647850	0.024070
3	7	0	2.743086	-0.431290	-0.020666
4	7	0	1.918603	0.643813	-0.052308
5	6	0	0.584392	0.484467	-0.047909
6	6	0	-0.053885	-0.795388	0.042838
7	7	0	-0.185339	1.626408	-0.189987
8	6	0	-1.552071	1.529361	0.301478
9	6	0	-2.196259	0.277541	-0.262288
10	7	0	-1.422785	-0.886244	0.151344
11	6	0	0.474179	2.911844	0.002846
12	6	0	-2.050562	-2.186704	-0.025190
13	1	0	0.444451	-2.909003	0.092206
14	1	0	2.893193	-2.475451	0.036257
15	1	0	-2.102415	2.409822	-0.044781
16	1	0	-1.597532	1.510178	1.401718
17	1	0	-3.209691	0.171835	0.137753
18	1	0	-2.265497	0.354592	-1.357515
19	1	0	-0.235818	3.695417	-0.270720
20	1	0	0.798125	3.062426	1.041879
21	1	0	1.350411	2.971143	-0.640711
22	1	0	-1.658208	-2.896334	0.706991
23	1	0	-3.121342	-2.074859	0.151878
24	1	0	-1.896137	-2.593891	-1.034274

rb3lyp/cc-pvtz

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.863281	-1.859900	0.044439
2	6	0	2.232841	-1.583229	0.017478
3	7	0	2.738757	-0.366482	-0.019755
4	7	0	1.895464	0.671641	-0.041175
5	6	0	0.583471	0.496435	-0.039285
6	6	0	-0.023422	-0.799875	0.036527
7	7	0	-0.216793	1.621920	-0.139056
8	6	0	-1.594338	1.493650	0.290556
9	6	0	-2.200527	0.218998	-0.272938
10	7	0	-1.393767	-0.926842	0.112271
11	6	0	0.394841	2.933267	-0.008932
12	6	0	-1.999185	-2.237578	0.003764
13	1	0	0.524123	-2.884052	0.070838
14	1	0	2.955333	-2.390026	0.027734
15	1	0	-2.154080	2.352286	-0.082133
16	1	0	-1.685749	1.490436	1.386263
17	1	0	-3.204818	0.085317	0.130593
18	1	0	-2.287117	0.304748	-1.364205
19	1	0	-0.312665	3.681790	-0.365014
20	1	0	0.666293	3.167035	1.027780
21	1	0	1.301517	2.975307	-0.603731
22	1	0	-1.580926	-2.916313	0.747377
23	1	0	-3.066519	-2.149275	0.196220
24	1	0	-1.862798	-2.689512	-0.987359

6-10. Acetylated 5,8-dimethyl-5,6,7,8-tetrahydropyrazino[2,3-c]pyridazine (**11a′-Ac**$^{+}$)

s-trans conformer

rb3lyp/6-31g(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.119048	-1.906303	0.079730
2	6	0	-1.241691	-1.691177	0.068781
3	7	0	-1.730384	-0.440513	0.012322
4	7	0	-0.959681	0.664376	-0.004447
5	6	0	0.352882	0.515180	-0.017412
6	6	0	0.991702	-0.804265	0.018599
7	7	0	1.129491	1.631029	-0.083305
8	6	0	2.515186	1.511311	0.365930
9	6	0	3.160862	0.276444	-0.245965
10	7	0	2.326263	-0.913196	-0.020448
11	6	0	2.970837	-2.230914	-0.053214
12	6	0	-3.202052	-0.238042	-0.009365
13	8	0	-3.889087	-1.221543	0.027389
14	6	0	0.497518	2.950109	-0.051256
15	6	0	-3.660504	1.186093	-0.077303
16	1	0	0.487975	-2.922356	0.107988
17	1	0	-1.983613	-2.479639	0.093410
18	1	0	3.062652	2.396693	0.034600
19	1	0	2.574355	1.471086	1.463360
20	1	0	3.316976	0.413914	-1.323327
21	1	0	4.133751	0.104066	0.220808
22	1	0	2.686379	-2.818182	0.825397
23	1	0	2.699010	-2.780834	-0.961481
24	1	0	4.051532	-2.091943	-0.039786
25	1	0	1.248045	3.697416	-0.314882
26	1	0	-0.313801	2.984900	-0.779889
27	1	0	0.086979	3.181929	0.940036
28	1	0	-3.285642	1.757502	0.777025
29	1	0	-3.283703	1.672219	-0.982527
30	1	0	-4.750745	1.183075	-0.079841

rb3lyp/6-31g(d) scrf=(iefpcm,solvent=benzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.118803	-1.907471	0.087227
2	6	0	-1.239821	-1.693982	0.076451
3	7	0	-1.731838	-0.442581	0.014824
4	7	0	-0.961105	0.664788	-0.004244
5	6	0	0.350406	0.515761	-0.017121
6	6	0	0.990568	-0.803692	0.019253
7	7	0	1.127262	1.630613	-0.082734
8	6	0	2.512952	1.509607	0.367136
9	6	0	3.157469	0.277422	-0.248509
10	7	0	2.321858	-0.912388	-0.027480
11	6	0	2.966179	-2.230148	-0.060280
12	6	0	-3.190510	-0.237822	-0.010989
13	8	0	-3.890605	-1.216113	0.033647
14	6	0	0.495302	2.947897	-0.041707
15	6	0	-3.646573	1.186888	-0.093486
16	1	0	0.489931	-2.922286	0.119265
17	1	0	-1.978448	-2.484342	0.104844
18	1	0	3.059946	2.395787	0.038418
19	1	0	2.570310	1.464835	1.464033
20	1	0	3.311875	0.415823	-1.325481
21	1	0	4.129418	0.102353	0.217661
22	1	0	2.695264	-2.809511	0.827522
23	1	0	2.676419	-2.785471	-0.959015
24	1	0	4.046376	-2.089969	-0.067359
25	1	0	1.247182	3.696694	-0.296179
26	1	0	-0.314469	2.988552	-0.771835
27	1	0	0.082017	3.171002	0.950580
28	1	0	-3.281508	1.760952	0.763148
29	1	0	-3.254858	1.667689	-0.994849
30	1	0	-4.736513	1.187012	-0.110323

rb3lyp/6-31g(d) scrf=(iefpcm,solvent=chloroform)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.118950	-1.908540	0.088158
2	6	0	-1.238392	-1.696332	0.077142
3	7	0	-1.732761	-0.444351	0.014996
4	7	0	-0.961934	0.664458	-0.003958
5	6	0	0.348918	0.515906	-0.018192
6	6	0	0.990304	-0.803414	0.018588
7	7	0	1.125503	1.630569	-0.085302
8	6	0	2.510570	1.509980	0.367768
9	6	0	3.156460	0.278284	-0.246173
10	7	0	2.319750	-0.911683	-0.029675
11	6	0	2.965147	-2.229012	-0.060503
12	6	0	-3.184054	-0.238176	-0.011060
13	8	0	-3.891910	-1.213599	0.032298
14	6	0	0.492682	2.946649	-0.041993
15	6	0	-3.638909	1.187422	-0.092342
16	1	0	0.491092	-2.922740	0.121508
17	1	0	-1.974834	-2.488191	0.105960
18	1	0	3.058150	2.395761	0.039659
19	1	0	2.564450	1.465189	1.464566
20	1	0	3.313966	0.415858	-1.322535
21	1	0	4.126272	0.102234	0.223358
22	1	0	2.697227	-2.805126	0.830075
23	1	0	2.671562	-2.786327	-0.956367
24	1	0	4.044837	-2.086855	-0.072340
25	1	0	1.244235	3.696341	-0.294565
26	1	0	-0.317344	2.987985	-0.771962
27	1	0	0.079225	3.167275	0.950876
28	1	0	-3.273424	1.759686	0.765217
29	1	0	-3.245259	1.668588	-0.992522
30	1	0	-4.728839	1.189556	-0.110093

rmp2/6-31g(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.127588	-1.905195	0.078425
2	6	0	-1.233943	-1.698532	0.062545
3	7	0	-1.722217	-0.443863	0.010308
4	7	0	-0.969279	0.665740	-0.008054
5	6	0	0.363738	0.503791	-0.023689
6	6	0	0.996333	-0.797299	0.014423
7	7	0	1.127860	1.622929	-0.114724
8	6	0	2.499085	1.507665	0.372638
9	6	0	3.152409	0.292171	-0.253416
10	7	0	2.334612	-0.898807	-0.003918
11	6	0	2.976893	-2.214118	-0.048709
12	6	0	-3.201478	-0.236498	-0.007538
13	8	0	-3.893751	-1.225452	0.033769
14	6	0	0.474550	2.928755	-0.035593
15	6	0	-3.640205	1.189531	-0.078010
16	1	0	0.498819	-2.922512	0.099718
17	1	0	-1.976026	-2.489116	0.085666
18	1	0	3.045037	2.404685	0.069568
19	1	0	2.531261	1.441237	1.469174
20	1	0	3.281393	0.437238	-1.332724
21	1	0	4.135361	0.127882	0.196232
22	1	0	2.655288	-2.818445	0.803137
23	1	0	2.740982	-2.735437	-0.982342
24	1	0	4.054674	-2.071212	0.015730
25	1	0	1.214356	3.688552	-0.289148
26	1	0	-0.342921	2.965535	-0.755451
27	1	0	0.074176	3.122448	0.966542
28	1	0	-3.259288	1.752668	0.776377
29	1	0	-3.259704	1.663851	-0.985245
30	1	0	-4.730050	1.192638	-0.079111

rmp2/6-31g(d) scrf=(iefpcm,solvent=benzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.128224	-1.905893	0.090377
2	6	0	-1.231542	-1.700936	0.074740
3	7	0	-1.723014	-0.446364	0.014149
4	7	0	-0.970219	0.664842	-0.009222
5	6	0	0.360982	0.504110	-0.025398
6	6	0	0.995438	-0.796120	0.013852
7	7	0	1.125650	1.623391	-0.119192
8	6	0	2.493937	1.505832	0.376670
9	6	0	3.150468	0.294996	-0.252725
10	7	0	2.330456	-0.897582	-0.016922
11	6	0	2.972005	-2.213420	-0.060185
12	6	0	-3.190133	-0.236564	-0.009957
13	8	0	-3.893547	-1.220088	0.042514
14	6	0	0.470944	2.926001	-0.021686
15	6	0	-3.626739	1.189325	-0.100205
16	1	0	0.501384	-2.922039	0.120561
17	1	0	-1.970167	-2.493578	0.105043
18	1	0	3.041253	2.404456	0.082056
19	1	0	2.518140	1.431968	1.472600
20	1	0	3.284518	0.444499	-1.330263
21	1	0	4.129762	0.126913	0.202027
22	1	0	2.676846	-2.803496	0.810862
23	1	0	2.703314	-2.747485	-0.976917
24	1	0	4.050723	-2.068444	-0.034842
25	1	0	1.209830	3.688973	-0.267436
26	1	0	-0.349803	2.970548	-0.737445
27	1	0	0.074169	3.105781	0.984665
28	1	0	-3.261413	1.756603	0.758207
29	1	0	-3.225662	1.657252	-1.001566
30	1	0	-4.716130	1.194758	-0.122269

rmp2/6-31g(d) scrf=(iefpcm,solvent= chloroform)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.128725	-1.906918	0.088745
2	6	0	-1.229938	-1.703032	0.073493
3	7	0	-1.723623	-0.448231	0.013427
4	7	0	-0.970679	0.663967	-0.010370
5	6	0	0.359368	0.504053	-0.029114
6	6	0	0.995273	-0.795621	0.012043
7	7	0	1.124300	1.623566	-0.126853
8	6	0	2.489246	1.506577	0.379568
9	6	0	3.150695	0.296634	-0.245233
10	7	0	2.328549	-0.896588	-0.019187
11	6	0	2.971507	-2.212024	-0.059016
12	6	0	-3.183911	-0.237152	-0.008895
13	8	0	-3.893662	-1.218095	0.040479
14	6	0	0.467860	2.924482	-0.025379
15	6	0	-3.620227	1.189411	-0.093408
16	1	0	0.502700	-2.922550	0.119873
17	1	0	-1.966339	-2.497276	0.103827
18	1	0	3.038635	2.404945	0.088788
19	1	0	2.504340	1.432425	1.475463
20	1	0	3.293429	0.445880	-1.321436
21	1	0	4.125566	0.127345	0.217834
22	1	0	2.678439	-2.798772	0.814770
23	1	0	2.699802	-2.748430	-0.973097
24	1	0	4.049786	-2.064701	-0.037537
25	1	0	1.205975	3.689018	-0.268420
26	1	0	-0.353286	2.969923	-0.740750
27	1	0	0.070874	3.100412	0.981675
28	1	0	-3.252938	1.752892	0.766603
29	1	0	-3.219508	1.660131	-0.993361
30	1	0	-4.709588	1.196070	-0.114012

s-cis conformer
rb3lyp/6-31g(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.406981	0.534587	0.012684
2	7	0	0.890299	0.771929	-0.001230
3	7	0	1.742818	-0.266649	-0.012066
4	6	0	1.334276	-1.546883	-0.068261
5	6	0	-0.009863	-1.858954	-0.080026
6	6	0	-0.958381	-0.822683	-0.019574
7	7	0	-2.282316	-1.020127	0.020832
8	6	0	-3.190689	0.114061	0.251619
9	6	0	-2.629556	1.389464	-0.362181
10	7	0	-1.252024	1.598148	0.075424
11	6	0	-0.704765	2.956674	0.035917
12	6	0	-2.838794	-2.376722	0.055037
13	6	0	3.183298	0.145544	0.034187
14	8	0	3.424593	1.309868	0.133327
15	6	0	4.194863	-0.967630	-0.051286
16	1	0	2.097139	-2.312248	-0.091835
17	1	0	-0.304041	-2.899207	-0.106526
18	1	0	-4.152902	-0.120997	-0.209840
19	1	0	-3.348932	0.240192	1.329985
20	1	0	-2.695419	1.348161	-1.459308
21	1	0	-3.230494	2.237241	-0.024725
22	1	0	-1.483803	3.649152	0.360782
23	1	0	0.149585	3.025469	0.709834
24	1	0	-0.370902	3.229062	-0.973338
25	1	0	-2.510676	-2.946873	-0.819645
26	1	0	-2.537315	-2.904557	0.967189
27	1	0	-3.926257	-2.309835	0.034057
28	1	0	4.090173	-1.541722	-0.978254
29	1	0	5.182008	-0.505045	-0.032008
30	1	0	4.113202	-1.655600	0.797601

rb3lyp/6-31g(d) scrf=(iefpcm,solvent=benzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.406630	0.538271	0.018607
2	7	0	0.888904	0.781258	0.002511
3	7	0	1.745349	-0.258261	-0.007574
4	6	0	1.338071	-1.541176	-0.061440
5	6	0	-0.002639	-1.856128	-0.073754
6	6	0	-0.954315	-0.821592	-0.014379
7	7	0	-2.274815	-1.023442	0.023217
8	6	0	-3.188823	0.105672	0.253893
9	6	0	-2.633816	1.382704	-0.358849
10	7	0	-1.257128	1.597794	0.080336
11	6	0	-0.715023	2.955808	0.025455
12	6	0	-2.827683	-2.381694	0.042199
13	6	0	3.173962	0.144935	0.033323
14	8	0	3.428725	1.310381	0.135273
15	6	0	4.184336	-0.968268	-0.061148
16	1	0	2.101100	-2.305735	-0.080790
17	1	0	-0.293427	-2.896851	-0.097795
18	1	0	-4.148486	-0.134136	-0.208745
19	1	0	-3.346947	0.228374	1.332235
20	1	0	-2.696863	1.340331	-1.455694
21	1	0	-3.238781	2.227092	-0.021254
22	1	0	-1.503462	3.650927	0.319692
23	1	0	0.124835	3.042383	0.715607
24	1	0	-0.361856	3.210072	-0.982149
25	1	0	-2.486101	-2.943066	-0.832390
26	1	0	-2.534288	-2.912938	0.954373
27	1	0	-3.914586	-2.316040	0.008878
28	1	0	4.060478	-1.552473	-0.978570
29	1	0	5.171606	-0.506458	-0.064040
30	1	0	4.116172	-1.647166	0.795588

rb3lyp/6-31g(d) scrf=(iefpcm,solvent=chloroform)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.406377	0.540542	0.020916
2	7	0	0.887982	0.787027	0.004409
3	7	0	1.747096	-0.253279	-0.007234
4	6	0	1.339938	-1.537732	-0.063922
5	6	0	0.001338	-1.854191	-0.076675
6	6	0	-0.952201	-0.820671	-0.013763
7	7	0	-2.270300	-1.025551	0.026132
8	6	0	-3.189324	0.100855	0.249195
9	6	0	-2.635108	1.378217	-0.361929
10	7	0	-1.260744	1.597143	0.084654
11	6	0	-0.722319	2.955228	0.029158
12	6	0	-2.819928	-2.385335	0.044359
13	6	0	3.168614	0.144656	0.031781
14	8	0	3.431209	1.311717	0.127312
15	6	0	4.179089	-0.968827	-0.055842
16	1	0	2.102754	-2.302027	-0.085811
17	1	0	-0.287543	-2.895217	-0.104174
18	1	0	-4.144970	-0.142845	-0.219028
19	1	0	-3.353403	0.223228	1.326417
20	1	0	-2.691147	1.334378	-1.458823
21	1	0	-3.243885	2.220917	-0.027765
22	1	0	-1.517227	3.649943	0.305953
23	1	0	0.105798	3.049301	0.732721
24	1	0	-0.354080	3.204464	-0.974467
25	1	0	-2.486176	-2.940992	-0.836671
26	1	0	-2.513620	-2.918893	0.950458
27	1	0	-3.906987	-2.321005	0.024362
28	1	0	4.059544	-1.552592	-0.973892
29	1	0	5.166772	-0.508105	-0.052776
30	1	0	4.103929	-1.648119	0.799602

rmp2/6-31g(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.431330	0.534426	0.015945
2	7	0	-0.910202	0.807684	0.028388
3	7	0	-1.771530	-0.271488	0.009807
4	6	0	-1.349349	-1.570999	0.049924
5	6	0	0.011645	-1.875022	0.071532
6	6	0	0.970102	-0.825565	0.006707
7	7	0	2.311988	-1.026448	-0.043193
8	6	0	3.229160	0.129010	-0.286634
9	6	0	2.683634	1.388149	0.401182
10	7	0	1.276588	1.608172	-0.013928
11	6	0	0.715336	2.985167	-0.005761
12	6	0	2.873813	-2.403768	-0.078666
13	6	0	-3.234461	0.133849	-0.066879
14	8	0	-3.498749	1.315201	-0.314390
15	6	0	-4.238194	-0.971125	0.182115
16	1	0	-2.108877	-2.346120	0.056802
17	1	0	0.308747	-2.920471	0.071131
18	1	0	4.211135	-0.129474	0.129096
19	1	0	3.334357	0.295848	-1.368919
20	1	0	2.763871	1.295404	1.496688
21	1	0	3.268908	2.260674	0.086092
22	1	0	1.522887	3.672526	-0.276245
23	1	0	-0.091746	3.046425	-0.741756
24	1	0	0.311446	3.249700	0.981870
25	1	0	2.513753	-2.978728	0.783673
26	1	0	2.598972	-2.917295	-1.010707
27	1	0	3.962659	-2.327377	-0.019415
28	1	0	-4.067220	-1.462076	1.148630
29	1	0	-5.227925	-0.504223	0.188817
30	1	0	-4.216986	-1.726585	-0.614945

rmp2/6-31g(d) scrf=(iefpcm,solvent=benzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.415186	0.526570	-0.025943
2	7	0	-0.900211	0.782786	-0.004972
3	7	0	-1.737571	-0.265720	0.002801
4	6	0	-1.328378	-1.551664	0.046115
5	6	0	0.015218	-1.855977	0.063400
6	6	0	0.960594	-0.814023	0.007287
7	7	0	2.286208	-1.006310	-0.008015
8	6	0	3.183022	0.127326	-0.254704
9	6	0	2.613316	1.382407	0.373359
10	7	0	1.252443	1.591321	-0.110754
11	6	0	0.687608	2.936648	-0.009298
12	6	0	2.838993	-2.361324	-0.039555
13	6	0	-3.176043	0.137808	-0.033447
14	8	0	-3.425173	1.310586	-0.155949
15	6	0	-4.172129	-0.977471	0.090813
16	1	0	-2.090712	-2.319375	0.054767
17	1	0	0.309622	-2.897835	0.075091
18	1	0	4.151607	-0.104738	0.194713
19	1	0	3.319945	0.263151	-1.333753
20	1	0	2.641519	1.311979	1.469500
21	1	0	3.217656	2.240932	0.070482
22	1	0	1.467828	3.645856	-0.286927
23	1	0	-0.153455	3.026062	-0.695986
24	1	0	0.336021	3.150170	1.006696
25	1	0	2.458897	-2.939040	0.806171
26	1	0	2.585877	-2.866005	-0.977342
27	1	0	3.922134	-2.290083	0.046331
28	1	0	-4.022507	-1.547237	1.010849
29	1	0	-5.159617	-0.517622	0.108629
30	1	0	-4.113827	-1.657249	-0.763217

rmp2/6-31g(d) scrf=(iefpcm,solvent= chloroform)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.414623	0.528500	-0.030523
2	7	0	-0.898937	0.787465	-0.007930
3	7	0	-1.739090	-0.260873	0.003741
4	6	0	-1.330308	-1.547858	0.051239
5	6	0	0.011228	-1.853985	0.067780
6	6	0	0.958445	-0.812899	0.006205
7	7	0	2.281646	-1.008464	-0.012376
8	6	0	3.184413	0.123030	-0.247333
9	6	0	2.612362	1.378012	0.377202
10	7	0	1.256570	1.590830	-0.121065
11	6	0	0.695090	2.936058	-0.015939
12	6	0	2.831722	-2.364964	-0.040890
13	6	0	-3.170929	0.137889	-0.029643
14	8	0	-3.427048	1.312625	-0.136539
15	6	0	-4.167172	-0.978629	0.076322
16	1	0	-2.092377	-2.315380	0.065148
17	1	0	0.303291	-2.896306	0.084262
18	1	0	4.147341	-0.113231	0.211322
19	1	0	3.331531	0.258913	-1.324758
20	1	0	2.628442	1.305335	1.473307
21	1	0	3.222084	2.234942	0.081465
22	1	0	1.479380	3.644823	-0.282851
23	1	0	-0.139765	3.032118	-0.709395
24	1	0	0.336030	3.145239	0.998568
25	1	0	2.455990	-2.937500	0.810074
26	1	0	2.569526	-2.871960	-0.974483
27	1	0	3.915332	-2.294188	0.036087
28	1	0	-4.026633	-1.553044	0.994714
29	1	0	-5.155365	-0.520415	0.085696
30	1	0	-4.096598	-1.653972	-0.779949

6-11. 4-Dimethylaminopyridazine (**10a**)

rb3lyp/6-31g(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.543112	0.006425	-0.087199
2	6	0	-0.171258	0.023206	-0.038441
3	6	0	0.587393	1.203508	-0.010767
4	6	0	0.604339	-1.168203	-0.014875
5	1	0	0.130824	2.186250	-0.005522
6	1	0	0.130922	-2.145021	-0.012521
7	7	0	2.645521	-0.072963	0.018757
8	7	0	1.931164	-1.204304	0.009556
9	6	0	1.973582	1.082988	0.011719
10	1	0	2.597570	1.974208	0.028491
11	6	0	-2.275485	1.257930	0.028802
12	6	0	-2.262234	-1.254115	0.034870
13	1	0	-3.342581	1.059866	-0.084434
14	1	0	-3.330619	-1.065195	-0.082181
15	1	0	-2.102315	-1.737383	1.009979
16	1	0	-1.960373	-1.957405	-0.749702
17	1	0	-1.979986	1.959707	-0.760563
18	1	0	-2.116465	1.748979	1.000811

rb3lyp/6-31g(d) scrf=(iefpcm,solvent=benzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.540009	0.006802	-0.049632
2	6	0	-0.173521	0.023667	-0.021766
3	6	0	0.587756	1.204498	-0.005456
4	6	0	0.602530	-1.169972	-0.007981
5	1	0	0.132051	2.187338	-0.001359
6	1	0	0.126752	-2.145441	-0.005899
7	7	0	2.645657	-0.073357	0.010016
8	7	0	1.929066	-1.205889	0.005304
9	6	0	1.973137	1.083520	0.006596
10	1	0	2.596062	1.975519	0.016290
11	6	0	-2.274280	1.262985	0.016057
12	6	0	-2.261413	-1.258239	0.019815
13	1	0	-3.342689	1.056917	-0.055885
14	1	0	-3.331265	-1.060273	-0.053794
15	1	0	-2.074733	-1.789327	0.963413
16	1	0	-1.984073	-1.920647	-0.808921
17	1	0	-2.000957	1.925110	-0.814955
18	1	0	-2.089399	1.799149	0.957708

rb3lyp/6-31g(d) scrf=(iefpcm,solvent=chloroform)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.538321	0.006984	-0.022046
2	6	0	-0.174906	0.023782	-0.009594
3	6	0	0.587897	1.204985	-0.002382
4	6	0	0.601563	-1.171174	-0.003179
5	1	0	0.132661	2.187872	-0.000434
6	1	0	0.124395	-2.145881	-0.001816
7	7	0	2.645767	-0.073531	0.004232
8	7	0	1.927815	-1.206821	0.002493
9	6	0	1.972687	1.083949	0.002731
10	1	0	2.594927	1.976402	0.006918
11	6	0	-2.273297	1.265489	0.007307
12	6	0	-2.261048	-1.260010	0.008468
13	1	0	-3.342481	1.055816	-0.026753
14	1	0	-3.331586	-1.057731	-0.027960
15	1	0	-2.051182	-1.827384	0.924704
16	1	0	-2.005341	-1.888456	-0.853496
17	1	0	-2.021605	1.894476	-0.856024
18	1	0	-2.063983	1.836343	0.922003

rmp2/6-31g(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.549626	0.002352	-0.212892
2	6	0	-0.174419	0.020634	-0.091497
3	6	0	0.578751	1.201737	-0.031539
4	6	0	0.597717	-1.165554	-0.054606
5	1	0	0.122888	2.185291	-0.029575
6	1	0	0.134553	-2.146686	-0.074745
7	7	0	2.646510	-0.067607	0.058200
8	7	0	1.933972	-1.211253	0.015786
9	6	0	1.964974	1.089534	0.036732
10	1	0	2.586214	1.981453	0.083103
11	6	0	-2.266063	1.239187	0.061785
12	6	0	-2.252743	-1.235305	0.100757
13	1	0	-3.329017	1.070321	-0.114902
14	1	0	-3.317876	-1.078527	-0.074150
15	1	0	-2.108544	-1.555062	1.142615
16	1	0	-1.925428	-2.038207	-0.562771
17	1	0	-1.938100	2.025345	-0.622320
18	1	0	-2.129974	1.590232	1.095294

rmp2/6-31g(d) scrf=(iefpcm,solvent=benzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.545680	0.003179	-0.194974
2	6	0	-0.175901	0.020747	-0.082455
3	6	0	0.580179	1.202175	-0.026053
4	6	0	0.596196	-1.167376	-0.047595
5	1	0	0.125321	2.185980	-0.019979
6	1	0	0.130258	-2.147207	-0.062445
7	7	0	2.647634	-0.068365	0.050198
8	7	0	1.932915	-1.212574	0.014046
9	6	0	1.965883	1.089654	0.033153
10	1	0	2.586060	1.982474	0.075592
11	6	0	-2.266181	1.244569	0.055209
12	6	0	-2.254867	-1.239071	0.091389
13	1	0	-3.327584	1.070073	-0.122177
14	1	0	-3.318648	-1.073376	-0.080087
15	1	0	-2.111842	-1.577835	1.126534
16	1	0	-1.930064	-2.029927	-0.587840
17	1	0	-1.936023	2.020220	-0.639682
18	1	0	-2.133411	1.609734	1.083299

rmp2/6-31g(d) scrf=(iefpcm,solvent= chloroform)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.543631	0.003685	-0.184462
2	6	0	-0.176718	0.020751	-0.077170
3	6	0	0.581003	1.202456	-0.023106
4	6	0	0.595360	-1.168436	-0.043257
5	1	0	0.126796	2.186448	-0.014869
6	1	0	0.128123	-2.147689	-0.054576
7	7	0	2.648230	-0.068811	0.045553
8	7	0	1.932322	-1.213278	0.013208
9	6	0	1.966353	1.089756	0.030845
10	1	0	2.585968	1.983065	0.070889
11	6	0	-2.266226	1.247474	0.051738
12	6	0	-2.256035	-1.241066	0.085515
13	1	0	-3.326759	1.069970	-0.126246
14	1	0	-3.319067	-1.070606	-0.084143
15	1	0	-2.113944	-1.591154	1.116558
16	1	0	-1.932065	-2.024457	-0.602788
17	1	0	-1.934387	2.017053	-0.649037
18	1	0	-2.135533	1.620586	1.076728

rb3lyp/cc-pvtz

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.534963	0.007010	-0.082068
2	6	0	-0.168875	0.022628	-0.035164
3	6	0	0.588324	1.197602	-0.008258
4	6	0	0.602843	-1.165145	-0.012635
5	1	0	0.135410	2.176836	-0.001580
6	1	0	0.131707	-2.137916	-0.009151
7	7	0	2.634617	-0.073645	0.015744
8	7	0	1.924027	-1.198353	0.008412
9	6	0	1.968497	1.078575	0.011167
10	1	0	2.589841	1.966175	0.026925
11	6	0	-2.269627	1.254422	0.025673
12	6	0	-2.257531	-1.248840	0.032481
13	1	0	-3.330083	1.055270	-0.100044
14	1	0	-3.319079	-1.058161	-0.097531
15	1	0	-2.112703	-1.728096	1.006786
16	1	0	-1.949819	-1.953342	-0.741906
17	1	0	-1.967919	1.956613	-0.754165
18	1	0	-2.124914	1.742085	0.996463

6-12. Acetylated 4-dimethylaminopyridazine (**10a-Ac**$^{+}$)

s-trans conformer

rb3lyp/6-31g(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.650537	-1.278005	-0.000363
2	6	0	0.717641	-1.272263	-0.000327
3	7	0	1.407843	-0.102468	-0.000107
4	7	0	0.810660	1.093892	-0.000060
5	6	0	-0.493659	1.134123	-0.000075
6	6	0	-1.345393	-0.034934	-0.000088
7	7	0	-2.676187	0.065196	0.000131
8	6	0	-3.505649	-1.151251	0.000424
9	6	0	-3.338903	1.381540	-0.000118
10	6	0	2.902450	-0.128822	0.000062
11	6	0	3.571476	1.209542	0.000131
12	8	0	3.416514	-1.211084	0.000226
13	1	0	-4.416648	1.230374	-0.000640
14	1	0	-3.071626	1.953276	-0.894569
15	1	0	-3.072411	1.953229	0.894606
16	1	0	-4.555225	-0.863722	0.001904
17	1	0	-3.309615	-1.752883	0.894053
18	1	0	-3.311789	-1.751916	-0.894349
19	1	0	4.648454	1.039810	-0.000715
20	1	0	3.282481	1.790804	0.881322
21	1	0	3.281065	1.791923	-0.879809
22	1	0	-0.908206	2.135043	-0.000056
23	1	0	1.330095	-2.166139	-0.000477
24	1	0	-1.169465	-2.227041	-0.000707

rb3lyp/6-31g(d) scrf=(iefpcm,solvent=benzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.650667	-1.281718	-0.005821
2	6	0	0.716020	-1.277225	-0.002282
3	7	0	1.408668	-0.107255	-0.004046
4	7	0	0.811779	1.091829	-0.014875
5	6	0	-0.491213	1.131316	-0.017442
6	6	0	-1.343109	-0.037647	-0.006936
7	7	0	-2.671319	0.065881	0.001304
8	6	0	-3.503272	-1.148032	0.001017
9	6	0	-3.327964	1.384513	0.017116
10	6	0	2.889830	-0.127479	0.004386
11	6	0	3.556028	1.212983	0.007519
12	8	0	3.420064	-1.205538	0.009351
13	1	0	-4.405479	1.237314	0.044873
14	1	0	-3.079169	1.954495	-0.883315
15	1	0	-3.032909	1.953765	0.903945
16	1	0	-4.551643	-0.857534	-0.003492
17	1	0	-3.310333	-1.747592	0.896274
18	1	0	-3.304068	-1.750316	-0.890829
19	1	0	4.633292	1.047469	0.016815
20	1	0	3.255992	1.794135	0.884556
21	1	0	3.270666	1.791388	-0.876179
22	1	0	-0.908394	2.130433	-0.028389
23	1	0	1.324215	-2.172899	0.002846
24	1	0	-1.170508	-2.229802	-0.003942

rb3lyp/6-31g(d) scrf=(iefpcm,solvent=chloroform)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.650516	-1.283115	-0.005693
2	6	0	0.715208	-1.279237	-0.001824
3	7	0	1.409387	-0.109129	-0.003992
4	7	0	0.812538	1.091496	-0.015742
5	6	0	-0.489651	1.130910	-0.018431
6	6	0	-1.341925	-0.038307	-0.007300
7	7	0	-2.668878	0.066251	0.000991
8	6	0	-3.501256	-1.147011	0.000182
9	6	0	-3.325124	1.384841	0.018800
10	6	0	2.883153	-0.126916	0.004599
11	6	0	3.549513	1.214115	0.007389
12	8	0	3.421704	-1.203065	0.009971
13	1	0	-4.402362	1.236894	0.047453
14	1	0	-3.076283	1.954872	-0.881290
15	1	0	-3.028373	1.952461	0.905821
16	1	0	-4.549111	-0.855379	-0.010024
17	1	0	-3.311539	-1.743889	0.897695
18	1	0	-3.297161	-1.751036	-0.889063
19	1	0	4.626847	1.049275	0.016894
20	1	0	3.249023	1.794942	0.884342
21	1	0	3.263989	1.791384	-0.876880
22	1	0	-0.907508	2.129543	-0.030360
23	1	0	1.321517	-2.175586	0.003873
24	1	0	-1.170417	-2.230976	-0.003359

rmp2/6-31g(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.653498	-1.274640	-0.000205
2	6	0	0.718053	-1.273540	-0.000261
3	7	0	1.404111	-0.103942	-0.000101
4	7	0	0.819655	1.098766	0.000083
5	6	0	-0.502990	1.130116	0.000130
6	6	0	-1.345588	-0.031967	0.000027
7	7	0	-2.677067	0.064580	0.000157
8	6	0	-3.495743	-1.155392	0.000296
9	6	0	-3.335782	1.379882	-0.000043
10	6	0	2.903175	-0.126049	-0.000119
11	6	0	3.555607	1.216411	0.000088
12	8	0	3.423820	-1.214822	-0.000143
13	1	0	-4.412154	1.224097	-0.000482
14	1	0	-3.066509	1.946147	-0.895486
15	1	0	-3.067196	1.946102	0.895640
16	1	0	-4.544982	-0.869257	0.001314
17	1	0	-3.294551	-1.751322	0.894953
18	1	0	-3.296020	-1.750622	-0.895169
19	1	0	4.632707	1.050558	-0.000203
20	1	0	3.260689	1.789170	0.881961
21	1	0	3.260245	1.789743	-0.881251
22	1	0	-0.907148	2.136166	0.000300
23	1	0	1.328529	-2.170569	-0.000449
24	1	0	-1.170467	-2.226393	-0.000430

rmp2/6-31g(d) scrf=(iefpcm,solvent=benzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.653705	-1.278246	0.000011
2	6	0	0.716327	-1.277703	-0.000155
3	7	0	1.404514	-0.107692	-0.000002
4	7	0	0.820314	1.096845	0.000412
5	6	0	-0.501169	1.127817	0.000551
6	6	0	-1.343494	-0.034446	0.000220
7	7	0	-2.672327	0.065270	0.000149
8	6	0	-3.493167	-1.152720	0.000042
9	6	0	-3.325064	1.383096	-0.000125
10	6	0	2.890920	-0.124796	-0.000246
11	6	0	3.542751	1.218402	-0.000175
12	8	0	3.425413	-1.209469	-0.000506
13	1	0	-4.401575	1.231554	-0.000623
14	1	0	-3.050239	1.947101	-0.894906
15	1	0	-3.051077	1.947103	0.894909
16	1	0	-4.541372	-0.864211	0.000464
17	1	0	-3.290685	-1.748172	0.894192
18	1	0	-3.291237	-1.747702	-0.894552
19	1	0	4.619802	1.054563	-0.000482
20	1	0	3.246146	1.789738	0.881581
21	1	0	3.245688	1.790053	-0.881571
22	1	0	-0.908383	2.131945	0.000937
23	1	0	1.323005	-2.176313	-0.000405
24	1	0	-1.171290	-2.229287	-0.000155

rmp2/6-31g(d) scrf=(iefpcm,solvent= chloroform)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.653593	-1.279482	-0.000010
2	6	0	0.715459	-1.279417	-0.000162
3	7	0	1.405142	-0.109208	-0.000004
4	7	0	0.821080	1.096376	0.000385
5	6	0	-0.499736	1.127682	0.000505
6	6	0	-1.342332	-0.034826	0.000192
7	7	0	-2.669896	0.065690	0.000140
8	6	0	-3.490945	-1.152001	0.000062
9	6	0	-3.322706	1.383398	-0.000115
10	6	0	2.884508	-0.124302	-0.000209
11	6	0	3.537191	1.218953	-0.000149
12	8	0	3.426256	-1.206956	-0.000480
13	1	0	-4.398887	1.230743	-0.000596
14	1	0	-3.047157	1.946725	-0.894816
15	1	0	-3.047961	1.946712	0.894840
16	1	0	-4.538725	-0.862563	0.000551
17	1	0	-3.287287	-1.746926	0.894019
18	1	0	-3.287946	-1.746426	-0.894387
19	1	0	4.614189	1.055201	-0.000444
20	1	0	3.240538	1.789723	0.881874
21	1	0	3.240096	1.790024	-0.881827
22	1	0	-0.907436	2.131433	0.000876
23	1	0	1.320336	-2.178677	-0.000405
24	1	0	-1.171161	-2.230359	-0.000175

s-cis conformer

rb3lyp/6-31g(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.567186	-1.166092	0.000123
2	7	0	-0.735081	-1.198664	0.000122
3	7	0	-1.406656	-0.040882	0.000055
4	6	0	-0.771871	1.159531	0.000061
5	6	0	0.595410	1.244784	0.000061
6	6	0	1.358725	0.044254	0.000041
7	6	0	-2.910541	-0.209543	-0.000067
8	8	0	-3.336045	-1.320811	-0.000163
9	6	0	-3.708340	1.065353	-0.000016
10	7	0	2.692484	0.015291	-0.000043
11	6	0	3.456632	1.273087	-0.000093
12	6	0	3.423258	-1.265141	-0.000045
13	1	0	1.033551	-2.144422	0.000215
14	1	0	-1.396035	2.043023	0.000107
15	1	0	1.056959	2.222979	0.000075
16	1	0	-3.503597	1.670486	-0.890308
17	1	0	-4.762225	0.785371	-0.000241
18	1	0	-3.503892	1.670111	0.890609
19	1	0	3.230930	1.863421	-0.894414
20	1	0	3.231026	1.863441	0.894240
21	1	0	4.519967	1.041233	-0.000147
22	1	0	3.186261	-1.849692	0.894493
23	1	0	3.185914	-1.849871	-0.894374
24	1	0	4.491518	-1.057204	-0.000277

rb3lyp/6-31g(d) scrf=(iefpcm,solvent=benzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.567329	-1.168714	0.000137
2	7	0	-0.733908	-1.205360	0.000138
3	7	0	-1.407916	-0.046090	0.000077
4	6	0	-0.773877	1.156547	0.000088
5	6	0	0.591496	1.243879	0.000091
6	6	0	1.355852	0.044463	0.000050
7	6	0	-2.896213	-0.206358	-0.000003
8	8	0	-3.335874	-1.316908	0.000045
9	6	0	-3.693986	1.068608	-0.000156
10	7	0	2.687490	0.016544	-0.000059
11	6	0	3.449486	1.275011	-0.000042
12	6	0	3.417309	-1.263336	-0.000222
13	1	0	1.038216	-2.144458	0.000211
14	1	0	-1.397646	2.039341	0.000089
15	1	0	1.049994	2.223166	0.000093
16	1	0	-3.486115	1.673459	-0.889538
17	1	0	-4.748083	0.790668	-0.000266
18	1	0	-3.486322	1.673526	0.889229
19	1	0	3.220198	1.863855	-0.893820
20	1	0	3.220126	1.863869	0.893706
21	1	0	4.512857	1.044967	0.000011
22	1	0	3.177551	-1.846433	0.893860
23	1	0	3.176905	-1.846549	-0.894054
24	1	0	4.485274	-1.056405	-0.000628

rb3lyp/6-31g(d) scrf=(iefpcm,solvent=chloroform)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.566999	-1.170591	0.000182
2	7	0	-0.733642	-1.209288	0.000165
3	7	0	-1.408908	-0.048845	0.000065
4	6	0	-0.774960	1.155170	0.000071
5	6	0	0.589300	1.242952	0.000090
6	6	0	1.354172	0.044041	0.000071
7	6	0	-2.888534	-0.204502	-0.000044
8	8	0	-3.336592	-1.314703	-0.000106
9	6	0	-3.686086	1.070402	-0.000093
10	7	0	2.684694	0.016992	-0.000041
11	6	0	3.445001	1.276333	-0.000049
12	6	0	3.415992	-1.261662	-0.000186
13	1	0	1.040649	-2.144785	0.000287
14	1	0	-1.398576	2.037570	0.000054
15	1	0	1.046774	2.222426	0.000086
16	1	0	-3.476519	1.675176	-0.888901
17	1	0	-4.740278	0.793443	-0.000268
18	1	0	-3.476791	1.675057	0.888861
19	1	0	3.213777	1.864246	-0.893676
20	1	0	3.213669	1.864317	0.893502
21	1	0	4.508369	1.046992	0.000035
22	1	0	3.176329	-1.844443	0.893918
23	1	0	3.175632	-1.844610	-0.893993
24	1	0	4.483389	-1.052634	-0.000628

rmp2/6-31g(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.574369	-1.161013	-0.000023
2	7	0	-0.745161	-1.203852	-0.000028
3	7	0	-1.403441	-0.036675	-0.000037
4	6	0	-0.770892	1.162513	-0.000018
5	6	0	0.601128	1.241681	-0.000006
6	6	0	1.359298	0.041654	-0.000026
7	6	0	-2.911874	-0.205516	-0.000045
8	8	0	-3.337674	-1.326971	0.000240
9	6	0	-3.697687	1.071486	-0.000015
10	7	0	2.693750	0.013412	-0.000039
11	6	0	3.448548	1.273242	0.000010
12	6	0	3.418070	-1.267330	-0.000054
13	1	0	1.029922	-2.145263	-0.000007
14	1	0	-1.392132	2.049621	-0.000008
15	1	0	1.062346	2.221697	0.000013
16	1	0	-3.488357	1.669290	-0.891356
17	1	0	-4.751474	0.793205	0.000114
18	1	0	-3.488165	1.669370	0.891229
19	1	0	3.217923	1.857858	-0.895121
20	1	0	3.217940	1.857781	0.895197
21	1	0	4.511232	1.041732	-0.000011
22	1	0	3.177696	-1.846431	0.895340
23	1	0	3.177515	-1.846504	-0.895350
24	1	0	4.485158	-1.057073	-0.000176

rmp2/6-31g(d) scrf=(iefpcm,solvent=benzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.574806	-1.164108	0.000016
2	7	0	0.744051	-1.209833	-0.000028
3	7	0	1.404464	-0.042309	-0.000081
4	6	0	0.772791	1.159121	-0.000124
5	6	0	-0.597074	1.240525	-0.000087
6	6	0	-1.356501	0.041129	0.000020
7	6	0	2.898018	-0.202388	-0.000091
8	8	0	3.337025	-1.322527	-0.000421
9	6	0	3.684097	1.074225	0.000268
10	7	0	-2.688726	0.014710	0.000105
11	6	0	-3.440709	1.275945	0.000041
12	6	0	-3.413210	-1.265193	0.000244
13	1	0	-1.034843	-2.145807	0.000033
14	1	0	1.393738	2.045540	-0.000197
15	1	0	-1.055188	2.221675	-0.000128
16	1	0	3.471723	1.671775	0.890749
17	1	0	4.738003	0.797671	0.000155
18	1	0	3.471652	1.672292	-0.889851
19	1	0	-3.205871	1.858880	0.894553
20	1	0	-3.205937	1.858747	-0.894576
21	1	0	-4.503506	1.046806	0.000094
22	1	0	-3.170311	-1.842952	-0.894658
23	1	0	-3.170011	-1.842916	0.895087
24	1	0	-4.479806	-1.055009	0.000424

rmp2/6-31g(d) scrf=(iefpcm,solvent= chloroform)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.574742	-1.166233	-0.000035
2	7	0	0.743797	-1.213335	-0.000079
3	7	0	1.405296	-0.045382	-0.000113
4	6	0	0.773810	1.157502	-0.000169
5	6	0	-0.594740	1.239507	-0.000135
6	6	0	-1.354802	0.040283	-0.000008
7	6	0	2.890531	-0.200595	-0.000084
8	8	0	3.337460	-1.319886	-0.000432
9	6	0	3.676468	1.075688	0.000336
10	7	0	-2.685838	0.015213	0.000122
11	6	0	-3.435819	1.277642	0.000089
12	6	0	-3.412340	-1.263309	0.000301
13	1	0	-1.037245	-2.146541	-0.000018
14	1	0	1.394630	2.043549	-0.000247
15	1	0	-1.051749	2.220898	-0.000175
16	1	0	3.462242	1.673138	0.890278
17	1	0	4.730398	0.800007	0.000450
18	1	0	3.462553	1.673523	-0.889422
19	1	0	-3.198759	1.859546	0.894411
20	1	0	-3.198864	1.859439	-0.894329
21	1	0	-4.498645	1.049411	0.000161
22	1	0	-3.169700	-1.840860	-0.894580
23	1	0	-3.169266	-1.840842	0.895075
24	1	0	-4.478257	-1.050569	0.000563

6-13. Pyridazine (**9**)

rb3lyp/6-31g(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.691878	1.180997	-0.000016
2	6	0	-1.322908	-0.067313	-0.000026
3	7	0	-0.668469	-1.232482	0.000074
4	7	0	0.668246	-1.232589	-0.000052
5	6	0	1.322889	-0.067560	-0.000006
6	6	0	0.692097	1.180885	0.000018
7	1	0	2.407007	-0.152381	-0.000066
8	1	0	1.272716	2.098769	0.000225
9	1	0	-2.407038	-0.151927	0.000013
10	1	0	-1.272331	2.098991	-0.000151

rb3lyp/6-31g(d) scrf=(iefpcm,solvent=benzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.668762	-1.232089	-0.000004
2	6	0	1.324374	-0.067615	-0.000002
3	6	0	0.692075	1.180384	0.000002
4	6	0	-0.692083	1.180379	0.000004
5	6	0	-1.324373	-0.067624	0.000002
6	7	0	-0.668755	-1.232094	-0.000002
7	1	0	1.271657	2.098387	0.000004
8	1	0	2.408447	-0.150306	-0.000004
9	1	0	-1.271670	2.098379	0.000007
10	1	0	-2.408446	-0.150321	0.000003

rb3lyp/6-31g(d) scrf=(iefpcm,solvent=chloroform)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.669221	-1.232108	-0.000004
2	6	0	1.324892	-0.067664	-0.000002
3	6	0	0.691938	1.180298	0.000002
4	6	0	-0.691935	1.180300	0.000004
5	6	0	-1.324893	-0.067661	0.000002
6	7	0	-0.669225	-1.232106	-0.000002
7	1	0	1.271476	2.098050	0.000004
8	1	0	2.408901	-0.149124	-0.000004
9	1	0	-1.271470	2.098053	0.000007
10	1	0	-2.408902	-0.149118	0.000003

rmp2/6-31g(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.674377	-1.238960	0.000005
2	6	0	-1.325822	-0.062894	0.000003
3	6	0	-0.693121	1.182864	-0.000002
4	6	0	0.693182	1.182829	-0.000004
5	6	0	1.325819	-0.062962	-0.000002
6	7	0	0.674312	-1.238994	0.000002
7	1	0	-1.270685	2.102922	-0.000005
8	1	0	-2.409569	-0.149496	0.000002
9	1	0	1.270793	2.102857	-0.000006
10	1	0	2.409562	-0.149619	-0.000004

rmp2/6-31g(d) scrf=(iefpcm,solvent=benzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.674669	-1.238580	-0.000004
2	6	0	1.327172	-0.063031	-0.000002
3	6	0	0.693194	1.182309	0.000002
4	6	0	-0.693172	1.182322	0.000004
5	6	0	-1.327174	-0.063007	0.000002
6	7	0	-0.674692	-1.238568	-0.000003
7	1	0	1.270974	2.101799	0.000004
8	1	0	2.410929	-0.147591	-0.000004
9	1	0	-1.270935	2.101822	0.000007
10	1	0	-2.410931	-0.147547	0.000003

rmp2/6-31g(d) scrf=(iefpcm,solvent= chloroform)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.674958	-1.238360	-0.000004
2	6	0	1.328059	-0.063018	-0.000002
3	6	0	0.693246	1.181935	0.000002
4	6	0	-0.693223	1.181948	0.000004
5	6	0	-1.328060	-0.062993	0.000002
6	7	0	-0.674982	-1.238348	-0.000003
7	1	0	1.270911	2.101227	0.000004
8	1	0	2.411827	-0.146403	-0.000004
9	1	0	-1.270870	2.101252	0.000007
10	1	0	-2.411829	-0.146357	0.000003

rb3lyp/cc-pvtz

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.664724	-1.225533	-0.000004
2	6	0	1.318670	-0.067488	-0.000002
3	6	0	0.688784	1.174277	0.000002
4	6	0	-0.688783	1.174277	0.000004
5	6	0	-1.318670	-0.067487	0.000002
6	7	0	-0.664726	-1.225532	-0.000002
7	1	0	1.265691	2.088822	0.000004
8	1	0	2.398388	-0.150834	-0.000004
9	1	0	-1.265690	2.088823	0.000007
10	1	0	-2.398388	-0.150832	0.000003

6-14. Acetylated pyridazine (**9-Ac**$^{+}$)

s-trans conformer

rb3lyp/6-31g(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.648158	-1.281689	0.000160
2	7	0	-0.328638	-1.159362	0.000115
3	7	0	0.158624	0.074461	-0.000047
4	6	0	-0.578513	1.194309	-0.000188
5	6	0	-1.969514	1.093966	-0.000163
6	6	0	-2.522274	-0.176888	0.000046
7	6	0	1.708008	0.209450	0.000010
8	8	0	2.114877	1.326835	0.000363
9	6	0	2.443681	-1.085912	-0.000281
10	1	0	-2.012070	-2.304176	0.000322
11	1	0	-0.020027	2.124166	-0.000282
12	1	0	-2.576861	1.992549	-0.000301
13	1	0	-3.596459	-0.331759	0.000117
14	1	0	3.510296	-0.858197	-0.000997
15	1	0	2.182773	-1.681487	-0.881013
16	1	0	2.184043	-1.680884	0.881275

rb3lyp/6-31g(d) scrf=(iefpcm,solvent=benzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.639493	-1.281882	0.000610
2	7	0	-0.321723	-1.157518	0.000471
3	7	0	0.161897	0.079285	-0.000110
4	6	0	-0.578350	1.196980	-0.000571
5	6	0	-1.968152	1.092148	-0.000577
6	6	0	-2.516346	-0.179324	0.000051
7	6	0	1.695219	0.209028	0.000046
8	8	0	2.116533	1.324130	0.001195
9	6	0	2.431451	-1.086742	-0.000998
10	1	0	-2.003448	-2.303525	0.001140
11	1	0	-0.025117	2.128740	-0.000788
12	1	0	-2.577071	1.988634	-0.001019
13	1	0	-3.589254	-0.337429	0.000072
14	1	0	3.498106	-0.861257	-0.002703
15	1	0	2.167124	-1.681500	-0.880799
16	1	0	2.170208	-1.680323	0.880640

rb3lyp/6-31g(d) scrf=(iefpcm,solvent=chloroform)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.635845	-1.281787	0.000298
2	7	0	-0.318933	-1.156745	0.000213
3	7	0	0.163512	0.081248	-0.000073
4	6	0	-0.578117	1.197967	-0.000320
5	6	0	-1.967404	1.091430	-0.000295
6	6	0	-2.513920	-0.180170	0.000060
7	6	0	1.688666	0.208646	0.000021
8	8	0	2.117778	1.322504	0.000634
9	6	0	2.426128	-1.086899	-0.000514
10	1	0	-1.999728	-2.303130	0.000609
11	1	0	-0.027890	2.130845	-0.000463
12	1	0	-2.576785	1.987122	-0.000517
13	1	0	-3.586214	-0.339801	0.000147
14	1	0	3.492528	-0.861048	-0.001668
15	1	0	2.162358	-1.680831	-0.880836
16	1	0	2.164410	-1.679830	0.881179

rmp2/6-31g(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.650070	-1.276496	0.000489
2	7	0	-0.313351	-1.162682	0.000475
3	7	0	0.160616	0.079657	0.000041
4	6	0	-0.575325	1.204436	-0.000390
5	6	0	-1.963433	1.095037	-0.000375
6	6	0	-2.518716	-0.179067	0.000085
7	6	0	1.699592	0.204840	-0.000002
8	8	0	2.125790	1.327118	0.000144
9	6	0	2.419417	-1.097336	-0.000325
10	1	0	-2.007897	-2.300773	0.000878
11	1	0	-0.019233	2.135875	-0.000742
12	1	0	-2.574870	1.990999	-0.000727
13	1	0	-3.593439	-0.329864	0.000133
14	1	0	3.486318	-0.875394	-0.000411
15	1	0	2.151469	-1.682394	-0.882592
16	1	0	2.151680	-1.682699	0.881805

rmp2/6-31g(d) scrf=(iefpcm,solvent=benzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.650292	-1.276528	0.000117
2	7	0	-0.313442	-1.162777	0.000032
3	7	0	0.160602	0.079629	-0.000098
4	6	0	-0.575392	1.204428	-0.000057
5	6	0	-1.963454	1.095163	-0.000072
6	6	0	-2.518779	-0.178946	0.000005
7	6	0	1.699692	0.204848	-0.000069
8	8	0	2.126090	1.327066	0.000187
9	6	0	2.419480	-1.097354	-0.000162
10	1	0	-2.008263	-2.300791	0.000265
11	1	0	-0.019066	2.135781	-0.000113
12	1	0	-2.574931	1.991137	-0.000023
13	1	0	-3.593562	-0.329535	-0.000037
14	1	0	3.486389	-0.875424	-0.001834
15	1	0	2.150184	-1.683815	-0.881113
16	1	0	2.152879	-1.681517	0.883252

rmp2/6-31g(d) scrf=(iefpcm,solvent= chloroform)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.646745	-1.276332	0.000418
2	7	0	-0.310538	-1.161530	0.000378
3	7	0	0.162034	0.081326	0.000013
4	6	0	-0.574939	1.205151	-0.000354
5	6	0	-1.962524	1.094296	-0.000347
6	6	0	-2.516260	-0.180066	0.000060
7	6	0	1.693274	0.204463	0.000091
8	8	0	2.126379	1.325295	0.000143
9	6	0	2.414621	-1.097179	-0.000278
10	1	0	-2.004347	-2.300339	0.000730
11	1	0	-0.021921	2.137748	-0.000584
12	1	0	-2.574302	1.989532	-0.000654
13	1	0	-3.590430	-0.332182	0.000107
14	1	0	3.481154	-0.874567	-0.000830
15	1	0	2.146427	-1.681609	-0.882702
16	1	0	2.147352	-1.681502	0.882507

s-cis conformer

rb3lyp/6-31g(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.841798	1.248937	-0.000150
2	6	0	0.448652	1.170963	-0.000046
3	7	0	-0.151808	-0.028679	0.000071
4	7	0	0.493486	-1.185392	0.000213
5	6	0	1.816992	-1.142658	0.000146
6	6	0	2.550702	0.059214	-0.000079
7	6	0	-1.726251	-0.222009	-0.000085
8	8	0	-2.096001	-1.342449	-0.000325
9	6	0	-2.517217	1.048288	0.000184
10	1	0	2.328786	2.217987	-0.000274
11	1	0	-0.187713	2.046448	0.000003
12	1	0	2.302207	-2.113710	0.000356
13	1	0	3.635809	0.039837	-0.000205
14	1	0	-2.308999	1.650321	-0.891433
15	1	0	-3.572540	0.771293	-0.000116
16	1	0	-2.309339	1.649506	0.892454

rb3lyp/6-31g(d) scrf=(iefpcm,solvent=benzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.830930	1.250527	0.000148
2	6	0	0.438663	1.167063	0.000338
3	7	0	-0.156604	-0.034802	0.000147
4	7	0	0.493897	-1.190847	-0.000090
5	6	0	1.815728	-1.139902	-0.000177
6	6	0	2.544234	0.065255	-0.000183
7	6	0	-1.709542	-0.219902	0.000024
8	8	0	-2.093902	-1.339977	0.000317
9	6	0	-2.504642	1.047814	-0.000418
10	1	0	2.311648	2.221788	0.000266
11	1	0	-0.198953	2.040513	0.000603
12	1	0	2.307737	-2.106673	-0.000281
13	1	0	3.628571	0.049719	-0.000429
14	1	0	-2.296048	1.650466	-0.891090
15	1	0	-3.558398	0.767664	-0.000595
16	1	0	-2.296617	1.650761	0.890197

rb3lyp/6-31g(d) scrf=(iefpcm,solvent=chloroform)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.825278	1.251426	-0.000187
2	6	0	0.433288	1.165085	-0.000187
3	7	0	-0.159231	-0.037848	-0.000005
4	7	0	0.494088	-1.194170	0.000192
5	6	0	1.814874	-1.138757	0.000213
6	6	0	2.540591	0.068451	0.000019
7	6	0	-1.700855	-0.218714	-0.000052
8	8	0	-2.093178	-1.338768	-0.000408
9	6	0	-2.497391	1.047881	0.000347
10	1	0	2.302719	2.223856	-0.000347
11	1	0	-0.204939	2.037518	-0.000337
12	1	0	2.310988	-2.103132	0.000396
13	1	0	3.624604	0.054697	0.000039
14	1	0	-2.288167	1.650855	-0.889753
15	1	0	-3.550853	0.767542	0.000615
16	1	0	-2.287628	1.650706	0.890415

rmp2/6-31g(d)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.845081	1.244702	-0.000012
2	6	0	0.451174	1.179189	0.000046
3	7	0	-0.151876	-0.022982	0.000010
4	7	0	0.480035	-1.193191	-0.000082
5	6	0	1.819350	-1.142500	-0.000141
6	6	0	2.553864	0.050981	-0.000107
7	6	0	-1.732120	-0.217977	0.000095
8	8	0	-2.101769	-1.348700	0.000190
9	6	0	-2.508124	1.057665	0.000000
10	1	0	2.339524	2.211105	0.000021
11	1	0	-0.182228	2.058072	0.000119
12	1	0	2.294832	-2.118845	-0.000222
13	1	0	3.639679	0.031829	-0.000155
14	1	0	-2.292918	1.651027	-0.892901
15	1	0	-3.564249	0.786123	-0.000003
16	1	0	-2.292961	1.651135	0.892840

rmp2/6-31g(d) scrf=(iefpcm,solvent=benzene)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.832847	1.246916	0.000013
2	6	0	-0.440179	1.174698	-0.000044
3	7	0	0.156254	-0.030234	-0.000006
4	7	0	-0.480834	-1.198053	0.000082
5	6	0	-1.819380	-1.138791	0.000139
6	6	0	-2.547279	0.057646	0.000109
7	6	0	1.715123	-0.216035	-0.000073
8	8	0	2.098437	-1.346070	-0.000212
9	6	0	2.496235	1.056292	0.000003
10	1	0	-2.320287	2.215973	-0.000017
11	1	0	0.195229	2.051034	-0.000119
12	1	0	-2.301813	-2.110829	0.000213
13	1	0	-3.632387	0.043385	0.000159
14	1	0	2.281633	1.651201	0.891709
15	1	0	3.550464	0.780182	0.000015
16	1	0	2.281684	1.651269	-0.891670

rmp2/6-31g(d) scrf=(iefpcm,solvent= chloroform)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.826492	1.248133	-0.000010
2	6	0	-0.434544	1.172675	-0.000052
3	7	0	0.158492	-0.033801	0.000023
4	7	0	-0.481278	-1.200595	0.000121
5	6	0	-1.819414	-1.137167	0.000160
6	6	0	-2.543632	0.060924	0.000103
7	6	0	1.706519	-0.215020	-0.000001
8	8	0	2.096926	-1.344773	-0.000337
9	6	0	2.489857	1.055605	0.000032
10	1	0	-2.310506	2.218461	-0.000063
11	1	0	0.202166	2.047485	-0.000141
12	1	0	-2.305767	-2.106911	0.000246
13	1	0	-3.628431	0.049225	0.000144
14	1	0	2.274706	1.650716	0.891292
15	1	0	3.543520	0.778278	-0.000029
16	1	0	2.274646	1.650801	-0.891155