Electronic Supplementary Material (ESI) for New Journal of Chemistry.

A green approach for A^3-coupling reactions: an experimental and theoretical study on NHC silver and gold catalysts

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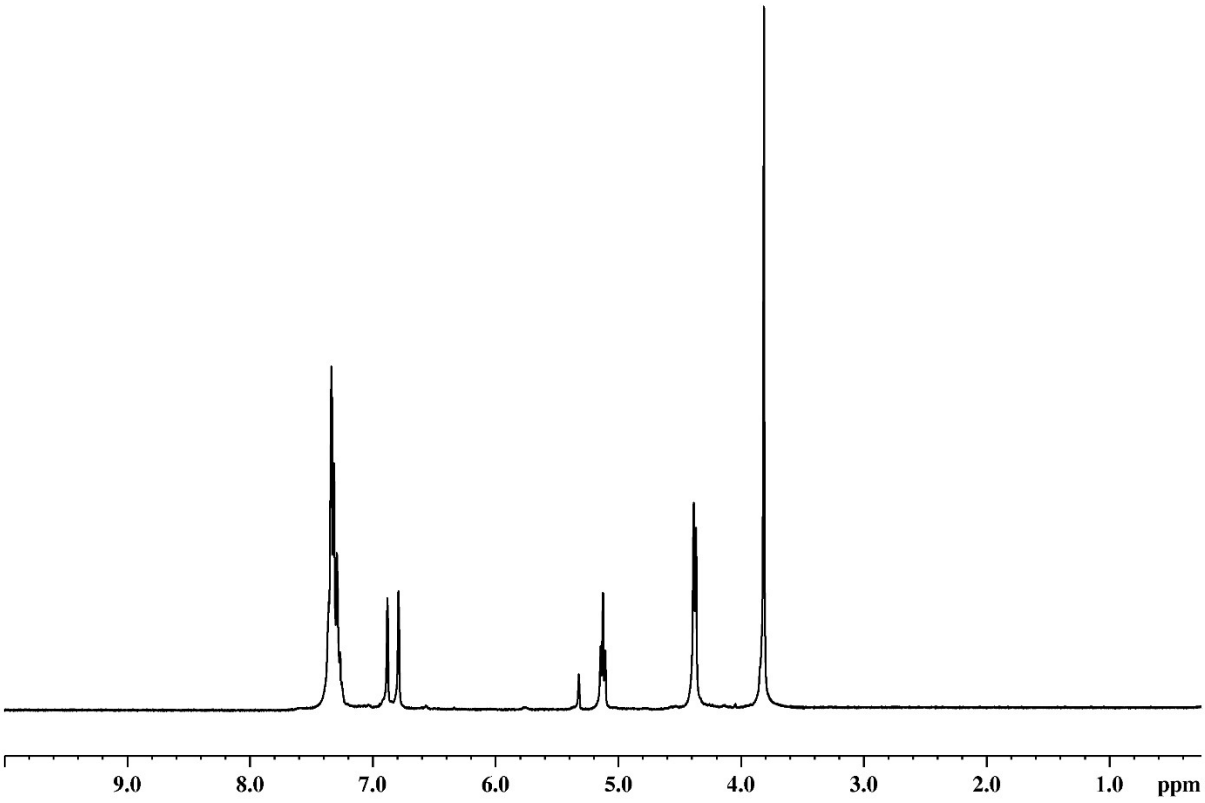
List of contents

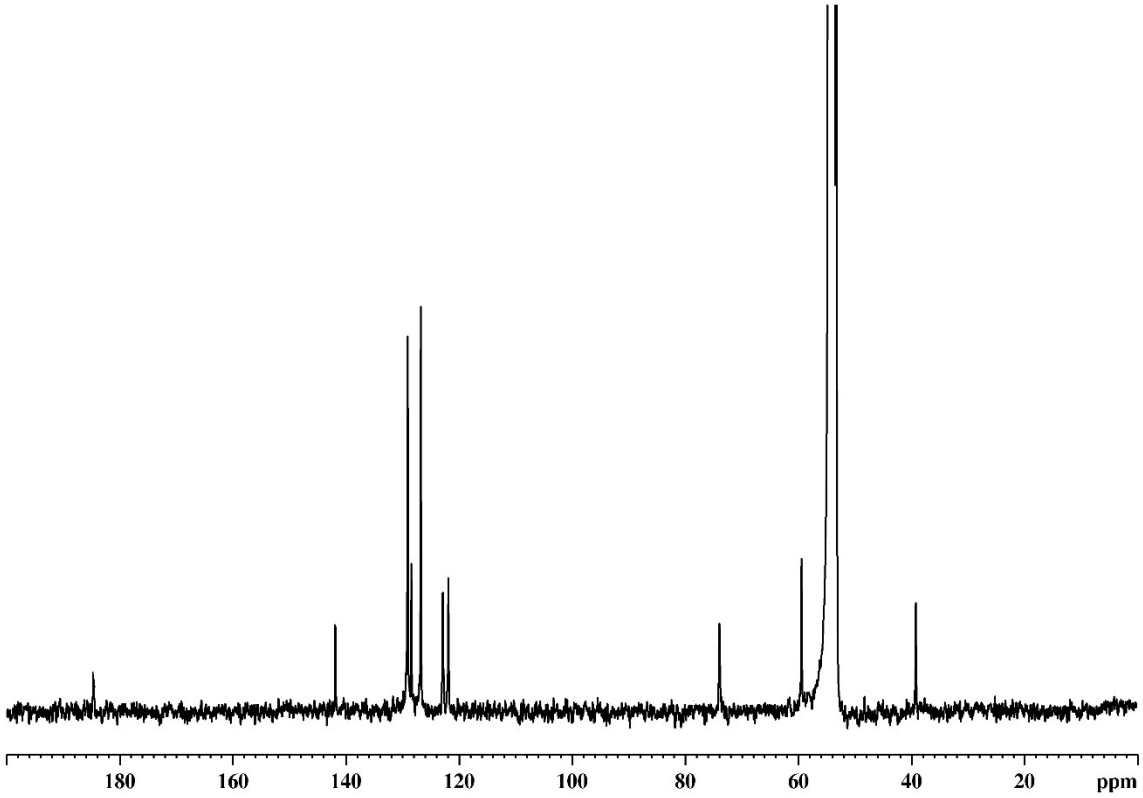
A: ^{1}H-NMR of 3a

^{1}H NMR (CD_2Cl_2, 400 MHz): ppm δ 7.33-7.00 (m, 5H, aromatic protons), 6.89 (s, 1H, C*H*$_{imidazole}$) 6.79 (s, 1H, C*H*$_{imidazole}$), 5.13 (t, 1H, C*H*O^{-}), 4.40 (d, 2H, NC*H*$_2$), 3.82 (s, 3H, NC*H*$_3$).



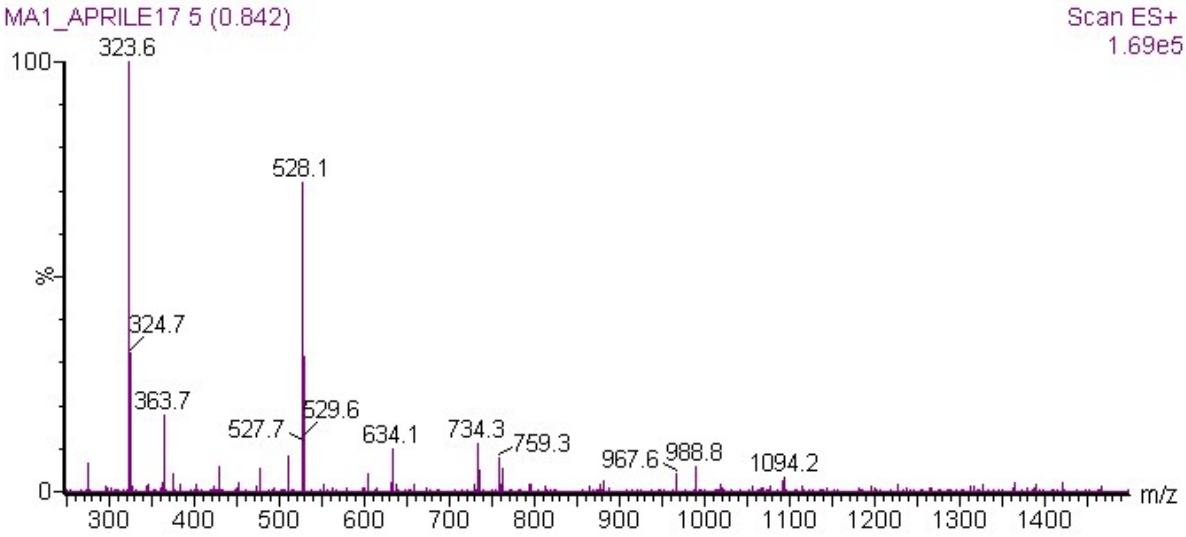
B:^{13}C-NMR of 3a

^{13}C {^{1}H} NMR (CD_2Cl_2, 100 MHz): ppm δ 184.6 (N*C*N), 141.8 (C_{Ar}) 129.1 (C_{Ar}), 128.4 (C_{Ar}), 126.7 (C_{Ar}), 122.8 (N*C*H), 121.8 (N*C*H), 73.9 (*C*HO$^-$), 59.4 (N*C*H$_2$), 39.2 (N*C*H$_3$).



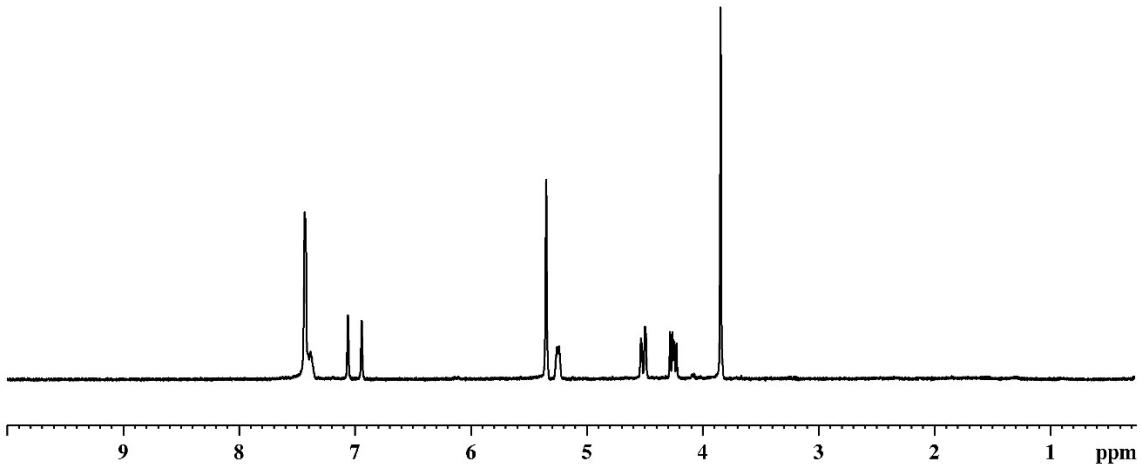
C: ESI-MS of 3a

(ESI): m/z: 528.1 Da attributable to $[C_{22}H_{22}AgN_4O_2Na_2]^+$



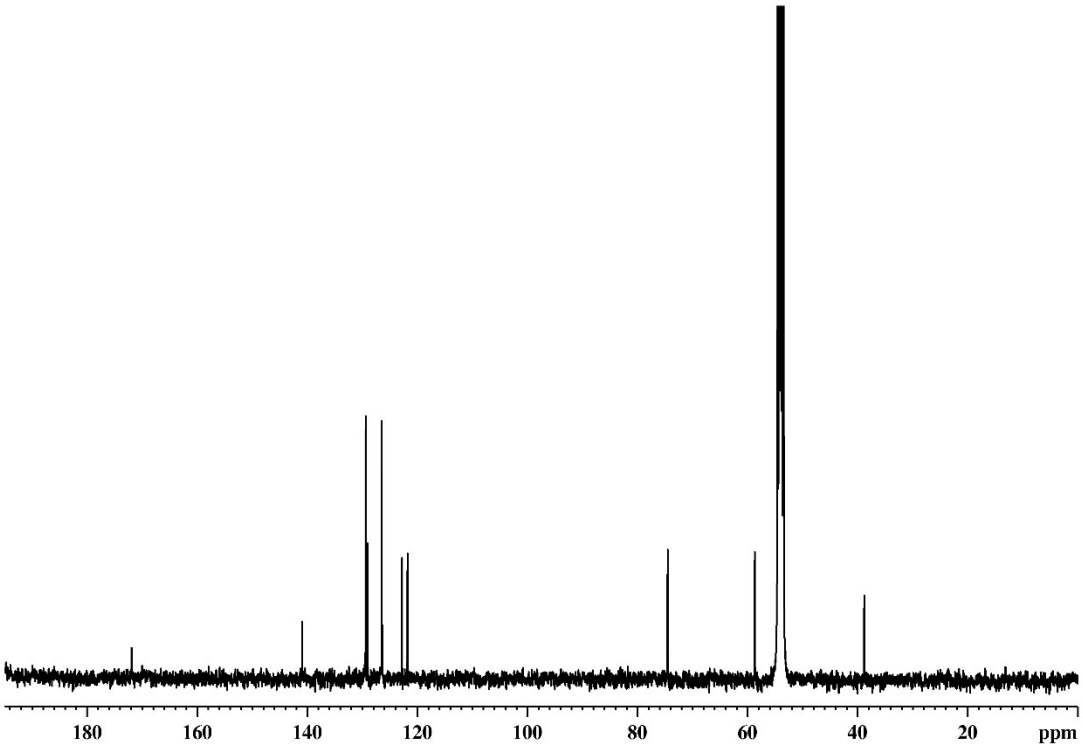
D:^{1}H-NMR of 4a

^{1}H NMR (CD_2Cl_2, 400 MHz): ppm δ 7.40-7.35 (m, 5H, aromatic protons), 7.04 (s, 1H, C$H_{imidazole}$) 6.92 (s, 1H, C$H_{imidazole}$), 5.23 (t, 1H, CHO^{-}), 4.10 (d, 2H, NCH_2), 3.81 (s, 3H, NCH_3).



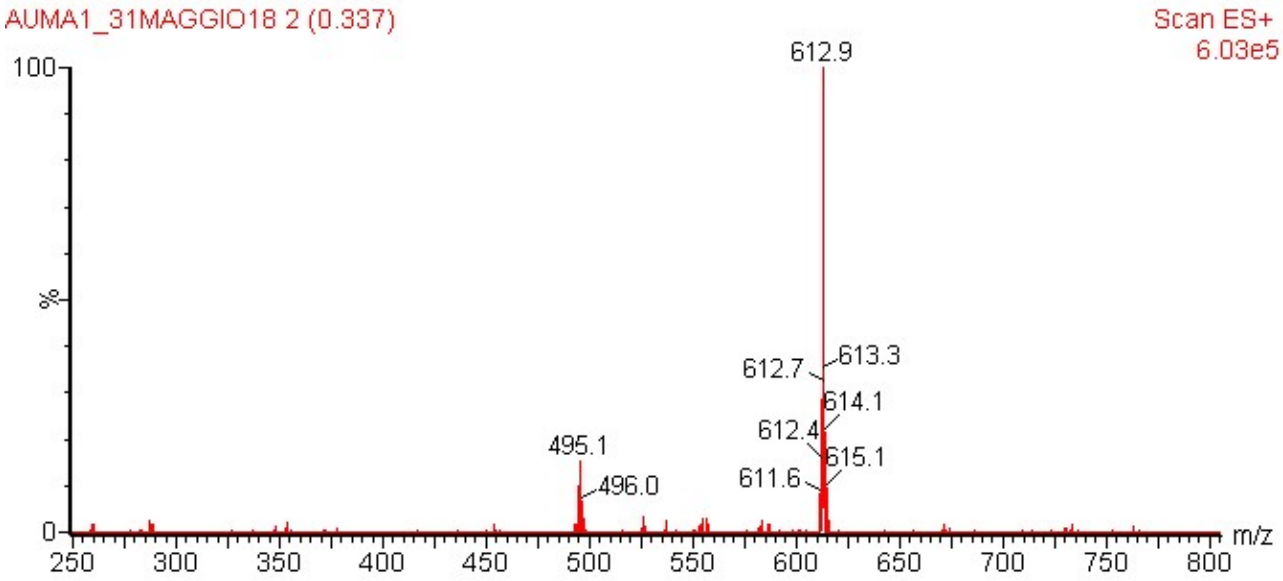
E:^{13}C-NMR of 4a

^{13}C {^{1}H} NMR (CD_2Cl_2, 100 MHz): ppm δ 171.8 (N*C*N), 141.8 (C_{Ar}) 129.5 (C_{Ar}), 129.3 (C_{Ar}), 129.1 (C_{Ar}), 122.9 (N*C*H), 121.8 (N*C*H), 74.5 (*C*HO$^-$), 58.7 (N*C*H$_2$), 38.8 (N*C*H$_3$).



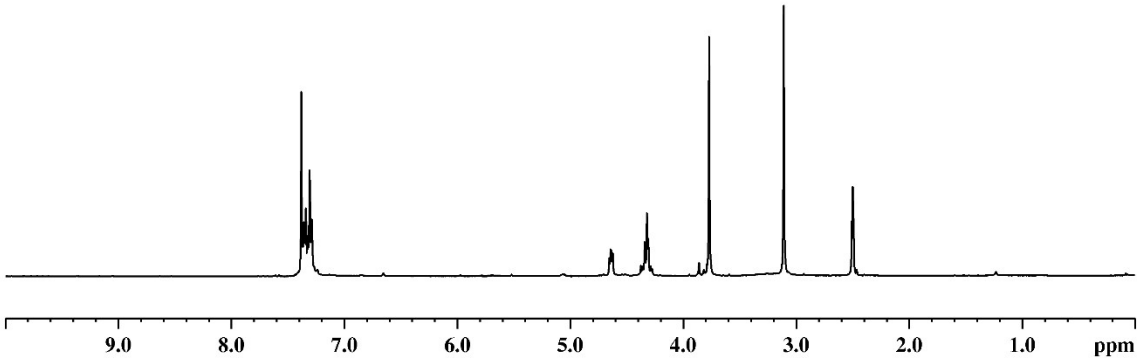
F: ESI-MS of 4a

(ESI): m/z: 612.3 Da attributable to $[C_{22}H_{18}AuN_4O_2Na_2]^+$.



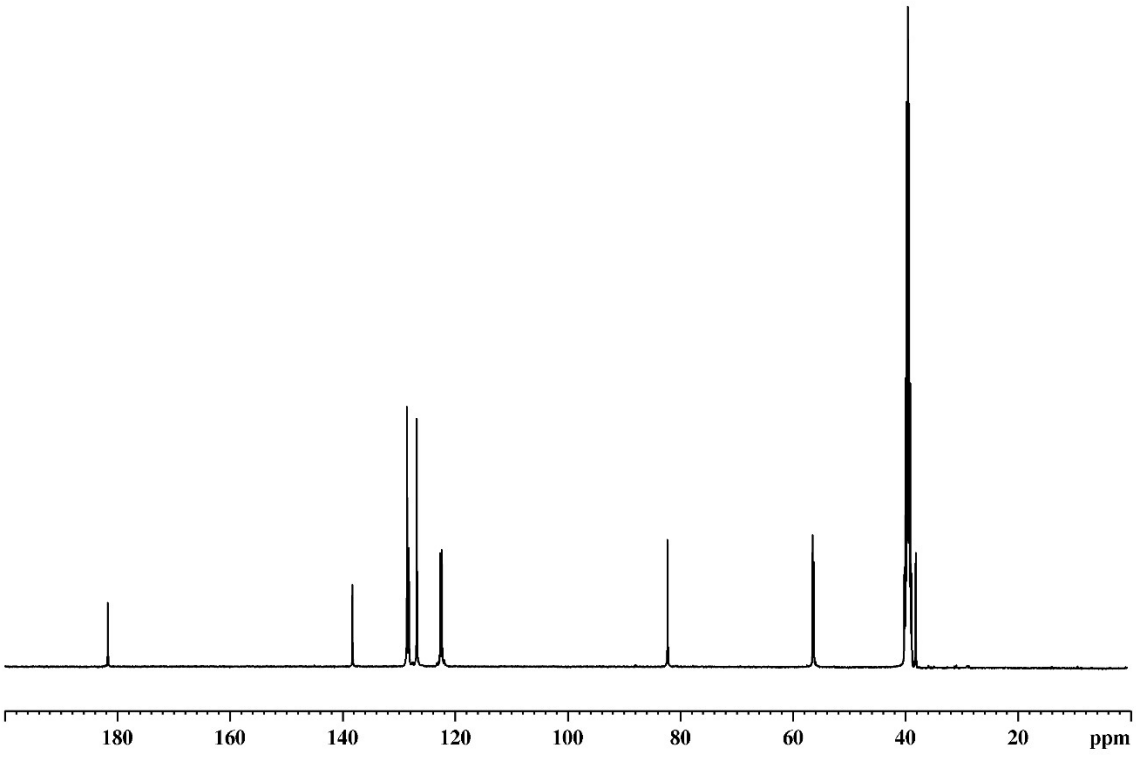
G:^{1}H-NMR of 3b

^{1}H NMR (400 MHz, DMSO-d_6) ppm δ 7.34-7.26 (m, 7H, *aromatic protons*), 4.60 (m, 1H, CH_2CHOCH_3), 4.28 (m, 2H, NCH_2CHOCH_3), 3.74 (s, 3H, CH_3N), 3.07 (s, 3H, $CHOCH_3$).



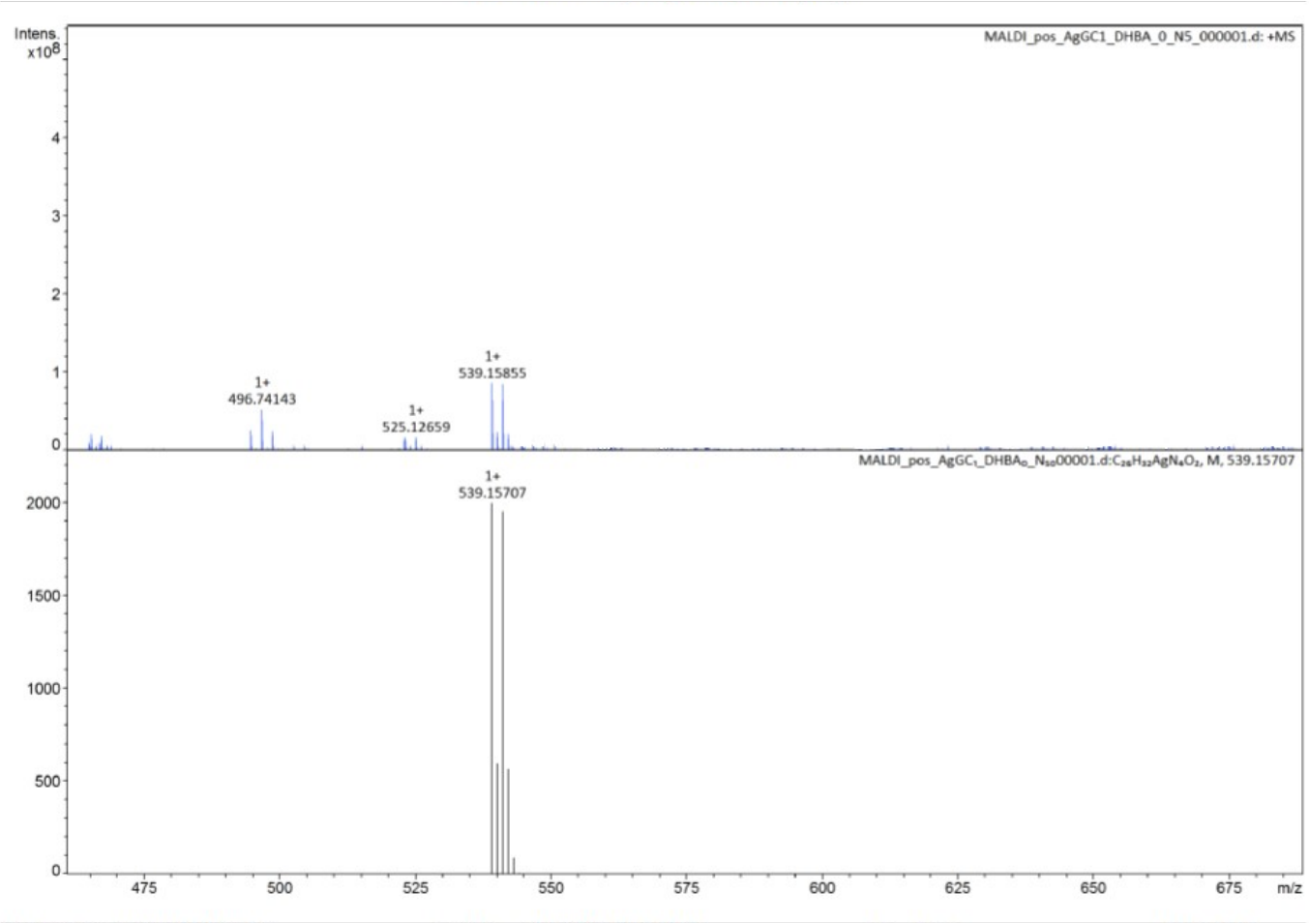
H:^{13}C-NMR of 3b

^{13}C NMR (100 MHz, DMSO-d_6) ppm δ 181.6 (N*C*N), 138.2 (*ipso carbon aromatic ring)*, 128.5, 128.2, 126.8 (*aromatic carbons)*, 122.6, 122.3 (NCH*C*HN), 82.2 (*C*HOCH$_3$), 56.4 (N*C*H$_2$), 56.2 (O*C*H$_3$), 38.1 (N*C*H$_3$).



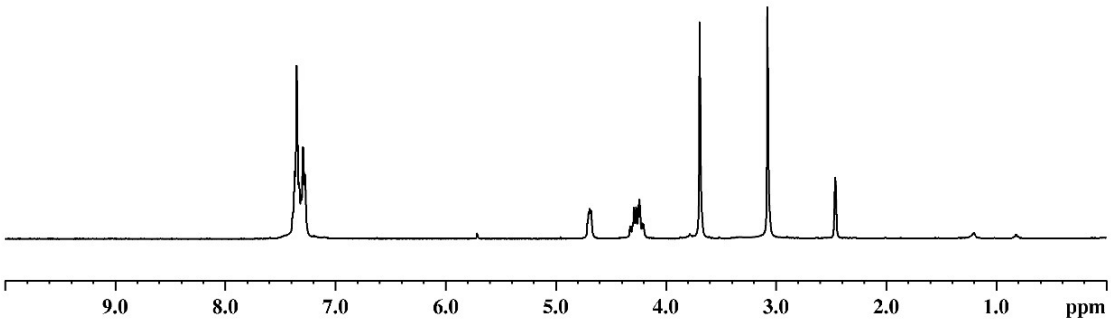
I: MALDI-MS of 3b

(MALDI, CH_2Cl_2): m/z = 539.1 Dalton attributable to $[(C_{26}H_{32}N_4O_2)Ag]^+$.



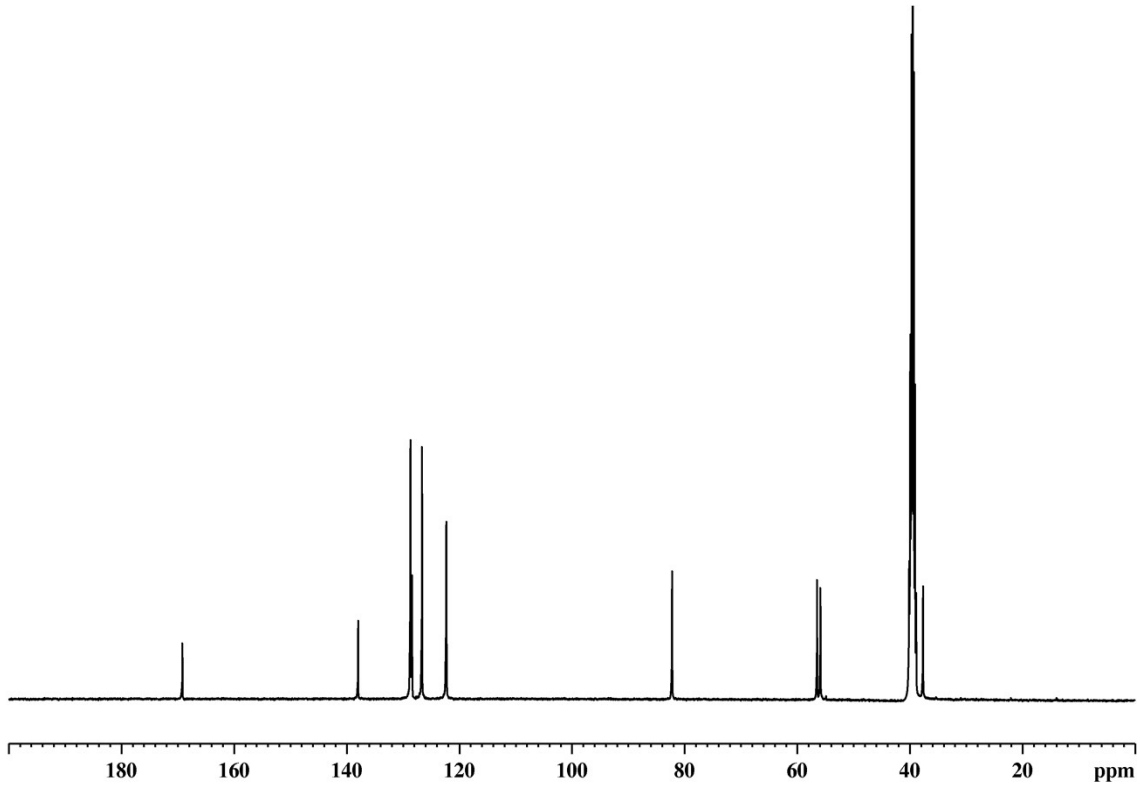
J:^{1}H-NMR of 4b

^{1}H NMR (400 MHz, DMSO-d_6) ppm δ 7.35-7.29 (m, 7H, *aromatic protons*), 4.69 (m, 1H, C*H*OCH$_3$), 4.26 (dd, 2H, NC*H$_2$*CHOCH$_3$), 3.70 (s, 3H, NC*H$_3$*), 3.07 (s, 3H, CHOC*H$_3$*).



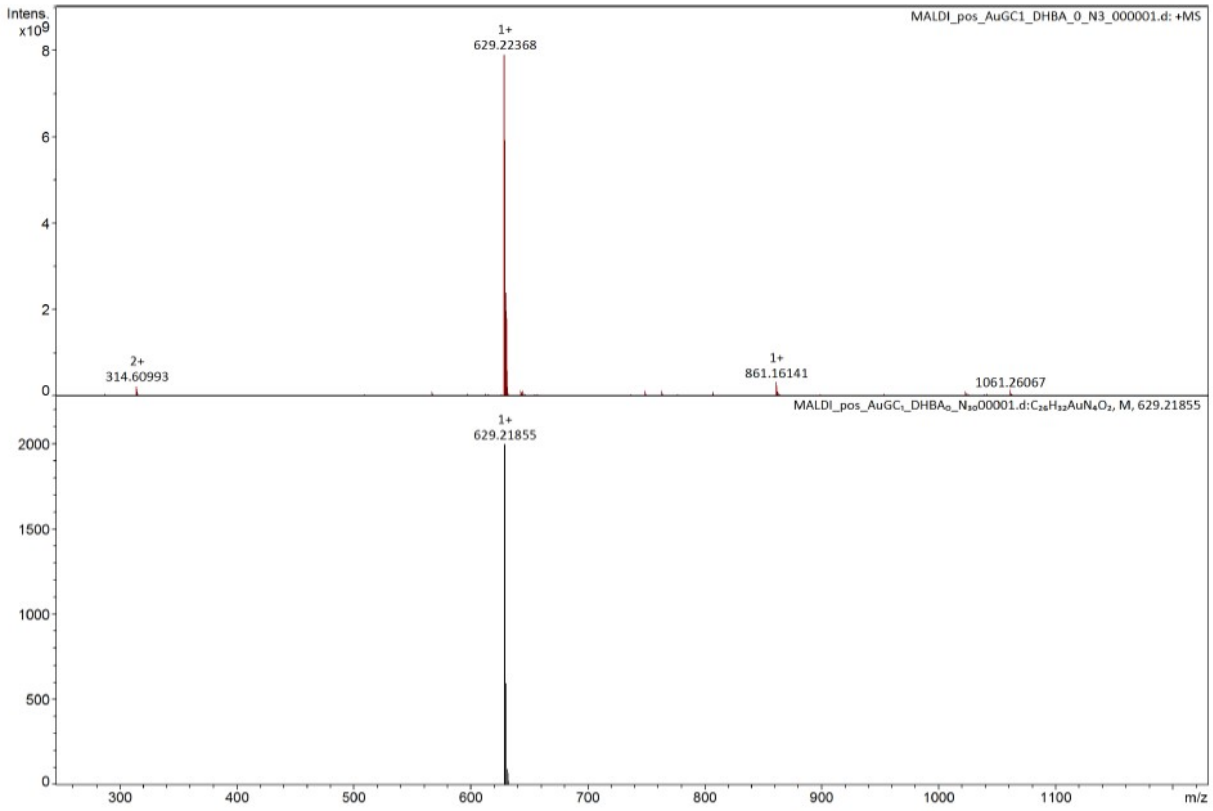
K:^{13}C-NMR of 4b

^{13}C NMR (100 MHz, DMSO-d_6) ppmδ 169.1 (N*C*N), 137.9 (*ipso carbon aromatic ring)*, 128.6, 128.3, 126.6 (*aromatic carbons)*, 122.3, 122.2 (NCH*C*HN), 82.2 (*C*HOCH_3), 56.4 (N*C*H_2), 55.8 (O*C*H_3), 37.6 (N*C*H_3)



L: MALDI-MS of 4b

(MALDI, CH_2Cl_2): m/z = 629.22 attributable to $[(C_{26}H_{32}N_4O_2)Au]^+$.



M: Single Crystal X-Ray Analysis check CIF/PLATON report

Structure factors have been supplied for datablock(s) **4b**

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 4b

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Bond precision:  C-C = 0.0043 A          Wavelength=0.71073

Cell:            a=9.012(3)    b=10.387(4)           c=16.294(5)
                 alpha=90      beta=105.724(13)      gamma=90
Temperature:     296 K

                Calculated                Reported
Volume          1468.2(9)                 1468.2(9)
Space group     P 21/n                    P 21/n
Hall group      -P 2yn                    -P 2yn
Moiety formula  C13 H16 Au Cl N2 O        ?
Sum formula     C13 H16 Au Cl N2 O        C13 H16 Au Cl N2 O
Mr              448.70                    448.69
Dx,g cm-3       2.030                     2.030
Z               4                         4
Mu (mm-1)       10.192                    10.192
F000            848.0                     848.0
F000'           841.31
h,k,lmax        11,13,20                  11,13,20
Nref            3198                      3192
Tmin,Tmax       0.100,0.361               0.125,0.532
Tmin'           0.012

Correction method= # Reported T Limits: Tmin=0.125 Tmax=0.532
AbsCorr = MULTI-SCAN

Data completeness= 0.998          Theta(max)= 26.956

R(reflections)= 0.0166( 2857)     wR2(reflections)= 0.0391( 3192)

S = 1.058                 Npar= 165
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The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT480_ALERT_4_C Long H...A H-Bond Reported H5B ..CL . 2.95 Ang.PLAT480_ALERT_4_C Long H...A H-Bond Reported H4B ..CL . 2.99 Ang.PLAT480_ALERT_4_C Long H...A H-Bond Reported H4C ..CL . 2.97 Ang.

Alert level G

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PLAT793_ALERT_4_G Model has Chirality at C6          (Centro SPGR)          R Verify
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          6 Note
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          3 Info
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0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
5 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
5 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT480_4b
;
PROBLEM: Long H...A H-Bond Reported H5B      ..CL       .       2.95 Ang.
RESPONSE: ...
;
# end Validation Reply Form
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It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

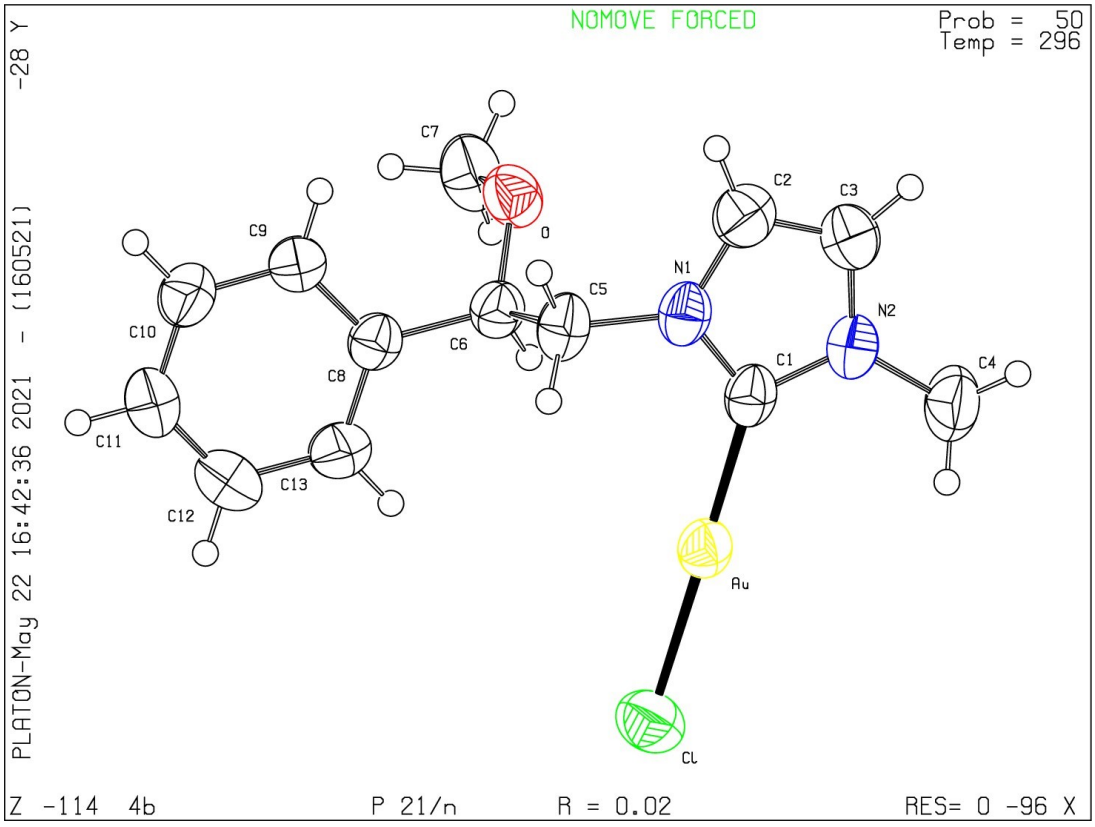
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 16/05/2021; check.def file version of 13/05/2021

Datablock 4b - ellipsoid plot



N: Computational details

Computational details relative to calculations on Ag and Au complexes and BDE of NHC and halogen ligands.

The DFT calculations were performed with the Gaussian09 set of programs,[1] using the PBE0 model.[2] The electronic configuration of the molecular systems was described with 6-311G(d,p) basis set for H, C, N, and O.[3] For Au we used the small-core, quasi-relativistic Stuttgart/Dresden effective core potential, with an associated (8s7p6d)/[6s5p3d] valence basis set contracted according to a (311111/22111/411) scheme (standard SDD keywords in gaussian09).[4] The geometry optimizations were performed without symmetry constraints and the characterization of the located stationary points was performed by analytical frequency calculations. Solvent effects including contributions of non electrostatic terms have been estimated in single-point calculations on the gas phase optimized structures, based on the polarizable continuous solvation model PCM using benzaldehyde as a solvent.[5]

[1] Gaussian 09, Revision A.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; N. Kudin, K.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2009**.

[2] C. Adamo and V. Barone, "Toward reliable density functional methods without adjustable parameters: The PBE0 model," *J. Chem. Phys.*, **110** (1999) 6158-69.

[3] (a) A. D. McLean and G. S. Chandler, "Contracted Gaussian-basis sets for molecular calculations. 1. 2nd row atoms, Z=11-18," *J. Chem. Phys.*, **72** (1980) 5639-48. (b) K. Raghavachari, J. S. Binkley, R. Seeger, and J. A. Pople, "Self-Consistent Molecular Orbital Methods. 20. Basis set for correlated wave-functions," *J. Chem. Phys.*, **72** (1980) 650-54.

[4] a) Haeusermann, U., Dolg, M., Stoll, H. and Preuss, H. *Mol. Phys.* **1993**, *78*, 1211– 1224. b) Kuechle, W., Dolg, M., Stoll, H. and Preuss, H. *J. Chem. Phys.* **1994**, *100*, 7535– 7542. c) Leininger, T., Nicklass, A., Stoll, H., Dolg, M. and Schwerdtfeger, P. *J. Chem. Phys.* 1996, 105, 1052– 1059.

[5] a) Barone, V. and Cossi, M. *J. Phys. Chem. A* **1998**, *102*, 1995– 2001. b) Tomasi, J. and Persico, M. *Chem. Rev.* **1994**, *94*, 2027– 2094.

Cartesian coordinates of calculated structures.

34
2a-A E(gas)=-862.649211575 G(gas)=-862.426149 E(Benzaldehyde)=-862.712289539

Au	1.611725	-0.791844	-0.066594
C	1.269567	1.199907	-0.179614
N	0.084701	1.791521	-0.438482
N	2.137985	2.207622	0.037988
C	0.208901	3.158324	-0.374259
C	1.504112	3.421179	-0.078044
C	3.550337	2.058773	0.347476
H	4.151008	2.565366	-0.409292
H	3.761629	2.482083	1.330560
H	3.795747	0.998245	0.351616
C	-1.174456	1.095436	-0.673364
C	-1.945812	0.814318	0.613706
H	-1.779966	1.707695	-1.342981
H	-0.955360	0.152802	-1.179148
C	-3.304144	0.240125	0.287358
O	-1.136102	-0.060562	1.375120
H	-2.082541	1.766565	1.148044
H	2.021448	4.358201	0.047349
H	-0.619189	3.823953	-0.555074
C	-3.450967	-1.118431	0.009825
C	-4.697759	-1.633329	-0.321636
C	-5.805344	-0.795525	-0.382205
C	-5.665253	0.559023	-0.104017
C	-4.419714	1.073407	0.232509
H	-2.588191	-1.774236	0.068931
H	-4.806501	-2.691944	-0.531439
H	-6.778614	-1.199205	-0.638661
H	-6.529079	1.213801	-0.138471
H	-4.318759	2.129994	0.466730
H	-1.617722	-0.288676	2.175222
C	2.269124	-2.840971	-0.552112
C	1.737741	-2.899495	0.550430
H	2.766971	-3.015147	-1.484890
H	1.324859	-3.179741	1.498615

33
4a-A E(gas)=-862.214952378 G(gas)=-862.001205 E(Benzaldehyde)=-862.232842022

Au	1.282789	-0.855256	0.011966
C	1.284450	1.221716	-0.136940
N	0.189533	1.952142	-0.426667
N	2.263692	2.129804	0.075730
C	0.476375	3.297485	-0.400249
C	1.787071	3.412636	-0.083245
C	3.627735	1.801826	0.430214
H	4.317041	2.165829	-0.335131
H	3.884940	2.245893	1.394307
H	3.699999	0.717758	0.501175
C	-1.133225	1.386812	-0.691995
C	-1.534549	0.332007	0.361147
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H	-1.130732	0.907135	-1.675338
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O	-0.844823	-0.838081	0.224575
H	-1.372822	0.815542	1.349659
H	2.408975	4.283204	0.043569
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C	-3.504722	-1.084661	-0.330781
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C	-5.321525	0.847157	0.499810
C	-3.956661	1.060814	0.644426
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H	-5.225349	-2.231459	-0.910785
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H	-6.027140	1.599952	0.837725
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C	1.935196	-2.817710	0.075135
H	4.007226	-1.969455	-0.278728
H	1.476880	-3.781176	0.206203

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2a-B E(gas)=-1114.33564403 G(gas)=-1113.963249 E(Benzaldehyde)=-1114.39242258

Au	-0.418759	0.387664	-0.773679
C	0.580455	1.827649	0.237388
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N	0.276095	3.138491	0.328342
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C	1.226707	3.805288	1.064397
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H	-0.567621	4.519458	-0.999743
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C	2.484369	0.437292	1.052989
C	3.560911	0.291473	-0.019587
H	2.939363	0.410808	2.044419
H	1.782289	-0.395066	0.974707
C	4.389191	-0.943711	0.245979
O	2.878560	0.251726	-1.255347
H	4.216676	1.174571	0.026513
H	1.166588	4.862319	1.265133
H	3.040561	2.985549	2.030592
C	3.931038	-2.198223	-0.155037
C	4.679222	-3.336029	0.118275
C	5.888213	-3.230347	0.796436
C	6.351073	-1.982294	1.196148
C	5.605101	-0.843635	0.919152
H	2.993289	-2.277086	-0.695831
H	4.319799	-4.308347	-0.201200
H	6.473116	-4.119102	1.006472
H	7.299408	-1.894161	1.714919
H	5.979486	0.131866	1.218648
H	3.528205	0.108096	-1.948916
C	-1.904201	-1.151735	-1.374424
C	-1.070567	-1.089407	-2.276452
H	-2.772085	-1.376350	-0.682134
H	-0.476913	-1.203174	-3.160473
N	-4.196984	-1.734978	0.303569
C	-5.404564	-1.633967	-0.527010
H	-4.128592	-2.684592	0.661711
C	-6.698325	-1.789421	0.265058
H	-5.383840	-0.648469	-1.010565
H	-5.335920	-2.380507	-1.323635
C	-6.740909	-0.805596	1.430662
H	-7.556082	-1.644657	-0.399193

H	-6.766322	-2.816972	0.645892
C	-5.488407	-0.936007	2.292859
H	-6.806166	0.218026	1.038175
H	-7.639101	-0.964733	2.033774
C	-4.230650	-0.807190	1.439695
H	-5.477577	-0.179307	3.083908
H	-5.484336	-1.913627	2.792489
H	-4.168137	0.209832	1.029187
H	-3.329108	-0.965995	2.039969

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2a-BC$^{\neq}$ E(gas)=-1114.32802812 G(gas)=-1113.955483 E(Benzaldehyde)=-1114.38859782

Au	-0.521440	0.731554	-0.577573
C	0.808471	1.950919	0.330281
N	1.967537	1.598136	0.928631
N	0.742088	3.293658	0.457896
C	2.621746	2.708231	1.414667
C	1.848685	3.777140	1.120008
C	-0.331201	4.130682	-0.044008
H	-0.773745	4.702317	0.773781
H	0.050417	4.814150	-0.804762
H	-1.088707	3.486599	-0.488110
C	2.507796	0.249119	0.978741
C	3.609978	0.019194	-0.053202
H	2.892127	0.059997	1.983285
H	1.685876	-0.442655	0.784610
C	4.182436	-1.370409	0.108609
O	3.016525	0.238265	-1.311864
H	4.412402	0.752226	0.127000
H	1.986370	4.825431	1.327703
H	3.564820	2.644831	1.932057
C	3.566598	-2.460686	-0.504460
C	4.076980	-3.741026	-0.330157
C	5.202158	-3.943399	0.460660
C	5.821065	-2.859805	1.072870
C	5.314092	-1.578915	0.894345
H	2.695675	-2.296243	-1.130831
H	3.597438	-4.583850	-0.816678
H	5.601982	-4.942941	0.592581
H	6.706597	-3.011013	1.680678
H	5.812304	-0.732483	1.360167
H	3.675887	0.061833	-1.987956
C	-1.976433	-0.560135	-1.396585
C	-1.581590	-0.536923	-2.564983
H	-3.065672	-1.155759	-0.382265
H	-1.279264	-0.551989	-3.591609
N	-3.903059	-1.579014	0.237727
C	-5.056870	-1.865500	-0.653908
H	-3.563166	-2.452728	0.639845
C	-6.248189	-2.378177	0.136552
H	-5.289940	-0.925072	-1.161911
H	-4.716685	-2.575479	-1.410458
C	-6.618883	-1.413779	1.259799
H	-7.087370	-2.522263	-0.548989
H	-6.014278	-3.366643	0.552642
C	-5.412328	-1.128415	2.149723
H	-6.983711	-0.473773	0.827607
H	-7.438630	-1.823345	1.854764
C	-4.233879	-0.630258	1.330968

H	-5.653619	-0.379660	2.908863
H	-5.122532	-2.038089	2.691469
H	-4.460777	0.325167	0.848659
H	-3.332016	-0.494057	1.931719

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2a-C E(gas)=-1114.34999001 G(gas)=-1113.973965 E(Benzaldehyde)=-1114.41661568

Au	-0.555473	0.683104	-0.733567
C	0.639771	1.941917	0.339467
N	1.771607	1.629051	1.008712
N	0.505735	3.277617	0.489713
C	2.340946	2.754383	1.560831
C	1.540975	3.794827	1.235807
C	-0.565031	4.077621	-0.074719
H	-1.099813	4.603178	0.718690
H	-0.158549	4.801263	-0.783559
H	-1.250202	3.412193	-0.598021
C	2.375359	0.307180	1.049081
C	3.511773	0.152072	0.039668
H	2.743811	0.117089	2.059278
H	1.593670	-0.419562	0.819453
C	4.136722	-1.217174	0.177992
O	2.937768	0.382907	-1.224759
H	4.277980	0.912372	0.260523
H	1.616708	4.843183	1.473089
H	3.250049	2.720949	2.138443
C	3.590110	-2.311035	-0.491762
C	4.149460	-3.573814	-0.339910
C	5.253692	-3.754988	0.484803
C	5.803295	-2.667444	1.153719
C	5.247979	-1.403845	0.997720
H	2.735963	-2.162295	-1.144737
H	3.725197	-4.418996	-0.871579
H	5.692066	-4.740515	0.598618
H	6.672974	-2.801495	1.787895
H	5.692750	-0.552910	1.507394
H	3.611924	0.241755	-1.894537
C	-1.688590	-0.517027	-1.853260
C	-2.341011	-1.230371	-2.598374
H	-3.022216	-1.313594	-0.662706
H	-2.857759	-1.828321	-3.316407
N	-3.608644	-1.543533	0.190205
C	-4.732361	-2.444694	-0.197667
H	-2.990187	-2.036267	0.836142
C	-5.601808	-2.762273	1.005261
H	-5.295192	-1.913590	-0.970277
H	-4.294172	-3.337173	-0.648694
C	-6.098460	-1.487006	1.680567
H	-6.438182	-3.382467	0.673185
H	-5.030565	-3.369343	1.719434
C	-4.929805	-0.574855	2.042619
H	-6.779504	-0.956683	1.003858
H	-6.675431	-1.734726	2.574450
C	-4.069207	-0.275768	0.829077
H	-5.285801	0.372014	2.456585
H	-4.315117	-1.042322	2.822852
H	-4.628689	0.264145	0.060323
H	-3.175209	0.305477	1.064263

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4a-B E(gas)=-1113.89417512 G(gas)=-1113.531252 E(Benzaldehyde)=-1113.90804885

Au	1.512771	-0.897299	-0.318114
C	2.551705	0.846774	0.116329
N	2.001866	2.077669	0.055674
N	3.784620	1.042735	0.637015
C	2.876834	3.029834	0.527094
C	4.004428	2.378130	0.894828
C	4.741401	-0.011665	0.894425
H	5.666409	0.173854	0.343809
H	4.958619	-0.075864	1.963013
H	4.296048	-0.947640	0.559470
C	0.649466	2.358327	-0.421283
C	-0.426991	1.493870	0.274175
H	0.471049	3.421950	-0.248565
H	0.600674	2.163048	-1.496775
C	-1.768145	2.147612	-0.031938
O	-0.396565	0.190212	-0.133707
H	-0.251324	1.610061	1.365643
H	4.927928	2.745624	1.310597
H	2.626545	4.077345	0.558242
C	-2.476822	1.779387	-1.173629
C	-3.682866	2.395949	-1.485531
C	-4.201390	3.382906	-0.653941
C	-3.505643	3.749174	0.492536
C	-2.296793	3.134700	0.797882
H	-2.071138	0.987529	-1.794417
H	-4.226048	2.099153	-2.377599
H	-5.147631	3.857521	-0.893018
H	-3.910455	4.508083	1.154991
H	-1.762016	3.414695	1.702632
C	2.099595	-2.877431	-0.781115
C	0.846336	-2.834896	-0.731224
H	3.045901	-3.360335	-0.932218
H	-0.215936	-3.075385	-0.721247
N	-2.081835	-2.268859	-0.066357
C	-2.288290	-2.680255	1.315692
H	-1.668276	-1.329045	-0.076743
C	-3.377983	-1.889234	2.039326
H	-2.558570	-3.746966	1.318632
H	-1.333413	-2.592990	1.844790
C	-4.684363	-1.941528	1.250730
H	-3.519944	-2.281017	3.053780
H	-3.051540	-0.846119	2.137710
C	-4.458042	-1.486621	-0.188892
H	-5.061928	-2.974268	1.249166
H	-5.453198	-1.328287	1.732911
C	-3.320862	-2.282060	-0.831514
H	-5.375778	-1.599524	-0.778831
H	-4.199070	-0.420712	-0.198067
H	-3.637045	-3.329403	-0.947895
H	-3.108315	-1.905043	-1.837340

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4a-BC$^{\neq}$ E(gas)=-1113.88736978 G(gas)=-1113.525878 E(Benzaldehyde)=-1113.90212604

Au	1.608976	-0.825748	-0.452137
C	2.473138	0.917442	0.154026
N	1.832004	2.105434	0.207969
N	3.650200	1.128139	0.789399

C	2.591638	3.041024	0.872817
C	3.741057	2.427358	1.238012
C	4.670813	0.120138	0.976748
H	5.630644	0.483060	0.602171
H	4.765036	-0.138164	2.034136
H	4.367467	-0.763871	0.416284
C	0.492939	2.344212	-0.312751
C	-0.603113	1.561710	0.457301
H	0.320606	3.422507	-0.271744
H	0.465963	2.020945	-1.356920
C	-1.937307	2.125294	-0.026455
O	-0.487897	0.223785	0.273035
H	-0.497516	1.867744	1.523339
H	4.604950	2.801776	1.761688
H	2.257547	4.054892	1.018251
C	-2.523422	1.613207	-1.183120
C	-3.722806	2.127705	-1.659582
C	-4.361458	3.159390	-0.978603
C	-3.789623	3.672217	0.179758
C	-2.585038	3.158063	0.648380
H	-2.023934	0.794024	-1.690847
H	-4.165661	1.720487	-2.563694
H	-5.302706	3.556488	-1.345038
H	-4.286950	4.469188	0.724245
H	-2.146411	3.554314	1.561472
C	1.735182	-2.835578	-1.347667
C	0.576211	-2.686210	-0.915302
H	2.607630	-3.249420	-1.808675
H	-0.643298	-2.515118	-0.425641
N	-1.775706	-2.097105	0.171393
C	-1.922846	-2.707645	1.491917
H	-1.501900	-1.085540	0.276614
C	-3.138566	-2.174403	2.240455
H	-2.012316	-3.794993	1.360568
H	-1.000884	-2.519008	2.048982
C	-4.402261	-2.339525	1.399745
H	-3.239374	-2.691251	3.201065
H	-2.978495	-1.111847	2.460315
C	-4.221334	-1.702693	0.024382
H	-4.618358	-3.410305	1.279111
H	-5.264552	-1.902143	1.913016
C	-2.969826	-2.243333	-0.658855
H	-5.096641	-1.888738	-0.607585
H	-4.126492	-0.615192	0.128685
H	-3.099781	-3.310568	-0.886089
H	-2.786219	-1.730993	-1.607773

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4a-C E(gas)=-1113.93967151 G(gas)=-1113.574277 E(Benzaldehyde)=-1113.95965933

Au	1.942812	-0.663424	-0.573554
C	2.176577	1.197938	0.217984
N	1.292961	2.218001	0.136862
N	3.187386	1.677937	0.976698
C	1.737266	3.311787	0.844291
C	2.935904	2.973630	1.371756
C	4.373529	0.926699	1.332708
H	5.268349	1.443155	0.978708
H	4.428107	0.797269	2.415726
H	4.308326	-0.051082	0.856828

C	0.009158	2.133098	-0.536009
C	-1.147242	1.878936	0.445322
H	-0.159860	3.062519	-1.087736
H	0.093062	1.317366	-1.255889
C	-2.472771	1.851661	-0.290679
O	-0.922614	0.755730	1.242118
H	-1.175578	2.731957	1.136755
H	3.623796	3.538391	1.978903
H	1.176167	4.229634	0.905022
C	-2.657842	1.084643	-1.442249
C	-3.894116	1.041542	-2.074816
C	-4.966977	1.762231	-1.563333
C	-4.795693	2.527047	-0.416021
C	-3.556720	2.570147	0.211399
H	-1.836622	0.501801	-1.847937
H	-4.019877	0.440207	-2.969353
H	-5.932600	1.726798	-2.056748
H	-5.628153	3.091313	-0.008277
H	-3.427576	3.163420	1.112270
C	1.328578	-3.586341	-1.729923
C	1.603164	-2.478865	-1.306144
H	1.116371	-4.558080	-2.111843
H	-0.552669	-2.127597	-0.178331
N	-1.340723	-1.862595	0.410971
C	-1.150923	-2.452035	1.737717
H	-1.120733	-0.096062	0.767312
C	-2.290813	-2.041388	2.659972
H	-1.104755	-3.553421	1.676325
H	-0.190367	-2.105864	2.129477
C	-3.637661	-2.445114	2.064466
H	-2.150185	-2.499707	3.644655
H	-2.254506	-0.954596	2.794925
C	-3.777817	-1.913335	0.640715
H	-3.710726	-3.541443	2.047498
H	-4.459832	-2.085473	2.692050
C	-2.581927	-2.327590	-0.205015
H	-4.700268	-2.281173	0.178906
H	-3.837521	-0.818812	0.655936
H	-2.578668	-3.426627	-0.316561
H	-2.654342	-1.900750	-1.209337