SUPPORTING INFORMATION – XYZ STRUCTURES

Reactants

17
LAuH scalar

C	4.393262	-1.762505	7.081148
C	4.812023	-1.670532	5.790757
N	3.735999	-1.196472	5.061225
C	2.644910	-0.984888	5.852851
N	3.075167	-1.341597	7.097599
C	3.746961	-0.948236	3.626919
Au	0.773863	-0.285601	5.295354
C	2.235546	-1.279403	8.285101
H	5.768119	-1.898692	5.338340
H	4.913089	-2.086372	7.973184
H	2.132661	-2.280441	8.723286
H	2.672256	-0.587056	9.016273
H	1.253295	-0.911260	7.966665
H	3.957667	-1.880615	3.087521
H	2.750618	-0.580133	3.355691
H	4.501864	-0.189326	3.384392
H	-0.682851	0.258578	4.861478

17
LAuH SOC

C	4.389227	-1.762564	7.079979
C	4.808536	-1.669984	5.789660
N	3.732955	-1.195894	5.059719
C	2.641387	-0.985025	5.851187
N	3.070248	-1.344873	7.095744
C	3.744014	-0.945433	3.625805
Au	0.775661	-0.285925	5.296031
C	2.231626	-1.275870	8.283583
H	5.764256	-1.899730	5.337293
H	4.908377	-2.087919	7.971855
H	2.182869	-2.261687	8.763225
H	2.633037	-0.531670	8.983582
H	1.231162	-0.971646	7.954483
H	3.975794	-1.872605	3.086201
H	2.741148	-0.597271	3.352101
H	4.483894	-0.170750	3.386783
H	-0.681376	0.259159	4.863910

Interatomic distance O2 scalar= 1.235 Å

Interatomic distance O2 SOC= 1.235 Å

Product

```
   19
LAuOOH scalar
C        -0.477504    0.939769    4.089054
C        -0.760308    0.921288    2.760313
N         0.057707   -0.038448    2.191407
C         0.854641   -0.630132    3.132372
N         0.508505   -0.007963    4.299854
C         0.077434   -0.382263    0.778179
Au        2.196879   -2.049090    2.854432
C         1.108234   -0.311215    5.588958
H        -0.886198    1.538654    4.891997
H        -1.464393    1.500641    2.178042
H         0.336089   -0.653797    6.289498
H         1.839346   -1.111284    5.428215
H         1.616813    0.577333    5.984325
H        -0.909859   -0.748262    0.469024
H         0.363980    0.494766    0.184010
H         0.821321   -1.175485    0.642995
O         3.573227   -3.482801    2.662746
O         3.614890   -3.858434    1.190555
H         4.311476   -4.550779    1.269828
```

Hydrogen abstraction mechanism

```
  19
MECP scalar
      N      0.9928576     -0.4992997      3.1689648
      C      0.9803817      0.1675716      4.3818120
      C     -0.1557383      0.9142829      4.4033807
      N     -0.8055822      0.6818941      3.2040869
      C     -0.1074079     -0.1929789      2.4290671
      C     -2.0691249      1.2921973      2.8103552
      Au    -0.6308949     -0.8629342      0.5628989
      C      2.0410856     -1.4125165      2.7350961
      O     -2.9078689     -1.3162569     -2.1676584
      O     -1.8660614     -1.9849536     -1.6433648
      H      1.7686683      0.0555462      5.1146775
      H     -0.5510617      1.5812837      5.1582191
      H      2.1056177     -2.2590522      3.4300397
      H      1.7692194     -1.7731188      1.7371048
      H      2.9994937     -0.8798426      2.6908793
      H     -2.8446567      1.0432614      3.5451690
      H     -1.9468964      2.3800303      2.7340319
      H     -2.3419959      0.8803152      1.8323865
      H     -1.0718177     -1.2631355     -1.1744368


   19
TS SOC
  N           0.989451629    -0.513158171     3.192442944
  C           1.025491766     0.217124868     4.368637460
  C          -0.106144000     0.973444047     4.392762368
```

N	-0.803633968	0.681286268	3.232512817
C	-0.138723609	-0.238772254	2.479419063
C	-2.079325882	1.275902324	2.853125039
AU	-0.634322754	-0.899651166	0.603592733
C	2.005227821	-1.469345358	2.771129502
O	-2.810715454	-1.575504877	-2.192774067
O	-1.588714867	-2.004264505	-1.766540307
H	1.840289231	0.137270447	5.077197412
H	-0.468991725	1.682739184	5.126037410
H	2.007501415	-2.336402450	3.444503811
H	1.750450357	-1.792543138	1.754709804
H	2.989815278	-0.984755505	2.768903064
H	-2.837185163	1.047903950	3.613665912
H	-1.964600958	2.361629351	2.740998989
H	-2.374891429	0.836578456	1.892994401
H	-1.051097402	-1.174744610	-1.318628388

Oxidative addition mechanism

19

MECP scalar

C	-0.6439697	0.6740444	4.0637058
C	-0.8451890	0.8530531	2.7312016
N	0.0857795	0.0634892	2.0790228
C	0.8724467	-0.6107496	2.9684884
N	0.4073001	-0.2166686	4.1906823
C	0.2159445	-0.0515508	0.6356450
Au	2.1580988	-2.1566720	2.5812259
O	4.5192289	-1.5538969	2.7204216
O	4.2077255	-2.8264531	2.4176978
C	0.9370264	-0.7051591	5.4533720
H	-1.1471420	1.1011514	4.9209873
H	-1.5559904	1.4706768	2.1984840
H	0.2233518	-1.3957851	5.9211722
H	1.8692032	-1.2377626	5.2393345
H	1.1450955	0.1404736	6.1201784
H	-0.7122797	-0.4493582	0.2058777
H	0.4517164	0.9273153	0.1994700
H	1.0348120	-0.7498235	0.4352231
H	1.4971395	-3.6226518	2.2695255

19

TS SOC

N	0.628222	-0.085118	4.150344
C	-0.425739	0.808901	4.110112
C	-0.891903	0.804881	2.832275
N	-0.116991	-0.099673	2.130093
C	0.834202	-0.659258	2.929823
C	-0.265108	-0.409085	0.716500
AU	2.076540	-2.238598	2.496476
O	4.102840	-2.982520	2.856796
O	4.279562	-1.842500	3.534481
C	1.404038	-0.410732	5.338251
H	-0.750125	1.365099	4.979767

H	-1.694033	1.364484	2.369385
H	0.871515	-1.155397	5.943958
H	2.367356	-0.822526	5.013274
H	1.571344	0.502596	5.921458
H	-1.331665	-0.464522	0.468152
H	0.228519	0.357844	0.105852
H	0.208881	-1.382666	0.542953
H	1.578794	-3.582934	1.710554

19

Struc 3 scalar

C	-0.485712	0.677233	4.138847
C	-0.905920	0.767404	2.849169
N	-0.107951	-0.087509	2.109064
C	0.806278	-0.705478	2.903738
N	0.564356	-0.221953	4.154497
C	-0.198648	-0.256262	0.664967
Au	2.229327	-2.081692	2.479456
O	3.935281	-1.916808	3.663993
O	3.980259	-3.053098	2.742279
C	1.295069	-0.624611	5.353684
H	-0.839821	1.167546	5.035674
H	-1.689334	1.360805	2.397185
H	0.673931	-1.300557	5.955121
H	2.213951	-1.143964	5.046739
H	1.552411	0.270899	5.931580
H	-1.248523	-0.398854	0.382353
H	0.216377	0.625105	0.159222
H	0.382903	-1.144562	0.397469
H	1.310712	-2.789857	1.362895

21

Struc 4 scalar

N	0.060738	-0.995938	3.357750
C	-1.095268	-0.475391	2.805792
C	-0.853645	-0.307104	1.479456
N	0.439161	-0.735764	1.249971
C	1.011099	-1.167075	2.400747
C	1.072953	-0.739273	-0.061731
Au	2.848956	-1.932823	2.748223
O	4.570481	-2.270285	3.778005
O	3.799786	-1.322042	4.522991
C	0.221448	-1.359092	4.761757
H	-1.978889	-0.279178	3.397608
H	-1.486863	0.056292	0.681956
H	-0.233712	-2.340455	4.946115
H	1.292424	-1.399396	4.994693
H	-0.258063	-0.594795	5.383882
H	0.425888	-1.282512	-0.761352
H	1.231899	0.293213	-0.397782
H	2.034560	-1.252042	0.027640
H	2.744516	-2.802828	1.412992
O	-0.801482	-3.421196	0.720442
O	-1.398081	-2.881214	-0.255592

21
Struc 5 scalar

N	0.329431	-0.380408	3.875975
C	-0.809862	0.352087	3.598606
C	-0.953359	0.352633	2.246490
N	0.093814	-0.389115	1.730476
C	0.892338	-0.846661	2.727829
C	0.338846	-0.586330	0.305645
Au	2.532715	-2.011568	2.649250
O	4.380302	-2.742421	3.079187
O	4.259696	-1.561418	3.864645
C	0.840269	-0.658632	5.214048
H	-1.412288	0.800771	4.376939
H	-1.697785	0.814169	1.611796
H	0.298466	-1.505824	5.653318
H	1.906309	-0.904743	5.135432
H	0.716503	0.235489	5.835559
H	-0.609001	-0.824397	-0.189770
H	0.779671	0.323058	-0.122688
H	1.024008	-1.429607	0.181442
H	1.758642	-2.975111	1.603004
O	0.833690	-4.082030	0.526346
O	0.758151	-3.638522	-0.667691

21
Struc 6 scalar

N	-0.062524	-0.867962	3.541942
C	-1.218499	-0.268989	3.080796
C	-1.007826	0.029568	1.771241
N	0.271079	-0.389982	1.467190
C	0.860440	-0.960415	2.548955
C	0.854971	-0.356461	0.133270
Au	2.646829	-1.848772	2.641996
O	4.480116	-2.762647	2.794584
O	4.929287	-2.520328	4.038719
C	0.113482	-1.403761	4.884818
H	-2.077966	-0.104903	3.716686
H	-1.651416	0.496965	1.038350
H	-0.507036	-2.300697	5.006730
H	1.168213	-1.669915	5.008314
H	-0.162427	-0.641507	5.623313
H	0.687033	0.631179	-0.312558
H	1.929466	-0.541724	0.229312
H	0.400761	-1.144731	-0.480851
H	1.379279	-3.280324	1.478714
O	0.733037	-3.700120	0.808702
O	-0.497740	-3.243509	1.203276

21
Struc 7 scalar

N	-0.106893	-0.855764	3.489343
C	-1.284945	-0.344649	2.980890
C	-1.062402	-0.086026	1.664898
N	0.245571	-0.441382	1.404837
C	0.840104	-0.937343	2.519455
C	0.847177	-0.464020	0.078303
Au	2.675210	-1.707682	2.677170
O	4.539255	-2.552840	2.846758

```
O          4.407071   -3.806680    3.314136
C          0.063483   -1.345101    4.850315
H         -2.165883   -0.204432    3.592625
H         -1.714366    0.316478    0.901526
H         -0.490766   -2.284289    4.973830
H          1.130572   -1.528227    5.012595
H         -0.294284   -0.589654    5.560015
H          0.566124    0.446821   -0.462937
H          1.934640   -0.503271    0.197440
H          0.503387   -1.358047   -0.458419
H          1.529692   -3.382074    1.755164
O          0.906197   -3.952637    1.187969
O         -0.336216   -3.421236    1.422785

   21
Struc  8  scalar
N          0.319297    0.251358    3.554064
C         -0.892266    0.771760    3.137000
C         -1.240360    0.095059    2.010282
N         -0.229953   -0.815005    1.762101
C          0.743754   -0.735370    2.713183
C         -0.220534   -1.771509    0.661066
Au         2.382864   -1.842164    2.865343
O          4.078568   -2.926424    3.085172
O          4.046633   -4.140835    2.277980
C          1.056500    0.702452    4.725955
H         -1.391873    1.571577    3.666934
H         -2.107147    0.184477    1.369292
H          0.433196    0.589258    5.621773
H          1.948639    0.073773    4.816595
H          1.355384    1.750586    4.597922
H         -0.660457   -1.300515   -0.225445
H          0.816391   -2.049237    0.452724
H         -0.789061   -2.668946    0.936458
H          3.637215   -3.833262    1.416614
O          2.873776   -3.318755   -0.074076
O          1.986438   -4.228171   -0.169197
```

2 O_2 molecules mechanism

```
   21
MECP scalar
  N      1.7332698      0.9943314      0.1934017
  C      3.0823735      0.6967634      0.2591880
  C      3.2048092     -0.6216835     -0.0537807
  N      1.9259642     -1.0887661     -0.3006022
  C      1.0021663     -0.1023810     -0.1441422
  C      1.5894769     -2.4618378     -0.6502880
  Au    -1.0629715     -0.2361697     -0.3060951
  C      1.1475841      2.2926066      0.4997473
  H      3.8285223      1.4371116      0.5171793
  H      4.0782639     -1.2564387     -0.1229578
  H      1.6793824      3.0749939     -0.0552839
  H      0.0989422      2.2624975      0.1864998
  H      1.1959260      2.4785106      1.5799326
```

```
  H      2.1863822     -2.7823345     -1.5128997
  H      1.7721395     -3.1220812      0.2071761
  H      0.5249325     -2.4803657     -0.9095219
  H     -2.6608605     -0.4013732     -0.8170737
  O     -4.0534742     -0.6618368     -1.3113637
  O     -4.7842101      0.3833864     -1.2327628
  O     -2.4020661      0.2957561      1.7141378
  O     -1.5934838      0.8828995      2.5052394
```

```
   21
TS SOC
    C           0.963509967     0.051503984    -0.048503853
    N           1.851566352     0.935505710     0.484428089
    C           3.153958562     0.526322889     0.264563093
    C           3.085244347    -0.643019520    -0.425639270
    N           1.742312306    -0.915299196    -0.606479195
    C           1.484752016     2.159937255     1.183247042
    C           1.218948298    -2.085830689    -1.297056543
    AU         -1.104221547     0.106160741    -0.053414954
    O          -2.617828568     1.643495478     0.959228473
    O          -1.870849356     2.504912050     1.549490086
    O          -4.014091808    -1.063007446    -0.706071870
    O          -4.331283552    -1.056128909    -1.940693648
    H           4.006787727     1.094454975     0.612565199
    H           3.865411778    -1.294886374    -0.796544937
    H           1.839049036     3.028985590     0.614632329
    H           0.391994322     2.195773324     1.265250624
    H           1.927897226     2.154461897     2.186768056
    H           1.601481169    -2.110777672    -2.324878086
    H           1.507700636    -2.996478426    -0.757532630
    H           0.126507169    -1.994159385    -1.310152678
    H          -2.663093059    -0.416069769    -0.445826770
```

XYZ OF STRUCTURES IN THE S.I.

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  19
Fig. S1 left- 1.35 singlet
N          1.089012   -0.612094    3.017696
C          1.099998    0.110730    4.196733
C         -0.060385    0.819411    4.233124
N         -0.750142    0.515820    3.074473
C         -0.050874   -0.372979    2.309673
C         -2.053569    1.060166    2.708957
Au        -0.629400   -1.104883    0.582947
C          2.147582   -1.508311    2.574455
O         -2.428554   -0.682935   -1.225227
O         -1.405849   -1.698876   -1.263153
H          1.922142    0.061188    4.897952
H         -0.448110    1.505036    4.974672
H          2.322323   -2.278949    3.335804
H          1.799910   -1.972121    1.642906
H          3.066392   -0.937963    2.388158
```

H	-2.280202	0.730815	1.686608
H	-2.820076	0.680950	3.396523
H	-2.014626	2.155687	2.745474
H	-1.883017	-2.905702	-0.891154

19

Fig. S1 right – 1.35 triplet

N	1.884836	0.205631	2.565903
C	2.061339	0.645426	3.866375
C	0.817449	0.810993	4.390733
N	-0.079117	0.466796	3.393893
C	0.563868	0.088664	2.254055
C	-1.528675	0.498303	3.529783
Au	-0.277438	-0.528672	0.448950
C	2.962427	-0.099464	1.635293
O	-2.675291	-1.590354	-2.294476
O	-1.400862	-1.440802	-2.252275
H	3.040055	0.800881	4.301178
H	0.500104	1.138979	5.371973
H	3.580845	-0.913578	2.034094
H	2.497992	-0.414633	0.693893
H	3.573689	0.795958	1.465652
H	-1.844078	-0.190874	4.323379
H	-1.859727	1.519401	3.757697
H	-1.952094	0.177183	2.571254
H	-0.973047	-1.038235	-1.036786

19

Fig. S2 – singlet 1.8

C	2.036103	-1.071919	-0.455808
N	1.325256	0.079590	-0.738135
C	1.570588	1.048773	0.191816
N	2.443833	0.469045	1.062209
C	2.738228	-0.828809	0.681978
C	0.466194	0.256746	-1.904649
Au	0.742346	2.910511	0.132153
C	2.958954	1.104312	2.266829
H	3.408362	-1.459165	1.250936
H	1.982433	-1.953135	-1.080984
H	4.053578	1.032124	2.279981
H	2.658308	2.156195	2.243167
H	2.534949	0.617906	3.154980
H	-0.161738	-0.633903	-2.025564
H	-0.170157	1.136623	-1.741937
H	1.081251	0.412304	-2.800648
H	2.060248	3.553741	0.787415
O	-0.378621	4.279288	-0.199358
O	-1.153537	3.127947	-0.711861

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MECP scalar oxidative addition_ experimental carbene

C	-3.0082233	4.6314585	-0.9322436
C	-3.0454607	4.6020373	0.4669129
C	-3.1805610	5.7485885	1.2590885
C	-3.2910698	6.9723267	0.5966275

C	-3.2636677	7.0361083	-0.7926438
C	-3.1259990	5.8779669	-1.5499707
N	-2.8729989	3.3391161	1.1207660
C	-3.8559276	2.3825245	1.3311871
C	-3.2493004	1.3332742	1.9480648
N	-1.9155552	1.6831802	2.1003092
C	-1.6629362	2.9275473	1.6007810
C	-0.8979116	0.8796374	2.7095328
C	-0.6816353	1.0142345	4.0852063
C	0.3248107	0.2312243	4.6542631
C	1.0819844	-0.6332186	3.8712127
C	0.8578023	-0.7241475	2.5013111
C	-0.1360308	0.0400802	1.8877904
C	-1.4758214	1.9831853	4.9316005
C	-2.2731074	1.2428885	6.0111877
C	-0.3672279	-0.0437061	0.3956431
C	0.9249251	0.2144869	-0.3836412
Au	0.1386915	3.8369758	1.4258190
C	-3.2548475	5.6725162	2.7676177
C	-2.3242045	6.6788698	3.4453783
C	-2.7941646	3.3793630	-1.7542685
C	-3.8757114	3.2180947	-2.8270085
C	-4.7087378	5.8606956	3.2223016
C	-1.3887848	3.3805707	-2.3674681
C	-0.9844962	-1.3969961	0.0227706
C	-0.5584588	3.0468933	5.5435157
H	-4.8812330	2.5413046	1.0222842
H	-3.6332533	0.3838678	2.2989365
H	1.0992798	3.5803244	0.1216267
H	-3.3925119	7.8894091	1.1760692
H	-3.3437399	8.0019118	-1.2909900
H	-3.0943073	5.9455376	-2.6374794
H	-3.7332664	2.2724548	-3.3710739
H	-4.8825914	3.2193963	-2.3831277
H	-3.8292531	4.0352358	-3.5626839
H	-2.9294123	4.6676252	3.0722054
H	-1.2208013	2.4517641	-2.9339368
H	-1.2700066	4.2308090	-3.0580900
H	-0.6204171	3.4636437	-1.5848597
H	1.4741600	-1.3901097	1.8973740
H	1.8660012	-1.2336677	4.3319260
H	0.5267608	0.3090259	5.7225026
H	-1.0800406	0.7464558	0.1189023
H	0.7182775	0.2187609	-1.4642854
H	1.3546152	1.1877182	-0.1067939
H	1.6708003	-0.5712925	-0.1874109
H	-1.1857094	-1.4423576	-1.0583081
H	-0.2958526	-2.2181951	0.2769494
H	-1.9279144	-1.5697057	0.5623111
H	-2.1931089	2.4979138	4.2757235
H	-2.8818403	1.9537741	6.5899013
H	-2.9401957	0.4871109	5.5699412
H	-1.5968206	0.7293774	6.7119935
H	-1.1528621	3.7680750	6.1247758
H	0.1724594	2.5844723	6.2254544
H	-0.0061618	3.5970885	4.7676271
H	-4.7838942	5.7631562	4.3159560

H	-5.0713352	6.8620788	2.9404683
H	-5.3744146	5.1178877	2.7571317
H	-2.3804719	6.5591684	4.5377021
H	-1.2796901	6.5241731	3.1383127
H	-2.6167813	7.7137284	3.2104758
H	-2.8609212	2.5124671	-1.0806506
O	1.5984715	5.1616807	2.2923372
O	0.7480775	5.3209232	3.3171180

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Fig. S4 left- MECP oxidative addition – LAuCH3

N	0.0749909	0.0752321	2.0846916
C	0.8715044	-0.5866198	2.9770907
N	0.3967339	-0.1970617	4.1990634
C	-0.6646869	0.6810903	4.0675732
C	-0.8658093	0.8552934	2.7348598
Au	2.1963086	-2.0735881	2.5934301
O	4.6510160	-1.6396559	2.7095530
O	4.1670452	-2.8601564	2.4022839
C	0.9291080	-0.6768292	5.4644662
C	0.2091435	-0.0357934	0.6410770
C	1.3556045	-4.0166698	2.1737319
H	-1.1735468	1.1075037	4.9218420
H	-1.5809898	1.4661742	2.2005239
H	0.2219483	-1.3746760	5.9319149
H	1.8697618	-1.1970292	5.2549988
H	1.1210705	0.1731524	6.1311532
H	-0.7234719	-0.4198425	0.2083650
H	0.4542949	0.9430288	0.2091602
H	1.0224741	-0.7406332	0.4387672
H	2.1805781	-4.7160423	1.9898500
H	0.7684000	-4.3204625	3.0505315
H	0.7065464	-3.9311016	1.2926069

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Fig. S4 middle – Product oxidative addition – LAuCH3

N	-0.103858	-0.148299	2.110016
C	0.832609	-0.699508	2.927639
N	0.576959	-0.170027	4.155514
C	-0.506681	0.688349	4.107075
C	-0.933162	0.707158	2.816235
Au	2.268256	-2.071785	2.565268
O	4.154009	-1.638316	3.359566
O	4.089130	-2.938667	2.694609
C	1.340783	-0.497926	5.355339
C	-0.181055	-0.372825	0.672830
C	0.964537	-3.421804	1.587678
H	-0.872742	1.208294	4.982131
H	-1.735677	1.255939	2.341671
H	0.838903	-1.300187	5.911204
H	2.340638	-0.834001	5.048211
H	1.425911	0.399481	5.978685
H	-1.155184	-0.806637	0.415660
H	-0.036291	0.578293	0.144300
H	0.615410	-1.070053	0.400043

H	1.176511	-4.419602	1.995793
H	-0.092916	-3.174186	1.751177
H	1.190980	-3.423260	0.511189

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Fig. S4 right – Max. Rearrang. – LAuCH3

C	-1.073508	0.389665	3.047430
N	-0.173188	-0.343417	2.293058
C	0.814732	-0.844860	3.078286
N	0.527740	-0.405931	4.329691
C	-0.633467	0.342828	4.332924
C	-0.253456	-0.517272	0.849622
Au	2.332365	-2.086448	2.592617
C	0.947595	-3.603067	1.943615
C	1.289255	-0.781135	5.514522
O	4.351308	-1.500651	2.808751
O	4.216298	-2.847870	2.346456
H	-1.041566	0.771861	5.238012
H	-1.929883	0.881816	2.606521
H	0.895951	-1.724038	5.915032
H	2.338058	-0.911176	5.225681
H	1.208782	0.020548	6.257068
H	-1.204860	-0.995788	0.586720
H	-0.167530	0.458281	0.353564
H	0.576711	-1.157984	0.539989
H	1.253495	-4.645816	2.077067
H	-0.132379	-3.431336	1.972622
H	1.211664	-3.411865	0.860873
O	0.627176	-3.886537	3.794824
O	-0.358128	-3.289176	4.353940

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Fig. S5 – LAuH SOC TZP

C	4.396210	-1.768036	7.083234
C	4.816660	-1.673693	5.790582
N	3.738515	-1.196567	5.057957
C	2.647184	-0.985904	5.853339
N	3.074349	-1.344839	7.101022
C	3.747996	-0.944302	3.621073
Au	0.773230	-0.285327	5.295202
C	2.232819	-1.275557	8.290739
H	5.774576	-1.904231	5.341281
H	4.918828	-2.095330	7.973363
H	2.164224	-2.263138	8.763273
H	2.642782	-0.550293	9.004809
H	1.238362	-0.949873	7.966376
H	3.973905	-1.868895	3.075500
H	2.748529	-0.588621	3.347591
H	4.492933	-0.177175	3.375359
H	-0.684550	0.257968	4.860887

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Fig. S5- TS SOC TZP Hydrogen Abstraction

N	0.995008074	-0.502706378	3.201111790
C	1.034253256	0.238114134	4.374383535

C	-0.105048335	0.985617475	4.402812754
N	-0.810708284	0.680555955	3.247114329
C	-0.142291372	-0.240417240	2.496171747
C	-2.096361563	1.262979011	2.871063572
AU	-0.667508551	-0.949004867	0.636351960
C	2.021186816	-1.447907323	2.770578873
O	-2.791014797	-1.288145788	-2.327654722
O	-1.747410490	-1.971231197	-1.784246029
H	1.855024359	0.172281739	5.078075672
H	-0.466602352	1.695849243	5.136436816
H	2.073061236	-2.294098420	3.466727713
H	1.739359883	-1.807539488	1.774753730
H	2.994328155	-0.945015723	2.720714031
H	-2.850913889	1.031080497	3.632436544
H	-1.998143677	2.349630900	2.760848507
H	-2.390803323	0.821850261	1.912547817
H	-1.069325303	-1.280309392	-1.325832179

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Fig. S5- TS SOC TZP Oxidative Addition

N	0.638686	-0.079798	4.155711
C	-0.407396	0.829427	4.118435
C	-0.888943	0.820095	2.843659
N	-0.129997	-0.101017	2.138107
C	0.822634	-0.665029	2.935197
C	-0.294605	-0.418360	0.724489
AU	2.078335	-2.243641	2.484981
O	4.108728	-2.958886	2.896523
O	4.247897	-1.830857	3.598017
C	1.425772	-0.404171	5.341153
H	-0.716670	1.399002	4.985765
H	-1.691256	1.385788	2.387079
H	0.876272	-1.103253	5.983785
H	2.361957	-0.870365	5.012737
H	1.645422	0.515375	5.894973
H	-1.362031	-0.488847	0.487480
H	0.175556	0.352042	0.100875
H	0.193060	-1.382726	0.544815
H	1.638391	-3.579032	1.651245

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Fig. S5- TS SOC TZP – 2 O_2 molecules

C	0.968018	0.044317	-0.047334
N	1.855618	0.937484	0.475445
C	3.161568	0.531836	0.244094
C	3.092274	-0.645487	-0.437784
N	1.745424	-0.925187	-0.608583
C	1.484436	2.163579	1.176826
C	1.217577	-2.103401	-1.289068
AU	-1.105644	0.107952	-0.049274
O	-2.611300	1.663487	0.966393
O	-1.873184	2.512708	1.587280
O	-4.026085	-1.044516	-0.736474
O	-4.325797	-1.101899	-1.971857
H	4.016640	1.105014	0.580097
H	3.874522	-1.295762	-0.809003
H	1.831193	3.036397	0.610621

H	0.392492	2.196787	1.266708
H	1.933767	2.167200	2.176861
H	1.582176	-2.135094	-2.322498
H	1.519636	-3.013450	-0.757146
H	0.125037	-2.020644	-1.285741
H	-2.664433	-0.412212	-0.451566