Chemistry – A European Journal

Metal Ion Coordination to Azole Nucleosides

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Supporting Information

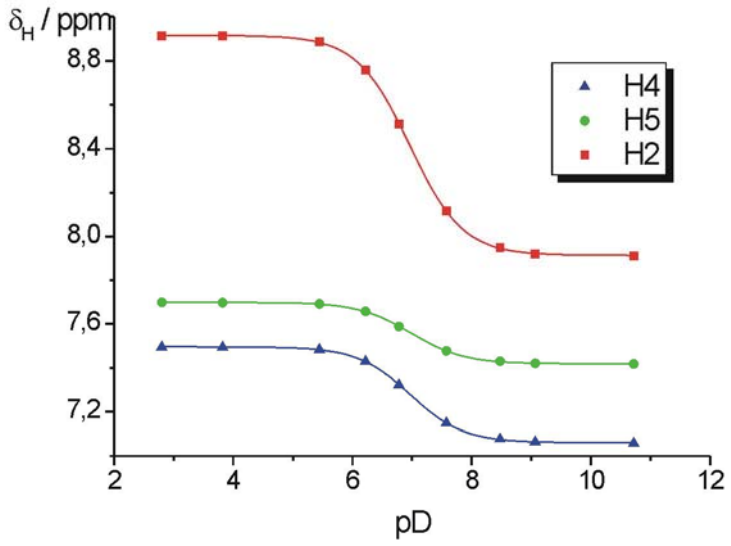


Figure S1: pD-dependent chemical shifts of imidazole α nucleoside **4a**

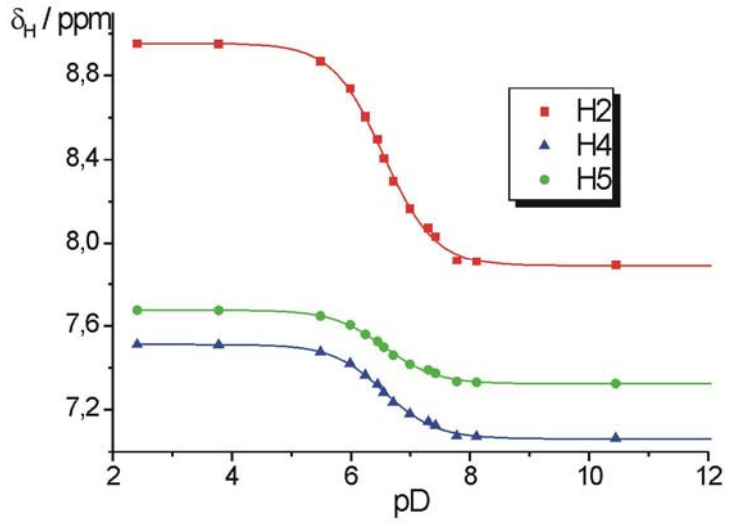


Figure S2: pD-dependent chemical shifts of imidazole β nucleoside **4b**

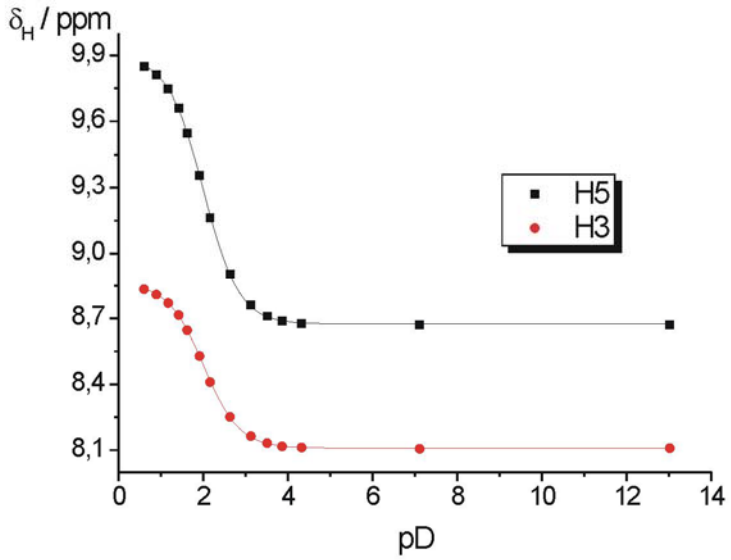


Figure S3: pD-dependent chemical shift of 1,2,4-triazole α nucleoside **5a**

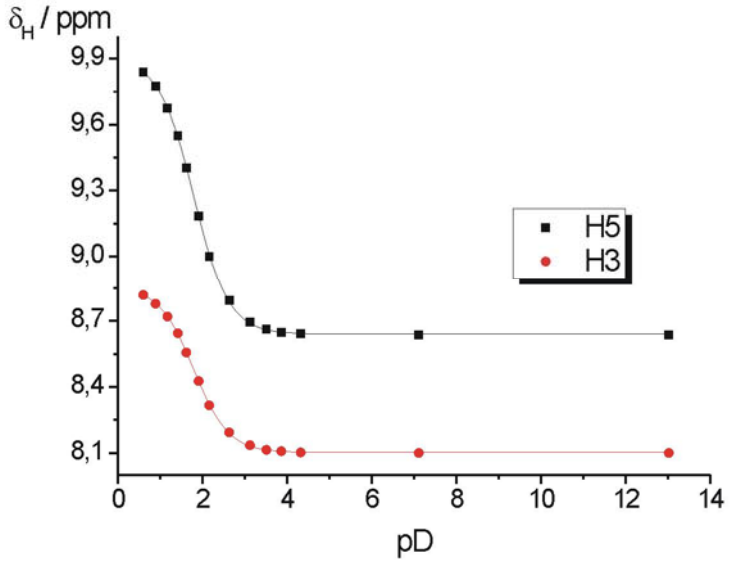


Figure S4: pD-dependent chemical shift of 1,2,4-triazole β nucleoside **5b**

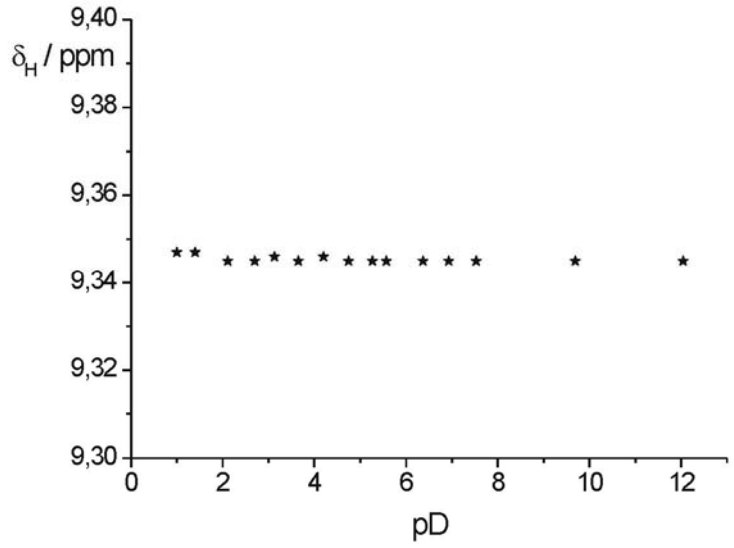
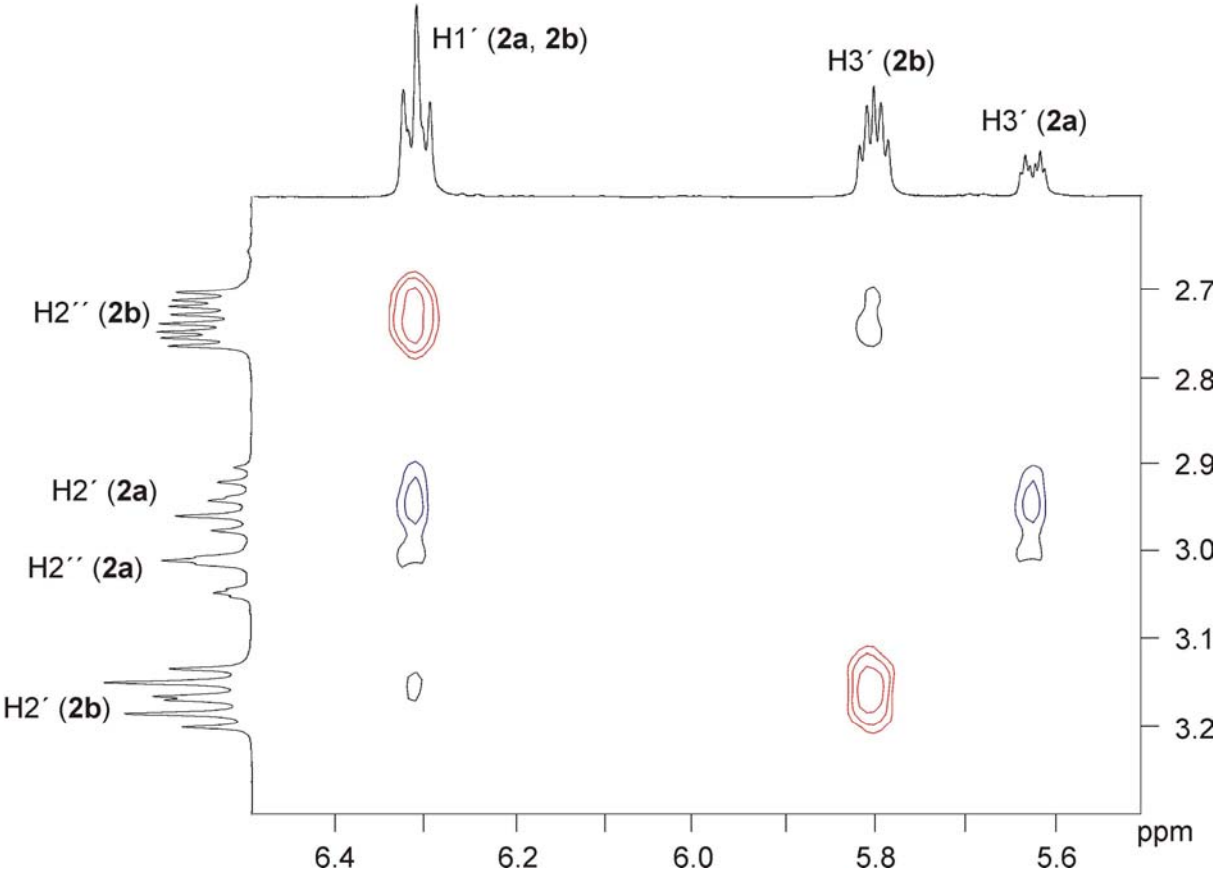
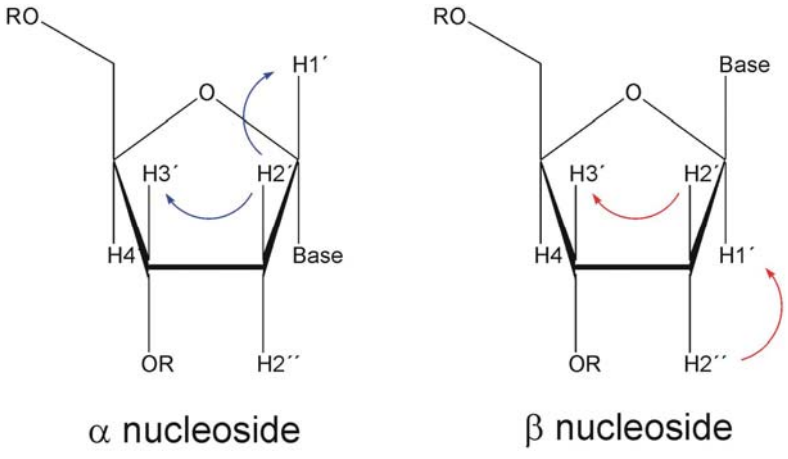


Figure S5: pD-dependent chemical shift of the H5 proton of tetrazole β nucleoside **6b**

Figure S6: Section of a ^{1}H,^{1}H NOESY spectrum of a mixture of **2a** and **2b** explaining the ^{1}H NMR spectroscopic differentiation of α and β nucleosides by the relative intensities of NOE based cross-peaks.





Calculations by WinEQNMR Version 1.20 by Michael J. Hynes
Program run at 15:19:12 on 04/01/2005

Titration Triazolnucleoside with Ag+ (H3)
Reactions: M + L = ML (beta1 = K1); M + 2L = ML2 (beta2 = K1K2)
FILE: Triazol_Ag.fit
IDEAL DATA: ?
File prepared by J. Mueller, March 31 2005

NO.	A	PARAMETER	DELTA	ERROR	CONDITION	DESCRIPTION
1	1	1.31993E+00	1.000E-03	1.344E-01	4.514E+00	logBETA1
2	1	4.26651E+00	1.000E-03	4.880E-02	1.951E+01	logBETA2
3	1	8.09404E+00	1.000E-03	1.325E-03	4.357E+00	SHIFT L
4	1	8.19064E+00	1.000E-03	8.999E-03	1.389E+01	SHIFT LAg
5	1	8.19540E+00	1.000E-03	2.544E-03	2.817E+01	SHIFT L2Ag

0RMS ERROR = 1.34E-03 MAX ERROR = 3.02E-03 AT OBS.NO. 16
RESIDUALS SQUARED = 3.58E-05
RFACTOR = 0.0147 PERCENT

NO.	A	EXPT. DEL	CALC. DEL	RESIDUAL	% DEV	WEIGHT	METAL	LIGAND	pH
1	1	8.1220E+00	8.1234E+00	-1.4238E-03	-1.7531E-02	1.0000E+00	3.5900E-03	1.7940E-02	0.0000E+00
2	1	8.1410E+00	8.1425E+00	-1.5182E-03	-1.8649E-02	1.0000E+00	7.1500E-03	1.7880E-02	0.0000E+00
3	1	8.1540E+00	8.1543E+00	-3.1853E-04	-3.9064E-03	1.0000E+00	1.0690E-02	1.7820E-02	0.0000E+00
4	1	8.1610E+00	8.1610E+00	2.0981E-05	2.5709E-04	1.0000E+00	1.4210E-02	1.7760E-02	0.0000E+00
5	1	8.1660E+00	8.1654E+00	6.4754E-04	7.9298E-03	1.0000E+00	1.7700E-02	1.7700E-02	0.0000E+00
6	1	8.1700E+00	8.1684E+00	1.5879E-03	1.9435E-02	1.0000E+00	2.1180E-02	1.7650E-02	0.0000E+00
7	1	8.1720E+00	8.1708E+00	1.2321E-03	1.5078E-02	1.0000E+00	2.4630E-02	1.7590E-02	0.0000E+00
8	1	8.1730E+00	8.1725E+00	4.5872E-04	5.6126E-03	1.0000E+00	2.8050E-02	1.7530E-02	0.0000E+00
9	1	8.1750E+00	8.1740E+00	1.0099E-03	1.2354E-02	1.0000E+00	3.1460E-02	1.7480E-02	0.0000E+00
10	1	8.1750E+00	8.1752E+00	-1.9360E-04	-2.3681E-03	1.0000E+00	3.4840E-02	1.7420E-02	0.0000E+00
11	1	8.1760E+00	8.1766E+00	-5.5122E-04	-6.7420E-03	1.0000E+00	3.9040E-02	1.7350E-02	0.0000E+00
12	1	8.1770E+00	8.1775E+00	-4.7684E-04	-5.8314E-03	1.0000E+00	4.3200E-02	1.7280E-02	0.0000E+00
13	1	8.1770E+00	8.1784E+00	-1.3752E-03	-1.6818E-02	1.0000E+00	4.7330E-02	1.7210E-02	0.0000E+00
14	1	8.1780E+00	8.1792E+00	-1.1673E-03	-1.4274E-02	1.0000E+00	5.1430E-02	1.7140E-02	0.0000E+00
15	1	8.1810E+00	8.1827E+00	-1.7424E-03	-2.1298E-02	1.0000E+00	8.3080E-02	1.6620E-02	0.0000E+00
16	1	8.1890E+00	8.1860E+00	3.0241E-03	3.6929E-02	1.0000E+00	1.5429E-01	1.5430E-02	0.0000E+00
17	1	8.1420E+00	8.1413E+00	7.0477E-04	8.6559E-03	1.0000E+00	1.6200E-02	1.8000E-03	0.0000E+00
18	1	8.1460E+00	8.1474E+00	-1.3924E-03	-1.7093E-02	1.0000E+00	1.4400E-02	3.6000E-03	0.0000E+00
19	1	8.1480E+00	8.1495E+00	-1.5430E-03	-1.8938E-02	1.0000E+00	1.2600E-02	5.4000E-03	0.0000E+00
20	1	8.1490E+00	8.1497E+00	-6.5708E-04	-8.0633E-03	1.0000E+00	1.0800E-02	7.2000E-03	0.0000E+00
21	1	8.1480E+00	8.1479E+00	1.1730E-04	1.4396E-03	1.0000E+00	9.0000E-03	9.0000E-03	0.0000E+00
22	1	8.1450E+00	8.1440E+00	1.0033E-03	1.2318E-02	1.0000E+00	7.2000E-03	1.0800E-02	0.0000E+00
23	1	8.1370E+00	8.1364E+00	5.5599E-04	6.8329E-03	1.0000E+00	5.4000E-03	1.2600E-02	0.0000E+00
24	1	8.1270E+00	8.1257E+00	1.2865E-03	1.5830E-02	1.0000E+00	3.6000E-03	1.4400E-02	0.0000E+00
25	1	8.1120E+00	8.1108E+00	1.2064E-03	1.4872E-02	1.0000E+00	1.8000E-03	1.6200E-02	0.0000E+00

TOLERANCE ON SUM OF SQUARES 0.0010
TOLERANCE ON EIGEN VALUES 0.0001
CONVERGANCE AFTER 8 ITERATIONS

Calculations by WinEQNMR Version 1.20 by Michael J. Hynes
Program run at 15:21:36 on 04/01/2005

Titration Triazolnucleoside with Ag+ (H5) JM128
Reactions: M + L = ML (beta1 = K1); M + 2L = ML2 (beta2 = K1K2)
FILE: Triazol_Ag.fit
IDEAL DATA: ?
File prepared by J. Mueller, April 1 2005

NO.	A	PARAMETER	DELTA	ERROR	CONDITION	DESCRIPTION
1	1	1.76238E+00	1.000E-02	4.214E-02	7.901E+00	logBETA1
2	1	4.26144E+00	1.000E-02	4.379E-02	1.990E+01	logBETA2
3	1	8.62628E+00	1.000E-03	2.202E-03	5.403E+00	SHIFT L
4	1	8.86418E+00	1.000E-03	6.593E-03	1.882E+01	SHIFT LAg
5	1	8.84587E+00	1.000E-03	4.216E-03	2.332E+01	SHIFT L2Ag

0RMS ERROR = 1.94E-03 MAX ERROR = 4.73E-03 AT OBS.NO. 2
RESIDUALS SQUARED = 7.50E-05
RFACTOR = 0.0197 PERCENT

NO.	A	EXPT. DEL	CALC. DEL	RESIDUAL	% DEV	WEIGHT	METAL	LIGAND	pH
1	1	8.6850E+00	8.6891E+00	-4.0588E-03	-4.6734E-02	1.0000E+00	3.5900E-03	1.7940E-02	0.0000E+00
2	1	8.7270E+00	8.7317E+00	-4.7264E-03	-5.4158E-02	1.0000E+00	7.1500E-03	1.7880E-02	0.0000E+00
3	1	8.7560E+00	8.7576E+00	-1.6499E-03	-1.8843E-02	1.0000E+00	1.0690E-02	1.7820E-02	0.0000E+00
4	1	8.7740E+00	8.7748E+00	-8.0395E-04	-9.1628E-03	1.0000E+00	1.4210E-02	1.7760E-02	0.0000E+00
5	1	8.7850E+00	8.7857E+00	-7.3051E-04	-8.3155E-03	1.0000E+00	1.7700E-02	1.7700E-02	0.0000E+00
6	1	8.7940E+00	8.7936E+00	4.2534E-04	4.8367E-03	1.0000E+00	2.1180E-02	1.7650E-02	0.0000E+00
7	1	8.8000E+00	8.7995E+00	5.2452E-04	5.9605E-03	1.0000E+00	2.4630E-02	1.7590E-02	0.0000E+00
8	1	8.8050E+00	8.8041E+00	8.8024E-04	9.9971E-03	1.0000E+00	2.8050E-02	1.7530E-02	0.0000E+00
9	1	8.8090E+00	8.8079E+00	1.0729E-03	1.2179E-02	1.0000E+00	3.1460E-02	1.7480E-02	0.0000E+00
10	1	8.8120E+00	8.8111E+00	8.9645E-04	1.0173E-02	1.0000E+00	3.4840E-02	1.7420E-02	0.0000E+00
11	1	8.8150E+00	8.8144E+00	5.7983E-04	6.5778E-03	1.0000E+00	3.9040E-02	1.7350E-02	0.0000E+00
12	1	8.8180E+00	8.8172E+00	7.9060E-04	8.9657E-03	1.0000E+00	4.3200E-02	1.7280E-02	0.0000E+00
13	1	8.8190E+00	8.8196E+00	-6.1226E-04	-6.9425E-03	1.0000E+00	4.7330E-02	1.7210E-02	0.0000E+00
14	1	8.8210E+00	8.8217E+00	-7.2193E-04	-8.1842E-03	1.0000E+00	5.1430E-02	1.7140E-02	0.0000E+00
15	1	8.8300E+00	8.8318E+00	-1.8110E-03	-2.0510E-02	1.0000E+00	8.3080E-02	1.6620E-02	0.0000E+00
16	1	8.8430E+00	8.8421E+00	9.0122E-04	1.0191E-02	1.0000E+00	1.5429E-01	1.5430E-02	0.0000E+00
17	1	8.7580E+00	8.7590E+00	-9.8133E-04	-1.1205E-02	1.0000E+00	1.6200E-02	1.8000E-03	0.0000E+00
18	1	8.7610E+00	8.7619E+00	-8.7929E-04	-1.0036E-02	1.0000E+00	1.4400E-02	3.6000E-03	0.0000E+00
19	1	8.7610E+00	8.7611E+00	-5.0545E-05	-5.7693E-04	1.0000E+00	1.2600E-02	5.4000E-03	0.0000E+00
20	1	8.7580E+00	8.7571E+00	9.4414E-04	1.0780E-02	1.0000E+00	1.0800E-02	7.2000E-03	0.0000E+00
21	1	8.7520E+00	8.7498E+00	2.1639E-03	2.4724E-02	1.0000E+00	9.0000E-03	9.0000E-03	0.0000E+00
22	1	8.7400E+00	8.7384E+00	1.6193E-03	1.8528E-02	1.0000E+00	7.2000E-03	1.0800E-02	0.0000E+00
23	1	8.7220E+00	8.7200E+00	1.9627E-03	2.2502E-02	1.0000E+00	5.4000E-03	1.2600E-02	0.0000E+00
24	1	8.6970E+00	8.6947E+00	2.2984E-03	2.6427E-02	1.0000E+00	3.6000E-03	1.4400E-02	0.0000E+00
25	1	8.6640E+00	8.6620E+00	2.0218E-03	2.3336E-02	1.0000E+00	1.8000E-03	1.6200E-02	0.0000E+00

TOLERANCE ON SUM OF SQUARES 0.0010
TOLERANCE ON EIGEN VALUES 0.0001
CONVERGANCE AFTER 4 ITERATIONS

Calculations by WinEQNMR Version 1.20 by Michael J. Hynes
Program run at 14:40:52 on 04/01/2005

Titration Triazolnucleoside with Hg2+ (H3)
Reaction: L + Ag = LAg
FILE: Triazol_Hg.fit
IDEAL DATA: ?
File prepared by J. Mueller, March 31 2005

NO.	A	PARAMETER	DELTA	ERROR	CONDITION	DESCRIPTION
1	1	1.54797E+00	1.000E-02	1.870E-02	7.489E+01	logBETA1
2	1	8.08755E+00	1.000E-02	1.163E-03	4.159E+00	SHIFT L
3	1	8.75689E+00	1.000E-02	1.225E-02	5.810E+01	SHIFT LAg

0RMS ERROR = 2.24E-03 MAX ERROR = 4.80E-03 AT OBS.NO. 1
RESIDUALS SQUARED = 1.10E-04
RFACTOR = 0.0255 PERCENT

NO.	A	EXPT. DEL	CALC. DEL	RESIDUAL	% DEV	WEIGHT	LIGAND	METAL	pH
1	1	8.1050E+00	8.1002E+00	4.7951E-03	5.9162E-02	1.0000E+00	8.9000E-04	1.7850E-02	0.0000E+00
2	1	8.1140E+00	8.1125E+00	1.4582E-03	1.7971E-02	1.0000E+00	1.7700E-03	1.7700E-02	0.0000E+00
3	1	8.1240E+00	8.1244E+00	-3.6526E-04	-4.4960E-03	1.0000E+00	2.6300E-03	1.7560E-02	0.0000E+00
4	1	8.1340E+00	8.1358E+00	-1.8482E-03	-2.2722E-02	1.0000E+00	3.4800E-03	1.7420E-02	0.0000E+00
5	1	8.1450E+00	8.1470E+00	-1.9970E-03	-2.4518E-02	1.0000E+00	4.3200E-03	1.7280E-02	0.0000E+00
6	1	8.1550E+00	8.1577E+00	-2.6922E-03	-3.3013E-02	1.0000E+00	5.1400E-03	1.7140E-02	0.0000E+00
7	1	8.1660E+00	8.1681E+00	-2.0599E-03	-2.5226E-02	1.0000E+00	5.9500E-03	1.7010E-02	0.0000E+00
8	1	8.1760E+00	8.1781E+00	-2.1200E-03	-2.5930E-02	1.0000E+00	6.7500E-03	1.6880E-02	0.0000E+00
9	1	8.1850E+00	8.1878E+00	-2.7781E-03	-3.3941E-02	1.0000E+00	7.5300E-03	1.6740E-02	0.0000E+00
10	1	8.1970E+00	8.1972E+00	-2.2984E-04	-2.8039E-03	1.0000E+00	8.3100E-03	1.6620E-02	0.0000E+00
11	1	8.2060E+00	8.2062E+00	-2.0409E-04	-2.4870E-03	1.0000E+00	9.0700E-03	1.6490E-02	0.0000E+00
12	1	8.2150E+00	8.2150E+00	-7.6294E-06	-9.2872E-05	1.0000E+00	9.8200E-03	1.6360E-02	0.0000E+00
13	1	8.2230E+00	8.2235E+00	-5.2452E-04	-6.3787E-03	1.0000E+00	1.0560E-02	1.6240E-02	0.0000E+00
14	1	8.2320E+00	8.2316E+00	4.1389E-04	5.0279E-03	1.0000E+00	1.1280E-02	1.6120E-02	0.0000E+00
15	1	8.2410E+00	8.2395E+00	1.4782E-03	1.7937E-02	1.0000E+00	1.2000E-02	1.6000E-02	0.0000E+00
16	1	8.2490E+00	8.2472E+00	1.7567E-03	2.1296E-02	1.0000E+00	1.2710E-02	1.5880E-02	0.0000E+00
17	1	8.2560E+00	8.2546E+00	1.3542E-03	1.6403E-02	1.0000E+00	1.3400E-02	1.5770E-02	0.0000E+00
18	1	8.2650E+00	8.2620E+00	2.9716E-03	3.5955E-02	1.0000E+00	1.4090E-02	1.5650E-02	0.0000E+00
19	1	8.2720E+00	8.2692E+00	2.8248E-03	3.4149E-02	1.0000E+00	1.4760E-02	1.5540E-02	0.0000E+00
20	1	8.2790E+00	8.2766E+00	2.4023E-03	2.9017E-02	1.0000E+00	1.5430E-02	1.5430E-02	0.0000E+00
21	1	8.3380E+00	8.3393E+00	-1.3180E-03	-1.5807E-02	1.0000E+00	2.2660E-02	1.5100E-02	0.0000E+00
22	1	8.3870E+00	8.3900E+00	-3.0212E-03	-3.6023E-02	1.0000E+00	3.0000E-02	1.5000E-02	0.0000E+00
23	1	8.4280E+00	8.4305E+00	-2.4595E-03	-2.9183E-02	1.0000E+00	3.7240E-02	1.4900E-02	0.0000E+00
24	1	8.4630E+00	8.4634E+00	-3.9959E-04	-4.7216E-03	1.0000E+00	4.4380E-02	1.4790E-02	0.0000E+00
25	1	8.4930E+00	8.4904E+00	2.5711E-03	3.0273E-02	1.0000E+00	5.1430E-02	1.4690E-02	0.0000E+00

TOLERANCE ON SUM OF SQUARES 0.0001
TOLERANCE ON EIGEN VALUES 0.0001
CONVERGANCE AFTER 9 ITERATIONS

Calculations by WinEQNMR Version 1.20 by Michael J. Hynes
Program run at 14:39:06 on 04/01/2005

Titration Triazolnucleoside with Hg2+ (H5)
Reaction: L + Ag = LAg
FILE: Triazol_Hg.fit
IDEAL DATA: ?
File prepared by J. Mueller, March 31 2005

NO.	A	PARAMETER	DELTA	ERROR	CONDITION	DESCRIPTION
1	1	1.57777E+00	1.000E-02	1.689E-02	6.742E+01	logBETA1
2	1	8.61407E+00	1.000E-02	2.004E-03	4.023E+00	SHIFT L
3	1	9.82664E+00	1.000E-02	1.948E-02	5.207E+01	SHIFT LAg

0RMS ERROR = 3.89E-03 MAX ERROR = 8.94E-03 AT OBS.NO. 1
RESIDUALS SQUARED = 3.32E-04
RFACTOR = 0.0409 PERCENT

NO.	A	EXPT. DEL	CALC. DEL	RESIDUAL	% DEV	WEIGHT	LIGAND	METAL	pH
1	1	8.6470E+00	8.6381E+00	8.9426E-03	1.0342E-01	1.0000E+00	8.9000E-04	1.7850E-02	0.0000E+00
2	1	8.6640E+00	8.6614E+00	2.6398E-03	3.0468E-02	1.0000E+00	1.7700E-03	1.7700E-02	0.0000E+00
3	1	8.6830E+00	8.6837E+00	-7.2193E-04	-8.3143E-03	1.0000E+00	2.6300E-03	1.7560E-02	0.0000E+00
4	1	8.7020E+00	8.7055E+00	-3.4962E-03	-4.0177E-02	1.0000E+00	3.4800E-03	1.7420E-02	0.0000E+00
5	1	8.7240E+00	8.7266E+00	-2.5711E-03	-2.9472E-02	1.0000E+00	4.3200E-03	1.7280E-02	0.0000E+00
6	1	8.7410E+00	8.7468E+00	-5.7774E-03	-6.6095E-02	1.0000E+00	5.1400E-03	1.7140E-02	0.0000E+00
7	1	8.7630E+00	8.7663E+00	-3.3474E-03	-3.8199E-02	1.0000E+00	5.9500E-03	1.7010E-02	0.0000E+00
8	1	8.7810E+00	8.7853E+00	-4.3163E-03	-4.9155E-02	1.0000E+00	6.7500E-03	1.6880E-02	0.0000E+00
9	1	8.8000E+00	8.8035E+00	-3.5143E-03	-3.9935E-02	1.0000E+00	7.5300E-03	1.6740E-02	0.0000E+00
10	1	8.8200E+00	8.8212E+00	-1.2026E-03	-1.3635E-02	1.0000E+00	8.3100E-03	1.6620E-02	0.0000E+00
11	1	8.8380E+00	8.8383E+00	-2.5749E-04	-2.9135E-03	1.0000E+00	9.0700E-03	1.6490E-02	0.0000E+00
12	1	8.8540E+00	8.8548E+00	-7.8487E-04	-8.8646E-03	1.0000E+00	9.8200E-03	1.6360E-02	0.0000E+00
13	1	8.8700E+00	8.8707E+00	-6.5136E-04	-7.3434E-03	1.0000E+00	1.0560E-02	1.6240E-02	0.0000E+00
14	1	8.8870E+00	8.8859E+00	1.0748E-03	1.2094E-02	1.0000E+00	1.1280E-02	1.6120E-02	0.0000E+00
15	1	8.9030E+00	8.9008E+00	2.1744E-03	2.4423E-02	1.0000E+00	1.2000E-02	1.6000E-02	0.0000E+00
16	1	8.9180E+00	8.9153E+00	2.7237E-03	3.0542E-02	1.0000E+00	1.2710E-02	1.5880E-02	0.0000E+00
17	1	8.9320E+00	8.9291E+00	2.9297E-03	3.2800E-02	1.0000E+00	1.3400E-02	1.5770E-02	0.0000E+00
18	1	8.9470E+00	8.9427E+00	4.2973E-03	4.8030E-02	1.0000E+00	1.4090E-02	1.5650E-02	0.0000E+00
19	1	8.9610E+00	8.9559E+00	5.1260E-03	5.7203E-02	1.0000E+00	1.4760E-02	1.5540E-02	0.0000E+00
20	1	8.9730E+00	8.9692E+00	3.7546E-03	4.1843E-02	1.0000E+00	1.5430E-02	1.5430E-02	0.0000E+00
21	1	9.0850E+00	9.0858E+00	-8.4209E-04	-9.2691E-03	1.0000E+00	2.2660E-02	1.5100E-02	0.0000E+00
22	1	9.1740E+00	9.1792E+00	-5.2404E-03	-5.7123E-02	1.0000E+00	3.0000E-02	1.5000E-02	0.0000E+00
23	1	9.2490E+00	9.2534E+00	-4.3564E-03	-4.7101E-02	1.0000E+00	3.7240E-02	1.4900E-02	0.0000E+00
24	1	9.3120E+00	9.3129E+00	-9.1934E-04	-9.8727E-03	1.0000E+00	4.4380E-02	1.4790E-02	0.0000E+00
25	1	9.3660E+00	9.3616E+00	4.3516E-03	4.6462E-02	1.0000E+00	5.1430E-02	1.4690E-02	0.0000E+00

TOLERANCE ON SUM OF SQUARES 0.0001
TOLERANCE ON EIGEN VALUES 0.0001
CONVERGANCE AFTER 6 ITERATIONS

Calculations by WinEQNMR Version 1.20 by Michael J. Hynes
Program run at 11:04:32 on 04/15/2005

Titration Tetrazolnucleoside with Ag+
Reaction: L + Ag = LAg
FILE: Jens11.fit
IDEAL DATA: ?
File prepared by J. Mueller, April 15 2005

NO.	A	PARAMETER	DELTA	ERROR	CONDITION	DESCRIPTION
1	1	8.60837E-01	1.000E-03	4.122E-03	6.346E+00	logBETA1
2	1	9.34342E+00	1.000E-02	3.582E-04	2.487E+00	SHIFT L
3	1	9.60646E+00	1.000E-02	9.014E-04	4.093E+00	SHIFT LAg

0RMS ERROR = 7.06E-04 MAX ERROR = 1.53E-03 AT OBS.NO. 16
RESIDUALS SQUARED = 7.48E-06
RFACTOR = 0.0068 PERCENT

NO.	A	EXPT. DEL	CALC. DEL	RESIDUAL	% DEV	WEIGHT	METAL	LIGAND	pH
1	1	9.3500E+00	9.3495E+00	5.1785E-04	5.5385E-03	1.0000E+00	3.5900E-03	1.6370E-02	0.0000E+00
2	1	9.3550E+00	9.3553E+00	-2.8801E-04	-3.0787E-03	1.0000E+00	7.1500E-03	1.6310E-02	0.0000E+00
3	1	9.3600E+00	9.3610E+00	-9.5654E-04	-1.0219E-02	1.0000E+00	1.0680E-02	1.6240E-02	0.0000E+00
4	1	9.3660E+00	9.3663E+00	-3.4714E-04	-3.7064E-03	1.0000E+00	1.4190E-02	1.6180E-02	0.0000E+00
5	1	9.3710E+00	9.3715E+00	-5.2452E-04	-5.5973E-03	1.0000E+00	1.7670E-02	1.6120E-02	0.0000E+00
6	1	9.3810E+00	9.3810E+00	1.5259E-05	1.6266E-04	1.0000E+00	2.4550E-02	1.5990E-02	0.0000E+00
7	1	9.3890E+00	9.3894E+00	-3.5381E-04	-3.7684E-03	1.0000E+00	3.1320E-02	1.5870E-02	0.0000E+00
8	1	9.3980E+00	9.3972E+00	7.7534E-04	8.2500E-03	1.0000E+00	3.7990E-02	1.5750E-02	0.0000E+00
9	1	9.4050E+00	9.4045E+00	5.4836E-04	5.8305E-03	1.0000E+00	4.4560E-02	1.5630E-02	0.0000E+00
10	1	9.4120E+00	9.4113E+00	6.8569E-04	7.2853E-03	1.0000E+00	5.1030E-02	1.5510E-02	0.0000E+00
11	1	9.4260E+00	9.4259E+00	8.6784E-05	9.2069E-04	1.0000E+00	6.6790E-02	1.5230E-02	0.0000E+00
12	1	9.4390E+00	9.4383E+00	7.3051E-04	7.7393E-03	1.0000E+00	8.1980E-02	1.4950E-02	0.0000E+00
13	1	9.4490E+00	9.4487E+00	2.8324E-04	2.9976E-03	1.0000E+00	9.6640E-02	1.4690E-02	0.0000E+00
14	1	9.4670E+00	9.4676E+00	-5.8556E-04	-6.1852E-03	1.0000E+00	1.2840E-01	1.4640E-02	0.0000E+00
15	1	9.4830E+00	9.4824E+00	6.2180E-04	6.5570E-03	1.0000E+00	1.5993E-01	1.4590E-02	0.0000E+00
16	1	9.5070E+00	9.5085E+00	-1.5297E-03	-1.6090E-02	1.0000E+00	2.3780E-01	1.4460E-02	0.0000E+00
17	1	9.5250E+00	9.5254E+00	-3.8242E-04	-4.0149E-03	1.0000E+00	3.1434E-01	1.4340E-02	0.0000E+00
18	1	9.5380E+00	9.5373E+00	6.9427E-04	7.2790E-03	1.0000E+00	3.8955E-01	1.4210E-02	0.0000E+00

TOLERANCE ON SUM OF SQUARES 0.0001
TOLERANCE ON EIGEN VALUES 0.0001
CONVERGANCE AFTER 8 ITERATIONS

Cartesian coordinates for 2:1 complex of 1-methylimidazole and Ag^+, fully optimized:

C	2.871385	1.067976	-0.893987
N	2.123494	0.192107	-0.128318
C	2.994440	-0.521072	0.582345
N	4.260469	-0.143362	0.307964
C	4.198063	0.867880	-0.630620
Ag	-0.000005	0.001511	-0.117774
N	-2.123420	-0.189891	-0.131230
C	-2.870830	-1.053582	-0.911072
C	-4.197631	-0.858355	-0.644693
N	-4.260604	0.137593	0.310066
C	-2.994777	0.511349	0.590720
C	-5.478620	0.687095	0.905150
C	5.478195	-0.703068	0.894052
H	2.749076	-1.300893	1.288021
H	5.086282	1.343468	-1.017529
H	2.411864	1.771041	-1.571703
H	6.036531	0.080078	1.412729
H	5.203158	-1.479644	1.609341
H	6.101880	-1.141472	0.111108
H	-2.749862	1.279704	1.309020
H	-5.085599	-1.327908	-1.039471
H	-2.410930	-1.745375	-1.600038
H	-6.104250	1.134408	0.128818
H	-6.034725	-0.103820	1.414365
H	-5.204101	1.454946	1.629977

Cartesian coordinates for 2:1 complex of 1-methylimidazole and Ag^+, cisoid geometry:

C	-2.946750	0.852946	-0.002257
N	-2.133125	-0.200370	-0.002682
N	2.133106	-0.200125	-0.001925
C	2.946939	0.853037	-0.001212
N	4.238402	0.461605	0.004141
C	4.253496	-0.919245	0.006547
C	2.945947	-1.318910	0.002881
C	5.410367	1.336799	0.002463
H	5.077705	2.375830	0.013535
H	6.006509	1.160739	-0.896325
H	6.018911	1.146238	0.889818
H	5.175375	-1.480437	0.011043
H	2.542199	-2.319773	0.003413
H	2.642939	1.889222	-0.005116
N	-4.238279	0.461659	0.001668
C	-4.253636	-0.919164	0.004165
C	-2.946134	-1.319016	0.001697
C	-5.410086	1.337046	0.006348
H	-5.077283	2.376005	-0.006950
H	-6.003126	1.162034	0.907379
H	-6.021727	1.145615	-0.878695
H	-2.642585	1.889086	-0.004666
H	-5.175609	-1.480217	0.007580
H	-2.542531	-2.319934	0.001692
Ag	-0.000050	-0.183505	-0.003722

Cartesian coordinates for 2:1 complex of 1-methylimidazole and Hg^{2+}, fully optimized:

C	-2.895653	-1.049796	-0.912988
N	-2.165946	-0.181046	-0.106712
C	-3.050098	0.522883	0.626327
N	-4.293052	0.137386	0.319213
C	-4.217839	-0.849837	-0.645786
Hg	-0.000011	0.001009	-0.079959
N	2.165968	0.183076	-0.102950
C	2.895829	1.066920	-0.892508
C	4.217993	0.861461	-0.629376
N	4.293029	-0.144133	0.316460
C	3.049996	-0.535063	0.616318
C	5.537767	-0.688112	0.891668
C	-5.537847	0.670049	0.904804
H	-2.816121	1.285105	1.355161
H	-5.100074	-1.320194	-1.054983
H	-2.434144	-1.736217	-1.606750
H	-6.081360	-0.141598	1.392513
H	-5.285620	1.435222	1.639366
H	-6.148038	1.108878	0.112834
H	2.815878	-1.311053	1.330426
H	5.100303	1.339444	-1.029474
H	2.434433	1.766695	-1.572873
H	6.148067	-1.111289	0.091324
H	6.081164	0.113842	1.395299
H	5.285495	-1.467542	1.611077

Cartesian coordinates for 2:1 complex of 1-methylimidazole and Hg^{2+}, cisoid geometry:

N	-2.174719	-0.158091	0.000788
C	-3.010481	0.897817	0.000502
N	-4.276382	0.466788	0.000348
C	-4.266359	-0.915463	0.000447
C	-2.960080	-1.307035	0.000568
N	2.174746	-0.157994	-0.001387
C	3.010465	0.897899	-0.001242
N	4.276351	0.466757	0.000789
C	4.266369	-0.915430	0.001677
C	2.960041	-1.306949	0.000266
C	5.483823	1.314081	0.001225
H	6.071578	1.100918	0.896304
H	6.071519	1.102100	-0.894184
H	5.182604	2.361928	0.001966
H	2.727095	1.940174	-0.001898
H	5.177587	-1.495685	0.003073
H	2.545487	-2.303693	0.000192
Hg	0.000002	-0.120107	-0.000492
H	-2.545613	-2.303828	0.000908
H	-5.177598	-1.495684	0.001203
C	-5.483797	1.314188	0.000803
H	-6.074079	1.098326	-0.891956
H	-6.068999	1.104998	0.898509
H	-5.182518	2.362005	-0.004080
H	-2.727087	1.940088	0.000122

Cartesian coordinates for 2:1 complex of 1-methyl-1,2,4-triazole and Ag^+, fully optimized:

C	3.011077	0.793749	0.309885
N	2.138491	-0.137382	-0.090962
N	-2.137961	-0.134451	0.093510
C	-3.013330	0.793102	-0.309545
N	-4.252922	0.354962	-0.071943
N	-4.218505	-0.878352	0.494842
C	-2.933256	-1.140824	0.578974
C	-5.533028	1.004057	-0.342884
H	-5.343278	1.991395	-0.766169
H	-6.090040	1.098110	0.591052
H	-6.101351	0.397005	-1.050373
H	-2.550654	-2.061808	0.993660
H	-2.778085	1.746994	-0.758039
N	4.252128	0.355927	0.079463
N	4.221410	-0.879930	-0.482072
C	2.936818	-1.144514	-0.569745
C	5.530354	1.008329	0.351349
H	5.337745	1.992588	0.780464
H	6.085558	1.109573	-0.582960
H	6.101950	0.399388	1.054503
H	2.772879	1.749499	0.752837
H	2.556931	-2.067757	-0.981912
Ag	-0.000042	-0.106464	-0.006407

Cartesian coordinates for 2:1 complex of 1-methyl-1,2,4-triazole and Ag^+, cisoid geometry:

C	2.994533	0.872435	0.000172
N	2.141350	-0.157443	0.000436
N	-2.141356	-0.157412	0.000035
C	-2.994552	0.872444	-0.000387
N	-4.245340	0.402486	-0.001742
N	-4.240700	-0.955092	-0.002106
C	-2.961162	-1.256636	-0.001166
C	-5.509905	1.133400	-0.001942
H	-5.297044	2.203360	-0.002066
H	-6.078487	0.865337	0.890531
H	-6.078344	0.865116	-0.894435
H	-2.600485	-2.274700	-0.001237
H	-2.736251	1.921035	0.000287
N	4.245322	0.402497	-0.001832
N	4.240711	-0.955072	-0.002937
C	2.961176	-1.256653	-0.001501
C	5.509889	1.133419	-0.001589
H	5.297107	2.203290	-0.016577
H	6.084218	0.853983	-0.886787
H	6.072510	0.876546	0.897996
H	2.736209	1.921020	0.001425
H	2.600491	-2.274712	-0.002002
Ag	0.000006	-0.132138	0.002306

Cartesian coordinates for 2:1 complex of 1-methyl-1,2,4-triazole and Hg^{2+}, fully optimized:

C	3.090195	-0.553528	0.618335
N	2.183042	0.161805	-0.088802
N	-2.183044	-0.161673	-0.088699
C	-3.090231	0.553657	0.618389
N	-4.298991	0.136553	0.272231
N	-4.221932	-0.851443	-0.660287
C	-2.943323	-1.017068	-0.865117
C	-5.615967	0.590410	0.747678
H	-5.469414	1.378315	1.486979
H	-6.134139	-0.260859	1.192502
H	-6.179955	0.967472	-0.107234
H	-2.539559	-1.739512	-1.560830
H	-2.883866	1.330681	1.340929
N	4.298975	-0.136471	0.272187
N	4.221946	0.851666	-0.660178
C	2.943348	1.017287	-0.865089
C	5.615926	-0.590332	0.747700
H	5.469361	-1.378987	1.486199
H	6.133680	0.260679	1.193509
H	6.180332	-0.966414	-0.107366
H	2.883804	-1.330632	1.340781
H	2.539607	1.739792	-1.560751
Hg	0.000006	-0.000077	-0.050516

Cartesian coordinates for 2:1 complex of 1-methyl-1,2,4-triazole and Hg^{2+}, cisoid geometry:

C	-3.062829	0.900168	-0.000095
N	-2.189977	-0.135076	-0.000134
N	2.189959	-0.134898	0.000550
C	3.062902	0.900257	0.000862
N	4.289921	0.400528	0.004238
N	4.258713	-0.959529	0.006609
C	2.989088	-1.263438	0.004253
C	5.584615	1.100737	0.007353
H	5.402099	2.175585	-0.006709
H	6.143301	0.795467	-0.879046
H	6.128780	0.816229	0.909637
H	2.620018	-2.279636	0.004916
H	2.820996	1.953612	-0.001437
N	-4.289886	0.400558	0.004724
N	-4.258809	-0.959500	0.008013
C	-2.989213	-1.263531	0.005006
C	-5.584511	1.100904	0.006655
H	-5.401862	2.175739	-0.006643
H	-6.129711	0.816014	0.908188
H	-6.142240	0.796126	-0.880521
H	-2.820827	1.953498	-0.003499
H	-2.620234	-2.279762	0.006101
Hg	-0.000001	-0.075725	-0.004540

Cartesian coordinates for 2:1 complex of 1-methyltetrazole and Ag^+, fully optimized:

C	3.132265	-0.815275	0.000120
N	2.153006	0.077679	-0.000125
N	-2.153001	-0.077795	0.000086
C	-3.132091	0.815348	0.000275
N	-4.288830	0.145246	0.000054
N	-4.016698	-1.182362	-0.000266
N	-2.740137	-1.310751	-0.000253
C	-5.672038	0.625815	0.000241
H	-5.661496	1.716138	-0.000953
H	-6.176561	0.256424	0.894595
H	-6.177347	0.254497	-0.892860
H	-3.029100	1.889913	0.000579
N	4.288879	-0.144953	0.000059
N	4.016488	1.182601	-0.000222
N	2.739898	1.310749	-0.000331
C	5.672178	-0.625262	0.000367
H	5.661840	-1.715588	-0.000664
H	6.176589	-0.255644	0.894689
H	6.177463	-0.253985	-0.892766
H	3.029479	-1.889860	0.000320
Ag	0.000000	-0.000182	-0.000042

Cartesian coordinates for 2:1 complex of 1-methyltetrazole and Ag^+, cisoid geometry:

C	3.154133	-0.886698	0.000714
N	2.156962	-0.014020	-0.001214
N	-2.156935	-0.013613	-0.000702
C	-3.153913	-0.886511	0.001464
N	-4.297231	-0.193540	0.005119
N	-3.998507	1.128425	0.005095
N	-2.720038	1.231156	0.001561
C	-5.690057	-0.645016	0.009233
H	-5.702760	-1.735306	0.002789
H	-6.191227	-0.258628	-0.879802
H	-6.183013	-0.269213	0.907396
H	-3.073873	-1.962842	0.000617
N	4.297291	-0.193468	0.005023
N	3.998247	1.128418	0.005711
N	2.719753	1.230893	0.001954
C	5.690220	-0.644631	0.009308
H	5.703158	-1.734920	0.003147
H	6.183015	-0.268495	0.907416
H	6.191389	-0.258367	-0.879785
H	3.074344	-1.963046	-0.000868
Ag	-0.000003	-0.070251	-0.007299

Cartesian coordinates for 2:1 complex of 1-methyltetrazole and Hg^{2+}, fully optimized:

C	3.232620	-0.885573	0.000021
N	2.195216	-0.042861	0.000123
N	-2.195212	0.042951	0.000061
C	-3.232593	0.885684	0.000035
N	-4.327379	0.130982	-0.001222
N	-3.966217	-1.180495	-0.001924
N	-2.693413	-1.237186	-0.001176
C	-5.755218	0.508193	-0.001451
H	-5.824580	1.595917	-0.004912
H	-6.219303	0.096290	0.896290
H	-6.220236	0.090601	-0.896050
H	-3.203248	1.966462	0.000793
N	4.327383	-0.130842	-0.001272
N	3.966181	1.180623	-0.001954
N	2.693374	1.237285	-0.001154
C	5.755234	-0.508013	-0.001425
H	5.824628	-1.595729	-0.006215
H	6.219013	-0.097199	0.896978
H	6.220531	-0.089307	-0.895355
H	3.203303	-1.966352	0.000759
Hg	0.000001	-0.000070	0.001053

Cartesian coordinates for 2:1 complex of 1-methyltetrazole and Hg^{2+}, cisoid geometry:

C	3.311283	-0.815155	0.000380
N	2.193442	-0.082516	-0.000081
N	-2.193426	-0.082399	0.000740
C	-3.311219	-0.815110	0.001618
N	-4.323652	0.046853	0.001068
N	-3.831070	1.315029	-0.000229
N	-2.559384	1.241985	-0.000485
C	-5.782503	-0.181962	0.001920
H	-6.202746	0.280644	-0.892698
H	-6.201279	0.276385	0.899435
H	-5.963566	-1.256763	-0.000516
H	-3.392907	-1.893011	0.002590
N	4.323660	0.046871	0.001051
N	3.830996	1.315019	0.000969
N	2.559313	1.241888	0.000295
C	5.782525	-0.181850	0.001906
H	5.963659	-1.256628	-0.003588
H	6.200930	0.273921	0.900910
H	6.203080	0.283369	-0.891203
H	3.393039	-1.893052	0.000407
Hg	0.000001	-0.226869	-0.000920