Supplementary Information for:

Hydration of alkynes at room temperature catalyzed by gold (I) isocyanide compounds

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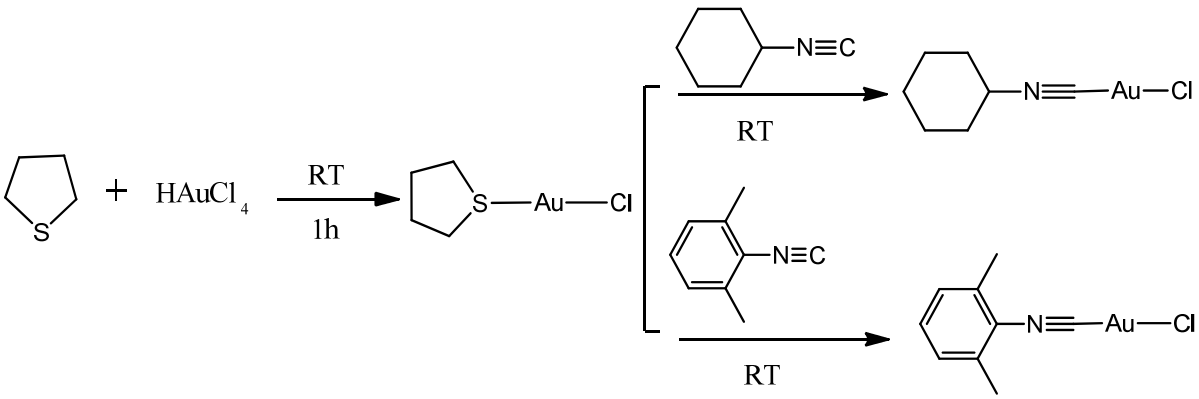
1. Experimental

1.1 Materials and methods

All solvents and chemicals were commercially available and used without further purification unless otherwise stated.

^{1}H NMR spectra were determined on a Bruker DPX 300 MHz spectrometer, using $CDCl_3$ as solvents with TMS as the internal standard. Elemental analysis was taken on an Elementar vario EL II. The purity of raw materials and the reaction solution was analyzed using a GC5890C gas chromatography fitted with a SE-50 column (50 m, 0.25 lm diameters) and a flame ionisation detector. The structure and content of the product and byproducts were further identified using a HP6890 GC/MS spectrometer by comparing retention times and fragmentation patterns with authentic samples.

1.2 Synthetic Procedures



(A) Preparation of (tht) AuCl: $HAuCl_4.4H_2O$ (1g, 2.4mmol) was dissolved in H_2O/C_2H_5OH (20ml, 4:1) and excessive amounts of tetrahydrothiophene were added slowly dropwise under stirring. The yellow solution became displayed white turbidity. (tht)

AuCl was filtered off and dried in thermostatic vacuum drier. (tht) AuCl was obtained as a colourless powder (Yield: 65%).

(B) Preparation of (CyNC)AuCl and (2,6-$Me_2C_6H_3NC$)AuCl: (tht) AuCl (0.5g,1.5mmol) was dissolved in THF (20ml), then a solution of cyclohexyl isonitrile (0.2g,1.8mmol) or 2,6-dimethyphenyl isocyanide (0.2g,1.5mmol) in THF was added. The reaction mixture was stirred for 12h at ambient temperature. The solvent was removed and the resulting precipitate was recrystallized with THF/light petroleum (1:10) (Yield: 55%, 67%).

Cat-1: ^{1}H NMR (300 MHz, $CDCl_3$): δ = 1.45-1.57 (m, 4H), 1.75-1.84 (m, 4H), 1.99-2.05 (m, 2H),3.88-3.94 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 22.6, 24.5, 31.5, 54.9; Elemental analysis of $C_7H_{11}AuClN$: Calc. C 24.61, H 3.25, N 4.10; Found C 24.99, H 3.41, N 4.10. MS (m/z): $[M+NH_4]^+$ calcd for $[C_7H_{11}AuClN+NH_4]^+$, 359.06; found, 359.10.

Cat-2: ^{1}H NMR (300 MHz, $CDCl_3$) δ = 2.47 (s, 6H), 7.18-7.20(d, 2H),7.34-7.39(t, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ = 18.7,128.5,131,136.2,144.9; Elemental analysis of C_9H_9AuClN: Calc. C 29.73, H 2.49, N 3.85; Found C 29.84, H 2.71, N 3.74. MS (m/z): $[M+NH_4]^+$ calcd for $[C_9H_9AuClN+NH_4]^+$, 381.04; found, 381.05.

All NMR data are in accordance with previous reports. [31, 34, 38]

2. General Procedures for Hydration Reactions

Akynes (1.0 mmol), methanol (1.0 ml), H_2O (1.0 ml), Cat-1 or Cat-2 (0.05mmol) and $KB(C_6F_5)_4$ (0.05mmol) were added to a 10ml screw-cap vial. The reaction mixture was stirred at room temperature for 24h. The product was isolated by extraction using ether (Note: for large practical application, separation by distillation is a more green choice),

followed by removing the solvent under reduced pressure at room temperature. Catalyst can be further separated by flash chromatography on silica gel (eluent: ether).

3. The ^{13}C NMR, ^{1}H NMR and MS data of the products

1b: ^{13}C NMR (75 MHz, $CDCl_3$) δ 197.71, 136.95, 132.93, 128.43, 128.14, 26.34; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.89 – 7.87 (d, 2H), 7.50 – 7.45 (t, 1H), 7.39 – 7.34 (t, 2H), 2.50 (s, 3H); MS calculated m/e for C_8H_8O: 120.1, found: 120.1 (Relative abundance: 30%). Calculated [M-CH_3]: 105.1, found: 105.0 (Relative abundance: 100%)

2b: ^{13}C NMR (75 MHz, $CDCl_3$) δ 198.07, 143.96, 134.93, 128.46, 128.06, 26.52, 21.62; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.87 – 7.84 (d, 2H), 7.27 – 7.24 (d, 2H), 2.58 (s, 3H), 2.41 (s, 3H). MS calculated m/e for $C_9H_{10}O$: 134.1, found: 134.1 (Relative abundance: 32%). Calculated [M-CH_3]: 119.1, found: 119.0 (Relative abundance: 100%)

3b: MS calculated m/e for $C_9H_{10}O$: 134.1, found: 134.2 (Relative abundance: 25%). Calculated [M-$COCH_3$]: 91.1, found: 91.2 (Relative abundance: 100%)

4b: MS calculated m/e for $C_{10}H_{12}O$: 148.1, found: 148.0 (Relative abundance: 24%). Calculated [M-CH_3]: 133.1, found: 132.9 (Relative abundance: 100%)

5b: ^{13}C NMR (75 MHz, $CDCl_3$) δ 197.28, 163.65, 130.64, 130.13, 113.71, 55.42, 26.24; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.92 – 7.89 (d, 2H), 6.91 – 6.88 (d, 2H), 3.83 (s, 3H), 2.53 (s, 3H). MS calculated m/e for $C_9H_{10}O_2$: 150.1, found: 150.1 (Relative abundance: 29%). Calculated [M-CH_3]: 135.1, found: 135.0 (Relative abundance: 100%)

6b: MS calculated m/e for C_8H_7ClO: 154.0, found: 154.0 (Relative abundance: 32%). Calculated [M-CH_3]: 139.0, found: 139.0 (Relative abundance: 100%)

7b: MS calculated m/e for $C_9H_7F_3O$: 188.0, found: 188.2 (Relative abundance: 10%). Calculated [M-CH_3]: 173.0, found: 173.1 (Relative abundance: 100%)

8b: ^{13}C NMR (75 MHz, $CDCl_3$) δ 200.47, 159.01, 133.99, 130.34, 127.93, 120.54, 111.72, 55.49, 31.73. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.73 – 7.70 (d, 1H), 7.49 – 7.43 (t, 1H), 7.00 – 6.95 (t, 2H), 3.89 (s, 3H), 2.61 (s, 3H). MS calculated m/e for $C_9H_{10}O_2$: 150.1, found: 150.4 (Relative abundance: 10%). Calculated [M-CH_3]: 135.1, found: 135.3 (Relative abundance: 100%)

9b: ^{13}C NMR (75 MHz, $CDCl_3$) δ 214.57, 51.52, 28.41, 27.87, 25.75, 25.51. ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.37-2.31 (br, 1H), 2.13 (s, 3H), 1.86 – 1.65 (m, 4H), 1.35 – 1.17 (m, 6H). MS calculated m/e for $C_8H_{14}O$: 126.1, found: 126.1 (Relative abundance: 21%). Calculated [M-CH_3]: 111.1, found: 111.1 (Relative abundance: 8%)

10b: ^{13}C NMR (75 MHz, $CDCl_3$) δ 199.81, 141.55, 139.49, 26.07, 25.02, 22.88, 21.83, 21.42. ^{1}H NMR (300 MHz, $CDCl_3$) δ 6.90 – 6.87 (t, 1H), 2.22 (s, 3H), 2.20 – 2.15 (m, 4H), 1.58 – 1.53 (m, 4H). MS calculated m/e for $C_8H_{12}O$: 124.1, found: 124.1 (Relative abundance: 68%). Calculated [M-CH_3]: 109.1, found: 109.1 (Relative abundance: 100%)

11b: MS calculated m/e for C_5H_9ClO: 120.0, found: 120.3 (Relative abundance: 20%). Calculated [M-CH_3]: 105.0, found: 105.3 (Relative abundance: 26%)

12b: ^{13}C NMR (75 MHz, $CDCl_3$) δ 210.06, 44.62, 42.68, 31.73, 29.85, 20.95. ^{1}H NMR (300 MHz, $CDCl_3$) δ 3.52 – 3.48 (t, 2H), 2.50 – 2.45 (t, 2H), 2.14 (s, 3H), 1.74 – 1.68 (m, 4H).

13b: ^{13}C NMR (75 MHz, $CDCl_3$) δ 208.31, 43.22, 29.31, 25.61, 21.95, 13.66. ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.35 – 2.30 (t, 2H), 2.03 (s, 3H), 1.50 – 1.40 (m, 2H), 1.27 – 1.15 (m,

2H), 0.83 – 0.78 (t, 3H). MS calculated m/e for $C_6H_{12}O$: 100.1, found: 100.1 (Relative abundance: 15%). Calculated [M-CH_3]: 85.1, found: 85.1 (Relative abundance: 11%). Calculated [M-C_4H_9]: 43.0, found: 43.1 (Relative abundance: 100%)

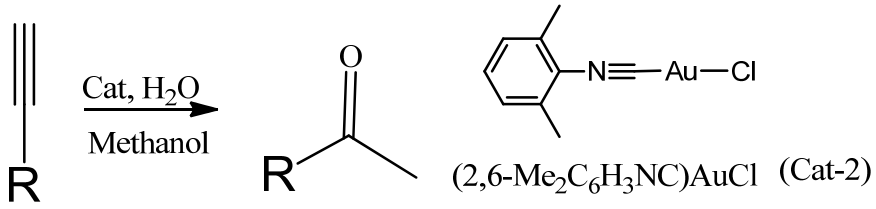
14b: ^{13}C NMR (75 MHz, $CDCl_3$) δ 207.92, 43.44, 31.33, 29.22, 28.73, 23.43, 22.17, 13.94. ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.34 – 2.29 (t, 2H), 2.02 (s, 3H), 1.48 – 1.41 (m, 2H), 1.18 (br, 6H), 0.80 – 0.75 (t, 3H). MS calculated m/e for $C_8H_{16}O$: 128.1, found: 128.1 (Relative abundance: 8%). Calculated [M-CH_3]: 113.1, found: 113.1 (Relative abundance: 4%). Calculated [M-C_6H_{13}]: 43.0, found: 43.0 (Relative abundance: 100%)

15b: ^{13}C NMR (75 MHz, $CDCl_3$) δ 210.03, 43.67, 31.73, 29.60, 29.28, 29.07, 29.05, 23.78, 22.54, 13.92. ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.38 – 2.33 (t, 2H), 2.06 (s, 3H), 1.51 – 1.47 (m, 2H), 1.20 (br, 10H), 0.83 – 0.78 (t, 3H). MS calculated m/e for $C_{10}H_{20}O$: 156.2, found: 156.2 (Relative abundance: 6%). Calculated [M-CH_3]: 141.1, found: 141.2 (Relative abundance: 3%).

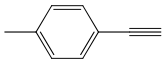
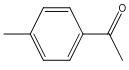
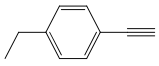
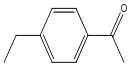
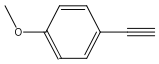
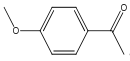
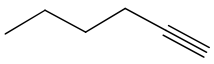
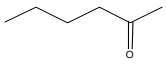
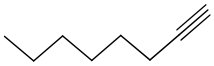
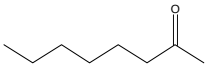
16b: ^{13}C NMR (75 MHz, $CDCl_3$) δ 209.92, 42.38, 29.79, 17.49. ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.47 – 2.42 (t, 4H), 2.10 (s, 6H), 1.81 – 1.71 (m, 2H). MS calculated m/e for $C_7H_{12}O_2$: 128.1, found: 128.4 (Relative abundance: 7%). Calculated [M-CH_3]: 113.1, found: 113.3 (Relative abundance: 5%).

17b: ^{13}C NMR (75 MHz, $CDCl_3$) δ 209.87, 43.20, 29.76, 22.95. ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.40 (br, 4H), 2.07 (s, 6H), 1.51– 1.44 (m, 4H).

4. Table S1 Hydration of various alkynes catalyzed by Cat-2 [a]



$(2,6\text{-}Me_2C_6H_3NC)AuCl$ (Cat-2)

Entry	Reactant	Product	Yield (%)[b]
1	 2a	 2b	99
2	 4a	 4b	>99 (95)
3	 5a	 5b	97
4	 11a	 11b	>99 (96)
5	 12a	 12b	96

[a] Reaction condition: alkyne (1.0 mmol), Cat-2 (0.05mmol), $KB(C_6F_5)_4$ (0.05mmol), H_2O(1.0 ml), methanol (1.0 ml), room temperature, 24h. [b] Yield determined by GC with biphenyl as internal standard. Isolated yields are shown in parenthesis

5. Computational Methods:

All the geometries were fully optimized with Gaussian 03 program using B3LYP method based on density functional theory [S1]. LANL2DZ basis set was used for Au and 6-31+G* basis set for other atoms. Energy calculations as well as Zero-point energies (ZPE) correction have been performed at the same theory. All energies reported in this work are corrected by ZPE. The computed stationary points have been characterized as minima or transition states by diagonalizing the Hessian matrix and analyzing the vibrational normal modes. In this way, the stationary points can be classified as minima if no imaginary frequencies are shown or as transition states if only one imaginary frequency is obtained.

The particular nature of the transition states has been determined by analyzing the motion described by the eigenvector associated with the imaginary frequency.

Reference:

(S1) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Pittsburgh PA, **2003**.

6. Cartesians coordinates of the optimized structures

Cat-1^+

C 0	1.132858	0.930649	-0.585648
C 0	1.132858	2.469803	-0.585648
C 0	-0.322464	0.418488	-0.585648
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Au 0	-0.314407	-4.134277	-0.479477
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H 0	1.666200	0.539520	-1.459412
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H 0	2.170425	2.819168	-0.542496
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H 0	0.813873	2.784866	1.534714
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H 0	-2.170441	0.580536	0.550827
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Rea

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N 0 0.013046 0.993011 -2.529053
C 0 -0.000137 -0.166504 -2.499756
Au 0 -0.052032 -2.162064 -2.472580
C 0 -0.532837 -5.590698 2.523941
C 0 0.793823 -5.793808 2.127350
C 0 1.178650 -5.524673 0.817734
C 0 0.231995 -5.047333 -0.117142
C 0 -1.104187 -4.846252 0.295883
C 0 -1.479706 -5.116257 1.606430
C 0 0.639816 -4.790482 -1.492050
C 0 -0.194885 -4.309784 -2.545990
O 0 1.921707 -5.038315 -1.725250
H 0 1.982529 2.583725 -1.648743
H 0 2.008011 2.569229 -3.418289
H 0 1.057724 4.863388 -3.496400
H 0 2.508713 4.853775 -2.503265
H 0 -0.467500 2.719528 -3.486359
H 0 0.638489 6.163956 -1.430893
H 0 1.152817 4.813721 -0.425797
H 0 -0.353836 2.604874 -0.424957
H 0 -1.823364 2.602798 -1.411072
H 0 -1.316803 4.884827 -2.252335
H 0 -1.326279 4.887329 -0.493820
H 0 -0.831085 -5.803421 3.546677
H 0 1.525574 -6.163956 2.838867
H 0 2.205536 -5.685898 0.510696
H 0 -1.849304 -4.476212 -0.399918
H 0 -2.508713 -4.961090 1.915924
H 0 0.152695 -4.583649 -3.546677
H 0 -1.257202 -4.515594 -2.423600
H 0 2.157364 -4.884247 -2.658020

TS2
C 0 0.955338 -5.240234 -0.932037

C 0	0.840347	-6.729752	-1.299194
C 0	-0.430862	-4.695511	-0.529922
C 0	-0.209763	-6.967987	-2.395203
C 0	-1.486618	-4.900833	-1.635162
C 0	-1.577820	-6.393570	-1.995651
N 0	-0.330902	-3.291855	-0.198227
C 0	-0.244720	-2.163834	0.047974
Au 0	-0.072357	-0.216263	0.482651
C 0	0.405396	7.032379	2.161560
C 0	1.658691	6.506042	1.819611
C 0	1.777832	5.165253	1.472153
C 0	0.633972	4.337387	1.464966
C 0	-0.623734	4.875214	1.810379
C 0	-0.734192	6.218719	2.157013
C 0	0.783279	2.937637	1.099411
C 0	-0.354416	1.934387	1.048538
O 0	1.872574	2.407272	0.785568
H 0	1.322998	-4.666916	-1.793365
H 0	1.664825	-5.093475	-0.109726
H 0	0.576660	-7.307434	-0.401535
H 0	1.823547	-7.090256	-1.622238
H 0	-0.764053	-5.186035	0.393539
H 0	-0.300200	-8.040985	-2.599030
H 0	0.124924	-6.498184	-3.331451
H 0	-1.190903	-4.317245	-2.517090
H 0	-2.457321	-4.520554	-1.296814
H 0	-1.977890	-6.952316	-1.137300
H 0	-2.300659	-6.516830	-2.810104
H 0	0.945679	1.260773	0.664780
H 0	0.316864	8.080719	2.432678
H 0	2.537048	7.144302	1.825974
H 0	2.740707	4.741928	1.205353
H 0	-1.510742	4.248138	1.808640
H 0	-1.701782	6.633240	2.422897
H 0	-0.823593	1.785080	2.027023
H 0	-1.113846	2.202393	0.306000

Int1’

C 0	-0.526718	3.232773	0.381622
C 0	-0.526718	4.771164	0.381622
C 0	-1.978912	2.713730	0.381622
C 0	-1.339996	5.341827	1.553772
C 0	-2.796555	3.253891	1.572388
C 0	-2.774780	4.791672	1.562302

N 0	-1.991562	1.267334	0.394028
C 0	-2.005325	0.109665	0.422852
Au 0	-2.047333	-1.827866	0.447159
C 0	2.761749	-3.855743	-0.382614
C 0	2.027985	-3.771561	0.804550
C 0	0.663971	-4.067581	0.808884
C 0	0.019791	-4.451660	-0.383453
C 0	0.763184	-4.524231	-1.575531
C 0	2.126938	-4.233566	-1.570892
C 0	-1.408432	-4.800476	-0.389969
C 0	-2.045456	-5.742416	-1.086105
O 0	-2.157500	-3.974960	0.514908
H 0	-0.017502	2.855820	1.278580
H 0	0.007874	2.841537	-0.491516
H 0	-0.941422	5.135712	-0.569366
H 0	0.509811	5.124496	0.423355
H 0	-2.469467	2.995438	-0.558945
H 0	-1.359879	6.436081	1.496567
H 0	-0.844208	5.086777	2.501770
H 0	-2.353668	2.876129	2.503616
H 0	-3.824402	2.877258	1.518387
H 0	-3.317230	5.158188	0.678787
H 0	-3.323181	5.158905	2.437134
H 0	3.824417	-3.630554	-0.382156
H 0	2.520508	-3.491760	1.731476
H 0	0.108673	-4.038589	1.742004
H 0	0.267929	-4.794830	-2.503632
H 0	2.692810	-4.294128	-2.496017
H 0	-3.124680	-5.868073	-1.057083
H 0	-1.483154	-6.436096	-1.699890
H 0	-3.041367	-4.353775	0.669174

TS2’

C 0	-0.473480	-3.036500	1.533783
C 0	-0.455475	-4.323608	2.375977
C 0	-1.926010	-2.549194	1.358200
C 0	-1.356400	-5.412567	1.772934
C 0	-2.832275	-3.623260	0.723541
C 0	-2.792984	-4.905197	1.572098
N 0	-1.955597	-1.345657	0.558000
C 0	-1.986786	-0.390991	-0.098251
Au 0	-2.046570	1.225372	-1.174515
C 0	2.691208	4.405228	-2.271469
C 0	2.061951	3.264236	-2.786789

C 0	0.673782	3.174713	-2.779541
C 0	-0.097458	4.229507	-2.239822
C 0	0.547668	5.379074	-1.728424
C 0	1.935333	5.462158	-1.746063
C 0	-1.534271	4.158356	-2.213303
C 0	-2.533051	5.131241	-2.228333
O 0	-2.181534	2.954422	-2.371918
H 0	-0.044144	-3.229324	0.541534
H 0	0.127213	-2.251129	2.006958
H 0	-0.786300	-4.094193	3.399338
H 0	0.577927	-4.679535	2.456894
H 0	-2.333969	-2.255356	2.333923
H 0	-1.359161	-6.296219	2.421265
H 0	-0.943359	-5.734924	0.805893
H 0	-2.471924	-3.831833	-0.292694
H 0	-3.856262	-3.241791	0.638794
H 0	-3.256363	-4.709579	2.550003
H 0	-3.407547	-5.671158	1.085693
H 0	3.775300	4.475189	-2.286972
H 0	2.655807	2.459778	-3.209991
H 0	0.177139	2.316620	-3.221222
H 0	-0.045944	6.183258	-1.304047
H 0	2.431778	6.342529	-1.349548
H 0	-3.337250	5.029495	-1.493210
H 0	-2.351578	6.145096	-2.572952
H 0	-3.065094	3.816025	-2.708420

Int1'-W

C 0	2.664642	-0.752060	3.377975
C 0	2.636169	-1.584671	4.671448
C 0	1.224182	-0.429169	2.932434
C 0	1.786560	-2.855042	4.513931
C 0	0.370605	-1.699173	2.742279
C 0	0.362854	-2.522049	4.041870
N 0	1.244598	0.337341	1.707123
C 0	1.263900	0.930191	0.711639
Au 0	1.280396	1.925369	-0.950333
C 0	-1.908875	-0.374283	-4.479263
C 0	-0.514404	-0.387344	-4.380219
C 0	0.178467	0.784409	-4.070236
C 0	-0.521042	1.987564	-3.856308
C 0	-1.924454	1.988739	-3.948013
C 0	-2.611084	0.816238	-4.262878
C 0	0.201859	3.238266	-3.563416

C 0	-0.100098	4.474411	-3.969330
O 0	1.358704	3.019730	-2.767990
H 0	3.162537	-1.315598	2.577591
H 0	3.225281	0.178314	3.524277
H 0	2.235153	-0.971039	5.491165
H 0	3.664642	-1.840698	4.950348
H 0	0.748840	0.225220	3.674362
H 0	1.747711	-3.398666	5.464798
H 0	2.265076	-3.528061	3.787567
H 0	0.800354	-2.292023	1.923798
H 0	-0.648163	-1.421051	2.448990
H 0	-0.165344	-1.960617	4.826157
H 0	-0.212967	-3.439728	3.876358
H 0	-2.446075	-1.285965	-4.725113
H 0	0.036362	-1.306580	-4.559418
H 0	1.263870	0.774429	-4.029419
H 0	-2.475433	2.905167	-3.756805
H 0	-3.695206	0.829758	-4.330872
H 0	0.471436	5.343811	-3.661316
H 0	-0.926559	4.633911	-4.651596
H 0	1.989456	3.792404	-2.782410
O 0	3.233154	4.925873	-2.746475
H 0	3.853928	5.019897	-3.487259
H 0	3.280411	5.749863	-2.235855

TS2’-W

C 0	2.716064	-1.867600	3.037628
C 0	3.803970	-2.949997	3.146225
C 0	1.883347	-2.088364	1.758865
C 0	4.686752	-3.000168	1.889740
C 0	2.756638	-2.112564	0.488190
C 0	3.843552	-3.192856	0.619888
N 0	0.872925	-1.062347	1.640793
C 0	0.081726	-0.221008	1.536133
Au 0	-1.237915	1.185181	1.338943
C 0	-1.441269	2.730957	-3.661362
C 0	-0.590500	2.910690	-2.566879
C 0	-1.120667	3.125458	-1.293167
C 0	-2.513290	3.174927	-1.104721
C 0	-3.362015	3.016296	-2.213196
C 0	-2.826965	2.783783	-3.481232
C 0	-3.073517	3.447693	0.243179
C 0	-4.049973	4.400970	0.461060
O 0	-2.691498	2.681686	1.275360

H 0	3.177612	-0.872253	2.989304
H 0	2.059540	-1.883713	3.915115
H 0	3.329391	-3.929489	3.303528
H 0	4.411774	-2.753510	4.036743
H 0	1.330048	-3.032715	1.840988
H 0	5.418793	-3.810959	1.979263
H 0	5.261948	-2.066223	1.808853
H 0	3.221115	-1.125229	0.362778
H 0	2.127579	-2.295395	-0.390594
H 0	3.371170	-4.185867	0.636658
H 0	4.479172	-3.167114	-0.272598
H 0	-1.027222	2.561127	-4.651062
H 0	0.486954	2.899139	-2.705597
H 0	-0.450241	3.309677	-0.457352
H 0	-4.439621	3.060486	-2.081619
H 0	-3.492752	2.647766	-4.328674
H 0	-4.148788	4.836044	1.457047
H 0	-4.366287	5.031082	-0.362015
O 0	-5.089905	2.509964	1.985748
H 0	-4.059494	2.351013	1.968796
H 0	-5.564316	1.707916	1.692032
H 0	-5.051666	3.268005	1.185867

Pro

C 0	1.129837	3.533783	1.742310
C 0	1.129837	5.072021	1.742310
C 0	-0.321274	3.011627	1.742310
C 0	0.316040	5.642014	2.914398
C 0	-1.138779	3.552979	2.932709
C 0	-1.118317	5.090942	2.921829
N 0	-0.326111	1.566177	1.758270
C 0	-0.321533	0.408203	1.803268
Au 0	-0.319504	-1.527863	1.886124
C 0	-0.322922	-4.698227	-2.778717
C 0	0.346756	-3.693039	-2.070251
C 0	0.283707	-3.661331	-0.680573
C 0	-0.440582	-4.645615	0.024200
C 0	-1.083755	-5.672195	-0.700653
C 0	-1.038589	-5.685394	-2.092468
C 0	-0.508759	-4.632431	1.491821
C 0	-0.777283	-5.899323	2.258011
O 0	-0.350510	-3.597015	2.187424
H 0	1.639145	3.157013	2.639328

H 0	1.665390	3.142563	0.869629
H 0	0.714615	5.436539	0.791519
H 0	2.166153	5.426102	1.784409
H 0	-0.812256	3.291931	0.801590
H 0	0.295731	6.736374	2.857849
H 0	0.811234	5.386673	3.862595
H 0	-0.694885	3.176407	3.863876
H 0	-2.166153	3.174911	2.880066
H 0	-1.659882	5.456482	2.037277
H 0	-1.667969	5.458572	3.795746
H 0	-0.277069	-4.718124	-3.863876
H 0	0.925797	-2.944458	-2.602768
H 0	0.837616	-2.899307	-0.140259
H 0	-1.640839	-6.445190	-0.181473
H 0	-1.554703	-6.466827	-2.641830
H 0	-1.837585	-6.169708	2.159775
H 0	-0.186111	-6.736389	1.875244
H 0	-0.565140	-5.737305	3.316162

Rea”

C	-4.96137000	1.30719900	0.03519400
C	-6.49686000	1.31238700	-0.03928400
C	-4.40801600	-0.05335200	-0.43315400
C	-7.10955300	0.14858000	0.75607100
C	-4.99894300	-1.22259800	0.37925000
C	-6.53444000	-1.20277000	0.30267200
N	-2.97510300	-0.06102600	-0.35244300
C	-1.81176000	-0.06140300	-0.27214700
Au	0.17370500	-0.04740800	-0.15138100
C	7.62280100	0.08346600	0.26303400
C	6.94898000	-1.13449600	0.12028700
C	5.55661200	-1.16601900	0.04387400
C	4.80454300	0.02675000	0.10895000
C	5.49665400	1.24858400	0.25320900
C	6.88915100	1.27312400	0.32900700
C	3.37895500	-0.00107700	0.03039200
C	2.15487100	-0.02270700	-0.03734700
H	-4.63239400	1.48078900	1.06859200
H	-4.53650000	2.10881100	-0.57993000
H	-6.81104700	1.24280000	-1.09148600
H	-6.87296300	2.27268200	0.33372700
H	-4.65339900	-0.19403000	-1.49454400
H	-8.20086600	0.14971200	0.64436200
H	-6.90329000	0.29109700	1.82721800

H	-4.67148300	-1.12375900	1.42299600
H	-4.60012600	-2.17148500	0.00228700
H	-6.85084000	-1.40707600	-0.73106900
H	-6.93673100	-2.01732000	0.91697700
H	8.70811500	0.10532200	0.32196000
H	7.51069700	-2.06420900	0.06787500
H	5.03324400	-2.11126700	-0.06733600
H	4.92676200	2.17182900	0.30440500
H	7.40408700	2.22451200	0.44014400

TS1”

C	5.20404900	-0.74998300	0.37272100
C	6.70348700	-0.42258100	0.28305600
C	4.38452600	0.27620700	-0.43450400
C	6.99976400	1.01736800	0.73198400
C	4.65637600	1.72046300	0.03076000
C	6.15890400	2.03406100	-0.05660300
N	2.98320300	-0.02203700	-0.34572000
C	1.84592500	-0.26555400	-0.26449400
Au	-0.10478200	-0.63682400	-0.13739000
C	-6.38857700	2.28008900	0.16644900
C	-5.09896100	2.63824300	-0.24230400
C	-4.08408200	1.68351800	-0.28846000
C	-4.34850400	0.34549000	0.07922000
C	-5.64685900	-0.00834500	0.48827400
C	-6.65437400	0.95602000	0.53027700
C	-3.24820600	-0.58059300	0.04245200
C	-2.06639800	-1.05257600	-0.01021200
O	-4.02821100	-2.46542500	0.28291900
H	4.87197100	-0.71807200	1.41907600
H	5.00063300	-1.75982500	-0.00188600
H	7.04537000	-0.56123400	-0.75347100
H	7.26621800	-1.13888500	0.89367900
H	4.64630100	0.18691700	-1.49753900
H	8.06757600	1.23742800	0.61068000
H	6.77835800	1.11663400	1.80495900
H	4.30862500	1.82531400	1.06727300
H	4.07396400	2.42012000	-0.57981100
H	6.47175300	2.02967200	-1.11136400
H	6.33718500	3.05024600	0.31532600
H	-7.17854000	3.02618500	0.19805000
H	-4.88256000	3.66412000	-0.53038300
H	-3.08339200	1.96041100	-0.60725300
H	-5.82608000	-1.03999300	0.76985200

H	-7.65357100	0.66981800	0.84927000
H	-4.44792000	-2.82006000	-0.52343400
H	-2.67722500	-2.19302700	0.11579100

Int1”

C	4.29022600	0.75755400	1.29864900
C	5.78695600	1.10257800	1.35664600
C	4.01008100	-0.22718900	0.14596900
C	6.29852700	1.64467800	0.01239800
C	4.50215000	0.31977500	-1.20884100
C	5.99756400	0.66817000	-1.13568300
N	2.60969000	-0.53215700	0.08294600
C	1.46535200	-0.75742200	0.03818300
Au	-0.50288400	-1.12598800	-0.01910000
C	-3.65084000	3.56747000	-0.13044900
C	-2.67174700	2.86319700	-0.83894000
C	-2.64438700	1.46794200	-0.80739700
C	-3.58602300	0.74422200	-0.05473000
C	-4.58162500	1.46306700	0.63308800
C	-4.60782100	2.85883100	0.60233400
C	-3.56525400	-0.73840900	0.00636500
C	-2.48992700	-1.55616800	-0.03209800
O	-4.86262000	-1.22591500	0.14070200
H	3.69859400	1.66772100	1.13160700
H	3.95154700	0.32058800	2.24514400
H	6.35866600	0.20315700	1.63037300
H	5.95838200	1.83390200	2.15581800
H	4.52073100	-1.17708700	0.35497000
H	7.37698900	1.83755700	0.06988400
H	5.81701500	2.61149300	-0.19664400
H	3.91761300	1.21612200	-1.45668300
H	4.31001900	-0.41962200	-1.99500600
H	6.58121900	-0.25385300	-0.99454600
H	6.31669400	1.09321400	-2.09505900
H	-3.67482400	4.65421600	-0.15936200
H	-1.93634600	3.40124100	-1.43294700
H	-1.90063400	0.92774500	-1.38452000
H	-5.32992900	0.91743000	1.19814600
H	-5.37999600	3.39360900	1.15061300
H	-4.81192500	-2.18692000	0.26676300
H	-2.73227300	-2.62480800	0.00117300

TS2”

C	-4.28765400	1.35834500	-0.81777600

C	-5.77630200	1.74132600	-0.79430900
C	-4.08136400	-0.03996500	-0.20212100
C	-6.36269700	1.65551800	0.62378800
C	-4.64981600	-0.12633900	1.22837500
C	-6.13628200	0.26577100	1.23972800
N	-2.68945100	-0.38586700	-0.20803000
C	-1.55229200	-0.65205200	-0.20258700
Au	0.40701600	-1.08463000	-0.22204300
C	4.35616800	3.37761000	0.00595200
C	3.28867400	2.84877500	-0.72859200
C	2.99665000	1.48664500	-0.65529200
C	3.76365400	0.63821900	0.16309800
C	4.83103800	1.18092200	0.90400300
C	5.12872000	2.54084400	0.81956000
C	3.49575200	-0.80835400	0.22951100
C	2.37861100	-1.58823900	-0.19073500
O	4.37545100	-1.58000800	0.81678600
H	-3.70226100	2.08460000	-0.23782800
H	-3.89594500	1.36981200	-1.84151900
H	-6.33642800	1.07080900	-1.46311100
H	-5.89591700	2.75376400	-1.19884400
H	-4.58496600	-0.78553300	-0.83244100
H	-7.43463200	1.88822100	0.60275600
H	-5.88814100	2.41711100	1.26026200
H	-4.07566500	0.55241200	1.87338800
H	-4.50868200	-1.14082300	1.61876700
H	-6.71571500	-0.48230900	0.67821400
H	-6.50974100	0.23729100	2.27054600
H	4.58523000	4.43886800	-0.05524000
H	2.69129400	3.49685100	-1.36492000
H	2.18305600	1.06267400	-1.23516800
H	5.41198500	0.52272600	1.54170400
H	5.95612900	2.95109200	1.39294200
H	2.67313400	-2.32330200	-0.95108000
H	3.35835500	-2.36149600	0.66928400