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Photophysical properties of the triangular [Au(HN=COH)]$_3$ complex and its dimer†

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1 [Au(HN=COH)]$_3$ Monomer

1.1 Ground state

```
18

Au   -1.9942323   -0.0359579    0.0000000
Au    0.9659757    1.7450347    0.0000000
Au    1.0282566   -1.7090769    0.0000000
N    -1.9202965    2.0355753    0.0000000
N     2.7230082    0.6452379    0.0000000
N    -0.8027117   -2.6808132    0.0000000
C    -0.7999723    2.6920720    0.0000000
C     2.7313889   -0.6532397    0.0000000
C    -1.9314166   -2.0388323    0.0000000
O    -0.8131602    4.0369454    0.0000000
O    -3.0895172   -2.7226901    0.0000000
O     3.9026774   -1.3142553    0.0000000
H    -2.7697675    2.5984329    0.0000000
H     3.6351926    1.0994726    0.0000000
H    -0.8654252   -3.6979055    0.0000000
H    -1.7220055    4.3792040    0.0000000
H    -2.9314991   -3.6809025    0.0000000
H     4.6535046   -0.6983015    0.0000000
```

1.2 Singlet excited state

```
18

Au   -2.0170508    0.0858690    0.2715483
Au    1.0168757    1.8462055    0.0644175
Au    0.9961777   -1.6005255   -0.0451515
N    -1.7842630    2.0647429    0.6380719
N     2.7657846    0.6977673    0.1395050
N    -0.8541109   -2.5410482   -0.1843806
C    -0.7375020    2.7888151    0.0137611
C     2.7299287   -0.5970930    0.0905098
C    -1.9811561   -1.9099650   -0.0799349
O    -1.1201864    3.6038932   -1.0187052
O    -3.1428098   -2.5746634   -0.1891334
O     3.8736308   -1.3063921    0.1360926
H    -2.0879308    2.4776233    1.5180665
H     3.6923146    1.1170321    0.2095819
H    -0.9175167   -3.5461771   -0.3433701
H    -2.0827975    3.6354704   -1.0713167
H    -2.9946987   -3.5207837   -0.3518588
H     4.6453107   -0.7207710    0.2022966
```

1.3 Triplet excited state

```
18

Au   -1.9393355    0.0778101    0.3101730
Au    0.9455143    1.8129878    0.0987083
Au    1.0038512   -1.6342200   -0.0659496
N    -1.7481923    2.0901228    0.6890661
N     2.7190768    0.6888112    0.1817355
N    -0.8475993   -2.5633911   -0.2145320
C    -0.7918913    2.8523969    0.0170901
C     2.7172635   -0.6054186    0.0939806
C    -1.9563044   -1.9046802   -0.0761347
O    -1.1329331    3.4657991   -1.1673780
O    -3.1357653   -2.5393251   -0.1754271
O     3.8792031   -1.2835202    0.1181129
H    -1.9615872    2.4441247    1.6188486
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H	3.6331877	1.1322093	0.2641092
H	-0.9368613	-3.5622106	-0.3972123
H	-2.0702658	3.6947897	-1.1401985
H	-3.0129956	-3.4864036	-0.3532100
H	4.6356344	-0.6798820	0.1982179

2 [Au(HN=COH)]$_3$ Dimer

2.1 Ground state

36

Au	-3.2459737	-0.6135668	-0.6942084
Au	-0.8442809	1.8438120	-0.9919543
Au	-0.1589370	-1.3479815	-2.0681466
Au	0.7371625	-1.7635695	1.0285569
Au	0.1317816	1.4541374	2.0864876
Au	3.2023716	0.6168551	0.7294242
N	-3.5769214	1.3523792	-0.1376679
N	0.9642474	1.3084338	-1.8474875
N	-1.0496090	-1.1812285	1.8932211
N	3.4717779	-1.3513023	0.1374390
N	1.6659259	2.8229932	1.8199421
N	-1.6495645	-2.7694765	-1.7898857
C	-2.6502471	2.2573690	-0.2266846
C	2.8094814	2.4934086	1.3217985
C	-1.2640358	0.0326196	2.2959185
C	1.2029405	0.1068691	-2.2695806
C	-2.7935206	-2.4858277	-1.2514858
C	2.5187016	-2.2275347	0.2352155
O	-2.8900721	3.5026827	0.2169385
O	-2.4641260	0.3608227	2.8078486
O	-3.6990212	-3.4629464	-1.0449285
O	2.4065707	-0.1892775	-2.7958118
O	3.7055658	3.5065345	1.2177771
O	2.7115400	-3.4749779	-0.2270509
H	-4.4542764	1.6505741	0.2850768
H	-1.8351668	-1.8249412	1.9670404
H	1.5846532	3.8051677	2.0723415
H	1.7315483	1.9738973	-1.9211183
H	-1.4934834	-3.7476408	-2.0288963
H	-3.7773705	3.5721044	0.6052411
H	-3.0787698	-0.3888121	2.7505940
H	-3.3644273	-4.3195116	-1.3571200
H	4.3297025	-1.6699511	-0.3093704
H	3.5896470	-3.5671194	-0.6312083
H	4.5251998	3.1483400	0.8648933
H	3.0009860	0.5766652	-2.7431487

2.2 Singlet excited state

36

Au	-3.3899511	-0.6219137	-0.7119353
Au	-0.8299751	1.7156773	-0.8357362
Au	-0.2570996	-1.3987783	-1.9036279
Au	0.8453183	-1.7422462	0.9337159
Au	0.1451931	1.4517697	1.7948502
Au	3.3603529	0.6806431	0.7067602
N	-3.6508664	1.3638175	-0.1684683
N	0.9886972	1.1913489	-1.6158108
N	-0.9902076	-1.2048508	1.8001484
N	3.6613299	-1.2982530	0.2778368
N	1.6220023	2.8714644	1.5553131
N	-1.8061564	-2.7967316	-1.7370355
C	-2.6721811	2.2064890	-0.1715168
C	2.8510335	2.5361803	1.2506212
C	-1.2309591	0.0143195	2.1212776
C	1.1919303	-0.0272420	-2.0399063
C	-2.9713991	-2.5044400	-1.2589163
C	2.6592112	-2.1600260	0.1987613
O	-2.8375669	3.4644244	0.2610030
O	-2.3921516	0.3894153	2.6903980
O	-3.9111608	-3.4573092	-1.1096519
O	2.4059171	-0.3856143	-2.4502875
O	3.7090525	3.5830139	1.2522256
O	2.8056004	-3.2524571	-0.6133822
H	-4.5436488	1.7114370	0.1759797
H	-1.7318421	-1.8804316	1.9726738
H	1.4704900	3.8668133	1.6899132
H	1.8079261	1.7916357	-1.5540928
H	-1.6466126	-3.7739034	-1.9789003
H	-3.7411045	3.6163921	0.5809346
H	-2.9945856	-0.3664592	2.7717224
H	-3.5851847	-4.3199458	-1.4135876
H	4.5228928	-1.6065471	-0.1623942
H	3.4628831	-3.0583004	-1.3021063
H	4.5708973	3.2577104	0.9711392
H	3.1019250	0.1428978	-1.9779181

2.3 Triplet excited state

36

Au	-3.3327442	-0.5781326	-0.5308397
Au	-0.8902589	1.8146354	-0.8250298
Au	-0.2704477	-1.3349461	-2.0011367
Au	1.0904657	-1.7548206	0.7795760
Au	0.3109453	1.3031875	2.1279272
Au	3.4310628	0.7831198	0.7074148
N	-3.6601566	1.4060331	-0.0326532
N	0.9013298	1.1811186	-1.5874497
N	-0.7210329	-1.3710161	1.7149304
N	3.7956285	-1.0902096	-0.0809204
N	1.7568166	2.7791498	1.9883508
N	-1.7586906	-2.7771948	-1.5810221
C	-2.7220535	2.2983722	-0.1239275
C	2.9215861	2.5700684	1.4704974
C	-1.0036958	-0.2067098	2.2105915
C	0.8600161	0.2229923	-2.5821391
C	-2.8922455	-2.4689336	-1.0357601
C	2.8920543	-2.0176032	-0.0679475
O	-2.9581381	3.5596907	0.2698796
O	-2.2176179	0.0210985	2.7379119

O	-3.8035136	-3.4312976	-0.7811405
O	1.9014031	0.0905844	-3.4651827
O	3.7462974	3.6427400	1.4627493
O	3.2509627	-3.1640278	-0.6857981
H	-4.5490872	1.7241886	0.3501303
H	-1.4707382	-2.0592220	1.7288240
H	1.6098970	3.7299231	2.3189942
H	1.6462402	1.0201287	-0.8888976
H	-1.6212865	-3.7624543	-1.8028353
H	-3.8600277	3.6586083	0.6168335
H	-2.8096440	-0.7341766	2.5872668
H	-3.4904445	-4.2979479	-1.0876304
H	4.6481066	-1.3446156	-0.5737963
H	2.5047922	-3.7700468	-0.6556530
H	4.5798411	3.3846972	1.0582133
H	2.1843780	0.9730184	-3.7403310