Electronic Supplementary Information

Chimeric GNA/DNA metal-mediated base pairs

Kristof Seubert,[a] Célia Fonseca Guerra,[b] F. Matthias Bickelhaupt*[b] and Jens Müller*[a]

a) University of Muenster, Institute for Inorganic and Analytical Chemistry, Corrensstr. 28/30, 48149 Muenster, Germany. Fax: 49 251 8336007; Tel: 49 251 8336006; E-mail: mueller.j@uni-muenster.de

b) Department of Theoretical Chemistry and Amsterdam Center for Multiscale Modeling (ACMM), Scheikundig Laboratorium der Vrije Universiteit, De Boelelaan 1083, 1081 HV Amsterdam, The Netherlands. Fax: 31 20 5987629; Tel: 31 20 5987617; E-mail: f.m.bickelhaupt@vu.nl.

Mass spectrometric characterization of the oligonucleotides **I** and **II**:
The desalted oligonucleotides were characterized by MALDI-TOF mass spectrometry.
d(GAGGGAAGAXAAG): calcd for $[M+H]^+$: 4128 Da; found: 4130 Da;
d(CTTYTCTTCCCTC); Y = im: calcd for $[M+H]^+$: 3745 Da; found: 3747 Da;
d(CTTYTCTTCCCTC); Y = tri: calcd for $[M+H]^+$: 3746 Da; found: 3747 Da;
d(CTTYTCTTCCCTC); Y = tet: calcd for $[M+H]^+$: 3747 Da; found: 3748 Da;
d(GAGGGAXAGAAAG): calcd for $[M+H]^+$: 4128 Da; found: 4130 Da;
d(CTTTCTYTCCCTC); Y = im: calcd for $[M+H]^+$: 3745 Da; found: 3747 Da;
d(CTTTCTYTCCCTC); Y = tri: calcd for $[M+H]^+$: 3746 Da; found: 3748 Da;
d(CTTTCTYTCCCTC); Y = tet: calcd for $[M+H]^+$: 3747 Da; found: 3748 Da.

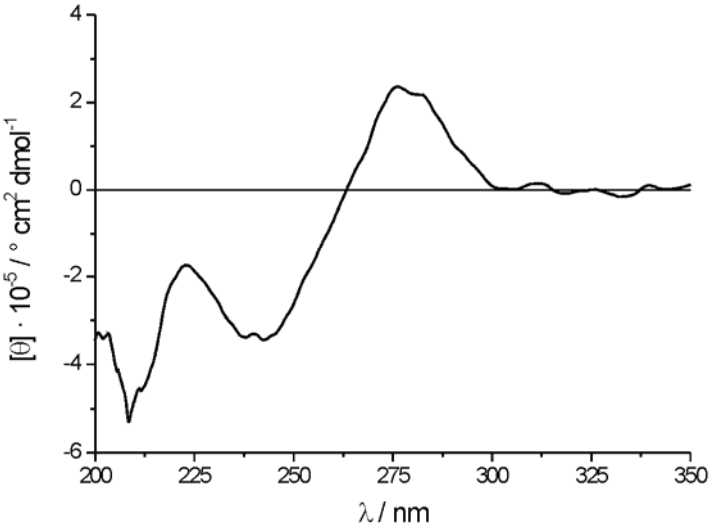

Figure S1: CD spectrum of 5'-d(GAG GGA AGA AAG)-3' · 3'-d(CTC CCT TCT TTC)-5', i.e. a dodecamer duplex analogous to **I** and **II** but lacking the artificial XY base pair (conditions: 0.5 µM oligonucleotide duplex, 150 mM $NaClO_4$, 5 mM MOPS (pH 6.8)). Except for the region below 225 nm, which is significantly influenced by the backbone of the nucleic acid, the CD spectrum of this GNA-free duplex closely resembles that of the GNA-containing **I** and **II**.

Table S1: Computed base pairing energies (kcal mol^{-1}) of various dipic–M^{2+}–azole base pairs.[a]

Y	Zn^{2+}			Hg^{2+}		
	gas phase	microsolvation[b]	COSMO	gas phase	microsolvation[b]	COSMO
im	–415	–301	–72	–367	–267	–80
tri	–403	–290	–67	–356	–256	–77
tet	–402	–289	–53	–357	–256	–73

[a] All geometries optimized without any constraint. [b] gas phase with one water molecule: dipic + azole + $[M(OH_2)]^{2+}$ → dipic–M^{2+}–azole + H_2O.

These base pairing energies indicate that under all conditions investigated, the formation of the metal complexes $[M(dipic)(azole)]^{2+}$ (M = Zn, Hg) from the metal ions and the respective ligands is thermodynamically favoured. The fact that the melting temperatures of oligonucleotide duplexes **I** and **II** in the presence of M^{2+} are – within error limits – identical to those in the absence of the transition metal ions (see Table 1) indicates that these metal ions do not form regular metal-mediated base pairs. This could have various reasons, including the increased charge compared with the stabilizing Ag^{+} ions, some extra stabilization of the Zn(II) and Hg(II) complexes that significantly distorts the duplex, and, particularly in the case of Zn^{2+} (see Table S2 for xyz coordinates), the preference for a tetrahedral coordination environment.

Table S2: Cartesian coordinates (in a.u.) and ADF total energies for each stationary point.

$[Ag(dipic)(im)]^{+}$ (gas phase), -5171.47 kcal mol^{-1}

C	-1.110480	2.231449	-0.359983
C	-1.947743	3.183892	-0.953946
C	-3.323468	3.089886	-0.733055
C	-3.803902	2.044305	0.063380
C	-2.891213	1.135502	0.612426
N	-1.560353	1.228061	0.411858
C	-3.364271	-0.050359	1.425511
N	-3.190814	-1.297095	0.633364
C	-3.649665	-2.509241	1.342520
C	-3.272547	-3.765802	0.574909
N	-2.058743	-3.781050	-0.020875
C	-1.673870	-4.893029	-0.680752
C	-2.475466	-6.031734	-0.775038
C	-3.732376	-6.015814	-0.163322
C	-4.135393	-4.864335	0.518112
Ag	-0.869485	-1.780667	-0.019199
N	1.095608	-0.876533	-0.167313
C	1.482575	0.254277	0.541156
C	2.803795	0.518802	0.285175
N	3.220653	-0.468878	-0.593193
C	2.166378	-1.291979	-0.840114
H	-0.032145	2.273330	-0.509392
H	-1.527132	3.976675	-1.567965
H	-4.009165	3.811146	-1.171704
H	-4.868566	1.932904	0.260103
H	-4.414479	0.092880	1.725463
H	-2.753261	-0.156141	2.329634
H	-3.704567	-1.205782	-0.246148
H	-4.734372	-2.505987	1.532744
H	-3.142486	-2.519250	2.317806
H	-0.690704	-4.859992	-1.143002
H	-2.120312	-6.903704	-1.317880
H	-4.388886	-6.880800	-0.220195
H	-5.108270	-4.808326	1.001526
H	0.770244	0.781294	1.158049
H	3.469306	1.293407	0.637074
H	4.149608	-0.564096	-0.987079
H	2.217252	-2.150379	-1.493947

$[Ag(dipic)(im)]^{+}$ (COSMO), -5207.38 kcal mol^{-1}

C	-0.767079	2.381351	0.717766
C	-0.880848	2.877794	-0.582706
C	-1.959082	2.453184	-1.365099
C	-2.867046	1.546273	-0.816380
C	-2.664375	1.080717	0.492306
N	-1.631741	1.497209	1.256311
C	-3.571065	0.019391	1.083376
N	-3.301821	-1.289454	0.424350
C	-3.908717	-2.443158	1.117177
C	-3.419383	-3.763047	0.541497
N	-2.112052	-3.859273	0.196376
C	-1.645324	-5.040510	-0.271191
C	-2.452993	-6.166819	-0.414139
C	-3.802471	-6.069731	-0.064607
C	-4.287701	-4.852458	0.416037
Ag	-0.874484	-1.973099	0.071285
N	0.777350	-0.641724	-0.275649
C	1.702530	-0.172838	0.652516
C	2.481104	0.793075	0.063945
N	2.018598	0.907869	-1.234228
C	0.994313	0.035994	-1.405338
H	0.056727	2.694842	1.355647
H	-0.144415	3.578022	-0.967676
H	-2.089786	2.820700	-2.379931
H	-3.720425	1.196444	-1.393930
H	-4.628681	0.310544	0.985115
H	-3.342291	-0.086114	2.146948
H	-3.659534	-1.256240	-0.533029
H	-5.007939	-2.425516	1.099664
H	-3.599038	-2.393929	2.169536
H	-0.592731	-5.069815	-0.534825
H	-2.029447	-7.091291	-0.795485
H	-4.466330	-6.923717	-0.169405
H	-5.332518	-4.737410	0.692143
H	1.738220	-0.555012	1.661428
H	3.296967	1.391109	0.438996
H	2.380513	1.533518	-1.944238
H	0.446962	-0.072697	-2.328462

$[Ag(dipic)(tri)]^{+}$ (gas phase), -5058.85 kcal mol^{-1}

C	-1.076814	2.234812	-0.359959
C	-1.924582	3.181878	-0.947110
C	-3.297811	3.078558	-0.715989
C	-3.764638	2.030934	0.085642
C	-2.842406	1.127412	0.627350
N	-1.513512	1.226003	0.413661
C	-3.305735	-0.056218	1.448605
N	-3.163335	-1.303821	0.649731
C	-3.638789	-2.509337	1.361765
C	-3.300361	-3.770144	0.583702
N	-2.092818	-3.812299	-0.024824
C	-1.743555	-4.929518	-0.696352
C	-2.575511	-6.046244	-0.789891
C	-3.825163	-6.002495	-0.164938
C	-4.191293	-4.845892	0.528526
Ag	-0.870155	-1.836456	-0.026831
N	1.097635	-0.922465	-0.186583
C	1.481707	0.224057	0.475252
N	2.733345	0.582685	0.240814
N	3.165360	-0.393599	-0.615913
C	2.189243	-1.287331	-0.863958
H	0.000134	2.292102	-0.515259
H	-1.512978	3.978690	-1.561795
H	-3.991635	3.795647	-1.148591
H	-4.826648	1.914679	0.293494
H	-4.347863	0.094758	1.771357
H	-2.676309	-0.169506	2.338888
H	-3.688907	-1.199689	-0.221549
H	-4.720362	-2.481684	1.565862
H	-3.119240	-2.533948	2.330160
H	-0.764953	-4.919351	-1.169008
H	-2.248720	-6.923075	-1.342559
H	-4.504397	-6.849818	-0.220876
H	-5.157342	-4.768363	1.022480
H	0.800053	0.774122	1.107957
H	4.115355	-0.371504	-0.971968
H	2.294298	-2.148087	-1.509637

$[Ag(dipic)(tri)]^{+}$ (COSMO), -5098.45 kcal mol^{-1}

C	-0.713696	2.324754	0.789689
C	-0.786074	2.786808	-0.526512
C	-1.847846	2.351553	-1.326655
C	-2.781682	1.470866	-0.777988
C	-2.618560	1.036224	0.547360
N	-1.600944	1.460897	1.327653
C	-3.547446	-0.007687	1.137894
N	-3.310871	-1.316547	0.462717
C	-3.912320	-2.475936	1.154200
C	-3.431378	-3.790686	0.556419
N	-2.133652	-3.874636	0.173778
C	-1.672434	-5.047219	-0.320439
C	-2.476475	-6.177842	-0.453470
C	-3.816118	-6.094040	-0.063066
C	-4.296082	-4.884973	0.445083
AG	-0.924519	-1.949346	0.048911
N	0.767143	-0.654460	-0.329935
C	1.659860	-0.116161	0.565695
N	2.490147	0.766885	0.023103
N	2.092151	0.784752	-1.289070
C	1.069952	-0.057148	-1.491501
H	0.092943	2.650467	1.442794
H	-0.032838	3.469476	-0.909578
H	-1.946301	2.691082	-2.354332
H	-3.622303	1.114983	-1.370017
H	-4.598498	0.306206	1.048599
H	-3.313595	-0.127405	2.198312
H	-3.689150	-1.270717	-0.485885
H	-5.010718	-2.454122	1.149655
H	-3.589058	-2.437414	2.202433
H	-0.627934	-5.066240	-0.614715
H	-2.058622	-7.094785	-0.857809
H	-4.476768	-6.951253	-0.158029
H	-5.333036	-4.781048	0.752334
H	1.686162	-0.382617	1.611456
H	2.563837	1.372681	-1.967065
H	0.589203	-0.215847	-2.444120

$[Ag(dipic)(tet)]^{+}$ (gas phase), -4933.65 kcal mol^{-1}

C	-1.142822	1.897983	0.061034
C	-1.664751	3.172199	-0.176429
C	-3.046895	3.356132	-0.090080
C	-3.853644	2.260648	0.234686
C	-3.258696	1.017668	0.467095
N	-1.920085	0.842753	0.379255
C	-4.096343	-0.185083	0.889239
N	-3.717270	-1.405688	0.156306
C	-4.048704	-2.684273	0.807469
C	-3.162002	-3.823262	0.314373
N	-1.831236	-3.589702	0.242860
C	-1.013526	-4.592339	-0.136444
C	-1.481686	-5.869326	-0.455064
C	-2.855834	-6.112801	-0.386176
C	-3.705751	-5.072620	0.002838
Ag	-1.143710	-1.355646	0.164633
N	1.083260	-1.212669	-0.508463
N	1.770677	-0.024239	-0.505481
C	3.037521	-0.359179	-0.680718
N	3.118053	-1.705907	-0.783891
N	1.874329	-2.237513	-0.672055
H	-0.076620	1.697041	-0.009707
H	-0.999267	3.993804	-0.428604
H	-3.491046	4.330964	-0.277515
H	-4.934504	2.361147	0.308432
H	-5.163715	0.068054	0.794470
H	-3.897034	-0.378292	1.952370
H	-4.064019	-1.380739	-0.802123
H	-5.104582	-2.974321	0.691569
H	-3.860155	-2.552359	1.881879
H	0.045403	-4.349015	-0.187183
H	-0.783307	-6.646560	-0.754331
H	-3.260449	-7.090913	-0.635619
H	-4.781810	-5.220482	0.066165
H	3.881621	0.315135	-0.735514
H	3.924131	-2.309234	-0.924637

$[Ag(dipic)(tet)]^{+}$ (COSMO), -4974.63 kcal mol^{-1}

C	-0.775854	2.261729	0.731661
C	-0.871489	2.765754	-0.567617
C	-1.955153	2.367940	-1.357711
C	-2.887124	1.479997	-0.816936
C	-2.699640	1.001638	0.489674
N	-1.660163	1.390075	1.260711
C	-3.617176	-0.060123	1.063790
N	-3.327132	-1.368088	0.400585
C	-3.923989	-2.538421	1.083726
C	-3.396326	-3.847069	0.512824
N	-2.088608	-3.899497	0.162770
C	-1.580952	-5.064027	-0.301925
C	-2.348452	-6.219863	-0.435586
C	-3.699475	-6.168601	-0.079803
C	-4.227368	-4.966616	0.397080
AG	-0.970555	-1.901516	0.041277
N	0.768265	-0.656186	-0.327069
N	1.609900	-0.201458	0.656417
C	2.424877	0.644110	0.040663
N	2.085033	0.700288	-1.259975
N	1.041382	-0.121583	-1.492707
H	0.047367	2.558716	1.377922
H	-0.120244	3.454111	-0.944725
H	-2.071450	2.741175	-2.371600
H	-3.743690	1.149992	-1.400904
H	-4.672892	0.221030	0.940886
H	-3.409053	-0.171070	2.130256
H	-3.687451	-1.333493	-0.556035
H	-5.021110	-2.536077	1.042334
H	-3.634638	-2.483092	2.140708
H	-0.529377	-5.055578	-0.570977
H	-1.894829	-7.130708	-0.814183
H	-4.332352	-7.046203	-0.177232
H	-5.274270	-4.888566	0.676974
H	3.231666	1.201967	0.489592
H	2.508651	1.226652	-2.018544

$[Hg(dipic)(im)]^{2+}$ (gas phase), -4901.70 kcal mol^{-1}

C	-1.088438	1.844689	-0.063326
C	-1.552766	3.154436	-0.145028
C	-2.925938	3.385352	-0.015725
C	-3.783993	2.301934	0.197047
C	-3.253190	1.012564	0.282226
N	-1.925016	0.805053	0.151213
C	-4.143683	-0.185822	0.617459
N	-3.717011	-1.439640	-0.055240
C	-4.141226	-2.703126	0.594240
C	-3.209323	-3.882738	0.303250
N	-1.885568	-3.646939	0.172473
C	-1.018132	-4.674745	0.013014
C	-1.448690	-5.996821	-0.018709
C	-2.817380	-6.257510	0.105389
C	-3.703815	-5.189066	0.266293
Hg	-1.200743	-1.435123	-0.061081
N	1.007668	-1.148865	-0.475090
C	1.940858	-0.737112	0.475787
C	3.170142	-0.663810	-0.124969
N	2.972011	-1.033741	-1.444433
C	1.662917	-1.321172	-1.630370
H	-0.035687	1.599744	-0.170925
H	-0.854343	3.968764	-0.313227
H	-3.325265	4.393645	-0.084856
H	-4.855634	2.454018	0.299612
H	-5.186561	0.060883	0.387618
H	-4.079915	-0.358571	1.698963
H	-4.007913	-1.430300	-1.035325
H	-5.166002	-2.976560	0.318135
H	-4.131637	-2.535011	1.678341
H	0.030132	-4.409975	-0.086614
H	-0.727058	-6.798606	-0.143586
H	-3.190306	-7.277756	0.074583
H	-4.772057	-5.364096	0.367948
H	4.141503	-0.391432	0.261002
H	3.691655	-1.083348	-2.160282
H	1.665987	-0.533611	1.499683
H	1.233923	-1.633937	-2.570468

$[Hg(dipic)(im)]^{2+}$ (COSMO), -5057.99 kcal mol^{-1}

C	-0.945685	1.991147	0.107445
C	-1.457355	3.284187	0.010247
C	-2.837920	3.464719	0.148226
C	-3.652598	2.353684	0.384271
C	-3.065460	1.088184	0.481587
N	-1.736463	0.926414	0.341312
C	-3.892550	-0.144608	0.829604
N	-3.421035	-1.369235	0.136494
C	-3.893808	-2.638079	0.740914
C	-3.061235	-3.838653	0.307152
N	-1.735554	-3.657110	0.152282
C	-0.938969	-4.696793	-0.169543
C	-1.443678	-5.983758	-0.340530
C	-2.819500	-6.185978	-0.186085
C	-3.637856	-5.100819	0.137951
Hg	-0.998165	-1.392358	0.057045
N	1.139278	-1.077532	-0.373041
C	1.662488	-0.276203	-1.384127
C	3.030541	-0.318185	-1.301648
N	3.323741	-1.151459	-0.235981
C	2.169006	-1.594545	0.305857
H	0.115474	1.785707	-0.000669
H	-0.791168	4.120929	-0.175280
H	-3.275273	4.455663	0.067125
H	-4.728373	2.460415	0.492975
H	-4.949333	0.048085	0.618303
H	-3.793775	-0.325088	1.905831
H	-3.696588	-1.333721	-0.847092
H	-4.949331	-2.820457	0.515030
H	-3.796028	-2.534656	1.826962
H	0.116622	-4.474244	-0.291015
H	-0.775080	-6.799550	-0.596405
H	-3.250610	-7.173314	-0.323869
H	-4.710469	-5.222959	0.258954
H	3.799895	0.157422	-1.888829
H	4.252354	-1.394163	0.090549
H	2.101516	-2.257659	1.152853
H	1.025318	0.254991	-2.072980

$[Hg(dipic)(tri)]^{2+}$ (gas phase), -4783.38 kcal mol^{-1}

C	-0.960301	1.936255	-0.029418
C	-1.434270	3.243032	-0.076518
C	-2.809015	3.460719	0.061472
C	-3.658244	2.366481	0.249733
C	-3.122046	1.077382	0.301129
N	-1.791426	0.884110	0.158695
C	-4.014109	-0.126959	0.619204
N	-3.575106	-1.380534	-0.040423
C	-3.941923	-2.647051	0.638321
C	-2.982502	-3.803118	0.337703
N	-1.665062	-3.536307	0.191600
C	-0.775182	-4.541944	0.018576
C	-1.173747	-5.874215	-0.008815
C	-2.533842	-6.167978	0.133288
C	-3.444222	-5.121347	0.305792
Hg	-1.052351	-1.308387	-0.046663
N	1.213127	-1.248085	-0.516065
C	2.240117	-1.213123	0.412022
N	3.435858	-1.183536	-0.143632
N	3.155441	-1.200456	-1.482076
C	1.835262	-1.238832	-1.708358
H	0.094330	1.703583	-0.141375
H	-0.741013	4.065730	-0.224178
H	-3.215671	4.467622	0.019449
H	-4.730392	2.508703	0.361205
H	-5.052501	0.120111	0.370697
H	-3.970768	-0.292861	1.702854
H	-3.882002	-1.396723	-1.015143
H	-4.964484	-2.956719	0.394320
H	-3.908251	-2.462628	1.719318
H	0.264452	-4.251098	-0.097534
H	-0.434622	-6.658090	-0.144698
H	-2.882315	-7.196975	0.106500
H	-4.506525	-5.322884	0.420030
H	2.085482	-1.210151	1.481943
H	3.918270	-1.183732	-2.155819
H	1.370477	-1.258443	-2.683906

$[Hg(dipic)(tri)]^{2+}$ (COSMO), -4947.85 kcal mol^{-1}

C	-0.976866	1.915675	-0.521603
C	-1.522958	3.193802	-0.637539
C	-2.807033	3.416159	-0.130048
C	-3.496875	2.358532	0.470633
C	-2.881901	1.106070	0.555159
N	-1.641811	0.904736	0.067156
C	-3.566632	-0.078022	1.230219
N	-3.337191	-1.331648	0.476192
C	-3.687459	-2.582679	1.176675
C	-3.045642	-3.797330	0.512956
N	-1.830239	-3.643382	-0.049854
C	-1.194494	-4.697714	-0.604292
C	-1.758918	-5.970076	-0.614169
C	-3.021097	-6.145524	-0.036276
C	-3.671747	-5.047013	0.529585
Hg	-0.959254	-1.473404	-0.086745
N	1.194616	-0.956543	-0.305697
C	1.896780	-0.060457	0.463959
N	3.178313	0.002182	0.137716
N	3.279426	-0.905498	-0.886816
C	2.100671	-1.474719	-1.148923
H	0.010936	1.680910	-0.907333
H	-0.958006	3.985688	-1.119284
H	-3.269848	4.395571	-0.209829
H	-4.499980	2.495768	0.864836
H	-4.634798	0.132288	1.349777
H	-3.135313	-0.214866	2.228254
H	-3.818476	-1.288776	-0.424571
H	-4.771191	-2.729763	1.236836
H	-3.302152	-2.506274	2.199642
H	-0.222315	-4.497617	-1.041410
H	-1.222704	-6.796912	-1.068641
H	-3.494750	-7.122881	-0.032321
H	-4.654677	-5.147443	0.980863
H	1.444604	0.530264	1.245791
H	4.170415	-1.070091	-1.343506
H	1.921268	-2.218217	-1.908839

$[Hg(dipic)(tet)]^{2+}$ (gas phase), -4660.03 kcal mol^{-1}

C	-1.102951	1.868892	0.096466
C	-1.560999	3.182080	0.083984
C	-2.931987	3.418213	0.219482
C	-3.800281	2.332756	0.370349
C	-3.289626	1.033449	0.388550
N	-1.956887	0.826072	0.249715
C	-4.213270	-0.161256	0.663461
N	-3.816863	-1.394908	-0.053855
C	-4.155443	-2.690675	0.577251
C	-3.173804	-3.819108	0.231341
N	-1.853198	-3.538474	0.110408
C	-0.951017	-4.527301	-0.105399
C	-1.342409	-5.858071	-0.202543
C	-2.700672	-6.168556	-0.086460
C	-3.620494	-5.138399	0.129722
Hg	-1.291568	-1.334586	0.028228
N	1.056517	-1.240749	-0.509221
N	1.732100	-0.056329	-0.571714
C	2.982641	-0.399213	-0.841920
N	3.045915	-1.748818	-0.934751
N	1.825065	-2.277375	-0.722571
H	-0.054158	1.619336	-0.021379
H	-0.853632	3.996933	-0.037870
H	-3.322616	4.432209	0.203338
H	-4.870724	2.489402	0.477947
H	-5.245147	0.130613	0.438257
H	-4.164289	-0.374004	1.738818
H	-4.130051	-1.368849	-1.025604
H	-5.170959	-3.016723	0.325936
H	-4.121414	-2.548322	1.664738
H	0.085606	-4.222881	-0.201992
H	-0.596310	-6.628408	-0.373085
H	-3.041320	-7.197336	-0.167662
H	-4.682060	-5.353430	0.223727
H	3.821586	0.272051	-0.969593
H	3.840248	-2.356874	-1.131459

$[Hg(dipic)(tet)]^{2+}$ (COSMO), -4822.22 kcal mol^{-1}

C	-1.147556	1.928661	-0.013523
C	-1.641100	3.228930	-0.073851
C	-3.016998	3.429416	0.078946
C	-3.848025	2.327191	0.292270
C	-3.289654	1.046983	0.353867
N	-1.960977	0.871083	0.198518
C	-4.156906	-0.169617	0.678055
N	-3.705215	-1.396652	-0.005530
C	-4.087355	-2.676486	0.621234
C	-3.155870	-3.827154	0.239806
N	-1.839557	-3.570997	0.089990
C	-0.971158	-4.570113	-0.178066
C	-1.392484	-5.891117	-0.301495
C	-2.754228	-6.174516	-0.152960
C	-3.643190	-5.131737	0.117624
Hg	-1.223714	-1.329541	0.012444
N	1.062356	-1.214449	-0.398488
N	1.808076	-0.081642	-0.251427
C	3.031584	-0.441103	-0.618629
N	3.009747	-1.740674	-0.969502
N	1.765815	-2.228738	-0.831453
H	-0.093350	1.704101	-0.133193
H	-0.961462	4.057777	-0.244205
H	-3.438120	4.429209	0.026297
H	-4.920934	2.449138	0.411374
H	-5.202484	0.065458	0.453001
H	-4.081302	-0.349168	1.756402
H	-3.976993	-1.381547	-0.988878
H	-5.119305	-2.958006	0.386783
H	-4.018757	-2.542835	1.706510
H	0.068207	-4.283300	-0.295608
H	-0.669786	-6.671543	-0.517160
H	-3.120196	-7.192141	-0.253501
H	-4.707025	-5.318213	0.234413
H	3.907928	0.187321	-0.641459
H	3.764409	-2.336001	-1.300477

$[Zn(dipic)(im)]^{2+}$ (gas phase), -4966.04 kcal mol^{-1}

C	-1.016510	1.272777	1.353300
C	-1.574962	2.453832	1.829338
C	-2.929499	2.703155	1.581794
C	-3.681768	1.760251	0.873876
C	-3.065722	0.589193	0.433989
N	-1.747780	0.358068	0.670337
C	-3.843366	-0.524749	-0.255888
N	-2.978860	-1.326095	-1.194181
C	-3.377148	-2.764951	-1.307961
C	-2.833677	-3.582556	-0.139014
N	-1.693103	-3.135099	0.450424
C	-1.138326	-3.847998	1.462965
C	-1.695317	-5.037124	1.919498
C	-2.870571	-5.502132	1.318772
C	-3.446955	-4.762658	0.281401
Zn	-1.062138	-1.323201	-0.236657
N	0.735710	-1.165821	-1.011435
C	1.360189	0.032791	-1.364881
C	2.595943	-0.250550	-1.879385
N	2.717322	-1.630253	-1.835773
C	1.589558	-2.155871	-1.312488
H	0.030848	1.031615	1.505661
H	-0.960190	3.162664	2.375636
H	-3.393934	3.621235	1.931622
H	-4.735268	1.930778	0.668277
H	-4.720113	-0.123034	-0.773692
H	-4.203328	-1.212744	0.519865
H	-2.998822	-0.897381	-2.120964
H	-2.945491	-3.148358	-2.240303
H	-4.464626	-2.880827	-1.377869
H	-0.236210	-3.434928	1.903378
H	-1.222658	-5.579752	2.732626
H	-3.336130	-6.423802	1.657589
H	-4.363191	-5.098371	-0.197656
H	3.377757	0.387473	-2.264038
H	3.523735	-2.163817	-2.148259
H	1.415017	-3.211223	-1.166857
H	0.875862	0.987648	-1.229701

$[Zn(dipic)(im)]^{2+}$ (COSMO), -5114.39 kcal mol^{-1}

C	-1.095543	0.951624	1.696496
C	-1.637551	2.041174	2.368087
C	-2.888622	2.521913	1.964642
C	-3.550289	1.905334	0.900075
C	-2.945451	0.824334	0.258254
N	-1.738991	0.357771	0.664723
C	-3.569467	0.152708	-0.957575
N	-3.101335	-1.257194	-1.095500
C	-3.853974	-2.228460	-0.232728
C	-2.983665	-3.395976	0.200784
N	-1.661955	-3.142149	0.360365
C	-0.833005	-4.111956	0.808613
C	-1.298061	-5.384194	1.121372
C	-2.660445	-5.658426	0.955471
C	-3.512201	-4.654119	0.488289
Zn	-1.130569	-1.313163	-0.339746
N	0.688797	-1.217254	-1.033450
C	1.461088	-2.266310	-1.530901
C	2.690363	-1.773056	-1.879059
N	2.654222	-0.419342	-1.587417
C	1.444197	-0.111795	-1.082165
H	-0.136118	0.526056	1.968891
H	-1.094717	2.494308	3.190781
H	-3.344902	3.364379	2.475870
H	-4.523208	2.253202	0.566304
H	-3.245444	0.689802	-1.854531
H	-4.660502	0.213857	-0.906733
H	-3.179858	-1.541042	-2.071374
H	-4.757338	-2.583392	-0.734288
H	-4.162109	-1.690678	0.671826
H	0.212435	-3.840112	0.904199
H	-0.606927	-6.140321	1.478138
H	-3.054032	-6.644954	1.181598
H	-4.572745	-4.837481	0.346404
H	3.563383	-2.248396	-2.296551
H	3.410480	0.240320	-1.731155
H	1.139853	0.873735	-0.768114
H	1.074082	-3.270567	-1.599252

$[Zn(dipic)(tri)]^{2+}$ (gas phase), -4847.19 kcal mol^{-1}

C	-1.082378	1.020862	1.558342
C	-1.621828	2.189089	2.083848
C	-2.816440	2.679052	1.543710
C	-3.429069	1.984782	0.495907
C	-2.831304	0.824574	0.003892
N	-1.672043	0.352617	0.534645
C	-3.412902	0.062715	-1.184441
N	-2.993731	-1.376044	-1.167792
C	-3.809169	-2.240046	-0.240664
C	-2.991317	-3.377510	0.359018
N	-1.663496	-3.149371	0.545309
C	-0.900009	-4.088346	1.158780
C	-1.433056	-5.290696	1.608911
C	-2.796284	-5.537266	1.410400
C	-3.582084	-4.569543	0.776585
Zn	-1.051224	-1.410657	-0.280305
N	0.730912	-1.257364	-1.138663
C	1.444688	-0.076102	-1.285346
N	2.595827	-0.239382	-1.902346
N	2.617091	-1.582518	-2.162111
C	1.514205	-2.190828	-1.712167
H	-0.165489	0.590324	1.948758
H	-1.120305	2.697193	2.901956
H	-3.268199	3.586054	1.936480
H	-4.360027	2.341465	0.062584
H	-3.025791	0.501998	-2.111635
H	-4.503725	0.165092	-1.203240
H	-3.051406	-1.751824	-2.115749
H	-4.699946	-2.627424	-0.745123
H	-4.147803	-1.600200	0.584344
H	0.151223	-3.847582	1.281884
H	-0.792749	-6.017348	2.099725
H	-3.241962	-6.471083	1.742738
H	-4.643520	-4.736065	0.612391
H	1.089592	0.880853	-0.930399
H	3.414774	-1.988380	-2.647327
H	1.300607	-3.246088	-1.803744

$[Zn(dipic)(tri)]^{2+}$ (COSMO), -5003.42 kcal mol^{-1}

C	-1.082378	1.020862	1.558342
C	-1.621828	2.189089	2.083848
C	-2.816440	2.679052	1.543710
C	-3.429069	1.984782	0.495907
C	-2.831304	0.824574	0.003892
N	-1.672043	0.352617	0.534645
C	-3.412902	0.062715	-1.184441
N	-2.993731	-1.376044	-1.167792
C	-3.809169	-2.240046	-0.240664
C	-2.991317	-3.377510	0.359018
N	-1.663496	-3.149371	0.545309
C	-0.900009	-4.088346	1.158780
C	-1.433056	-5.290696	1.608911
C	-2.796284	-5.537266	1.410400
C	-3.582084	-4.569543	0.776585
Zn	-1.051224	-1.410657	-0.280305
N	0.730912	-1.257364	-1.138663
C	1.444688	-0.076102	-1.285346
N	2.595827	-0.239382	-1.902346
N	2.617091	-1.582518	-2.162111
C	1.514205	-2.190828	-1.712167
H	-0.165489	0.590324	1.948758
H	-1.120305	2.697193	2.901956
H	-3.268199	3.586054	1.936480
H	-4.360027	2.341465	0.062584
H	-3.025791	0.501998	-2.111635
H	-4.503725	0.165092	-1.203240
H	-3.051406	-1.751824	-2.115749
H	-4.699946	-2.627424	-0.745123
H	-4.147803	-1.600200	0.584344
H	0.151223	-3.847582	1.281884
H	-0.792749	-6.017348	2.099725
H	-3.241962	-6.471083	1.742738
H	-4.643520	-4.736065	0.612391
H	1.089592	0.880853	-0.930399
H	3.414774	-1.988380	-2.647327
H	1.300607	-3.246088	-1.803744

$[Zn(dipic)(tet)]^{2+}$ (gas phase), -4722.43 kcal mol^{-1}

C	-1.002775	1.374578	1.155634
C	-1.531320	2.600248	1.547096
C	-2.890639	2.848261	1.330785
C	-3.682699	1.861268	0.732700
C	-3.099574	0.648449	0.373308
N	-1.775469	0.417094	0.586196
C	-3.907088	-0.506853	-0.206808
N	-3.085335	-1.346131	-1.155172
C	-3.505015	-2.782014	-1.226788
C	-2.902381	-3.601808	-0.087455
N	-1.751577	-3.142249	0.472133
C	-1.138151	-3.866404	1.442740
C	-1.649486	-5.079095	1.888034
C	-2.837316	-5.556032	1.322118
C	-3.471143	-4.805812	0.327121
Zn	-1.181990	-1.330589	-0.208068
N	0.694084	-1.212793	-0.983172
N	1.620965	-0.349873	-0.467101
C	2.700153	-0.547416	-1.206213
N	2.417539	-1.498628	-2.131843
N	1.151794	-1.918411	-1.988747
H	0.047886	1.132761	1.273778
H	-0.886620	3.345646	2.002718
H	-3.329344	3.800612	1.616494
H	-4.739964	2.032391	0.548637
H	-4.816784	-0.140951	-0.692823
H	-4.210064	-1.162186	0.619961
H	-3.124606	-0.935033	-2.089434
H	-3.134957	-3.180874	-2.178784
H	-4.596064	-2.883230	-1.229718
H	-0.227401	-3.444504	1.855254
H	-1.130870	-5.632089	2.665236
H	-3.266899	-6.497517	1.653807
H	-4.395788	-5.153122	-0.126724
H	3.652790	-0.044579	-1.102103
H	3.004650	-1.898828	-2.863974

$[Zn(dipic)(tet)]^{2+}$ (COSMO), -4866.84 kcal mol^{-1}

C	-0.565851	2.198542	0.802950
C	-0.713747	2.921564	-0.384594
C	-1.854500	2.703241	-1.162484
C	-2.799974	1.774089	-0.719741
C	-2.565610	1.086388	0.479216
N	-1.462063	1.287940	1.234270
C	-3.506313	0.001105	0.955763
N	-3.222540	-1.279146	0.198014
C	-3.943715	-2.474769	0.754803
C	-3.247597	-3.777158	0.390084
N	-1.922111	-3.716477	0.115750
C	-1.222935	-4.844593	-0.152925
C	-1.832943	-6.092321	-0.148020
C	-3.203496	-6.168797	0.128565
C	-3.918863	-4.999754	0.397098
Zn	-1.261960	-1.859632	0.006424
N	0.382376	-0.866378	-0.348830
N	1.376275	-0.687420	0.567358
C	2.240379	0.107389	-0.046438
N	1.765574	0.388774	-1.278193
N	0.595158	-0.224936	-1.473111
H	0.308371	2.345256	1.433381
H	0.046318	3.636517	-0.686648
H	-2.006081	3.244499	-2.091963
H	-3.702111	1.578860	-1.294685
H	-4.554424	0.278013	0.811527
H	-3.324821	-0.200973	2.011612
H	-3.546570	-1.141125	-0.763754
H	-4.984698	-2.490432	0.424450
H	-3.935453	-2.380538	1.845133
H	-0.169721	-4.713979	-0.371355
H	-1.247788	-6.979707	-0.364415
H	-3.710184	-7.129147	0.129658
H	-4.982771	-5.027171	0.610345
H	3.169636	0.478798	0.355627
H	2.180053	0.947841	-2.019503

Imidazole (gas phase), -1267.42 kcal mol^{-1}

C	-0.432676	-0.162948	0.019849
C	-1.713378	0.343146	0.042126
N	-1.559528	1.720218	-0.020315
C	-0.209761	1.977664	-0.076492
N	0.498021	0.861516	-0.054248
H	-0.128955	-1.200641	0.054238
H	-2.685138	-0.125219	0.094965
H	-2.305228	2.404549	-0.023499
H	0.184941	2.983430	-0.132075

Imidazole (COSMO), -1278.10 kcal mol^{-1}

C	-0.434691	-0.169383	0.020668
C	-1.712119	0.345437	0.042609
N	-1.554202	1.718545	-0.020432
C	-0.216600	1.983790	-0.076500
N	0.500035	0.861098	-0.053850
H	-0.134886	-1.208156	0.054146
H	-2.685294	-0.119226	0.095246
H	-2.299320	2.405730	-0.023980
H	0.174228	2.990035	-0.131465

1,2,4-Triazole (gas phase), -1160.08 kcal mol^{-1}

C	-0.461750	-0.110532	0.029783
N	-1.718765	0.332757	0.052262
N	-1.532705	1.688392	-0.023045
C	-0.207722	1.981059	-0.085358
N	0.504127	0.860575	-0.054017
H	-0.235187	-1.167375	0.075115
H	-2.333420	2.308276	-0.026397
H	0.176765	2.990488	-0.149797

1,2,4-Triazole (COSMO), -1171.69 kcal mol^{-1}

C	-0.459611	-0.117706	0.029968
N	-1.714269	0.334782	0.051883
N	-1.529373	1.691879	-0.023871
C	-0.216655	1.984977	-0.085003
N	0.502226	0.857011	-0.053643
H	-0.234702	-1.174650	0.076371
H	-2.322902	2.323351	-0.025274
H	0.164241	2.994303	-0.148918

Tetrazole (gas phase), -1036.58 kcal mol^{-1}

N	-0.471173	-0.146026	0.042376
N	-1.677249	0.339778	0.059483
N	-1.532022	1.699656	-0.026611
C	-0.211622	1.987429	-0.093579
N	0.474749	0.859351	-0.052833
H	-2.344358	2.306509	-0.031716
H	0.195470	2.985615	-0.167717

Tetrazole (COSMO), -1049.41 kcal mol^{-1}

N	-0.467656	-0.147027	0.042457
N	-1.676548	0.348609	0.058767
N	-1.528009	1.694059	-0.026700
C	-0.218680	1.988555	-0.093251
N	0.472926	0.855566	-0.052531
H	-2.334144	2.311870	-0.029755
H	0.180289	2.988489	-0.166709

Dipicolylamine (gas phase), -3948.78 kcal mol^{-1}

N	0.945577	-1.381866	0.059530
C	1.621211	-0.201840	0.628476
C	0.862830	1.057105	0.255868
N	-0.369474	1.175416	0.793488
C	-1.095968	2.257426	0.470513
C	-0.641204	3.269967	-0.381980
C	0.636285	3.145377	-0.932775
C	1.397977	2.019172	-0.612333
C	1.509832	-2.654993	0.541790
C	0.640295	-3.812362	0.090209
N	-0.610608	-3.833527	0.596476
C	-1.430527	-4.823240	0.208213
C	-1.055221	-5.836236	-0.681658
C	0.241565	-5.812814	-1.199901
C	1.100838	-4.782276	-0.811341
H	-0.042063	-1.347071	0.325158
H	2.644154	-0.158285	0.232001
H	1.696700	-0.250430	1.733705
H	-2.088255	2.317932	0.918057
H	-1.273368	4.126562	-0.605350
H	1.029848	3.905995	-1.603888

H	2.391755	1.880590	-1.033289
H	1.589756	-2.689212	1.647512
H	2.524714	-2.765037	0.137613
H	-2.434809	-4.806041	0.632140
H	-1.761818	-6.615730	-0.958017
H	0.575984	-6.577319	-1.898124
H	2.113525	-4.723309	-1.205064

Dipicolylamine (COSMO), -3961.84 kcal mol^{-1}

N	0.908258	-1.385173	0.146365
C	1.577888	-0.196034	0.736033
C	0.852043	1.060019	0.298421
N	-0.340765	1.295466	0.895297
C	-1.043680	2.376016	0.497628
C	-0.602116	3.263656	-0.489099
C	0.632141	3.019003	-1.098094
C	1.367474	1.898235	-0.700341
C	1.464785	-2.665530	0.657636
C	0.628808	-3.819488	0.142297
N	-0.578725	-3.988706	0.731977
C	-1.376697	-4.971773	0.266481
C	-1.019394	-5.823482	-0.783952
C	0.230233	-5.647980	-1.385454
C	1.064424	-4.628471	-0.916740
H	-0.078742	-1.348491	0.418016
H	2.615492	-0.176957	0.387107
H	1.593919	-0.238662	1.839740
H	-1.998632	2.536810	0.994469
H	-1.210677	4.119862	-0.766979
H	1.013450	3.683551	-1.869001
H	2.328014	1.671621	-1.156326
H	1.481220	-2.694924	1.761772
H	2.497400	-2.756849	0.305254
H	-2.340815	-5.081286	0.759557
H	-1.703181	-6.600137	-1.115457
H	0.548129	-6.287937	-2.204449
H	2.040125	-4.456979	-1.364479