CHEMISTRY
A EUROPEAN JOURNAL

1FULL PAPER

DOI: 10.1002/chem.200((will be filled in by the editorial staff))

Binap-gold(I) *vs* Binap-silver trifluoroacetate complexes as catalysts in 1,3-dipolar cycloadditions of azomethine ylides

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Dedication ((optional))

Abstract: The 1,3-dipolar cycloaddition between azomethine ylides and alkenes is efficiently catalyzed by [(S_a)-Binap-AuTFA]$_2$. Maleimides, 1,2-bis(phenylsulfonyl)-ethylene, chalcone and nitrostyrene were suitable dipolarophiles even using sterically hindered 1,3-dipole precursors. The results obtained in these transformations improve the analogous ones obtained in the same reactions catalyzed by Binap-AgTFA. In addition, computational studies have also been carried out in order to demonstrate both the high enantioselection exhibited by de chiral gold(I) complex, and the NLE observed in this transformation.

Keywords: Au • Ag • 1,3-dipolar cycloaddition • azomethine • asymmetric synthesis • NLE•

Introduction

The application of soluble gold complexes as catalysts for organic transformations has been widely explored for the last ten years.[1] Spite of the numerous published gold(III)-catalysed processes, the diverse range of transformations developed by gold(I) complexes have demonstrated particular interest as catalysts. Gold(I) complexes catalyze reactions under very mild conditions giving, wide functional group compatibility and high efficiency. They act as soft carbophilic Lewis acids towards C-C multiple bonds. This high carbophilicity translates to a relative low oxophilic character of the gold(I) cation. However, recent advances in synthetic catalytic organic transformations have demonstrated that the weak heteroatom-gold(I) interaction is appropriate for the reaction succeed.[1] Its size, together with the already mentioned chemoselectivity and functional group compatibility are crucial features for application in complex crowded molecular structures. There are many processes which are sensitive to steric hindrance, the 1,3-dipolar cycloaddition (1,3-DC)[2] being one of them. The enantioselective version of 1,3-DC of stabilized azomethine ylides[3] employing substoichiometric amounts[4] of catalysts has been studied extensively since 2002[5]. Silver(I)[6] and copper(I)[7] catalyzed 1,3-dipolar cycloadditions offer excellent complementary results in terms of endo/*exo*-diastereoselection and are the most frequently employed metals nowadays.

This work, focused on the activity and efficiency of Binap-silver(I) salts complexes, can be considered as a evolution from the first attempt for the enantioselective 1,3-DC of azomethine ylides with dimethyl maleate described in 2002 by Zhang *et al.* using 3 mol % of (S_a)-Binap and AgOAc and Et_3N as base with very poor results.[5] Our research group has found out that the very stable and recoverable (S_a)- or (R_a)-Binap-$AgClO_4$ complexes are able to catalyze the enantioselective 1,3-DC of azomethine ylides with maleimides.[8] Using a less coordinating anion such as $AgSbF_6$, instead of $AgClO_4$, it was possible to achieve better results for bulky substrates and even with 1,3-bis(phenylsulfonyl)ethylene as a dipolarophile.[6e]

Toste *et al.* published the first enantioselective 1,3-dipolar cycloaddition between mesoionic azomethine ylides (münchnones) with electron-poor alkenes catalyzed by Cy-Segphos$(AuCl)_2$. The reaction afforded in all cases only the *exo*-adduct in high yields and very good enantioselections.[9] However, the classical 1,3-dipolar cycloaddition of iminoesters and electrophilic olefins was not described using gold complexes. In this article, we present the general scope of this transformation using Binap-gold(I) complexes

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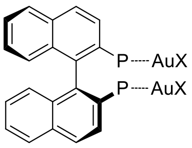
and a comparison with the analogous reactions performed with chiral Binap-silver(I) salts.[10][11

Results and Discussion

The gold(I) cation has only two coordination sites and its linear geometry makes asymmetric catalysis extremely difficult. Fortunately, a key to the development of enantioselecive gold(I)-catalyzed transformations has been the identification of enantiomerically pure bis(gold)-chiral diphosphine complexes of the form $[(AuX)_2(P\text{-}P)^*]$ as catalysts for enantioselective transformations.[1] A clear and recent example of the isolation, identification, and characterization of two chiral Binap-gold(I) complexes **1** and **2**, bearing trifluoroacetate as counteranion, have been reported by Puddephatt *et al.*[12] These complexes were prepared by mixing $(Me_2S)AuCl$ and the corresponding amount of the chiral Binap ligand. The resulting gold(I) chloride complexes were treated with different silver salts for 1 h in toluene and the suspension was filtered through a celite plug. The remaining solution was evaporated obtaining **1** or **2** in 89 and 96% yields, respectively. These cationic complexes were immediately employed without any other purification in the catalytic enantioselective 1,3-DC of the imino ester **3a** and *N*-methylmaleimide **4** (NMM) in toluene at rt (Scheme 1 and Table 1).



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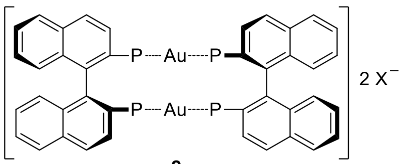

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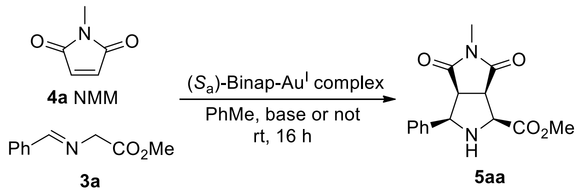
P = PPh_2 X = CF_3CO_2

According to our experience, the model reaction between the imino ester (1,3-dipole precursor) **3a** and *N*-methylmaleimide (NMM) **4a**, in toluene at rt (Scheme 1 and Table 1), was selected for the initial optimization of the gold(I) catalytic efficiency. When this cycloaddition was performed in the presence of 10 mol% of diisopropylethylamine (DIPEA) and 10 mol% of complexes $(BinapAuX)_2$ **1** (X = Cl or TFA), product *endo*-**5aa** was obtained with high conversion but in racemic form (Table 1, entries 1 and 2). These two examples demonstrated that the chiral environment of the bisgold(I) complexes type **1** hardly participated in the enantiodiscriminating step. However, dimeric complexes type $(BinapAuX)_2$ **2** resulted to be the appropriate catalysts. Thus, in the case of the chiral complex **2** (X = OAc) product *endo*-**5aa** was obtained with high conversion and 60% *ee* in the presence of DIPEA (Table 1, entry 3). Interestingly, in the absence of base a 70% *ee* was obtained working the complex as a bifunctional catalyst (Table 1, entries 3 and 4). Better results were achieved when using complex **2** (X = OBz) in the presence of DIEA or in the absence of added base affording cycloadduct *endo*-**5aa** in 74% and 94% *ee*, respectively (Table 1, entries 5 and 6). Although product *endo*-**5aa** was obtained in higher 94% *ee* in the absence of DIPEA, it was contaminated with secondary byproducts. The same inconvenience was detected when triethylamine was used as base in this cycloaddition reaction. When the gold(I) trifluoroacetate complex **2** (X = TFA) was used as catalyst, 74% *ee* of compound *endo*-**5aa** was obtained in the presence of DIPEA (Table 1, entry 7), whereas without base, 99% *ee* was obtained (Table 1, entry 8). This last reaction was performed introducing a previously synthesized (isolated and recrystallized) complex **2** (X = TFA)[12] obtaining identical results (Table 1, entry 9). The enantiomeric form of cycloadduct *endo*-**5aa** was generated in 99% *ee* by the employment of the corresponding (*R*,*R*)-dimeric complex **2** (X = TFA) (Table 1, entry 10). Attempts to reduce the catalyst loading to a 5 mol% werenot successful such as reveals the lower 60% *ee* obtained (Table 1, entry 11). At this point, an identical result was obtained independently of using the chiral complex **2** (X = TFA) (Table 1, entry 8) and the chiral complex (S_a)-Binap-AgTFA **6** in the absence of base (Table 1, entry 12). In every example the major cycloadduct obtained was the *endo* (>98:2 *dr*) according to the NMR experiments of the crude products. Analogously, the absolute configuration was confirmed by comparison of their retention times using analytical chiral HPLC columns, and especific optical rotations with those described for enantiomerically pure samples.



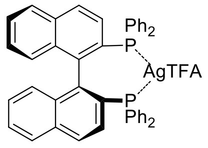
Scheme 1. Optimization of the 1,3-dipolar cycloaddition of **3a** and **4a**.

Table 1. Optimization of the 1,3-dipolar cycloaddition of **3a** and **4a**.

Entry	Cat. (10 mol%)[a]	Base (10 mol%)	Conv (%)[b]	*ee* (%)[c]
1	**1**-Cl	DIPEA	>95	*rac*
2	**1**-TFA	DIPEA	>95	*rac*
3	**2**-OAc	DIPEA	>95	62
4	**2**-OAc	—	>95	70
5	**2**-OBz	DIPEA	>95	74
6	**2**-OBz	—	>95	94[d]
7	**2**-TFA	DIPEA	>95	74
8	**2**-TFA	—	>95	99
9	**2**-TFA[e]	—	>95	99
10	**2**-TFA[f]	—	>95	*ent*-99
11	**2**-TFA[g]	—	90	60
12	(S_a)-Binap-AgTFA **6**	—	>95	99

[a] The generation of gold catalysts was achieved by mixing tantamount equivalents of gold(I) complex **1** and the corresponding silver(I) salt. [b] Determined by ^{1}H NMR of the crude sample obained by using the filtered solution of the gold complex after anionic interchange. The observed *endo:exo* ratio was always >98:2 (^{1}H NMR). [c] Determined by using analytical chiral HPLC columns (Daicel, Chiralpak AS). [d]

Notable amounts of unidentified side products were observed (^{1}H NMR). [e] The reaction was carried out with the chiral complex isolated by recrystallization. [f] The reaction was performed with (R_a)-Binap as ligand. [g] Reaction performed with 5 mol % of catalyst.



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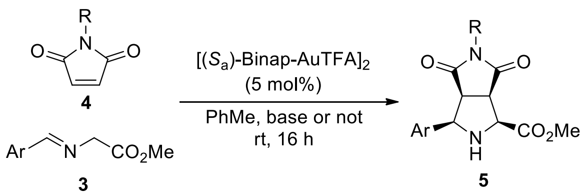
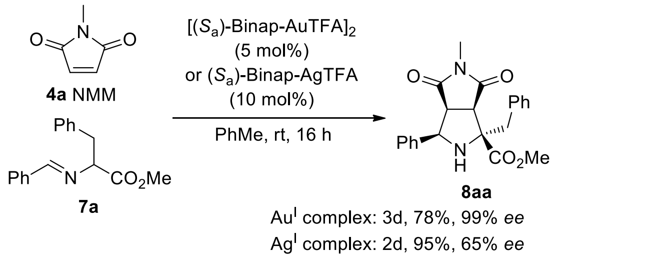
Comparative studies for this catalyzed enantioselective 1,3-DC were performed using gold(I) and silver(I) complexes together with different iminoesters and maleimides under the best reaction conditions depicted on Table 1 (Scheme 2 and Table 2). In the first example, the absence of base, (including the above described reaction of **3aa** with NMM) performed with *N*-ethylmaleimide (NEM) **4b** and *N*-phenylmaleimide (NPM) **4c** products **5ab** and **5ac** were isolated with higher enantioselectivity when the reaction was catalyzed by the chiral gold complex (Table 2, entries 1, 3, and 5). However, in the presence of DIPEA (10 mol%) the chiral silver(I) catalyzed process is more efficient except in the reaction done with NPM (Table 2, compare entries 1 with 2, 3 with 4 and 5 with 6). In fact, the result obtained when NPM was employed as a dipolarophile (Table 2, entry 5) is particularly noteworthy because it is the best *ee* (80% *ee*) achieved till date with chiral Binap ligands. When (S_a)-Binap-AgTFA **6** was used as catalyst, racemic product **5ac** was obtained. For the 1,3-DC of other arylideneaminoesters **3b-h**, and maleimides the conversions are identical independently of the metal cation employed. In the case of 2-naphthyl derived iminoester the enantioselections were very close to each other, but with NPM chiral gold(I) catalysts **2** (X = TFA) (Table 2, entries 7-9) again was much more efficient generating the highest enantioselections. The dipole precursors **3c**, and **3d**, containing an *ortho*-substituent in the aryl moiety, were appropriate sterically hindered starters in the gold(I)-catalyzed 1,3-DC with NMM affording *endo*-compounds **5ca** and **5da** with 99 and 88% *ee*, respectively. In both examples the resulting enantioselections induced with the corresponding chiral silver(I) complex were very poor (Table 2, entries 10 and 11). The *para*-substituted methyl iminoglycinates **3e**, **3f**, and **3g** underwent the gold(I) and the silver(I)- mediated 1,3-DC obtaining no rational results in terms of enantioselection (Table 2, entries 12-14).



4a, R = Me (NMM); **4b**, R = Et (NEM); **4c**, R = Ph (NPM)

Scheme 2. [(*S*)-Binap-AuTFA]$_2$ Catalyzed 1,3-dipolar cycloaddition of iminoesters **3** and maleimides **4**.

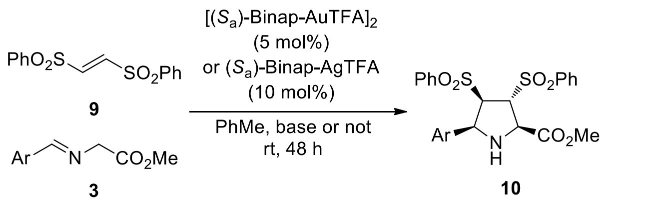
The insertion of a substituent at the α-position of the 1,3-dipole precursor was next evaluated. Thus, when methyl benzylidenephenylalaninate **7a** was allowed to react with NMM under the standard reaction conditions, the reaction performed with the gold(I) complex needed 24 h more than the corresponding reaction using the analogous silver(I) complex for achieving almost total conversions (Scheme 3). The enantioselection showed by [(S_a)-Binap-AuTFA]$_2$ complex (99% *ee*) was higher than in the case of using (S_a)-BinapAgTFA (65% *ee*) as a catalyst. Product **8aa** was obtained as *endo*-diastereoisomer (>98:2, determined by ^{1}H NMR spectroscopy).



Scheme 3. [(*S*)-Binap-AuTFA]$_2$ versus (*S*)-Binap-AgTFA Catalyzed 1,3-dipolar cycloaddition of iminoester **7a** and NMM **4a**.

According to the published results, obtained from chiral Binap-silver(I) complexes,[8] we also tested the efficiency of the Binap-gold(I) trifluoroacetate complexes in the enantioselective cycloaddition of azomethine ylides and *trans*-1,2-bis(phenylsulfonyl)ethylene **9**, a synthetic equivalent of acetylene (Scheme 4 and Table 3). The reaction, performed with 5 mol % of the gold(I) **2** (X = TFA) catalyst, afforded cycloadducts **10** in a non predictable enantioselectivities in the absence or in the presence of DIPEA (10 mol%) as base. In the case of product **10a**, a lower enantiomeric excess was obtained when (S_a)-Binap-AgTFA **6** was used as catalyst and better results were obtained in the absence of base (Table 3, compare entries 1 and 2). Compound *endo*-**10b** was obtained in better enantiomeric excesses in the absence of base (compare in Table 3, entries 3 and 4). The rest of the examples gave the best enantioselections in the absence of base (compare entries 5 and 6, 7 and 8, 9 and 10). Again, the *p*-chloro substituted iminoester gave very poor *ee* (Table 3, entries 11 and 12).

The absolute configuration of the *endo*-cycloadducts was assigned according to the retention times using analytical chiral HPLC columns, and by comparison of the physical properties of the isolated samples with the properties published in the literature for the analogous compounds.



Scheme 4. [(*S*)-Binap-AuTFA]$_2$ versus (*S*)-Binap-AgTFA Catalyzed 1,3-dipolar cycloaddition of iminoesters **3** and disulfone **9**.

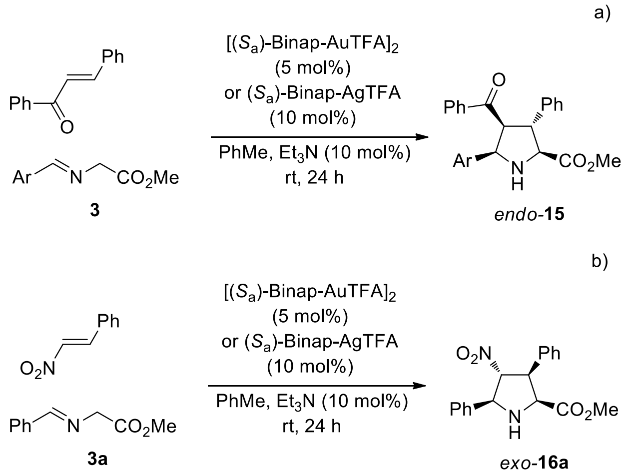
Table 3. 1,3-DC of iminoesters **3a** and disulfone **9** catalyzed by chiral complex **2** (X = TFA).

				Gold catalysis		Silver catalysis	
Entry	Ar, **3**	Base (10 mol%)	10	Yield (%)[a][b]	*ee* (%)[c]	Yield (%)[a][b]	*ee* (%)[c][d]
1	Ph, **3a**	DIPEA	**10a**	81	80	80	86
2	Ph, **3a**	—	**10a**	74	99	81	96

3	2-Naphthyl, **3b**	DIPEA	**10b**	91	90	88	64
4	2-Naphthyl, **3b**	—	**10b**	<40	*rac*	<40	*rac*
5	2-(MeO)C_6H_4, **3i**	DIPEA	**10i**	80	30	83	20
6	2-(MeO)C_6H_4, **3i**	—	**10i**	<40	40	<40	20
7	3-Pyridyl, **3e**	DIPEA	**10e**	73	96	70	92
8	3-Pyridyl, **3e**	—	**10e**	73	96	70	96
9	4-MeC_6H_4, **3f**	DIPEA	**10f**	91	88	90	96
10	4-MeC_6H_4, **3f**	—	**10f**	67	99	75	96
11	4-ClC_6H_4, **3h**	DIPEA	**10h**	81	22	80	*rac*
12	4-ClC_6H_4, **3h**	—	**10h**	<40	*rac*	<40	*rac*

[a] Isolated yields after flash chromatography (silica gel). [b] The observed *endo*:*exo* ratio was always >98:2 (^{1}H NMR). [c] Determined by using analytical chiral HPLC columns. [d] Reaction performed with (S_a)-Binap-AgTFA **6**.

Searching for another appropriate dipolarophiles for this enantioselective catalyzed 1,3-DC of azomethine ylides, chalcone and β-nitrostyrene were used. As well as occurred in the 1,3-DC catalyzed by chiral phosphoramidites and silver perchlorate, chalcones reacted efficently affording exclusively very clean *en*do-cycloadducts **14** after 24 h, at room temperature and in the presence of Et_3N (10 ml%) as base, rather than DIPEA, independently of the selected metal. The most important difference consisted of the enantioselection achieved. Whilst chiral dimeric gold catalyst furnished very high *ee* of **15**, silver complex gave always lower enantiodiscriminations (Scheme 5a, and Table 4, entries 1-3). The reaction between iminoester **3a** and β-nitrostyrene afforded very complex mixtures of unidentified compounds when chiral silver complexes were employed. However, very clean crude reaction products were obtained when dimeric [(*S*)-Binap-AuTFA]$_2$ was used. The diastereoselectivity was not so high than in precedent cycloadditions, obtaining in these examples 20:80 *endo*:*exo* mixtures of **16a**, spite of runnig the reaction at −20 ºC. Cycloadduct *exo*-**16a** was obtained in 70% or 60% *ee* whether the reaction was performed at 25 ºC or −20 ºC, respectively (Scheme 5b, and Table 4, entries 4 and 5). The lowering of the temperature in the reactions involving chalcone or β-nitrostyrene afforded incomplete crude reaction mixtures after 48 h, furnishing a lower enantioselectivity in products **15** or **16a**, respectively.



Scheme 5. [(*S*)-Binap-AuTFA]$_2$ versus (*S*)-Binap-AgTFA Catalyzed 1,3-dipolar cycloaddition of iminoesters **3** and chalcone or β-nitrostyrene.

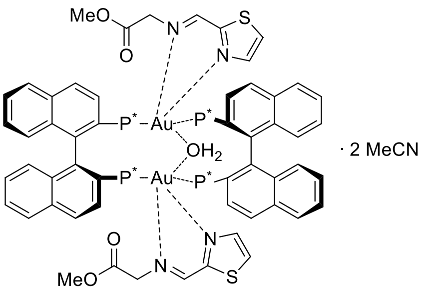
Table 4. 1,3-DC of iminoesters **3** with chalcone and β-nitrostyrene

			Gold catalysis		Silver catalysis	
Entry	Ar, **3**	Product	Yield (%)[a][b]	*ee* (%)[c]	Yield (%)[a][b]	*ee* (%)[c][d]
1	Ph, **3a**	**15a**	95	80	80	20
2	2-Naphthyl, **3b**	**15b**	90	60	81	50
3	4-MeC_6H_4, **3f**	**15f**	80	80	80	74
4	Ph, **3a**	**16a**	78[e]	70	—[f]	—
5	Ph, **3a**[g]	**16a**	77[e]	60	—[f]	—

[a] Isolated yields after flash chromatography (silica gel). [b] The observed *endo*:*exo* ratio was always >98:2 (^{1}H NMR). [c] Determined by using analytical chiral HPLC columns. [d] Reaction performed with (S_a)-Binap-AgTFA **6**. [e] The observed *endo*:*exo* ratio was 20:80 (^{1}H NMR and using analytical chiral HPLC columns). [f] The reaction failed. [g] Reaction performed at −20 ºC.

When conjugated esters were used as dipolarophiles, such as methyl or *tert*-butyl acrylate, dimethyl maleate, and diisopropyl fumarate, were allowed to react with inimoester **3a**, under the optimized reaction conditions, high yields of the corresponding *endo*-cycloadducts were obtained but with very low enantioselections.

The interest for identifying the catalytic species structure several analyses were carried out. The ^{31}P NMR analysis of [(S_a)-Binap-AuTFA]$_2$ complex **2** revealed a singlet at 41.1 ppm, whereas the a singlet at 23.3 ppm corresponded to (S_a)-Binap-AuCl complex according to the literature. The dimeric complex is assumed to be a non-reactive complex but, in our case, the existence of the dipole would induce a reorganization of **2**. For this study, the strongly coordinating thiazole-derived iminoester was selected. In the case of ESI-MS experiments peaks at 819, 819.2 and 819.6 were observed on elution with a mixture of acetonitrile and water, demonstrating the existence of such a dimeric complex. However, apart from the already described M^+ at 819, a very intense one was observed at 1053, which was possibly originated by the formation of the cluster **17** involving two molecules of the corresponding dipole. Efforts to obtain crystals from the mixture of equimolar amounts of chiral complex and the dipole derived from thiazole in dichloromethane resulted unfruitful. This analysis also revealed the existence (in less proportion) of fragments and peaks originated by the analogous complex **18** coordinated just with one equivalent of the iminoester (M^+ 966.4).



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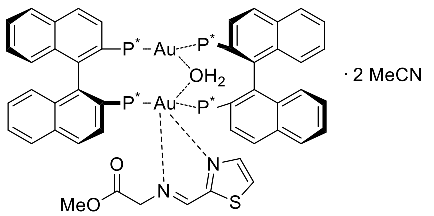

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$P^* = PPh_2$

We observed a strong positive NLE (Figure 1) when the reaction of iminoester **3a** was allowed to react with NMM employing different enantiomeric purity of the catalytic chiral complex **2** (X = TFA). This behavior can be justified by a generation of a reservoir of unproductive non-chiral heterodimer complex,[13] increasing the concentration of the chiral catalytic active species in solution.

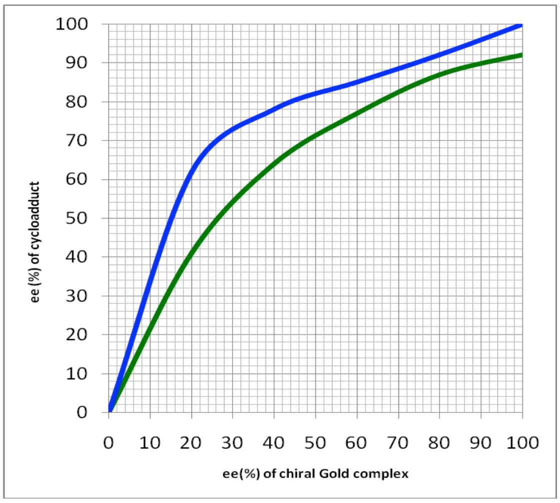


Figure 1. Experimental (blue line) and theoretical (green line) NLE observed in the chiral complex **2**-catalyzed 1,3-DC between the iminoester **3a** and NMM.

Next, we performed DFT calculations to shed light on the origins of the great stereocontrol obtained in these (S_a)-Binap Au(I) catalyzed 1,3-DC reactions. In a previous work, we demonstrated that the stereoselectivity obtained employing chiral ligand-metallated azomethine ylide in 1,3-DC is a consequence of the blockage of one of the ylide stereogenic faces by the chiral ligand.[14]

We calculated the geometries of the most stable (S_a)-Binap silver(I) or gold(I) ylide **I** reactive complexes (Figure 2**).** As expected, in the case of the silver complex (Figure 2A) the metallic centre adopts a tetrahedral environment. This Ag(I) is surrounded by both phosphorous atoms of the ligand and by the nitrogen and oxygen atoms of the ylide (Figure 2A). Due to this coordination pattern, the distance between the chiral ligand and the prochiral faces is short enough to induce a proper stereoselectivity allowing the attack of the dipolarophile only by the (2*Si*,5*Re*) face of the ylide. This is in good agreement with the experimental evidence of the major formation of the (*S*, *S*, *S*, *R*) cycloadducts.[8b]

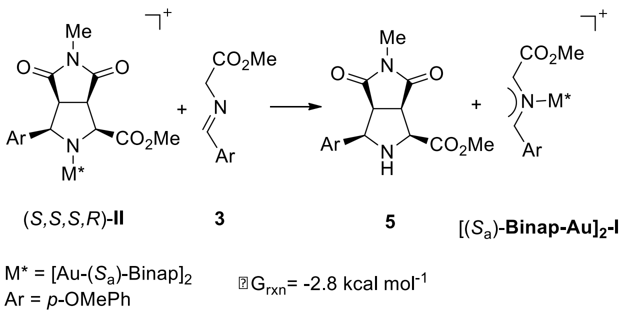
In the case of monomeric (S_a)-Binap-Au-ylide **I** complex (Figure 2B), the gold atom presents a linear coordination and it is surrounded only by one phosphorous atom of the ligand and the nitrogen atom of the ylide. In this case, the carboxy-gold distance is *c.a.* 0.3 Å larger than the carboxy-silver distance as one may expect from the known low oxophilicity of the gold(I) cation. This geometry makes the two prochiral faces approximately equivalent. Therefore, no significant enantioselection should be expected in the [3+2] reaction.

We also considered the existence of (S_a)-Binap-Au dimeric units as the actual catalytic complex (Figures 2B and 2C). Under these conditions only two significant conformations are energetically accessible. In [(S_a)-Binap-Au]$_2$-ylide-**I** only the (2*Si*,5*Re*) face is accessible. By contrast, in [(S_a)-Binap-Au]$_2$-ylide-**I-b** the accessible face is the opposite one [named (2*Re*,5*Si*)]. However, the difference in energy of the less stable one is enough to assume that only **I** is present in solution at room temperature. Therefore, the major product corresponds to the (*S*, *S*, *S*, *R*) cycloadducts. In previous works focused on catalyzed 1,3-DC of azomethine ylides and maleimides we demonstrated the exclusive preference of the reaction for *endo*-cycloadducts. Therefore, only this approach will be considered in the following study.[8b]

The main geometric features and relative energies of the stationary points corresponding to the 1,3-DC of (S)-Binap-Au-ylide dimers are gathered in Figure 3. As expected from the previous analysis, *endo*-saddle points corresponding to the reaction of the dipolarophile through the hindered (2*Re*,5*Si*) face of ylide [(S_a)-BinapAu]$_2$**I** are of much higher energy than the obtained from suprafacial approach through (2*Si*,5*Re*) of ylide [(S_a)-BinapAu]$_2$**I-b** (see the supporting information for further details). Our calculations also indicate that the reaction presents a concerted but slightly asynchronous transition structure in which the critical distance of the forming C2-C_{nmm} bond is shorter than that associated with formation of the C5-C'_{nmm} bond.

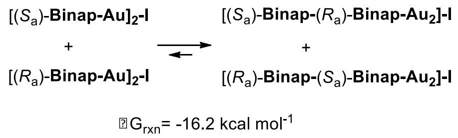
The activation Gibbs free energy barrier associated with the formation of of (*S*, *S*, *S*, *R*)-**II** is c.a. 4.5 kcal mol^{-1} higher than the one associated with the formation of the corresponding enantiomer. If we assume a preequilibrium between both possible reactive ylides, Curtin-Hammet kinetics show that the product ratio should depend on the free Gibbs activation energy difference of both corresponding transition structures. Under this kinetic framework, our calculations predict the major formation of (*S*, *S*, *S*, *R*)-**II** with *ee* 90% *c.a.* in good agreement with the experimental results.

The formation of the major complexed cycloadduct is thermodynamically favored (*c.a.* 6 kcal mol^{-1}, Figure 3). The catalytic cycle is completed because the final step (**3i** + (*S*,*S*,*S*,*R*)-**II** to release the cycloadduct **5i**) is endothermic (3 kcal mol^{-1}) and the recovery of the reactive ylide is ensured (Scheme 6).



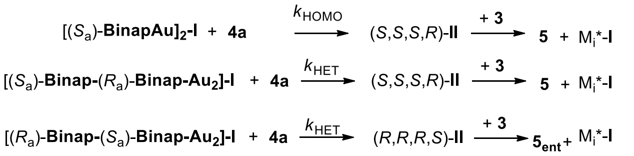
Scheme 6. Last step in the catalytic cycle to generate compound **5**.

Finally we studied computationally the strong positive NLE observed in the reaction of the iminoester **3a** and NMM catalyzed by gold(I) complexes. We calculated the stability of the possible azomethine ylide complexes with hetero Binap-gold(I) dimers. Our results indicate that there is only one energetically feasible geometry for the [(*S_a*)-Binap,(*R_a*)-Binap-Au_2]-**I** reactive complex and this complex is much more stable than the possible homodimeric species. Our results also indicate that all of the (R_a)-Binap present in solution would be involved in the generation of the heterodimeric form. Therefore the presence of [(R_a)-Binap-Au]$_2$-**I** complex can be neglected.



Scheme 7. Equilibrium between all the possible reactive dimeric gold (I) azomethine ylide complexes when non-enantiopure Binap ligand is employed.

We also studied the reaction mechanism when the heterochiral gold(I) complexes are involved. The calculated activation free energy barrier associated with the reaction of [(S_a)-Binap,(R_a)-Binap-Au_2]-**I** and NMM is 20.2 kcal mol^{-1}, *c. a.* 1 kcal mol^{-1} higher than the value associated with the reaction of [(S_a)-Binap-Au]$_2$-**I** complex (see supporting information for further geometrical details of the transition structure).



Scheme 8. Reaction framework for the reaction of chiral complex **2**-catalyzed 1,3-DC between the iminoester **3a** and NMM when non-enantiopure Binap ligand is employed.

The kinetic constants of the [3+2] cycloaddition process within the framework indicated in Scheme 8 have been calculated employing the Eyring equations and using the previously computed activation free energy barriers. We have analysed the kinetic system employing numerical integration assuming the total recovery of the catalyst and the irreversibility of the process. Within this framework the expected stereochemical outcome of the reaction employing different non-enantiopure catalyst mixtures shown in Figure 1 (*vide supra*) was surveyed. Our calculations show that the generation of the heterodimer produces less reactive complexes, which avoids the formation of the non-desired homodimer [(R_a)-BinapAu]$_2$.**I**. Therefore an increase of the *ee* of the cycloadduct is observed. Our results are in qualitative agreement with the experimental evidences (Figure 1).

Conclusion

The enantioselective 1,3-DC of azomethine ylides and electrophilic alkenes has been successfully catalysed by [(S_a)-Binap-AuTFA]$_2$ complex. The results obtained with this catalyst improved the analogous ones described for the reactions carried out in the presence of (S_a)-Binap-AgTFA, especially when a hindered component (dipole or dipolarophile) are involved. In some examples, [(S_a)-Binap-AuTFA]$_2$ catalyst, once ligaed to the 1,3-dipole, acted as a bifunctional complex activating the dipolarophile and as an internal base. Even unreactive dipolarohiles under silver catalysis, such as nitrostyrene, were appropriate under the gold(I) catalysis. The origin of the enantioselection was confirmed by DFT calculations, revealing very interesting geometric data of the transition states. Computational studies of the strong positive NLE showed important differences between all of the possible catalytic species demonstrating the existance of very stable and unreactive heterodiemric complexes. Finally, regarding the observed positive NLE, calculations predicted a very close NLE plot with respect to the experimental data. To the best of our knowledge this is the first work in which NLE is analysed using computational tools.

Experimental Section

General. All reactions were carried out in the absence of light. Anhydrous solvents were freshly distilled under an argon atmosphere. Aldehydes were also distilled prior to use for the elaboration of the iminoesters. Melting points were determined with a Reichert Thermovar hot plate apparatus and are uncorrected. Only the structurally most important peaks of the IR spectra (recorded on a Nicolet 510 P-FT and on a Jasco FTIR 4100) are listed. ^{1}H NMR (300 MHz) and ^{13}C NMR (75 MHz) spectra were obtained on a Bruker AC-300 using $CDCl_3$ as solvent and TMS as internal standard, unless otherwise stated. Optical rotations were measured on a Perkin Elmer 341 polarimeter. HPLC analyses were performed on a JASCO 2000-series equipped with a chiral column (detailed for each compound in the main text), using mixtures of *n*-hexane/isopropyl alcohol as mobile phase, at 25 ºC. Low-resolution electron impact (EI) mass spectra were obtained at 70eV on a Shimadzu QP-5000 and high-resolution mass spectra were obtained on a Finnigan VG Platform. HRMS (EI) were recorded on a Finnigan MAT 95S. Microanalyses were performed on a Perkin Elmer 2400 and a Carlo Erba EA1108. Analytical TLC was performed on Schleicher & Schuell F1400/LS silica gel plates and the spots were visualized under UV light (λ=254 nm). For flash chromatography we employed Merck silica gel 60 (0.040-0.063 mm). Complexes **1**, and **2** were prepared according to the reported procedure.[12] Silver complex was ready prepared just by mixing equimolar amounts of the Binap chiral ligand and AgTFA. All of the transformations performed with this catalyst were performed in the absence of light.

Hybrid QM/MM calculations for optimizations of saddle points were performed in terms of ONIOMc[15] method implemented in GAUSSIAN09 suite of programs.[16] Ball & stick model in Figure 2 shows atoms included in the high-level layer, and a wire model is used to represent atoms included in the low-level layer. In the high level layer, the electron correlation was partially taken into account by using the hybrid functional B3LYP[17] combined with Hay-Wadt small core effective potential (ECP)[18] basis set. UFF[19] molecular mechanics force field was employed in the low-level layer. This combination has offered excellent results in studies of organocatalytic mechanisms.[20] Thermal corrections of Gibbs free energies were computed at the same level of theory and were not scaled. All stationary points were characterized by harmonic analysis. Reactant intermediates and cycloadducts have positive definite Hessian matrices. Transition structures show only one negative eiganvalue in their diagonalysed force constant matrices, and their associated eigenvectors were confirmed to correspond to the motion along the reaction coordinate under consideration.

1,3-Dipolar cycloaddition of iminoesters 3 or 7 and dipolarophiles. General procedure. To a solution of the in situ prepared chiral gold complex or chiral silver complex (0.05 mmol) in toluene (2 mL) was added, at room temperature, a solution of the iminoester (0.5 mmol) and dipolarophile (0.5 mmol) in toluene (2 mL). In some cases DIPEA or triethylamine (0.05 mmol) was added (see, Tables) and the mixture stirred at room temperature for 16-48 h (see, Tables). The reaction was filtered off through a celite pad and the organic filtrate was directly evaporated and the residue was purified by recrystallization or by flash chromatography yielding pure *endo*-cycloadducts **5**, **8**, **10**, **15** or **16**.

Methyl (1S,3R,3aS,6aR)-5-methyl-3-phenyl-4,6-dioxooctahydropyrrolo[3,4-c]pyrrole-1-carboxylate ***5aa***. [21][22]

*Methyl (1S,3R,3aS,6aR)-5-ethyl-3-phenyl-4,6-dioxooctahydropyrrolo[3,4-c]pyrrole-1-carboxylate **5ab**.*[21][22]
*Methyl (1S,3R,3aS,6aR)-3,5-diphenyl-4,6-dioxooctahydropyrrolo[3,4-c]pyrrole-1-carboxylate **5ac**.*[21,22]
*Methyl (1S,3R,3aS,6aR)-5-methyl-3-(2-naphthyl)-4,6-dioxooctahydropyrrolo[3,4-c]pyrrole-1-carboxylate **5ba**.*[8]
*Methyl (1S,3R,3aS,6aR)-5-ethyl-3-(2-naphthyl)-4,6-dioxooctahydropyrrolo[3,4-c]pyrrole-1-carboxylate **5bb***: Colourless solid; mp: 196-197 ºC (*n*-hexane/ethyl acetate); $[\alpha]_D^{20}$ = 7.0 (*c* 0.5, CH_2Cl_2, 50% *ee* by HPLC); IR (neat) ν_{max}: 3330, 2946, and 1748 cm^{-1}; ^{1}H NMR δ_H: 1.05 (t, *J* = 7.2 Hz, 1H, CH_2CH_3), 2.45 (s, 1H, NH), 3.39 (m, 2H, CH_2), 3.47 (dd, *J* = 7.6, and 8.0 Hz, 1H, C*H*CCO_2), 3.55 (dd, *J* = 7.0 and 8.0 Hz, 1H, C*H*CCAr), 3.91 (s, 3H, OCH_3), 4.08 (dd, *J* = 7.0, and 5.2 Hz, 1H, $CHCO_2$), 4.63 (dd, *J* = 7.6, and 5.2 Hz, 1H, C*H*Ar), 7.46 (dd, *J* = 6.2, 3.3 Hz, 3H, Ar *H*), 7.95 – 7.65 (m, 4H, Ar*H*); ^{13}C NMR δ_C: 13.1 (CH_3CH_2), 33.9 (CH_3), 48.1, 49.1, 52.3 (2x*C*HCON and CO_2CH_3), 61.6, 63.9 (*C*HCO_2Me), 67.9 (ArC*H*N), 125.3, 125.4, 125.9, 126.1, 126.2, 127.8, 127.9, 133.2, 134.2 and 134.2 (Ar*C*), 170.15, 174.33, 175.70 (3xCO); MS (EI) *m/z* (%): 352 (20), 293 (45), 127 (34), 91 (100); HRMS for $C_{20}H_{20}N_2O_4$ requires 352.3838; found 352.3830; HPLC (Chiralpak AS), 1 mL *n*-hexane/*i*–PrOH: 20/80, λ 225 nm, t_{maj} = 7.4 min, t_{min} = 20 min.

*Methyl (1S,3R,3aS,6aR)-3-(2-naphthyl)-5-phenyl-4,6-dioxooctahydropyrrolo[3,4-c]pyrrole-1-carboxylate **5bc**.*[7f]
*Methyl (1S,3R,3aS,6aR)-5-methyl-4,6-dioxo-3-o-tolyloctahydropyrrolo[3,4-c]pyrrole-1-carboxylate **5ca**.*[8]
*Methyl (1S,3R,3aS,6aR)-3-(2-chlorophenyl)-5-methyl-4,6-dioxooctahydropyrrolo[3,4-c]pyrrole-1-carboxylate **5da**.*[8]
*Methyl (1S,3R,3aS,6aR)-5-methyl-3-(4-methylphenyl)-4,6-dioxooctahydropyrrolo[3,4-c]pyrrole-1-carboxylate **5ea**.*[8]
*Methyl (1S,3R,3aS,6aR)-3-(4-methoxyphenyl)-5-methyl-4,6-dioxooctahydropyrrolo[3,4-c]pyrrole-1-carboxylate **5fa**.*[8]
*Methyl (1S,3R,3aS,6aR)-3-(4-chlorophenyl)-5-methyl-4,6-dioxooctahydropyrrolo[3,4-c]pyrrole-1-carboxylate **5ga**.*[8]
*Methyl (1S,3R,3aS,6aR)-1-benzyl-5-methyl-4,6-dioxo-3-phenyloctahydropyrrolo[3,4-c]pyrrole-1-carboxylate **8aa**.*[8]
*Methyl (2R,3R,4R,5S)-5-phenyl-3,4-bis(phenylsulfonyl)pyrrolidine-2-carboxylate **10a***: Colourless viscous oil; $[\alpha]_D^{20}$ = +1.2º (*c* 1.0, CH_2Cl_2, 90% *ee* by HPLC); IR (neat) ν_{max}: 3311, and 1753 cm^{-1}; ^{1}H RMN δ_H: 3.00 (br. s, 1H, NH) 3.68 (s, 3H, CH_3); 4,33 (br. s, 1H, NCHCO), 4.41, 4.47 (2xdd, *J* = 2.4 and 6.3 Hz, 2H, 2xCHS), 4.64 (m, 1H, PhC*H*N), 7.28-7.26 (m, 2H, Ar*H*), 7.34-7.32 (m, 2H, Ar*H*), 7.46-7.42 (m, 2H, Ar*H*), 7.61-7.52 (m, 3H, Ar*H*), 7.72-7.65 (m, 5H, Ar*H*), ^{13}C RMN δ_C: 37.4 (OCH_3), 48.6 (*C*HCO), 49.1, 52.7 (2xCHS), 56.0 (*C*HPh), 112.3, 112.9, 113.2, 113.4, 113.7, 113.9, 114.1, 114.2, 119.2, 121.9, 122.8, 123.1 (Ar), 152.4 (CO_2); MS (EI) *m/z* (%): 485 (M$^+$, <1%), 284 (11), 203 (15), 202 (100), 170 (18), 144 (27), 143 (60), 115 (14), 77 (14); HRMS for $C_{24}H_{23}NO_6S_2$ requires: 485.5725; found: 485.5717; HPLC (Chiralpak IA), 1 mL/min, *n*-hexane/*i*-PrOH: 80/20, λ 224 nm, t_{maj} = 50.23 min, t_{min} = 30.92 min.
*Methyl (2R,3R,4R,5S)-5-(naphth-2-yl)-3,4-bis(phenylsulfonyl)pirrolidine-2-carboxylate **10b***: Colluorless viscous oil; $[\alpha]_D^{20}$ = +17.1º (*c* 0.5, CH_2Cl_2, 92% *ee* by HPLC); IR (neat) ν_{max}: 3340, 1741.45 cm^{-1}; ^{1}H RMN δ_H: 3.15 (br. s, 1H, NH), 3.69 (s, 3H, CH_3); 4.38 (br. s, 1H, NCHCO), 4.45 (dd, *J* = 2.4 Hz, 6.4 Hz, 1H, CHS), 4.49 (dd, *J* = 2.4 Hz, 6.0 Hz, 1H, CHS), 4.79 (br. s, 1H, PhC*H*N), 7.39-7.35 (m, 2H, Ar*H*), 7.56-7.45 (m, 6H, Ar*H*), 7.72-7.60 (m, 7H, Ar*H*), 7.81-7.77 (m, 2H, Ar*H*); ^{13}C RMN δ_C: 38.5 (O*C*H_3), 48.6 (CHCO), 49.1, 52.7 (2xCHS), 55.9 (Ar*C*H), 109.3, 109.4, 111.2, 111.3, 112.0, 112.3, 112.4, 112.5, 113.0, 113.3, 113.4, 113.5, 113.8, 114.0, 114.2, 114.3, 119.3, 119.2, (Ar*C*), 152.5 (CO_2); MS (EI) *m/z* (%)**:** 535 (M$^+$, <1%), 394 (26), 392 (11), 391 (35), 359 (28), 268 (21), 267 (19), 266 (17), 253 (19), 252 (100), 251 (31), 250 (13), 220 (31), 219 (31), 194 (35), 193 (62), 192 (22), 191 (31), 190 (41), 167 (15), 166 (11), 165 (47), 164 (13), 163 (15), 155 (11), 153 (11), 152 (22), 142 (11), 127 (17), 125 (14), 78 (20), 77 (46), 51 (15); HRMS for $C_{28}H_{25}NO_6S_2$ requires: 535.6312; found: 535.6315; HPLC (Chiralpak AD), 1 mL/min, *n*-hexane/*i*-PrOH: 75/25, λ 227 nm, t_{maj} = 57.01 min, t_{min} = 51.97 min.
*Methyl (2R,3R,4R,5S)-3,4-bis(phenylsulfonyl)-5-(pyrid-3-yl)pirrolidine-2-carboxylate **10e***: Pale yellow oil; $[\alpha]_D^{20}$ = –63.9º (*c* 1.2, CH_2Cl_2, 92% *ee* by HPLC); IR (neat) ν_{max}: 3310, 1753 cm^{-1}; ^{1}H RMN δ_H**:** 1.90 (br. s, 1H, NH), 3.68 (s, 3H, CH_3); 4.33 (dd, *J* = 2.3 Hz, 6.4 Hz, 1H, CHS), 4.35 (m, 1H, NCHCO), 4.43 (dd, *J* = 2.3 Hz, 5.9 Hz, 1H, CHS), 4.66 (d, *J* = 6.2 Hz, 1H, ArC*H*N), 7.46 (t, *J* = 7.7 Hz, 8.0 Hz, 2H, Ar*H*), 7.53 (t, *J* = 7.4 Hz, 8.2 Hz, 2*H*, ArH), 7.61-7.65 (m, 2H, Ar*H*), 7.70 (t, *J* = 7.3 Hz, 7.9 Hz, 6H, Ar*H*), 8.36 (s, 1H, Ar*H*), 8.52 (s, 1H, Ar*H*); ^{13}C RMN δ_C: 34.6 (OCH_3), 45.8 (*C*HCO), 48.9, 52.4, (2xCHS), 55.7 (Ar*C*H), 108.7 113.3, 113.4, 114.3, 114.6, 119.3, 119.5, 119.6, 119.8, 121.5, 122.5, 134.0, 134.7 (ArC), 152.3 (CO_2Me); MS (EI) *m/z* (%): 486 (M$^+$, < 1%), 285 (10), 204 (14), 203 (100), 171 (10), 145 (19), 144 (30), 77 (18); HRMS for $C_{28}H_{25}NO_6S_2$ requires: 486.5606; found: 486.5601; HPLC (Chiralpak AD), 1 mL/min, *n*-hexane/*i*-PrOH: 50/50, λ 222 nm, t_{maj} = 15.05 min, t_{min} = 7.91 min.
*Methyl (2R,3R,4R,5S)-5-(4-methylphenyl)-3,4-bis(phenylsulfonyl)pyrrolidine-2-carboxylate **10f***: Colourless viscous oil; $[\alpha]_D^{20}$ = +2.3º (*c* 1.0, CH_2Cl_2, 88% *ee* by HPLC); IR (neat) ν_{max}: 3341, 1747 cm^{-1}; ^{1}H RMN δ_H: 2.30 (s, 3H, ArC*H*$_3$); 2.95 (br. s, 1H, NH), 3.66 (s, 3H, OC*H*$_3$), 4.31-4.27 (m, 1H, CHCO), 4.35 (dd, *J* = 2.4 Hz, 6.4 Hz, 1H, CHS), 4.41 (dd, *J* = 2.4 Hz, 6.0 Hz, 1H, CHS), 4.61-4.57 (br. s, 1H, ArC*H*N), 7.06 (d, *J* = 8.1 Hz, 1H, Ar*H*), 7.20 (d, *J* = 8.1 Hz, 1H, Ar*H*), 7.54-7.40 (m, 6H, Ar*H*), 7.64-7.57 (m, 2H, Ar*H*), 7.70-7.66 (m, 4H, Ar*H*); ^{13}C RMN δ_C: 21.2 (CH_3Ph) 53.6 (OCH_3), 63.5 (*C*HCO), 64.2 67.9 (2xCHS), 71.2 (Ar*C*HN), 127.3 128.5, 128.6, 129.1, 129.2, 129.3, 129.4, 129.5, 134.3, 135.0, 138.1, 138.2 (ArC), 167.6 (*C*O); (EI) *m/z* (%): 499 (M$^+$, < 1%), 358 (24), 217 (15), 216 (100), 184 (22), 158 (22), 157 (48), 156 (14), 77 (15); HRMS for $C_{25}H_{25}NO_6S_2$ requires: 499.5991; found: 499.6000; HPLC (Chiralpak AD), 1 mL/min, *n*-hexane/*i*-PrOH: 75/25, λ 220 nm, t_{maj} = 50.08 min, t_{min} = 26.11 min.

*Methyl (2R,3R,4R,5S)-5-(4-chlorophenyl)-3,4-bis(phenylsulfonyl)pyrrolidine-2-carboxylate **10h***: Colourless viscous oil; $[\alpha]_D^{20}$ = +91.6º (*c* 1.0, CH_2Cl_2, 45% *ee* by HPLC); IR (neat) ν_{max}: 3341, 1750 cm^{-1}; ^{1}H RMN δ_H: 2.90 (deform. t, 1H, NH), 3.67 (s, 3H, CH_3); 4.30 (dd, *J* = 2.3 Hz, 6.3 Hz, 1H, CHS), 4.34 (br. s, 1H, CHCO), 4.38 (dd, *J* = 2.3 Hz, 5.9 Hz, 1H, CHS), 4.66-4.61 (m, 1H, ArC*H*N), 7.30-7.21 (m, 3H, Ar*H*), 7.53-7.43 (m, 4H, Ar*H*), 7.71-7.59 (m, 7H, Ar*H*); ^{13}C RMN δ_C: 37.5 (OCH_3), 45.2 (*C*HCO), 48.9, 52.6 (2xCHS), 55.9 (Ar*C*H), 113.2, 113.7, 113.8, 114.0, 114.1, 114.3, 114.5, 114.8, 119.4, 119.5, 121.7, 123.0 (Ar*C*), 152.3 (CO); MS (EI) *m/z* (%): 519 (M$^+$, < 1%), 238 (32), 237 (17), 236 (100), 235 (12), 204 (19), 203 (15), 179 (17), 178 (19), 177 (48), 143 (21), 140 (14), 125 (16), 115 (13), 77 (29), 152 (13); HRMS for $C_{24}H_{22}ClNO_6S_2$ requires: 520.0176; found: 520.0170; HPLC (Chiralpak AD), 1 mL/min, *n*-hexane/*i*-PrOH: 70/30, λ 220 nm), t_{maj} = 41.08 min, t_{min} = 34.69 min.

*Methyl (2R,3R,4R,5S)-5-(4-chlorophenyl)-3,4-bis(phenylsulfonyl)pyrrolidine-2-carboxylate **10i***: Pale yellow oil; $[\alpha]_D^{20}$= -3º (*c* 0.5, CH_2Cl_2, 40% *ee*); IR (neat) ν_{max}: 2957, 1747, 1308, 1249 cm^{-1}; ^{1}H NMR δ_H: 2.98 (br. t, 1H, NH). 3.66 (s, 3H, CO_2CH_3), 3.78 (s, 3H, ArOC*H*$_3$), 3.83 (t, *J* = 6.5 Hz, 1H $CHCO_2$), 4.33 (dd, *J* = 7.0, 2.5 Hz, 1H, CHS), 4.42 (dd, *J* = 6.5, 2.5 Hz, 1H, CHS), 4.59 (dd, *J* = 10.0, 7.0 Hz, 1H, ArC*H*N), 6.79-6.75 (m, 2H, Ar*H*), 7.43 (t, *J* = 7.7 Hz, 2H, Ar*H*), 7.53 (td, *J* = 13.5, 6.6 Hz, 5H, Ar*H*), 7.67 (dt, *J* = 10.5, 4.1 Hz, 5H, Ar*H*); ^{13}C NMR δ_C: 52.5, 55.2 (2xOCH_3), 63.2, 64.1, 67.8 (2xCHS, and $CHCO_2$), 71.1 (ArCHN), 114.1, 128.4, 128.5, 128.6, 129.3, 129.4, 130.1, 134.3, 134.5, 136.9, 138.1, 159.5 (Ar*C*), 167.55 (CO); MS (EI) *m/z* (%): 515 (0.03), 277 (23), 141 (56), 91 (22), 77 (100); HRMS for $C_{25}H_{25}NO_7S_2$ requires 515.5985; found 5155991; HPLC (Chiralpak AD), *n*-hexane/*i*-PrOH:70/30, 1 mL/min, t_{maj} = 31.3 min, t_{min} = 36.4 min.
*Methyl (2S,3R,4S,5R)-4-benzoyl-3,5-diphenylpyrrolidine-2-carboxylate **15a**.*[6b]
*Methyl (2S,3R,4S,5R)-4-benzoyl-5-(naphth-2-yl)-3-phenylpyrrolidine-2-carboxylate **15b***: Colourless solid, mp: 128-129 ºC (*n*-hexane/ethyl acetate); $[\alpha]_D^{20}$ = -37 (*c* 0.8, CH_2Cl_2, 60% *ee* by HPLC). IR (neat) ν_{max}: 3345, 1736, 1677 cm^{-1}; ^{1}H NMR δ_H 3.35 (br. s, NH), 3.76 (s, 3H, CH_3). 4.19 (deform. t, *J* = 7.5 Hz, 1H, C*H*$CHCO_2$) 4.25 (d, *J* = 8.0 Hz, 1H, $CHCO_2$), 4.62 (dd, *J* = 15.0, 7.5 Hz, 1H, C*H*COPh), 5.17 (d, *J* = 8.5 Hz, 1H, ArC*H*N), 7.83-7.10 (m, 17H, Ar*H*); ^{13}C NMR δ_C: 52.3, 52.7 (CH_3, *C*Ph), 60.5 (*C*HCO_2), 66.7, 67.8 (2xCHN), 125.0, 125.1, 125.8, 125.9, 126.3, 126.4, 127.1, 127.6, 127.7, 127.8, 127.9, 128.1, 128.5, 128.8, 132.8, 136.4, 137.4, 140.7 (Ar*C*), 173.3 (CO_2), 198.8 (*C*OPh); MS (EI): *m/z* (%): 435 (M$^+$, 10); HRMS-ESI for $C_{29}H_{25}NO_3$ requires: 435.5135; found: 435. 5137; HPLC (Chiralcel OD-H), *n*-hexane/*i*-PrOH: 99/1, 1 mL/min, t_{maj} = 17.3 min, t_{min} 25.8 min.
*2-Methyl (2S,3R,4R,5S)-4-nitro-3,5-diphenyl-2-pyrrolidinocarboxylate **16a**.*[7f]

Acknowledgements

This work has been supported by the DGES of the Spanish Ministerio de Ciencia e Innovación (MICINN) (Consolider INGENIO 2010 CSD2007-00006, FEDER-CTQ2007-62771/BQU, CTQ2007/67528, CTQ2010-20387 and by the Hispano-Brazilian project PHB2008-0037-PC), Generalitat Valenciana (PROMETEO/ 2009/039), the Basque government (Grant IT-324-07) and by the University of Alicante. M. M.-R. Also thanks DGES for a grant. The authors also thank the SGI/IZO-SGIker of UPV/EHU for allocation of computational resources.

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Table 2. 1,3-DC of iminoesters **3a** and maleimides **4** catalyzed by chiral complex **2** (X = TFA).

						Gold catalysis		Silver catalysis	
Entry	3	Ar	R	Base	endo-**5**	Yield (%)[a][b]	*ee* (%)[c]	Yield (%)[a][b]	*ee* (%)[c][,d]
1	**3a**	Ph	Me	—	**5aa**	95	99	89	99
2	**3a**	Ph	Me	DIPEA	**5aa**	90	70	89	99
3	**3a**	Ph	Et	—	**5ab**	78	99	78	99
4	**3a**	Ph	Et	DIPEA	**5ab**	80	70	81	99
5	**3a**	Ph	Ph	—	**5ac**	81	80	80	*Rac*
6	**3a**	Ph	Ph	DIPEA	**5ac**	89	64	88	*Rac*
7	**3b**	2-Naphthyl	Me	—	**5ba**	87	90	88	99
8	**3b**	2-Naphthyl	Et	—	**5bb**	85	50	81	50
9	**3b**	2-Naphthyl	Ph	—	**5bc**	82	99	84	46
10	**3c**	2-MeC_6H_4	Me	—	**5ca**	90	99	92	50
11	**3d**	2-ClC_6H_4	Me	—	**5da**	88	88	89	60
12	**3e**	4-MeC_6H_4	Me	—	**5ea**	88	88	88	99
13	**3f**	4-(MeO)C_6H_4	Me	—	**5fa**	88	99	88	99
14	**3g**	4-ClC_6H_4	Me	—	**5ga**	85	22	81	*Rac*

[a] Isolated yields after flash chromatography (silica gel). [b] The observed *endo*:*exo* ratio was >98:2 (^{1}H NMR). [c] Determined by using analytical chiral HPLC columns. [d] The reaction was performed exclusively with (S_a)-Binap-AgTFA **6** (10 mol%).

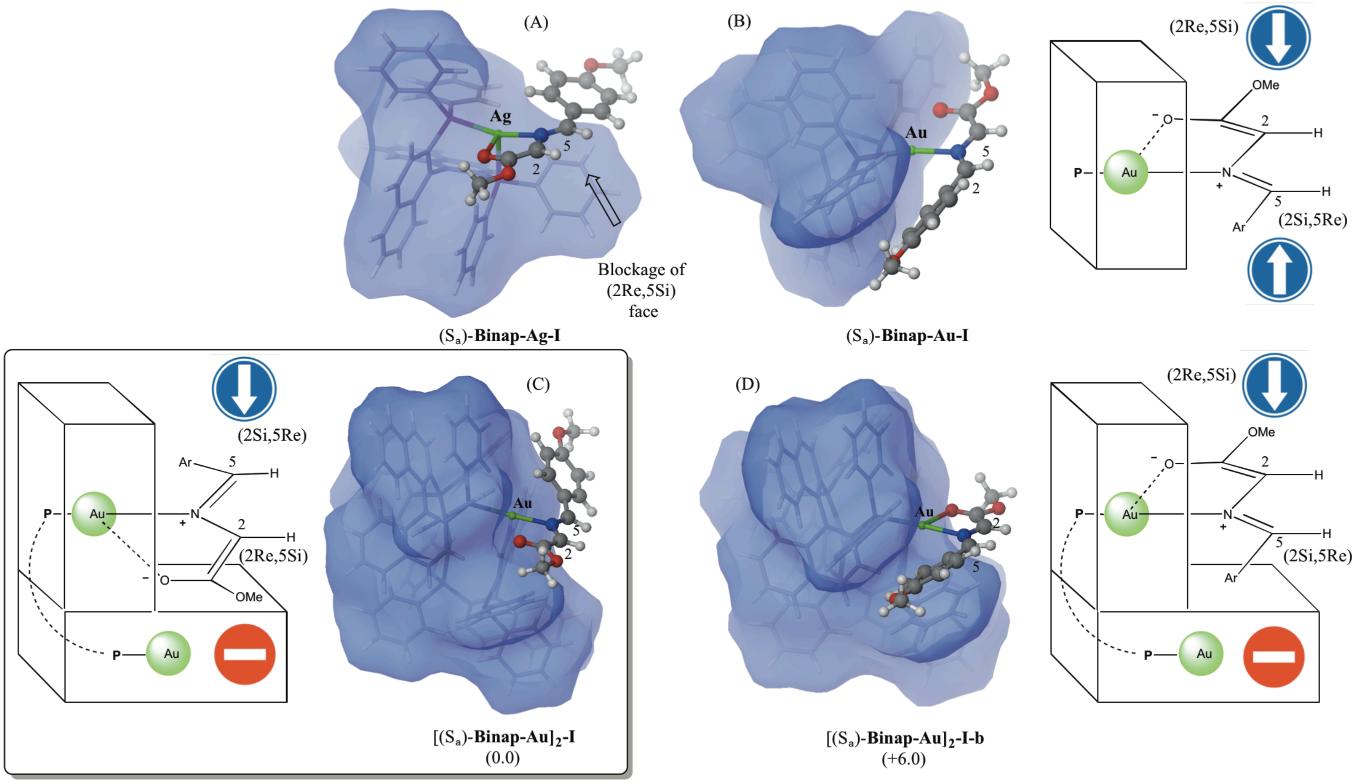

Figure 2. Geometry of the most stable (S_a)-Binap Ag(I) or Au(I) complexes computed at ONIOM(B3LYP/LanL2DZ:UFF) level of theory. The B3LYP/LanL2DZ and UFF levels in the ONIOM calculation are depicted in ball & stick and tube representations respectively. Number in parentheses correspond to the relative Gibbs free energies at 298K and are given in kcal mol^{-1}. Surfaces represent e solvent accessible surface with a probe radius of 1.9 Å. For panels (B), (C) and (D) a schematic cartoon of the possible stereochemical course of the corresponding (3+2) cycloaddition is also displayed.

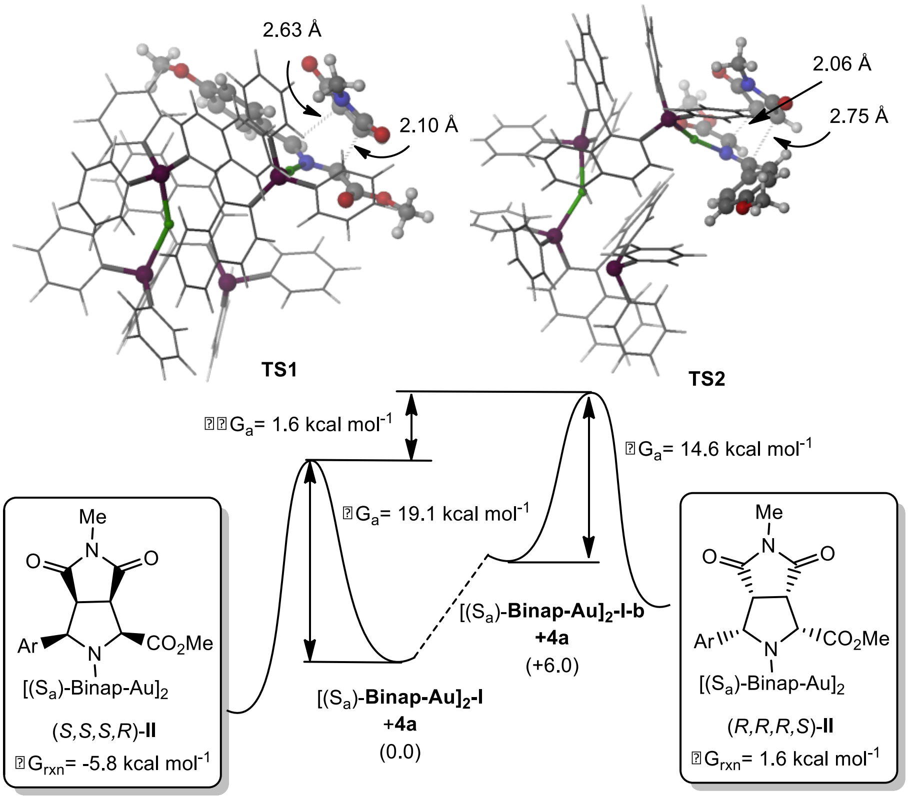

Figure 3. Gibbs activation energy and main geometrical features of the transition structures computed reaction paths corresponding for the two possible 1,3-DC of Au(I) ylide dimeric complexes and *N*-Methyl maleimide computed at ONIOM(B3LYP/LanL2DZ:UFF) level of theory. High level and low-level layers were represented as ball & stick and wireframe models respectively.

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Entry for the Table of Contents (Please choose one layout only)

Layout 1:

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Title Text

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Layout 2:

Chiral gold(I)-catalyzed 1,3-DC shows NLE

María Martín-Rodríguez, Carmen Nájera, José M. Sansano, Abel de Cózar, and Fernando P. Cossío.**

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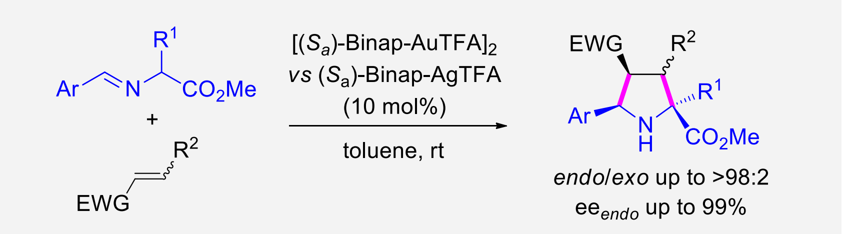
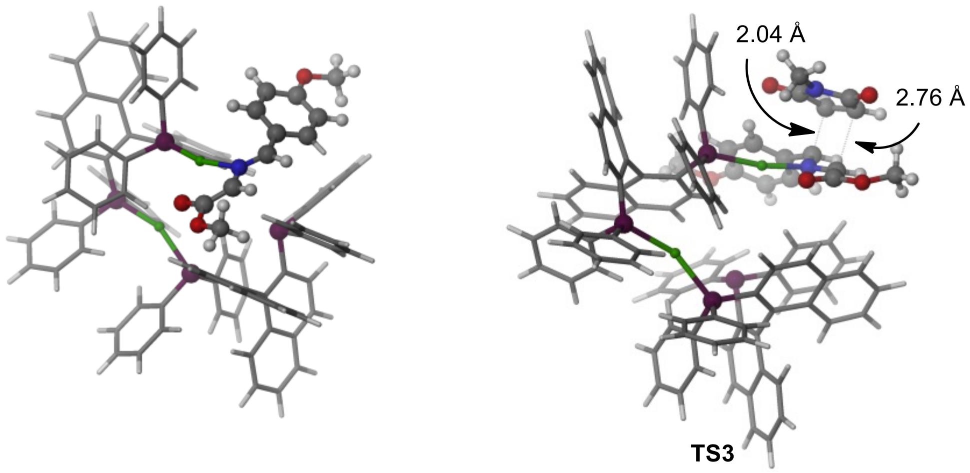
Binap-gold(I) *vs* Binap-silver trifluoroacetate complexes as catalysts in 1,3-dipolar cycloadditions of azomethine ylides



The enantioselective 1,3-DC of azomethine ylides and electrophilic alkenes has been successfully catalysed by [(S_a)-Binap-AuTFA]$_2$ complex. The origin of the enantioselection, as well as the observed NLE, are analyzed using computational tools.

SUPPORTING INFORMATION



ΔG_a= 20.2 kcal mol^{-1}

FigureS1. Geometrical features of the most stable ylide heterodimer complex [(S_a)-Binap,(R_a)-Binap-Au_2]-**I** and the TS corresponding to the reaction of that ylide and NMM computed at ONIOM(B3LYP/LanL2DZ:UFF) level of theory. High level and low-level layers were represented as ball & stick and wireframe models respectively.

Table S1. Total electronic energies[a] (E, in a.u.), thermal corrections to Gibbs free energies[b] (TCGE, in a.u.) and number of imaginary frequencies[c] (NIMAG) of all stationary points discussed in the main text.

Structure	E	TCGE	NIMAG(ν)
3	-707.2881858	0.181147	0
4a	-398.6789855	0.064225	0
5	-1106.0113219	0.275834	0
[(S_a)-Binap Ag]-**I**	-868.862405	0.795801	0
[(S_a)-Binap Au]-**I**	-858.551914	0.796065	0
[(S_a)-Binap Au]$_2$-**I**	-1010.201625	1.430058	0
[(S_a)-Binap Au]$_2$-**I-b**	-1010.191870	1.429869	0
[(S_a)-Binap-(R_a)-Binap-Au_2]-**I**	-1010.215705	1.418365	0
(*S*, *S*, *S*, *R*)-**II**	-1408.921851	1.526251	0
(*R*, *R*, *R,* S)-**II**	-1408.911811	1.527335	0
TS1	-1408.878344	1.522479	1 (-300.875)
TS2	-1408.875365	1.521839	1 (-292.414)
TS3	-1408.89197	1.512060	1 (-342.801)

[a]Computed at level ONIOM(B3LYP/LanL2DZ:UFF) of theory. [b]Computed at 298 K at ONIOM(B3LYP/LanL2DZ:UFF) level of theory. [c]If NIMAG=1, the imaginary frequency ν (in parentheses) is given in cm^{-1}

Table S2. Calculated kinetic constants calculated employing Eyring equations and the computed activation free energy barriers.

	K (s^{-1})
k_{HOMO}	6.1 10^{-2}
k_{HET}	9.6 10^{-3}

Cartesian coordinates (optimized at the ONIOM(B3LYP/LanL2DZ:UFF) level) of all the stationary points discussed in the main text.

3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.537234	0.893114	-0.433045
2	6	0	2.846655	0.658035	-0.954946
3	6	0	3.720396	0.110894	0.174168
4	8	0	3.405569	0.046550	1.370620
5	6	0	-0.856158	0.442350	-0.288241
6	6	0	-1.240443	-0.889960	-0.593911
7	6	0	-1.840999	1.344122	0.165038
8	6	0	-2.566430	-1.297937	-0.449752
9	1	0	-0.477047	-1.580456	-0.939479
10	6	0	-3.181828	0.947109	0.316013
11	1	0	-1.560709	2.368255	0.406873
12	6	0	-3.543574	-0.380356	0.006174
13	1	0	-2.878535	-2.312713	-0.677210
14	1	0	-3.917679	1.662542	0.668705
15	7	0	1.484681	0.119065	-0.860462
16	8	0	-4.835130	-0.890646	0.115478
17	8	0	4.955327	-0.279192	-0.306295
18	6	0	-5.900142	-0.013933	0.584987
19	1	0	-6.800464	-0.631212	0.587155
20	1	0	-5.696668	0.348109	1.602238
21	1	0	-6.038404	0.840506	-0.091891
22	6	0	5.923325	-0.791334	0.682408
23	1	0	6.130966	-0.028007	1.439123
24	1	0	5.521915	-1.684920	1.170232
25	1	0	6.817823	-1.026519	0.104307
26	1	0	3.292656	0.358619	-1.907317
27	1	0	0.729482	1.943886	-0.153644
28	1	0	2.889556	1.762130	-0.877653

4a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.682413	-1.636126	0.000024
2	6	0	0.669064	-1.641522	0.000016
3	1	0	1.353465	-2.479251	-0.000015
4	1	0	-1.373952	-2.467929	-0.000017
5	7	0	0.003488	0.596717	-0.000056
6	6	0	0.010785	2.061590	0.000027
7	1	0	0.522033	2.443482	-0.889946
8	1	0	-1.028200	2.402197	-0.000372
9	1	0	0.521354	2.443394	0.890419
10	6	0	1.157632	-0.213904	-0.000017
11	8	0	2.331923	0.197276	0.000005
12	6	0	-1.159813	-0.205206	-0.000003
13	8	0	-2.330753	0.214235	0.000000

5

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	0.141184	-0.796526	1.160526
2	6	0	-2.185796	-1.077005	0.734155
3	6	0	-3.281259	-1.397757	-0.274713
4	8	0	-3.115675	-1.910592	-1.389327
5	6	0	1.530470	-0.717383	0.549767
6	6	0	1.710272	-0.517615	-0.839036
7	6	0	2.670958	-0.835084	1.362705
8	6	0	2.992847	-0.431954	-1.391273
9	1	0	0.836349	-0.445912	-1.480530
10	6	0	3.968762	-0.742407	0.826025
11	1	0	2.555286	-0.995183	2.433707
12	6	0	4.127948	-0.537085	-0.559338
13	1	0	3.142766	-0.283001	-2.456393
14	1	0	4.827549	-0.831294	1.483743
15	7	0	-0.848161	-1.374628	0.237511
16	8	0	5.360969	-0.432785	-1.207274
17	8	0	-4.511170	-1.089879	0.260821
18	6	0	6.576371	-0.493622	-0.408083
19	1	0	7.395392	-0.368924	-1.119254
20	1	0	6.604666	0.315638	0.334876
21	1	0	6.672589	-1.464160	0.098887
22	6	0	-5.672811	-1.181099	-0.642675
23	1	0	-5.553451	-0.454661	-1.451826
24	1	0	-5.754429	-2.191153	-1.056045
25	1	0	-6.534656	-0.937968	-0.019879
26	1	0	0.215075	-1.371933	2.104632
27	1	0	-2.452101	-1.619208	1.664385
28	6	0	-2.040329	0.426398	1.105407
29	6	0	-0.561907	0.578119	1.568520
30	1	0	-2.779227	0.727203	1.853696
31	1	0	-0.441707	0.749326	2.641091
32	7	0	-0.989952	2.142709	-0.169817
33	6	0	-0.791056	3.211393	-1.154205
34	1	0	0.137760	3.730117	-0.904191
35	1	0	-0.721845	2.789800	-2.162574
36	1	0	-1.633342	3.909890	-1.125560
37	6	0	-0.043564	1.803964	0.819581
38	8	0	1.008998	2.430357	1.025775
39	6	0	-2.151902	1.364341	-0.107509
40	8	0	-3.108397	1.467884	-0.897595
41	1	0	-0.668810	-2.295082	-0.150958

[(S_a)-Binap Ag]-**I**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	10471001	1.125667	1.459323	1.250834
2	6	10061000	-0.739450	-1.593572	0.920844
3	6	10061002	0.167026	-2.688173	1.357491
4	6	10061002	0.416350	-3.751212	0.583626
5	6	10061000	-0.206593	-3.870390	-0.743391
6	6	10061002	0.069743	-5.039846	-1.606638
7	6	10061000	-0.491174	-5.124786	-2.824331
8	6	10061000	-1.343873	-4.122714	-3.307813
9	6	10061002	-1.634783	-3.032650	-2.576406
10	6	10061000	-1.051268	-2.860096	-1.217286
11	6	10061000	-1.298597	-1.647577	-0.382468
12	6	10061002	-2.176320	-0.580185	-0.940564
13	6	10061002	-1.676621	0.545928	-1.528235
14	6	10061002	-2.619900	1.469269	-2.228950
15	6	10061000	-3.939711	1.234136	-2.252229
16	6	10061000	-4.480571	0.100357	-1.644291
17	6	10061000	-3.647630	-0.830807	-1.007720
18	6	10061002	-4.282417	-2.034227	-0.405811
19	6	10061000	-5.614956	-2.199733	-0.467276
20	6	10061000	-6.442951	-1.260020	-1.097507
21	6	10061002	-5.940008	-0.153420	-1.670865
22	6	10061000	-4.866264	0.438665	2.027355
23	6	10061000	-4.998749	1.756863	1.583515
24	6	10061000	-3.860953	2.508232	1.278927
25	6	10061000	-2.590909	1.941304	1.416803
26	6	10061000	-2.450690	0.614805	1.847163
27	6	10061000	-3.596695	-0.133105	2.159106

28	15	10151003	-0.763301	-0.085285	1.981290
29	6	10061000	-0.736240	-0.707361	3.708177
30	6	10061000	-0.020363	0.019333	4.668778
31	6	10061000	0.025482	-0.419069	5.995631
32	6	10061000	-0.639817	-1.589711	6.369224
33	6	10061000	-1.347658	-2.325316	5.415000
34	6	10061000	-1.395956	-1.888720	4.087632
35	15	10151003	0.133461	0.947502	-1.441151
36	6	10061000	0.820246	-0.362720	-2.523195
37	6	10061000	1.818056	-1.207528	-2.023822
38	6	10061000	2.315691	-2.250860	-2.809666
39	6	10061000	1.816028	-2.454318	-4.099027
40	6	10061000	0.812634	-1.619316	-4.599908
41	6	10061000	0.307241	-0.581132	-3.811224
42	6	10061000	0.347036	2.512727	-2.386740
43	6	10061000	1.161306	2.592180	-3.530682
44	6	10061000	1.359667	3.819613	-4.170833
45	6	10061000	0.771961	4.979911	-3.661751
46	6	10061000	-0.005754	4.916866	-2.503973
47	6	10061000	-0.205707	3.691996	-1.861807
48	1	10011000	2.184562	-1.075892	-1.016403
49	1	10011000	3.078256	-2.909334	-2.415028
50	1	10011000	2.197465	-3.265673	-4.705066
51	1	10011000	0.416973	-1.785281	-5.593350
52	1	10011000	-0.482719	0.048576	-4.200062
53	1	10011000	-0.798451	3.660207	-0.956584
54	1	10011000	-0.448027	5.818129	-2.099885
55	1	10011000	0.930612	5.929369	-4.156417
56	1	10011000	1.982009	3.873392	-5.054760
57	1	10011000	1.668490	1.723551	-3.921883
58	1	10011000	0.499212	0.927616	4.389967
59	1	10011000	0.577127	0.148415	6.733912
60	1	10011000	-0.602704	-1.929232	7.396247
61	1	10011000	-1.854112	-3.237538	5.702702
62	1	10011000	-1.925011	-2.487426	3.359709
63	1	10011000	-2.256501	2.340281	-2.755410
64	1	10011000	-4.590337	1.932782	-2.764443
65	1	10011000	-6.609677	0.553755	-2.151591
66	1	10011000	-7.511575	-1.431586	-1.122498
67	1	10011000	-6.061370	-3.077165	-0.016866
68	1	10011000	-3.681509	-2.781399	0.102116
69	1	10011000	-2.286682	-2.277302	-3.001597
70	1	10011000	-1.771168	-4.226647	-4.297061
71	1	10011000	-0.278845	-5.983708	-3.448097
72	1	10011000	0.729919	-5.829316	-1.260188
73	1	10011000	1.093552	-4.523764	0.935688
74	1	10011000	0.663690	-2.624913	2.318990
75	1	10011000	-5.982353	2.193913	1.471261
76	1	10011000	-5.748293	-0.146525	2.252874
77	1	10011000	-3.521027	-1.163034	2.467609
78	1	10011000	-1.716203	2.530837	1.174020
79	1	10011000	-3.962719	3.528431	0.932503
80	6	10061000	4.255909	1.423589	0.306231
81	1	10011000	5.099077	1.869258	-0.235267
82	6	10061000	3.227918	3.558632	0.501765
83	6	10061000	2.070811	4.291324	0.838518
84	8	10081000	0.955803	3.829250	1.301245
85	6	10061000	4.303562	-0.023750	0.515504
86	6	10061000	3.605942	-0.683943	1.567810
87	6	10061000	5.065450	-0.833734	-0.364071
88	6	10061000	3.622241	-2.077130	1.689207
89	1	10011000	3.081984	-0.086848	2.310100
90	6	10061000	5.079359	-2.235900	-0.260227
91	1	10011000	5.629369	-0.357771	-1.164536
92	6	10061000	4.333979	-2.863632	0.758794
93	1	10011000	3.111128	-2.581357	2.504390
94	1	10011000	5.656949	-2.817050	-0.972812
95	7	10071000	3.247672	2.195108	0.680654
96	1	10011000	4.093120	4.086190	0.106824
97	8	10081003	4.245772	-4.250696	0.944410
98	8	10081003	2.197196	5.670007	0.611486
99	6	10061003	4.903902	-5.117618	-0.019551
100	1	10011000	4.674441	-6.136023	0.301396
101	1	10011000	4.514008	-4.952583	-1.034580
102	1	10011000	5.992923	-4.967714	-0.016939
103	6	10061003	1.044226	6.496519	0.969480
104	1	10011000	1.304967	7.504212	0.636836
105	1	10011000	0.136279	6.142904	0.468690
106	1	10011000	0.875390	6.479671	2.052566

[(S_a)-Binap Au]-**I**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	10791004	1.655741	1.428819	0.135546
2	6	10061000	-0.017751	-1.619508	-0.563837
3	6	10061002	0.779623	-1.982376	-1.762660
4	6	10061002	0.230457	-2.598876	-2.816697
5	6	10061000	-1.203827	-2.929950	-2.824259
6	6	10061002	-1.823394	-3.590526	-3.994699
7	6	10061000	-3.140892	-3.854028	-4.000053
8	6	10061000	-3.958018	-3.518298	-2.911681
9	6	10061002	-3.459814	-2.919189	-1.816093
10	6	10061000	-2.009056	-2.591962	-1.730692
11	6	10061000	-1.410737	-1.884709	-0.561145
12	6	10061002	-2.323501	-1.422514	0.514795
13	6	10061002	-2.811835	-0.151664	0.531595
14	6	10061002	-3.863695	0.196686	1.538554
15	6	10061000	-4.308911	-0.707046	2.424227
16	6	10061000	-3.827723	-2.017463	2.421325
17	6	10061000	-2.868051	-2.419524	1.481934
18	6	10061002	-2.422595	-3.838102	1.502988
19	6	10061000	-2.922434	-4.690532	2.414330
20	6	10061000	-3.873914	-4.279953	3.359286
21	6	10061002	-4.330816	-3.016186	3.393175
22	6	10061000	-0.840511	-2.069886	4.260131
23	6	10061000	-1.318659	-0.883067	4.822445
24	6	10061000	-1.108729	0.333777	4.167786
25	6	10061000	-0.429032	0.362493	2.946708
26	6	10061000	0.017926	-0.827061	2.359702
27	6	10061000	-0.168951	-2.043250	3.033674
28	15	10151003	0.909110	-0.743539	0.768419
29	6	10061000	2.387445	-1.778601	1.069701
30	6	10061000	3.585981	-1.155985	1.442596
31	6	10061000	4.740364	-1.917058	1.648960
32	6	10061000	4.704336	-3.303430	1.477992
33	6	10061000	3.511006	-3.931014	1.109296
34	6	10061000	2.353655	-3.172829	0.906766
35	15	10151003	-2.215377	1.084781	-0.737241
36	6	10061000	-3.401138	0.568391	-2.054277
37	6	10061000	-2.895353	0.257132	-3.323425
38	6	10061000	-3.752676	-0.181420	-4.336493
39	6	10061000	-5.121868	-0.308358	-4.087997
40	6	10061000	-5.635147	0.005727	-2.826623
41	6	10061000	-4.779970	0.442998	-1.810895
42	6	10061000	-3.006900	2.658711	-0.172671
43	6	10061000	-3.779462	3.446908	-1.045542
44	6	10061000	-4.325464	4.657872	-0.608765
45	6	10061000	-4.083762	5.107828	0.690941
46	6	10061000	-3.277711	4.357407	1.548937
47	6	10061000	-2.722225	3.152168	1.111214
48	1	10011000	-1.834000	0.337810	-3.521930
49	1	10011000	-3.354254	-0.430862	-5.311284
50	1	10011000	-5.784255	-0.652098	-4.871719
51	1	10011000	-6.695786	-0.091802	-2.635188
52	1	10011000	-5.194663	0.686236	-0.843071
53	1	10011000	-2.089969	2.591026	1.783110
54	1	10011000	-3.072094	4.715590	2.549322
55	1	10011000	-4.505976	6.045903	1.027096
56	1	10011000	-4.928449	5.252853	-1.282390
57	1	10011000	-3.952178	3.142299	-2.068093
58	1	10011000	3.628039	-0.081118	1.565859
59	1	10011000	5.665287	-1.430852	1.930870
60	1	10011000	5.600680	-3.890655	1.629868
61	1	10011000	3.483392	-5.004909	0.977796
62	1	10011000	1.438868	-3.673173	0.617282
63	1	10011000	-4.325622	1.173717	1.548840
64	1	10011000	-5.071385	-0.415374	3.136484
65	1	10011000	-5.068991	-2.731860	4.137402
66	1	10011000	-4.248805	-4.998901	4.076634
67	1	10011000	-2.581386	-5.717981	2.422068
68	1	10011000	-1.680500	-4.194759	0.796021
69	1	10011000	-4.135944	-2.666423	-1.006717
70	1	10011000	-5.016425	-3.741135	-2.958969
71	1	10011000	-3.583259	-4.332863	-4.864339

72	1	10011000	-1.216357	-3.858235	-4.854244
73	1	10011000	0.848744	-2.849027	-3.673593
74	1	10011000	1.836952	-1.745339	-1.791240
75	1	10011000	-1.846739	-0.905963	5.766730
76	1	10011000	-1.000634	-3.012001	4.768107
77	1	10011000	0.181549	-2.971228	2.606613
78	1	10011000	-0.250580	1.309517	2.455789
79	1	10011000	-1.468477	1.254668	4.607898
80	6	10061000	4.282048	2.731950	-0.725024
81	1	10011000	4.981619	3.572206	-0.743136
82	6	10061000	2.533192	4.289436	-0.319253
83	6	10061000	1.204307	4.521921	0.098751
84	8	10081000	0.330683	3.644354	0.435964
85	6	10061000	4.842630	1.405841	-0.993328
86	6	10061000	4.145574	0.382542	-1.698952
87	6	10061000	6.165637	1.117772	-0.574545
88	6	10061000	4.723118	-0.873910	-1.915001
89	1	10011000	3.163522	0.596174	-2.111192
90	6	10061000	6.753698	-0.142548	-0.777594
91	1	10011000	6.732476	1.886366	-0.052473
92	6	10061000	6.020537	-1.151313	-1.436160
93	1	10011000	4.203096	-1.650291	-2.468709
94	1	10011000	7.761748	-0.324650	-0.417938
95	7	10071000	3.009046	3.004822	-0.440020
96	1	10011000	3.176215	5.130419	-0.557440
97	8	10081003	6.487721	-2.450082	-1.672785
98	8	10081003	0.879749	5.888146	0.118128
99	6	10061003	7.796469	-2.818727	-1.155617
100	1	10011000	7.931301	-3.867383	-1.428866
101	1	10011000	8.592739	-2.213859	-1.611927
102	1	10011000	7.835864	-2.712834	-0.061897
103	6	10061003	-0.483706	6.227788	0.521940
104	1	10011000	-0.517969	7.319805	0.514037
105	1	10011000	-1.212313	5.815214	-0.185568
106	1	10011000	-0.701836	5.840449	1.523352

[(S_a)-Binap Au]$_2$-**I**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	10061000	-1.773665	1.952728	0.078611
2	6	10061002	-0.323228	1.800377	0.371861
3	6	10061002	0.103889	1.197734	1.491043
4	6	10061000	-0.858101	0.671161	2.474498
5	6	10061002	-0.398773	0.078050	3.745277
6	6	10061000	-1.290431	-0.372418	4.643131
7	6	10061000	-2.667269	-0.342679	4.383318
8	6	10061002	-3.153549	0.162916	3.236756
9	6	10061000	-2.229480	0.735485	2.220865
10	6	10061000	-2.709932	1.371692	0.969341
11	6	10061002	-4.164741	1.394033	0.683550
12	6	10061000	-4.726833	0.530808	-0.205984
13	6	10061000	-6.089460	0.647403	-0.556350
14	6	10061002	-6.891444	1.579781	-0.019397
15	6	10061000	-6.372264	2.484921	1.017928
16	6	10061000	-5.033472	2.379565	1.394279
17	6	10061002	-4.555218	3.240370	2.508454
18	6	10061000	-5.396307	4.108743	3.099093
19	6	10061000	-6.734723	4.227203	2.692856
20	6	10061002	-7.237568	3.468854	1.702863
21	6	10061000	-4.192249	5.754663	0.323536
22	6	10061000	-5.309567	5.962794	-0.487459
23	6	10061000	-5.518152	5.154573	-1.606748
24	6	10061000	-4.606462	4.142234	-1.918986
25	6	10061000	-3.483326	3.921461	-1.109051
26	6	10061000	-3.286208	4.733068	0.022003
27	15	10151003	-2.319325	2.571645	-1.588448
28	6	10061000	-0.935932	3.661190	-2.137433
29	6	10061000	-0.294487	4.579350	-1.286671
30	6	10061000	0.635480	5.485586	-1.802124
31	6	10061000	0.965437	5.458918	-3.158388
32	6	10061000	0.353768	4.533473	-4.005311
33	6	10061000	-0.603394	3.649785	-3.499785
34	15	10151003	-3.780383	-0.886669	-0.901143
35	6	10061000	-4.708383	-2.295539	-0.190319

36	6	10061000	-4.239717	-2.862699	1.000958
37	6	10061000	-4.903061	-3.951055	1.573977
38	6	10061000	-6.047538	-4.471208	0.964298
39	6	10061000	-6.533654	-3.897111	-0.213721
40	6	10061000	-5.871200	-2.808173	-0.788729
41	6	10061000	-4.103323	-0.960564	-2.702528
42	6	10061000	-4.446230	0.196484	-3.417344
43	6	10061000	-4.730160	0.124864	-4.783920
44	6	10061000	-4.685543	-1.105262	-5.444093
45	6	10061000	-4.345370	-2.262369	-4.739586
46	6	10061000	-4.034404	-2.188314	-3.378265
47	1	10011000	-3.358300	-2.459831	1.481981
48	1	10011000	-4.531394	-4.389985	2.490657
49	1	10011000	-6.560999	-5.314500	1.407572
50	1	10011000	-7.424709	-4.295609	-0.681150
51	1	10011000	-6.266228	-2.376055	-1.697439
52	1	10011000	-3.762578	-3.091789	-2.849268
53	1	10011000	-4.311866	-3.215737	-5.250488
54	1	10011000	-4.914570	-1.161947	-6.500259
55	1	10011000	-4.995383	1.021846	-5.328456
56	1	10011000	-4.507984	1.151258	-2.920022
57	1	10011000	-0.499756	4.603000	-0.229681
58	1	10011000	1.096038	6.213872	-1.148784
59	1	10011000	1.686456	6.161370	-3.554841
60	1	10011000	0.601604	4.518009	-5.058678
61	1	10011000	-1.108792	2.975664	-4.178737
62	1	10011000	-6.514897	-0.027945	-1.285558
63	1	10011000	-7.932071	1.639711	-0.323398
64	1	10011000	-8.278190	3.576265	1.412536
65	1	10011000	-7.375994	4.943233	3.190827
66	1	10011000	-5.031883	4.736395	3.902338
67	1	10011000	-3.525513	3.188837	2.845648
68	1	10011000	-4.225608	0.155304	3.070306
69	1	10011000	-3.351878	-0.742582	5.120413
70	1	10011000	-0.938707	-0.786018	5.578952
71	1	10011000	0.660131	0.000185	3.949625
72	1	10011000	1.167250	1.085115	1.669578
73	1	10011000	0.417402	2.152594	-0.332976
74	1	10011000	-6.016835	6.745050	-0.244562
75	1	10011000	-4.040857	6.368883	1.201668
76	1	10011000	-2.469305	4.553449	0.702996
77	1	10011000	-4.775157	3.533494	-2.797154
78	1	10011000	-6.384710	5.314368	-2.235016
79	79	10791004	3.047570	2.185344	0.390830
80	79	10791004	-1.428525	-1.336184	-0.190583
81	6	10061000	1.939162	-0.500217	-1.747435
82	6	10061002	1.099293	0.437168	-2.536296
83	6	10061002	0.143408	-0.001618	-3.365341
84	6	10061000	-0.097185	-1.443062	-3.529169
85	6	10061002	-0.987372	-1.944822	-4.597615
86	6	10061000	-1.136512	-3.267354	-4.784438
87	6	10061000	-0.474112	-4.199544	-3.975280
88	6	10061002	0.354450	-3.811366	-2.991238
89	6	10061000	0.587450	-2.363688	-2.730412
90	6	10061000	1.604312	-1.881169	-1.754257
91	6	10061000	2.334343	-2.893821	-0.971369
92	6	10061000	1.790779	-3.452179	0.204168
93	6	10061002	2.575857	-4.501371	0.907874
94	6	10061000	3.705438	-5.000637	0.386686
95	6	10061000	4.192122	-4.562877	-0.847552
96	6	10061000	3.536305	-3.546123	-1.559259
97	6	10061002	4.073404	-3.175312	-2.894536
98	6	10061000	5.184168	-3.766218	-3.366960
99	6	10061000	5.857967	-4.753497	-2.634260
100	6	10061002	5.414246	-5.162333	-1.433370
101	6	10061000	6.424936	-2.283016	0.288976
102	6	10061000	6.020223	-2.588256	1.590644
103	6	10061000	4.835171	-2.049724	2.096929
104	6	10061000	4.048873	-1.213210	1.298493
105	6	10061000	4.431062	-0.926947	-0.017273
106	6	10061000	5.639570	-1.448302	-0.511811
107	15	10151003	3.434091	0.272793	-0.969430
108	6	10061000	4.512405	0.809233	-2.350602
109	6	10061000	5.638636	1.591187	-2.055240
110	6	10061000	6.485554	2.025865	-3.078593
111	6	10061000	6.213106	1.682307	-4.404899
112	6	10061000	5.092096	0.905781	-4.708480
113	6	10061000	4.241400	0.471616	-3.687439
114	15	10151003	0.066143	-3.107361	0.771572
115	6	10061000	-0.805672	-4.639655	0.272363

116	6	10061000	-1.827668	-4.551023	-0.682062
117	6	10061000	-2.538945	-5.690329	-1.065868
118	6	10061000	-2.234944	-6.928140	-0.494450
119	6	10061000	-1.220870	-7.025105	0.462538
120	6	10061000	-0.508279	-5.885190	0.847968
121	6	10061000	0.040539	-3.206320	2.604424
122	6	10061000	-1.103208	-3.673972	3.270852
123	6	10061000	-1.105496	-3.807346	4.662683
124	6	10061000	0.031418	-3.467159	5.400320
125	6	10061000	1.164891	-2.978031	4.747020
126	6	10061000	1.165654	-2.839590	3.356371
127	1	10011000	-2.069560	-3.600116	-1.134896
128	1	10011000	-3.326215	-5.612376	-1.804544
129	1	10011000	-2.787724	-7.810615	-0.789240
130	1	10011000	-0.993101	-7.982522	0.912885
131	1	10011000	0.247960	-5.976195	1.612596
132	1	10011000	2.046646	-2.459472	2.869205
133	1	10011000	2.043404	-2.706809	5.316902
134	1	10011000	0.030039	-3.570888	6.477546
135	1	10011000	-1.987637	-4.177528	5.168645
136	1	10011000	-1.984020	-3.960671	2.715299
137	1	10011000	5.859905	1.863283	-1.030712
138	1	10011000	7.352934	2.628738	-2.843175
139	1	10011000	6.869765	2.018033	-5.197031
140	1	10011000	4.881405	0.640370	-5.736385
141	1	10011000	3.383037	-0.126133	-3.952320
142	1	10011000	2.236970	-4.886480	1.861702
143	1	10011000	4.237823	-5.771108	0.931287
144	1	10011000	5.956808	-5.934159	-0.895252
145	1	10011000	6.751354	-5.201573	-3.050237
146	1	10011000	5.566322	-3.476862	-4.337673
147	1	10011000	3.574290	-2.430738	-3.501751
148	1	10011000	0.852963	-4.570773	-2.398037
149	1	10011000	-0.629276	-5.256297	-4.152102
150	1	10011000	-1.783928	-3.622847	-5.575447
151	1	10011000	-1.512098	-1.245655	-5.241689
152	1	10011000	-0.425381	0.706997	-3.956044
153	1	10011000	1.296570	1.503293	-2.483608
154	1	10011000	6.626689	-3.238011	2.207932
155	1	10011000	7.344829	-2.697614	-0.102237
156	1	10011000	5.971979	-1.231140	-1.516827
157	1	10011000	3.147253	-0.774870	1.705672
158	1	10011000	4.529877	-2.277132	3.109626
159	6	10061000	2.434726	3.880173	2.877671
160	1	10011000	2.111238	4.832345	3.305158
161	6	10061000	3.092984	5.094703	0.948268
162	6	10061000	3.587556	5.126875	-0.383940
163	8	10081000	3.788313	4.131001	-1.166232
164	6	10061000	2.471466	2.747020	3.792606
165	6	10061000	3.361421	1.640255	3.654866
166	6	10061000	1.667919	2.787681	4.963386
167	6	10061000	3.413733	0.625006	4.612690
168	1	10011000	4.055556	1.612073	2.820133
169	6	10061000	1.713533	1.775204	5.935106
170	1	10011000	0.996400	3.630996	5.113221
171	6	10061000	2.586192	0.679495	5.756345
172	1	10011000	4.113983	-0.200078	4.524255
173	1	10011000	1.079410	1.849844	6.812893
174	7	10071000	2.856949	3.908853	1.608115
175	1	10011000	3.002919	6.029340	1.491743
176	8	10081003	2.710708	-0.392549	6.639045
177	8	10081003	3.863820	6.428604	-0.802218
178	6	10061003	1.904082	-0.401468	7.853005
179	1	10011000	2.177168	-1.321434	8.372962
180	1	10011000	2.133063	0.463948	8.488833
181	1	10011000	0.830825	-0.413629	7.615705
182	6	10061003	4.501616	6.593889	-2.113395
183	1	10011000	5.581743	6.428767	-2.023499
184	1	10011000	4.088952	5.887240	-2.838872
185	1	10011000	4.298538	7.626285	-2.404856

[(S_a)-Binap Au]$_2$-**I-b**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	10061002	1.564350	-2.083639	0.427410
2	6	10061002	0.424275	-1.404476	1.112495
3	6	10061002	0.596116	-0.740937	2.265251
4	6	10061000	1.928749	-0.657853	2.878570
5	6	10061002	2.129218	-0.034029	4.203152
6	6	10061000	3.370699	0.107496	4.697936
7	6	10061000	4.496726	-0.324584	3.982319
8	6	10061002	4.380253	-0.928824	2.786598
9	6	10061000	3.035903	-1.156214	2.190891
10	6	10061002	2.831930	-1.890406	0.907681
11	6	10061002	4.027642	-2.391919	0.180367
12	6	10061000	4.505947	-1.753933	-0.922896
13	6	10061000	5.568495	-2.309414	-1.668273
14	6	10061002	6.178100	-3.449719	-1.308876
15	6	10061000	5.782499	-4.133842	-0.067778
16	6	10061000	4.737354	-3.604346	0.688623
17	6	10061002	4.402528	-4.271720	1.974702
18	6	10061000	5.082562	-5.365328	2.364271
19	6	10061000	6.117322	-5.904048	1.583508
20	6	10061002	6.480456	-5.344103	0.416153
21	6	10061000	2.711244	-6.503415	0.129985
22	6	10061000	3.453177	-6.952369	-0.964269
23	6	10061000	3.540808	-6.167414	-2.115632
24	6	10061000	2.881812	-4.936252	-2.175493
25	6	10061000	2.140424	-4.471641	-1.079515
26	6	10061000	2.062782	-5.265551	0.078248
27	15	10151003	1.256395	-2.857915	-1.244587
28	6	10061000	-0.437782	-3.580374	-1.098330
29	6	10061000	-0.956622	-4.099480	0.103001
30	6	10061000	-2.155814	-4.817360	0.100365
31	6	10061000	-2.861424	-5.002190	-1.089598
32	6	10061000	-2.374665	-4.458014	-2.279369
33	6	10061000	-1.164933	-3.758427	-2.284701
34	15	10151003	3.896777	-0.082705	-1.397671
35	6	10061000	5.331464	0.947851	-0.919291
36	6	10061000	5.246952	1.700091	0.258541
37	6	10061000	6.323606	2.489922	0.670826
38	6	10061000	7.495389	2.525228	-0.089336
39	6	10061000	7.592696	1.765388	-1.258428
40	6	10061000	6.517128	0.973041	-1.671309
41	6	10061000	3.827774	-0.002605	-3.224484
42	6	10061000	3.421570	-1.122933	-3.962196
43	6	10061000	3.402280	-1.079530	-5.359105
44	6	10061000	3.783750	0.086461	-6.027898
45	6	10061000	4.170783	1.213889	-5.298924
46	6	10061000	4.174979	1.177088	-3.901352
47	1	10011000	4.348586	1.665255	0.860037
48	1	10011000	6.252169	3.070334	1.581338
49	1	10011000	8.329219	3.136932	0.229750
50	1	10011000	8.502002	1.790145	-1.844840
51	1	10011000	6.609248	0.397908	-2.581346
52	1	10011000	4.459983	2.064330	-3.352597
53	1	10011000	4.454041	2.121311	-5.816226
54	1	10011000	3.771361	0.119129	-7.109520
55	1	10011000	3.093990	-1.950489	-5.922686
56	1	10011000	3.129463	-2.030953	-3.458273
57	1	10011000	-0.438693	-3.973238	1.040754
58	1	10011000	-2.532909	-5.242234	1.020549
59	1	10011000	-3.791559	-5.555593	-1.087254
60	1	10011000	-2.925165	-4.594430	-3.201103
61	1	10011000	-0.776761	-3.383147	-3.223008
62	1	10011000	5.914391	-1.812640	-2.563440
63	1	10011000	6.987879	-3.845370	-1.914277
64	1	10011000	7.286558	-5.779211	-0.166522
65	1	10011000	6.634327	-6.789421	1.930932
66	1	10011000	4.821660	-5.846660	3.298177
67	1	10011000	3.600640	-3.896635	2.601473
68	1	10011000	5.278252	-1.245210	2.266453
69	1	10011000	5.481094	-0.172964	4.406638
70	1	10011000	3.506604	0.571212	5.666583
71	1	10011000	1.274286	0.304621	4.779490
72	1	10011000	-0.241649	-0.237895	2.733526
73	1	10011000	-0.562901	-1.417456	0.665764
74	1	10011000	3.965131	-7.904629	-0.917368
75	1	10011000	2.657054	-7.104294	1.028492
76	1	10011000	1.546050	-4.919321	0.957997
77	1	10011000	2.944605	-4.349693	-3.081503
78	1	10011000	4.115747	-6.514700	-2.964152
79	79	10791004	-3.345745	-1.256329	1.317588
80	79	10791004	1.972035	0.983592	-0.238912

81	6	10061000	−1.844094	1.098259	−0.892981
82	6	10061002	−1.503826	−0.077765	−1.732578
83	6	10061002	−0.646619	0.012541	−2.757680
84	6	10061000	−0.030497	1.304393	−3.100767
85	6	10061002	0.741758	1.466399	−4.351306
86	6	10061000	1.213882	2.675416	−4.699396
87	6	10061000	1.008062	3.801612	−3.891796
88	6	10061002	0.316569	3.724366	−2.742006
89	6	10061000	−0.248552	2.423629	−2.290246
90	6	10061000	−1.127298	2.308780	−1.092996
91	6	10061002	−1.327121	3.512078	−0.256888
92	6	10061002	−0.431085	3.879707	0.701052
93	6	10061002	−0.732874	5.080917	1.535452
94	6	10061000	−1.786817	5.867561	1.275809
95	6	10061000	−2.636236	5.595829	0.202331
96	6	10061000	−2.432099	4.458861	−0.593949
97	6	10061002	−3.314017	4.273154	−1.774495
98	6	10061000	−4.323227	5.129190	−2.009513
99	6	10061000	−4.559962	6.230579	−1.174509
100	6	10061002	−3.773624	6.490695	−0.115792
101	6	10061000	−4.749462	4.101408	2.310491
102	6	10061000	−3.978486	4.065148	3.473956
103	6	10061000	−2.995535	3.085549	3.627604
104	6	10061000	−2.771443	2.151282	2.610935
105	6	10061000	−3.521389	2.195145	1.430196
106	6	10061000	−4.531085	3.164978	1.295603
107	15	10151003	−3.309051	0.844931	0.212243
108	6	10061000	−4.793247	0.907837	−0.863755
109	6	10061000	−6.053116	0.698795	−0.281556
110	6	10061000	−7.210434	0.742180	−1.063762
111	6	10061000	−7.117125	0.979257	−2.436957
112	6	10061000	−5.865030	1.158201	−3.030405
113	6	10061000	−4.705034	1.113302	−2.250536
114	15	10151003	1.240095	3.094699	0.872387
115	6	10061000	2.320022	4.339172	0.067958
116	6	10061000	3.069879	3.959364	−1.053724
117	6	10061000	3.918686	4.874903	−1.680797
118	6	10061000	4.027527	6.177231	−1.187899
119	6	10061000	3.289924	6.562472	−0.065289
120	6	10061000	2.440377	5.647300	0.563907
121	6	10061000	1.742209	3.201223	2.633651
122	6	10061000	3.080030	3.447622	2.982492
123	6	10061000	3.449471	3.566217	4.325587
124	6	10061000	2.487564	3.433926	5.330209
125	6	10061000	1.158738	3.167880	4.991638
126	6	10061000	0.792214	3.038407	3.649020
127	1	10011000	2.989705	2.957449	−1.451103
128	1	10011000	4.490922	4.574799	−2.548960
129	1	10011000	4.685969	6.886216	−1.672713
130	1	10011000	3.382323	7.568686	0.322484
131	1	10011000	1.904599	5.956846	1.447715
132	1	10011000	−0.230722	2.821197	3.399926
133	1	10011000	0.414520	3.051310	5.768682
134	1	10011000	2.773575	3.526447	6.369792
135	1	10011000	4.481034	3.762966	4.587065
136	1	10011000	3.835413	3.568536	2.220043
137	1	10011000	−6.137980	0.508921	0.781091
138	1	10011000	−8.178600	0.585099	−0.606396
139	1	10011000	−8.013149	1.007343	−3.043309
140	1	10011000	−5.792430	1.323392	−4.097460
141	1	10011000	−3.750537	1.233116	−2.739300
142	1	10011000	−0.094292	5.336529	2.372406
143	1	10011000	−1.966125	6.733815	1.901012
144	1	10011000	−3.977553	7.358391	0.504727
145	1	10011000	−5.386570	6.893266	−1.397159
146	1	10011000	−4.962521	4.971514	−2.868963
147	1	10011000	−3.140508	3.460272	−2.467203
148	1	10011000	0.172721	4.625860	−2.155604
149	1	10011000	1.410912	4.756285	−4.205422
150	1	10011000	1.763806	2.784973	−5.625022
151	1	10011000	0.909930	0.613540	−5.001260
152	1	10011000	−0.440878	−0.862534	−3.365824
153	1	10011000	−1.985836	−1.029765	−1.533930
154	1	10011000	−4.148588	4.789818	4.259413
155	1	10011000	−5.515123	4.857137	2.192642
156	1	10011000	−5.139128	3.218671	0.404388
157	1	10011000	−2.031098	1.376264	2.753038
158	1	10011000	−2.414646	3.043757	4.539748
159	6	10061000	−5.399567	−3.569940	1.385362
160	1	10011000	−5.955066	−4.338177	1.930776

161	6	10061000	-3.734366	-3.680024	3.081570
162	6	10061000	-2.564385	-3.116967	3.628993
163	8	10081000	-1.966378	-2.053971	3.203471
164	6	10061000	-5.964709	-3.166467	0.099972
165	6	10061000	-5.203038	-2.642260	-0.984248
166	6	10061000	-7.349870	-3.374065	-0.127071
167	6	10061000	-5.795670	-2.326208	-2.208071
168	1	10011000	-4.130511	-2.520520	-0.873730
169	6	10061000	-7.963577	-3.041257	-1.345104
170	1	10011000	-7.959664	-3.790414	0.672397
171	6	10061000	-7.183905	-2.508785	-2.394204
172	1	10011000	-5.207998	-1.955623	-3.043224
173	1	10011000	-9.029774	-3.203450	-1.466170
174	7	10071000	-4.280816	-3.118581	1.946756
175	1	10011000	-4.166109	-4.575332	3.515673
176	8	10081003	-7.674413	-2.140915	-3.644486
177	8	10081003	-2.044209	-3.816656	4.713941
178	6	10061003	-9.102185	-2.281361	-3.908934
179	1	10011000	-9.241594	-1.924257	-4.930708
180	1	10011000	-9.417609	-3.330866	-3.837573
181	1	10011000	-9.693945	-1.666728	-3.216765
182	6	10061003	-0.812495	-3.286313	5.305998
183	1	10011000	-0.594211	-3.953246	6.142211
184	1	10011000	0.004610	-3.299872	4.575073
185	1	10011000	-0.960292	-2.258676	5.655554

[(S_a)-Binap-(R_a)-Binap-Au_2]-**I**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	10061000	-2.232152	-0.995464	0.579621
2	6	10061000	-0.925945	-1.271079	1.214214
3	6	10061000	-0.623922	-0.821435	2.494462
4	6	10061000	-1.548933	-0.093897	3.239122
5	6	10061000	-1.246605	0.347786	4.532437
6	6	10061000	-2.200262	1.021237	5.302912
7	6	10061000	-3.492437	1.262402	4.825379
8	6	10061000	-3.870941	0.866438	3.543889
9	6	10061002	-2.882916	0.200838	2.666282
10	6	10061000	-3.187061	-0.210098	1.269174
11	6	10061000	-4.443678	0.252402	0.637784
12	6	10061000	-4.501787	1.467534	-0.075779
13	6	10061000	-5.736122	1.800585	-0.828451
14	6	10061000	-6.875712	1.001795	-0.756386
15	6	10061000	-6.908638	-0.128259	0.059595
16	6	10061002	-5.702928	-0.511723	0.829645
17	6	10061000	-5.847296	-1.591136	1.829010
18	6	10061000	-7.045337	-2.299162	1.903609
19	6	10061000	-8.128556	-1.970946	1.081809
20	6	10061000	-8.071463	-0.897174	0.186182
21	6	10061000	-4.687066	5.973557	-1.954869
22	6	10061000	-3.757482	6.178502	-2.978042
23	6	10061000	-2.656816	5.327204	-3.101350
24	6	10061000	-2.488811	4.268068	-2.205506
25	6	10061000	-3.424846	4.045007	-1.186862
26	6	10061000	-4.518950	4.915696	-1.055822
27	15	10151003	-3.118520	2.680351	-0.009579
28	6	10061000	-3.221369	3.480938	1.624698
29	6	10061000	-4.456410	3.801475	2.208023
30	6	10061000	-4.499471	4.408316	3.467295
31	6	10061000	-3.312516	4.689938	4.150723
32	6	10061000	-2.080833	4.363139	3.576307
33	6	10061000	-2.035614	3.761035	2.316100
34	15	10151003	-2.513510	-1.842528	-1.029507
35	6	10061000	-3.775110	-3.136888	-0.751538
36	6	10061000	-4.408751	-3.744623	-1.846500
37	6	10061000	-5.304147	-4.799877	-1.648165
38	6	10061000	-5.533462	-5.289761	-0.360231
39	6	10061000	-4.850778	-4.738468	0.726213
40	6	10061000	-3.961714	-3.677732	0.529289
41	6	10061000	-3.138378	-0.594046	-2.211462
42	6	10061000	-2.223228	0.317384	-2.755169
43	6	10061000	-2.632498	1.236142	-3.725242
44	6	10061000	-3.962069	1.257160	-4.151952
45	6	10061000	-4.880468	0.350676	-3.616781

46	6	10061000	-4.472674	-0.572984	-2.648703
47	1	10011000	-4.207502	-3.405633	-2.854472
48	1	10011000	-5.807735	-5.248169	-2.494759
49	1	10011000	-6.221942	-6.110630	-0.207300
50	1	10011000	-5.003673	-5.137630	1.720494
51	1	10011000	-3.412923	-3.291311	1.377035
52	1	10011000	-5.208404	-1.241362	-2.227635
53	1	10011000	-5.912489	0.371839	-3.941993
54	1	10011000	-4.280005	1.974487	-4.897293
55	1	10011000	-1.917698	1.929339	-4.149051
56	1	10011000	-1.187993	0.303229	-2.439803
57	1	10011000	-5.383394	3.561083	1.705479
58	1	10011000	-5.453065	4.649519	3.918491
59	1	10011000	-3.347644	5.153177	5.128112
60	1	10011000	-1.161665	4.574122	4.107533
61	1	10011000	-1.077788	3.515566	1.878130
62	1	10011000	-5.761819	2.651946	-1.488781
63	1	10011000	-7.748054	1.283621	-1.333998
64	1	10011000	-8.953619	-0.653149	-0.393747
65	1	10011000	-9.044015	-2.542748	1.162794
66	1	10011000	-7.139767	-3.112450	2.611458
67	1	10011000	-5.035408	-1.844989	2.496708
68	1	10011000	-4.877877	1.064077	3.201845
69	1	10011000	-4.208545	1.769995	5.458584
70	1	10011000	-1.936824	1.349153	6.300188
71	1	10011000	-0.268206	0.161278	4.958884
72	1	10011000	0.338344	-1.067850	2.915267
73	1	10011000	-0.184474	-1.854034	0.682063
74	1	10011000	-3.887024	6.999633	-3.671064
75	1	10011000	-5.536606	6.636821	-1.856110
76	1	10011000	-5.247649	4.777003	-0.271972
77	1	10011000	-1.622668	3.626382	-2.301212
78	1	10011000	-1.929727	5.491640	-3.886098
79	79	10791004	-0.800300	1.981390	-0.308543
80	79	10791004	-0.529092	-2.873009	-1.798286
81	6	10061000	2.673824	1.345111	-1.282832
82	6	10061000	2.170294	0.839322	-2.579634
83	6	10061000	2.966604	0.090199	-3.439409
84	6	10061000	4.276144	-0.238979	-3.099214
85	6	10061000	5.077619	-0.991980	-3.965092
86	6	10061000	6.393346	-1.321885	-3.624632
87	6	10061000	6.963989	-0.910800	-2.416346
88	6	10061000	6.236766	-0.156856	-1.497720
89	6	10061002	4.834056	0.212274	-1.802574
90	6	10061000	3.980176	0.997830	-0.867130
91	6	10061000	4.545158	1.379262	0.446934
92	6	10061000	4.331345	0.579421	1.590491
93	6	10061000	5.096052	0.877805	2.829805
94	6	10061000	5.978043	1.953758	2.905552
95	6	10061000	6.211082	2.774093	1.802707
96	6	10061002	5.528617	2.490221	0.519914
97	6	10061000	5.831372	3.370324	-0.630805
98	6	10061000	6.715330	4.434253	-0.464306
99	6	10061000	7.329158	4.675494	0.769250
100	6	10061000	7.088734	3.861742	1.882088
101	6	10061000	3.369927	4.617383	2.623400
102	6	10061000	2.807903	4.027803	3.758245
103	6	10061000	1.899122	2.975999	3.620287
104	6	10061000	1.573644	2.493049	2.349059
105	6	10061000	2.145703	3.068635	1.207531
106	6	10061000	3.025490	4.153761	1.350619
107	15	10151003	1.560624	2.535980	-0.436011
108	6	10061000	1.597224	4.074608	-1.424763
109	6	10061000	0.697707	5.100057	-1.100281
110	6	10061000	0.682589	6.285649	-1.839856
111	6	10061000	1.571064	6.456721	-2.904391
112	6	10061000	2.475910	5.442190	-3.228982
113	6	10061000	2.490670	4.252904	-2.493687
114	15	10151003	3.125735	-0.835948	1.495493
115	6	10061000	4.289016	-2.007717	0.681632
116	6	10061000	3.892007	-2.637270	-0.503469
117	6	10061000	4.762919	-3.508497	-1.164885
118	6	10061000	6.032697	-3.761300	-0.640351
119	6	10061000	6.438155	-3.133545	0.540209
120	6	10061000	5.573543	-2.253975	1.197892
121	6	10061000	3.126561	-1.512827	3.220404
122	6	10061000	3.403963	-2.867608	3.485215
123	6	10061000	3.311957	-3.368195	4.787313
124	6	10061000	2.902321	-2.536521	5.830986
125	6	10061000	2.575417	-1.204591	5.571744

126	6	10061000	2.674114	-0.701095	4.272264
127	1	10011000	2.918060	-2.429544	-0.925974
128	1	10011000	4.460142	-3.978686	-2.090264
129	1	10011000	6.706206	-4.434195	-1.154725
130	1	10011000	7.424692	-3.323531	0.942345
131	1	10011000	5.902359	-1.774187	2.109643
132	1	10011000	2.397846	0.323210	4.083354
133	1	10011000	2.236567	-0.563752	6.375409
134	1	10011000	2.822599	-2.928401	6.836655
135	1	10011000	3.541719	-4.407340	4.984139
136	1	10011000	3.670601	-3.551258	2.693041
137	1	10011000	0.001986	4.976549	-0.279322
138	1	10011000	-0.019931	7.069961	-1.589380
139	1	10011000	1.559095	7.375050	-3.476922
140	1	10011000	3.165981	5.576950	-4.051816
141	1	10011000	3.201468	3.485509	-2.762375
142	1	10011000	5.021550	0.240893	3.695616
143	1	10011000	6.498283	2.135880	3.838513
144	1	10011000	7.594585	4.088246	2.813154
145	1	10011000	8.011050	5.510733	0.864151
146	1	10011000	6.930026	5.084066	-1.302849
147	1	10011000	5.369931	3.207780	-1.594903
148	1	10011000	6.703715	0.132776	-0.566229
149	1	10011000	7.984510	-1.188899	-2.187073
150	1	10011000	6.985233	-1.909602	-4.314373
151	1	10011000	4.685725	-1.328467	-4.917148
152	1	10011000	2.554350	-0.223647	-4.390295
153	1	10011000	1.165190	1.090406	-2.893771
154	1	10011000	3.066386	4.394246	4.743096
155	1	10011000	4.064604	5.440528	2.728796
156	1	10011000	3.450166	4.638975	0.482411
157	1	10011000	0.859432	1.686056	2.252774
158	1	10011000	1.442807	2.538082	4.498609
159	7	10071000	1.135359	-4.190522	-2.103383
160	6	10061000	1.564375	-5.039611	-1.178108
161	6	10061000	1.757183	-4.046706	-3.334308
162	1	10011000	2.489134	-5.582888	-1.392675
163	1	10011000	2.543832	-4.747125	-3.589776
164	6	10061000	0.990051	-5.254415	0.153653
165	6	10061000	1.872578	-5.533993	1.226816
166	6	10061000	-0.402490	-5.223940	0.445859
167	6	10061000	1.412712	-5.700689	2.544392
168	1	10011000	2.941001	-5.602125	1.029077
169	6	10061000	-0.873999	-5.388410	1.751310
170	1	10011000	-1.114666	-5.118152	-0.366754
171	6	10061000	0.031160	-5.604854	2.813323
172	1	10011000	2.125156	-5.907024	3.336697
173	1	10011000	-1.936523	-5.393775	1.975809
174	8	10081000	-0.545599	-5.732482	4.076198
175	6	10061003	0.311573	-6.040520	5.214665
176	1	10011000	-0.363925	-6.131254	6.067101
177	1	10011000	0.846524	-6.987881	5.064968
178	1	10011000	1.032271	-5.232178	5.399224
179	6	10061000	1.384071	-2.980733	-4.188486
180	8	10081000	0.479458	-2.102322	-3.930174
181	8	10081003	2.032305	-2.815046	-5.416795
182	6	10061003	3.047571	-3.770325	-5.856353
183	1	10011000	2.627289	-4.779756	-5.953848
184	1	10011000	3.370620	-3.409581	-6.834813
185	1	10011000	3.904627	-3.789338	-5.169138

(*S*, *S*, *S*, *R*)-**II**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	10061000	-1.031173	2.381041	-0.221093
2	6	10061002	0.178792	1.533083	-0.060719
3	6	10061002	0.461970	0.932534	1.105556
4	6	10061000	-0.424781	1.094250	2.269634
5	6	10061002	-0.097150	0.472647	3.567229
6	6	10061000	-0.906575	0.648531	4.624834
7	6	10061000	-2.098809	1.377646	4.518893
8	6	10061002	-2.470228	1.949795	3.360610
9	6	10061000	-1.598642	1.840639	2.159859
10	6	10061000	-1.933249	2.483477	0.865686

11	6	10061002	-3.219330	3.205715	0.731667
12	6	10061000	-4.288348	2.637560	0.110638
13	6	10061000	-5.467392	3.381791	-0.111243
14	6	10061002	-5.599188	4.655193	0.291805
15	6	10061000	-4.512804	5.303237	1.043614
16	6	10061000	-3.344520	4.583551	1.292281
17	6	10061002	-2.297891	5.224624	2.130791
18	6	10061000	-2.478453	6.474073	2.596324
19	6	10061000	-3.645495	7.201712	2.314627
20	6	10061002	-4.639658	6.676216	1.577283
21	6	10061000	-1.029847	6.873982	-0.489790
22	6	10061000	-2.053251	7.556917	-1.150420
23	6	10061000	-2.902541	6.868748	-2.019454
24	6	10061000	-2.724019	5.499281	-2.234282
25	6	10061000	-1.699679	4.804288	-1.576113
26	6	10061000	-0.857933	5.500977	-0.691498
27	15	10151003	-1.527234	2.998288	-1.904312
28	6	10061000	0.047370	3.080901	-2.861930
29	6	10061000	1.253221	3.575958	-2.333422
30	6	10061000	2.375908	3.715524	-3.154804
31	6	10061000	2.320143	3.331984	-4.495450
32	6	10061000	1.129776	2.834432	-5.026806
33	6	10061000	-0.005069	2.727910	-4.218604
34	15	10151003	-4.289653	0.861584	-0.375629
35	6	10061000	-5.623348	0.211410	0.695743
36	6	10061000	-5.265686	-0.367844	1.919407
37	6	10061000	-6.245793	-0.895232	2.764428
38	6	10061000	-7.591945	-0.836261	2.394878
39	6	10061000	-7.958507	-0.242122	1.183939
40	6	10061000	-6.979246	0.286004	0.336838
41	6	10061000	-4.941150	0.738355	-2.082839
42	6	10061000	-4.820510	1.813628	-2.976060
43	6	10061000	-5.354323	1.724938	-4.264666
44	6	10061000	-6.023627	0.566731	-4.666639
45	6	10061000	-6.149248	-0.507837	-3.783262
46	6	10061000	-5.592471	-0.431406	-2.502940
47	1	10011000	-4.225762	-0.409914	2.215404
48	1	10011000	-5.962288	-1.347795	3.705733
49	1	10011000	-8.351021	-1.245449	3.048827
50	1	10011000	-9.002059	-0.190539	0.901693
51	1	10011000	-7.284012	0.743980	-0.593712
52	1	10011000	-5.691598	-1.275419	-1.834322
53	1	10011000	-6.668244	-1.405068	-4.094145
54	1	10011000	-6.444539	0.501873	-5.661527
55	1	10011000	-5.258019	2.558759	-4.947920
56	1	10011000	-4.327399	2.725390	-2.677161
57	1	10011000	1.341646	3.847006	-1.294672
58	1	10011000	3.287633	4.134007	-2.756456
59	1	10011000	3.194839	3.433602	-5.124765
60	1	10011000	1.079519	2.551871	-6.070314
61	1	10011000	-0.933645	2.387108	-4.657337
62	1	10011000	-6.299416	2.925563	-0.629235
63	1	10011000	-6.520683	5.193891	0.092950
64	1	10011000	-5.534499	7.258390	1.379600
65	1	10011000	-3.747439	8.206885	2.703401
66	1	10011000	-1.703577	6.932767	3.197199
67	1	10011000	-1.377153	4.700269	2.363700
68	1	10011000	-3.407219	2.495132	3.318629
69	1	10011000	-2.736677	1.474758	5.388183
70	1	10011000	-0.643166	0.203143	5.574891
71	1	10011000	0.794731	-0.133704	3.662682
72	1	10011000	1.342710	0.307808	1.193625
73	1	10011000	0.836763	1.360832	-0.899670
74	1	10011000	-2.193876	8.616562	-0.981631
75	1	10011000	-0.385445	7.403250	0.200096
76	1	10011000	-0.103276	4.987094	-0.117098
77	1	10011000	-3.385708	4.980509	-2.915417
78	1	10011000	-3.699041	7.396380	-2.527758
79	79	10791004	3.120795	0.403785	-0.465720
80	79	10791004	-2.379156	-0.631733	0.154060
81	6	10061000	0.583394	-1.726686	-1.952208
82	6	10061002	0.119355	-0.626901	-2.835283
83	6	10061002	-1.068983	-0.669886	-3.451203
84	6	10061000	-1.956485	-1.828528	-3.278788
85	6	10061002	-3.169283	-1.981798	-4.110125
86	6	10061000	-3.933845	-3.080333	-3.990581
87	6	10061000	-3.611681	-4.099804	-3.085282
88	6	10061002	-2.517316	-4.028939	-2.308320
89	6	10061000	-1.615953	-2.845353	-2.382568
90	6	10061000	-0.327283	-2.771642	-1.636803

91	6	10061002	0.012101	-3.900540	-0.747659
92	6	10061002	-0.477915	-3.988098	0.520405
93	6	10061002	-0.129733	-5.190088	1.336884
94	6	10061000	0.564551	-6.213289	0.819842
95	6	10061000	0.977462	-6.198807	-0.512588
96	6	10061000	0.707387	-5.089549	-1.327311
97	6	10061002	1.109633	-5.164713	-2.756525
98	6	10061000	1.763375	-6.243186	-3.221474
99	6	10061000	2.068300	-7.330850	-2.390711
100	6	10061002	1.706178	-7.349101	-1.096514
101	6	10061000	4.128025	-5.073931	-0.024193
102	6	10061000	3.879912	-4.975110	1.346560
103	6	10061000	3.160819	-3.888315	1.848139
104	6	10061000	2.679425	-2.904749	0.978190
105	6	10061000	2.895447	-3.011913	-0.401097
106	6	10061000	3.647057	-4.092720	-0.896165
107	15	10151003	2.374881	-1.623664	-1.474467
108	6	10061000	3.332457	-1.841321	-3.023784
109	6	10061000	4.723853	-1.669720	-2.978248
110	6	10061000	5.493292	-1.816590	-4.135637
111	6	10061000	4.878096	-2.137368	-5.347897
112	6	10061000	3.492938	-2.310776	-5.402983
113	6	10061000	2.720085	-2.162223	-4.247329
114	15	10151003	-1.713919	-2.789039	1.209175
115	6	10061000	-3.272359	-3.745292	1.086931
116	6	10061000	-4.306287	-3.246791	0.283387
117	6	10061000	-5.519319	-3.932292	0.183421
118	6	10061000	-5.709119	-5.121455	0.891004
119	6	10061000	-4.686811	-5.621705	1.702122
120	6	10061000	-3.472475	-4.935571	1.804142
121	6	10061000	-1.463441	-2.676353	3.023492
122	6	10061000	-2.558580	-2.454966	3.873742
123	6	10061000	-2.382717	-2.425565	5.260477
124	6	10061000	-1.110959	-2.610845	5.808647
125	6	10061000	-0.012754	-2.808777	4.968766
126	6	10061000	-0.187208	-2.830831	3.582329
127	1	10011000	-4.169204	-2.332680	-0.275342
128	1	10011000	-6.310922	-3.541440	-0.442733
129	1	10011000	-6.649072	-5.652429	0.814809
130	1	10011000	-4.838494	-6.537260	2.258972
131	1	10011000	-2.709493	-5.321923	2.461822
132	1	10011000	0.669957	-2.978977	2.949294
133	1	10011000	0.973691	-2.944979	5.390870
134	1	10011000	-0.974735	-2.589619	6.882041
135	1	10011000	-3.233237	-2.263551	5.909751
136	1	10011000	-3.552205	-2.330472	3.468597
137	1	10011000	5.212356	-1.423780	-2.043545
138	1	10011000	6.566303	-1.681978	-4.092270
139	1	10011000	5.474187	-2.251904	-6.243946
140	1	10011000	3.017031	-2.560161	-6.342558
141	1	10011000	1.653249	-2.303696	-4.321593
142	1	10011000	-0.439383	-5.254824	2.372348
143	1	10011000	0.791038	-7.067503	1.446365
144	1	10011000	1.951739	-8.210307	-0.482014
145	1	10011000	2.599996	-8.178048	-2.804835
146	1	10011000	2.058320	-6.275847	-4.262629
147	1	10011000	0.877481	-4.355929	-3.437943
148	1	10011000	-2.303506	-4.849403	-1.631484
149	1	10011000	-4.256233	-4.966889	-3.015957
150	1	10011000	-4.817530	-3.182504	-4.607169
151	1	10011000	-3.438635	-1.211262	-4.826085
152	1	10011000	-1.360564	0.131279	-4.119811
153	1	10011000	0.780745	0.210173	-3.031719
154	1	10011000	4.250001	-5.736789	2.020260
155	1	10011000	4.689745	-5.913446	-0.412651
156	1	10011000	3.850676	-4.194768	-1.952362
157	1	10011000	2.151801	-2.049345	1.378326
158	1	10011000	2.984397	-3.805059	2.912364
159	6	10061003	4.009685	2.471787	1.745570
160	6	10061003	4.840433	2.941960	-0.399921
161	6	10061000	5.303434	2.495537	-1.782409
162	8	10081002	5.056604	1.413912	-2.343030
163	6	10061000	3.705010	1.454686	2.835274
164	6	10061000	4.157120	0.116584	2.773837
165	6	10061000	3.041289	1.874980	4.001771
166	6	10061000	3.936935	-0.769452	3.834987
167	1	10011000	4.697719	-0.220741	1.893995
168	6	10061000	2.831453	1.007005	5.090168
169	1	10011000	2.698975	2.905840	4.079871
170	6	10061000	3.273976	-0.327912	4.999104

171	1	10011000	4.296279	-1.793661	3.802004
172	1	10011000	2.331880	1.375410	5.980585
173	7	10071003	4.115513	1.940638	0.378747
174	8	10081003	3.096634	-1.291787	5.996372
175	8	10081000	6.001787	3.510001	-2.388191
176	6	10061003	2.490755	-0.884479	7.256737
177	1	10011000	2.486718	-1.781611	7.878823
178	1	10011000	3.080839	-0.098036	7.745722
179	1	10011000	1.459180	-0.532804	7.108261
180	6	10061003	6.645319	3.203139	-3.679495
181	1	10011000	7.391512	2.417613	-3.529791
182	1	10011000	5.896480	2.875295	-4.407432
183	1	10011000	7.114506	4.137556	-3.988890
184	1	10011000	3.239752	3.268039	1.809369
185	1	10011000	4.255156	3.870901	-0.565176
186	6	10061003	6.015014	3.339321	0.542483
187	6	10061003	5.405582	3.254696	1.961962
188	1	10011000	6.432380	4.317263	0.283842
189	1	10011000	5.216177	4.220639	2.436553
190	7	10071000	7.364622	1.913851	1.885081
191	6	10061003	8.450661	1.018635	2.297189
192	1	10011000	8.425464	0.939890	3.386868
193	1	10011000	8.318148	0.029164	1.846841
194	1	10011000	9.416082	1.420846	1.973671
195	6	10061002	6.442571	2.494827	2.783387
196	8	10081002	6.508476	2.384741	4.019496
197	6	10061002	7.146293	2.300798	0.558007
198	8	10081002	7.796345	1.874278	-0.415554

(*R*, *R, R,* S)-**II**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	10061002	1.792542	-2.170521	0.223949
2	6	10061002	0.607857	-1.533441	0.872692
3	6	10061002	0.676703	-1.029932	2.113630
4	6	10061000	1.947966	-1.055442	2.851146
5	6	10061002	2.035101	-0.592680	4.251938
6	6	10061000	3.227240	-0.544905	4.870705
7	6	10061000	4.407509	-0.924129	4.214976
8	6	10061002	4.392775	-1.383555	2.951301
9	6	10061000	3.106332	-1.502579	2.213521
10	6	10061002	3.010767	-2.084563	0.842724
11	6	10061002	4.253924	-2.578284	0.192968
12	6	10061000	4.871584	-1.869285	-0.791073
13	6	10061000	5.974595	-2.414361	-1.483631
14	6	10061002	6.489714	-3.615904	-1.181242
15	6	10061000	5.941452	-4.386566	-0.054514
16	6	10061000	4.852519	-3.870113	0.647439
17	6	10061002	4.359406	-4.634084	1.824394
18	6	10061000	4.944794	-5.795687	2.168330
19	6	10061000	6.026024	-6.317447	1.440945
20	6	10061002	6.529893	-5.673618	0.373462
21	6	10061000	2.823652	-6.582053	-0.450090
22	6	10061000	3.638107	-6.949481	-1.522870
23	6	10061000	3.851860	-6.054892	-2.573225
24	6	10061000	3.246526	-4.795222	-2.554232
25	6	10061000	2.433285	-4.411926	-1.477856
26	6	10061000	2.228436	-5.316983	-0.421506
27	15	10151003	1.625561	-2.751323	-1.543678
28	6	10061000	-0.099692	-3.405735	-1.631590
29	6	10061000	-0.738816	-4.044308	-0.551967
30	6	10061000	-1.961185	-4.694468	-0.740282
31	6	10061000	-2.568772	-4.695809	-1.996619
32	6	10061000	-0.729889	-3.397052	-2.884552
33	15	10151003	4.404592	-0.126083	-1.149455
34	6	10061000	5.833154	0.759107	-0.424232
35	6	10061000	5.662636	1.401598	0.808290
36	6	10061000	6.729311	2.078632	1.405553
37	6	10061000	7.976818	2.109213	0.777209
38	6	10061000	8.159174	1.456823	-0.445333
39	6	10061000	7.093455	0.777465	-1.043550
40	6	10061000	4.534535	0.138781	-2.955040
41	6	10061000	4.143331	-0.872563	-3.842850
42	6	10061000	4.283320	-0.694720	-5.222132

43	6	10061000	4.809885	0.498529	−5.723506
44	6	10061000	5.181902	1.520015	−4.845700
45	6	10061000	5.027741	1.349496	−3.466588
46	1	10011000	4.704002	1.369623	1.308234
47	1	10011000	6.590863	2.575447	2.356887
48	1	10011000	8.802896	2.633821	1.239465
49	1	10011000	9.126811	1.477758	−0.929743
50	1	10011000	7.252813	0.285523	−1.992186
51	1	10011000	5.304136	2.157285	−2.802705
52	1	10011000	5.576704	2.449787	−5.234230
53	1	10011000	4.920393	0.635391	−6.791300
54	1	10011000	3.985794	−1.482683	−5.901673
55	1	10011000	3.740909	−1.800610	−3.468254
56	1	10011000	−0.300157	−4.057764	0.432954
57	1	10011000	−2.434521	−5.204567	0.087977
58	1	10011000	−3.517222	−5.197555	−2.138607
59	1	10011000	−0.250184	−2.924214	−3.732160
60	1	10011000	6.431759	−1.858084	−2.289389
61	1	10011000	7.335365	−4.000097	−1.743469
62	1	10011000	7.368654	−6.097960	−0.169728
63	1	10011000	6.463460	−7.258844	1.747993
64	1	10011000	4.569178	−6.346009	3.021558
65	1	10011000	3.516844	−4.274961	2.405245
66	1	10011000	5.329600	−1.663821	2.481094
67	1	10011000	5.350387	−0.850107	4.741742
68	1	10011000	3.280364	−0.198577	5.894926
69	1	10011000	1.136640	−0.294777	4.783024
70	1	10011000	−0.199945	−0.581099	2.566614
71	1	10011000	−0.331445	−1.459955	0.336515
72	1	10011000	4.108354	−7.924048	−1.536882
73	1	10011000	2.671617	−7.269125	0.372160
74	1	10011000	1.654789	−5.039756	0.447176
75	1	10011000	3.406290	−4.122968	−3.385594
76	1	10011000	4.482684	−6.339060	−3.405397
77	79	10791004	−3.332023	−1.101872	0.400493
78	79	10791004	2.453907	0.946597	−0.085576
79	6	10061000	−1.192540	1.369714	−1.139242
80	6	10061002	−0.789578	0.262134	−2.040710
81	6	10061002	0.174669	0.417126	−2.957810
82	6	10061000	0.854486	1.714580	−3.109939
83	6	10061002	1.754200	1.969919	−4.254887
84	6	10061000	2.304711	3.184643	−4.421531
85	6	10061000	2.057718	4.229796	−3.521504
86	6	10061002	1.245020	4.067903	−2.463463
87	6	10061000	0.586654	2.756619	−2.215876
88	6	10061000	−0.425838	2.564020	−1.142118
89	6	10061002	−0.665150	3.673488	−0.195046
90	6	10061002	0.113708	3.853847	0.906567
91	6	10061002	−0.227813	4.961339	1.848237
92	6	10061000	−1.196989	5.844336	1.568575
93	6	10061000	−1.912898	5.767256	0.372818
94	6	10061000	−1.664458	4.728742	−0.537411
95	6	10061002	−2.389893	4.755001	−1.832577
96	6	10061000	−3.316807	5.698235	−2.072476
97	6	10061000	−3.606962	6.697074	−1.131859
98	6	10061002	−2.953603	6.768221	0.040766
99	6	10061000	−4.261352	4.140697	2.127221
100	6	10061000	−3.663250	3.841657	3.352609
101	6	10061000	−2.792046	2.755751	3.455139
102	6	10061000	−2.506551	1.976703	2.329081
103	6	10061000	−3.083963	2.281080	1.090974
104	6	10061000	−3.982583	3.359241	1.002049
105	15	10151003	−2.825082	1.116615	−0.298921
106	6	10061000	−4.116432	1.507309	−1.540593
107	6	10061000	−5.464642	1.415823	−1.160940
108	6	10061000	−6.478957	1.700829	−2.078657
109	6	10061000	−6.155427	2.046260	−3.392615
110	6	10061000	−4.817706	2.094907	−3.791750
111	6	10061000	−3.800458	1.817461	−2.873512
112	15	10151003	1.708393	2.947653	1.166379
113	6	10061000	2.932214	4.201978	0.629703
114	6	10061000	3.777233	3.905185	−0.448514
115	6	10061000	4.732377	4.831238	−0.874842
116	6	10061000	4.851790	6.061208	−0.223788
117	6	10061000	4.017213	6.363547	0.855612
118	6	10061000	3.060810	5.437709	1.283846
119	6	10061000	2.007628	2.824976	2.971025
120	6	10061000	3.302308	2.971311	3.495149
121	6	10061000	3.514355	2.923303	4.876143
122	6	10061000	2.437165	2.722211	5.742984

123	6	10061000	1.150256	2.551180	5.227163
124	6	10061000	0.940768	2.587407	3.845678
125	1	10011000	3.689703	2.961717	−0.968462
126	1	10011000	5.378335	4.595578	−1.710637
127	1	10011000	5.592380	6.778294	−0.553278
128	1	10011000	4.116023	7.313225	1.365217
129	1	10011000	2.445777	5.679686	2.137036
130	1	10011000	−0.051397	2.441504	3.457261
131	1	10011000	0.316848	2.379706	5.895898
132	1	10011000	2.601484	2.686372	6.812000
133	1	10011000	4.513436	3.044813	5.274059
134	1	10011000	4.145970	3.142180	2.842558
135	1	10011000	−5.728551	1.135922	−0.148895
136	1	10011000	−7.515877	1.641698	−1.774390
137	1	10011000	−6.941303	2.259649	−4.105359
138	1	10011000	−4.568440	2.343239	−4.815200
139	1	10011000	−2.776756	1.843345	−3.214814
140	1	10011000	0.313896	5.069581	2.780313
141	1	10011000	−1.409434	6.636965	2.275695
142	1	10011000	−3.193582	7.561647	0.742520
143	1	10011000	−4.363766	7.435755	−1.363320
144	1	10011000	−3.844065	5.694570	−3.018087
145	1	10011000	−2.163442	4.029978	−2.603159
146	1	10011000	1.073966	4.908823	−1.799402
147	1	10011000	2.527398	5.191007	−3.687433
148	1	10011000	2.952508	3.362629	−5.270092
149	1	10011000	1.955292	1.182549	−4.974077
150	1	10011000	0.423741	−0.405397	−3.621076
151	1	10011000	−1.316475	−0.684982	−1.985881
152	1	10011000	−3.881851	4.445073	4.223843
153	1	10011000	−4.940730	4.979318	2.047604
154	1	10011000	−4.456389	3.616487	0.066343
155	1	10011000	−1.856624	1.118732	2.427288
156	1	10011000	−2.347529	2.509859	4.410719
157	6	10061000	−5.647391	−3.042851	0.397091
158	1	10011000	−5.868883	−4.124133	0.287956
159	6	10061000	−4.108773	−3.603175	2.004915
160	6	10061000	−2.774470	−3.469699	2.711938
161	8	10081000	−1.875056	−2.652456	2.454785
162	6	10061000	−6.105856	−2.381094	−0.896612
163	6	10061000	−5.206235	−2.237162	−1.980081
164	6	10061000	−7.449572	−2.019276	−1.112069
165	6	10061000	−5.622297	−1.734152	−3.218287
166	1	10011000	−4.173567	−2.533088	−1.847222
167	6	10061000	−7.888201	−1.516500	−2.351664
168	1	10011000	−8.172278	−2.095821	−0.307088
169	6	10061000	−6.970476	−1.369737	−3.410411
170	1	10011000	−4.929864	−1.629137	−4.048629
171	1	10011000	−8.930265	−1.237633	−2.469219
172	7	10071000	−4.200317	−2.935651	0.705328
173	1	10011000	−4.289502	−4.685962	1.893926
174	8	10081003	−7.287310	−0.868185	−4.675228
175	8	10081003	−2.669752	−4.406373	3.710804
176	6	10061003	−8.661804	−0.462129	−4.938146
177	1	10011000	−8.664473	−0.102504	−5.968884
178	1	10011000	−9.352933	−1.310427	−4.840806
179	1	10011000	−8.973305	0.346700	−4.262430
180	6	10061003	−1.504321	−4.300129	4.607220
181	1	10011000	−1.620101	−5.119861	5.316902
182	1	10011000	−0.576457	−4.401645	4.034885
183	1	10011000	−1.525641	−3.331588	5.115778
184	6	10061002	−6.387006	−2.665966	1.770134
185	6	10061002	−5.334326	−3.049855	2.852843
186	1	10011000	−7.328026	−3.218373	1.856758
187	1	10011000	−5.673150	−3.791252	3.582016
188	7	10071003	−5.819866	−0.731856	3.051341
189	6	10061002	−5.011719	−1.744798	3.582471
190	8	10081002	−4.179542	−1.575031	4.495929
191	6	10061003	−5.831581	0.647263	3.543428
192	1	10011000	−6.777843	0.866563	4.049749
193	1	10011000	−5.003487	0.761416	4.247544
194	1	10011000	−5.724778	1.343272	2.705359
195	6	10061000	−1.961789	−4.032228	−3.064735
196	1	10011000	−2.437150	−4.025145	−4.036979
197	6	10061002	−6.671942	−1.184552	2.023943
198	8	10081002	−7.519682	−0.450239	1.483395

TS1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	10061000	1.481585	-2.253307	-0.021667
2	6	10061002	0.200398	-1.599027	0.359419
3	6	10061002	0.032568	-1.031778	1.563017
4	6	10061000	1.129108	-1.027116	2.549160
5	6	10061002	0.945148	-0.449061	3.895374
6	6	10061000	1.959638	-0.442720	4.775758
7	6	10061000	3.222073	-0.947765	4.438209
8	6	10061002	3.463648	-1.478273	3.227389
9	6	10061000	2.376117	-1.558644	2.214550
10	6	10061000	2.575240	-2.164461	0.874817
11	6	10061002	3.925845	-2.639178	0.498032
12	6	10061000	4.743335	-1.893185	-0.292928
13	6	10061000	5.972588	-2.418933	-0.747839
14	6	10061002	6.410004	-3.636149	-0.389259
15	6	10061000	5.628210	-4.447092	0.557233
16	6	10061000	4.410773	-3.950697	1.021512
17	6	10061002	3.676180	-4.748739	2.038383
18	6	10061000	4.174949	-5.924565	2.461556
19	6	10061000	5.388784	-6.428320	1.967714
20	6	10061002	6.111524	-5.751647	1.057687
21	6	10061000	2.651174	-6.634553	-0.552738
22	6	10061000	3.688648	-6.978044	-1.421707
23	6	10061000	4.133654	-6.058155	-2.373122
24	6	10061000	3.536934	-4.797288	-2.460445
25	6	10061000	2.498443	-4.439156	-1.588686
26	6	10061000	2.062043	-5.368556	-0.628311
27	15	10151003	1.727784	-2.773804	-1.792285
28	6	10061000	0.066426	-3.402088	-2.295625
29	6	10061000	-0.805740	-4.067536	-1.414236
30	6	10061000	-1.970617	-4.668478	-1.896629
31	6	10061000	-2.295714	-4.582605	-3.251891
32	6	10061000	-1.454439	-3.894898	-4.127865
33	6	10061000	-0.273148	-3.318033	-3.653931
34	15	10151003	4.357093	-0.134720	-0.682946
35	6	10061000	5.608267	0.723342	0.341753
36	6	10061000	5.187317	1.337654	1.527497
37	6	10061000	6.106779	1.999534	2.345577
38	6	10061000	7.456177	2.043627	1.986144
39	6	10061000	7.886675	1.420757	0.811313
40	6	10061000	6.968114	0.757058	-0.007834
41	6	10061000	4.857981	0.175485	-2.415371
42	6	10061000	4.675465	-0.817756	-3.387508
43	6	10061000	5.110174	-0.610418	-4.699570
44	6	10061000	5.725875	0.593863	-5.050191
45	6	10061000	5.892364	1.597071	-4.091916
46	6	10061000	5.443053	1.397397	-2.783108
47	1	10011000	4.146787	1.295614	1.819342
48	1	10011000	5.774503	2.474586	3.259378
49	1	10011000	8.168401	2.556551	2.619288
50	1	10011000	8.932454	1.453367	0.534503
51	1	10011000	7.319545	0.291265	-0.917010
52	1	10011000	5.567614	2.189682	-2.057938
53	1	10011000	6.357483	2.535000	-4.366155
54	1	10011000	6.065289	0.753144	-6.065369
55	1	10011000	4.972929	-1.384750	-5.443087
56	1	10011000	4.210454	-1.756054	-3.128077
57	1	10011000	-0.596661	-4.132990	-0.358388
58	1	10011000	-2.621978	-5.202864	-1.217841
59	1	10011000	-3.199290	-5.048374	-3.622193
60	1	10011000	-1.705817	-3.828064	-5.178390
61	1	10011000	0.391230	-2.825487	-4.352365
62	1	10011000	6.594158	-1.835605	-1.411615
63	1	10011000	7.358996	-4.004163	-0.767234
64	1	10011000	7.049254	-6.161891	0.695681
65	1	10011000	5.750810	-7.381934	2.330182
66	1	10011000	3.625128	-6.500016	3.195353
67	1	10011000	2.729460	-4.400276	2.437369
68	1	10011000	4.459213	-1.846942	3.003995
69	1	10011000	4.020553	-0.903298	5.167875
70	1	10011000	1.805519	-0.021623	5.760856
71	1	10011000	-0.004789	-0.015713	4.168933
72	1	10011000	-0.910264	-0.551215	1.801234

73	1	10011000	-0.614335	-1.546827	-0.351840
74	1	10011000	4.152262	-7.953475	-1.352719
75	1	10011000	2.318406	-7.341182	0.196437
76	1	10011000	1.305877	-5.110719	0.094374
77	1	10011000	3.881369	-4.103288	-3.214790
78	1	10011000	4.938387	-6.323221	-3.046411
79	79	10791004	-3.204808	-1.013608	-0.113524
80	79	10791004	2.237662	0.954715	-0.005028
81	6	10061000	-1.066946	1.333234	-1.836997
82	6	10061002	-0.486022	0.238486	-2.653497
83	6	10061002	0.635879	0.408832	-3.365054
84	6	10061000	1.327311	1.707707	-3.363016
85	6	10061002	2.426092	1.982387	-4.313206
86	6	10061000	2.995306	3.199087	-4.351800
87	6	10061000	2.581902	4.227530	-3.494998
88	6	10061002	1.583548	4.048104	-2.613539
89	6	10061000	0.889626	2.734109	-2.519905
90	6	10061000	-0.316121	2.526901	-1.669681
91	6	10061002	-0.769412	3.652469	-0.827688
92	6	10061002	-0.229222	3.894441	0.398689
93	6	10061002	-0.737895	5.058234	1.184421
94	6	10061000	-1.622163	5.921918	0.665457
95	6	10061000	-2.094164	5.767855	-0.638800
96	6	10061000	-1.685491	4.674692	-1.417046
97	6	10061002	-2.173264	4.599757	-2.819164
98	6	10061000	-3.023667	5.527233	-3.291690
99	6	10061000	-3.460916	6.595413	-2.495310
100	6	10061002	-3.036801	6.746912	-1.228835
101	6	10061000	-5.006993	4.219543	0.141832
102	6	10061000	-4.673744	4.226971	1.498434
103	6	10061000	-3.756675	3.298587	1.996248
104	6	10061000	-3.164034	2.370315	1.135197
105	6	10061000	-3.469150	2.374311	-0.229960
106	6	10061000	-4.415900	3.290865	-0.720198
107	15	10151003	-2.801916	1.023931	-1.263564
108	6	10061000	-3.852259	0.995790	-2.764492
109	6	10061000	-5.200386	0.635439	-2.629179
110	6	10061000	-6.034641	0.580506	-3.748605
111	6	10061000	-5.527435	0.888299	-5.013178
112	6	10061000	-4.185527	1.250148	-5.157774
113	6	10061000	-3.347721	1.302157	-4.039434
114	15	10151003	1.244301	2.976851	1.047725
115	6	10061000	2.580401	4.206993	0.801660
116	6	10061000	3.624049	3.903062	-0.083187
117	6	10061000	4.669327	4.808374	-0.282407
118	6	10061000	4.681445	6.023514	0.406141
119	6	10061000	3.649474	6.331417	1.296686
120	6	10061000	2.602481	5.426539	1.497242
121	6	10061000	1.110499	2.884202	2.875506
122	6	10061000	2.266508	2.922836	3.671592
123	6	10061000	2.165853	2.902934	5.065926
124	6	10061000	0.910976	2.832230	5.676183
125	6	10061000	-0.242908	2.777853	4.891489
126	6	10061000	-0.142428	2.794653	3.497506
127	1	10011000	3.623887	2.969875	-0.628494
128	1	10011000	5.469032	4.568075	-0.970811
129	1	10011000	5.491870	6.724249	0.253101
130	1	10011000	3.664715	7.268584	1.837837
131	1	10011000	1.832778	5.670732	2.213000
132	1	10011000	-1.040733	2.752914	2.908201
133	1	10011000	-1.215367	2.721003	5.362513
134	1	10011000	0.833211	2.813458	6.755425
135	1	10011000	3.061062	2.940077	5.672888
136	1	10011000	3.244479	2.991646	3.218238
137	1	10011000	-5.602769	0.397046	-1.654106
138	1	10011000	-7.073507	0.298876	-3.635245
139	1	10011000	-6.173382	0.846073	-5.880506
140	1	10011000	-3.793252	1.488630	-6.137916
141	1	10011000	-2.315607	1.583053	-4.181760
142	1	10011000	-0.395282	5.221951	2.198625
143	1	10011000	-1.960429	6.756589	1.267375
144	1	10011000	-3.390167	7.589082	-0.641086
145	1	10011000	-4.149555	7.318100	-2.914209
146	1	10011000	-3.377059	5.451037	-4.312180
147	1	10011000	-1.846447	3.802159	-3.474684
148	1	10011000	1.289946	4.878038	-1.979362
149	1	10011000	3.073386	5.190539	-3.551167
150	1	10011000	3.791116	3.391271	-5.059817
151	1	10011000	2.760656	1.207922	-4.995783
152	1	10011000	1.012404	-0.402254	-3.980004

153	1	10011000	-1.009760	-0.709188	-2.717039
154	1	10011000	-5.131513	4.946494	2.164539
155	1	10011000	-5.722647	4.934347	-0.242909
156	1	10011000	-4.692376	3.303346	-1.764674
157	1	10011000	-2.483755	1.628653	1.531169
158	1	10011000	-3.513502	3.291979	3.050600
159	6	10061000	-3.824801	-3.042065	2.111416
160	6	10061002	-4.755145	-3.567914	0.039424
161	6	10061000	-4.909416	-3.336074	-1.401292
162	8	10081002	-4.438218	-2.377450	-2.069645
163	6	10061000	-3.243571	-2.208722	3.166134
164	6	10061000	-3.376020	-0.794102	3.212116
165	6	10061000	-2.622116	-2.844191	4.268690
166	6	10061000	-2.883104	-0.055676	4.288038
167	1	10011000	-3.928172	-0.282233	2.432428
168	6	10061000	-2.118561	-2.115090	5.357317
169	1	10011000	-2.533414	-3.929047	4.276120
170	6	10061000	-2.252409	-0.710126	5.367671
171	1	10011000	-3.027745	1.018534	4.347244
172	1	10011000	-1.649082	-2.640902	6.182448
173	7	10071000	-3.907351	-2.753396	0.798029
174	8	10081003	-1.786668	0.122676	6.384070
175	8	10081000	-5.718184	-4.295075	-1.963881
176	6	10061003	-1.179679	-0.478158	7.565585
177	1	10011000	-0.922252	0.360907	8.214525
178	1	10011000	-1.887175	-1.140475	8.081203
179	1	10011000	-0.270248	-1.037775	7.304396
180	6	10061003	-6.249134	-4.005996	-3.311265
181	1	10011000	-6.888577	-3.120467	-3.251057
182	1	10011000	-5.430849	-3.833344	-4.016547
183	1	10011000	-6.822383	-4.893563	-3.581704
184	1	10011000	-4.039723	-4.073596	2.394150
185	1	10011000	-4.833275	-4.611097	0.342456
186	6	10061000	-6.646796	-3.174664	0.862722
187	6	10061000	-6.453329	-2.953514	2.246867
188	1	10011000	-7.096175	-4.055839	0.418518
189	1	10011000	-6.478493	-3.684997	3.041376
190	7	10071003	-6.770644	-0.878559	1.240595
191	6	10061003	-7.009924	0.552315	1.088404
192	1	10011000	-7.353791	0.951847	2.047084
193	1	10011000	-6.095878	1.089183	0.796515
194	1	10011000	-7.768383	0.712184	0.315707
195	6	10061002	-6.533422	-1.521937	2.515549
196	8	10081002	-6.444869	-0.870520	3.583876
197	6	10061002	-6.955474	-1.833558	0.237262
198	8	10081002	-7.303835	-1.587901	-0.942453

TS2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	10061000	-2.554313	-2.072210	-0.000034
2	6	10061002	-1.107056	-1.999796	0.316594
3	6	10061002	-0.217885	-1.557456	-0.581342
4	6	10061000	-0.647826	-1.175835	-1.936488
5	6	10061002	0.341660	-0.861947	-2.985559
6	6	10061000	-0.065799	-0.549534	-4.226652
7	6	10061000	-1.428938	-0.484016	-4.552465
8	6	10061002	-2.383011	-0.745062	-3.641209
9	6	10061000	-2.006245	-1.150965	-2.261055
10	6	10061000	-3.003895	-1.576835	-1.246234
11	6	10061002	-4.451566	-1.510567	-1.566723
12	6	10061000	-5.255066	-0.552524	-1.024998
13	6	10061000	-6.643807	-0.549494	-1.277199
14	6	10061002	-7.235714	-1.477870	-2.043712
15	6	10061000	-6.426144	-2.526140	-2.684821
16	6	10061000	-5.046902	-2.536454	-2.475057
17	6	10061002	-4.246085	-3.572218	-3.179178
18	6	10061000	-4.854917	-4.476961	-3.967070
19	6	10061000	-6.245864	-4.470847	-4.153893
20	6	10061002	-7.029533	-3.554000	-3.559886
21	6	10061000	-4.321176	-6.058973	-0.918536
22	6	10061000	-5.667322	-6.346467	-0.682449
23	6	10061000	-6.424285	-5.511753	0.142748
24	6	10061000	-5.833892	-4.393347	0.738122

25	6	10061000	-4.482427	-4.099035	0.511688
26	6	10061000	-3.730987	-4.934053	-0.334392
27	15	10151003	-3.785415	-2.583782	1.292031
28	6	10061000	-2.765966	-3.371185	2.610495
29	6	10061000	-1.835039	-4.396754	2.363495
30	6	10061000	-1.111853	-4.961528	3.418508
31	6	10061000	-1.321157	-4.521144	4.727165
32	6	10061000	-2.256636	-3.516177	4.983110
33	6	10061000	-2.976541	-2.945497	3.929388
34	15	10151003	-4.581055	0.809833	0.012173
35	6	10061000	-5.285757	2.288242	-0.810527
36	6	10061000	-4.777364	2.650211	-2.064554
37	6	10061000	-5.245220	3.794564	-2.715477
38	6	10061000	-6.240255	4.576361	-2.124097
39	6	10061000	-6.773651	4.207706	-0.886221
40	6	10061000	-6.302816	3.065585	-0.230379
41	6	10061000	-5.355260	0.727327	1.670417
42	6	10061000	-6.200309	-0.332999	2.039488
43	6	10061000	-6.787438	-0.358819	3.307670
44	6	10061000	-6.550078	0.679854	4.210419
45	6	10061000	-5.718440	1.741300	3.847947
46	6	10061000	-5.108893	1.756281	2.590078
47	1	10011000	-4.019153	2.041534	-2.536362
48	1	10011000	-4.837168	4.074008	-3.678125
49	1	10011000	-6.602179	5.463503	-2.627252
50	1	10011000	-7.552334	4.807949	-0.433831
51	1	10011000	-6.744808	2.795958	0.716713
52	1	10011000	-4.467490	2.584338	2.322272
53	1	10011000	-5.542768	2.551795	4.543150
54	1	10011000	-7.012922	0.664040	5.188548
55	1	10011000	-7.432458	-1.181596	3.587689
56	1	10011000	-6.407940	-1.144759	1.359175
57	1	10011000	-1.634648	-4.741730	1.363807
58	1	10011000	-0.386614	-5.740005	3.220484
59	1	10011000	-0.759425	-4.958903	5.542095
60	1	10011000	-2.421541	-3.175843	5.997127
61	1	10011000	-3.700826	-2.168627	4.141382
62	1	10011000	-7.265097	0.218068	-0.832753
63	1	10011000	-8.309123	-1.444175	-2.203594
64	1	10011000	-8.102527	-3.569065	-3.724997
65	1	10011000	-6.695903	-5.219850	-4.792954
66	1	10011000	-4.259622	-5.231583	-4.465206
67	1	10011000	-3.169534	-3.619437	-3.055307
68	1	10011000	-3.425516	-0.669459	-3.931700
69	1	10011000	-1.717564	-0.206570	-5.558257
70	1	10011000	0.672073	-0.329309	-4.987864
71	1	10011000	1.396996	-0.909046	-2.757105
72	1	10011000	0.828706	-1.488244	-0.307774
73	1	10011000	-0.746609	-2.282964	1.291203
74	1	10011000	-6.125747	-7.210266	-1.146001
75	1	10011000	-3.740222	-6.694554	-1.574163
76	1	10011000	-2.704741	-4.703675	-0.580264
77	1	10011000	-6.432495	-3.752490	1.373020
78	1	10011000	-7.469336	-5.730109	0.319942
79	79	10791004	3.290268	-0.844689	-0.887986
80	79	10791004	-2.141136	1.253229	-0.011636
81	6	10061000	1.534335	0.544742	1.982534
82	6	10061002	1.010627	-0.693186	2.613354
83	6	10061002	-0.075211	-0.682243	3.393486
84	6	10061000	-0.827003	0.561677	3.607755
85	6	10061002	-1.934915	0.613260	4.585828
86	6	10061000	-2.549326	1.778444	4.843734
87	6	10061000	-2.192272	2.957687	4.175259
88	6	10061002	-1.205692	2.977267	3.262459
89	6	10061000	-0.446879	1.735600	2.947112
90	6	10061000	0.769043	1.739410	2.081020
91	6	10061002	1.285634	3.052634	1.638318
92	6	10061002	0.884095	3.650415	0.481926
93	6	10061002	1.446611	4.991170	0.139043
94	6	10061000	2.243040	5.656971	0.985938
95	6	10061000	2.562482	5.125316	2.235039
96	6	10061000	2.096524	3.855236	2.606233
97	6	10061002	2.402835	3.380593	3.983533
98	6	10061000	3.144229	4.136016	4.812189
99	6	10061000	3.638540	5.387884	4.419607
100	6	10061002	3.381816	5.893600	3.201256
101	6	10061000	5.630639	3.610641	1.910848
102	6	10061000	5.713258	4.201245	0.647535
103	6	10061000	5.030246	3.635908	-0.431477
104	6	10061000	4.253986	2.489852	-0.242491

105	6	10061000	4.120403	1.922545	1.029808
106	6	10061000	4.845680	2.468992	2.101722
107	15	10151003	3.189726	0.355719	1.171531
108	6	10061000	4.155536	-0.630546	2.373891
109	6	10061000	4.974585	-1.663045	1.902569
110	6	10061000	5.700703	-2.452453	2.798981
111	6	10061000	5.595724	-2.226785	4.173729
112	6	10061000	4.767580	-1.207965	4.652593
113	6	10061000	4.047122	-0.412335	3.756898
114	15	10151003	-0.469353	2.998278	-0.599783
115	6	10061000	-1.609397	4.434873	-0.646813
116	6	10061000	-2.672547	4.470231	0.264825
117	6	10061000	-3.593094	5.520765	0.239662
118	6	10061000	-3.461553	6.542295	-0.703656
119	6	10061000	-2.406768	6.514571	-1.619785
120	6	10061000	-1.482610	5.465306	-1.594790
121	6	10061000	0.122104	2.911841	-2.331431
122	6	10061000	-0.805706	2.660391	-3.351090
123	6	10061000	-0.416594	2.715442	-4.692458
124	6	10061000	0.907408	3.008788	-5.023958
125	6	10061000	1.840274	3.252668	-4.013528
126	6	10061000	1.451186	3.200348	-2.672573
127	1	10011000	-2.796947	3.675263	0.985693
128	1	10011000	-4.414615	5.536156	0.944154
129	1	10011000	-4.179087	7.352075	-0.727840
130	1	10011000	-2.307223	7.304797	-2.352540
131	1	10011000	-0.678467	5.462989	-2.317241
132	1	10011000	2.181197	3.421400	-1.914469
133	1	10011000	2.863180	3.496270	-4.267925
134	1	10011000	1.208042	3.054048	-6.062482
135	1	10011000	-1.142127	2.531154	-5.474006
136	1	10011000	-1.835066	2.447047	-3.107558
137	1	10011000	5.052037	-1.853963	0.841388
138	1	10011000	6.340032	-3.242891	2.428392
139	1	10011000	6.152829	-2.843038	4.867353
140	1	10011000	4.681090	-1.036982	5.717738
141	1	10011000	3.400144	0.363712	4.142401
142	1	10011000	1.204779	5.452231	-0.811044
143	1	10011000	2.619719	6.631773	0.700670
144	1	10011000	3.775776	6.868921	2.930814
145	1	10011000	4.236648	5.960938	5.116617
146	1	10011000	3.366561	3.769919	5.806466
147	1	10011000	2.039691	2.420418	4.332641
148	1	10011000	-0.960037	3.915856	2.777107
149	1	10011000	-2.724178	3.873143	4.401279
150	1	10011000	-3.340663	1.807433	5.581399
151	1	10011000	-2.231987	-0.282027	5.122494
152	1	10011000	-0.395672	-1.600152	3.873026
153	1	10011000	1.537538	-1.632563	2.472906
154	1	10011000	6.317028	5.087434	0.502313
155	1	10011000	6.171634	4.039613	2.744244
156	1	10011000	4.804583	2.030824	3.085422
157	1	10011000	3.774801	2.025531	-1.091940
158	1	10011000	5.114266	4.075222	-1.416954
159	6	10061000	4.155081	-3.427899	-2.107764
160	6	10061002	4.330764	-1.663897	-3.640560
161	6	10061000	3.967695	-0.299982	-4.039948
162	8	10081002	3.389254	0.570970	-3.340179
163	6	10061000	3.744120	-4.037257	-0.825500
164	6	10061000	2.389385	-3.970245	-0.406812
165	6	10061000	4.677075	-4.678857	0.017445
166	6	10061000	1.991215	-4.463930	0.839162
167	1	10011000	1.649993	-3.567160	-1.092893
168	6	10061000	4.285574	-5.183143	1.271479
169	1	10011000	5.724758	-4.722545	-0.266010
170	6	10061000	2.946993	-5.051521	1.696352
171	1	10011000	0.955951	-4.425269	1.162203
172	1	10011000	5.034228	-5.642854	1.908209
173	7	10071000	3.836582	-2.171355	-2.434133
174	8	10081003	2.463344	-5.467938	2.935864
175	8	10081000	4.421191	-0.054174	-5.318453
176	6	10061003	3.387736	-6.099322	3.872439
177	1	10011000	2.788674	-6.332311	4.754572
178	1	10011000	3.805458	-7.024180	3.453553
179	1	10011000	4.202839	-5.415165	4.145543
180	6	10061003	4.420864	1.340137	-5.788462
181	1	10011000	3.400187	1.655112	-6.026189
182	1	10011000	4.854289	1.985786	-5.019829
183	1	10011000	5.037439	1.332605	-6.688457
184	6	10061000	6.378487	-1.624657	-3.379952

185	6	10061000	6.775143	-2.763744	-2.636365
186	1	10011000	4.607548	-4.061426	-2.867080
187	1	10011000	4.400557	-2.365708	-4.470356
188	1	10011000	6.996772	-3.750191	-3.017056
189	1	10011000	6.558867	-1.479715	-4.440279
190	6	10061002	7.111945	-2.366923	-1.281875
191	8	10081002	7.497836	-3.035704	-0.288849
192	6	10061002	6.588184	-0.423428	-2.473248
193	8	10081002	6.468868	0.792743	-2.757445
194	7	10071003	6.949711	-0.925265	-1.224335
195	6	10061003	7.378144	-0.111589	-0.092311
196	1	10011000	8.202518	0.551441	-0.380038
197	1	10011000	6.559941	0.514676	0.283714
198	1	10011000	7.714570	-0.793507	0.694434

TS3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	10061000	-2.041199	0.924479	0.928679
2	6	10061000	-1.204944	0.038974	1.766504
3	6	10061000	-0.763140	0.425695	3.026882
4	6	10061000	-1.062626	1.686235	3.537534
5	6	10061000	-0.658018	2.056079	4.825345
6	6	10061000	-1.010975	3.298283	5.361785
7	6	10061000	-1.799489	4.206946	4.649940
8	6	10061000	-2.245209	3.916533	3.362161
9	6	10061002	-1.850948	2.641170	2.723137
10	6	10061000	-2.293936	2.249153	1.356782
11	6	10061000	-3.038544	3.223946	0.527904
12	6	10061000	-2.385028	4.061008	-0.403272
13	6	10061000	-3.207981	4.903956	-1.308021
14	6	10061000	-4.594316	4.969723	-1.193859
15	6	10061000	-5.264908	4.269547	-0.193460
16	6	10061002	-4.499642	3.409141	0.737847
17	6	10061000	-5.229221	2.838683	1.891254
18	6	10061000	-6.608550	3.013796	1.985194
19	6	10061000	-7.307613	3.755050	1.027629
20	6	10061000	-6.651122	4.383889	-0.035771
21	6	10061000	-0.093277	7.579480	-2.826562
22	6	10061000	0.593831	7.072331	-3.932341
23	6	10061000	0.927265	5.717146	-3.984186
24	6	10061000	0.576076	4.870131	-2.929734
25	6	10061000	-0.118455	5.367190	-1.819667
26	6	10061000	-0.448024	6.732473	-1.771830
27	15	10151003	-0.546799	4.205769	-0.469352
28	6	10061000	-0.049653	5.084140	1.050770
29	6	10061000	-0.813170	6.139744	1.572564
30	6	10061000	-0.407526	6.786699	2.744275
31	6	10061000	0.752136	6.373873	3.406879
32	6	10061000	1.508371	5.315024	2.896825
33	6	10061000	1.109127	4.674538	1.720603
34	15	10151003	-2.829867	0.112405	-0.521238
35	6	10061000	-4.623496	0.011713	-0.178124
36	6	10061000	-5.543718	-0.143952	-1.226493
37	6	10061000	-6.900873	-0.337522	-0.952551
38	6	10061000	-7.340808	-0.434845	0.369416
39	6	10061000	-6.420300	-0.359173	1.416734
40	6	10061000	-5.064920	-0.153758	1.143516
41	6	10061000	-2.489089	1.150853	-1.986705
42	6	10061000	-1.219978	1.059403	-2.569479
43	6	10061000	-0.921175	1.772037	-3.733280
44	6	10061000	-1.889756	2.590978	-4.318168
45	6	10061000	-3.159328	2.688897	-3.743007
46	6	10061000	-3.461056	1.970769	-2.580920
47	1	10011000	-5.213526	-0.136365	-2.256126
48	1	10011000	-7.607733	-0.435982	-1.766097
49	1	10011000	-8.390150	-0.593441	0.581159
50	1	10011000	-6.755085	-0.465112	2.440452
51	1	10011000	-4.362195	-0.130048	1.965550
52	1	10011000	-4.436602	2.091028	-2.135153
53	1	10011000	-3.906799	3.331422	-4.189887
54	1	10011000	-1.655689	3.151622	-5.213736
55	1	10011000	0.062040	1.692101	-4.178876
56	1	10011000	-0.467596	0.424142	-2.123238

57	1	10011000	-1.736605	6.441225	1.097157
58	1	10011000	-1.001796	7.595900	3.148173
59	1	10011000	1.059801	6.868794	4.318749
60	1	10011000	2.403861	4.991126	3.411331
61	1	10011000	1.702933	3.862629	1.328415
62	1	10011000	-2.748509	5.455832	-2.112409
63	1	10011000	-5.146072	5.592546	-1.888000
64	1	10011000	-7.231958	4.983719	-0.726353
65	1	10011000	-8.379520	3.867610	1.127191
66	1	10011000	-7.146493	2.568634	2.812178
67	1	10011000	-4.712701	2.274607	2.655625
68	1	10011000	-2.870547	4.630866	2.844319
69	1	10011000	-2.070943	5.149729	5.107018
70	1	10011000	-0.682966	3.554097	6.361023
71	1	10011000	-0.079587	1.372139	5.433320
72	1	10011000	-0.213331	-0.286482	3.625370
73	1	10011000	-0.968311	-0.958837	1.419177
74	1	10011000	0.866168	7.728529	-4.748767
75	1	10011000	-0.355117	8.628954	-2.788333
76	1	10011000	-0.993632	7.145121	-0.939195
77	1	10011000	0.843644	3.824427	-2.980123
78	1	10011000	1.458255	5.322561	-4.840744
79	79	10791004	0.934367	2.266608	-0.768568
80	79	10791004	-2.037035	-2.095706	-0.780042
81	6	10061000	3.014545	-0.662853	-1.541071
82	6	10061000	2.090910	-1.121269	-2.604363
83	6	10061000	2.028625	-2.449787	-3.010260
84	6	10061000	2.832564	-3.418747	-2.417294
85	6	10061000	2.765980	-4.756716	-2.823719
86	6	10061000	3.591870	-5.726140	-2.246008
87	6	10061000	4.516692	-5.402583	-1.248658
88	6	10061000	4.641925	-4.096110	-0.780510
89	6	10061002	3.781063	-3.030713	-1.347098
90	6	10061000	3.827139	-1.615094	-0.880819
91	6	10061000	4.732760	-1.276789	0.240279
92	6	10061000	4.269332	-1.252028	1.573498
93	6	10061000	5.256933	-1.111398	2.675950
94	6	10061000	6.620415	-0.972184	2.424872
95	6	10061000	7.119089	-0.985636	1.123025
96	6	10061002	6.191384	-1.166442	-0.016373
97	6	10061000	6.767797	-1.179768	-1.379765
98	6	10061000	8.141579	-1.014341	-1.542587
99	6	10061000	8.983280	-0.843309	-0.438441
100	6	10061000	8.487174	-0.831104	0.870086
101	6	10061000	6.584515	2.352955	0.491433
102	6	10061000	6.182390	2.636239	1.799016
103	6	10061000	4.848557	2.455864	2.173428
104	6	10061000	3.918838	1.977732	1.244554
105	6	10061000	4.318465	1.672589	-0.061305
106	6	10061000	5.654592	1.883345	-0.440670
107	15	10151003	3.056755	1.159012	-1.276619
108	6	10061000	3.674543	1.897337	-2.834732
109	6	10061000	3.664512	3.292964	-2.964680
110	6	10061000	4.143903	3.897792	-4.129742
111	6	10061000	4.647335	3.111896	-5.169062
112	6	10061000	4.681288	1.721015	-5.038996
113	6	10061000	4.203013	1.112937	-3.874182
114	15	10151003	2.447813	-1.428490	1.907083
115	6	10061000	2.412947	-3.261720	1.743794
116	6	10061000	1.492294	-3.843555	0.863349
117	6	10061000	1.487417	-5.227713	0.664497
118	6	10061000	2.383382	-6.040099	1.362953
119	6	10061000	3.301195	-5.467886	2.246717
120	6	10061000	3.325275	-4.082761	2.430561
121	6	10061000	2.346398	-1.239247	3.747098
122	6	10061000	1.803095	-2.241357	4.573077
123	6	10061000	1.657196	-2.026209	5.946637
124	6	10061000	2.024658	-0.801867	6.507289
125	6	10061000	2.525123	0.214350	5.691923
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127	1	10011000	0.798947	-3.221593	0.311735
128	1	10011000	0.794210	-5.672933	-0.034555
129	1	10011000	2.374611	-7.111268	1.209613
130	1	10011000	4.001744	-6.096481	2.780721
131	1	10011000	4.048709	-3.654377	3.110655
132	1	10011000	3.024126	0.809427	3.698961
133	1	10011000	2.788250	1.172345	6.121219
134	1	10011000	1.905611	-0.634954	7.569906
135	1	10011000	1.243785	-2.805044	6.574342
136	1	10011000	1.465002	-3.180813	4.166196

137	1	10011000	3.288632	3.912439	-2.159987
138	1	10011000	4.127910	4.975769	-4.225085
139	1	10011000	5.019708	3.580729	-6.070640
140	1	10011000	5.085701	1.113728	-5.838409
141	1	10011000	4.268630	0.038365	-3.787602
142	1	10011000	4.947405	-1.151533	3.707529
143	1	10011000	7.295876	-0.862302	3.265049
144	1	10011000	9.182056	-0.695133	1.690332
145	1	10011000	10.045979	-0.716922	-0.600664
146	1	10011000	8.563317	-1.015332	-2.539337
147	1	10011000	6.137909	-1.296758	-2.251761
148	1	10011000	5.355019	-3.883703	0.004265
149	1	10011000	5.137795	-6.181260	-0.825223
150	1	10011000	3.514764	-6.752467	-2.581015
151	1	10011000	2.070883	-5.058499	-3.598168
152	1	10011000	1.357422	-2.717213	-3.816571
153	1	10011000	1.481839	-0.396727	-3.127057
154	1	10011000	6.902610	3.000107	2.520069
155	1	10011000	7.616820	2.496039	0.199786
156	1	10011000	5.983465	1.673170	-1.449279
157	1	10011000	2.887816	1.839276	1.540831
158	1	10011000	4.535654	2.689237	3.182646
159	7	10071000	-1.682202	-4.170832	-0.700849
160	6	10061002	-2.099178	-4.907495	0.400351
161	6	10061000	-1.380447	-4.849935	-1.831774
162	1	10011000	-1.723939	-5.935806	0.403220
163	6	10061000	-2.098023	-4.320063	1.777347
164	6	10061000	-1.242865	-4.908710	2.744491
165	6	10061000	-2.883490	-3.217165	2.177602
166	6	10061000	-1.107663	-4.367410	4.027331
167	1	10011000	-0.667828	-5.795437	2.485213
168	6	10061000	-2.759296	-2.662769	3.464568
169	1	10011000	-3.635389	-2.825467	1.501394
170	6	10061000	-1.845505	-3.218756	4.383326
171	1	10011000	-0.444471	-4.809198	4.764655
172	1	10011000	-3.390233	-1.824451	3.744301
173	8	10081003	-1.604598	-2.723777	5.664290
174	6	10061003	-2.359757	-1.568597	6.128323
175	1	10011000	-1.986130	-1.366610	7.133761
176	1	10011000	-2.185082	-0.693092	5.486494
177	1	10011000	-3.435199	-1.786890	6.169820
178	6	10061000	-1.172142	-4.117222	-3.083224
179	8	10081002	-1.250680	-2.859683	-3.173120
180	8	10081000	-0.841862	-4.812293	-4.221078
181	6	10061003	-0.940269	-6.282029	-4.307919
182	1	10011000	-1.962859	-6.603529	-4.088817
183	1	10011000	-0.693687	-6.506060	-5.346607
184	1	10011000	-0.209491	-6.762162	-3.644559
185	1	10011000	-1.113855	-5.897809	-1.767830
186	6	10061000	-3.716610	-6.262525	-1.433607
187	6	10061000	-3.937241	-5.506675	-0.255722
188	1	10011000	-3.374403	-7.286299	-1.496373
189	1	10011000	-4.199352	-5.937580	0.707354
190	6	10061002	-4.232412	-5.548266	-2.592662
191	8	10081002	-4.274068	-5.865554	-3.806153
192	6	10061002	-4.698601	-4.259660	-0.701501
193	8	10081002	-5.157156	-3.325393	0.006305
194	7	10071000	-4.794380	-4.318062	-2.085059
195	6	10061003	-5.439747	-3.320514	-2.934419
196	1	10011000	-4.763730	-2.482850	-3.146742
197	1	10011000	-5.701657	-3.802987	-3.880126
198	1	10011000	-6.341821	-2.944772	-2.441730

Complete reference 16:

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