Supplemental Material

Ammonia Elimination from Protonated Nucleobases and Related Synthetic Substrates

Ming Qian, Shuo Yang, Hong Wu, Papiya Majumdar, Nathan Leigh, and Rainer Glaser*

Department of Chemistry, University of Missouri-Columbia, Columbia, Missouri, USA

Content

* Address reprint requests to Professor Rainer Glaser, Department of Chemistry, University of Missouri-Columbia, 321 Chemistry Building, Columbia, Missouri 65211, USA. E-mail: GlaserR@missouri.edu

Table S1. Summary of major electron-impact fragmentation of nucleobases.

Molecular Ion		Fragmentation					
$[M]^+$ with *m/e*		looses to give *m/e*		looses to give *m/e*		looses to give *m/e*	
$[A]^+$	135	-HCN	108	-HCN	81	-HCN	54
		-HCN	108	$-CH_2N_2$	66		
$[G]^+$	151	$-NH_3$	134				
		$-CHN_2$	110				
		$-CH_2N_2$	109				
		-HNCO	108				
$[C]^+$	111	$-NH_2$	95	-HCN	68		
		-CO	83				
		-NCO	69				
		-HNCO	68				
		-HNCO-H	67				

Table S2. Summary of major ESI-CID fragmentations of nucleosides.

Molecular Ion		Fragmentation			
$[M\pm H]^{\pm}$ with *m/z*		loses to give *m/z*		loses to give *m/z*	
$[A+H]^+$	136	$-NH_3+H_2O$	137	-HCN	110
		$-NH_3$	119		
		-HCN	109		
		$-H_2NCN$	94		
$[rA+H]^+$	268	-ribosyl	136		
$[dA+H]^+$	252	-deoxyribosyl	136		
$[rG+H]^+$	284	-ribosyl	152		
$[dG+H]^+$	268	-deoxyribosyl	152		
$[A-H]^-$	266	-ribosyl-NH_3+H_2O	135		
$[dA-H]^-$	250	-ribosyl-NH_3+H_2O	135		
	250	-ribosyl	134		
$[G-H]^-$	282	-ribosyl	150		
	262	-ribosyl-NH_3	133		
$[dG-H]^-$	266	-ribosyl	150		
	266	-ribosyl-NH_3	133		
$[C-H]^-$	110				
$[rC-H]^-$	242	-ribosyl	110		
$[dC-H]^-$	226	-deoxyribosyl	110		

Table S3. Total energies and thermodynamical data of neutral and protonated aniline and of neutral and protonated nucleobases and related models computed at B3LYP/6-31++G**.

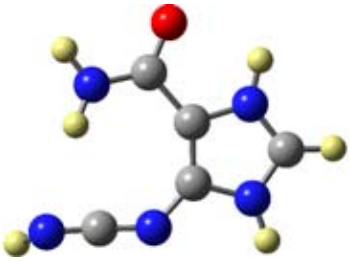
Molecule	*E*	*VZPE*	*TE*	*S*	N
Aniline	-287.631131	73.36	77.03	75.75	0
NH_2	-287.979063	82.40	86.36	82.49	0
Adenine, **1h**	-467.353339	70.02	74.85	89.10	0
15 (NH_2)	-467.688791	79.12	83.84	96.70	0
16 (N1)	-467.724393	78.83	83.39	83.91	0
17 (N3)	-467.721995	78.83	83.37	83.89	0
18 (N7)	-467.711187	78.48	83.20	85.23	0
19 (N9)	-467.651361	77.86	82.50	84.59	0
60, IMPT(**16**,**15**)	-467.646853	75.81	80.08	82.40	1
61, IMPT(**18**,**15**)	-467.644426	75.82	80.10	83.56	1
62, POTS(**16**,**63**)	-467.617884	74.88	80.15	89.32	1
63	-467.617954	74.99	80.77	93.45	0
64, RTS(**63**,**65**)	-467.594861	74.72	79.95	89.08	"1"
65	-467.594955	74.83	80.56	93.91	"0"
Guanine, **2h**	-542.591699	73.20	78.39	88.93	0
20 (NH_2)	-542.905299	91.50	86.89	90.72	0
21 (N1)	-542.910925	79.30	85.55	98.12	0
22 (N3)	-542.940077	80.55	86.25	92.29	0
23 (N7)	-542.968851	81.57	86.92	89.97	0
24 (N9)	-542.893358	80.50	85.93	90.50	0
25 (C6-O, N1 side)	-542.945100	80.44	86.17	92.74	0
26 (C6-O, N7 side)	-542.959365	81.18	86.60	90.19	0
74	-542.853347	79.13	84.79	93.48	1
75	-542.918888	78.85	85.14	98.66	0
76, RTS(**75**,**77**)	-542.906700	78.57	84.52	96.48	1
77	-542.915859	78.77	85.01	98.22	0
78, IMPT(**77**,**79**)	-542.883585	76.06	82.04	96.34	1
79	-542.900961	78.76	85.17	99.26	0
80, IMPT(**23**,**81**)	-542.866637	77.39	82.80	91.56	1
81, N3(1*H*,7*H*)	-542.960408	81.20	86.71	90.98	0

Molecule	*E*	*VZPE*	*TE*	*S*	N
82, IMPT(**81**,**83**)	-542.876568	78.54	83.56	88.10	1
83, NH_2(1*H*,7*H*)	-542.912126	81.71	87.07	90.46	0
84, IMPT(**81**,**85**)	-542.870854	78.56	83.61	88.39	1
85, NH_2(3*H*,7*H*)	-542.900900	81.46	86.96	91.70	0
86, IMPT(**23**,**87**)	-542.886972	78.93	83.88	87.69	1
87	-542.921476	82.07	87.46	92.06	0
88, IMPT(**22**,**89**)	-542.847458	77.87	83.11	89.58	1
89	-542.876170	80.55	86.35	94.00	0
90, IMPT(**22**,**20**)	-542.865486	78.14	83.22	88.55	1
91, RTS(**22**,**92**)	-542.874317	78.91	84.65	94.37	1
92	-542.882684	79.97	85.7	95.18	0
93, IMPT(**21**,**94**)	-542.819927	76.15	82.18	98.31	1
94	-542.862825	79.5	85.84	99.41	0
95	-486.249733	53.78	58.98	90.46	0
TS(**95**,**10'**)	-486.175883	50.05	55.23	90.83	0
Cyanoamine (*E*,*Z*)-13h	-542.559084	71.26	77.41	97.79	0
27 (NH_2)	-542.888433	79.75	86.09	99.02	0
28 (N7)	-542.903909	79.26	85.66	101.05	0
29 (C6-O, NH_2 side)	-542.900724	79.31	85.61	98.17	0
30 (NCN, cyano-N)	turns into **103**				
31 (NCN, amino-N)	-542.894173	79.90	85.95	97.94	0
103	-542.921524	79.05	85.15	96.88	0
104	-542.902469	77.76	83.88	97.72	0
105	-542.911201	78.51	84.85	98.96	0
106, IMPT(**105**,**107**)	-542.841342	75.44	81.68	98.71	0
107	-542.896519	78.59	85.07	100.41	0
108, RTS(**103**,**109**)	-542.892129	78.77	84.55	95.28	1
109	-542.921873	79.03	85.16	97.35	0
110, IMPT(**109**,**111**)	-542.901244	76.39	82.30	96.03	1
111	-542.921173	78.92	85.18	98.48	0
112, RTS(**111**,**113**)	-542.904135	78.62	84.53	96.30	1
113	-542.904857	78.60	85.02	100.71	0
114, IMPT(**113**,**107**)	-542.877548	75.90	81.95	97.52	1

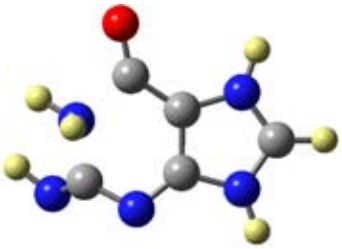
Molecule	*E*	*VZPE*	*TE*	*S*	N
121, IMPT(**28**,**27**)	-542.867598	76.90	82.84	96.34	1
Cyanoamine (*Z*,*Z*)-13h	-542.536039	71.23	77.38	98.07	0
32 (NH_2)	-542.888433	79.75	86.09	99.02	0
33 (N7)	-542.899510	79.62	85.91	99.21	0
34 (C6-O, N7 side)	-542.895675	79.56	85.78	99.44	0
35 (C6-O, NH_2 side)	-542.879170	79.26	85.52	100.85	0
36 (NCN, cyano-N)	-542.885169	78.61	84.97	99.38	0
37 (NCN, amino-N	-542.862141	79.11	85.47	98.94	0
118	-542.885169	78.61	84.97	99.39	0
122, IMPT(**33**,**123**)	-542.877557	77.13	82.92	95.14	1
123	-542.883713	79.90	85.96	96.58	0
9	-486.272824	52.50	57.91	92.49	0
TS(**9**,**125**)	-486.160681	51.22	55.93	85.65	1
Thioether (*Z*)-14h	-924.727236	80.49	86.96	101.02	0
38 (N3)	-925.070724	88.16	94.87	102.43	0
39 (N7)	-925.098721	89.01	95.51	100.69	0
40 (C6-O, N1 side)	-925.079108	88.24	94.91	101.61	0
41 (C6-O, N7 side)	-925.091752	88.74	95.25	100.52	0
42 (S)	-925.024478	86.30	92.99	102.92	0
(*Z*)-**129**	-925.091586	88.78	95.33	101.13	0
(*Z*)-**132**	turns into (*E*)-**132**				
(*Z*)-**134**	-925.032477	86.58	93.20	101.98	0
128	-924.996769	84.78	91.37	103.21	1
130	-925.085792	88.76	94.83	97.26	1
(*Z*)-**131**	-925.003522	84.74	91.19	100.32	1
135	-924.987004	86.16	93.2	105.43	1
136	-925. 052201	85.93	93.60	112.50	0
Thioether (*E*)-14h	-924.723031	80.47	86.90	101.03	0
43 (N3)	-925.073373	88.23	94.93	102.45	0
44 (N7)	-925.095124	88.99	95.43	100.09	0
45 (C6-O, N1 side)	-925.072554	88.08	94.74	101.48	0

Molecule	*E*	*VZPE*	*TE*	*S*	N
46 (C6-O, N7 side)	-925.086460	88.67	95.13	100.10	0
47 (S)	turns into (Z)-rotamer				
(*E*)-**129**	-925.092009	88.75	95.33	101.63	0
(*E*)-**132**	-925.023397	86.42	93.14	102.61	0
(*E*)-**134**	-925.026754	86.42	93.12	103.54	0
(*E*)-**133**	-925.011113	84.66	91.09	100.12	1
Cytosine, **3h**	-394.963350	61.61	65.91	81.60	0
48 (NH_2**)**	-395.287718	70.45	74.78	82.48	0
49 (N1)	-395.307348	68.87	74.02	88.93	0
50 (N3)	-395.339256	70.55	74.71	80.33	0
51 (C6-O, N1 side)	-395.325894	70.18	74.40	80.55	0
52 (C6-O, N3 side)	-395.339815	70.63	74.70	79.60	0
138, IMPT(**50**,**48**)	-395.251445	67.30	71.24	79.34	1
139	-395.206931	67.03	71.83	87.38	1
140	-395.255328	69.53	73.85	82.55	0
141	-395.222941	67.07	71.89	86.20	1
142	-395.310922	68.74	73.83	88.37	0
143, IMPT(**142**,1**43**)	-395.223511	65.59	70.45	87.60	1
144	-395.258673	68.74	73.93	90.07	0
145	-395.214979	67.15	71.89	84.98	1
146	-395.307348	68.87	74.02	88.93	0

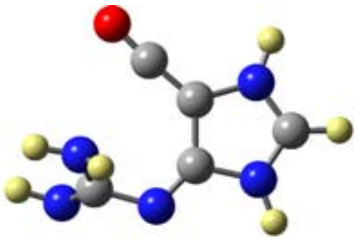
[a] Total energies, E, in atomic units. Vibrational zero-point energies, *VZPE*, and thermal energies, *TE*, in kcal mol^{-1}. Molecular entropies, *S*, in cal $mol^{-1}\cdot K^{-1}$.



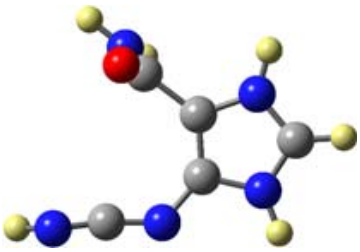
75



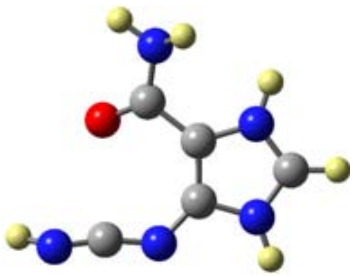
on path **74** → **75**



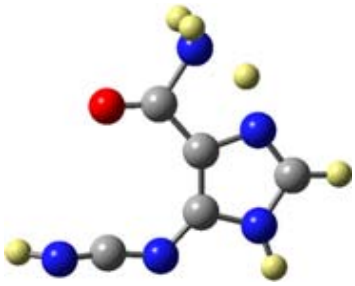
74, RTS(**23**,**75**)



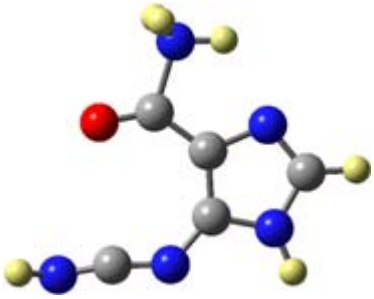
76, RTS(**75**,**77**)



77

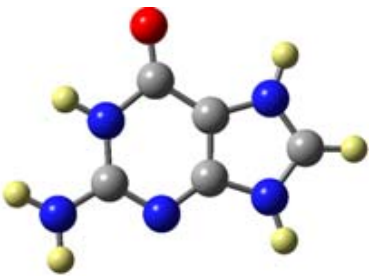


78, IMPT(**77**,**79**)

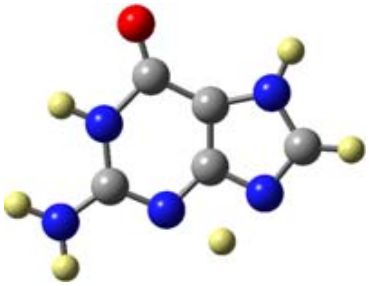


79

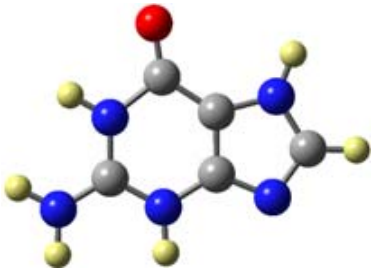
Scheme S1. (This is the left half.) N7-Protonated guanine **23** (bold single-lined) is the most stable structure of [**2h** + H]$^+$. The paths are shown for the formations of isomeric ammonium ion precursors **77** and **81** (single-lined) and of their ammonium ions **79**, **83**, **85**, and **87** (double-lined).



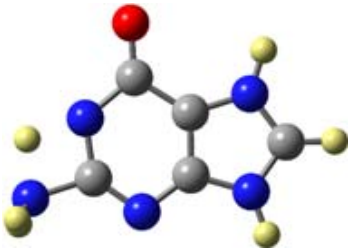
23



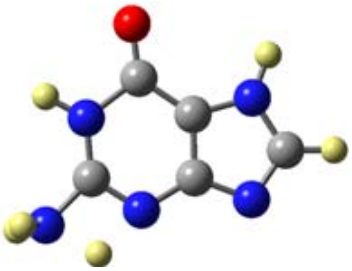
80, IMPT(**23**,**81**)



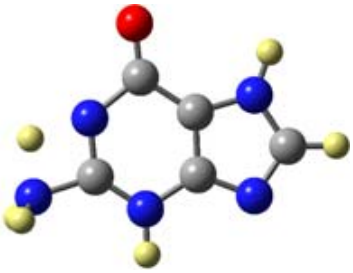
81



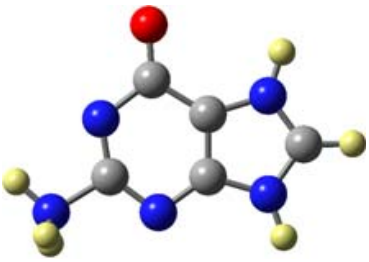
86, IMPT(**23**,**87**)



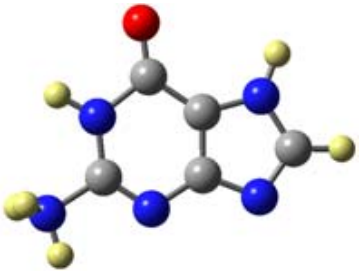
82, IMPT(**81**,**83**)



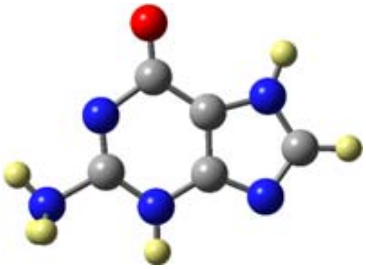
84, IMPT(**81**,**85**)



87

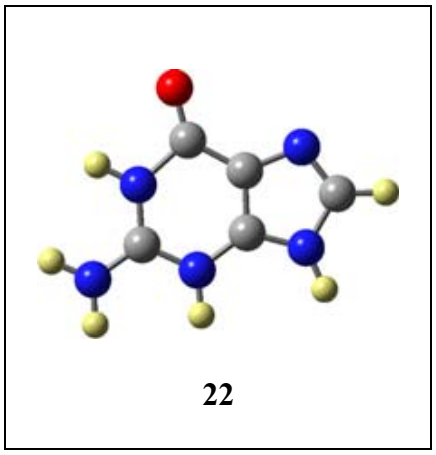


83

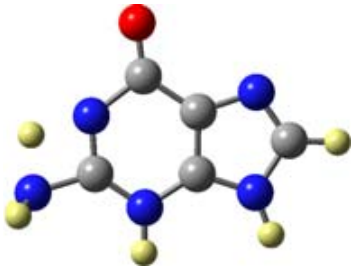


85

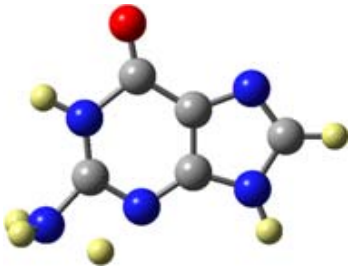
Scheme S1. (Continued. This is the right half.)



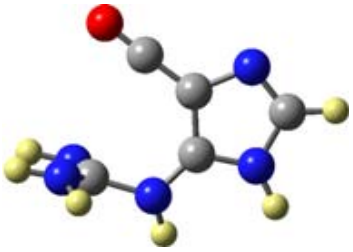
22



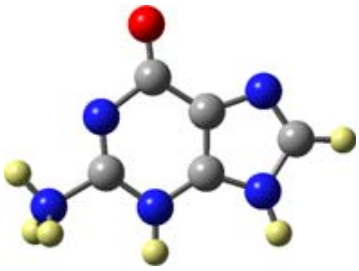
88, IMPT(**22**,**87**)



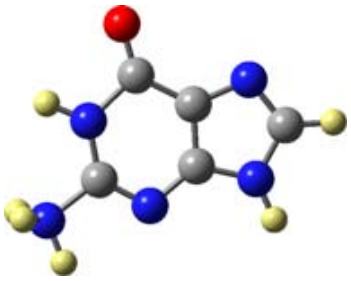
90, IMPT(**22**,**20**)



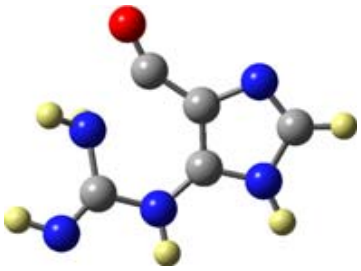
91, IMPT(**22**,**92**)



89

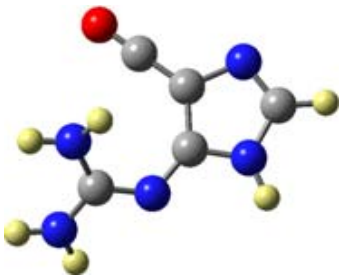


20

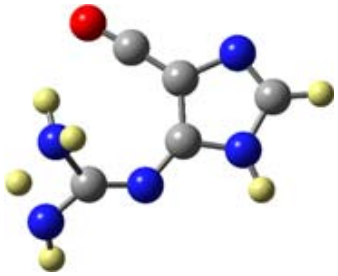


92

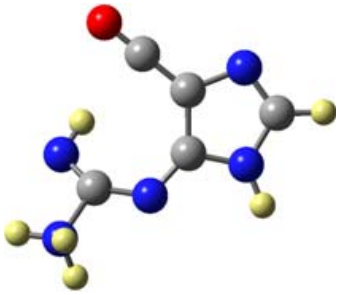
Scheme S2. (Continued on the next page.) The N3- and N1-protonated guanines **22** and **21** (single-lined) are potential intermediates in the fragmentation of [**2h** + H]$^+$, and they are precursors on the paths to ammonium ions **20**, **89**, and **94** (double-outlined).



21

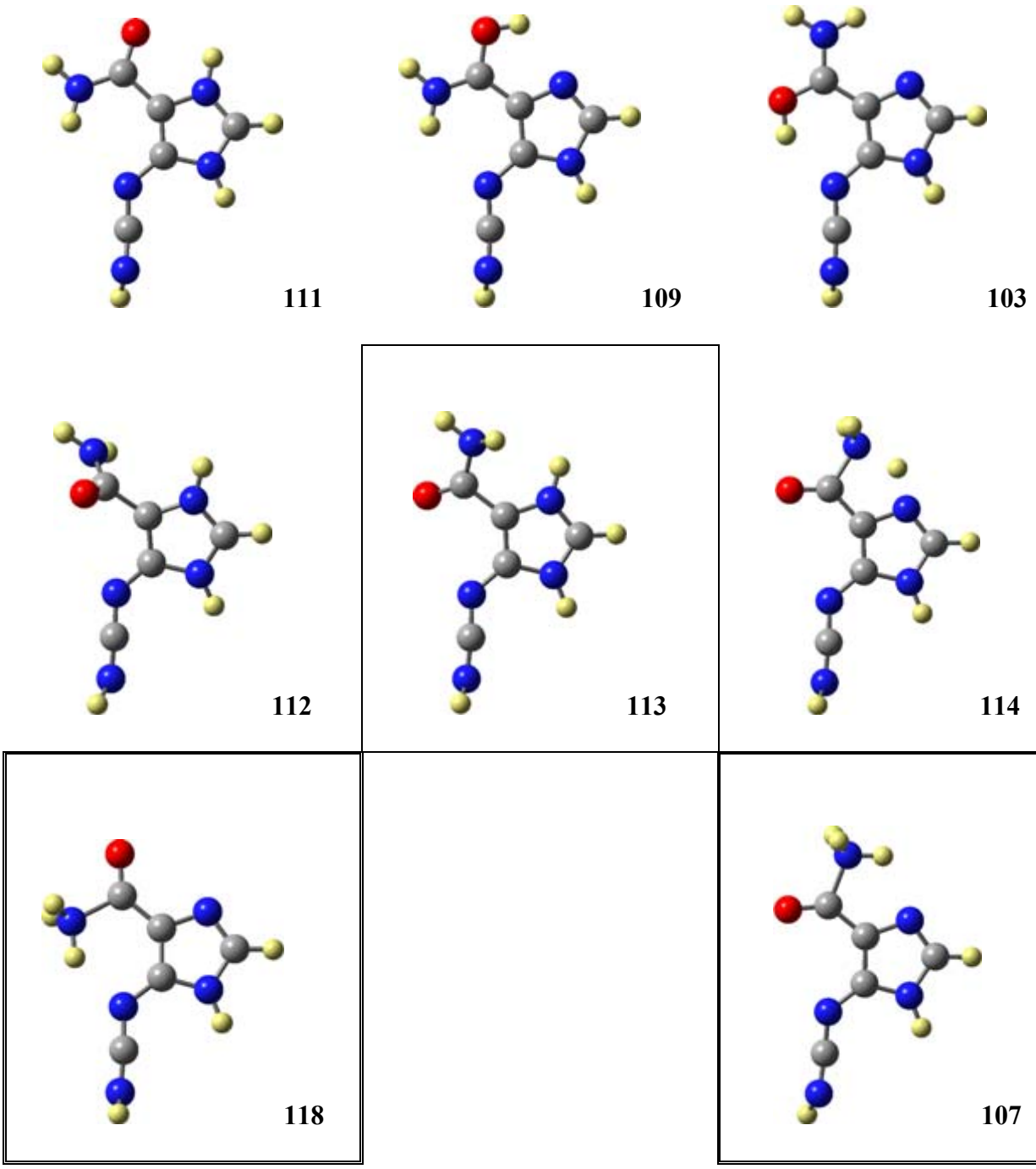


93, IMPT(**21**,**94**)

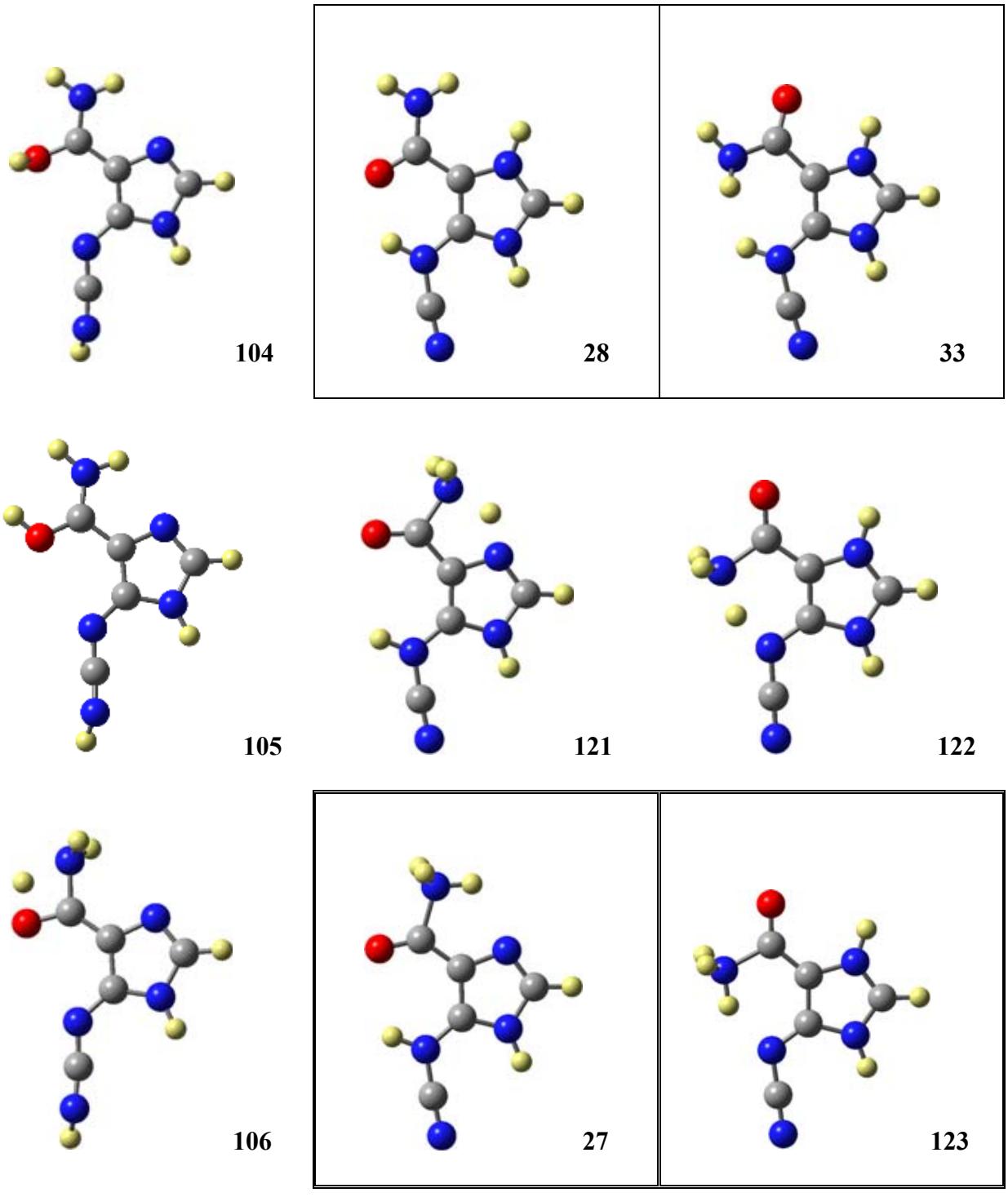


94

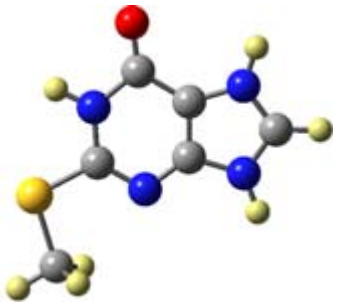
Scheme S2 (Continued. Attach to the right-most column.)



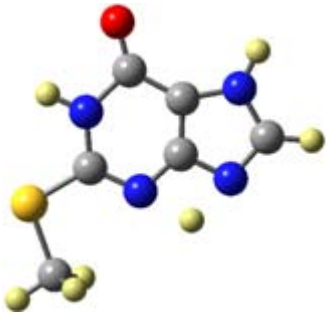
Scheme S3. (This is the left half.) Paths to ammonium ions from nitrilium and imidazolium ions formed by protonation of (*E*,*Z*)- and (*Z*,*Z*)-**13h**.



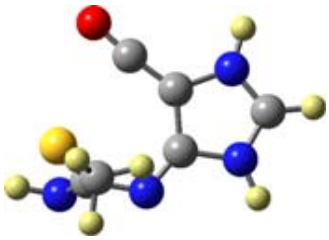
Scheme S3. (Continued. This is the right half.)



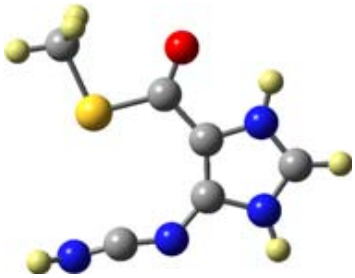
(*Z*)-**39**



128, IMPT((*Z*)-**39**,(*Z*)-**129**)

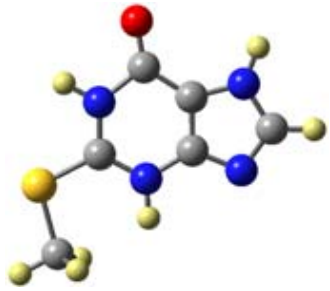


135

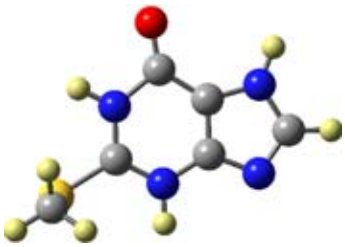


136

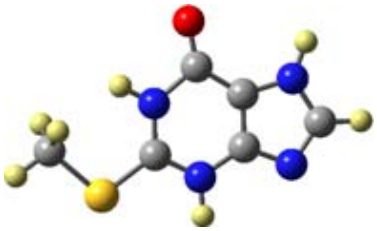
Scheme S4. (This is the left part.) Paths to sulfonium ions (double-lined) from the conjugate acids of **14h**.



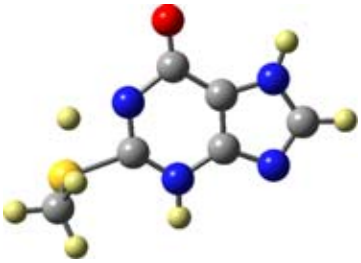
(*Z*)-**129**



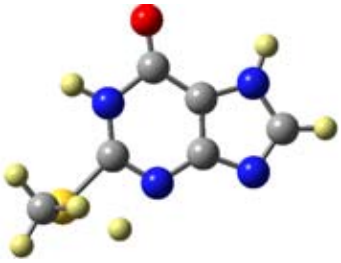
130, RTS((*Z*)-**129**,(*E*)-**129)**



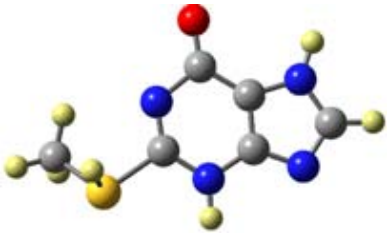
(*E*)-**129**



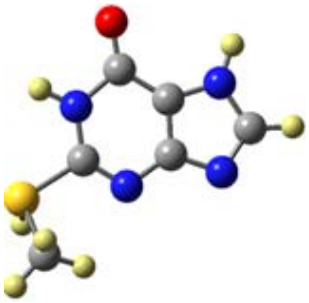
131, IMPT((*Z*)-**129**,(*E*)-**132)**



133, IMPT((*E*)-**129**,(*E*)-**134)**



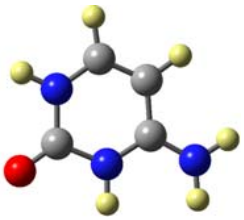
(*E*)-**132**



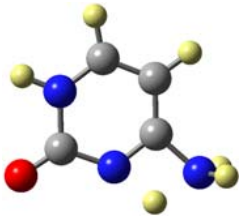
(*Z*)-**134**

(*E*)-**134**

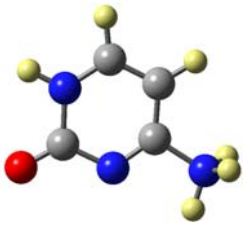
Scheme S4. (Continued. This is the right part.)



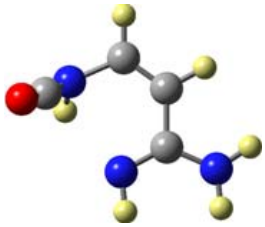
50



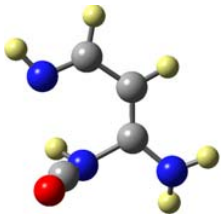
138, IMPT(**50**,**48**)



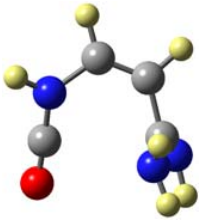
48



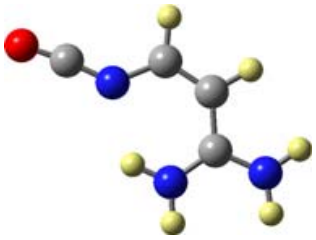
141, RTS(**50**,**142**)



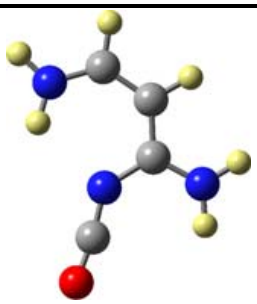
145, RTS(**50**,**146**)



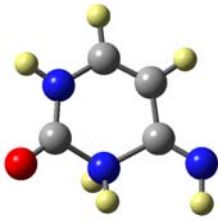
139, RTS(**50**,**140**) = "**49**"



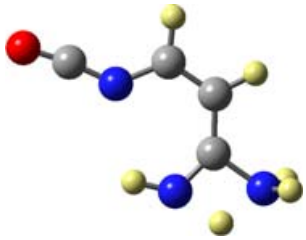
142



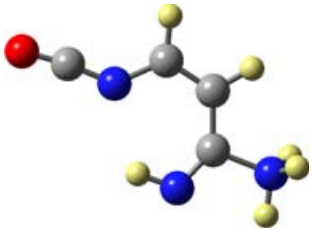
146 = "**49**"



140



143, IMPT(**142**,**144**)



144

Scheme S5. The N3-protonated cytosine **50** (single-lined) leads to NH_3 elimination from [**3h** + H]$^+$ via ammonium ion **48** (double-lined). Paths involving CN cleavage and rotation via **139**, **141**, and **145** also have been explored.

Aniline and Derivatives

Aniline

0,1
C,-1.5724206322,0.592426974,-0.0468020471
C,-1.6855060014,-0.7066494933,0.4578632703
C,-0.5267520037,-1.4734044849,0.614230325
C,0.7232174236,-0.9556720099,0.2747065018
C,0.8398654283,0.3510515788,-0.231467301
C,-0.3271655515,1.1194728555,-0.3893058804
N,2.0842634433,0.854416572,-0.6268514672
H,-2.4606923188,1.2048774151,-0.175586103
H,-2.6561635765,-1.1127882815,0.7240709681
H,-0.592927695,-2.48509342,1.0051443323
H,1.6158250559,-1.564904587,0.3962370836
H,-0.2541619854,2.1294566985,-0.785898495
H,2.1610671962,1.8619138637,-0.6560100266
H,2.8897772412,0.4222697865,-0.1953467006

N-Protonated Aniline

1,1
C,-1.2723361999,-0.2009678269,1.149751228
C,-1.9052416992,-0.2340825195,-0.0959884619
C,-1.1622544612,-0.1036288458,-1.2726286864
C,0.2238855818,0.0632328838,-1.2138707731
C,0.8224901633,0.0914909974,0.0410536906
C,0.1128124589,-0.0349825723,1.2303076815
N,2.303880345,0.3016320918,0.1168187264
H,-1.8504864451,-0.3063969567,2.0614129587
H,-2.9807977796,-0.3654379558,-0.1501439572
H,-1.6550858289,-0.1336164835,-2.2384018653
H,0.8049621648,0.1652235775,-2.1267610088
H,0.6084603694,-0.0085321471,2.1972895893
H,2.7023026502,-0.1570501281,0.9441016004
H,2.7772100399,-0.0905203517,-0.7051917102
H,2.5501373529,1.2985331018,0.1682152369

Adenine and Derivatives

Adenine, 1h

0,1
C,-0.7288577484,1.1351574392,0.2514897165
N,-1.9360041472,0.5654899857,0.0813724031
C,-1.9936908481,-0.7405755664,-0.2321971343
N,-0.9848897938,-1.6004611299,-0.4094537774

C,0.2017908624,-1.0045548032,-0.2342030548
C,0.4252456986,0.3377203016,0.0927811381
N,1.7795507298,0.612849242,0.1953722634
C,2.3594926844,-0.5354617469,-0.0632194765
N,1.4631873287,-1.5517016229,-0.3304847272
N,-0.6646349888,2.4497934301,0.5704438751
H,-2.9944837339,-1.145814677,-0.3570921644
H,3.4275067628,-0.7052067184,-0.0747087554
H,1.6755461696,-2.513078829,-0.5543966008
H,0.2269183533,2.9031900256,0.6890156434
H,-1.5198353468,2.9754071182,0.6585244838

15, NH_3^+-Adenine

1,1
C,-0.848798204,0.8451465991,-0.4377312404
N,-1.9731761141,0.2134201693,-0.1928551461
C,-1.8777925672,-1.0068229402,0.3862929501
N,-0.7480841444,-1.633113436,0.7341260708
C,0.3525174224,-0.9459945612,0.4620186109
C,0.4000929272,0.3386789936,-0.140764753
N,1.6903435038,0.7856978349,-0.2909754815
C,2.4162478152,-0.1951592398,0.2048965996
N,1.6722911003,-1.2584532135,0.670884321
N,-0.9747854811,2.1891488974,-1.0764984923
H,-2.812421552,-1.5194084185,0.5839388867
H,3.4970714116,-0.1957239097,0.2556815456
H,2.0271629803,-2.1106062366,1.0887934801
H,-0.0423437111,2.5988414141,-1.2277616327
H,-1.4611666985,2.1147942257,-1.9792954448
H,-1.5280288434,2.8201080508,-0.4823987418

16, N1-Protonated Adenine

1,1
C,-0.6237074925,1.1975124948,0.1672288879
N,-1.7576732943,0.5524391032,0.5915960939
C,-1.8651205524,-0.825222276,0.6879269526
N,-0.9109033437,-1.6556799878,0.389371075
C,0.2197921349,-1.0475046938,-0.0322731175
C,0.4328139632,0.3322758273,-0.165638642
N,1.697964688,0.6064340262,-0.620077858
C,2.2473640743,-0.5785636398,-0.7618373429
N,1.3967880351,-1.6140811674,-0.4200295773
N,-0.5568288874,2.5255398626,0.0871986891
H,-2.5725486741,1.0985704859,0.8534352133
H,-2.8242608322,-1.1902925256,1.0391784671
H,3.2558740085,-0.7612428372,-1.1069907567
H,1.601178853,-2.6064595662,-0.4492502838

H,0.3079841916,2.9445484068,-0.2334709798
H,-1.3205106957,3.141326904,0.3282489532

17, N3-Protonated Adenine

1,1
C,-0.8887130644,0.9839837294,-0.4080278429
N,-2.0038025762,0.326600833,0.0350715959
C,-1.893926658,-0.8364527691,0.6112128275
N,-0.7121723797,-1.4943039261,0.8253806455
C,0.4238299542,-0.8711028339,0.3974436117
C,0.3787218518,0.3725077888,-0.2258230422
N,1.6480893975,0.7871455534,-0.5617996483
C,2.4328161521,-0.1746476025,-0.1546009207
N,1.7359425018,-1.2233809648,0.4443351281
N,-1.0465663965,2.1652865934,-0.9885781695
H,-2.7876290575,-1.3462274208,0.9577098288
H,-0.7107842925,-2.4000510902,1.2825146225
H,3.5096855291,-0.2006258303,-0.2489439699
H,2.145474343,-2.0658279609,0.8287094771
H,-0.2477974098,2.6842695356,-1.3303055584
H,-1.975752355,2.5532962687,-1.0917790621

18,N7-Protonated Adenine

1,1
C,0.811792862,0.8332242978,-0.8034178417
N,-0.1674101288,1.1614667064,-1.6607513738
C,-1.4026417351,0.6717824472,-1.5042331047
N,-1.8380968419,-0.1605052304,-0.5454136539
C,-0.8687333039,-0.479953564,0.2957766102
C,0.4592652901,-0.0468126468,0.2553411305
N,1.1008060257,-0.6461857211,1.3435010949
C,0.2209491344,-1.3997927432,2.0095153217
N,-0.9689660497,-1.3205302503,1.4055197322
N,2.035028227,1.3550787094,-1.0090011641
H,-2.1356312033,0.9864703044,-2.2404879807
H,2.0710794376,-0.5520050232,1.6184664088
H,0.4402763347,-1.979239738,2.894594362
H,-1.8177518377,-1.793540754,1.7000883312
H,2.8342678134,1.171352879,-0.4245552988
H,2.15443734,1.9710061016,-1.8029809552

19, N9-Protonated Adenine

1,1
N,-1.9685580505,0.4965869042,-0.2962908541
C,-1.9772659568,-0.8254940943,-0.3334117182
N,-0.9075854444,-1.6631522918,-0.1877642936

C,0.1831141746,-0.9782487699,0.0023638169
C,0.3690382203,0.3892388053,0.0685921005
C,-0.8049353789,1.1687705446,-0.0950358575
N,1.5384549407,-1.5770968915,0.1994059068
C,2.3998431012,-0.3237131041,0.3688098863
N,1.7116809744,0.7384594822,0.2892654703
N,-0.8339826265,2.5025809024,-0.0635394239
H,-2.9362712825,-1.3066133887,-0.4973085983
H,1.8258594674,-2.1464639096,-0.6097964663
H,1.5684170618,-2.1906940231,1.0265635486
H,3.4625458447,-0.4467489937,0.5326720884
H,0.0007947412,3.051644602,0.0826486644
H,-1.720179352,2.973908686,-0.190226242

60, IMPT(16 → 15)

1,1
C,0.0072239381,0.0001290515,0.0197553024
N,0.0027154897,0.0001658085,1.3660314714
C,1.1519783633,-0.000093524,2.0755452616
N,2.3529016093,-0.0003993767,1.5028101413
C,2.3386231495,-0.0004310991,0.1730868534
C,1.1881448075,-0.0001754171,-0.6853120361
N,1.5531800998,-0.0002986957,-2.0083790184
C,2.8658315204,-0.0006152991,-1.9719786602
N,3.3930299648,-0.0007090515,-0.6934007885
N,-1.4104357989,0.0004648807,-0.2620532643
H,-1.3174780731,0.0004780014,1.0920353963
H,1.0802951021,-0.0000474399,3.1569316426
H,3.5057078609,-0.0007931411,-2.8448504782
H,4.3743087932,-0.000939938,-0.4388198659
H,-1.7583325953,-0.8343436249,-0.7411210031
H,-1.7579280417,0.8354155971,-0.7411667724

61, IMPT(18 → 15)

1,1
C,-0.0024067758,0.0001604515,0.0015095373
N,-0.0011703414,-0.0000650127,1.3164822897
C,1.249631525,-0.0000303926,1.887884759
N,2.4611275913,0.0002403458,1.2957162008
C,2.3952909075,0.0004714285,-0.0368506753
C,1.1820183669,0.0003925552,-0.672290131
N,1.2525205548,0.000766254,-2.0266994314
C,2.5608082824,0.0010529084,-2.2763567877
N,3.290806608,0.0008839646,-1.1089375013
N,-1.0501096919,0.0003014289,-1.0187769693
H,1.2558852633,-0.0002353363,2.9722371419
H,-0.0558140081,0.0006660427,-2.0874751657

H,3.0234758751,0.0013842866,-3.2533508048
H,4.3049798617,0.0010471376,-1.062687749
H,-1.6522554174,0.8267039341,-0.9803384098
H,-1.6520590511,-0.826263922,-0.9807606646

62, IMPT(16 → 63), Pyrimidine Ring-Opened N1-Protonated Adenine,
1,1
C,0.0066412355,0.0000136904,0.0052261823
C,0.0012471434,0.0000887644,1.4029097389
C,1.1776854732,0.0000690531,2.3055777567
C,-2.0495512698,0.0001720074,0.7433687919
C,2.1464546119,-0.0001762245,-1.2324635133
H,3.1328362005,-0.0002562913,-1.662266603
H,3.1045627595,-0.000036796,2.4097039823
H,-0.1009626399,0.0002294821,3.9223867784
H,1.585583791,0.000153836,4.3310791976
H,-1.6676980198,0.0000380926,-1.3475150762
H,-3.1308947867,0.0002341527,0.7367978564
N,2.3390165039,-0.0000286725,1.7342219492
N,1.0684623981,-0.0000917495,-0.8188496774
N,-1.3152607643,0.0000685367,-0.3976482443
N,-1.2864088589,0.0001859154,1.8277908235
N,0.8648660779,0.0001577695,3.6253947985

63, Pyrimidine Ring-Opened N1-Protonated Adenine
1,1
C,0.0779602938,-0.0121126532,-0.1587723483
C,0.0814120642,0.0922839111,1.2363872122
C,1.2625766124,0.1111818088,2.1319371437
C,-1.9726916121,0.1274418784,0.588642655
C,2.1199945155,-0.2005366012,-1.5655059437
H,3.0516140241,-0.2782971581,-2.0980738883
H,3.1887130475,0.0388806404,2.215874764
H,-0.0029812298,0.2838551935,3.751008452
H,1.6853977265,0.2447113094,4.1500711859
H,-1.6100587395,-0.0436235332,-1.4970981523
H,-3.0532517349,0.1713844359,0.5875065109
N,2.4136118201,0.0206993481,1.5514786473
N,1.1160241859,-0.1177404899,-1.004868673
N,-1.2488438006,0.0124593389,-0.5522534312
N,-1.2010483611,0.17671152,1.665758934
N,0.9595727103,0.2224707473,3.4501392818

64, RTS(**63**,**65**)
1,1
C,-0.0104983097,-0.0861715109,0.0402959157
C,-0.050215449,0.0078205768,1.4403128969

C,1.1169452642,0.0231388596,2.377383334
C,-2.0705550133,0.1589703995,0.7193606611
C,2.0125200718,-0.2633608852,-1.4108078394
H,2.9089713604,-0.3304622545,-2.0025891963
H,2.1374679587,1.0867536382,3.6110375618
H,1.3714574254,-2.0164938456,2.2704376024
H,2.6278023236,-1.1909167997,3.0287531451
H,-1.6529438563,0.0096767627,-1.3580738153
H,-3.1475337055,0.2554018548,0.6858568122
N,1.3279639998,1.121223913,2.9862034292
N,1.0491100149,-0.1825829222,-0.778100378
N,-1.3204983153,0.0224239706,-0.401074939
N,-1.3361562385,0.1524947784,1.825421833
N,1.8786437463,-1.1414850866,2.3467630558

65
1,1
C,0.0217545811,-0.0847295475,-0.0393026711
C,0.0452179205,0.0482883463,1.3601939861
C,1.228364388,-0.0797358429,2.260751463
C,-1.9985142375,0.2459621871,0.7208401926
C,1.9285032843,-0.6149962758,-1.5606797633
H,2.7737924269,-0.8555651989,-2.1817100586
H,1.9627605358,-0.9569387306,3.8034105928
H,2.1646648444,1.5951429704,1.5260081596
H,3.1460155492,0.5950133541,2.4456934143
H,-1.681499887,-0.0180116892,-1.363852113
H,-3.0703618601,0.3925963597,0.728336254
N,1.1196669604,-0.9019000674,3.226362098
N,1.0185459048,-0.3686464377,-0.8928185614
N,-1.3044874197,0.0370810839,-0.4250271793
N,-1.217258542,0.2556737423,1.792570518
N,2.344627782,0.6416304229,1.8249247674

Guanine and Derivatives

Guanine, 2h
0,1
C,-1.5053069017,-0.9224100022,0.1130516922
N,-2.6649887284,-1.6485585378,0.2605452047
N,-1.59314007,0.4350014148,0.2927398306
C,-0.5073823902,1.37581373,0.2391973037
C,0.723902037,0.6803840642,-0.0320366434
C,0.6881192017,-0.7067525996,-0.1868312736
N,-0.3785993559,-1.5467279648,-0.1393782139

O,-0.7391436474,2.56072549,0.422874019
N,2.0137537712,1.1580142493,-0.1655695658
N,1.9880728628,-1.0709308996,-0.4207479715
C,2.7392131189,0.093342313,-0.3956446402
H,-3.5401025643,-1.2093145708,0.0115747019
H,-2.5797511781,-2.6131647037,-0.0296779287
H,-2.4790077959,0.8574029263,0.5460862003
H,2.3164494129,-2.0130152168,-0.5766981801
H,3.8086015516,0.0824347793,-0.5538205658

20, NH_3^+-Guanine

1,1
C,-1.3113870894,-0.4134431139,0.9577670253
N,-2.4229738582,-0.8442688064,1.8558791317
N,-1.587968205,0.5401782403,0.0414922739
C,-0.58919928,1.063491157,-0.91181899
C,0.6749435971,0.3924501088,-0.6859583446
C,0.7871620273,-0.5783242385,0.3130762034
N,-0.1936842681,-1.0130349091,1.1641918593
O,-0.9297059618,1.9143336815,-1.6925298704
N,1.8669848655,0.5599853952,-1.3327853136
N,2.084071111,-1.0038145912,0.262308236
C,2.6878712668,-0.2845975451,-0.7468625868
H,-2.7836241677,-0.078695735,2.4428004712
H,-3.2145789497,-1.2583939601,1.3435299957
H,-2.0247811516,-1.5660004281,2.4743515192
H,-2.5031025295,0.9704129043,-0.0620149148
H,2.5135874395,-1.7073328285,0.8499444741
H,3.7287964068,-0.4254349163,-1.0031957377

21, N1-Protonated Guanine

1,1
C,-1.7300305799,-0.7713575741,0.5197858425
N,-2.8552411267,-1.3867622681,0.1369224434
N,-1.8257072521,0.3830909784,1.2369671314
C,0.1704936654,1.7572974733,-0.6151660294
C,0.9575823081,0.6910426029,-0.342041814
C,0.560675747,-0.6645068881,0.0074557546
N,-0.5719480502,-1.3269499029,0.1793438999
O,-0.4805768409,2.6747573221,-0.8470144603
N,2.3539418856,0.7835954701,-0.5041067526
N,1.7637196102,-1.3072437092,0.0379995211
C,2.7834011043,-0.4135994957,-0.270433621
H,-2.7772834098,-2.2043091362,-0.4524315362
H,-3.7667509458,-1.1382145732,0.4930313043
H,-2.7327851734,0.7256399369,1.5272484671
H,-1.0643895718,0.6207225727,1.859155147

H,1.8589951069,-2.2955791264,0.2416950685
H,3.8207397847,-0.7196889391,-0.3000672673

22, N3-Protonated Guanine

1,1
C,-1.5884138687,-0.811040278,-0.3463082214
N,-2.7050039724,-1.4987421779,-0.6194256511
N,-1.626029676,0.4886249447,-0.0207844084
C,-0.4966976128,1.3881694281,0.3072528971
C,0.7483333853,0.6598424219,0.2334643555
C,0.7540193487,-0.6807416172,-0.1053377153
N,-0.3821158885,-1.4262530999,-0.3949251661
O,-0.7487417121,2.5313802824,0.5742392438
N,2.0318695555,1.096245052,0.4578581695
N,2.0533657092,-1.0797979665,-0.0910200337
C,2.7884921708,0.05130859,0.2605365055
H,-3.6123620827,-1.0549861023,-0.5875416817
H,-2.6865830439,-2.4783047213,-0.865874836
H,-2.5231955206,0.964909911,0.0200069796
H,-0.3249789565,-2.4073090204,-0.6377291145
H,2.4326508224,-1.9971346942,-0.2895471874
H,3.8654018436,0.0160138317,0.347204589

23, N7-Protonated Guanine

1,1
C,-0.4305056879,-0.0307483321,-1.7602678749
N,-0.7886504144,-0.0519721931,-3.0534784529
N,0.9159218227,-0.0658275591,-1.4584589104
C,1.4845909003,-0.0509712787,-0.1546522451
C,0.4237973782,0.0071751728,0.8179985676
C,-0.9011336324,0.0390255881,0.4147513931
N,-1.3814747362,0.0228504231,-0.8306273562
O,2.6844442969,-0.0842138511,0.0350139094
N,0.4381026126,0.0416150165,2.2009059556
N,-1.6475679879,0.0922758675,1.5871298669
C,-0.8151271747,0.0926272277,2.6476221532
H,-0.1256299186,-0.0923065607,-3.8121942529
H,-1.774178874,-0.026453698,-3.2741944814
H,1.6054174274,-0.1064616758,-2.203446108
H,1.2718275747,0.0297861527,2.7804501906
H,-2.6604337559,0.1255844885,1.634639058
H,-1.1166066087,0.1283209506,3.6836246327

24, N9-Protonated Guanine

1,1
N,-1.4479968188,0.9478614901,-0.0941124852
C,-1.7678105783,-0.3401806763,0.2195654619

N,-0.8273102361,-1.2951128933,0.3564581702
C,0.3890565884,-0.8290627564,0.1535577998
C,0.8532849534,0.4216159109,-0.1634780112
C,-0.123141389,1.4834548001,-0.3213144532
N,1.596713846,-1.6961571813,0.2491305757
C,2.7162759369,-0.6894336653,-0.066660329
N,2.2466813072,0.4654718844,-0.2864565748
O,0.0266535432,2.6495729674,-0.5939015604
N,-3.0487910158,-0.6825594908,0.4001057604
H,-2.1790017016,1.647790164,-0.1910781585
H,1.5643621688,-2.4726892808,-0.4264687531
H,1.6953178906,-2.1125830577,1.1858003066
H,3.738494625,-1.0429770587,-0.070735939
H,-3.26103729,-1.6432472878,0.6319010944
H,-3.8124366842,-0.0277655591,0.3158929978

25, (C6)O-Protonated (N1 side) Guanine

1,1
N,-1.5408507607,0.5732389072,-0.2475935129
C,-1.5551861476,-0.818585505,-0.3435480309
N,-0.4648214294,-1.5451607241,-0.1898920898
C,0.6411183258,-0.8399411864,0.0626245614
C,0.7617395069,0.5705403469,0.1796886989
C,-0.3995757634,1.3001485431,0.0130457249
N,1.9003733149,-1.3036206835,0.2652568352
C,2.7120713976,-0.1909330109,0.4906154129
N,2.0658480074,0.9403063776,0.4465956841
O,-0.431044264,2.6148996594,0.0953847081
N,-2.733538837,-1.4124264384,-0.6023907724
H,-2.4144136695,1.0727122839,-0.3767916097
H,2.1858926046,-2.2756047496,0.2530062195
H,3.7716067394,-0.2982738132,0.6800832669
H,-1.2988266271,3.0270934672,-0.037970621
H,-2.7428956064,-2.4209328868,-0.6711669193
H,-3.6030853113,-0.9179287747,-0.7286292136

26, (C6)O-Protonated (N7 side) Guanine

1,1
C,-1.5590713456,-0.8702514912,-0.1878231813
N,-2.7327902071,-1.5077239721,-0.3239046144
N,-1.5881404759,0.4533907494,0.2371977354
C,-0.4569775262,1.2039864499,0.4116000779
C,0.7435076779,0.5810892866,0.1426926245
C,0.6728653779,-0.7674790807,-0.2845283989
N,-0.42667666,-1.5031515435,-0.4559685755
O,-0.6661923014,2.4395311482,0.818899927

N,2.048777633,1.0273408467,0.2096643663
N,1.9730053721,-1.1217691237,-0.4733072062
C,2.7517470625,-0.0082882971,-0.1623713275
H,-3.6283312314,-1.0843877271,-0.1348883495
H,-2.7116149989,-2.4701324433,-0.6318178401
H,-2.4727052843,0.9128349043,0.4353392603
H,0.1745895148,2.9205846237,0.9239426857
H,2.3053725282,-2.0275853053,-0.7823134606
H,3.8305707692,-0.0385131407,-0.23465242

74

1,1
C,0.0141403085,0.3976740654,0.0313764494
N,0.556629132,-0.2388712778,1.15598011
N,0.5542033516,1.2056610734,-0.7842266352
C,0.6857974117,-2.5697700409,-0.6661562598
C,-0.6252315232,-2.395357615,-0.8977883365
C,-1.485549855,-1.2219578703,-0.6390596774
N,-1.3162634125,-0.0376582091,-0.2373013105
O,1.8083399796,-2.7926903512,-0.5205932577
N,-1.4736142758,-3.4055679262,-1.4347881622
N,-2.7765773921,-1.7112151741,-1.0162836049
C,-2.7154718193,-2.9530881799,-1.4807363839
H,1.4391213917,0.1439807237,1.4790030157
H,-0.09098524,-0.3869083616,1.9240918883
H,1.4959023077,1.4831362956,-0.504145057
H,-1.186057604,-4.326497366,-1.7434379861
H,-3.6055733465,-1.1267993804,-0.9805811679
H,-3.5573983932,-3.523494348,-1.8509482467

75

1,1
C,-0.0362211268,-0.2716899844,-0.1354413845
C,0.0563337088,-0.0146471837,1.2243872323
C,1.0871111577,0.1065962281,2.3066635981
C,-2.1030198098,0.0916546217,0.6524740851
C,2.0019868063,-0.9254642076,-1.1510429181
H,-1.763209674,-0.3244764501,-1.3822306109
H,-1.431780145,0.3888368476,2.6397735573
H,3.0576295873,0.1492164335,2.7459624252
H,2.7607494556,0.006086553,1.04819662
H,-3.1749362679,0.2089141038,0.704811756
H,3.6895210326,-1.9940490502,-1.3903968035
N,2.3965163487,0.0282484762,1.9887446365
N,0.8310916234,-0.5255804781,-1.1523025859
N,-1.3896839355,-0.1874734148,-0.4485216227
N,-1.2441343522,0.1945829229,1.6553892131

N,3.1873869423,-1.1264601731,1.2440753636
O,0.6598312375,0.2692646405,3.4462459439

76, RTS(75,77)

1,1
C,-0.0016043485,-0.0018048099,0.0040229638
C,-0.0024231263,0.0121746189,1.3855692845
C,1.146376486,0.0108897556,2.3743182561
C,-2.0942637059,0.4126479603,0.6914895876
C,2.1693492493,-0.2431167255,-0.8766322535
H,-1.6223506528,0.2795478954,-1.349880712
H,-1.6271271408,0.3983317613,2.7210748603
H,-3.153286776,0.6201280788,0.6914535612
H,2.1861044554,-1.2375636214,3.6117746498
H,0.9467167758,-2.0385204597,2.6904467721
H,4.1088560815,-0.8338271413,-0.9044578027
N,0.9300846739,-0.1810907965,-0.9684493775
N,-1.3190547154,0.2321030828,-0.3825692173
N,-1.3115120101,0.2825090294,1.7640972014
N,1.434571434,-1.1890366801,2.9343688367
N,3.3632206478,-0.1537034542,-0.9512015997
O,1.7237785869,1.0571205527,2.6145019924

77

1,1
C,0.1080603113,0.180010386,-0.0678233261
C,0.0708071866,0.2841510717,1.318137328
C,1.2213902643,0.4004466694,2.2470851558
C,-2.0257542117,-0.0390765525,0.5962164205
C,2.2784252742,0.4651275572,-0.9085043848
H,-1.4954576819,-0.1135573299,-1.4359786451
H,-1.6172806025,0.0867416512,2.6278027632
H,-3.0941532123,-0.191808533,0.5790548867
H,1.7523602957,0.8720075192,4.1388368025
H,0.1829230826,1.4203682332,3.7341744482
H,4.3017550086,0.4616016763,-0.7981121829
N,1.0623419157,0.1938795515,-1.019863696
N,-1.2124727232,-0.0089167298,-0.4668557406
N,-1.2695922837,0.1404655905,1.6771286114
N,0.947710542,0.7920487826,3.5272352313
N,3.401698178,0.8485440295,-1.0441834117
O,2.3356696728,0.0867678734,1.8468869463

78, IMPT(77,79)

1,1
C,-0.0026896665,-0.001125999,-0.0017678854
C,-0.0073816942,-0.0006328014,1.3926075225

C,0.949224076,0.0012414149,2.480409565
C,-2.1119871037,-0.0769689592,0.7807090714
C,2.1663861615,0.1812753605,-0.8643691753
H,-1.679435995,-0.0628957819,-1.3006587155
H,-1.0656984773,-0.0511033667,3.0579798772
H,-3.1911822415,-0.1156302146,0.7788208305
H,0.3629810652,-0.831435801,4.3118555529
H,0.3079622563,0.8147303372,4.3021859113
H,4.1975086787,0.000996638,-0.8244882788
N,0.9324823214,0.0190108781,-0.9756391205
N,-1.3417753698,-0.0527255036,-0.3437933372
N,-1.3240382914,-0.0466994729,1.8305974929
N,0.1213544538,-0.0189573639,3.740180662
N,3.3190772569,0.4846166221,-0.9420478856
O,2.1527046511,0.004997206,2.456787559

79

1,1
C,0.193627029,0.2245426991,-0.1204049175
C,0.1965322331,0.4008333981,1.2808643171
C,1.2827947473,0.7029303605,2.1396774539
C,-1.8555480836,0.0378833377,0.7470483221
C,2.3582982888,0.2791251726,-1.060339682
H,-1.4703822137,-0.1667296935,-1.3555933453
H,-2.9251710429,-0.1162877704,0.7634540389
H,1.2334343816,0.1143122375,4.2093859314
H,0.9797481986,1.7399061127,4.0011814735
H,-0.2647173377,0.6506835635,3.6247155981
H,4.3320246542,0.7558705623,-1.1675446316
N,1.1128481085,0.2520027717,-1.1082469859
N,-1.1209067811,0.0027781727,-0.4189849496
N,-1.0966894146,0.2755793561,1.7811225623
N,0.7579137558,0.8116303299,3.6281992699
N,3.5377459782,0.1337888869,-1.2027524354
O,2.4563230313,0.8881294367,1.9625373485

80, IMPT(23→81)

1,1
C,0.0057153026,0.0341487201,0.0006000288
N,-0.0055476377,-0.0557126933,1.3343987337
N,1.1996857248,0.0408473218,-0.6849477323
C,1.4552234907,0.0347323333,-2.1317567902
C,0.1889892008,0.1383658135,-2.8237227045
C,-0.9106466607,0.182668326,-2.0312595778
N,-1.1267141908,0.1325233949,-0.7057560744
O,2.5863057914,-0.0576554521,-2.5413798586
N,-0.3678850522,-0.0101062237,-4.099459688

N,-2.0748762522,0.0624746011,-2.6899957683
C,-1.7221577332,-0.0547388498,-3.9792593973
H,0.8377969088,-0.1534031939,1.8801978195
H,-0.8877727202,-0.0271073225,1.8264707144
H,2.0654884099,-0.0077539468,-0.1555390009
H,0.1385890927,-0.0482151483,-4.9774590007
H,-2.4004078447,-0.0393336064,-1.321607295
H,-2.3917964967,-0.1559947749,-4.8208748597

81, N3(1*H*,7*H*)-Protonated Guanine

1,1
C,-0.0135435879,0.0064499027,0.0306243002
C,-0.0307818171,0.1083979305,2.3963692877
C,1.3488550428,0.1830685073,2.4476342817
C,2.1756043573,0.1756786898,1.2792801186
C,0.4363676007,0.2220196314,4.4459074656
H,-1.7209908597,-0.0324734435,1.1956028528
H,1.869872997,0.070282328,-0.7738538076
N,1.3335299987,0.0797371072,0.0891968848
N,-0.7078625654,0.0201546049,1.1839395178
N,-0.6011226879,0.1314200315,3.6148320139
N,1.6290612261,0.2563651376,3.7953699253
N,-0.6456862284,-0.0779062702,-1.1463405405
O,3.3762851951,0.2332597254,1.1539966739
H,0.3592239608,0.2648032523,5.5232379016
H,-1.6529970506,-0.1336062037,-1.2048308087
H,-0.136384711,-0.0890974348,-2.0187665226
H,2.5502730557,0.3228370961,4.212056545

82, IMPT(81 → 83)

1,1
C,-0.011141539,0.0003663361,0.0262363468
C,0.0060382711,0.0000255513,2.3171686826
C,1.4043114224,-0.0004917754,2.2839645498
C,2.2023715453,-0.0006235153,1.0875222373
C,0.6171953119,-0.0004966262,4.3353404357
H,-1.6860452277,0.0010072791,0.1801373211
H,1.7947140157,-0.0001666213,-0.9843059521
N,1.3205922186,-0.0001178947,-0.0848799252
N,-0.7064521432,0.0004588196,1.1332038075
N,-0.4730425942,0.0000198355,3.5797246606
N,1.7715977272,-0.0008222599,3.6053076137
N,-1.0463914767,0.0009422503,-0.9875774906
O,3.4026083023,-0.0010592415,0.9408271503
H,0.6193083707,-0.0006533421,5.4165669251
H,-1.1063503685,-0.8394372524,-1.5698924737
H,-1.1056602104,0.8415444919,-1.5696413211

H,2.7202982155,-0.0012274978,3.9623005865

83, NH_2(1*H*,7*H*)-Protonated Guanine

```
1,1
C,0.0403682949,0.0315559571,0.1403027633
C,-0.0317517243,0.1109400667,2.3629451781
C,1.3648663955,0.0900057385,2.4346373335
C,2.2230842329,0.0351899835,1.2854700199
C,0.4444318706,0.1754502725,4.4241617503
N,1.3988153537,0.0069175557,0.0882016321
N,-0.719176807,0.0804008142,1.1665449631
N,0.5897106338,0.1638100324,3.5995582256
N,1.647975393,0.1323335756,3.7730165563
N,-0.6878400326,-0.0020983747,-1.1642747185
O,3.4319523908,0.0117502301,1.1957580475
H,0.3775180851,0.2145108428,5.5026320407
H,-1.6885317979,0.0233886066,-0.915403844
H,-0.5104074133,-0.859940599,-1.7051402167
H,1.9304238077,-0.0324227689,-0.7770063241
H,2.5705970094,0.1315660336,4.1916749978
H,-0.4824859486,0.8092800361,-1.763780299
```

84, IMPT(81 → 85)

```
1,1
C,0.0350146757,0.0000650195,0.0033348283
C,0.0067227499,0.0007232245,2.2972156574
C,1.3961182099,0.0009844056,2.2770164418
C,2.2125250591,0.0008075752,1.0782253692
C,0.574138582,0.0014418919,4.3215411324
H,-1.7327289084,0.0000684882,1.1102144079
H,0.9309878195,-0.0001627176,1.417422966
N,1.3413203291,0.0002865212,-0.0789477227
N,-0.7174000877,0.0002325278,1.1028511092
N,-0.5041949972,0.0009983186,3.5430073159
N,1.7354467883,0.001457023,3.6092982908
N,-0.369129258,-0.0004001487,-1.3903480244
O,3.4176592601,0.0010336406,0.9848735088
H,0.5536261867,0.0017623536,5.4022851361
H,-0.8501672481,0.8414278611,-1.7210308488
H,-0.8498421359,-0.8425967259,-1.7205651796
H,2.6795281927,0.001732313,3.9785045112
```

85, NH_2(3*H*,7*H*)-Protonated Guanine

```
1,1
C,0.0266087174,0.2890340961,0.1798002694
C,-0.0074595389,0.3895380037,2.4812003542
C,1.3683372987,0.229601465,2.4471290693
C,2.140066468,0.089670261,1.2314819432
C,0.5845829951,0.4060368768,4.4985676955
```

N,1.2838591264,0.1392052601,0.0618863777
N,-0.733559575,0.4233073621,1.2939145745
N,-0.4993120373,0.4987115051,3.7317723935
N,1.7272113145,0.2440764301,3.7764727683
N,-0.7152973484,0.3196064493,-1.1306319536
O,3.3383764591,-0.0526854817,1.1286764591
H,0.5792323017,0.4519931508,5.5784224577
H,-1.3915894153,-0.4491697957,-1.233050765
H,-1.199706687,1.2109736615,-1.30 29505573
H,2.6702240157,0.150495359,4.1349238541
H,0.0197425781,0.2046311982,-1.8450309909
H,-1.7408493852,0.5407884705,1.3226016482

86, IMPT(23,87)

1,1
C,0.0199441263,-0.0003658324,-0.0069194036
N,-0.0108082734,0.0001389529,1.4535293302
N,1.3460148265,-0.0006001663,-0.2117554969
C,1.9007982584,-0.0011156892,-1.5080839895
C,0.8006369595,-0.0013103792,-2.4737583298
C,-0.5300641648,-0.0010138053,-2.09085936
N,-1.0045921844,-0.0005189072,-0.8211886009
O,3.0851928237,-0.0013575038,-1.7792607193
N,0.8190494615,-0.0017880956,-3.8553984298
N,-1.2717822582,-0.0013252789,-3.2636298878
C,-0.4326099851,-0.0017912834,-4.3158557146
H,-0.4270179637,0.8356424835,1.8710279627
H,-0.4272301159,-0.8349722816,1.8716008576
H,1.2684860999,-0.0001225346,1.1503601717
H,1.6619043696,-0.0020880258,-4.423107892
H,-2.284992297,-0.00121913,-3.3205101899
H,-0.7269185191,-0.002112078,-5.3547392159

87

1,1
C,0.0017460879,0.0009062236,-0.0000589634
N,0.0024191142,0.0002011879,1.5111941941
N,1.2043658612,-0.0005216109,-0.4914461371
C,1.3585830159,-0.0005685119,-1.8962904799
C,0.0606394759,0.00120003,-2.5625726225
C,-1.1239221769,0.002616465,-1.847951167
N,-1.2284624966,0.0025614954,-0.5044144796
O,2.4325999451,-0.0018762645,-2.4720774591
N,-0.2802660629,0.0018570678,-3.9027009946
N,-2.1471201342,0.0041084972,-2.7880267557
C,-1.607584464,0.0036079051,-4.0233512895
H,-0.4842378216,0.8257961086,1.8782260631

H,-0.4736470174,-0.8319172009,1.8774179422
H,0.9820132922,0.005752104,1.8205182788
H,0.3876415277,0.0011449923,-4.668082248
H,-3.140383857,0.0053572014,-2.5843015012
H,-2.1617884728,0.0044618352,-4.9496644602

88, IMPT(22,89)

1,1
C,0.0390725231,0.00372256,-0.0155347525
N,-0.0221761924,-0.0007924234,1.4354903052
N,1.3162354953,0.0037781242,-0.2579938647
C,1.8886271402,0.0076925154,-1.6070840398
C,0.8081003815,0.0113848103,-2.5957293921
C,-0.5316999756,0.0109637989,-2.2259292846
N,-0.9682081215,0.0070558573,-0.9020949379
O,3.0786428612,0.0075511891,-1.7704408451
N,0.9057298336,0.0156201972,-3.9642399625
N,-1.259714211,0.0149697462,-3.3761547364
C,-0.3249605453,0.0176793705,-4.4050164997
H,-0.4039218261,-0.8448556038,1.8729881943
H,-0.402994023,0.8409308465,1.8782729856
H,1.2402965923,-0.0006020007,1.1521835529
H,-1.9444793378,0.0067470647,-0.6313868599
H,-2.2659690149,0.0158660975,-3.4855752547
H,-0.6311858759,0.0210976589,-5.4419223443

89

1,1
C,0.0700171605,0.009982365,-0.0031434178
N,-0.0553319512,0.0070750311,1.5019701338
N,1.257224568,-0.0486711592,-0.4301249713
C,1.5540497955,-0.0549725708,-1.8693553331
C,0.3346115791,0.0129836548,-2.6694950432
C,-0.9151683816,0.073790673,-2.0728312215
N,-1.1059655959,0.0750051468,-0.6953922624
O,2.6970069077,-0.1116480678,-2.2399065331
N,0.1929887378,0.0288380267,-4.037243511
N,-1.8334294939,0.1274652424,-3.0767842968
C,-1.0922590932,0.0965601052,-4.2557415726
H,0.9212360886,-0.0458250198,1.8307716708
H,-0.5646579731,-0.8069091081,1.8718040316
H,-2.0236395792,0.1199617919,-0.2702216661
H,-2.8414665819,0.1790661051,-3.0086589294
H,-1.5759719966,0.1275713015,-5.2220738477
H,-0.4775652368,0.8649067538,1.8822414707

90, IMPT(22,20)

1,1
C,0.0012497168,0.0002648966,0.00038669
N,-0.0009940944,-0.0000386018,1.4484176775
N,0.993864545,-0.0000533682,-0.881405711
C,0.7698427593,0.0003666042,-2.3560036453
C,-0.6551656755,0.0011453756,-2.6355672404
C,-1.6042704181,0.0014122103,-1.610906709
N,-1.2840575937,0.0009715517,-0.2752942985
O,1.7298797087,0.0000308281,-3.0765843884
N,-1.2794453004,0.0017138814,-3.8534771219
N,-2.8203259812,0.0021534893,-2.2200950629
C,-2.5627408847,0.0023058337,-3.5805691159
H,0.3784406042,0.8392876505,1.8961525382
H,0.3775963265,-0.8399347097,1.895798397
H,1.9715871536,-0.0006045975,-0.6011638643
H,-1.2966257044,0.0006938075,1.0727306651
H,-3.7301400078,0.0025204161,-1.775659693
H,-3.3620170072,0.0028612026,-4.3086567649

91 RTS(22,92)

1,1
C,0.0404556238,-0.0072750046,0.1342505695
N,0.0585379014,0.3220976312,1.4643923706
N,0.9618362567,-0.3286259244,-0.6758692169
C,-0.6073673133,-2.8946933468,0.8595774186
C,-1.7258020557,-2.4943556703,0.1972381716
C,-2.0054050121,-1.2210696142,-0.3954762879
N,-1.3268957738,-0.0621667547,-0.3819634175
O,0.3137230706,-3.2671462877,1.4265800464
N,-2.7677129581,-3.4025303144,-0.0594979559
N,-3.2045967591,-1.4131578367,-0.9969397445
C,-3.6152468291,-2.7336649147,-0.7652287659
H,0.9535521881,0.4932418369,1.904540684
H,-0.7239938603,0.8305321975,1.8544420774
H,1.9017266667,-0.2339693479,-0.2875504985
H,-3.7297893534,-0.7137829444,-1.509466749
H,-4.55137209,-3.1098644664,-1.1555165045
H,-1.5153383655,0.5986667321,-1.1299231416

92

1,1
C,-0.0050855389,0.008575314,0.022564281
N,0.1521515802,-0.144231,1.4632488967
N,0.8822589557,0.089509718,-0.8655258886
C,-1.0856248407,0.7638670475,2.6853983318
C,-2.2276564169,0.8472041466,1.8918220873

C,-2.3176768591,0.5121168679,0.5250836077
N,-1.3589662103,0.0569748118,-0.3315954418
O,-0.5731736611,0.9408510825,3.7155746269
N,-3.4559905367,1.301469309,2.3647848477
N,-3.6073581447,0.7558349389,0.1969509234
C,-4.2523672262,1.2338264734,1.3474472849
H,0.0244978956,-1.1228136608,1.7409499561
H,1.0805346162,0.153038325,1.7684913272
H,1.8428010157,-0.0182538989,-0.5440836889
H,-4.0357731757,0.6278971667,-0.7125616458
H,-5.3004265244,1.4996454802,1.3347620795
H,-1.5207550259,0.0656647164,-1.333848135

93, IMPT(21,94)

1,1
C,-0.0000468281,0.0001265622,0.0001090698
N,-0.0001340179,0.000574842,1.2998309284
N,1.5005665336,-0.000322107,-0.2174574559
C,0.4802214233,2.2096825352,-2.5662432101
C,-0.3656477245,1.2462643707,-2.9832912294
C,-0.9964963467,0.228474731,-2.1526638635
N,-0.9604447985,-0.1325380639,-0.8874922376
O,1.2062126954,3.009710531,-2.165469481
N,-0.8520102742,1.2001041305,-4.3026168349
N,-1.8536717481,-0.3582304543,-3.0392769527
C,-1.7245176347,0.2449345442,-4.2851114628
H,-0.870486018,-0.015245367,1.8275201821
H,1.344261442,-0.0249106785,1.0483738955
H,1.8683387481,-0.8286107682,-0.6906342421
H,1.9173695836,0.8455265924,-0.6081657824
H,-2.477954211,-1.1174255871,-2.7904937575
H,-2.309679901,-0.0763104706,-5.13687224

94

1,1
C,-0.0012450057,0.0006003225,-0.0002088352
N,0.0005805713,-0.0000689372,1.2718296722
N,1.4333521046,-0.0008637283,-0.5402406816
C,-2.5970255717,1.81410536,0.9736801568
C,-2.9578827461,1.0615475943,-0.0902611975
C,-2.1211760836,0.2482845418,-0.9601639225
N,-0.8413684374,-0.0772234096,-1.0419423838
O,-2.3090157727,2.4548896308,1.8838791743
N,-4.2855086677,1.1060254148,-0.5627888859
N,-3.0150376339,-0.1500927151,-1.9126844073
C,-4.2690270781,0.3791613262,-1.6319007763
H,-0.9194640469,-0.0996004154,1.6976201124

H,2.0752431008,0.02765611,0.2598915055
H,1.5972093036,-0.8516079565,-1.0896732133
H,1.5987704129,0.8016501981,-1.1566797539
H,-2.7682418882,-0.7515099375,-2.6895195624
H,-5.1256331872,0.1818861833,-2.26276224

95
1,1
C,-0.0022567948,0.0001894537,0.0802227475
C,-0.0279798436,-0.0000294298,1.5403610679
C,0.9984817892,-0.0001034474,2.419515003
C,-2.1446023894,-0.0000427459,0.8197704839
C,2.179706218,0.0003778234,-0.3593780439
H,-1.6946405171,0.0002873912,-1.228836477
H,-1.7654497506,-0.0003243355,2.8579487403
H,-3.2270608445,-0.0001035093,0.8144494024
N,0.9231288552,0.0003738467,-0.8072015306
N,-1.3711091658,0.0001632424,-0.2654246413
N,-1.3999388694,-0.0001631864,1.9117843379
N,3.2809753654,0.0003810087,0.0339456336
O,1.8190042988,-0.0001724012,3.2234202831

TS(95,10')
1,1
C,-0.0228636676,-0.0008183343,0.0028556731
C,-0.0109342116,-0.0006762015,1.433505909
C,1.0408480711,-0.0002777071,2.2822806452
C,-2.124221857,-0.0014244912,0.6635415069
C,1.9802148432,-0.0005314293,-1.3000857081
H,-0.6980544861,-0.0012572194,-1.5620235763
H,-1.7676328068,-0.0011052148,2.7348865458
H,-3.2069043924,-0.0017735768,0.6569561219
N,0.6589728035,-0.0008330168,-1.1200799265
N,-1.3394215374,-0.0012336316,-0.3984379838
N,-1.393568414,-0.0010923269,1.7925656371
N,3.1311531982,-0.0002792939,-1.4909579908
O,1.9441403028,0.0000712939,2.9883348387

Cyanoamine 13h and Derivatives

Cyanoamine (*E*,*Z*)-13h
0,1
C,0.0276358338,-0.025819046,-0.0665763097
C,-0.0129743173,-0.0088036795,1.3142794272
C,1.1816311899,-0.0060227778,2.1589195859
C,-2.0573875964,-0.0038777625,0.655514818

C,1.0756179636,-0.0604029143,-2.2186697356
H,-1.5903356267,-0.0324497189,-1.4470496577
H,2.0256480293,-0.0420407677,-0.3662705045
H,0.035500329,0.0215599902,3.8680214415
H,1.7701325836,0.0139004538,4.1175207543
H,-3.1363090332,0.0022629526,0.6040289664
N,1.1427483609,-0.0425291903,-0.88818819
N,-1.2721281784,-0.0226737565,-0.4870870071
N,1.3302485044,0.0047277912,1.7422889533
N,0.9747131699,0.0112748555,3.4977153805
N,0.9645333253,-0.0754279141,-3.381711152
O,2.3147309365,-0.0191933008,1.6423314209

27, NH_3^+-Cyanoamine (*E*,*Z*)-13h

1,1
C,0.116259403,0.0057011977,-0.1202224397
C,0.1337069337,-0.0036486746,1.283491127
C,1.2691718771,-0.0938560202,2.1176306235
C,-1.9324179264,0.1553708003,0.7218415238
C,0.9520623528,-0.0447201569,-2.3413516178
H,-1.564991078,0.1397392561,-1.4020625409
H,2.0958031464,-0.1404673092,-0.6388312481
H,1.2863375709,0.7244903813,4.0988176105
H,-0.1884241311,0.0064729535,3.6847177346
H,1.1617687039,-0.9289180759,4.0889477664
H,-3.0101049249,0.2366993281,0.7149007835
N,1.1513267708,-0.0672761187,-1.0095554088
N,-1.1939614477,0.1064061025,-0.4574001496
N,-1.1666231698,0.0916388949,1.7710512423
N,0.8409626909,-0.0705667215,3.6278966503
N,0.7128934228,-0.0202502931,-3.4804302333
O,2.4452246156,-0.1807119,1.8709088033

28, N7-Protonated Cyanoamine (*E*,*Z*)-13h

1,1
C,0.0477792543,0.020234589,-0.0293167854
C,-0.0101475023,-0.0292322978,1.3539321238
C,1.1958362904,-0.0585987556,2.2144764946
C,-2.1018642918,-0.0102704753,0.5481020057
C,1.0232428988,0.1039179979,-2.178861407
H,-1.5225367961,0.067745313,-1.4742661608
H,2.043501286,0.0199175657,-0.3509347456
H,0.2021882319,-0.0132929518,4.064109551
H,1.9265338113,-0.0936517483,4.1024089892
H,-1.780959666,-0.0953632883,2.5855851928
H,-3.1795317272,-0.0150629996,0.4842349015
N,1.1429471478,0.0503278335,-0.841916597

N,-1.2512558139,0.0330125623,-0.4944499063
N,-1.3733201637,-0.0477804441,1.6593953754
N,1.0717318266,-0.0846169403,3.5591946829
N,0.8274063463,0.1501893973,-3.3262468188
O,2.2829809349,-0.0667250838,1.6314160076

29, (C)O-Protonated (NH2 side)-Cyanoamine (*E*,*Z*)-13h

1,1
C,0.0980390355,0.0242438924,-0.1208452725
C,0.0730582979,-0.0189295125,1.2841048149
C,1.1420648291,-0.0326011759,2.204148174
C,-1.9783755961,-0.0272927606,0.6607094116
C,0.9454489809,0.1034180319,-2.3391624396
H,-1.5473456202,0.0428922679,-1.4521070001
H,2.0886792382,0.0662534784,-0.642992667
H,-0.0581232408,-0.0976231049,3.8095873141
H,1.6407850207,-0.0869255573,4.2071379251
H,3.0847230905,-0.0110830897,2.3565068651
H,-3.0585018316,-0.0405065036,0.6216956363
N,1.1424605329,0.0652189124,-1.0077600656
N,-1.2051617773,0.0183288358,-0.4966190043
N,-1.2433274701,-0.0501094775,1.7299539729
N,0.9121685804,-0.075332709,3.5056921925
N,0.7129129053,0.1353069647,-3.4795784483
O,2.3712216408,-0.0006516327,1.697812816

30, cyano-N Protonated Cyanoamine (*E*,*Z*)-13h

1,1
C,-0.116654489,0.0373076095,-0.1809333066
C,-0.0560611175,-0.0067100486,1.2112346909
C,1.1251015135,-0.0111090117,2.0167219483
C,-2.1373321324,-0.0144357984,0.7358326225
C,0.9730694695,0.0739067593,-2.2806688891
H,-1.8751795594,0.0746082033,-1.3891357065
H,2.2868458066,0.0718463064,0.5100184978
H,0.1331578614,-0.0895440131,3.767125109
H,1.8847502915,-0.0558606238,3.8990219111
H,1.2330697254,-0.4082503437,-4.2265256788
H,-3.2174049945,-0.0266669714,0.7803128678
N,0.9550204935,0.0886567428,-1.032919059
N,-1.4539672495,0.0314193756,-0.4690667283
N,-1.3242013467,-0.0393341424,1.7562052504
N,1.0474390924,-0.0573785356,3.329189043
N,1.0922576727,0.2416942122,-3.4629945398
O,2.3285612887,0.0313537022,1.4899489963

31, amino-N Protonated Cyanoamine (*E*,*Z*)-13h

1,1
C,-0.07622019,-0.2121148663,-0.1945966402
C,-0.0212213486,-0.0681196901,1.1823366968
C,1.1505130932,0.0494708684,2.0154990934
C,-2.0983322135,-0.0754614563,0.6873078986
C,1.0688039028,0.5812318698,-2.1236754827
H,-1.8143516307,-0.2730627,-1.4245261167
H,1.2170301033,-1.2860400103,-1.4067843699
H,0.0960789593,0.1890873088,3.7196729774
H,1.8427635313,0.2799531253,3.907280315
H,2.3586228553,-0.0126213684,0.5442130192
H,-3.1782439293,-0.040557526,0.7266976888
N,0.9962929889,-0.3336991735,-1.1122185023
N,-1.4086105416,-0.2129058613,-0.4961312498
N,-1.2874236536,0.0058715627,1.7140109305
N,1.0271035928,0.1763513631,3.3134054887
N,1.14350576,1.3858567851,-2.9597428418
O,2.3652805073,0.043963097,1.5222109225

103

1,1
C,-0.116654489,0.0373076095,-0.1809333066
C,-0.0560611175,-0.0067100486,1.2112346909
C,1.1251015135,-0.0111090117,2.0167219483
C,-2.1373321324,-0.0144357984,0.7358326225
C,0.9730694695,0.0739067593,-2.2806688891
H,-1.8751795594,0.0746082033,-1.3891357065
H,2.2868458066,0.0718463064,0.5100184978
H,0.1331578614,-0.0895440131,3.767125109
H,1.8847502915,-0.0558606238,3.8990219111
H,1.2330697254,-0.4082503437,-4.2265256788
H,-3.2174049945,-0.0266669714,0.7803128678
N,0.9550204935,0.0886567428,-1.032919059
N,-1.4539672495,0.0314193756,-0.4690667283
N,-1.3242013467,-0.0393341424,1.7562052504
N,1.0474390924,-0.0573785356,3.329189043
N,1.0922576727,0.2416942122,-3.4629945398
O,2.3285612887,0.0313537022,1.4899489963

104

1,1
C,-0.0011469064,0.0001860988,-0.0032562386
C,0.0009523662,-0.0005219991,1.4053527135
C,1.0937973684,0.0044794563,2.3038331171
C,-2.0662455728,-0.015144491,0.8398910303
C,1.0850986457,-0.1114537762,-2.0904071434

H,-1.7080240869,0.0038333465,-1.2740363794
H,2.8349416567,0.7294067577,1.7896516758
H,-3.1475933884,-0.0226163117,0.8369233193
H,1.6621432044,-0.0453505807,4.2550097474
H,-0.0667357267,0.0475700466,3.954355092
H,1.4713989991,-0.7821302792,-3.9632674289
N,1.0490552178,0.0449577983,-0.8580957817
N,-1.3293305674,-0.0128886355,-0.3345880816
N,-1.300277748,-0.0087858793,1.8905855638
N,0.8880918206,0.0292436362,3.6064507223
N,1.207305459,-0.0796081873,-3.2855686944
O,2.3511120416,-0.1091132564,1.8593724226

105

1,1
C,-0.0961096768,0.0793208625,-0.1117899647
C,0.0088417057,0.0310138469,1.2868344902
C,1.156977279,0.0175183565,2.1261875294
C,-2.0947462051,0.0320770248,0.8784782968
C,0.8264797656,0.0750695507,-2.2803436228
H,-1.8947355479,0.1278141119,-1.2509044929
H,3.0877962954,0.0433701165,2.1853969935
H,-3.1728129263,0.0238950048,0.9592452014
H,1.7611678034,-0.0296250007,4.0994638516
H,0.0408686699,-0.0258550978,3.7916448727
H,1.0317334336,-0.4787690438,-4.2137570907
N,0.8874747274,0.1406524118,-1.0425219367
N,-1.4482815434,0.0775485259,-0.3431535064
N,-1.2494552083,0.001723568,1.8685978414
N,0.9950002066,-0.0133260914,3.4397790209
N,0.8646614358,0.193984969,-3.4774329215
O,2.3458069858,0.0368810328,1.559172504

106, IMPT(105,107)

1,1
C,0.002668431,0.0000183019,-0.0022694168
C,0.0053080036,-0.0001194982,1.4153659235
C,1.0986844334,-0.0000432203,2.2825625476
C,-2.0606479218,0.0068894653,0.849791722
C,1.1350165468,-0.0975645962,-2.0704257612
H,-1.7023224015,0.02513952,-1.2690297731
H,2.2883723817,0.0049205418,3.3814226848
H,-3.1420758247,0.0118311368,0.8426397552
H,0.5580590674,0.8137259192,4.1505013826
H,0.5631752903,0.8499484612,4.1356500997
H,1.5877091134,-0.6921881905,-3.9734879772
N,1.0611447375,0.0223522359,-0.8340157968

N,-1.3214180054,0.0036781623,-0.3301664018
N,1.3000354616,0.0031265278,1.9017073579
N,1.0037528142,0.0131532383,3.7432689445
N,1.2993901575,-0.043450629,-3.2551638269
O,2.3483197395,-0.0081123406,2.0877344944

107

1,1
C,-0.0759810085,0.0831496947,-0.127081022
C,0.0828348488,0.0511703852,1.2669629914
C,1.2881330874,0.0487516713,2.0289896411
C,-2.0407694054,0.0344267223,0.9335982902
C,0.8040335146,0.0415033399,-2.3171365685
H,-1.9173248929,0.1079551403,-1.199050002
H,-3.114922935,0.0205842654,1.05380724
H,-0.114684927,0.0043293346,3.6768353708
H,1.3388153041,-0.7980962894,4.0182982649
H,1.3033642123,0.8592275563,4.0335634836
H,1.0255938163,-0.5520880931,-4.2418171804
N,0.8774548461,0.1460506242,-1.0826222795
N,-1.4370733682,0.0704061024,-0.3077287471
N,-1.1574025916,0.0203875857,1.8934675655
N,0.9144352041,0.02588775,3.5821763374
N,0.8207578918,0.1217296798,-3.5165638377
O,2.4515314896,0.0608803105,1.760842717

108, RTS(103,109)

1,1
C,-0.018256062,0.0059583424,0.0139280998
C,-0.0471342784,-0.0187384596,1.3999938625
C,1.0908963449,-0.0376414371,2.3300477497
C,-2.0972133983,-0.0238423924,0.8090444618
C,1.1292017257,0.0193855526,-2.0494517187
H,-1.7128600447,0.0381208854,-1.2882110451
H,1.1783145308,1.929605035,2.3643765756
H,2.3696345031,1.0285639183,3.4865377212
H,1.2214780636,1.9579891987,2.5514449863
H,-3.1780333141,-0.0305072242,0.8022515742
H,1.4576751055,-0.5221777626,-3.9464835603
N,1.6042190149,1.0585709135,2.8172796633
N,1.0725611455,0.0492713573,-0.8116994899
N,-1.3502968839,0.0020017188,-0.343393939
N,-1.3400379857,-0.0378184182,1.8811232185
N,1.2875953146,0.1806038277,-3.2369847982
O,1.6336472019,-1.1553139045,2.7391300607

109
1,1
C,0.0107823845,0.0669918936,-0.1562126205
C,0.0351420484,-0.0002700553,1.2368820996
C,1.1327252546,-0.0243944224,2.1523338288
C,-2.0395383866,0.002740219,0.7107779443
C,1.1014815451,0.136622166,-2.2459687507
H,-1.7213775261,0.126508344,-1.400945696
H,-0.0928225602,-0.1185210081,3.57096 55055
H,3.1294196725,0.0048514162,2.4944984616
H,2.6478330312,0.0833721477,0.8106358766
H,-3.1202502231,-0.0086947248,0.7300464439
H,1.373209807,-0.3133251461,-4.1992314901
N,2.3999610555,0.0206282992,1.7914288501
N,1.0819940527,0.1306552335,-0.9998986718
N,-1.3238494134,0.0676856076,-0.4710329822
N,-1.2482637619,-0.0404046855,1.7475644042
N,1.2271891593,0.3230761019,-3.4259428009
O,0.8793621495,-0.0939651138,3.4358938719

110, IMPT(109,111)
1,1
C,0.0001078914,0.0004165302,0.0013371605
C,0.0014899125,-0.0000001869,1.379607611
C,0.8712841719,-0.0002697592,2.5659913778
C,-2.1042601008,0.0169552704,0.7988846826
C,1.1008746628,-0.0732288582,-2.0832229884
H,-1.7248204616,0.0338696619,-1.2817509066
H,-0.9831991748,0.0062305935,3.0436890957
H,2.7225634744,0.0054021646,3.3849247434
H,2.6920410517,0.008313971,1.6403707285
H,-3.18419494,0.0275111942,0.8140284522
H,1.4099974324,-0.6644441859,-3.9883913083
N,2.1945435418,0.0001186095,2.5206283036
N,1.0666985681,0.0087036032,-0.8432757389
N,-1.351315438,0.0112491982,-0.3395757218
N,-1.2978317279,0.0082804725,1.834257677
N,1.2380749101,0.0314069485,-3.273818234
O,0.189841322,0.0009475352,3.6342929877

111
1,1
C,0.0235040144,0.0822023054,-0.1600260324
C,0.0889258033,-0.0219794586,1.2141025184
C,1.1588023027,-0.0917394892,2.2547665833
C,-2.0669076158,0.0094778138,0.6503382768
C,1.0690221009,0.156123579,-2.2754903162

H,-1.7305693931,0.1879470015,-1.4083191645
H,-1.421267969,-0.1460063032,2.659974899
H,3.1726039132,-0.0648842716,2.5183845698
H,2.6762055862,0.0814413262,0.8519680377
H,-3.1449008592,0.0016042472,0.7092919307
H,1.3523132602,-0.3240721886,-4.2157767152
N,2.4348656377,-0.0292268138,1.8270935846
N,1.0634072023,0.1757623291,-1.0326105807
N,-1.3377023629,0.0996647247,-0.4776185923
N,-1.2161170822,-0.0653527081,1.6639026215
N,1.1667796818,0.3258946456,-3.4621328993
O,0.7933838982,-0.2012869585,3.4217123873

112, RTS(111,113)
1,1
C,-0.0197559063,-0.1502448269,-0.0601329368
C,0.0250982628,-0.2147291222,1.3157588336
C,1.2043135835,-0.051915318,2.2544007212
C,-2.1286433425,-0.1551304596,0.706602683
C,1.1029798954,0.2020617119,-2.1089905076
H,-1.7452837986,-0.1043679056,-1.3464561034
H,-1.5874139293,-0.2155447568,2.7165549666
H,-3.2071049373,-0.1428566532,0.7489038838
H,2.3789253348,-1.1073637608,3.5388558677
H,1.2663227699,-2.0906316158,2.6445736418
H,1.5888214537,1.1623397886,-3.8044196861
N,1.0222228692,-0.1666307376,-0.9290876008
N,-1.3762194958,-0.1240733798,-0.4020328689
N,-1.2939976279,-0.2108199087,1.745544501
N,1.5757967774,-1.1707091798,2.9242960385
N,1.2392327347,0.3590901154,-3.2966828296
O,1.6980838167,1.0529713736,2.3895694255

113
1,1
C,0.0033640268,-0.1000948785,-0.0629844712
C,0.0149596758,-0.1222861066,1.3210800901
C,1.1676054799,-0.2665460589,2.2659591288
C,-2.1249837614,-0.0588064319,0.6599760777
C,1.1357103742,0.031308342,-2.1347694614
H,-1.6938085632,-0.0389445327,-1.3847224873
H,-1.6293353915,-0.1631831665,2.6806941713
H,-3.2044660797,-0.0552854602,0.6738198474
H,1.7432720852,0.1856350617,4.1495544527
H,0.441851303,1.1469504615,3.6042156408
H,1.5987609696,0.7090687779,-3.9829061127
N,1.0527966383,-0.1330416823,-0.9101931763

N,-1.3459819868,-0.0507089728,-0.4321630909
N,-1.3176593059,-0.0902439285,1.7178665937
N,0.9628100113,0.2841335634,3.5089230974
N,1.2959443317,0.0011019763,-3.3273714816
O,2.1480948496,-0.9066261948,1.9406668936

114, IMPT(113,107)
1,1
C,0.0033438331,-0.0011518552,0.0008492249
C,0.0068561042,-0.0008307974,1.3894100158
C,0.9718396771,-0.0001693567,2.4831904661
C,-2.1060715506,-0.0032834348,0.7954844844
C,1.1135112267,0.1283549628,-2.0799696578
H,-1.7151263391,-0.0233065743,-1.2821974634
H,-1.0576186135,-0.0042535521,3.0522899094
H,-3.1860673267,-0.0070106984,0.8048051205
H,0.3543550518,-0.8431719708,4.2989499786
H,0.363363781,0.8022410841,4.3202958191
H,1.5548303455,0.7995628447,-3.941649356
N,1.0492703873,-0.0332442596,-0.8512211618
N,-1.346437263,-0.0017023891,-0.337903883
N,-1.3052038486,-0.0004552689,1.8359548807
N,0.1397159109,-0.0118323395,3.7437649616
N,1.2583295065,0.1019914729,-3.2725231843
O,2.1706186737,0.0098020047,2.4649143789

121, IMPT(28,27) Cyanoamine (*E*,*Z*)-13h
1,1
C,-0.0028595036,0.000027576,-0.0010262544
C,-0.0056785751,-0.000116265,1.3842840963
C,0.9532365406,0.0000612902,2.4683154937
C,-2.1081299556,-0.0006858089,0.7609375598
C,0.817642675,0.0005045784,-2.2246839816
H,-1.6734132161,-0.0003396974,-1.3235413971
H,1.9843369381,0.0006823258,-0.5370855574
H,0.3437062778,0.8231920904,4.2927119467
H,0.3442012915,-0.82381559,4.2925404775
H,-1.0742866172,-0.0006084186,3.0343276013
H,-3.1879607012,-0.0010097597,0.7453884532
N,1.0334412011,0.0004324036,-0.8957848957
N,-1.3277813117,-0.0003340947,-0.3674178088
N,-1.3261016317,-0.0005585312,1.8121112171
N,0.1308336531,-0.0003166415,3.724418726
N,0.5502258728,0.0005409851,-3.357887328
O,2.1563340645,0.0004296094,2.4207051625

Cyanoamine (*Z*,*Z*)-13h

0,1
C,0.0458728994,-0.0529997774,-0.1138584301
C,0.0189499541,-0.0636962843,1.272937011
C,1.1516928341,-0.3269721341,2.1817356554
C,-2.0089398664,0.2367157365,0.6263579794
C,0.9324155869,-0.3042533701,-2.3279206082
H,-1.567162989,0.1702810447,-1.4815933714
H,1.9888470886,-0.5256852261,-0.588273751
H,3.1595764186,-0.1648633666,2.2895934093
H,2.4669970383,0.9210925909,1.2034618723
H,-3.0751420836,0.406931683,0.5860981949
N,2.4080629388,-0.0001338051,1.6270992577
N,1.1058022514,-0.2418848071,-1.0059046684
N,-1.243053562,0.1387793752,-0.5236200634
N,-1.2850522123,0.1110798456,1.7040384763
N,0.7371481706,-0.32580392,-3.4793910193
O,1.051528364,-0.8561245868,3.2744277832

32, NH_3^+-Cyanoamine (*Z*,*Z*)-13h

1,1
C,-0.1956256579,0.2185192211,-0.2653455343
C,-0.0377111174,-0.0760487808,1.0973727925
C,1.0877561922,-0.4164627606,1.9495434705
C,-2.1353680769,0.2917664524,0.7968725613
C,1.718946597,-0.5641268924,-1.4464314685
H,-1.9947547905,0.6215845052,-1.3176297811
H,0.5610721673,0.9756088006,-2.0784308211
H,2.7198958018,0.8364448405,1.2154854372
H,3.1710184114,-0.476493093,2.132311192
H,2.7661183204,-0.6798514462,0.5102716708
H,-3.1972949596,0.4396258651,0.9364115949
N,2.5427274072,-0.160112562,1.3839247352
N,0.6840720078,0.2731871528,-1.3553595583
N,-1.5266445301,0.4471380539,-0.4354152914
N,-1.2767168991,-0.0349322989,1.716508766
N,2.6334365733,-1.288041255,-1.3826559626
O,1.0776305977,-0.8310640302,3.0667612107

33, N7-Protonated Cyanoamine (*Z*,*Z*)-13h

1,1
C,0.0886575079,-0.0117098509,-0.1604925509
C,0.1334093013,0.0066859992,1.2174169672
C,1.1884065621,-0.0860421453,2.265993611
C,-2.0087487794,0.0693485195,0.5908097527
C,0.8187513611,-0.0039208176,-2.4137406845
H,-1.597569205,0.043562535,-1.4750581598

H,1.9873122178,-0.500667106,-0.8147631867
H,-1.4438803586,0.0006025838,2.6170239828
H,3.1672206534,0.1186085539,2.6008473173
H,2.6491767895,0.8622011203,1.151685732
H,3.0872476384,0.1166799539,0.6136498118
N,2.4702783697,0.1651996566,1.8643610693
N,1.099050622,-0.0982349259,-1.099477339
N,-1.2459265486,0.0402346014,-0.520378283
N,-1.1907062709,0.0346556631,1.6305117394
N,0.4938411728,0.1026727038,-3.5269525219
O,0.8510095029,-0.4285106672,3.3887784173

34, (C)O-Protonated (N7 side)-Cyanoamine (*Z*,*Z*)-13h

1,1
C,0.0832353988,-0.0943977213,-0.1558680974
C,0.1078023921,-0.05556826,1.237885262
C,1.1609624602,0.0350654339,2.2055811154
C,-1.9681622417,-0.0238605281,0.6845653776
C,0.8860054139,0.2025674512,-2.3707288703
H,-1.6101149071,-0.072457306,-1.4322251381
H,1.8022602677,-0.9089769511,-0.96609907
H,-0.1375501393,-0.1060611494,3.5521026753
H,3.108666699,0.2719159524,2.6946296214
H,2.7682906651,0.3799689541,0.9941688438
H,-3.0482748081,0.0167753882,0.6903657791
N,2.4453824693,0.1841495399,1.9318922014
N,1.1178596315,-0.1667516487,-1.0885098535
N,-1.2367235824,-0.062892231,-0.4874637222
N,-1.1876734662,-0.0368985319,1.7286510855
N,0.6514248268,0.5462626958,-3.4574936084
O,0.8392179488,-0.0186008977,3.4706706418

35, (C)O-Protonated (NH2 side)-Cyanoamine (*Z*,*Z*)-13h

1,1
C,0.0553882096,-0.1607856469,-0.1159228163
C,0.0382591243,-0.0726218284,1.2785297819
C,1.1488069665,0.0321826573,2.1814976101
C,-2.0083225111,-0.0208723383,0.6619595251
C,1.0487215159,0.3025810245,-2.2265977012
H,-1.5960063133,-0.1509429202,-1.4448346186
H,1.6033520792,-1.1927547825,-1.0141336223
H,1.6043747424,0.1251866175,4.0582506785
H,3.1824657233,0.2679990411,2.3887878324
H,2.5761687422,0.3301310555,0.7664643248
H,-3.0872499363,0.0426128909,0.6348969412
N,2.3956426944,0.1904841692,1.755732152
N,1.1422129773,-0.2831865558,-1.0035874425

N,-1.2493423328,-0.1216959591,-0.4908327868
N,-1.2641581501,-0.0066502511,1.7324855172
N,0.9602189933,0.8320998878,-3.258691821
O,0.8564848337,-0.0234922502,3.45522747

36, 'cyano-N'-Protonated Cyanoamine (*Z*,*Z*)-13h
1,1
C,-0.3219317644,-0.1866158921,-0.3618006029
C,-0.0696884906,0.1021597964,0.9878848635
C,1.1147342715,0.4246518476,1.763642879
C,-2.1874615295,-0.2366326198,0.8271075929
C,1.5186176339,0.5752495655,-1.6675475509
H,-2.1923858015,-0.5627483861,-1.2926479943
H,0.303497445,-0.9504304809,-2.2215612741
H,2.6780861008,-0.8445688591,0.9165716813
H,3.2062005038,0.4589693485,1.8052666961
H,2.6951258458,0.673924128,0.2150001619
H,-3.2396641667,-0.3704964584,1.0368078697
N,2.5249228688,0.1533173504,1.1000263536
N,0.4826592943,-0.2504321628,-1.5079333312
N,-1.6643071256,-0.3968491777,-0.4432503079
N,-1.2651112205,0.0759933744,1.6881188013
N,2.4436390988,1.2885104207,-1.6645284867
O,1.1851570194,0.8341707069,2.8805555611

37, amino-N- Protonated Cyanoamine (*Z*,*Z*)-13h
1,1
C,-0.3219317644,-0.1866158921,-0.3618006029
C,-0.0696884906,0.1021597964,0.9878848635
C,1.1147342715,0.4246518476,1.763642879
C,-2.1874615295,-0.2366326198,0.8271075929
C,1.5186176339,0.5752495655,-1.6675475509
H,-2.1923858015,-0.5627483861,-1.2926479943
H,0.303497445,-0.9504304809,-2.2215612741
H,2.6780861008,-0.8445688591,0.9165716813
H,3.2062005038,0.4589693485,1.8052666961
H,2.6951258458,0.673924128,0.2150001619
H,-3.2396641667,-0.3704964584,1.0368078697
N,2.5249228688,0.1533173504,1.1000263536
N,0.4826592943,-0.2504321628,-1.5079333312
N,-1.6643071256,-0.3968491777,-0.4432503079
N,-1.2651112205,0.0759933744,1.6881188013
N,2.4436390988,1.2885104207,-1.6645284867
O,1.1851570194,0.8341707069,2.8805555611

118
1,1

C,0.0046121477,0.0138605284,-0.1021314962
C,-0.0467329784,-0.0267636856,1.3011147454
C,1.0228087856,-0.0957469578,2.2555048619
C,-2.0818602951,0.0557117225,0.6502459782
C,1.1594010374,0.0811639851,-2.1597297354
H,-1.6417778033,0.0870621363,-1.4497458342
H,3.0337542075,0.5949740243,1.9394547893
H,2.423211777,-0.1232083452,0.5316253876
H,2.9069446995,-1.0511611898,1.859769095
H,-3.1617306442,0.0883607081,0.60464796
H,1.4410191995,0.6695507011,-4.0693742809
N,2.4665796455,-0.1730333059,1.5663432985
N,1.1167564585,-0.000467172,-0.9145361019
N,-1.3002904222,0.0661460829,-0.4962402895
N,-1.360435692,0.002959948,1.7314174364
N,1.2975322361,-0.0272820979,-3.3480484997
O,1.041426915,-0.1135741219,3.4458394343

122, IMPT(33,123)

1,1
C,-0.0002159347,-0.0000351122,0.0002493908
C,-0.0000987814,-0.0000464041,1.4033518166
C,1.1530265759,0.0000603304,2.2559825791
C,-2.1176254579,-0.0002491422,0.7249200207
C,1.0543324898,0.000085479,-2.0860206152
H,-1.6710251128,-0.0001885537,-1.3381756271
H,2.0299586169,0.0001635724,0.1652417342
H,-1.6579375145,-0.0002202883,2.7576680994
H,2.9679541351,-0.8199404051,1.6599403779
H,2.9677930813,0.820427256,1.6599539811
H,-3.1978968093,-0.0003553038,0.7238537809
N,2.4043404672,0.0001901321,1.4146255714
N,1.1026969732,0.0000793792,-0.7491326889
N,-1.3341215148,-0.0001632109,-0.3793168263
N,-1.3378143319,-0.0001810677,1.7934220595
N,1.0096509263,0.0000905831,-3.2520426466
O,1.1850487567,0.0000538929,3.4624919094

123

1,1
C,-0.0004506778,-0.0002507245,0.0142400591
C,-0.0052204587,-0.0001599415,1.4368739917
C,1.0715469144,-0.0000813054,2.3477397677
C,-2.1295933223,-0.0002805007,0.7632874079
C,0.8642747936,-0.0003663562,-2.0959984759
H,-1.6991118366,-0.0003928724,-1.2996477824
H,2.2995361612,-0.000162592,0.555007103

H,-1.6693400922,-0.0001377984,2.7934552384
H,2.9728601659,-0.826803965,1.8943765295
H,2.9727656378,0.8267811891,1.8942273019
H,-3.2104673672,-0.0003196403,0.7714774247
N,2.438819695,-0.0000682254,1.6041973873
N,1.0490588323,-0.0002666878,-0.7725254017
N,-1.3592376249,-0.0003224622,-0.3417068561
N,-1.3509866968,-0.0001855276,1.8294725063
N,0.7136289892,-0.0004523247,-3.2547794162
O,1.0862650957,-0.0000260863,3.554229631

9

1,1
C,0.0191235783,-0.1310602683,0.1849528414
C,-0.1310547003,0.0224893386,1.6045268066
C,0.8302227197,-0.0773161507,2.564208441
C,-2.0894033689,0.2864003093,0.8061056082
C,2.2584951259,-0.4893002866,-0.459194985
H,-1.5011722188,-0.0067134527,-1.252489166
H,-3.1495351759,0.4569204857,0.6742067647
H,4.3272200116,-0.3299566868,-0.5021628817
N,1.0272547385,-0.3994862275,-0.656132217
N,-1.2430438408,0.0419809668,-0.2714707825
N,-1.4643780538,0.2828722173,1.9414845923
N,3.4161675858,-0.7382919551,-0.3555572951
O,1.6401743281,-0.1619580355,3.3666613812

TS(9,125)

1,1
C,-0.0214025817,-0.0108905523,-0.0526975913
C,0.024303441,0.0156823688,1.4689659519
C,1.2039618097,-0.076237784,2.0319763308
C,-1.9928983849,0.4127679787,0.9132214157
C,1.9503613352,-0.9300824084,-0.3841002814
H,-1.71405092,0.4366075098,-1.2244050503
H,-3.0524108089,0.6385915632,0.9496678488
H,2.9217977835,-0.8098465932,1.9790309492
N,0.8497329298,-0.4236640344,-0.9173526472
N,-1.312027816,0.3576048833,-0.295083486
N,-1.2685815932,0.1937567862,1.9697486275
N,2.8177946088,-1.4320021468,0.2260959887
O,2.3789522968,-0.0213089013,2.3674566392

2-Methylthiohypoxanthine, 14h, and Derivatives

Thioether (*Z*)-14h

0,1
C,0.3689746653,0.376899717,-0.4124128356
C,0.1267961114,0.361679911,1.7972822548
C,1.3792545591,-0.18353072,2.0791927131
C,2.2612344531,-0.4983458262,0.9804669765
C,0.4430181423,0.1121136176,3.968770562
C,-1.782969444,1.364687664,-1.8542937963
H,-1.3862346345,0.9285363495,3.1793067288
H,2.1885126264,-0.3578855187,-1.0779041747
H,-2.1539034295,1.5752694313,-2.8596198085
H,-2.4303350883,0.640830536,-1.3589807205
H,-1.7344849487,2.2846227494,-1.2714087105
H,0.2217466116,0.1494320406,5.026329106
N,1.6211893299,-0.1613114578,-0.2599172373
N,-0.423222652,0.6589394848,0.588146847
N,-0.464828847,0.546961887,3.020264845
N,1.556707352,-0.3311069202,3.4390449184
O,3.3847216295,-0.9732882903,0.9682606703
S,-0.1138271711,0.6708213419,-2.0929702765

38, N3-Protonated-Thioether (*Z*)-14h

1,1
C,-0.0021809382,0.2062234254,-0.2753074427
C,-0.0453678139,0.1248486727,2.0777839199
C,1.3197159888,-0.07240838,2.1992461924
C,2.1545515136,-0.1464526432,1.0201791719
C,0.547174945,-0.0370392346,4.1820616387
C,-2.4875690784,0.6032492777,-1.5166439573
H,-1.5074797185,0.273287748,3.6380751952
H,1.8649000035,-0.0286653025,-1.0482455812
H,-2.9392312622,0.7038037974,-2.5063334157
H,-2.924639671,-0.2731040504,-1.0322042293
H,-2.6703031593,1.5285842412,-0.9652171564
H,-1.7140319622,0.4067842339,0.8312281924
H,0.4333630515,-0.0609255847,5.2568917626
N,1.3198776079,0.0163528234,-0.1891434742
N,-0.7128864673,0.264003285,0.8698844514
N,-0.5472119293,0.1486764237,3.3429364092
N,1.6674498931,-0.1706903674,3.5223207027
O,3.335819275,-0.3080227855,0.8797760171
S,-0.7082732458,0.3649812436,-1.8639604004

39, N7-Protonated-Thioether (*Z*)-14h

1,1

C,-0.1130648203,0.0660073667,-0.2476078038
C,-0.048344227,0.0372645955,1.978008665
C,1.3309396389,-0.0234330164,2.0486106067
C,2.1315442465,-0.0441649596,0.8460271096
C,0.5672678514,-0.0144801311,4.1232845665
C,-2.6483045743,0.1891640953,-1.3647135429
H,-1.4646526254,0.0799917158,3.5871549309
H,1.7447344542,-0.0038486697,-1.1736815944
H,-3.1750700655,0.2233603518,-2.3203000862
H,-2.936876263,-0.7039965709,-0.8111348454
H,-2.8587899819,1.0907196938,-0.7899518626
H,2.6257511235,-0.0994367668,3.7460220942
H,0.5240651831,-0.025186277,5.202106433
N,1.2654297549,0.0064932581,-0.2761264205
N,-0.8113990457,0.0832343088,0.8757236247
N,-0.4934796191,0.0412199473,3.2956676126
N,1.6770218805,-0.0540512872,3.3857821041
O,3.3414484542,-0.0955769059,0.7520916451
S,-0.8805055145,0.1175898811,-1.815745962

40, (C6)O-Protonated(N1 side) Thioether (*Z*)-14h

1,1
C,-0.0711132152,0.2558591091,-0.2528634421
C,-0.064773611,0.1596994054,1.9803121502
C,1.3340019398,-0.0271184319,2.0965618798
C,2.0506404058,-0.0695023262,0.9069242723
C,0.5981074694,-0.016120382,4.0799330822
C,-2.5339983819,0.6273351873,-1.4535909798
H,-1.4763232562,0.2758597238,3.5579912259
H,1.7900386447,0.0516001195,-1.1365056566
H,-3.0220487732,0.7322559332,-2.4243365013
H,-2.9136592724,-0.2527481185,-0.9352847837
H,-2.6820503862,1.5285097808,-0.8592046997
H,3.7594822,-0.2527948303,-0.0034541199
H,0.5059054054,-0.0501255535,5.1572001741
N,1.314976303,0.0750122471,-0.2379226894
N,-0.7771303046,0.3004791447,0.8520961214
N,-0.5138055057,0.1633380392,3.2625127164
N,1.7168919674,-0.1331891685,3.4150914895
O,3.3552727762,-0.2379208129,0.8788804156
S,-0.7633560138,0.4140584662,-1.850406143

41, (C6)O-Protonated(N7 side) Thioether (*Z*)-14h

1,1
C,-0.0604482868,0.2532877238,-0.2493409972
C,-0.072226614,0.1675328238,1.9868512829
C,1.322685749,-0.0162042992,2.103222087

C,2.041887424,-0.0623720451,0.9187480224
C,0.5986230136,-0.0007004428,4.0893199229
C,-2.5207831978,0.6164467832,-1.4560323202
H,-1.475130443,0.2856920432,3.5771010333
H,1.8356499535,0.043103944,-1.1053717216
H,-3.0057416841,0.7167217023,-2.4288404342
H,-2.9019854813,-0.261745189,-0.9355940289
H,-2.6731089152,1.5198350079,-0.8660503435
H,3.7882432434,-0.314205811,1.6230687699
H,0.5106110084,0.0314514459,5.1669484028
N,1.3211945414,0.0749274344,-0.2271441298
N,-0.7767571905,0.3022159039,0.8548947091
N,-0.5144304328,0.1740705811,3.274925761
N,1.7163704955,-0.1181144231,3.4186148642
O,3.33853178,-0.2228801598,0.763334696
S,-0.7489854884,0.404084395,-1.8468435276

42, S--Protonated Thioether (*Z*)-14h
1,1
C,-0.0099673093,0.0715846993,-0.1671319789
C,-0.023822067,0.0595693919,2.0377646926
C,1.366397548,-0.0401485232,2.1629340091
C,2.2002349289,-0.0906684833,0.9778048909
C,0.5993191444,-0.0036170237,4.1437409734
C,-2.0905968712,1.4693689045,-1.5640817317
H,-1.4704986559,0.1420802532,3.6035907987
H,1.8565715701,-0.0544011023,-1.0883255617
H,-1.6532428602,-0.9325078654,-1.6384181841
H,-1.5536196527,2.4161980552,-1.6345887344
H,-2.8066354807,1.3755031402,-2.383312711
H,-2.5566156493,1.3373038952,-0.5877326901
H,0.5061382596,-0.0077100314,5.2210229712
N,1.3424933112,-0.0218837849,-0.2119440371
N,-0.7535840079,0.1188056117,0.8839306459
N,-0.5010670147,0.0820732222,3.3194768236
N,1.7323651497,-0.0770620915,3.4777620411
O,3.3937329435,-0.1718840656,0.8316806151
S,-0.8446991166,0.1435880829,-1.8022140823

(*Z*)-**129** 1,1
C,0.0335870909,0.241062957,-0.0499065908
C,0.0656574231,0.1768602574,2.3143236173
C,1.4330106794,-0.0326209268,2.3341289867
C,2.2284034153,-0.1243472755,1.144520226
C,0.5703397764,0.0485754525,4.3535183378
C,-2.4874937863,0.6552174632,-1.1962703098
H,1.8715891071,-0.0184530059,-0.9025640211

H,-2.976921071,0.7544518713,-2.1677683798
H,-2.9101072304,-0.2131546493,-0.6860265416
H,-2.6353113599,1.5840456372,-0.6408890596
H,0.519031436,0.0293371071,5.4331139999
N,1.3660708607,0.0366775224,-0.0206621632
N,-0.6247743988,0.3124489307,1.1156804792
N,-0.4735196976,0.2283220409,3.5480176969
N,1.7384868925,-0.1128939535,3.6730722233
O,3.4144926779,-0.3019315021,0.9972971059
S,-0.7252836217,0.3962263368,-1.6122187536
H,2.6596114733,-0.2635829218,4.0680278344
H,-1.6267619802,0.4647574025,1.1483360332

(*Z*)-**134**
1,1
C,0.0943485458,0.2374633492,0.0924538708
C,-0.0353413766,0.0432227855,2.3092510602
C,1.3473290095,-0.1483486015,2.4025529806
C,2.2302666723,-0.1502812156,1.269211798
C,0.379249828,-0.2029866989,4.3707419172
C,-2.0676897126,1.6259714851,-1.1641617515
H,1.9907477657,0.1051565436,-0.7869938647
H,-2.7797575853,1.5501332376,-1.9883650341
H,-2.4952621875,1.3189678968,-0.2087350247
H,-1.6415525262,2.6287245935,-1.1165492087
H,0.2844266916,-0.2908439302,5.4442388438
N,1.4474302391,0.0699181734,0.0712449227
N,-0.6818964638,0.2380381543,1.1082656252
N,-0.6229142642,0.0070928059,3.5349369446
N,1.5912564896,-0.3038900362,3.739035058
O,3.433301994,-0.2942904732,1.2042892061
S,-0.6844168741,0.4898528202,-1.5641286784
H,2.4946915834,-0.463153716,4.1690510217
H,-1.3794064535,-0.673985967,-1.6112116664

128
1,1
C,-0.0001436487,0.0078893855,0.0073018106
C,-0.02873774,0.1095325543,2.2369062094
C,1.2948266403,0.0829766263,2.52597657
C,2.1842648294,0.0206710762,1.382631452
C,0.0004205008,-0.0454508506,4.3519783004
C,-2.4261556918,-0.0144029764,-1.3192713737
H,1.942470905,-0.0133370978,-0.6740235674
H,-2.8665262588,-0.0361231709,-2.3179076123
H,-2.7582720468,-0.8870818769,-0.7563083408
H,-2.7004533309,0.9154124659,-0.8199897105

H,-0.2769673745,-0.1128466719,5.3938285112
N,1.3667290154,0.0191768019,0.164443754
N,-0.7538382089,0.0700810779,1.1054910052
N,-0.8357343409,0.0292114287,3.3065454224
N,1.2924987482,-0.0122114827,3.9197565078
O,3.3869183211,-0.0325322104,1.3101814205
S,-0.6221223811,-0.0807722145,-1.6124883027
H,2.1072287709,-0.0361378752,4.5239488933
H,-1.6855761388,-0.0417710983,2.1835399336

130
1,1
C,-0.0369555277,-0.0006218578,0.0202319492
C,-0.0083888487,0.0218541136,2.3811715323
C,1.378613883,0.010045807,2.4008761473
C,2.1847993826,0.0340336432,1.2141044754
C,0.5113145787,-0.0332136576,4.4200224057
C,-1.2525013131,1.7256656333,-1.7961175204
H,1.7917629151,0.0276792129,-0.8465329021
H,-1.785455303,1.7521757786,-2.7491859065
H,-1.8944329476,2.1293487043,-1.0130712418
H,-0.3234751265,2.2886978808,-1.8866664648
H,0.4658518974,-0.0464442297,5.5001565965
N,1.3029221147,0.0282223117,0.0469354815
N,-0.7000436821,-0.0312785438,1.1793116984
N,-0.5470218718,-0.0480800923,3.6167203029
N,1.6918693594,0.0019196939,3.7375791766
O,3.3837483417,0.0571416233,1.0698816132
S,-0.9142739443,-0.0729355581,-1.5250584349
H,2.625388589,0.0163296609,4.1328182556
H,-1.7149355893,-0.0975827745,1.1780044896

(*Z*)-**131**
1,1
C,0.0115664009,-0.1174360272,0.0090045045
C,-0.0158750551,-0.0611195174,2.313396179
C,1.3683155009,0.0456428405,2.2906017905
C,2.1725956204,0.0726090967,1.0867384581
C,0.5509504447,0.0333245444,4.3364381168
C,-1.0600638717,1.4196880788,-2.1698117264
H,0.9762092461,-0.1525355269,-1.5930426554
H,-1.0933810285,1.4244524239,-3.2620132062
H,-2.0601452206,1.6006204143,-1.7740683967
H,-0.3362893808,2.1467293929,-1.8003754421
H,0.531843469,0.0581975328,5.4169233828
N,1.3163180737,-0.0165856434,-0.0782122182
N,-0.7312023134,-0.1508284159,1.1232427059

N,-0.5249680063,-0.0685314067,3.5623376198
N,1.709004361,0.1052988764,3.6212916368
O,3.3767552675,0.1591432327,0.9917465504
S,-0.5416482474,-0.2837993834,-1.7072383931
H,2.6507960171,0.1852120947,3.9868666074
H,-1.7376410125,-0.2795732724,1.1366929276

135

1,1
C,0.0208860733,0.0762583588,0.009511115
N,0.04566867 28,0.0834254439,1.2752106574
C,2.9884600503,0.0637866008,-1.06652801
C ,2.4319245292,1.2386498201,-1.4117335124
C,1.053149721,1.7304162694,-1.2371565811
N,-0.0021282386,1.3052627749,-0.6870147271
O,3.5897165063,-0.8777982964,-0.7750003566
N,3.1408455924,2.2687760516,-2.0943988349
N,1.1021404072,3.0028964361,-1.8851200551
C,2.3187569104,3.2733816226,-2.3450899294
H,0.0090802001,-0.8565566472,1.673418004
H,4.1225735657,2.2533824936,-2.3440050862
H,0.3007991686,3.6246892561,-1.9169959617
H,2.6067766502,4.1858224136,-2.8505607954
S,0.1068329587,-1.4112248463,-1.0222524614
C,-0.9914851625,-1.0200958281,-2.4396550215
H,-0.5936952396,-0.2112204722,-3.0534749635
H,-1.0286071881,-1.9360410102,-3.0328966297
H,-1.9944728447,-0.7776383211,-2.0867956974

136

1,1
C,-1.28308 40828,0.4533593641,0.5568942178
N,-1.031295544,0.2143423171,1.7044788546
C,1.2859602644,-0.0128997997,-2.2132008069
C,0.0210565627,0.7298935985,-2.4475379852
C,-1.1378364323,1.0803035849,-1.7593987949
N,-1.6689937014,0.9091178385,-0.5306126156
O,2.0634336723,-0.1156808778,-3.1529308148
N,-0.1293244562,1.2430495208,-3.7300984968
N,-1.916390786,1.7830826274,-2.6794237253
C,-1.2877573209,1.8710729486,-3.8596161915
H,-1.0398289434,-0.6335979362,2.2529346731
H,0.5949896604,1.1117092167,-4.4344392574
H,-2.8284533672,2.168998476,-2.4578306809
H,-1.6601172892,2.3630643132,-4.7455306874
S,1.5585046735,-0.6787957893,-0.6085840375
C,3.1775695235,-1.4833240339,-0.877860887

H,3.4522079838,-1.9199782581,0.0833566587
H,3.0858620732,-2.260658366,-1.6364505917
H,3.9137604234,-0.738614749,-1.1802553141

2-Methylthiohypoxanthine, 14h, s-(*E*)-rotamer, and Derivatives

Thioether (*E*)-14h

0,1
C,-0.1977866346,0.0669503735,-0.1764109892
C,-0.0476198853,0.0013761645,2.0410123676
C,1.3481554534,0.0118530691,2.0968410401
C,2.0865004534,0.0555684036,0.8615481055
C,0.6925279229,-0.0550066081,4.1214723642
C,0.0299768028,0.1528826666,-2.9984216287
H,-1.4135282058,-0.0596401509,3.6669381075
H,1.6385869181,0.1122258018,-1.1452139852
H,-0.5657370509,0.1751747873,-3.9136522641
H,0.6408615173,1.058968879,-2.9683786577
H,0.6556743676,-0.7432255211,-3.0218199484
H,0.6501799275,-0.0879970192,5.2012592804
N,1.16871581,0.0810460614,-0.2492659549
N,-0.857655041,0.0271509201,0.9527858427
N,-0.4549239026,-0.0416822311,3.3492041794
N,1.7885481894,-0.0237855449,3.4040108206
O,3.286412524,0.0727912775,0.6385668659
S,-1.1947295944,0.102580264,-1.6441200435

43, N3-Protonated Thioether (*E*)-14h

1,1
C,-0.1116214451,0.0774402684,-0.2151286081
C,-0.0329780825,0.0001772262,2.139292237
C,1.3520328674,0.0138755448,2.1976576275
C,2.1311390551,0.0629670346,0.9837460602
C,0.6747323564,-0.0607293879,4.2138102888
C,0.1433903184,0.1728501527,-3.0030144068
H,-1.4272162103,-0.069470992,3.762498054
H,1.7357931156,0.126524861,-1.0667314788
H,-0.4592700122,0.1963665906,-3.9137170447
H,0.7381612104,1.0874456634,-2.9570422261
H,0.7585748187,-0.7291954797,-3.01743844
H,-1.7814525369,0.0192831254,0.970688872
H,0.6144317598,-0.0972391632,5.292580889
N,1.222762651,0.091680299,-0.1908353826
N,-0.7673090492,0.0308118715,0.9671834681
N,-0.4727571672,-0.0474994165,3.4253474236
N,1.770887694,-0.0247768209,3.5038819483

O,3.3141032287,0.0831522506,0.7782341788
S,-1.0941192524,0.1142003804,-1.6575281649

44, N7-Protonated Thioether (*E*)-14h

1,1
C,-0.206036301,0.180458081,-0.1719448751
C,-0.032840451,0.003813054,2.0408560108
C,1.3509420942,0.0509378623,2.0519948535
C,2.0882957062,0.1869424351,0.8218244504
C,0.6828126836,-0.1572379461,4.1497743512
C,-0.0502348523,0.4288997842,-2.9749026628
H,-1.3734039397,0.201280671,3.7013922027
H,1.6101150498,0.3397583893,-1.1689431386
H,-0.6833396001,0.4801064634,-3.8634280874
H,0.5236599231,1.3570308053,-2.9150667632
H,0.5963680885,-0.4469224069,-3.0708364706
H,2.7216240971,-0.035509563,3.6911280227
H,0.69005729,-0.2499129555,5.2255747737
N,1.1642024433,0.2434264817,-0.2621891185
N,-0.8449339504,0.0549938874,0.9821808892
N,-0.4156039677,-0.1342748054,3.3722239443
N,1.7582027488,-0.0465536729,3.3699817799
O,3.2908954421,0.2492956281,0.6605781251
S,-1.2281047217,0.2616409844,-1.587723703

45, (C6)O-Protonated (N1 side) Thioether (*E*)-14h

1,1
C,-0.20857707,0.1084495251,-0.1825053757
C,-0.07532121,0.008561807,2.047114685
C,1.342964713,0.0085450336,2.0892988155
C,1.9919685179,0.0643009175,0.8661623515
C,0.7143384633,-0.0828425211,4.1072005453
C,0.0359342722,0.2345692043,-2.9869638079
H,-1.406045556,-0.0671431586,3.6949159759
H,1.6154807654,0.154719979,-1.159805596
H,-0.5684024507,0.2745047039,-3.896181801
H,0.6433208837,1.1436831982,-2.9553656322
H,0.6457692615,-0.6720885015,-3.0367479588
H,3.6593390074,0.111601895,-0.1379108556
H,0.6841172664,-0.1313652531,5.1875248318
N,1.182350289,0.1130214622,-0.2433236831
N,-0.8527259773,0.0562385289,0.9619058258
N,-0.4529546289,-0.0504519852,3.350986652
N,1.8038250198,-0.0490409226,3.3861152113
O,3.3057016673,0.0706053691,0.7645029653
S,-1.1881425726,0.1721817279,-1.6319265904

46, (C6)O-Protonated (N7 side) Thioether (*E*)-14h

1,1
C,-0.2003432148,0.0689308509,-0.1816883738
C,-0.0901940872,0.0014258247,2.0528499073
C,1.3241826374,0.0002790053,2.0984333773
C,1.9782169171,0.0371788249,0.8808954964
C,0.7021034836,-0.0608496967,4.1180191965
C,0.0696544282,0.1535509867,-2.9824705891
H,-1.4154939145,-0.0488886489,3.7107532744
H,1.6625340965,0.0978536149,-1.1285602124
H,-0.5270351604,0.181038118,-3.8970229445
H,0.6790691586,1.0609307949,-2.954906662
H,0.6793888676,-0.7536254703,-3.0096524484
H,3.7812866582,0.0192849873,1.482592631
H,0.6730820662,-0.0935167595,5.1988898272
N,1.1861367549,0.0706722875,-0.2317298175
N,-0.8576600549,0.0342634347,0.9620205914
N,-0.4638796416,-0.0381992182,3.3621247932
N,1.7919879973,-0.038774535,3.3933695294
O,3.275535097,0.0443656392,0.6500563066
S,-1.1667662322,0.1127387356,-1.6371023626

(*E*)-**129** 1,1
C,0.1199709619,0.0406308995,-0.0144752433
C,0.0279345527,0.0014714941,2.3505256757
C,1.4101167735,0.0073623378,2.4483124974
C,2.2733096798,0.030666075,1.3078835491
C,0.4335813853,-0.0300447622,4.4161328376
C,0.5724621423,0.0872878181,-2.7809482088
H,2.0239396331,0.0631619991,-0.7541995221
H,0.0335847403,0.0994837166,-3.7310596362
H,1.1707001059,0.9983429251,-2.7123129532
H,1.1800454937,-0.8192748468,-2.7409200769
H,0.3249675823,-0.0481898167,5.4915720592
N,1.46013955,0.0461988707,0.0900208093
N,-0.6052672311,0.0181701697,1.1170230129
N,-0.5789624844,-0.0214483517,3.5529130381
N,1.649022699,-0.0134637438,3.8039097611
O,3.4786726228,0.0386644167,1.2175715575
S,-0.7553171785,0.0606472389,-1.5238327037
H,2.5580706491,-0.0158331054,4.2516838579
H,-1.6211925966,0.0130371232,1.0861596658

(*E*)-**132** 1,1
C,-0.3644263963,0.8301218664,0.5373097154
C,0.3388356907,0.8081297476,2.7324439954
C,0.9735110316,-0.3941939969,2.4544964643

C,0.9443784928,-1.049462063,1.1661459272
C,1.245189554,0.243741861,4.5454182561
C,-1.9511912721,0.3513554797,-1.7940393184
H,-2.1597941424,0.7446551237,-2.7906199736
H,-1.1869497691,-0.4285294566,-1.8001980376
H,-2.8712190789,0.0183550864,-1.3124257134
H,1.5806666902,0.2234505904,5.572752848
N,0.1872563851,-0.2622595531,0.208576153
N,-0.3736520404,1.4621798069,1.7380058734
N,0.4999852259,1.2070885272,4.0122769855
N,1.5548108277,-0.7386981995,3.6535495284
O,1.4567371842,-2.1024450114,0.8578440294
S,-1.3151157054,1.75241666,-0.7976639542
H,2.1073697587,-1.5701149849,3.8256998174
H,-0.2330214663,2.0644286438,-1.5518505566
H,-0.8677781754,2.3255342544,1.9384643579

(*E*)-**133**
1,1
C,-0.0191458094,-0.0590377999,0.0272443227
C,0.0068810953,-0.0083487335,2.3109141085
C,1.4057589708,0.0055775937,2.2898299577
C,2.202952831,-0.0160976299,1.0942982022
C,0.6074172933,0.033007535,4.3357313335
C,-1.4628069746,1.5054858512,-1.9131655707
H,1.797629665,-0.1097516917,-0.9621847336
H,-2.4013514664,1.4989561166,-2.4726377686
H,-1.5058583585,2.2212791105,-1.0919360735
H,-0.6357384546,1.7151188899,-2.5928126395
H,0.605072775,0.0513669042,5.4168160001
N,1.320112617,-0.0530361782,-0.0669276754
N,-0.7196821845,-0.0360015929,1.1382257975
N,-0.4771957918,0.0109958151,3.575937883
N,1.7671204239,0.0311563388,3.6110354109
O,3.4047550684,-0.0118674829,0.9483288686
S,-1.2733074977,-0.2060944158,-1.263552065
H,2.7140485705,0.043684359,3.9721084982
H,-1.866787836,-0.1375260497,0.1759304118

(*E*)-**134**
1,1
C,0.1237862352,0.2993206406,-0.0331206721
C,0.0253494223,-0.1036605879,2.1602132791
C,1.4042544033,0.1005364252,2.293151296
C,2.2670817958,0.4379534408,1.1955201481
C,0.4614128747,-0.3843962095,4.2137238527
C,-0.2605191984,-1.1550950879,-2.520636436

H,2.0120607327,0.7727465008,-0.8344268213
H,-0.691920823,-1.0755451759,-3.5210710589
H,0.8255405383,-1.2337958497,-2.5579651105
H,-0.7053018977,-1.9961640699,-1.9864527741
H,0.3804880089,0.5800589812,5.2740919962
N,1.4762761984,0.5085616923,-0.0138414533
N,-0.6348434335,0.0014696434,0.959535487
N,-0.5445428298,-0.4047086435,3.3590863713
N,1.6623693022,-0.0835632012,3.6215763079
O,3.4619844475,0.6493936788,1.1646806179
S,-0.7877558183,0.3561889671,-1.6076734214
H,2.5659950963,-0.0073433846,4.0735511933
H,-0.0465027449,1.2721877538,-2.2812467592

Cytosine and Derivatives

Cytosine

0,1
N,-0.0450357456,-1.038919365,-0.1743109527
C,1.0883441249,-0.3597204809,-0.1875150865
C,1.1788448674,1.059515198,0.0500019878
C,0.0049062361,1.7016649815,0.2965773405
N,-1.1588734453,1.0053235227,0.3076038416
C,-1.2330508068,-0.3998448433,0.0700015074
N,2.223402456,-1.0590265478,-0.4622339105
O,-2.3338676094,-0.9338272788,0.1023007307
H,2.1210267556,1.5920133795,0.0287664077
H,-0.0583583567,2.7674260697,0.4895922277
H,-2.0451501288,1.4580157831,0.4880373113
H,3.1348269059,-0.6457540888,-0.3555180091
H,2.1478763133,-2.0624153147,-0.5410911278

48, NH_3^+-Cytosine

1,1
N,-0.0554259959,-0.9910838905,-0.2168672439
C,0.946508154,-0.3601890212,0.2870732054
C,1.0728061934,1.0049319491,0.6046959382
C,-0.0644596269,1.7336878716,0.318266443
N,-1.1401758459,1.1259192004,-0.209031352
C,-1.2218604614,-0.2697757942,-0.5158094713
N,2.1130456054,-1.2864194639,0.5455490286
O,-2.2228054462,-0.7429816123,-0.9882085024
H,1.9555251081,1.4637950242,1.0295104348
H,-0.1382643853,2.8006261321,0.5012121985
H,-1.9812648852,1.6556029011,-0.4227004193
H,2.3681764143,-1.3224787796,1.5404514056

H,1.8102843597,-2.2247779234,0.2454908918
H,2.9479150594,-1.0197554103,0.008793788

49, N1-Protonated Cytosine

1,1
N,-0.4163840997,-0.5571559942,0.1954473012
C,-0.918337725,-1.6478703841,0.4702636146
N,-1.0929177718,2.2326479395,0.1686143651
C,0.1580330696,2.2694813016,-0.2660912988
C,1.0503201235,1.2187653599,-0.475749058
C,0.8134305384,-0.1457634184,-0.2668627862
N,1.7604155349,-1.0634729271,-0.5077582633
O,-1.5061076531,-2.6039326085,0.7620915183
H,-1.5486964161,1.361400178,0.4069679744
H,-1.6235003561,3.0871627629,0.2718694513
H,0.5284398531,3.267298638,-0.4868154266
H,2.0313829798,1.4982894076,-0.8400223607
H,1.6123622261,-2.0527500934,-0.3644991092
H,2.6704012565,-0.7817503059,-0.8477193262

50, N3-Protonated Cytosine

1,1
N,-0.0116675388,-0.9395283505,0.2180117016
C,1.1763986958,-0.2990773899,0.0551988344
C,1.1454429806,1.0854477914,-0.2655484611
C,-0.0730406632,1.6909820798,-0.3913139422
N,-1.2317777223,1.0068392523,-0.2186930977
C,-1.2914314468,-0.3518211535,0.0971324238
N,2.3112826415,-0.9797668266,0.1994764139
O,-2.3082629822,-0.975752939,0.2540945641
H,-0.0507531555,-1.9290525249,0.4479840604
H,2.0622285082,1.6415743647,-0.4055727194
H,-0.1695024656,2.7435543389,-0.6342732779
H,-2.1326868839,1.4655910444,-0.3142323427
H,3.2023458382,-0.5164319971,0.0813356476
H,2.3353929553,-1.9652082076,0.4276238648

51, (C6)O-Protonated (N1 side) Cytosine

1,1
N,0.0047114992,-0.9836794345,-0.2424171286
C,-1.1110306061,-0.3618009265,0.022814557
N,-1.1559923797,0.9664875093,0.3540550618
C,0.010002204,1.6953729091,0.4160149908
C,1.1979399739,1.0973499279,0.1493743463
C,1.1677744206,-0.2979265509,-0.190796153
N,2.2760538797,-0.9791801055,-0.4699275612
O,-2.226304394,-1.0694854019,-0.0390013508

H,-2.0358118653,1.4286056085,0.5562891823
H,-0.0930125942,2.7398872691,0.6833154887
H,2.1226999645,1.6588352777,0.1944343999
H,2.2045066761,-1.9620371042,-0.7044637363
H,3.1905661057,-0.5503631981,-0.4564718824
H,-3.0400400837,-0.5824125798,0.1624883033

52, (C6)O-Protonated (N3 side) Cytosine
1,1
N,0.5026460432,-0.8779086921,0.0427893321
C,1.1255659233,0.2838536646,0.358314069
C,0.4293610772,1.5373125489,0.3034272258
C,-0.8757311831,1.5139285353,-0.0763713307
N,-1.4737450926,0.3208149288,-0.3883891507
C,-0.7541994429,-0.8313178279,-0.3148956075
N,2.4043293933,0.2027003443,0.7182268324
O,-1.4360664166,-1.9128940348,-0.6380709803
H,0.9160439976,2.471770832,0.5530784075
H,-1.4961269251,2.3985289812,-0.1524018251
H,-2.4468738378,0.274197372,-0.6748756797
H,2.9431688374,1.0192888738,0.9694295847
H,2.8586032675,-0.7015797589,0.7442508324
H,-0.8688746597,-2.7009616142,-0.5661487132

138, IMPT(50 → 48)1,1
N,0.0015054359,-0.0003717114,-0.0140280353
C,0.004133701,-0.0004088615,1.3096939504
C,1.1226744848,-0.0004304475,2.1349560669
C,2.3203117484,-0.000408889,1.4287465814
N,2.3355801873,-0.00037101,0.0872059001
C,1.1811273421,-0.0003489691,-0.766164537
N,-1.4293222616,-0.0004184547,1.569063412
O,1.2696050603,-0.0003156963,-1.9631021828
H,-1.3269474223,-0.0003804103,0.2375504698
H,1.0883374802,-0.0004608062,3.2151830815
H,3.28514652,-0.0004216565,1.9264285422
H,3.2210995478,-0.0003559304,-0.4146207569
H,-1.7887071684,0.8368760669,2.0355496561
H,-1.7887041031,-0.837739081,2.0355051343

139
1,1
N,0.106194576,-0.8928924417,0.0403829199
C,-0.0139491284,-0.3286537204,1.1777616314
C,1.2712789883,0.0208500247,1.8742012971
C,1.7706255861,1.2469006089,1.9903367196
N,1.1051655959,2.4352070659,1.4407738618

C,0.3026659547,2.4657855899,0.4486292912
N,-1.1590329812,0.1245229893,1.8238816237
O,-0.4022321808,2.5580264477,-0.44479835
H,-0.7870420486,-1.1215779677,-0.4035869404
H,1.8767085256,-0.7978576222,2.254293241
H,2.7162238591,1.5117637402,2.4452725778
H,1.3040367913,3.3413621919,1.8729049574
H,-1.1382207786,0.1597405709,2.8372905357
H,-2.0434165299,-0.2170022512,1.4616504058

140
1,1
C,-0.427853105,0.0188797435,-0.0480370869
C,-0.2038211636,0.0681910937,1.2785131136
C,1.1228846733,-0.0315078553,1.8429778365
C,1.9058352387,-0.2172323352,-0.7411563124
H,3.0780003614,-0.3430506618,0.9615924069
H,-1.4265349635,0.0686223358,-0.4642702909
H,-1.028474826,0.1372682567,1.9765553158
H,2.4093020263,0.2511457053,3.3134888594
N,2.2164427016,0.16582718,0.726646269
N,0.5826930251,-0.13437455,-1.0054238423
N,1.4271801749,-0.1998434651,3.044802254
O,2.824606963,-0.491546261,-1.4531975635
H,2.4646896184,1.1661144453,0.7154466486
H,0.3277200175,-0.3094744225,-1.9731659927

141
1,1
N,-0.3987055054,-0.563277511,0.1637218254
C,-0.1861481821,0.0077581181,1.3084779222
C,1.2234414153,0.1531799006,1.7761237038
C,2.3144596233,-0.3108914356,1.1635203864
N,2.2085036436,-1.1078260474,-0.0790157742
C,2.0305266649,-0.4680856963,-1.1738488794
N,-1.1147309812,0.5157822812,2.1613805409
O,1.9960015896,0.0966413519,-2.1633517351
H,-1.3898888021,-0.612815801,-0.0760684971
H,1.4007872807,0.6838920027,2.7084588083
H,3.3331280974,-0.1937685643,1.5100370756
H,1.6234875251,-1.9522945445,-0.0189759468
H,-0.8673652905,0.9240547892,3.0502767225
H,-2.0993445434,0.4676338164,1.9407580124

142
1,1
N,-0.1564728167,0.0121330737,-0.0616215512

C,-0.0692958551,0.0109548462,1.2648590538
C,1.2092653776,0.0044039841,1.9537319081
C,2.4416144193,-0.0012041224,1.3907403621
N,2.667303661,-0.0015112982,0.0326456931
H,1.1670660222,0.0039794298,3.0365888645
H,3.3107538241,-0.0057661922,2.0442018277
C,3.7136427079,-0.0061681095,-0.6240091132
O,4.6098266541,-0.0100579237,-1.3593697017
N,-1.1789790295,0.0158947386,2.0074485077
H,-2.1052338879,0.0204595648,1.6011414384
H,-1.12378882,0.0150134334,3.0160846341
H,-1.0450532315,0.0167180625,-0.5449370346
H,0.69300166,0.0083569421,-0.614699338

143

1,1
N,0.0078579142,0.0005818275,-0.0189018407
C,0.00685595,0.0003563766,1.2744367935
C,1.0006596632,0.0001517755,2.3015520423
C,2.3421867311,0.0001630902,2.0577501176
N,2.8631319039,0.0003689001,0.7941962744
H,0.6697488121,-0.0000218371,3.332973013
H,3.0341207209,0.0000005775,2.8973319581
C,4.0249066356,0.0004203141,0.3731246404
O,5.0524929765,0.000472154,-0.1626324
N,-1.4462708497,0.0003545381,1.5263253039
H,-1.8070939088,-0.8362817139,1.9920104488
H,-1.8070457997,0.8368281254,1.992339653
H,-1.3221478423,0.000580418,0.2173574538
H,0.8686177932,0.0006398933,-0.5638521813

144

1,1
N,-0.2410645776,0.0733542203,-0.0010970522
C,0.0844232028,0.1101529603,1.2163029249
C,1.3222266215,0.096797453,1.9702964122
C,2.5548122207,0.0315040023,1.4048485413
N,2.7502271485,-0.0288540519,0.0491695301
H,1.2772787306,0.1411648422,3.0534460278
H,3.432759049,0.0262554796,2.0467186577
C,3.7623082585,-0.0918256123,-0.6517260458
O,4.6216150328,-0.1525142853,-1.4296582023
N,-1.1610688409,0.189001513,2.1098829946
H,-1.9675631783,0.1913574711,1.4712772264
H,-1.2392611896,-0.6161331263,2.7423097966
H,0.5669699622,0.0205343792,-0.624013728
H,-1.1817605695,1.0455759809,2.6757229011

145

1,1
N,-0.2041902183,-0.0508028091,-0.0693065754
C,-0.088641023,-0.0040460259,1.4200820829
C,1.153292073,-0.0801937279,1.9528183238
C,2.4082930114,-0.0191941258,1.200425251
H,1.2250691227,-0.1831561879,3.0310936614
H,3.3093964441,-0.1093917974,1.8140512543
N,-1.2962739599,0.1891779556,2.0072609742
H,-1.3182106956,0.3353858211,3.0086283839
C,-0.0126193713,1.0707592097,-0.6715685285
O,0.0130990413,2.0899913932,-1.1791167364
N,2.4587524701,0.1274901692,-0.0793821731
H,3.420104045,0.154931374,-0.4207361843
H,0.3297683353,-0.8106321675,-0.5125458636
H,-2.1199840413,-0.247411605,1.6105625302

146

1,1
N,0.5271875466,0.1306023293,-0.1104397806
C,0.2868715079,0.0057142015,1.2393993676
C,1.3653034912,-0.0133008973,2.1328963834
C,2.7203424565,0.0825875581,1.8185540581
H,1.1309816244,-0.1131070728,3.1857231274
H,3.412648309,0.0484144489,2.6558737677
N,-0.978446181,-0.0952802641,1.6704040201
H,-1.771898277,-0.0839898119,1.0447724741
H,-1.1760832663,-0.1877751816,2.6580259287
C,-0.1822647217,0.1777351138,-1.1162272926
O,-0.7319998715,0.2342332858,-2.1356834946
N,3.2988403413,0.211081498,0.6336368392
H,4.3056145355,0.269001339,0.5599795573
H,2.7589823259,0.2545207058,-0.2209258278