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Supporting Information

69451 Weinheim, Germany

A Highly Stabilizing Silver(I)-Mediated Base Pair in Parallel-Stranded DNA**

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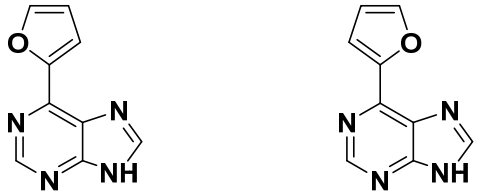
Table S1. Relative energies of different conformations of 9*H*-**6FP** (E / kcal mol^{-1}).

	Relative energy	
Species	Gas phase	COSMO
FP1 (with O facing towards N1)	0	0
FP2 (with O facing towards N7)	0.9	0.6



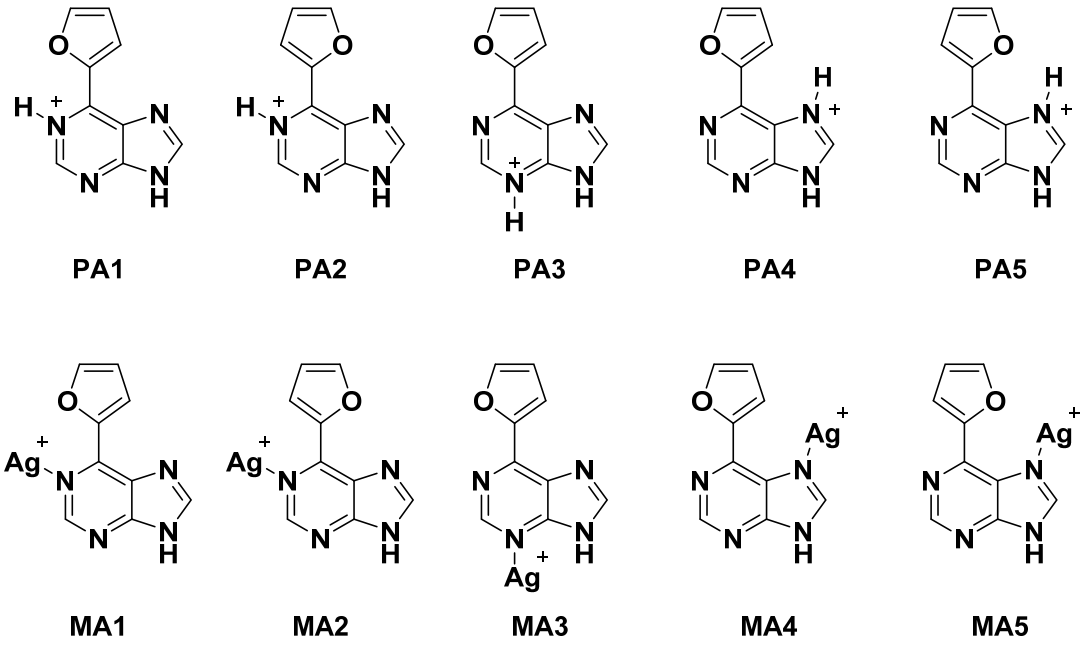
FP1 **FP2**

Scheme S1. Structural representation of the different conformations of 9*H*-**6FP**.

Table S2. Normalized proton and Ag^+ affinities of 9*H*-**6FP** (*E* / kcal mol^{-1}).

			Proton affinity		**Ag^+ affinity**	
Species	Position of protonation / metalation	Furyl oxygen atom facing towards	Gas phase	COSMO	Gas phase	COSMO
PA1 / MA1	N1	N1	0	0	0	0
PA2/ MA2	N1	N7	5.5	1.6	9.3	0.9
PA3 / MA3	N3	N1	10.1	4.5	10.0	1.1
PA4 / MA4	N7	N1	14.8	4.2	4.8	1.4
PA5 / MA5	N7	N7	7.9	2.7	3.0	0.3
	O	N1	*a*	*a*	*a*	*a*
	O	N7	*a*	*a*	*a*	*a*

[a] not stable, proton / Ag^+ migrates to N1 / N7.

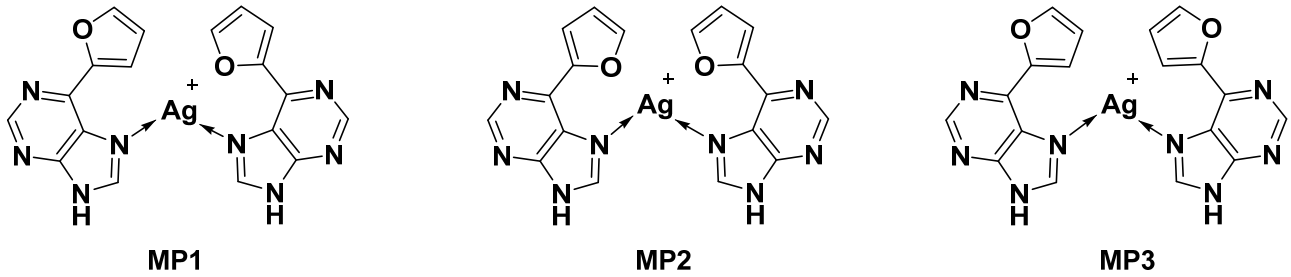


Scheme S2. Structural representation of the different protonated / metalated species.

Table S3. Normalized base pair formation energies of **6FP**–Ag^+–**6FP** base pairs (E / kcal mol^{-1}) and corresponding N9–N9' distances (d / Å). [a]

Species	Gas phase		COSMO	
	E	*d*	*E*	*d*
MP1	0.9	7.0	0.9	6.9
MP2	0	6.7	3.2	6.5
MP3	6.0	7.1	0	7.1

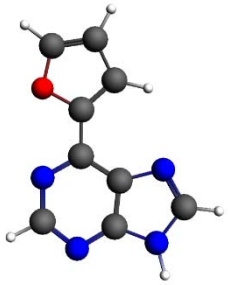
[a] Energy of most stable base pair has been set to 0 kcal/mol. Base pairs have been optimized in *C*s symmetry.



Scheme S3. Structural representation of the different **6FP**–Ag^+–**6FP** base pairs.

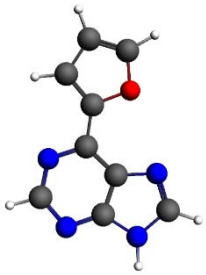
Cartesian coordinates (a. u.) and total bonding energies (kcal mol^{-1}) of the geometry-optimized structures of all computed compounds.

FP1 (Gas phase, C_1), -3118.2 kcal mol^{-1}, n_{imag} = 0:



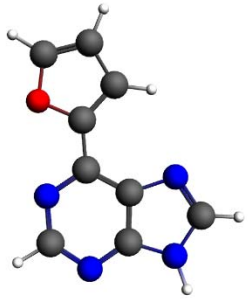
N	-0.248957	-0.623683	0.075050
C	2.075601	2.046541	0.143197
N	3.259411	1.387527	0.068626
C	3.253950	0.046359	-0.004338
N	2.193488	-0.788045	-0.015024
C	1.040551	-0.117729	0.059498
C	0.883513	1.285585	0.140960
N	-0.470150	1.621341	0.204296
C	-1.102400	0.464990	0.162472
H	1.133111	6.651261	0.419971
H	4.230635	-0.428516	-0.062323
H	-2.176569	0.339753	0.191562
C	2.066010	3.487974	0.221797
O	3.280507	4.158709	0.222964
C	2.990971	5.493663	0.303627
C	1.636346	5.696583	0.353586
C	1.035821	4.403642	0.301186
H	-0.499463	-1.603749	0.030914
H	3.843024	6.156826	0.315484
H	-0.014121	4.149839	0.317735

FP2 (Gas phase, C_1), -3117.3 kcal mol^{-1}, n_{imag} = 0:



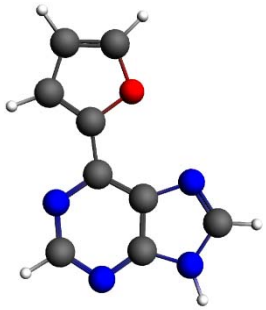
N	-0.235066	-0.674855	0.071785
C	1.999404	2.067371	0.147046
N	3.204933	1.439154	0.073143
C	3.241928	0.101488	-0.000751
N	2.205128	-0.762676	-0.013494
C	1.034162	-0.126446	0.059705
C	0.829420	1.276567	0.142683
N	-0.536360	1.563181	0.203315
C	-1.125563	0.387471	0.158879
H	3.051595	6.648055	0.361195
H	4.232067	-0.344744	-0.057662
H	-2.194917	0.224460	0.185304
C	2.033996	3.509204	0.224238
O	0.838868	4.207810	0.301622
C	1.162602	5.536272	0.363115
C	2.522648	5.705646	0.327446
C	3.087567	4.399149	0.237828
H	-0.450901	-1.663022	0.025220
H	0.328171	6.218310	0.427699
H	4.130711	4.124125	0.188470

FP1 (COSMO, C_1), -3132.9 kcal mol^{-1}, n_{imag} = 0:



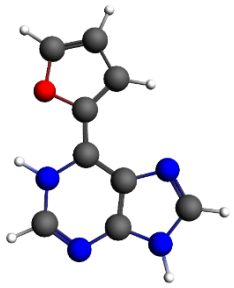
N	-0.246057	-0.631680	0.074362
C	2.060776	2.049004	0.143765
N	3.253458	1.393993	0.070018
C	3.257192	0.050743	-0.001491
N	2.198140	-0.784073	-0.011121
C	1.034358	-0.123376	0.061664
C	0.877036	1.282388	0.141085
N	-0.478493	1.609518	0.200102
C	-1.104384	0.440698	0.157265
H	1.152748	6.664575	0.426318
H	4.235295	-0.419329	-0.058552
H	-2.175888	0.304469	0.181582
C	2.053084	3.489583	0.221956
O	3.277672	4.152350	0.215685
C	3.000363	5.496762	0.298649
C	1.648733	5.706624	0.356945
C	1.035882	4.417926	0.307809
H	-0.507928	-1.610204	0.029534
H	3.857992	6.152061	0.303868
H	-0.018699	4.186841	0.331797

FP2 (COSMO, C_1), -3132.3 kcal mol^{-1}, n_{imag} = 0:



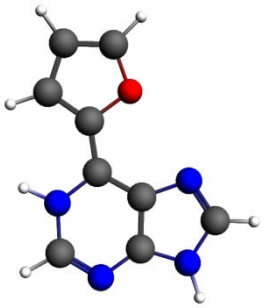
N	-0.238183	-0.666712	0.074081
C	2.007739	2.064334	0.145233
N	3.213961	1.428897	0.070480
C	3.246565	0.089552	-0.002059
N	2.203114	-0.766609	-0.012291
C	1.028264	-0.128555	0.061108
C	0.838438	1.277367	0.142056
N	-0.527787	1.568095	0.202128
C	-1.122742	0.385069	0.158409
H	3.040239	6.653748	0.364000
H	4.233547	-0.361601	-0.059923
H	-2.190498	0.221818	0.183335
C	2.043371	3.505526	0.222495
O	0.840192	4.200346	0.299525
C	1.157496	5.536739	0.362991
C	2.515637	5.709247	0.328623
C	3.088893	4.405161	0.238212
H	-0.475512	-1.651447	0.029186
H	0.319897	6.214313	0.428524
H	4.137764	4.151232	0.190676

PA1 (Gas phase, C_1), -3068.6 kcal mol^{-1}, n_{imag} = 0:



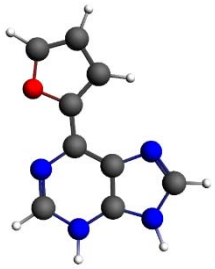
N	-0.268445	-0.525178	0.100912
C	2.004433	2.174594	0.150738
N	3.175297	1.443582	0.068586
C	3.227558	0.072627	-0.003087
N	2.168350	-0.702545	-0.001764
C	1.006116	-0.024238	0.077377
C	0.843217	1.383035	0.155149
N	-0.493946	1.720638	0.223701
C	-1.128121	0.563068	0.189255
H	1.327408	6.797071	0.411651
H	4.221341	-0.359298	-0.063234
H	-2.201894	0.436189	0.224081
C	2.056652	3.586867	0.220495
O	3.318923	4.176183	0.201923
C	3.110249	5.527874	0.278629
C	1.767034	5.811800	0.344687
C	1.083627	4.569559	0.307831
H	-0.521896	-1.508320	0.060696
H	4.000365	6.140431	0.275543
H	0.018114	4.389424	0.339633
H	4.050838	1.964731	0.061415

PA2 (Gas phase, C_1), -3063.1 kcal mol^{-1}, n_{imag} = 0:



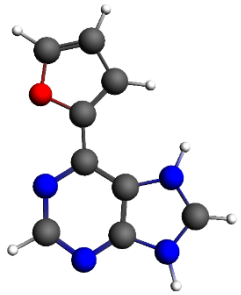
N	-0.216332	-0.656679	0.072154
C	1.984792	2.106499	0.149654
N	3.170833	1.391928	0.071703
C	3.256060	0.023426	-0.005458
N	2.216002	-0.774849	-0.014514
C	1.040123	-0.120868	0.059811
C	0.839901	1.287608	0.142937
N	-0.509250	1.581996	0.203443
C	-1.107715	0.409347	0.159479
H	3.019805	6.674909	0.363703
H	4.260614	-0.383761	-0.060723
H	-2.177658	0.251259	0.186190
C	2.039544	3.523609	0.224838
O	0.837551	4.206508	0.301595
C	1.142138	5.529850	0.363441
C	2.505535	5.724965	0.329060
C	3.087816	4.438685	0.239968
H	-0.439434	-1.646928	0.025716
H	0.298983	6.202640	0.427811
H	4.148062	4.224752	0.193365
H	4.043899	1.912521	0.071181

PA3 (Gas phase, C_1), -3058.5 kcal mol^{-1}, n_{imag} = 0:



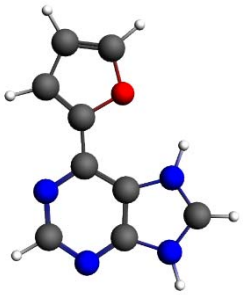
N	-0.288854	-0.606339	0.075313
C	2.062880	2.064356	0.144399
N	3.268067	1.397278	0.069955
C	3.309142	0.099464	-0.001385
N	2.197194	-0.721726	-0.010224
C	0.982278	-0.109331	0.061580
C	0.870647	1.288552	0.140571
N	-0.471172	1.640546	0.202371
C	-1.133219	0.508976	0.162432
H	1.159161	6.646850	0.420501
H	4.265281	-0.413515	-0.059568
H	-2.208207	0.394096	0.190527
C	2.065039	3.474880	0.220442
O	3.289284	4.136529	0.217089
C	3.009448	5.460744	0.297471
C	1.646629	5.684321	0.353012
C	1.035869	4.414216	0.303961
H	-0.578336	-1.578143	0.032109
H	3.864674	6.122148	0.305877
H	-0.018406	4.177312	0.324811
H	2.306391	-1.731945	-0.068219

PA4 (Gas Phase, C_1), -3053.8 kcal mol^{-1}, n_{imag} = 0:



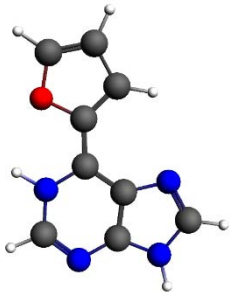
N	-0.263493	-0.638800	0.073922
C	2.049729	2.094035	0.147128
N	3.222305	1.422531	0.071994
C	3.235125	0.083875	-0.002484
N	2.175345	-0.756179	-0.014872
C	1.029920	-0.095099	0.060045
C	0.872668	1.297752	0.142927
N	-0.507039	1.527384	0.203642
C	-1.162326	0.354645	0.160727
H	1.227612	6.724571	0.414385
H	4.214368	-0.382929	-0.060051
H	-2.235025	0.235469	0.191456
C	2.052015	3.525643	0.224473
O	3.282108	4.156250	0.226953
C	3.045109	5.494378	0.304136
C	1.695326	5.752393	0.351570
C	1.053875	4.488482	0.300528
H	-0.477989	-1.632103	0.025892
H	3.920974	6.126935	0.316009
H	-0.016562	4.333612	0.316777
H	-0.967167	2.428507	0.271847

PA5 (Gas phase, C_1), -3060.7 kcal mol^{-1}, n_{imag} = 0:



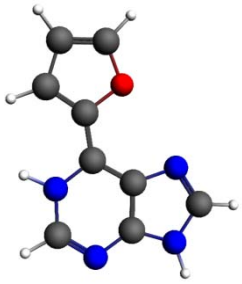
N	-0.285896	-0.589555	0.078147
C	2.090115	2.077320	0.144556
N	3.255318	1.392279	0.068822
C	3.236771	0.051728	-0.003417
N	2.159198	-0.767277	-0.012314
C	1.024271	-0.086557	0.062185
C	0.902109	1.307742	0.141994
N	-0.464208	1.586345	0.202287
C	-1.153987	0.436460	0.162593
H	2.948452	6.688838	0.366799
H	4.204919	-0.437220	-0.061982
H	-2.229677	0.348406	0.193356
C	2.102089	3.503618	0.221671
O	0.856879	4.139050	0.297354
C	1.118676	5.488404	0.362031
C	2.468740	5.720786	0.330044
C	3.103506	4.450757	0.240049
H	-0.535643	-1.574442	0.032878
H	0.254585	6.133334	0.425635
H	4.162272	4.239186	0.193562
H	-0.859431	2.521402	0.266163

PA1 (COSMO, C_1), -3124.9 kcal mol^{-1}, n_{imag} = 0:



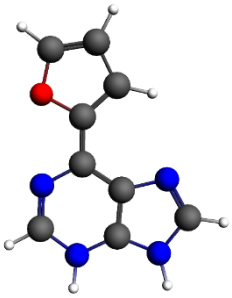
N	-0.203529	-0.651659	0.067458
C	2.000454	2.097997	0.157617
N	3.184005	1.401680	0.079549
C	3.276479	0.044772	-0.005767
N	2.234887	-0.764176	-0.019823
C	1.054315	-0.117854	0.058607
C	0.858701	1.285225	0.148630
N	-0.493440	1.582142	0.208897
C	-1.091159	0.399337	0.157607
H	1.220830	6.710556	0.413622
H	4.280897	-0.354109	-0.062693
H	-2.158211	0.235634	0.180629
C	2.022771	3.516350	0.232505
O	3.269121	4.135482	0.221265
C	3.032116	5.483857	0.294980
C	1.683848	5.736307	0.351994
C	1.029552	4.474857	0.312058
H	-0.439103	-1.637394	0.015637
H	3.908284	6.113947	0.295078
H	-0.031815	4.276981	0.336197
H	4.049563	1.936982	0.080008

PA2 (COSMO, C_1), -3123.3 kcal mol^{-1}, n_{imag} = 0:



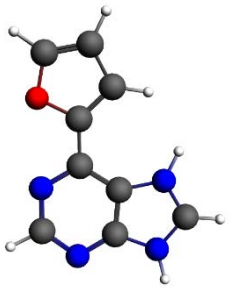
N	-0.214035	-0.662917	0.068993
C	1.972481	2.104124	0.157358
N	3.157436	1.404769	0.077930
C	3.256170	0.050011	-0.006982
N	2.218557	-0.763693	-0.019911
C	1.037446	-0.119899	0.059036
C	0.833117	1.286147	0.148482
N	-0.524753	1.567853	0.209826
C	-1.110770	0.381267	0.159561
H	3.048770	6.661814	0.353377
H	4.262922	-0.342782	-0.064508
H	-2.176291	0.208012	0.183909
C	2.030401	3.524631	0.232080
O	0.832150	4.222569	0.305859
C	1.158002	5.550323	0.360659
C	2.520367	5.720013	0.324717
C	3.086501	4.420766	0.242172
H	-0.440356	-1.650923	0.018720
H	0.325744	6.234642	0.422285
H	4.139813	4.180949	0.194945
H	4.027596	1.929745	0.076848

PA3 (COSMO, C_1), -3120.4 kcal mol^{-1}, n_{imag} = 0:



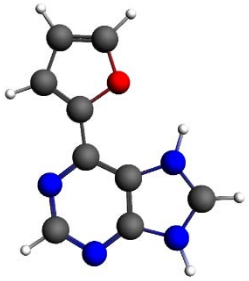
N	-0.266817	-0.640986	0.071989
C	2.053227	2.036550	0.146713
N	3.260426	1.382948	0.071024
C	3.300109	0.071864	-0.001157
N	2.198789	-0.731470	-0.009073
C	0.990154	-0.132726	0.061673
C	0.867669	1.268720	0.143456
N	-0.482943	1.602041	0.202679
C	-1.122181	0.446647	0.157621
H	1.161248	6.636649	0.422475
H	4.252460	-0.439557	-0.061785
H	-2.193126	0.312251	0.180772
C	2.053118	3.460958	0.223454
O	3.280774	4.119810	0.213569
C	3.005873	5.457145	0.293825
C	1.650558	5.675591	0.354617
C	1.035023	4.396975	0.309575
H	-0.533345	-1.618577	0.024060
H	3.863427	6.112852	0.295685
H	-0.019984	4.168455	0.335553
H	2.300096	-1.742420	-0.067329

PA4 (COSMO, C_1), -3120.5 kcal mol^{-1}, n_{imag} = 0:



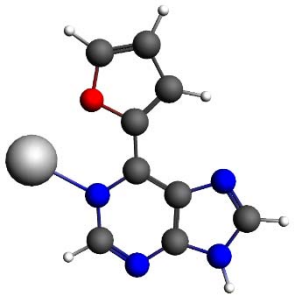
N	-0.265050	-0.623717	0.084573
C	2.055250	2.080654	0.138827
N	3.236275	1.414103	0.058090
C	3.238185	0.071985	-0.016386
N	2.177597	-0.760046	-0.022812
C	1.021988	-0.098670	0.058730
C	0.883092	1.296217	0.140900
N	-0.484182	1.544140	0.214945
C	-1.146499	0.381876	0.177409
H	1.200531	6.705246	0.397417
H	4.214208	-0.399089	-0.079499
H	-2.217273	0.274584	0.214419
C	2.052186	3.515774	0.219250
O	3.285308	4.156432	0.253072
C	3.031425	5.501816	0.329771
C	1.681846	5.739370	0.343936
C	1.049237	4.465801	0.272831
H	-0.509789	-1.607935	0.039985
H	3.900105	6.141318	0.365892
H	-0.016846	4.295574	0.254183
H	-0.940624	2.445716	0.284108

PA5 (COSMO, C_1), -3122.2 kcal mol^{-1}, n_{imag} = 0:



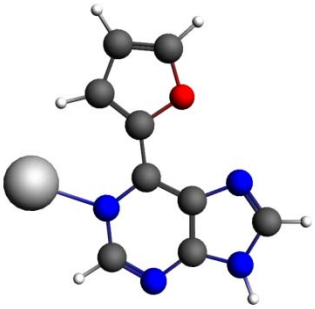
N	-0.282931	-0.585208	0.080974
C	2.086222	2.069894	0.143352
N	3.260217	1.390541	0.065747
C	3.238432	0.048561	-0.005464
N	2.163371	-0.768293	-0.011531
C	1.016573	-0.090609	0.064402
C	0.904334	1.306136	0.142957
N	-0.455467	1.589479	0.203627
C	-1.142725	0.443578	0.163470
H	2.943011	6.689603	0.368820
H	4.206145	-0.439651	-0.065599
H	-2.215829	0.358405	0.190083
C	2.101112	3.501613	0.221320
O	0.861762	4.137348	0.295324
C	1.115063	5.485709	0.360826
C	2.465132	5.721064	0.330759
C	3.102351	4.448732	0.241024
H	-0.552536	-1.562744	0.035332
H	0.247165	6.124065	0.424593
H	4.162499	4.245955	0.196879
H	-0.864842	2.516425	0.265520

MA1 (Gas Phase, C_1), -3007.7 kcal mol^{-1}, n_{imag} = 0:



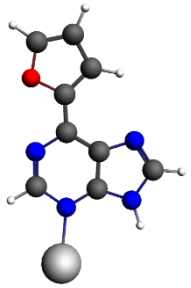
N	-0.254091	-0.607461	0.075167
C	2.073086	2.052180	0.143895
N	3.254265	1.355475	0.068315
C	3.252300	-0.007567	-0.004944
N	2.184911	-0.795148	-0.013138
C	1.031304	-0.119618	0.060239
C	0.889795	1.287626	0.140642
N	-0.448607	1.641102	0.202659
C	-1.096536	0.491682	0.161417
H	1.096812	6.642541	0.423227
H	4.225521	-0.484384	-0.061858
H	-2.172224	0.380165	0.189865
C	2.056199	3.485868	0.221883
O	3.273853	4.175810	0.220453
C	2.967750	5.522881	0.303088
C	1.614670	5.696099	0.355520
C	1.026562	4.397900	0.304004
H	-0.521196	-1.585760	0.030962
H	3.812896	6.194480	0.312589
H	-0.022749	4.140456	0.323473
Ag	5.143397	2.475098	0.066965

MA2 (Gas Phase, C_1), -2998.4 kcal mol^{-1}, n_{imag} = 0:



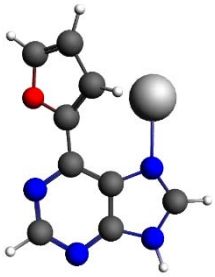
N	-0.258429	-0.606677	0.075448
C	2.064668	2.066014	0.144900
N	3.242822	1.353342	0.068653
C	3.238253	-0.011409	-0.004759
N	2.171043	-0.792484	-0.012586
C	1.019868	-0.113263	0.060992
C	0.876952	1.299627	0.141735
N	-0.465488	1.641885	0.203293
C	-1.106159	0.492313	0.161907
H	2.910069	6.708705	0.367988
H	4.210187	-0.491976	-0.061874
H	-2.181421	0.375520	0.190142
C	2.088278	3.502943	0.221591
O	0.859303	4.135568	0.295156
C	1.091438	5.475379	0.359916
C	2.438874	5.737093	0.330751
C	3.079189	4.472730	0.242040
H	-0.518376	-1.586920	0.030962
H	0.213709	6.101956	0.421875
H	4.155749	4.332698	0.199920
Ag	5.213049	2.259385	0.054216

MA3 (Gas phase, C_1), -2997.6 kcal mol^{-1}, n_{imag} = 0:



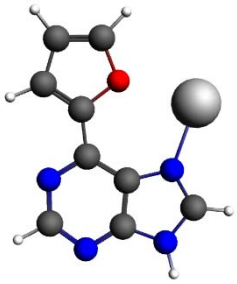
N	-0.252874	-0.623893	0.072708
C	2.071482	2.058174	0.142911
N	3.262868	1.389347	0.067017
C	3.303110	0.079849	-0.006088
N	2.218244	-0.765132	-0.016612
C	1.026148	-0.124439	0.057805
C	0.886312	1.278315	0.139305
N	-0.457454	1.618163	0.202354
C	-1.106919	0.478030	0.161337
H	1.150840	6.644438	0.424212
H	4.277725	-0.397151	-0.064316
H	-2.181062	0.355819	0.190151
C	2.067266	3.477226	0.220696
O	3.288011	4.141706	0.216874
C	3.003957	5.469526	0.298894
C	1.644151	5.685100	0.355463
C	1.037295	4.407497	0.305506
H	-0.533227	-1.596905	0.028846
H	3.857579	6.132218	0.307055
H	-0.015899	4.166905	0.326985
Ag	2.508041	-2.887367	-0.144400

MA4 (Gas phase, C_1), -3002.9 kcal mol^{-1}, n_{imag} = 0:



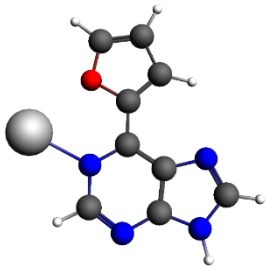
N	-0.288245	-0.674278	0.185450
C	2.025891	2.005878	0.049595
N	3.194475	1.369801	-0.152705
C	3.189196	0.027688	-0.288137
N	2.125042	-0.800995	-0.247451
C	0.989957	-0.157369	-0.003010
C	0.852507	1.236487	0.162965
N	-0.475653	1.534710	0.480763
C	-1.118831	0.369498	0.486047
H	1.253888	6.687096	-0.145851
H	4.155392	-0.438821	-0.455540
H	-2.168287	0.237590	0.706736
C	2.005213	3.464380	0.160754
O	3.022002	4.079670	0.828332
C	2.796819	5.440705	0.778887
C	1.655105	5.710462	0.084937
C	1.113347	4.434393	-0.316190
H	-0.544282	-1.655971	0.133773
H	3.531008	6.050807	1.283096
H	0.380090	4.270381	-1.100034
Ag	-0.738130	3.665988	1.135988

MA5 (Gas phase, C_1), -3004.7 kcal mol^{-1}, n_{imag} = 0:



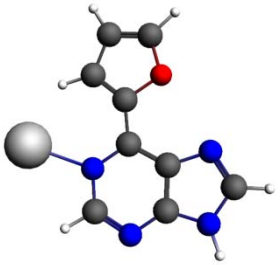
N	-0.187151	-0.751092	0.064411
C	1.948861	2.090391	0.158846
N	3.165160	1.495925	0.079082
C	3.258007	0.161681	-0.005800
N	2.247475	-0.731520	-0.023895
C	1.062218	-0.140910	0.055694
C	0.811323	1.248410	0.149732
N	-0.578841	1.436853	0.212741
C	-1.130251	0.225592	0.159011
H	3.102570	6.645999	0.380026
H	4.262549	-0.247278	-0.067219
H	-2.190289	0.021255	0.186162
C	1.985644	3.534351	0.242569
O	0.797551	4.285618	0.331725
C	1.177888	5.622546	0.394841
C	2.534452	5.726840	0.348786
C	3.051730	4.399927	0.251976
H	-0.352295	-1.751487	0.009305
H	0.371748	6.337007	0.467177
H	4.086985	4.097335	0.194308
Ag	-1.488081	3.400579	0.366402

MA1 (COSMO, C_1), -3073.5 kcal mol^{-1}, n_{imag} = 0:



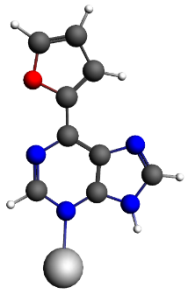
N	-0.249214	-0.618841	0.077648
C	2.060555	2.057885	0.142024
N	3.246827	1.378644	0.065567
C	3.254248	0.024802	-0.006719
N	2.191547	-0.785313	-0.012606
C	1.030110	-0.118285	0.062304
C	0.881259	1.287705	0.140574
N	-0.468676	1.623677	0.201235
C	-1.101777	0.458618	0.160495
H	1.105075	6.657931	0.428707
H	4.231295	-0.440673	-0.065101
H	-2.173832	0.328854	0.186466
C	2.043290	3.494330	0.220446
O	3.257372	4.175366	0.216124
C	2.968121	5.517991	0.300886
C	1.613953	5.707101	0.358307
C	1.016532	4.412387	0.307048
H	-0.515895	-1.596380	0.033572
H	3.820505	6.179385	0.307158
H	-0.035022	4.169487	0.330343
Ag	5.211487	2.425099	0.063982

MA2 (COSMO, C_1), -3072.5 kcal mol^{-1}, n_{imag} = 0:



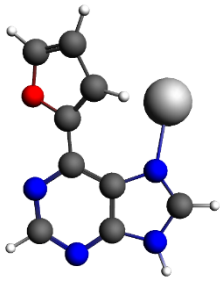
N	-0.247586	-0.628214	0.106519
C	2.043462	2.069702	0.124369
N	3.230952	1.388251	0.031208
C	3.243972	0.034148	-0.028154
N	2.185290	-0.779578	-0.016989
C	1.023985	-0.115888	0.066667
C	0.866432	1.293529	0.141867
N	-0.488971	1.611797	0.231579
C	-1.109102	0.441621	0.205195
H	2.933538	6.687366	0.507197
H	4.222544	-0.426989	-0.095145
H	-2.179007	0.300816	0.253712
C	2.065853	3.509118	0.206372
O	0.841538	4.168448	0.143193
C	1.101183	5.510240	0.255856
C	2.446267	5.729839	0.392380
C	3.066884	4.448118	0.362101
H	-0.503546	-1.609090	0.074565
H	0.239370	6.159056	0.220676
H	4.128996	4.256601	0.464455
Ag	5.231523	2.303540	-0.155355

MA3 (COSMO, C_1), -3072.4 kcal mol^{-1}, n_{imag} = 0:



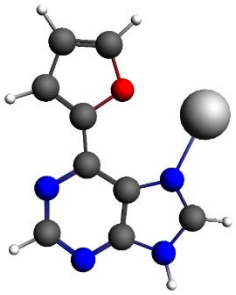
N	-0.227179	-0.632487	0.073154
C	2.069847	2.056407	0.146571
N	3.266982	1.403583	0.071671
C	3.293435	0.073503	-0.001789
N	2.221844	-0.759143	-0.011844
C	1.041519	-0.118952	0.061886
C	0.889552	1.284655	0.143755
N	-0.465726	1.606918	0.202951
C	-1.091109	0.440237	0.157910
H	1.154255	6.664308	0.420206
H	4.265468	-0.403133	-0.059803
H	-2.161565	0.298834	0.181340
C	2.060673	3.491500	0.223326
O	3.284415	4.155928	0.216361
C	3.004143	5.497516	0.296200
C	1.650754	5.706559	0.353388
C	1.040515	4.419326	0.306841
H	-0.483068	-1.613141	0.023457
H	3.860060	6.155198	0.300558
H	-0.013696	4.186617	0.330487
Ag	2.394856	-2.927216	-0.144252

MA4 (COSMO, C_1), -3072.1 kcal mol^{-1}, n_{imag} = 0:



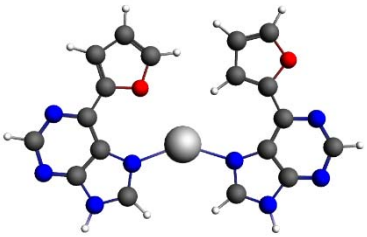
N	-0.253230	-0.652547	0.050455
C	2.063062	2.022760	0.116016
N	3.254000	1.375002	0.039019
C	3.254428	0.032706	-0.076698
N	2.191552	-0.796654	-0.137589
C	1.030887	-0.146186	-0.010580
C	0.889913	1.250750	0.134650
N	-0.456865	1.559161	0.319385
C	-1.102031	0.395873	0.265992
H	1.149904	6.646526	-0.138034
H	4.230659	-0.438835	-0.137396
H	-2.166128	0.267170	0.386643
C	2.024869	3.470119	0.174957
O	3.090260	4.133846	0.757978
C	2.809534	5.483041	0.689731
C	1.610209	5.691054	0.068580
C	1.094176	4.396385	-0.265297
H	-0.521640	-1.628411	-0.018440
H	3.547553	6.136352	1.128524
H	0.222820	4.183473	-0.871231
Ag	-1.007430	3.476515	1.291741

MA5 (COSMO, C_1), -3073.2 kcal mol^{-1}, n_{imag} = 0:



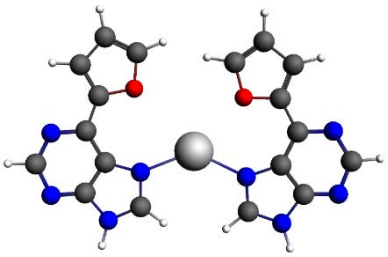
N	-0.202464	-0.709847	0.062328
C	1.988305	2.077856	0.156166
N	3.201825	1.459575	0.077158
C	3.262110	0.123237	-0.006716
N	2.234480	-0.750131	-0.026175
C	1.051057	-0.135275	0.053730
C	0.836096	1.263438	0.148059
N	-0.543694	1.492648	0.213000
C	-1.118768	0.294523	0.158551
H	3.072335	6.653164	0.388893
H	4.257357	-0.307908	-0.066903
H	-2.181407	0.112833	0.184717
C	2.027611	3.518824	0.237716
O	0.834810	4.238676	0.299562
C	1.171336	5.573842	0.366130
C	2.530769	5.718794	0.348166
C	3.082976	4.405184	0.265394
H	-0.409423	-1.701033	0.005205
H	0.341853	6.261647	0.419835
H	4.128164	4.135817	0.230017
Ag	-1.629302	3.382940	0.430939

MP1 (Gas phas, *Cs* symm.), -6156.8 kcal mol^{-1}, n_{imag} = 0:



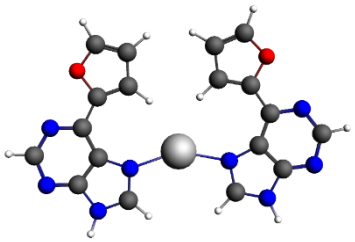
N	3.369067	3.315237	0.000000
C	4.016527	-0.181244	0.000000
N	5.370723	-0.175633	0.000000
C	6.045057	0.980457	0.000000
N	5.530791	2.224868	0.000000
C	4.202236	2.205913	0.000000
C	3.349239	1.075029	0.000000
N	2.011938	1.531473	0.000000
C	2.087755	2.866151	0.000000
C	2.117858	-3.348355	0.000000
H	7.129244	0.905572	0.000000
H	1.242740	3.536498	0.000000
O	4.226867	-2.572779	0.000000
C	3.380514	-1.477084	0.000000
C	2.073400	-1.923008	0.000000
C	3.445984	-3.686946	0.000000
N	-5.699704	2.037003	0.000000
H	1.297148	-4.050386	0.000000
H	3.969550	-4.631518	0.000000
C	-2.316641	2.977043	0.000000
C	-4.375928	2.148205	0.000000
C	-3.428358	1.097412	0.000000
H	1.196573	-1.289927	0.000000
C	-2.467713	-3.564334	0.000000
N	-2.137892	1.655750	0.000000
N	-3.634626	3.322270	0.000000
C	-3.964944	-0.211286	0.000000
H	-7.165998	0.572444	0.000000
H	-1.527596	3.713037	0.000000
O	-1.821033	-1.399353	0.000000
C	-3.217959	-1.439873	0.000000
C	-3.637470	-2.750502	0.000000
C	-1.400523	-2.712901	0.000000
H	-4.669656	-3.068256	0.000000
H	-2.423633	-4.644360	0.000000
H	-0.337846	-2.858449	0.000000
C	-6.093556	0.747057	0.000000
N	-5.315472	-0.343264	0.000000
H	3.682521	4.280204	0.000000
H	-4.021749	4.260152	0.000000
Ag	-0.087436	0.877683	0.000000

MP2 (Gas phase, *Cs* symm.), -6157.8 kcal mol^{-1}, n_{imag} = 2 (-23 cm^{-1}, -82 cm^{-1}):



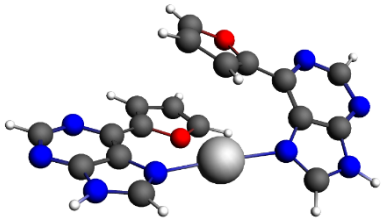
N	3.658413	3.205789	0.000000
C	4.087962	-0.314449	0.000000
N	5.440732	-0.413234	0.000000
C	6.188888	0.698869	0.000000
N	5.760832	1.977838	0.000000
C	4.434064	2.054546	0.000000
C	3.516231	0.978131	0.000000
N	2.209483	1.494287	0.000000
C	2.349862	2.818427	0.000000
C	2.635262	-3.689227	0.000000
H	7.265671	0.553258	0.000000
H	1.540962	3.532387	0.000000
O	1.966171	-1.531162	0.000000
C	3.363508	-1.556388	0.000000
C	3.796674	-2.862130	0.000000
C	1.560444	-2.847514	0.000000
N	-5.290686	2.581316	0.000000
H	2.602541	-4.769656	0.000000
H	0.497529	-2.996024	0.000000
C	-1.798281	2.846220	0.000000
C	-3.972431	2.421914	0.000000
C	-3.241846	1.205029	0.000000
H	4.832069	-3.169401	0.000000
C	-3.451577	-3.591373	0.000000
N	-1.865156	1.514343	0.000000
N	-3.025420	3.434295	0.000000
C	-4.034094	0.028880	0.000000
H	-7.019858	1.437915	0.000000
H	-0.886797	3.422611	0.000000
O	-2.243585	-1.675031	0.000000
C	-3.598229	-1.343810	0.000000
C	-4.356834	-2.494834	0.000000
C	-2.196298	-3.053254	0.000000
H	-5.436031	-2.520879	0.000000
H	-3.695593	-4.644379	0.000000
H	-1.219458	-3.501911	0.000000
C	-5.933914	1.396983	0.000000
N	-5.385596	0.178420	0.000000
H	4.016757	4.154892	0.000000
H	-3.232570	4.427289	0.000000
Ag	0.160200	0.611020	0.000000

MP3 (Gas phase, *Cs* symm.), -6151.8 kcal mol^{-1}, n_{imag} = 3 (-31 cm^{-1}, -35 cm^{-1}, -81 cm^{-1}):



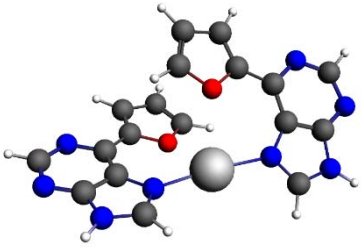
N	-3.312194	-3.572927	0.000000
C	-3.976912	-0.077674	0.000000
N	-5.331127	-0.091034	0.000000
C	-5.999655	-1.250381	0.000000
N	-5.479567	-2.492708	0.000000
C	-4.151379	-2.467222	0.000000
C	-3.305259	-1.332054	0.000000
N	-1.966699	-1.783807	0.000000
C	-2.033632	-3.120218	0.000000
C	-2.092200	3.097182	0.000000
H	-7.084183	-1.180755	0.000000
H	-1.185144	-3.786369	0.000000
O	-4.197585	2.311912	0.000000
C	-3.346084	1.219891	0.000000
C	-2.041314	1.674958	0.000000
C	-3.421887	3.430126	0.000000
N	5.796022	-1.628677	0.000000
H	-1.268907	3.791518	0.000000
H	-3.951340	4.371486	0.000000
C	2.486122	-2.774390	0.000000
C	4.479487	-1.806060	0.000000
C	3.470149	-0.813213	0.000000
H	-1.155023	1.058000	0.000000
C	1.594768	3.378273	0.000000
N	2.216124	-1.463840	0.000000
N	3.818757	-3.026810	0.000000
C	3.942652	0.528930	0.000000
H	7.181796	-0.087480	0.000000
H	1.749031	-3.562035	0.000000
O	3.795511	2.924307	0.000000
C	3.121090	1.714929	0.000000
C	1.762091	1.965051	0.000000
C	2.857852	3.910730	0.000000
H	0.980674	1.219710	0.000000
H	0.674899	3.938344	0.000000
H	3.237075	4.921992	0.000000
C	6.120575	-0.321571	0.000000
N	5.283045	0.722285	0.000000
H	-3.620963	-4.539596	0.000000
H	4.271390	-3.935073	0.000000
Ag	0.081946	-1.065727	0.000000

MP1 (Gas phase, C_1), -6170.5 kcal mol^{-1}, n_{imag} = 0:



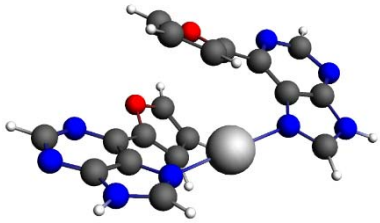
N	-7.384304	-6.068305	1.446775
C	-7.935891	-2.769966	0.241158
N	-9.165124	-2.513300	0.759286
C	-9.791452	-3.443327	1.491938
N	-9.353866	-4.681987	1.798748
C	-8.139779	-4.910526	1.308605
C	-7.345667	-4.022399	0.545677
N	-6.122487	-4.656690	0.259990
C	-6.194545	-5.866579	0.812242
C	-6.915854	0.098522	-1.822098
H	-10.770868	-3.172267	1.876812
H	-5.414479	-6.612097	0.777868
O	-6.176783	-1.953182	-1.253108
C	-7.383321	-1.732763	-0.590960
C	-7.858952	-0.483461	-0.925420
C	-5.918581	-0.820831	-1.993802
C	-2.032851	-1.795527	-1.324671
H	-6.968651	1.074610	-2.283093
H	-5.006663	-0.835028	-2.570933
C	-4.769929	-1.028124	2.190464
C	-1.665274	-3.766374	-2.192643
C	-0.976878	-1.649818	-2.247424
H	-8.783291	-0.057061	-0.564461
Ag	-4.337219	-3.804657	-0.547946
N	-2.458908	-3.133360	-1.329097
N	-0.750524	-2.924331	-2.757205
C	-2.449358	-0.625194	-0.650069
H	-0.499043	1.520171	-2.202792
H	-1.729916	-4.814773	-2.442749
O	-4.221620	0.467782	0.596289
C	-3.423316	-0.645295	0.419905
C	-3.728446	-1.584860	1.387508
C	-5.037506	0.208577	1.665552
N	-0.372430	-0.512859	-2.580209
H	-5.242142	-1.475705	3.053362
H	-5.737329	0.989968	1.920339
C	-0.913098	0.548906	-1.946395
N	-1.891147	0.548632	-1.023162
H	-3.199468	-2.512267	1.561346
H	-7.680166	-6.906822	1.935416
H	-0.046224	-3.167551	-3.446336

MP2 (Gas phase, C_1), -6173.9 kcal mol^{-1}, n_{imag} = 0:



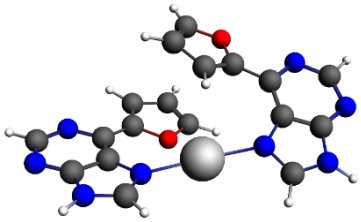
N	-7.194166	-6.240623	1.582143
C	-8.014734	-3.019433	0.323854
N	-9.265469	-2.860509	0.828803
C	-9.819656	-3.833826	1.563766
N	-9.281886	-5.027448	1.888452
C	-8.047739	-5.158296	1.412715
C	-7.324662	-4.215998	0.643487
N	-6.044366	-4.741996	0.386616
C	-6.017238	-5.943243	0.960947
C	-7.140459	-0.038194	-1.644983
H	-10.822514	-3.642584	1.935859
H	-5.172435	-6.615297	0.953153
O	-6.330692	-2.090047	-1.185450
C	-7.530098	-1.937216	-0.493779
C	-8.050726	-0.690093	-0.762481
C	-6.118670	-0.917901	-1.875519
C	-2.014126	-1.746810	-1.382978
H	-7.233302	0.954814	-2.061568
H	-5.220532	-0.881853	-2.473215
C	-4.830963	0.452059	1.772450
C	-1.776122	-3.760609	-2.208601
C	-0.916553	-1.711265	-2.275489
H	-8.978934	-0.307458	-0.364284
Ag	-4.334706	-3.791457	-0.479649
N	-2.537157	-3.053791	-1.375063
N	-0.789044	-3.003722	-2.767415
C	-2.323266	-0.524363	-0.734777
H	-0.040980	1.369891	-2.174709
H	-1.910583	-4.807701	-2.434241
O	-4.026872	-1.405138	0.781875
C	-3.343132	-0.309781	0.259416
C	-3.812584	0.841232	0.853891
C	-4.926833	-0.910467	1.698588
N	-0.172581	-0.655851	-2.590321
H	-5.414998	1.098766	2.411894
H	-5.535736	-1.646275	2.201595
C	-0.587842	0.457632	-1.952346
N	-1.589724	0.568390	-1.069951
H	-3.454015	1.837948	0.642859
H	-7.418900	-7.091586	2.086926
H	-0.085280	-3.312319	-3.429941

MP3 (Gas phase, C_1), -6168.1 kcal mol^{-1}, n_{imag} = 0:



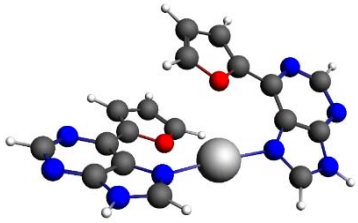
N	-7.489761	-5.980287	1.451206
C	-7.691667	-2.677161	0.160786
N	-8.792206	-2.206391	0.789778
C	-9.480315	-3.019861	1.610481
N	-9.226963	-4.313807	1.898867
C	-8.106303	-4.738810	1.321811
C	-7.265850	-3.987653	0.476991
N	-6.138318	-4.759316	0.155097
C	-6.317272	-5.937244	0.753188
C	-5.951878	-0.930867	-2.584706
H	-10.356507	-2.587934	2.086148
H	-5.625454	-6.765448	0.715613
O	-7.130563	-0.483392	-0.717224
C	-7.025251	-1.856130	-0.825858
C	-6.312207	-2.168630	-1.970654
C	-6.462898	0.056013	-1.783920
C	-2.206377	-1.669830	-1.193340
H	-5.407348	-0.791135	-3.507724
H	-6.433028	1.134227	-1.821148
C	-4.932840	-1.257570	2.390794
C	-1.578182	-3.580919	-2.047953
C	-1.173274	-1.391795	-2.109730
H	-6.164302	-3.160776	-2.375689
Ag	-4.306346	-3.881077	-0.516497
N	-2.454105	-3.051513	-1.193642
N	-0.777465	-2.628993	-2.610452
C	-2.766770	-0.563507	-0.514402
H	-1.110392	1.812607	-2.072171
H	-1.503014	-4.630216	-2.291490
O	-4.580710	0.329561	0.830729
C	-3.707294	-0.709157	0.574446
C	-3.890213	-1.701574	1.522188
C	-5.321050	-0.029294	1.925007
N	-0.718485	-0.186988	-2.443110
H	-5.326148	-1.769148	3.257698
H	-6.075606	0.678464	2.232569
C	-1.394755	0.796500	-1.813069
N	-2.363199	0.671730	-0.888277
H	-3.278047	-2.585223	1.642971
H	-7.847882	-6.763824	1.987727
H	-0.037083	-2.781931	-3.287588

MP1 (COSMO, C_1), -6232.1 kcal mol^{-1}, n_{imag} = 0:



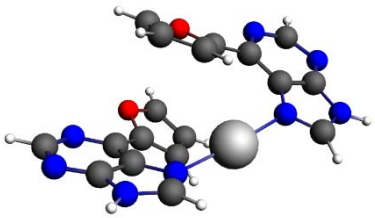
N	-7.269177	-6.276548	1.385203
C	-7.996861	-2.964953	0.344025
N	-9.225704	-2.775951	0.905346
C	-9.791172	-3.766916	1.609568
N	-9.296068	-4.999502	1.845095
C	-8.079516	-5.162307	1.316470
C	-7.351133	-4.199184	0.575065
N	-6.106908	-4.752147	0.236365
C	-6.106888	-5.986229	0.739422
C	-6.996738	0.040327	-1.534264
H	-10.769533	-3.556005	2.032009
H	-5.292578	-6.688419	0.661326
O	-6.350927	-2.094115	-1.225441
C	-7.484450	-1.875779	-0.448073
C	-7.907304	-0.575632	-0.624432
C	-6.074053	-0.912625	-1.872574
C	-2.009346	-1.738672	-1.346040
H	-7.020522	1.060000	-1.891103
H	-5.215085	-0.927547	-2.525730
C	-4.944766	-0.491346	1.884706
C	-1.638430	-3.788068	-1.996227
C	-0.897435	-1.713589	-2.220356
H	-8.762671	-0.122232	-0.145590
Ag	-4.332680	-3.828364	-0.534300
N	-2.461395	-3.060657	-1.238984
N	-0.682365	-3.025010	-2.592058
C	-2.410791	-0.502106	-0.797913
H	-0.272458	1.434401	-2.394123
H	-1.710278	-4.853648	-2.143636
O	-4.043770	0.881747	0.339226
C	-3.441639	-0.364439	0.203630
C	-3.965969	-1.223021	1.148803
C	-4.961678	0.771155	1.355844
N	-0.227731	-0.624309	-2.610302
H	-5.551059	-0.854657	2.702000
H	-5.533088	1.661304	1.569128
C	-0.746732	0.505688	-2.090238
N	-1.770328	0.620359	-1.227137
H	-3.646523	-2.239205	1.333166
H	-7.490636	-7.152557	1.845999
H	0.043966	-3.362348	-3.214584

MP2 (COSMO, C_1), -6232.0 kcal mol^{-1}, n_{imag} = 0:



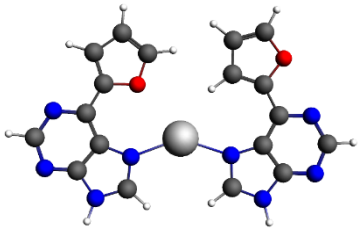
N	-7.212003	-6.273372	1.505268
C	-8.039703	-3.023189	0.350463
N	-9.292801	-2.872497	0.868366
C	-9.839570	-3.866747	1.582024
N	-9.300253	-5.069153	1.869351
C	-8.063231	-5.195824	1.380198
C	-7.352188	-4.225000	0.630013
N	-6.078556	-4.738956	0.339734
C	-6.045377	-5.956511	0.879724
C	-7.104667	-0.000488	-1.534775
H	-10.838881	-3.685886	1.967530
H	-5.203803	-6.629218	0.841479
O	-6.375721	-2.099172	-1.171316
C	-7.547374	-1.924202	-0.441968
C	-8.020615	-0.645788	-0.651411
C	-6.127800	-0.914531	-1.824229
C	-1.985773	-1.739677	-1.365807
H	-7.160031	1.012537	-1.906905
H	-5.241913	-0.896378	-2.440362
C	-4.882437	0.477498	1.679445
C	-1.733489	-3.775997	-2.113138
C	-0.887569	-1.735612	-2.262566
H	-8.912874	-0.225602	-0.211088
Ag	-4.322082	-3.809687	-0.469417
N	-2.499527	-3.044733	-1.304371
N	-0.753949	-3.036059	-2.700950
C	-2.306348	-0.503062	-0.763274
H	-0.036103	1.363358	-2.263713
H	-1.858844	-4.830301	-2.300439
O	-3.967613	-1.377024	0.789868
C	-3.337165	-0.276420	0.218560
C	-3.874678	0.876425	0.751505
C	-4.904418	-0.891129	1.671438
N	-0.152999	-0.675219	-2.610945
H	-5.513125	1.122003	2.274946
H	-5.479537	-1.635743	2.200095
C	-0.577018	0.455839	-2.011073
N	-1.579941	0.591160	-1.132032
H	-3.583364	1.883899	0.493267
H	-7.412270	-7.144431	1.984809
H	-0.057794	-3.381392	-3.352740

MP3 (COSMO, C_1), -6232.7 kcal mol^{-1}, n_{imag} = 0:



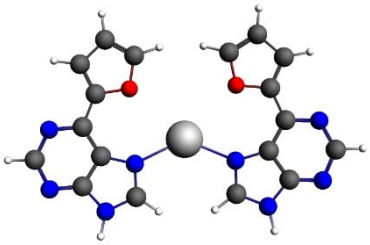
N	-7.261122	-5.862538	1.915165
C	-7.659971	-2.745391	0.273623
N	-8.772481	-2.253615	0.882734
C	-9.389747	-2.996249	1.818942
N	-9.055478	-4.229444	2.251149
C	-7.932074	-4.677678	1.680903
C	-7.164471	-3.988694	0.715730
N	-6.027674	-4.750605	0.419618
C	-6.129948	-5.857364	1.156368
C	-6.027002	-1.185850	-2.644490
H	-10.273460	-2.555486	2.270922
H	-5.409798	-6.659515	1.175829
O	-7.270530	-0.625644	-0.848268
C	-7.060355	-1.997783	-0.807233
C	-6.310226	-2.373822	-1.904068
C	-6.620432	-0.156727	-1.964816
C	-2.260818	-1.657320	-1.327496
H	-5.462097	-1.108678	-3.562464
H	-6.669952	0.909556	-2.121412
C	-4.957711	-1.032722	2.252281
C	-1.596641	-3.606661	-2.045236
C	-1.272374	-1.429977	-2.311027
H	-6.055728	-3.386210	-2.183545
Ag	-4.208874	-3.968626	-0.398658
N	-2.452795	-3.037896	-1.195866
N	-0.859745	-2.682584	-2.722284
C	-2.827074	-0.520466	-0.716355
H	-1.286571	1.779073	-2.504536
H	-1.494544	-4.667783	-2.206127
O	-4.600910	0.473216	0.612013
C	-3.739298	-0.595724	0.401062
C	-3.926158	-1.531065	1.399563
C	-5.337827	0.175228	1.733101
N	-0.868273	-0.233713	-2.751467
H	-5.359200	-1.507296	3.136196
H	-6.079797	0.906330	2.013883
C	-1.537649	0.778970	-2.163639
N	-2.465280	0.701740	-1.192851
H	-3.344566	-2.430105	1.545704
H	-7.544305	-6.599385	2.552472
H	-0.153226	-2.885086	-3.421568

MP1 (COSMO, *Cs* symm.), -6223.6 kcal mol^{-1}, n_{imag} = 2 (-90 cm^{-1}, -41 cm^{-1}):



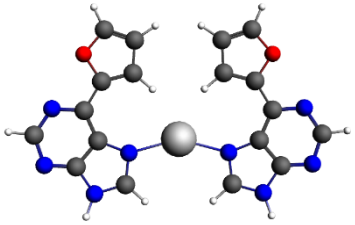
N	3.350676	3.319853	0.000000
C	4.045040	-0.157999	0.000000
N	5.407694	-0.145822	0.000000
C	6.065795	1.022238	0.000000
N	5.537983	2.260547	0.000000
C	4.201818	2.236435	0.000000
C	3.371505	1.085717	0.000000
N	2.031430	1.508375	0.000000
C	2.079514	2.843505	0.000000
C	2.132340	-3.318018	0.000000
H	7.150542	0.961358	0.000000
H	1.222826	3.497166	0.000000
O	4.251185	-2.559763	0.000000
C	3.406259	-1.452322	0.000000
C	2.099029	-1.890899	0.000000
C	3.453503	-3.673466	0.000000
N	-5.681062	2.069110	0.000000
H	1.302233	-4.008577	0.000000
H	3.967754	-4.622267	0.000000
C	-2.270108	2.913981	0.000000
C	-4.347613	2.156022	0.000000
C	-3.432989	1.072203	0.000000
H	1.225466	-1.253352	0.000000
C	-2.521146	-3.589237	0.000000
N	-2.129897	1.588401	0.000000
N	-3.576074	3.298330	0.000000
C	-3.998232	-0.218951	0.000000
H	-7.182718	0.642157	0.000000
H	-1.461231	3.626516	0.000000
O	-1.876321	-1.427726	0.000000
C	-3.269593	-1.460906	0.000000
C	-3.691532	-2.773217	0.000000
C	-1.452965	-2.736149	0.000000
H	-4.720407	-3.101576	0.000000
H	-2.476542	-4.669020	0.000000
H	-0.389260	-2.879326	0.000000
C	-6.106356	0.789270	0.000000
N	-5.358118	-0.322881	0.000000
H	3.622156	4.297180	0.000000
H	-3.916200	4.253855	0.000000
Ag	-0.066379	0.819256	0.000000

MP2 (COSMO, *Cs* symm.), -6221.2 kcal mol^{-1}, n_{imag} = 2 (-39 cm^{-1}, -43 cm^{-1}):



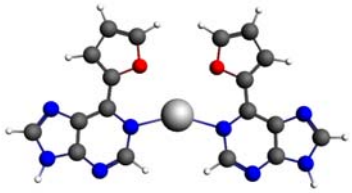
N	3.469189	3.105064	0.000000
C	4.097441	-0.380659	0.000000
N	5.462008	-0.401192	0.000000
C	6.142635	0.752597	0.000000
N	5.641189	2.004413	0.000000
C	4.304931	2.009864	0.000000
C	3.453862	0.873877	0.000000
N	2.121300	1.313226	0.000000
C	2.188080	2.644291	0.000000
C	2.877322	-3.849664	0.000000
H	7.225928	0.670343	0.000000
H	1.343118	3.312736	0.000000
O	2.064362	-1.743050	0.000000
C	3.455852	-1.669757	0.000000
C	3.979595	-2.945372	0.000000
C	1.746551	-3.081229	0.000000
N	-5.343008	2.694068	0.000000
H	2.914895	-4.929683	0.000000
H	0.698667	-3.316822	0.000000
C	-1.836753	2.889660	0.000000
C	-4.016884	2.529705	0.000000
C	-3.317174	1.294665	0.000000
H	5.031087	-3.191320	0.000000
C	-3.340204	-3.462692	0.000000
N	-1.939561	1.561031	0.000000
N	-3.048715	3.509818	0.000000
C	-4.115140	0.132182	0.000000
H	-7.084562	1.572428	0.000000
H	-0.913006	3.443851	0.000000
O	-2.270076	-1.474401	0.000000
C	-3.641316	-1.227502	0.000000
C	-4.320715	-2.427519	0.000000
C	-2.122135	-2.841703	0.000000
H	-5.394732	-2.539818	0.000000
H	-3.512712	-4.529511	0.000000
H	-1.111591	-3.205462	0.000000
C	-5.999569	1.516151	0.000000
N	-5.471261	0.285107	0.000000
H	3.753141	4.078744	0.000000
H	-3.206697	4.511642	0.000000
Ag	0.034663	0.511900	0.000000

MP3 (COSMO, *Cs* symm.), -6224.5 kcal mol^{-1}, n_{imag} = 3 (-23 cm^{-1}, -58 cm^{-1}, -95 cm^{-1}):



N	-3.288837	-3.562698	0.000000
C	-4.003057	-0.087731	0.000000
N	-5.365557	-0.108176	0.000000
C	-6.016847	-1.280069	0.000000
N	-5.482059	-2.515345	0.000000
C	-4.146094	-2.483642	0.000000
C	-3.323125	-1.328286	0.000000
N	-1.981445	-1.745303	0.000000
C	-2.020644	-3.081261	0.000000
C	-2.105159	3.080520	0.000000
H	-7.101926	-1.225576	0.000000
H	-1.159211	-3.728981	0.000000
O	-4.220912	2.313706	0.000000
C	-3.371078	1.209620	0.000000
C	-2.066320	1.655641	0.000000
C	-3.427686	3.431340	0.000000
N	5.798206	-1.649232	0.000000
H	-1.273765	3.765785	0.000000
H	-3.947180	4.377381	0.000000
C	2.463103	-2.733918	0.000000
C	4.472999	-1.820358	0.000000
C	3.484127	-0.803331	0.000000
H	-1.186753	1.029438	0.000000
C	1.615473	3.373299	0.000000
N	2.221404	-1.419440	0.000000
N	3.789716	-3.017070	0.000000
C	3.968242	0.526002	0.000000
H	7.204146	-0.129314	0.000000
H	1.710281	-3.505213	0.000000
O	3.822283	2.932504	0.000000
C	3.147686	1.713310	0.000000
C	1.790669	1.958508	0.000000
C	2.870420	3.918384	0.000000
H	1.015030	1.207450	0.000000
H	0.691367	3.927456	0.000000
H	3.241899	4.931741	0.000000
C	6.139800	-0.347350	0.000000
N	5.318195	0.712095	0.000000
H	-3.555295	-4.541436	0.000000
H	4.202269	-3.943733	0.000000
Ag	0.075638	-1.006715	0.000000

Base pair in Watson-Crick like geometry (Gas phase, *C*s symm.), -6173.1 kcal mol^{-1}, n_{imag} = 0:



N	5.654813	-2.965958	0.000000
C	3.178011	-0.437267	0.000000
N	2.032486	-1.189882	0.000000
C	2.122822	-2.552404	0.000000
N	3.227893	-3.290347	0.000000
C	4.342552	-2.548846	0.000000
C	4.404185	-1.136154	0.000000
N	5.725241	-0.707668	0.000000
C	6.435495	-1.819764	0.000000
C	3.487539	3.220986	0.000000
H	1.178710	-3.086959	0.000000
H	7.516000	-1.870341	0.000000
O	1.887116	1.627996	0.000000
C	3.127889	0.996244	0.000000
C	4.127235	1.948644	0.000000
C	2.141786	2.978905	0.000000
C	-4.658407	-1.911364	0.000000
H	3.963689	4.191334	0.000000
H	1.277582	3.621189	0.000000
C	-2.998723	3.680346	0.000000
C	-6.627733	-0.894586	0.000000
C	-4.520379	-0.504075	0.000000
H	5.185464	1.732142	0.000000
H	-6.467370	-3.047983	0.000000
N	-5.767832	0.106331	0.000000
N	-6.016375	-2.139367	0.000000
C	-3.207975	0.014995	0.000000
H	-1.601950	-2.889944	0.000000
H	-7.704584	-0.792339	0.000000
O	-1.638962	1.877564	0.000000
C	-2.956364	1.427113	0.000000
C	-3.811455	2.510914	0.000000
C	-1.700531	3.250869	0.000000
C	-2.461328	-2.227691	0.000000
H	-3.333384	4.708131	0.000000
H	-0.754357	3.764735	0.000000
N	-3.659364	-2.802518	0.000000
N	-2.179868	-0.891492	0.000000
H	-4.889656	2.445881	0.000000
H	5.973244	-3.929067	0.000000
Ag	-0.033157	-0.468304	0.000000