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Electronic Supplementary Information

Mechanistic study of C–H bond activation by O_2 on negatively charged Au clusters: α,β-dehydrogenation of 1-methyl-4-piperidone by supported Au catalysts

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S1. Surface Structure of the (100) Surface of OMS-2

K atoms are at the hollow site of the (100) surface of OMS-2 if (100) surface is simply cut from the bulk structure as shown in Figure S1a (8-hollow structure). However, once a K atom is moved from the hollow site to the terrace site, such structure (7-hollow_1-terrace structure) is more stable than the 8-hollow structure by 24.0 kcal/mol. Furthermore, when 8-terrace structure (i.e. all K atoms were put on the terrace site) was used as initial surface structure, half of K atoms occupied the terrace site, and the other half K atoms occupied hollow site after the geometry optimization (Figure S1b: 4-hollow_4-terrace structure). The 4-hollow_4-terrace structure is more stable than the 8-hollow structure by 47.1 kcal/mol. Although other surface structures (e.g. the 5-hollow_3-terrace structure or the 3-hollow_5-terrace structure) were also constructed, these structures are unstable than the 4-hollow_4-terrace structure. From these results, the 4-hollow_4-terrace structure was adopted in this study.

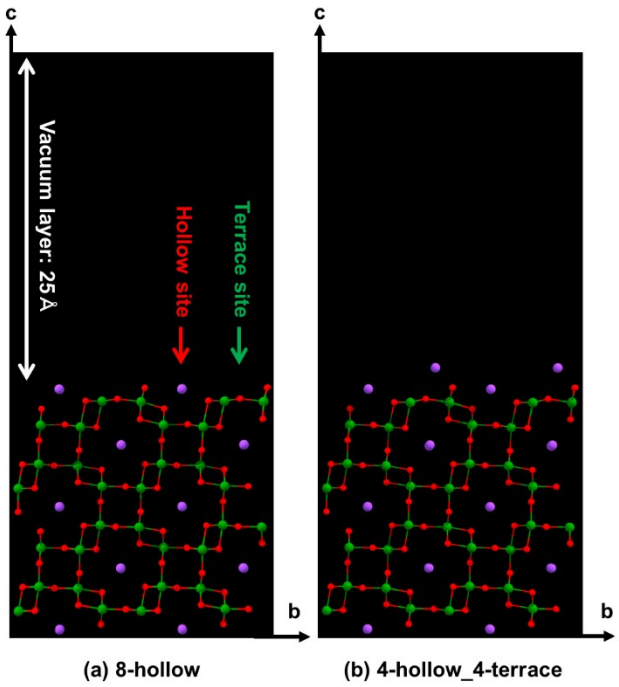


Figure S1. Slab models of the (100) surface of OMS-2 ($K_{40}Mn_{128}O_{256}$). (a) 8-hollow structure (b) 4-hollow_4-terrace structure. Red: oxygen, green: manganese, purple: potassium.

S2. Adsorption Structures of 1-methyl-4-piperidone on the Au_{20} Model

Adsorption structures of 1-methy-4-piperidone on each Au_{20} model were investigated. Because 1-methyl-4-piperidone is adsorbed on the Au_{20} model by nitrogen atom, there are three possible adsorption sites in the Au_{20} model: OT1, OT2 and OT3 sites (cf. Figure S2). Adsorption energies of 1-methyl-4-piperidone are summarized in Table S1. In the $Au_{20}^{0\pm}$ model, OT1 site is the most stable adsorption site (adsorption energy = −22.8 kcal/mol). In the Au_{20}^{1-} model and Au_{20}^{2-} model, both OT2 and OT3 sites are the most stable adsorption sites (adsorption energies of OT2 and OT3 sites are −20.6 kcal/mol in the Au_{20}^{1-} model and −30.0 kcal/mol in the Au_{20}^{2-} model). Thus, the OT1 site was adopted with the $Au_{20}^{0\pm}$ model although both the OT2 and OT3 sites

were adopted with the Au_{20}^{1-} and Au_{20}^{2-} models as the reactant states of the direct C–H activation pathway at the first C–H bond cleavage step.

Table S1. Adsorption energies of 1-methyl-4-piperidone on the Au_{20} models[a]

E_{ads} (kcal/mol)	OT1	OT2	OT3
$Au_{20}^{0\pm}$model	−22.8	−20.5	−21.0
Au_{20}^{1-}model	−18.5	−20.6	−20.6
Au_{20}^{2-}model	−23.0	−30.0	−30.0

[a]For the definitions of each adsorption site (i.e. OT1, OT2 and OT3), see Figure S2.

S3. Adsorption Structures of O_2 on the Au_{20} Model

Adsorption structures of O_2 on the Au_{20} model were investigated in the same way as that in a previous theoretical study.[1] Adsorption sites of O_2 on the Au_{20} model considered in the present study are shown in Figure S2, and adsorption energies of O_2 on these adsorption sites are summarized in Table S2. In the $Au_{20}^{0\pm}$ model, adsorption energies for any adsorption sites were calculated to be positive values. This result indicated that O_2 is not adsorbed on $Au_{20}^{0\pm}$ model stably. On the other hand, adsorption energies showed negative values both in the Au_{20}^{1-} model and Au_{20}^{2-} model (except for that of OT2 site in the Au_{20}^{2-} model). This result indicated that O_2 is adsorbed on the negatively charged Au_{20} models stably. The most stable adsorption site is BR1 site in both models. Comparing adsorption energies for BR1 site in both models, O_2 is adsorbed on the Au_{20}^{1-} model stronger than on the Au_{20}^{2-} model by 8.6 kcal/mol. In addition, O–O bond distance is elongated as negative charge of the Au_{20} model increases. More details for electronic structure of adsorbed O_2 are discussed in Section 3.4.

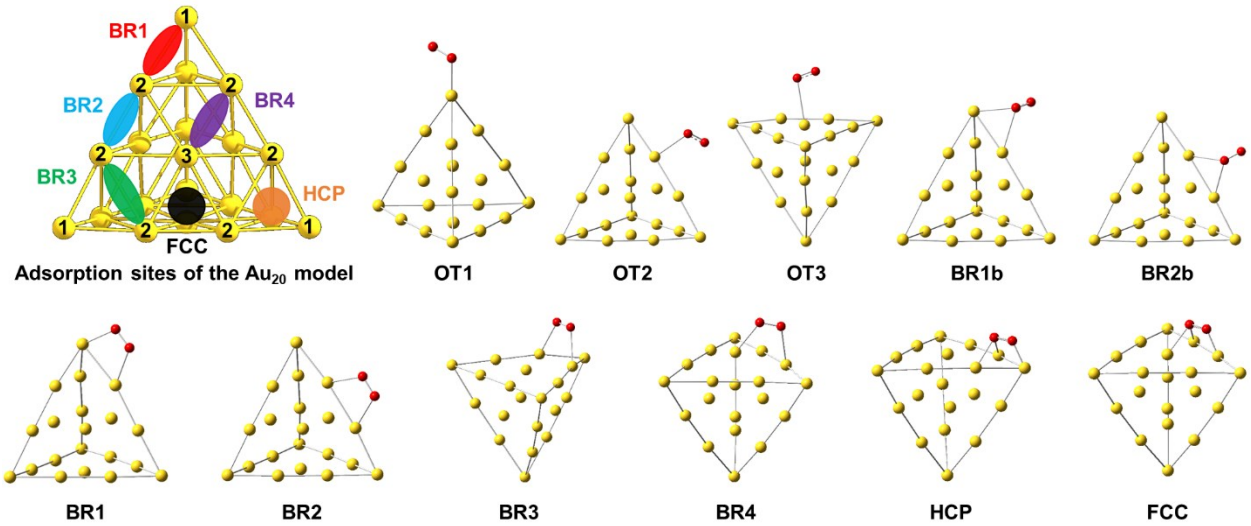


Figure S2. Adsorption sites of the Au_{20} model (numbers on each Au atom represent OT1 site, OT2 site and OT3 site, respectively), and examples of adsorption structures of O_2 on each adsorption site. Yellow: gold, red: oxygen.

Table S2. Adsorption energies and O–O bond distances of O_2 on each Au_{20} model

		OT1	OT2	OT3	HCP	FCC
$Au_{20}^{0\pm}$model	E_{ads} (kcal/mol)	27.4	28.5	30.4	27.4[a]	Converged to OT2
	O–O distance (Å)	1.23	1.23	1.20	1.23[a]	
Au_{20}^{1-}model	E_{ads} (kcal/mol)	−18.0	−11.2[a]	−7.6	Converged to BR1	Converged to BR4
	O–O distance (Å)	1.29	1.28[a]	1.23		
Au_{20}^{2-}model	E_{ads} (kcal/mol)	−0.1	4.1[a]	Converged to BR2	−6.2	−3.9
	O–O distance (Å)	1.31	1.32[a]		1.41	1.38
		BR1	BR2	BR3	BR4	
$Au_{20}^{0\pm}$model	E_{ads} (kcal/mol)	25.3[b]	31.4	28.6	29.0	
	O–O distance (Å)	1.25[b]	1.20	1.22	1.22	
Au_{20}^{1-}model	E_{ads} (kcal/mol)	−21.1	−16.1	−12.5	−11.7	
	O–O distance (Å)	1.30	1.29	1.29	1.29	
Au_{20}^{2-}model	E_{ads} (kcal/mol)	−12.5	−5.1	Converged to HCP	Converged to FCC	
	O–O distance (Å)	1.40	1.35			

[a]Converged to BR1b. [b]Converged to BR2b.

In the present study, adsorption structures of O_2 on the $Au_{20}^{0\pm}$ model and Au_{20}^{2-} model were calculated as singlet state, and O_2 on the Au_{20}^{1-} model was calculated as doublet state. When adsorption structure was calculated as triplet state in the $Au_{20}^{0\pm}$ model, O_2 is adsorbed as physisorbed (or desorbed) structure with long Au–O distance (> 2.6 Å) although adsorption energies showed small negative values (−5 ~ −6 kcal/mol). These results suggested that O_2 is not adsorbed on the $Au_{20}^{0\pm}$ model both in singlet and triplet states. When adsorption structures were calculated as quartet state in the Au_{20}^{1-} model, similar physisorbed (or desorbed) adsorption structures were also obtained with smaller adsorption energies (−5 ~ −6 kcal/mol) than those in doublet state. This result indicated that O_2 is adsorbed on the Au_{20}^{1-} model stably in doublet state. When adsorption structures were calculated as triplet state in the Au_{20}^{2-} model, chemisorption structures were obtained. The most stable adsorption site in triplet state is also BR1 site, and adsorption energy is −21.7 kcal/mol which is larger than that in singlet state by 9.2 kcal/mol. Co-adsorption structure of O_2 and 1-methyl-4-piperidone on the Au_{20}^{2-} in triplet state is also stable than that in singlet state by 9.5 kcal/mol. On the other hand, transition state for the indirect C–H activation by O_2 and its product state in triplet state are unstable than those in singlet state by 5.9 kcal/mol and 17.3 kcal/mol, respectively. Thus, apparent activation energy for the indirect C–H activation is 21.3 kcal/mol in singlet state from the reactant state in triplet state. This apparent activation energy is lower than that in triplet state and also that with the Au_{20}^{1-} model by 5.9 kcal/mol and 8.5 kcal/mol, respectively. From these results, the $Au_{20}^{0\pm}$ model and Au_{20}^{2-} model were calculated as singlet state, and the Au_{20}^{1-} model was calculated as doublet state in the present study.

S4. C–H$^{\beta}$ bond Activation Pathways at the First C–H Bond Cleavage Step

Potential energy diagram of the C–H$^{\beta}$ bond activation at the first C–H bond cleavage step is shown in FigureS3. In addition, optimized structures of reactant, product and transition states along the direct and the indirect C–H$^{\beta}$ bond activation pathways are shown in Figure S4 and Figure S5, respectively.

Calculated activation energies of the direct C–H$^{\beta}$ bond activation are 0.7 kcal/mol and 8.7 kcal/mol higher than those of the C–H$^{\alpha}$ bond with the Au_{20}^{1-} and Au_{20}^{2-} models, respectively (cf. E_{aB3} and E_{aC3} in Figure S3). Activation energy of the direct C–H$^{\beta}$ bond activation with the $Au_{20}^{0\pm}$ model is lower than that of the C–H$^{\alpha}$ bond by 11.8 kcal/mol. However, this low activation energy originates from unstability of the reactant state where the reactant is physisorbed (A3 in Figure S4). The reactant state A3 is unstable than A1 state (reactant state of the C–H$^{\alpha}$ bond activation: Figure 6) by 3.9 kcal/mol. We could not obtain a transition state for the direct C–H$^{\beta}$ bond activation which is connected to chemisorbed 1-methyl-4-piperidone on the OT1 site of the $Au_{20}^{0\pm}$ model. Additionally, product states of the direct C–H$^{\beta}$ bond activation pathways (A4, C6 and B5 in Figure S3 and S4) are unstable than reactant states (A3, B1 and C5 in Figure S3 and S4) by 41.3 kcal/mol, 34.5 kcal/mol and 51.8 kcal/mol, respectively.

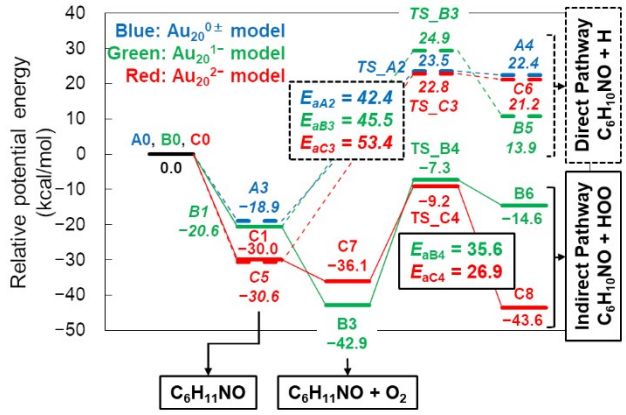


Figure S3. Potential energy diagram of C–H$^{\beta}$ bond activation at the first C–H bond cleavage step. Broken lines: the direct C–H$^{\beta}$ activation pathways, solid lines: the indirect C–H$^{\beta}$ bond activation pathways. Energies of A0, B0, and C0 states are defined as the sum of the energies of the isolated species: $Au_{20}^{0\pm}$, O_2, and 1-methyl-4-piperidone for A0; Au_{20}^{1-}, O_2, and 1-methyl-4-piperidone for B0; Au_{20}^{2-}, O_2, and 1-methyl-4-piperidone for C0.

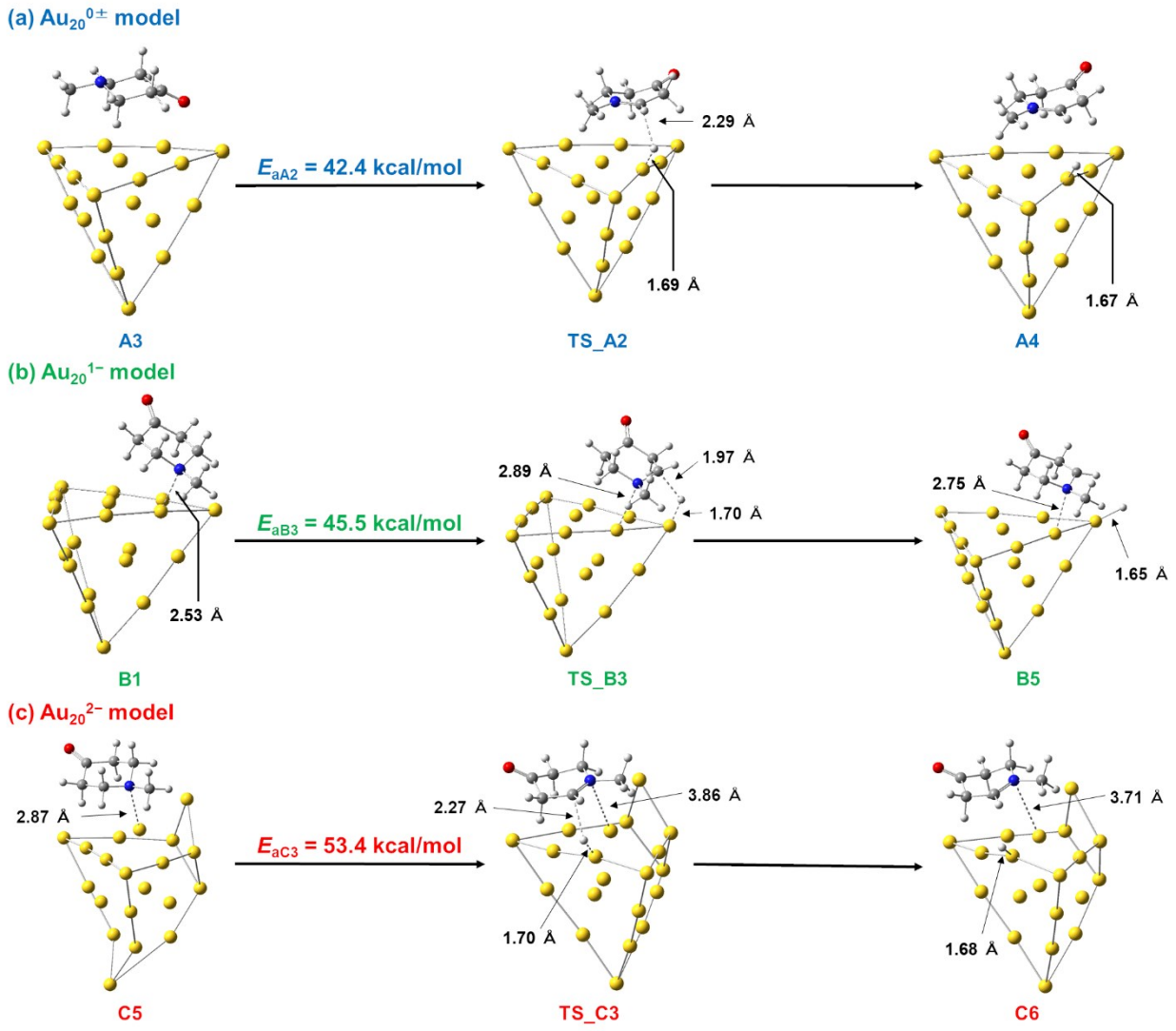


Figure S4. Optimized structures of the reactant, product and transition states of the direct C–H$^{\beta}$ bond activation at the first C–H bond cleavage step on the (a) $Au_{20}^{0\pm}$ model, (b) Au_{20}^{1-} model and (c) Au_{20}^{2-} model. Red: oxygen, blue: nitrogen, gray: carbon, white: hydrogen, yellow: gold.

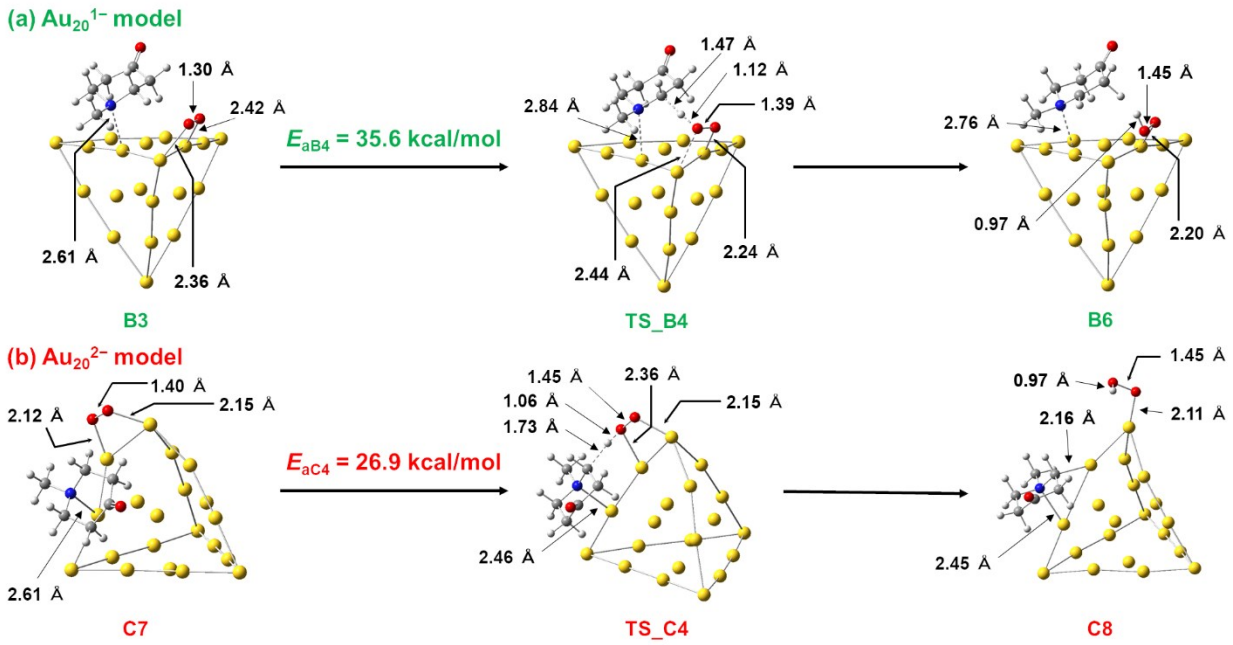


Figure S5. Optimized structures of the reactant, product and transition states of the indirect C–H$^{\beta}$ bond activation at the first C–H bond cleavage step on the (a) Au_{20}^{1-} model and (b) Au_{20}^{2-} model. Red: oxygen, blue: nitrogen, gray: carbon, white: hydrogen, yellow: gold.

S5. Comparison of Calculation Settings

As shown in Section 2, computational settings are different between the Au_{10}/OMS-2 model (PBE functional with FHI-aims code) and the Au_{20} model (M06 functional with Gaussian 09 code). Thus, difference between these computational settings were investigated by using adsorption structure of O_2 on the Au_{20} model. Optimized adsorption structures by using the calculation setting for the Au_{10}/OMS-2 model were shown in Figure S6. Comparing the result in Figure 8, maximum difference for Au–O bond is 0.2 Å, and for O–O bond is 0.04 Å, respectively. In addition, root-mean-square-deviation (RMSD: see equation S1) between optimized structures in Figure 8 and Figure S6 is less than 0.16 Å in each model.

$$RMSD = \sqrt{\frac{1}{N}\sum_{t=1}^{N} d_i^2} \quad \ldots \text{(S1)}$$

Here, N is total number of atoms in the system, and d_i is distance between corresponding atoms between two models. These results indicated that adsorption structures of O_2 on each model are almost same between the two settings. Furthermore, results of Hirshfeld charge analysis for adsorbed O_2 are shown in Table S3. Although difference of Hirshfeld charge in the Au_{20}^{1-} model and Au_{20}^{2-} model is slightly large, tendency of Hirshfeld charge of O_2 is same between two settings (i.e. Hirshfeld charge of O_2 becomes more negative as negative charge of the Au_{20} model increases). These results indicated that qualitative tendency of O_2 adsorption on the Au_{20} model are consistent in each calculation setting.

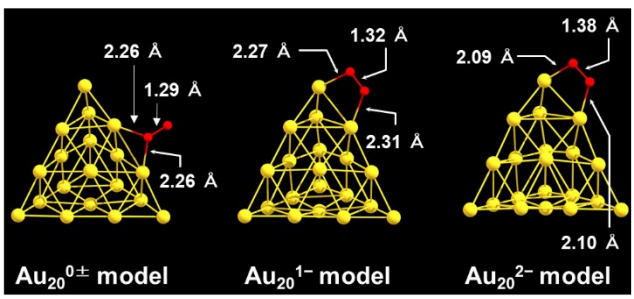


Figure S6. Adsorption structures of O_2 on each Au_{20} model optimized by using the calculation setting for the Au_{10}/OMS-2 model. Yellow: gold, red: oxygen.

Table S3. Hirshfeld charge of O_2 on each Au_{20} model

	$Au_{20}^{0\pm}$ model	Au_{20}^{1-} model	Au_{20}^{2-} model
FHI-aims[a]	−0.24	−0.31	−0.51
Gaussian[b]	−0.31	−0.50	−0.78

[a]Result with calculation setting for the Au_{10}/OMS-2 model. [b]Result with calculation setting for the Au_{20} model.

S6. Definition of the Relative Potential Energies at the Second C–H Bond Cleavage Step

At the second C–H bond cleavage step, the relative potential energies of the HOO generation pathway (ΔE_{HOO}) and the other pathways ($\Delta E_{\mathrm{Others}}$) are defined by equation S2 and S3, respectively.

$$\Delta E_{HOO} = \{E[HOO] + E[Au_{20}_HOO]\} - \{E[Au_{20}] + E[R] + E[O_2] + E[Au_{20}_O_2]\} \ \ldots \ (S2)$$

$$\Delta E_{Others} = \{E[Others] + E[Au_{20}_O_2]\} - \{E[Au_{20}] + E[R] + E[O_2] + E[Au_{20}_O_2]\} \ \ldots \ (S3)$$

Here, E[HOO] and E[Others] are potential energies of each state along the HOO generation pathway and the other pathways, respectively. E[Au_{20}_HOO] and E[Au_{20}_O_2] are potential energies of adsorbed state of HOO on the Au_{20}^{1-} model and O_2 on the Au_{20}^{1-} model, respectively. E[Au_{20}], E[R] and E[O_2] are potential energies of the isolated Au_{20}^{1-} model, 1-methyl-4-piperidone and O_2, respectively.

S7. Optimized Structures along the C–H$^{\alpha}$ Bond Cleavage by the Adsorbed O and OH

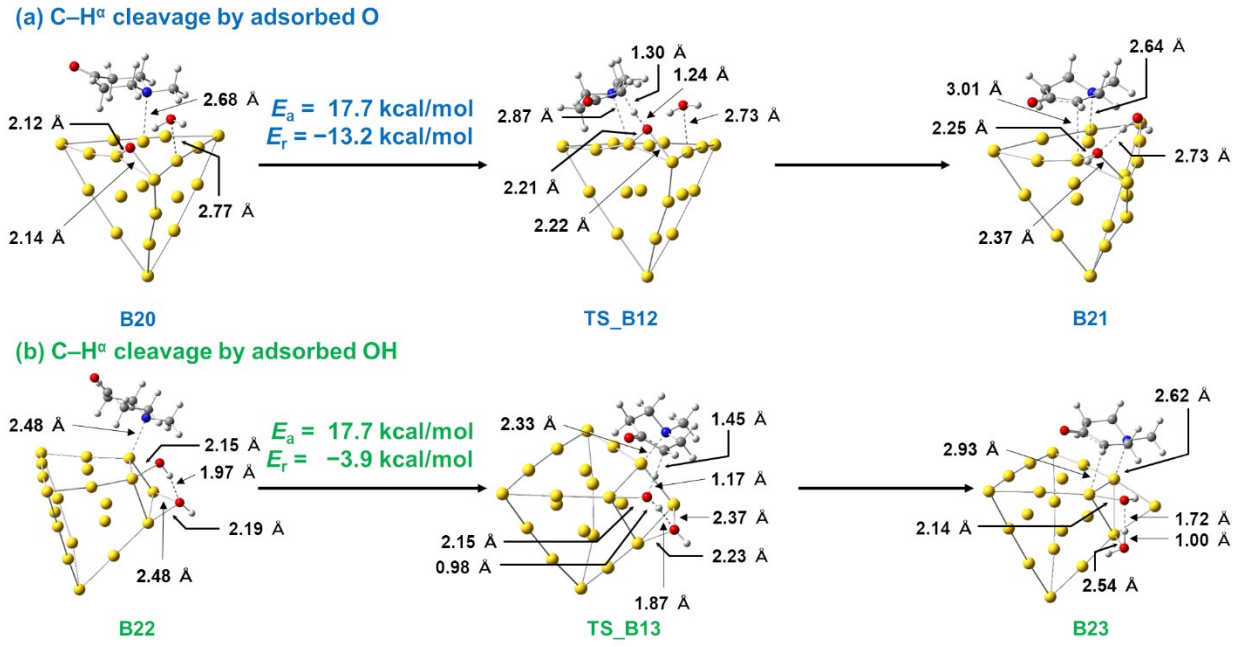


Figure S7. Optimized structures of the reactant, product and transition states of the C–H$^{\alpha}$ bond activation by the adsorbed (a) O and (b) OH with the Au_{20}^{1-} model. Red: oxygen, blue: nitrogen, gray: carbon, white: hydrogen, yellow: gold.

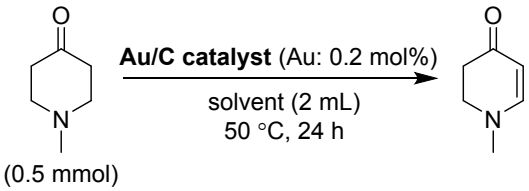
S8. Experimental Results for α,β-Dehydrogenation of 1-Methyl-4-piperidone by the Au/C Catalyst

The α,β-dehydrogenation of 1-methyl-4-piperidone by the Au/C catalyst was carried out according to the following procedure. Au/C (Haruta Gold Inc. RR2C, Au: 1 wt%, 0.2 mol%), 1-methyl-4-piperidone (0.5 mmol), solvent (2 mL), and a Teflon-coated magnetic stir bar were successively placed in a Pyrex glass reactor (volume *ca.* 20 mL). When the reaction was carried out under an Ar atmosphere, a Schlenk tube containing the aforementioned materials was

degassed by three freeze-pump-thaw cycles and refilled with 1 atm of Ar. The reaction mixture was vigorously stirred at 50 °C, under 1 atm of air or Ar. After the reaction was completed, an internal standard (biphenyl) and a large amount of acetone were added to the reaction mixture, and the product yield was determined by GC analysis.

When H_2O was used as a solvent, the reaction proceeded on the Au/C catalyst in the presence of O_2 in air to give the desired product in 36% yield (Table S4, entry 1). This result suggested that lattice oxygen or its vacancy of the OMS-2 support are not essential factors for the reaction to proceed. On the other hand, the reaction did not proceed on the Au/C catalyst without the existence of O_2 (Table S4, entry 2). This result suggested that O_2 is essential factor for the catalytic cycle in the case of the Au/C catalyst. In addition, when toluene was used as a solvent, the reaction hardly proceeded even in the presence of O_2, suggesting that H_2O is also essential factor for the reaction by the Au/C catalyst (Table S4, entry 3).

Table S4. The α,β-dehydrogenation of 1-methyl-4-piperidone by the Au/C catalyst

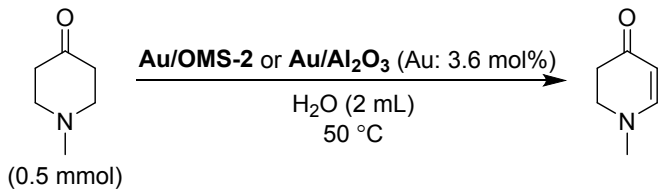


Entry	Solvent	Atmosphere	Yield (%)
1	H_2O	Air (1 atm)	36
2	H_2O	Ar (1 atm)	<1
3	Toluene	Air (1 atm)	1

Yields were determined by GC analysis.

S9. Experimental Measurements for Reaction Rates of α,β-Dehydrogenation of 1-Methyl-4-piperidone by the Au/OMS-2 or Au/Al_2O_3 Catalyst under Different Reaction Environments

The reaction profiles (Figure S8) and the $P(O_2)$ dependence of the initial rate (Figure S9) of α,β-dehydrogenation of 1-methyl-4-piperidone were measured according to the following procedure. Au/OMS-2 or Au/Al_2O_3 (Au: 3.6 mol%), H_2O (1.5 mL), and a Teflon-coated magnetic stir bar were successively placed in a Schlenk tube (volume *ca.* 20 mL). The Schlenk tube was degassed by three freeze-pump-thaw cycles, refilled with 1 atm of air ($P(O_2) = 0.21$) or O_2/Ar mixture ($P(O_2) = 1.0, 0.79, 0.48, 0$), stirred for 3 min at 50 °C. The reaction was started by adding a H_2O solution (0.5 mL) containing 1-methyl-4-piperidone (0.5 mmol) and an internal standard (*N*-methylpyrrolidone, 0.15 mmol) to the reaction mixture. The concentration of the product was determined by GC analysis. The initial rates of the reaction were calculated from the slope of the concentration of the product as shown in Figure S8.



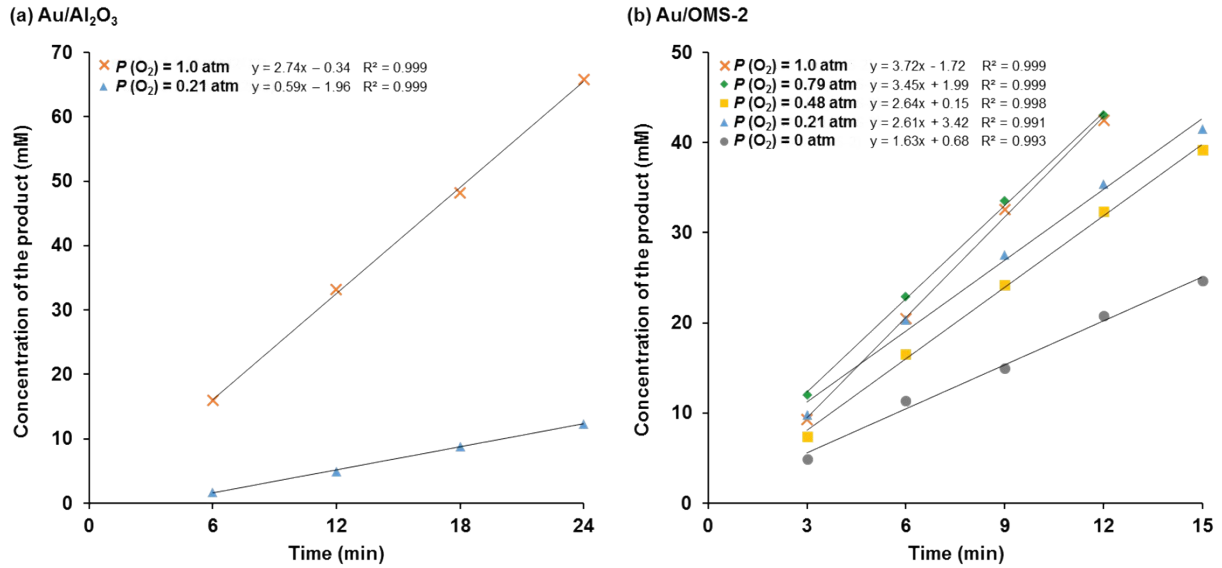


Figure S8. Reaction profiles and calculation of initial rates with different partial pressure of O_2 in the presence of (a) Au/Al_2O_3 and (b) Au/OMS-2.

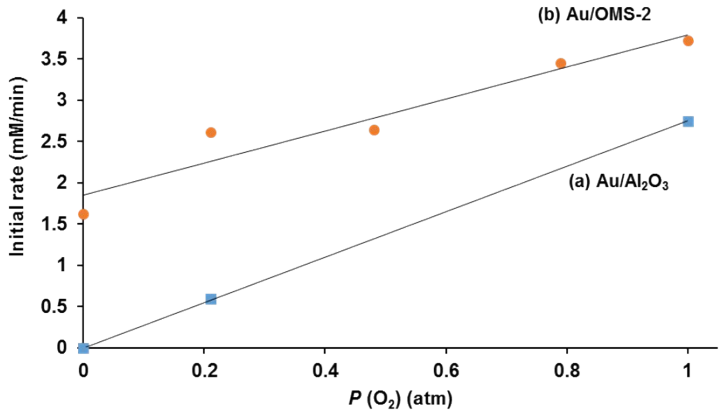


Figure S9. $P(O_2)$ dependence of the initial rate of the reaction in the presence of (a) Au/Al_2O_3 and (b) Au/OMS-2.

S10. Comparison Between the Different Sized Au Cluster Models

The model size effect to the amount of the charge transfer from OMS-2 to Au was investigated by using the Au_5/OMS-2 model. As shown in Table S5, Hirshfeld charge of the Au_5 cluster on OMS-2 was calculated to be −0.41, and this value is almost the same with that of the Au_{10}/OMS-2 model (−0.42). Additionally, adsorption structure of O_2 on the Au_5/OMS-2 model was also investigated. As shown in Table S5, Hirshfeld charge of the adsorbed O_2 on the Au_5/OMS-2 model was calculated to be −0.42, and this value is very close to that of the Au_{10}/OMS-2 model (−0.46). Furthermore, O−O bond distance of the adsorbed O_2 on the both models is also similar (1.39 Å in the Au_5/OMS-2 model and 1.43 Å in the Au_{10}/OMS-2 model). These results suggested that the electronic structures of the Au cluster on the OMS-2 support and adsorbed O_2 were not drastically changed if the different sized Au cluster models were adopted.

Table S5. Comparison between the Au_5/OMS-2 and Au_{10}/OMS-2 models.[a]

Model		q(Au)	q(O_2)	Adsorption energy of O_2 (kcal/mol)	O−O bond distance (Å)
Au_5/OMS-2	w/o O_2	−0.41	-	-	-
	w/ O_2	−0.08	−0.42	−18.5	1.39
Au_{10}/OMS-2	w/o O_2	−0.42	-	-	-
	w/ O_2	−0.24	−0.46	−33.6	1.43

[a]q(Au): Hirshfeld charge of the Au_5 or Au_{10} cluster. q(O_2): Hirshfeld charge of the adsorbed O_2.

The model size effect on the indirect C−H bond activation mechanism was investigated with the Au_{10} cluster models. First, the adsorption energies of O_2 on the Au_{10} model were calculated. As shown in Table S6, O_2 adsorption on the neutral charged Au_{10} cluster was unfavorable (i.e., endothermic adsorption). On the other hand, O_2 adsorption on the negatively charged Au_{10}

cluster models were calculated to be exothermic adsorption. This tendency is the same as that of the Au_{20} models, and the calculated adsorption energies were also similar in both models (see Table S6). Additionally, O−O bond distance of the adsorbed O_2 was also very close value between each Au_{10} and Au_{20} model (see Table S6). Furthermore, the reaction energies of the indirect C−H$^{\alpha}$ bond activation of 1-methyl-4-piperidone were calculated with the Au_{10} models. As shown in Table S6, the reaction energy was slightly endothermic with the Au_{10}^{1-} model (+2.4 kcal/mol), but that with the Au_{10}^{2-} model was exothermic (−10.6 kcal/mol). This tendency is the same as that of the Au_{20} models (see Table S6). These results suggested that the activity for the indirect C−H bond activation is not drastically changed if the different sized models are adopted.

Table S6. Comparison between the Au_{10} and Au_{20} models.

Model	Charge	Adsorption energy of O_2 (kcal/mol)	O−O bond distance (Å)	Reaction energy of the indirect C−H activation (kcal/mol)
Au_{10}	±0	+23.6	1.29	-
	−1	−21.5	1.30	+ 2.4
	−2	−16.2	1.39	−10.6
Au_{20}	±0	+25.3	1.25	-
	−1	−21.1	1.30	+5.8
	−2	−12.5	1.40	−5.5

S11. Cartesian Coordinates of Optimized Structures along the Catalytic Cycle

B3			
Au	-3.84457	-3.04618	-0.89770
Au	-0.27414	4.57194	-2.26812
Au	4.47007	-2.31200	-1.89220
Au	0.93563	0.70931	5.06109
Au	-1.26334	0.78896	0.69990
Au	0.02515	-0.26421	-1.95264
Au	1.94731	1.14770	0.34362
Au	0.36148	-1.78883	0.83443
Au	-2.88553	-0.39632	-1.43088
Au	3.30796	-1.42612	0.49712
Au	2.18204	-0.41135	2.79067
Au	-1.61449	2.09426	-1.90507
Au	-2.53082	-1.77817	1.40917
Au	2.94129	0.01398	-2.15426
Au	1.41975	2.32243	-2.26956
Au	-0.77739	-0.56957	3.21872
Au	-1.18072	-2.82855	-1.43362
Au	1.61866	-2.69677	-1.63377
Au	0.06304	3.38658	0.25556
Au	0.48414	2.12689	2.67492
C	-4.87583	2.57777	-0.22143
C	-5.43216	1.89845	-1.46413
C	-6.10987	-0.04167	-0.22069
C	-5.55187	0.50807	1.08277
C	-5.40979	2.00711	1.06965
H	-6.49142	2.19849	-1.61604
H	-4.87044	2.22318	-2.35166
H	-3.78008	2.43088	-0.19896
H	-5.05842	3.65733	-0.24070
H	-7.17433	0.25617	-0.33490
H	-6.07532	-1.13891	-0.20355
H	-6.15992	0.20029	1.93925
H	-4.54235	0.08567	1.24130
O	-5.65780	2.70427	2.03307
N	-5.35567	0.43893	-1.38273
C	-5.88228	-0.15601	-2.60412
H	-5.29829	0.18973	-3.46541
H	-5.80046	-1.24821	-2.54713
H	-6.94436	0.11571	-2.76129
O	-4.74657	-2.62193	1.89040
O	-5.37050	-3.16741	0.89186

TS_B2

Au	-3.91826	-3.06608	-0.29202
Au	0.06396	3.79085	-3.44791
Au	4.47873	-2.84625	-0.90487
Au	0.64623	2.01886	4.71717
Au	-1.22254	1.03052	0.34823
Au	0.11601	-0.78603	-1.81400
Au	1.98857	1.14957	0.13817
Au	0.26247	-1.50894	1.29952
Au	-2.80569	-0.68052	-1.43222
Au	3.21702	-1.32202	1.07336
Au	1.98767	0.30216	2.92675
Au	-1.42335	1.55352	-2.51688
Au	-2.64988	-1.23556	1.56007
Au	3.04964	-0.65580	-1.88909
Au	1.64071	1.57344	-2.72553
Au	-1.01560	0.34687	3.16528
Au	-1.22401	-3.08541	-0.68607
Au	1.59572	-3.07870	-0.75386
Au	0.24320	3.34976	-0.68307
Au	0.44787	2.77357	2.01759
C	-4.69425	2.23214	-0.09788
C	-5.10198	1.81802	-1.49821
C	-6.30225	-0.12853	-0.73931
C	-6.28340	0.42280	0.64592
C	-5.58719	1.65509	0.97829
H	-6.06822	2.29334	-1.77552
H	-4.35023	2.15278	-2.22892
H	-3.66239	1.89106	0.10243
H	-4.68666	3.32246	0.01149
H	-7.28336	0.09911	-1.21601
H	-6.24206	-1.23649	-0.68865
H	-7.19178	0.24930	1.22909
H	-5.62742	-0.68221	1.42141
O	-5.70123	2.20629	2.06998
N	-5.22693	0.36380	-1.60644
C	-5.50108	-0.03079	-2.98169
H	-4.68332	0.29517	-3.63538
H	-5.57984	-1.12293	-3.04189
H	-6.44827	0.41140	-3.34919
O	-5.25560	-1.63989	1.80204
O	-5.73905	-2.60554	0.95582

B4

Au	4.70136	-1.34421	0.54164
Au	-0.62416	4.69148	-2.08126
Au	-2.68198	0.01569	4.55145
Au	-2.73386	-3.34389	-3.10010
Au	0.67555	-0.05041	-1.65456
Au	0.58775	1.25724	1.16912
Au	-2.29301	0.52855	-0.25392
Au	-0.26138	-1.84217	0.78111
Au	3.08350	0.84928	-0.31077
Au	-2.83404	-1.19684	2.02678
Au	-2.84574	-2.31836	-0.50882
Au	1.27199	2.77401	-1.23417
Au	2.31140	-2.23882	-0.60864
Au	-2.03113	1.70368	2.41131
Au	-1.36041	3.25269	0.22005
Au	-0.13492	-2.85120	-1.92450
Au	2.27428	-0.99996	1.99892
Au	-0.13424	-0.48937	3.36490
Au	-1.30498	1.99487	-2.56596
Au	-1.93785	-0.66707	-2.89108
C	6.48012	1.04262	-1.45585
C	6.04241	2.33133	-0.78191
C	5.97041	1.32269	1.38572
C	6.49808	0.01063	0.84690
C	6.97163	-0.03087	-0.50195
H	6.93124	2.91563	-0.46127
H	5.47529	2.95969	-1.48250
H	5.64190	0.60790	-2.02262
H	7.27819	1.23497	-2.18235
H	6.80131	1.97834	1.73399
H	5.31895	1.15318	2.25453
H	7.09983	-0.55796	1.56164
H	7.71473	-2.25717	-0.18055
O	7.69698	-0.93475	-0.98551
N	5.20008	2.07363	0.38680
C	4.71489	3.32199	0.96047
H	4.13439	3.87430	0.21240
H	4.05452	3.10461	1.80868
H	5.55109	3.95790	1.30972
O	7.60833	-3.13170	0.35377
O	6.32099	-3.40461	0.31065

B9

Au	-4.68745	-1.30062	1.26285
Au	0.31188	4.81344	-1.83909
Au	2.53847	-3.09931	-3.44160
Au	3.08421	-0.08481	4.34808
Au	-0.63758	1.18241	1.32264
Au	-0.72237	0.00377	-1.54580
Au	2.22308	0.62227	-0.33972
Au	0.24445	-1.83285	0.67995
Au	-3.12735	0.71736	-0.06043
Au	2.81152	-2.19632	-0.79036
Au	2.93718	-1.23393	1.78832
Au	-1.46158	2.78492	-0.96149
Au	-2.09661	-1.16257	2.25314
Au	1.79814	-0.42030	-3.03990
Au	1.04999	2.18139	-2.51186
Au	0.44813	-0.67136	3.36224
Au	-2.33627	-2.30268	-0.59284
Au	0.09418	-2.72217	-2.04489
Au	1.22078	3.28101	0.33999
Au	2.06317	1.64923	2.39541
C	-6.33878	1.87548	0.43234
C	-5.97579	1.90602	-1.04364
C	-6.04248	-0.48389	-1.23772
C	-6.48559	-0.65295	0.19745
C	-6.94262	0.55562	0.90012
H	-6.89512	1.96114	-1.66399
H	-5.37212	2.79466	-1.27492
H	-5.43337	2.04743	1.03666
H	-7.04460	2.67585	0.68095
H	-6.93302	-0.38713	-1.89997
H	-5.48018	-1.36343	-1.58217
H	-7.16125	-1.50143	0.34424
H	-4.76559	-4.31604	-0.03868
O	-7.73465	0.54188	1.83458
N	-5.21400	0.71623	-1.43192
C	-4.77625	0.80087	-2.82115
H	-4.13370	1.67880	-2.95625
H	-4.19828	-0.09546	-3.07449
H	-5.63931	0.87578	-3.50916
O	-5.12941	-3.54138	-0.49106
O	-4.11063	-3.23711	-1.44216

TSB6

Au	-4.63029	-0.96721	1.59975
Au	0.47708	4.50137	-2.47918
Au	2.03757	-3.70332	-3.09219
Au	3.39168	0.28933	4.13434
Au	-0.44940	1.38371	1.21391
Au	-0.80387	-0.09966	-1.53293
Au	2.23595	0.41926	-0.53533
Au	0.19820	-1.72507	0.95887
Au	-3.06257	0.91689	0.01029
Au	2.57819	-2.47435	-0.61601
Au	2.95815	-1.17293	1.79515
Au	-1.33179	2.75646	-1.19694
Au	-2.03364	-0.71905	2.49984
Au	1.56287	-0.94034	-3.04079
Au	1.04578	1.77127	-2.83748
Au	0.60081	-0.19290	3.42319
Au	-2.49136	-2.06958	-0.12042
Au	-0.26995	-2.94466	-1.62842
Au	1.47082	3.20598	-0.17218
Au	2.36044	1.80560	2.02945
C	-6.28637	2.02982	0.61273
C	-6.04106	1.98227	-0.88375
C	-6.05350	-0.43038	-0.92871
C	-6.54977	-0.49121	0.44470
C	-6.88283	0.74451	1.17017
H	-7.00475	2.00619	-1.43335
H	-5.45296	2.85231	-1.20877
H	-5.33244	2.20815	1.13668
H	-6.95759	2.85338	0.88051
H	-6.80978	-0.67781	-1.70367
H	-5.27052	-1.46444	-1.16469
H	-7.24410	-1.30882	0.65178
H	-5.09378	-3.35056	0.27905
O	-7.60767	0.77441	2.15813
N	-5.30843	0.76710	-1.25895
C	-4.93200	0.77852	-2.66711
H	-4.29561	1.64616	-2.87649
H	-4.36472	-0.12970	-2.90165
H	-5.82387	0.81831	-3.32015
O	-5.36844	-3.47195	-0.64861
O	-4.57980	-2.51850	-1.33908

B10

Au	-4.21738	-1.86291	-1.60466
Au	0.08066	0.93336	5.07867
Au	1.31363	4.41487	-2.41637
Au	4.10879	-3.47064	-0.98231
Au	-0.04197	-1.75979	0.96936
Au	-1.65039	1.75269	0.49831
Au	1.98797	0.69720	0.61188
Au	0.46018	-0.39146	-2.03334
Au	-2.81793	-0.93532	0.70549
Au	2.35568	1.79784	-2.04338
Au	3.31594	-0.78854	-1.51004
Au	-1.43826	-0.09970	2.91699
Au	-1.48813	-2.51100	-1.47707
Au	0.82804	3.32488	0.12407
Au	0.43231	2.17183	2.57721
Au	1.28344	-3.05405	-1.24245
Au	-2.37002	0.26256	-1.95009
Au	-0.58701	2.31792	-2.28353
Au	1.49663	-0.61487	3.14850
Au	2.87375	-2.02892	1.14480
C	-6.42298	-2.25383	1.11416
C	-6.58985	-0.80911	1.55514
C	-6.27573	-0.16369	-0.75983
C	-6.60099	-1.43521	-1.24435
C	-6.89138	-2.51843	-0.30915
H	-7.64251	-0.59344	1.80652
H	-5.99301	-0.61177	2.45490
H	-5.35381	-2.52515	1.14862
H	-6.95227	-2.92945	1.79302
H	-6.05216	0.65310	-1.45007
H	-3.50905	2.93685	-0.80213
H	-6.92008	-1.53883	-2.27958
H	-3.96795	2.37314	-2.87838
O	-7.39118	-3.58649	-0.62854
N	-6.17167	0.14519	0.52906
C	-5.77273	1.46415	0.98529
H	-4.83510	1.39550	1.55752
H	-5.60180	2.12561	0.13127
H	-6.55612	1.89029	1.62673
O	-4.67561	2.40249	-2.20941
O	-4.21318	3.40697	-1.31083

B11

Au	5.03961	-1.67620	0.16142
Au	-2.02317	0.42983	4.81158
Au	-3.35897	-3.25524	-2.57599
Au	-0.55636	4.62514	-2.26254
Au	0.79996	1.22284	0.95616
Au	-0.21283	-1.79202	0.83557
Au	-2.31288	0.71643	-0.02396
Au	0.48712	-0.21536	-1.77300
Au	2.49435	-1.05707	1.70285
Au	-2.35520	-0.62571	-2.61462
Au	-1.44012	1.95887	-2.51615
Au	0.28526	-0.37381	3.33151
Au	3.08653	0.50303	-0.72531
Au	-3.00717	-2.11660	-0.04156
Au	-2.53630	-0.90758	2.39482
Au	1.31586	2.55908	-1.60553
Au	2.00329	-2.49760	-0.93241
Au	-0.63618	-2.91242	-1.79383
Au	-1.55432	1.95845	2.51419
Au	-1.04604	3.34415	0.17388
O	4.02167	-3.45848	-0.55120
O	3.86540	-4.33585	0.58887
C	6.51195	1.15248	-1.48479
C	5.85338	2.33280	-0.79091
C	5.65105	1.13143	1.27931
C	6.33404	-0.10478	0.71986
C	7.11805	0.14645	-0.51504
H	6.62870	2.98933	-0.34199
H	5.28928	2.94145	-1.51107
H	5.75967	0.61673	-2.08500
H	7.29945	1.48717	-2.16855
H	6.40766	1.80470	1.74192
H	4.93786	0.86265	2.07029
H	6.98715	-0.56009	1.47536
H	3.67493	-5.16861	0.13493
O	8.16135	-0.42809	-0.79124
N	4.93068	1.90035	0.26065
C	4.27902	3.05430	0.86864
H	3.71429	3.60767	0.10846
H	3.57044	2.71840	1.63541
H	5.01896	3.73220	1.33473

TS_B7

Au	5.10041	-1.93975	0.30647
Au	-3.03465	-0.29219	4.35905
Au	-2.96861	-2.32818	-3.75746
Au	0.24919	4.97383	-1.26240
Au	0.75238	0.77806	1.40188
Au	-0.59492	-1.89703	0.45034
Au	-2.12063	0.90499	-0.25517
Au	0.78405	0.05559	-1.61449
Au	1.83744	-1.81881	2.08949
Au	-1.82058	0.13500	-3.05185
Au	-0.75839	2.54088	-2.23981
Au	-0.54341	-1.00549	3.25892
Au	3.20460	0.23045	-0.02719
Au	-3.11200	-1.73687	-1.03087
Au	-3.14257	-1.05382	1.65101
Au	1.77525	2.61176	-0.66142
Au	1.94579	-2.48866	-0.91560
Au	-0.45354	-2.46066	-2.37880
Au	-1.88432	1.57887	2.58175
Au	-0.73599	3.27759	0.75095
O	3.60196	-3.44085	0.21133
O	3.08125	-3.73516	1.84602
C	6.28817	1.08687	-1.36805
C	5.86417	2.12248	-0.33997
C	6.17645	0.60363	1.48322
C	6.64507	-0.52562	0.57626
C	7.05691	-0.08949	-0.77941
H	6.74520	2.70387	0.00570
H	5.15563	2.83689	-0.78165
H	5.39202	0.67300	-1.85832
H	6.90418	1.53882	-2.15303
H	7.04157	1.21778	1.82254
H	5.69491	0.20678	2.38695
H	7.46992	-1.08294	1.03794
H	3.96060	-3.67145	2.24778
O	7.91929	-0.64966	-1.43970
N	5.22380	1.49725	0.81913
C	4.73303	2.50578	1.74787
H	4.00585	3.15377	1.24195
H	4.22136	2.01665	2.58538
H	5.55862	3.12834	2.14248

B12

Au	5.17094	1.37553	-1.36157
Au	-3.61594	-2.84079	-2.78483
Au	-2.55883	4.54206	1.01905
Au	0.62122	-2.41604	4.42844
Au	0.48679	-1.65766	-0.41244
Au	-0.52112	0.92060	-1.74112
Au	-2.04262	-0.25924	1.00540
Au	0.98449	1.06251	0.94054
Au	1.58147	-0.72603	-2.95669
Au	-1.39717	2.29890	2.26526
Au	-0.38139	0.00947	3.39797
Au	-1.03601	-1.65497	-2.88803
Au	3.14908	-0.44361	-0.23587
Au	-3.02292	2.12105	-0.35385
Au	-3.34935	-0.29493	-1.60034
Au	1.91382	-1.41369	2.11647
Au	1.97706	2.39707	-1.45357
Au	-0.34055	3.38257	-0.30379
Au	-2.21328	-2.84988	-0.35264
Au	-0.81673	-2.71107	2.02714
O	3.93923	2.88668	-2.02903
O	3.55756	-0.65995	-3.59399
C	6.08224	-1.11772	1.31322
C	5.52234	-2.36199	0.64292
C	5.94292	-1.50592	-1.55599
C	6.52685	-0.20163	-1.03419
C	6.91452	-0.22766	0.39804
H	6.32702	-3.10943	0.48511
H	4.75900	-2.83264	1.27921
H	5.25036	-0.49861	1.68684
H	6.69745	-1.38025	2.18099
H	6.73757	-2.27800	-1.65408
H	5.47503	-1.36393	-2.53711
H	7.40285	0.09742	-1.62544
H	3.75125	0.27206	-3.76060
O	7.81891	0.44689	0.86681
N	4.91557	-2.04742	-0.65470
C	4.29856	-3.23131	-1.24804
H	3.50690	-3.60668	-0.58832
H	3.85906	-2.95711	-2.21358
H	5.04658	-4.03102	-1.40222

TS_B8

Au	5.19198	1.29890	-1.23444
Au	-3.13168	-3.37695	-2.70996
Au	-2.87691	4.48900	0.14993
Au	0.23767	-1.75889	4.78585
Au	0.59895	-1.64569	-0.08424
Au	-0.26907	0.69701	-1.84244
Au	-2.12253	-0.22625	0.83519
Au	0.77746	1.30942	0.96654
Au	1.93017	-1.07889	-2.63685
Au	-1.79172	2.50467	1.81211
Au	-0.77959	0.44070	3.34235
Au	-0.64267	-2.05564	-2.67708
Au	3.10774	-0.17211	0.16455
Au	-3.00280	1.89882	-0.94500
Au	-3.11692	-0.67149	-1.86187
Au	1.73981	-0.98415	2.49873
Au	2.10199	2.35927	-1.41775
Au	-0.42952	3.33093	-0.74983
Au	-2.03198	-2.98686	-0.14937
Au	-0.91202	-2.44838	2.31927
O	4.02068	2.74553	-1.96906
O	4.02227	-1.10728	-3.29477
C	6.17785	-0.88176	1.43508
C	5.53257	-2.19410	1.03532
C	5.63678	-1.67266	-1.32106
C	6.44660	-0.47522	-1.07269
C	6.96668	-0.24371	0.30387
H	6.30661	-2.98054	0.91645
H	4.83444	-2.53180	1.81407
H	5.40199	-0.16533	1.74952
H	6.85895	-1.01860	2.28202
H	6.20034	-2.53425	-1.73819
H	4.85055	-1.41219	-2.32441
H	7.22775	-0.31335	-1.82217
H	4.23119	-0.16899	-3.43626
O	7.98796	0.38758	0.52439
N	4.78542	-2.07175	-0.22348
C	4.07368	-3.30742	-0.52178
H	3.35298	-3.52276	0.27607
H	3.52156	-3.19941	-1.46312
H	4.77396	-4.15833	-0.61591

B13

Au	4.92192	0.76315	-1.97388
Au	-4.97243	-0.69926	-2.18880
Au	-0.54091	4.14838	3.01634
Au	0.74144	-4.11460	2.86378
Au	-0.24626	-1.55589	-1.26521
Au	-0.67316	1.54403	-1.15792
Au	-1.80728	-0.27045	1.45876
Au	1.43551	0.31928	0.73544
Au	0.48006	0.15620	-3.47687
Au	-0.04133	1.38607	3.08221
Au	0.47246	-1.32088	2.97412
Au	-2.23633	-0.19866	-2.88114
Au	2.55128	-1.01135	-1.65415
Au	-2.10295	2.61942	1.23960
Au	-3.52913	1.04548	-0.51004
Au	1.72368	-2.58263	0.60452
Au	2.17506	2.12790	-1.47836
Au	0.80830	3.13984	0.72821
Au	-3.07395	-1.96389	-0.56499
Au	-1.17596	-3.09204	1.08650
O	3.61439	1.88031	-3.02521
O	2.27168	0.75231	-4.87119
C	5.20174	-0.11053	1.44491
C	5.21692	-1.63064	1.37866
C	6.13202	-1.41000	-0.86949
C	6.52132	-0.06577	-0.69391
C	6.30797	0.54044	0.63732
H	5.96929	-2.05739	2.06147
H	4.23360	-2.02843	1.67873
H	4.24094	0.26296	1.04749
H	5.26990	0.22439	2.48388
H	6.37654	-1.92182	-1.80136
H	2.73275	-0.07642	-5.04233
H	7.39775	0.27131	-1.24982
H	2.85844	1.23294	-4.16106
O	6.93161	1.50489	1.03931
N	5.50509	-2.14516	0.03374
C	5.11043	-3.51618	-0.22244
H	4.01408	-3.60659	-0.15451
H	5.42569	-3.81493	-1.22565
H	5.56950	-4.18153	0.52026

B20

Au	1.31427	4.79735	-1.16923
Au	0.44863	-1.02160	4.97024
Au	2.19834	-3.63486	-2.79097
Au	-5.29449	-0.29564	-1.09762
Au	-1.19762	1.31924	1.06724
Au	1.95781	0.05613	0.40359
Au	-0.96462	-1.76925	0.39351
Au	-0.32738	0.51457	-1.72700
Au	1.23452	2.87858	0.98486
Au	-0.37152	-2.52448	-2.36723
Au	-2.79822	-1.38535	-1.82051
Au	0.87966	0.98763	3.01007
Au	-0.97652	3.30002	-1.05095
Au	1.64208	-2.88174	-0.14163
Au	1.11783	-1.98127	2.41413
Au	-3.06419	1.48519	-1.18908
Au	2.31009	1.87814	-1.88496
Au	2.08092	-0.83876	-2.39300
Au	-1.62105	-0.79242	3.06968
Au	-3.50594	-0.51055	1.05534
O	3.13791	3.81985	-1.70214
O	3.84051	3.82410	0.91311
H	3.65636	4.72918	1.18377
H	3.69530	3.82898	-0.07559
C	5.51902	0.00147	-0.97589
C	5.39280	0.76709	0.33119
C	4.99427	-1.23272	1.59980
C	5.12871	-2.11650	0.37062
C	5.82891	-1.45962	-0.79182
H	6.39433	0.87473	0.80138
H	5.01463	1.78037	0.14919
H	4.54985	0.04885	-1.50819
H	6.26833	0.45141	-1.63547
H	5.98046	-1.13903	2.10448
H	4.30390	-1.69580	2.32054
H	5.62967	-3.06155	0.60576
H	4.11588	-2.37146	0.00402
O	6.53387	-2.08525	-1.55981
N	4.49422	0.10367	1.28118
C	4.41788	0.89917	2.50385
H	4.06481	1.90887	2.26680
H	3.72052	0.42948	3.21037
H	5.41289	0.97265	2.98568

TS_B12

Au	-3.33275	-3.70356	-0.26808
Au	2.16030	0.37362	4.76234
Au	-1.45008	4.65493	-1.47208
Au	4.11861	-1.34744	-3.19300
Au	1.00719	-1.74374	0.55900
Au	-1.12900	0.52491	1.14111
Au	1.76639	1.36361	0.02666
Au	-0.60687	-0.30599	-1.72890
Au	-1.65249	-2.32063	1.57906
Au	0.41348	2.64677	-2.19792
Au	2.15452	0.61740	-2.75741
Au	0.19143	-1.00885	3.24029
Au	-0.81417	-3.18271	-1.18107
Au	-0.28672	3.32476	0.71957
Au	0.89573	1.89985	2.77283
Au	1.55127	-2.22927	-2.28093
Au	-3.32159	-0.48393	-0.50649
Au	-2.25364	1.97550	-1.14777
Au	2.97352	-0.24524	2.14494
Au	3.59872	-0.84723	-0.48683
O	-4.78540	-2.05201	0.02413
O	-4.12408	-1.96706	2.67574
H	-4.27029	-2.85554	3.01558
H	-4.44582	-2.00049	1.73623
C	-6.90478	-0.72164	0.21390
C	-6.38051	0.25245	1.24418
C	-5.94886	1.91955	-0.41042
C	-6.37102	1.01144	-1.55565
C	-7.21772	-0.16875	-1.11720
H	-7.21712	0.85905	1.66723
H	-5.92698	-0.29074	2.08400
H	-5.90529	-1.51628	-0.01247
H	-7.69233	-1.38751	0.57876
H	-6.81988	2.50952	-0.04423
H	-5.19398	2.64126	-0.75860
H	-6.91531	1.55815	-2.33377
H	-5.46340	0.59187	-2.02390
O	-8.05500	-0.65600	-1.86230
N	-5.37657	1.14207	0.67594
C	-4.78667	1.98036	1.69937
H	-4.31516	1.34896	2.46328
H	-4.00846	2.61905	1.25951
H	-5.54064	2.62956	2.19155

B21

Au	2.31904	4.24910	-0.40665
Au	-0.38059	-1.78373	4.77385
Au	1.83422	-3.61516	-3.09258
Au	-5.08374	0.84503	-1.63533
Au	-1.20936	1.33075	1.19112
Au	1.86042	-0.35159	0.60400
Au	-1.25565	-1.59522	0.01881
Au	0.05470	0.87093	-1.52200
Au	1.46556	2.44271	1.54595
Au	-0.52121	-2.08878	-2.74078
Au	-2.72116	-0.55784	-2.25548
Au	0.62213	0.36916	3.20197
Au	-0.32161	3.60754	-0.46122
Au	1.18425	-3.11593	-0.39354
Au	0.47167	-2.47707	2.18806
Au	-2.59208	2.17861	-1.20569
Au	2.97767	1.52140	-1.39570
Au	2.13728	-0.94231	-2.26921
Au	-2.14010	-0.98138	2.73136
Au	-3.69526	-0.10337	0.60422
O	4.33032	3.31855	-1.23586
O	5.15202	3.58458	1.38658
H	4.30852	3.91126	1.72024
H	5.01727	3.55437	0.41578
C	5.42923	0.41813	-0.03945
C	5.02122	0.37113	1.38436
C	4.86900	-2.02536	1.25342
C	5.02589	-2.05785	-0.25617
C	5.54115	-0.76617	-0.85285
H	5.94459	0.37944	2.01225
H	4.48501	1.29139	1.65843
H	4.54870	3.64269	-2.11666
H	5.82005	1.35315	-0.44059
H	5.86370	-2.10522	1.74421
H	4.27195	-2.88314	1.59220
H	5.68785	-2.87435	-0.56730
H	4.04744	-2.25343	-0.72824
O	6.00901	-0.73648	-1.99448
N	4.21136	-0.80210	1.71453
C	3.99717	-0.86219	3.15342
H	3.50793	0.05899	3.49520
H	3.34105	-1.70646	3.39850
H	4.95511	-0.97953	3.69698

B14

Au	-5.01045	-1.73454	-0.51020
Au	0.76041	4.81389	-1.79419
Au	3.65886	-3.00285	-2.49119
Au	1.45084	-0.00724	4.99457
Au	-0.95979	1.15081	0.92946
Au	-0.27722	-0.05227	-1.83895
Au	2.28887	0.71925	0.27119
Au	0.13175	-1.86298	0.67048
Au	-3.00327	0.54119	-1.10619
Au	2.99478	-2.10823	0.07617
Au	2.25973	-1.11462	2.54456
Au	-1.16556	2.70489	-1.51974
Au	-2.64997	-1.19897	1.27406
Au	2.62844	-0.38799	-2.40980
Au	1.67975	2.17876	-2.18330
Au	-0.66646	-0.65616	3.19962
Au	-1.87961	-2.38234	-1.39705
Au	0.84952	-2.74306	-1.99482
Au	0.97508	3.31508	0.55857
Au	1.21810	1.72095	2.80134
C	-5.23883	1.45265	1.49578
C	-5.21534	2.44836	0.34803
C	-6.31778	0.92022	-1.13254
C	-6.38788	-0.18728	-0.09212
C	-6.18095	0.27503	1.30209
H	-6.12639	3.08290	0.37490
H	-4.34880	3.11793	0.43875
H	-4.23015	1.02742	1.63766
H	-5.50192	1.94851	2.43628
H	-7.22756	1.56036	-1.07416
H	-6.28885	0.50485	-2.14825
H	-7.35345	-0.70719	-0.14900
H	-3.33242	-5.11612	-0.55738
O	-6.68489	-0.27128	2.27243
N	-5.14952	1.79028	-0.96269
C	-5.10374	2.79179	-2.02164
H	-4.21749	3.42523	-1.89336
H	-5.03081	2.29623	-2.99619
H	-6.00728	3.43067	-2.00992
O	-3.80076	-4.38813	-0.12492
O	-3.89444	-3.45295	-1.22396

TS_B9

Au	5.06542	-1.55466	1.19631
Au	0.10900	4.92737	-1.48769
Au	-3.43326	-0.19588	4.09055
Au	-2.45838	-2.67915	-3.84520
Au	1.01465	-0.03616	-1.41076
Au	0.53613	0.97144	1.45132
Au	-2.11778	0.78555	-0.47047
Au	-0.54829	-1.86979	0.56928
Au	3.20897	0.54106	0.42585
Au	-3.22584	-1.11769	1.45966
Au	-2.91782	-1.93047	-1.16990
Au	1.68100	2.69850	-0.60165
Au	2.03707	-2.61716	-0.57553
Au	-2.21686	1.61528	2.32790
Au	-1.03968	3.30973	0.49829
Au	-0.13179	-2.54706	-2.27234
Au	1.81463	-1.47622	2.28788
Au	-0.76165	-0.87043	3.27091
Au	-0.59591	2.35698	-2.40487
Au	-1.50693	-0.09930	-3.18444
C	5.77587	0.08429	-1.91975
C	5.67353	1.54070	-1.49742
C	6.49750	1.07111	0.70570
C	6.65994	-0.41262	0.41816
C	6.67931	-0.75438	-1.02466
H	6.61793	2.07427	-1.73663
H	4.86611	2.04459	-2.04627
H	4.77447	-0.37639	-1.89483
H	6.14076	0.00141	-2.94923
H	7.43519	1.61920	0.45950
H	6.29860	1.24305	1.77162
H	7.56593	-0.80643	0.89576
H	4.14211	-4.13585	0.48184
O	7.32132	-1.68284	-1.49586
N	5.40688	1.67848	-0.06269
C	5.25514	3.08295	0.29204
H	4.42077	3.51992	-0.27262
H	5.02476	3.17156	1.35974
H	6.17582	3.65687	0.07330
O	3.22759	-4.01434	0.77983
O	3.56876	-2.82515	1.99108

B15

Au	4.84462	-1.01288	1.80242
Au	0.02888	4.60334	-2.30361
Au	-3.68748	0.33815	3.87356
Au	-2.08873	-3.40757	-3.44251
Au	1.07337	-0.20828	-1.32789
Au	0.44071	1.24340	1.31005
Au	-2.07761	0.56853	-0.68672
Au	-0.31939	-1.73000	0.88279
Au	3.17039	0.87310	0.45705
Au	-3.22093	-1.04199	1.46359
Au	-2.68973	-2.27019	-0.93287
Au	1.57952	2.66782	-0.95430
Au	2.32128	-2.58183	-0.10056
Au	-2.41284	1.88839	1.90452
Au	-1.21287	3.30165	-0.12730
Au	0.11098	-2.90273	-1.73174
Au	1.68970	-0.88327	2.84805
Au	-0.98328	-0.33581	3.31184
Au	-0.58749	1.89700	-2.81494
Au	-1.28561	-0.72333	-3.18591
C	5.17036	-0.59908	-1.93586
C	5.31873	0.91180	-1.99657
C	6.44894	0.98423	0.11194
C	6.31941	-0.50999	0.34989
C	5.99377	-1.29070	-0.86090
H	6.26350	1.18576	-2.51221
H	4.49342	1.35476	-2.57141
H	4.11923	-0.86690	-1.72862
H	5.41813	-1.05850	-2.89900
H	7.38432	1.21844	-0.44525
H	6.49830	1.52473	1.06491
H	7.22980	-0.91735	0.80991
H	4.73060	-3.39590	0.15494
O	6.28178	-2.47523	-1.00040
N	5.32412	1.51513	-0.66098
C	5.39109	2.96574	-0.75413
H	4.52570	3.34036	-1.31584
H	5.35984	3.40171	0.25076
H	6.31744	3.29735	-1.26113
O	4.03905	-3.30439	0.82967
O	3.64810	-1.32781	3.44539

B16

Au	5.07190	1.63587	-1.08842
Au	0.30137	-2.96406	4.16194
Au	-2.90051	-2.66713	-3.56907
Au	-3.12176	4.13230	1.32143
Au	0.77689	1.02625	1.24302
Au	0.69874	-1.50262	-0.51666
Au	-2.10744	-0.55097	0.72424
Au	-0.45151	1.15162	-1.59354
Au	3.19888	-0.18289	0.21307
Au	-3.05819	-0.31531	-2.02491
Au	-3.15150	1.91462	-0.42163
Au	1.76518	-1.52324	2.21438
Au	1.85913	2.74540	-0.82871
Au	-1.85368	-2.92072	-0.98064
Au	-0.77833	-3.01670	1.56249
Au	-0.63229	3.39043	0.18799
Au	2.01070	0.00553	-2.69689
Au	-0.44560	-1.27722	-3.13519
Au	-0.78739	-0.49432	3.33215
Au	-1.88312	1.83992	2.39140
C	6.31521	-0.82915	1.40389
C	5.71396	-2.10415	0.83633
C	5.81277	-1.28760	-1.41742
C	6.43024	0.03315	-0.99953
C	7.01000	0.04533	0.36607
H	6.51656	-2.83172	0.59333
H	5.05412	-2.58124	1.57452
H	5.51693	-0.21893	1.85677
H	7.03667	-1.05211	2.19772
H	6.60619	-2.04042	-1.62168
H	5.22529	-1.14688	-2.33296
H	7.19699	0.34837	-1.72013
H	4.12886	3.98280	-0.54447
O	7.96390	0.73608	0.69373
N	4.93620	-1.83887	-0.37654
C	4.28321	-3.05399	-0.84805
H	3.60678	-3.43827	-0.07519
H	3.69259	-2.82842	-1.74338
H	5.02596	-3.83535	-1.09627
O	3.88282	3.40580	-1.27772
O	3.90848	0.60547	-3.13075

TS_B10

Au	5.13155	1.37178	-1.26711
Au	0.21332	-1.73868	4.80061
Au	-3.01894	-3.44117	-2.73795
Au	-2.98125	4.43093	0.11586
Au	0.76876	1.31148	0.97396
Au	0.62323	-1.61817	-0.07816
Au	-2.12369	-0.26256	0.81307
Au	-0.21517	0.66527	-1.86376
Au	3.13510	-0.16017	0.23242
Au	-3.05164	-0.74230	-1.90088
Au	-3.08842	1.81845	-0.96417
Au	1.72737	-0.93233	2.54395
Au	2.00918	2.47466	-1.37383
Au	-1.96693	-3.02005	-0.17052
Au	-0.88923	-2.45530	2.31298
Au	-0.55537	3.29237	-0.77906
Au	2.05548	-1.05387	-2.59921
Au	-0.53588	-2.06538	-2.68813
Au	-0.81544	0.44147	3.33806
Au	-1.84041	2.47863	1.79286
C	6.26121	-0.87425	1.42091
C	5.57472	-2.16937	1.03309
C	5.54805	-1.60232	-1.30847
C	6.33405	-0.34792	-1.07280
C	6.98895	-0.22061	0.25619
H	6.33040	-2.96016	0.84605
H	4.92484	-2.52298	1.84619
H	5.51251	-0.15629	1.79195
H	6.98406	-1.03855	2.22754
H	6.15877	-2.44871	-1.68516
H	4.77555	-1.37071	-2.27776
H	7.08066	-0.19937	-1.86332
H	4.23391	3.78620	-1.00362
O	8.03083	0.38873	0.44064
N	4.74685	-2.01791	-0.17264
C	4.04334	-3.26600	-0.45173
H	3.37180	-3.50667	0.38131
H	3.44754	-3.15636	-1.36515
H	4.75801	-4.09771	-0.59165
O	4.05529	3.15705	-1.71320
O	4.00686	-1.06207	-3.21995

B17

Au	5.30967	1.26918	-1.18073
Au	-0.07970	-0.85017	5.04542
Au	-2.66039	-4.01995	-2.24562
Au	-3.19646	4.20897	-0.82843
Au	0.50865	1.59696	0.84271
Au	0.77397	-1.59339	0.23587
Au	-2.29197	-0.26950	0.78154
Au	-0.18428	0.32696	-1.87103
Au	3.00605	0.23326	0.35960
Au	-2.82851	-1.22186	-1.92019
Au	-3.00405	1.46325	-1.45541
Au	1.59397	-0.35145	2.75271
Au	2.01764	2.17783	-1.63456
Au	-1.77654	-3.09455	0.25135
Au	-0.87869	-2.04177	2.63343
Au	-0.59765	3.15583	-1.33421
Au	2.25705	-1.19452	-2.28972
Au	-0.22745	-2.54326	-2.29433
Au	-1.12194	0.94664	3.17128
Au	-2.19657	2.61751	1.24580
C	6.09516	-0.73152	1.82573
C	5.62692	-2.11635	1.40288
C	5.89884	-1.40349	-0.91316
C	6.70857	-0.27610	-0.57131
C	7.06443	-0.09127	0.85012
H	6.37738	-2.88552	1.64512
H	4.70299	-2.38259	1.93354
H	5.21909	-0.06295	1.89377
H	6.55816	-0.76725	2.81645
H	5.61684	-1.58834	-1.96331
H	4.16922	-1.08337	-3.99589
H	7.51024	-0.05054	-1.28133
H	4.27787	3.61108	-1.41840
O	8.02450	0.55600	1.22832
N	5.34889	-2.21187	-0.03478
C	4.47090	-3.29862	-0.45212
H	3.48039	-3.16555	0.00555
H	4.35920	-3.27833	-1.54083
H	4.89300	-4.25710	-0.12350
O	4.16762	2.84323	-1.99281
O	4.15834	-1.59477	-3.17978

B22

Au	-2.38188	-3.55469	-1.26634
Au	-2.56012	0.31508	4.31806
Au	1.96043	4.79077	-1.15502
Au	4.30964	-2.97901	0.95111
Au	-0.61509	-1.76200	0.18415
Au	-1.24724	1.26714	-0.30261
Au	1.27911	0.70863	1.42567
Au	1.28837	-0.07904	-1.69921
Au	-3.10977	-0.80561	-1.13782
Au	2.87787	2.20504	-0.50418
Au	3.68323	-0.33358	0.18717
Au	-2.82013	-0.37936	1.57706
Au	0.07288	-2.54818	-2.62823
Au	0.41464	3.43269	0.75727
Au	-1.12742	1.94687	2.52772
Au	2.21463	-2.64729	-0.93750
Au	-1.16449	0.58761	-3.13417
Au	0.47316	2.62591	-2.26660
Au	-0.38492	-0.99877	3.11201
Au	1.81101	-2.11628	1.91895
H	-2.50744	-1.54055	-3.80642
H	-1.48979	-4.18380	-4.03260
O	-1.70782	-3.33060	-3.64051
O	-2.85725	-0.66186	-3.56326
C	-4.89242	2.15050	-2.08480
C	-5.42132	0.87814	-2.73174
C	-6.30683	0.06289	-0.64348
C	-5.85492	1.30908	0.10519
C	-5.60644	2.48938	-0.80205
H	-6.45226	1.04395	-3.11065
H	-4.78174	0.58508	-3.57192
H	-3.82658	2.00095	-1.83375
H	-4.95251	3.00341	-2.76853
H	-7.34874	0.19711	-1.00523
H	-6.30309	-0.80441	0.03064
H	-6.57488	1.59544	0.87880
H	-4.89318	1.09041	0.60727
O	-5.92546	3.62193	-0.50047
N	-5.44123	-0.24092	-1.78275
C	-5.88664	-1.45906	-2.45473
H	-5.19767	-1.68649	-3.27509
H	-5.87422	-2.29526	-1.74552
H	-6.91304	-1.34033	-2.85278

TS_B13

Au	-3.12570	-3.07384	-0.70943
Au	-1.57248	1.20759	4.73288
Au	2.45517	4.24758	-1.97046
Au	3.87766	-3.56065	0.72786
Au	-0.98538	-1.54478	0.53793
Au	-1.09967	1.44503	-0.18920
Au	1.61507	0.62894	1.19675
Au	0.96126	-0.43668	-1.71617
Au	-3.44635	-0.29390	-0.36657
Au	3.07086	1.62605	-1.13115
Au	3.57414	-0.93507	-0.25338
Au	-2.52110	0.51009	2.15350
Au	-0.67469	-2.72452	-2.31874
Au	1.10080	3.38960	0.34460
Au	-0.27235	2.39617	2.51976
Au	1.68092	-3.08802	-1.00607
Au	-1.55958	0.43643	-2.89002
Au	0.43519	2.31681	-2.44132
Au	-0.04613	-0.63069	3.24779
Au	1.61368	-2.24085	1.78244
H	-3.13304	-1.56966	-3.66678
H	-2.71569	-4.18494	-3.35179
O	-2.71369	-3.27430	-3.03574
O	-3.17164	-0.60777	-3.85679
C	-5.48938	0.44421	-3.25037
C	-6.16371	-0.25555	-2.09795
C	-5.86142	1.67478	-0.68897
C	-5.01859	2.39877	-1.71765
C	-5.15478	1.83980	-3.13565
H	-7.26862	-0.11382	-2.09337
H	-5.98867	-1.34300	-2.13453
H	-4.19540	-0.15653	-3.52491
H	-5.92943	0.19566	-4.22050
H	-6.93689	1.89608	-0.84497
H	-5.60317	1.98696	0.33310
H	-5.28150	3.46235	-1.75157
H	-3.95303	2.35053	-1.43386
O	-4.87260	2.57999	-4.08095
N	-5.68301	0.21455	-0.77811
C	-6.43115	-0.44953	0.29016
H	-6.29146	-1.53407	0.21640
H	-6.06105	-0.11719	1.26690
H	-7.50891	-0.21879	0.21378

B23

Au	-4.42047	-2.58663	-0.96739
Au	-0.50436	1.08618	5.00144
Au	2.37131	4.09502	-2.27004
Au	3.51717	-3.97060	-0.31139
Au	-0.69806	-1.60970	0.83993
Au	-0.96003	1.40445	0.09832
Au	1.97010	0.43374	0.90386
Au	0.45835	-0.42679	-1.88131
Au	-3.25515	-0.38062	0.26060
Au	2.82869	1.36906	-1.73318
Au	3.20966	-1.28687	-1.09711
Au	-1.93361	0.39332	2.62408
Au	-1.73068	-2.38095	-1.70750
Au	1.40840	3.22648	0.23221
Au	0.43632	2.23306	2.61360
Au	0.88836	-3.17516	-1.10661
Au	-2.12999	0.76606	-2.56346
Au	0.07072	2.43878	-2.35272
Au	0.75136	-0.75536	3.28470
Au	2.07098	-2.41929	1.53022
H	-2.78117	-1.60358	-4.14017
H	-1.33883	-2.06027	-4.50992
O	-2.18636	-2.40396	-4.20673
O	-3.69944	-0.26593	-3.58323
C	-4.37149	2.57443	-2.04501
C	-5.40677	1.63785	-1.54186
C	-5.12537	2.50902	0.67857
C	-3.91904	3.35276	0.30423
C	-3.71226	3.52434	-1.18444
H	-6.40872	2.11178	-1.68200
H	-5.40885	0.72543	-2.15303
H	-4.12482	-0.79686	-2.88960
H	-4.27309	2.70939	-3.12142
H	-6.05752	3.10342	0.55874
H	-5.06547	2.21035	1.73411
H	-3.97794	4.34636	0.76312
H	-2.99927	2.88532	0.69785
O	-2.99500	4.42413	-1.62784
N	-5.23811	1.29184	-0.13009
C	-6.37153	0.49586	0.32276
H	-6.45516	-0.40982	-0.29047
H	-6.21384	0.18913	1.36335
H	-7.31862	1.06677	0.25556

References

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