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Natural Bond Orbital (NBO) Study of (5H-tetrazol-1-yl)(triphenylphosphine)gold [Au(tetz)(PPh₃)]

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In this research work, we studied theoretically the structural properties of (5H-tetrazol-1-yl)(triphenylphosphine)gold or [Au(tetz)(PPh₃)] by density functional theory (DFT) method at LANL2DZ level. All calculations were performed at 298.15 K and 1 atmosphere. Firstly, the bond lengths, bond angles, dihedral angles and natural charge density on atoms of the compound were calculated. The dependence between the experimental and calculated indicates a great convergence. The results have provided that the molecular structure of the compound is linear environment around gold atom. According to the calculations, the total natural charge of gold atom is consistent with the total number of electrons in the isolated gold atom. Natural bond orbitals (NBOs) analysis was then calculated at studied level of B3LYP (Becke, 3 parameter, Lee-Yang-Parr) theory. The NBO analysis revealed that the largest negative and positive charges are located on nitrogen (that coordinating to the gold) and phosphorus atoms, respectively. And also, it showed that the phosphorus atom uses more p orbital for formation of $\sigma(\text{Au-P})$ bond to formation of $\sigma(\text{P-C})$ bond.

Keywords: Density functional theory, Natural bond orbital, Natural charge, Theoretical study, Gold(I) complexes

INTRODUCTION

For many centuries gold has occupied a special place in medicine as a potential "cure-all" for diseases [1]. As early as 2500 BC gold was used in Chinese and Arabic medicine [2]. In 1890, Koch discovered that the gold(I) dicyanide ion had antitubercular activity [3]. During the search for non-toxic gold(I) complexes with antitubercular activity, gold(I) thiolate complexes were synthesized [4]. There is potential for more extensive use of gold in therapy based on the rational design of new gold compounds [5]. The molecular design and structural determination of gold(I) complexes composed of the ligands are an intriguing aspect of bioinorganic chemistry, inorganic syntheses and metal-based drugs [6-8]. Kenji Nomia and her coworkers synthesized and characterized (5H-tetrazol-1-yl) (triphenylphosphine)gold in 1999 [9].

In theoretical chemistry, a natural bond orbital (NBO) is

a computed bonding orbital with maximum electron density [10]. The NBOs are one of a sequence of natural localized orbital sets that contain "natural atomic orbitals" (NAO), "natural hybrid orbitals" (NHO), "natural bonding orbitals" (NBO) and "natural (semi-)localized molecular orbitals" (NLMO) [11]. Natural orbitals are used in theoretical chemistry to compute the distribution of electron density in atoms and in bonds between atoms [12]. NBOs contain the highest possible percentage of the electron density [13]. The NBO analysis is a powerful analysis technique capable of generating chemical representations of quantum mechanical electronic structure results and reactivity [14]. The bonding NBOs are of the "Lewis orbital"-type (occupation numbers near 2); antibonding NBOs are of the "non-Lewis orbital"-type (occupation numbers near 0) [15]. In an idealized Lewis structure, full Lewis orbitals (two electrons) are complemented by formally empty non-Lewis orbitals [16]. An optimal Lewis structure can be defined as that one with the maximum amount of electronic charge in Lewis orbitals (Lewis charge). A low amount of electronic charge in Lewis

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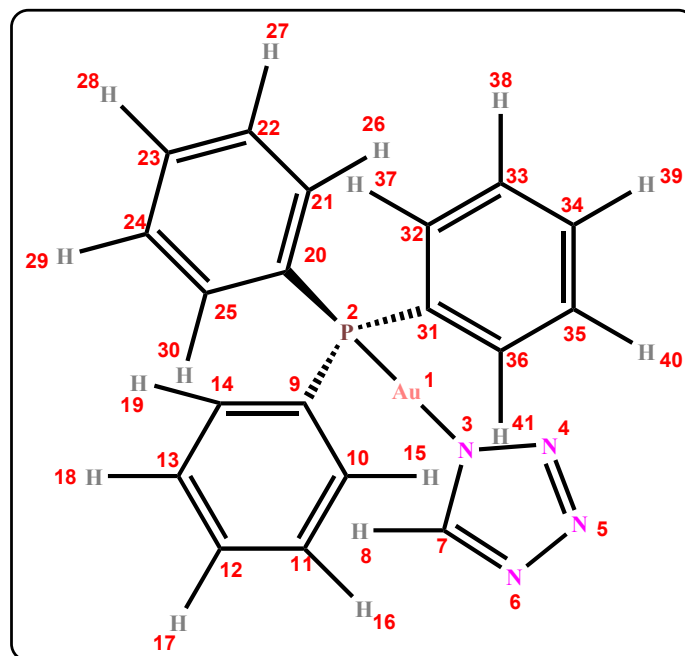


Fig. 1. The chemical structure of (5H-tetrazol-1-yl)(triphenylphosphine)gold with atomic numbering.

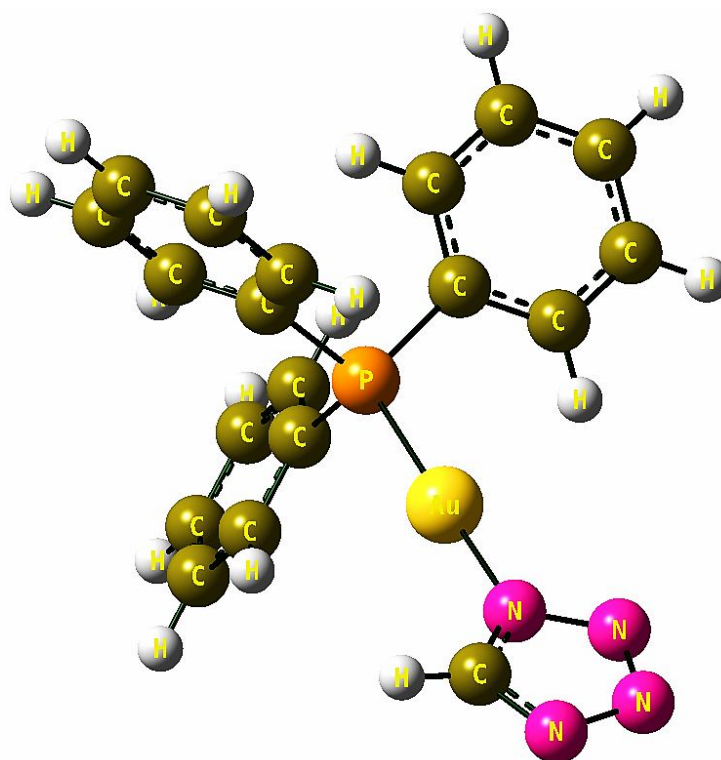


Fig. 2. The geometric structure of the (5H-tetrazol-1-yl)(triphenylphosphine)gold compound.

Table 1. The Experimental (Exp.) and Calculated Bond Lengths (Angstrom), Bond Angles (Degree) and Dihedral Angles (Degree) of the (5H-Tetrazol-1-yl)(triphenylphosphine)gold Molecule

Bond	Exp.	B3LYP/6-31G(d)	Angle	Exp.	B3LYP/6-31G(d)
Au-P	2.239	2.381	P-Au-N3	178.4	178.975
Au-N3	2.043	2.039	Au-N3-N4	124.5	120.484
P-C	1.811-1.815	1.871-1.872	Au-N3-C7	129.0	132.662
N3-N4	1.339	1.402	N3-N4-N5	108.4	106.944
N3-C7	1.310	1.366	N3-C7-N6	110.1	110.643
N4-N5	1.342	1.342	N4-N3-C7	106.3	106.855
N5-N6	1.322	1.401	N4-N5-N6	106.4	110.153
N6-C7	1.298	1.350	N5-N6-C7	108.8	105.405
C9-C10	-	1.412	Au-P-C9	-	112.179
C10-C11	-	1.407	Au-P-C20	-	112.910
C11-C12	-	1.409	Au-P-C31	-	112.914
C12-C13	-	1.408	C9-P-C20	-	106.015
C13-C14	-	1.408	C9-P-C31	-	106.248
C9-C14	-	1.410	C20-P-C31	-	106.017
C10-H15	-	1.088	C10-C9-C14	-	119.919
C11-H16	-	1.087	C9-P-C20-C25	-	-84.186
C12-H17	-	1.087	C9-P-C31-C32	-	-20.538
C13-H18	-	1.087	C20-P-C31-C32	-	91.959
C14-H19	-	1.087	P-C9-C14-H19	-	1.685

orbitals indicates strong effects of electron delocalization. These orbitals are localized electron pair orbitals for bonding pairs and lone pairs [17].

NBO analysis shows the intermolecular orbital interactions in the complex. This is performed by studying all possible interactions between donor and acceptor natural bond orbitals and guesstimating their energetic value by second-order perturbation theory [18]. The stabilization energy (E^2) for natural bond orbitals (donor NBO = I and

acceptor NBO = j) is guessed as follows:

$$E^2 = -q_i \times (F_{ij})^2 / (\epsilon_j - \epsilon_i)$$

Where

q_i = orbital occupancy

ϵ_j, ϵ_i = diagonal elements

F_{ij} = off-diagonal natural bond orbital Fock matrix element

COMPUTATIONAL METHOD

All theoretical studies were carried out with the Gaussian 03 computational package [19]. The computational method employed for the tetrazole derivatives calculations is the B3LYP/LANL2DZ level of theory. The term of B3LYP consists of the Vosko, Wilk, Nusair (VWN3) local correlation functional [20] and Lee, Yang, Parr (LYP) correlation correction functional [21]. The geometry of molecule was optimized without any structural or symmetry restrictions in the gas phase.

RESULTS AND DISCUSSION

In present study, we performed the theoretical investigation on (5H-tetrazol-1-yl)(triphenylphosphine)gold (Fig. 1), using B3LYP method. The global optimized structure of molecule can be seen in Fig. 2. The computed bond lengths and bond angles were compared with the experimental data which some of the data listed in Table 1. The dependence between the experimental and calculated data is presented for molecule (Figs. 3 and 4). Higher correlation coefficients for bond lengths ($R^2 = 0.988$) and bond angles ($R^2 = 0.9867$) show a great convergence. In the experimental data, the bond lengths of the Au-P, Au-N3, P-C, N3-N4, N3-C7, N4-N5, N5-N6 and N6-C7 are 2.239, 2.043, 1.811-1.815, 1.339, 1.31, 1.342, 1.322 and 1.298 Angstrom, respectively. The B3LYP/LANL2DZ level of theory indicates the related bond lengths in 2.381, 2.039, 1.871-1.872, 1.402, 1.366, 1.342, 1.401 and 1.35 Angstrom, respectively. And also, in the calculated data, the bond lengths of the C-C and C-H bonds in the phenyl groups occur in the range of 1.407-1.412 and 1.087-1.088 Å, respectively. The experimental bond angles indicate P-Au-N3 (178.4), Au-N3-N4 (124.5), Au-N3-C7 (129), N3-N4-N5 (108.4), N3-C7-N6 (110.1), N4-N3-C7 (106.3), N4-N5-N6 (106.4) and N5-N6-C7 (108.8) degree. The calculated data indicate the related bond angles in 178.975, 120.484, 132.662, 106.944, 110.643, 106.855, 110.153 and 105.405 degree, respectively. The computed bond angles show Au-P-C9 (112.179), Au-P-C20 (112.91), Au-P-C31 (112.914), C9-P-C20 (106.015), C9-P-C31 (106.248), C20-P-C31 (106.017) and C10-C9-C14 (119.919) degree. The computed dihedral angles C9-P-C20-C25, C9-P-C31-C32,

C20-P-C31-C32 and P-C9-C14-H19 are 84.186, 20.538, 91.959 and 1.685 degree, respectively.

The natural charges on atoms are listed in Table 2. The largest negative and positive charges (-0.558 and 0.883) are located on N3 and phosphorus atoms, respectively. The natural charge of gold atom is 0.415. As can be seen from the NBO calculation of the molecule, the electron configuration of Au is: [core] 6s (0.86) 5d (9.71) 6p (0.01). Thus, 68 core electrons and 10.58 valence electrons give the total of 78.58 electrons. This is consistent with the computed natural charge on Au atom of the molecule, which corresponds to the difference between 78.58 e^- and the total number of electrons in the isolated gold atom (79 e^-). It should be emphasized that the computed natural charges on the C9, C20 and C31 atoms of the phenyl groups are more negative than the charge on the other carbon atoms.

Table 3 follows the main listing of NBOs that displays the form and occupancy of the complete set of natural bond orbitals of the (5H-tetrazol-1-yl)(triphenylphosphine)gold. And also, the computed natural hybrids on atoms are given in this table. According to the data, the gold (Au) atom forms a single bond (sigma bond) with phosphorus atom of triphenylphosphine ligand. We can see the σ (Au-P) bond is formed from an $sd^{0.19}$ hybrid on gold atom and an $sp^{3.19}$ hybrid on phosphorus atom. While the sigma bonds between phosphorus atom and carbon atoms of the phenyl groups are formed from an $sp^{2.9}$ hybrid on phosphorus atom and an $sp^{2.8}$ hybrid on carbon atoms (C9, C20 and C31). Comparing the NBO of σ (Au-P) bond with the NBO of σ (P-C) bond indicates that the phosphorus atom uses more p orbital for formation of σ (Au-P) bond to formation of σ (P-C) bond. This result is consistent with the bond lengths of them (the Au-P bond length is more than P-C bond length). Table 4 collects the selected values of the computed second order interaction energy (E^2) between donor-acceptor orbitals in (5H-tetrazol-1-yl)(triphenylphosphine)gold. The strongest interactions are related to the electron transitions of the σ (C9-C14) \rightarrow π^* (C10-C11), σ (C9-C14) \rightarrow π^* (C13-C14), σ (C10-C11) \rightarrow π^* (C9-C14), σ (C10-C11) \rightarrow π^* (C12-C13), σ (C12-C13) \rightarrow π^* (C9-C14), σ (C12-C13) \rightarrow π^* (C10-C11), LP (1) N3 \rightarrow σ^* (Au-P), σ (N6-C7) \rightarrow σ^* (N4-N5), LP (2) N6 \rightarrow π^* (C7-N6) and LP (2) N6 \rightarrow π^* (N4-N5). It should be emphasized that the Au-N3 bond is

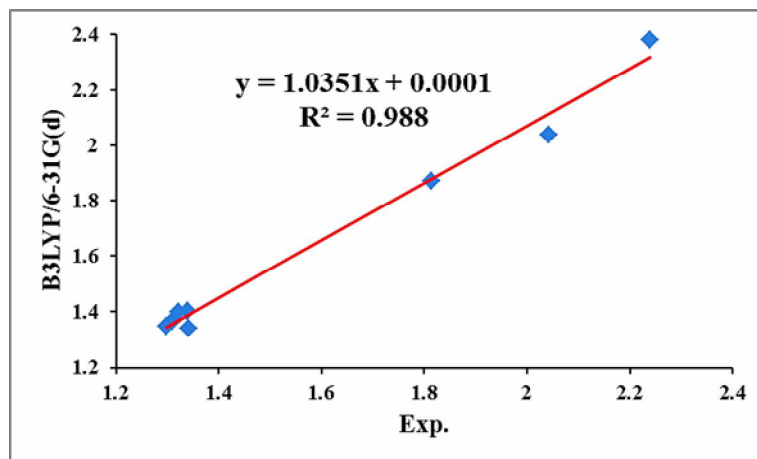


Fig. 3. The bond length correlation between the experimental and calculated data for the (5H-tetrazol-1-yl)(triphenylphosphine)gold compound.

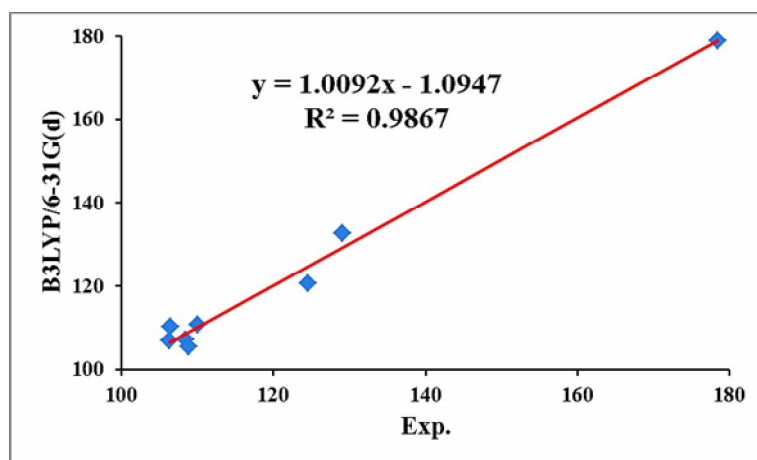


Fig. 4. The bond angle correlation between the experimental and calculated data for the (5H-tetrazol-1-yl)(triphenylphosphine)gold compound.

formed from an electron donation of a lone pair orbital on the nitrogen atom of the tetrazole ring, LP(1)N3 to the antibonding acceptor $\sigma^*(\text{Au-P})$ orbital. As shown in Table 3, the LP(1)N3 orbital is formed from an $sp^{1.59}$ hybrid that is occupied by 1.71 electrons (this is consistent with a delocalization of electron density from the idealized occupancy of 2.0 electrons). As seen from the calculated (E^2) values, the Au-P bond is stronger than P-C bond in molecule. As follows from the data of Table 4, the carbon

atoms in each phenyl ring are strongly conjugated by the above mentioned electron density donations. And also, the tetrazole ring aromaticity can be explained by the electron donations of a lone pair orbital on nitrogen atom, LP(2)N6 to the antibonding acceptor $\pi^*(\text{C7-N6})$ and $\pi^*(\text{N4-N5})$ orbitals. The carbon atom in tetrazole ring is conjugated by the following electron density donations: $\sigma(\text{N6-C7}) \rightarrow \sigma^*(\text{N4-N5})$.

Table 2. The NBO Atomic Charges of (5H-Tetrazol-1-yl)(triphenylphosphine)gold Calculated by the B3LYP Method with 6-31G(d) Basis Set

Atom	Natural charge	Atom	Natural charge	Atom	Natural charge	Atom	Natural charge
Au1	0.415	C12	-0.196	C23	-0.197	C34	-0.196
P2	0.883	C13	-0.203	C24	-0.202	C35	-0.202
N3	-0.558	C14	-0.212	C25	-0.210	C36	-0.209
N4	-0.105	H15	0.238	H26	0.235	H37	0.233
N5	-0.094	H16	0.231	H27	0.229	H38	0.229
N6	-0.356	H17	0.227	H28	0.226	H39	0.227
C7	0.165	H18	0.227	H29	0.227	H40	0.227
H8	0.216	H19	0.231	H30	0.232	H41	0.232
C9	-0.339	C20	-0.337	C31	-0.339	-	-
C10	-0.192	C21	-0.194	C32	-0.194	-	-
C11	-0.198	C22	-0.199	C33	-0.199	-	-

CONCLUSIONS

According to the results, the following conclusions are obtained:

- The molecular structure of (5H-tetrazol-1-yl)(triphenylphosphine)gold computed by the DFT method indicates the linear environment around gold atom.
- The calculations show that the experimental bond lengths and bond angles are consistent with corresponding computational data.
- The calculated total natural charge of gold atom is consistent with the total number of electrons in the isolated gold atom.
- The natural bond orbital (NBO) analysis shows the largest negative and positive charges are located on N3 and phosphorus atoms, respectively.
- The NBO analysis has provided the phosphorus atom uses more p orbital for formation of $\sigma(\text{Au-P})$ bond to formation of $\sigma(\text{P-C})$ bond.

f. Our calculations show the Au-P bond is longer than P-C bond.

g. The delocalization of electron density in each ring has explained by electron donation between donor-acceptor orbitals.

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Table 3. Natural Bond Orbital Population Analysis of (5H-Tetrazol-1-yl)(triphenylphosphine)gold

Donor Lewis type NBOs	Occupancy	Population/Bond orbital/Hybrids
σ (Au-P)	1.94267	22.22% Au ($sd^{0.19}$), 77.78% P ($sp^{3.19}$)
σ (P-C9)	1.95922	41.12% P ($sp^{2.92}$), 58.88% C9 ($sp^{2.83}$)
σ (P-C31)	1.95901	40.97% P ($sp^{2.95}$), 59.03% C31 ($sp^{2.82}$)
σ (P-C20)	1.95914	40.99% P ($sp^{2.93}$), 59.01% C20 ($sp^{2.82}$)
LP (1) Au	1.99915	$sp^{0.04}d^{99.99}$
LP (2) Au	1.99911	$sp^{0.03}d^{99.99}$
LP (3) Au	1.98917	$sd^{5.40}$
LP (4) Au	1.97026	$sp^{1.91}d^{99.99}$
LP (5) Au	1.96310	$pd^{99.99}$
LP (1) N3	1.71010	$sp^{1.59}$
LP (2) N3	1.46109	p
LP (1) N6	1.93890	$sp^{1.22}$
LP (1) N5	1.93130	$sp^{0.91}$
LP (1) N4	1.94098	$sp^{0.90}$
σ (C9-C14)	1.97753	50.95% C9 ($sp^{1.68}$), 49.05% C14 ($sp^{1.81}$)
π (C9-C14)	1.69257	54.36% C9 (p), 45.64% C14 (p)
σ (C9-C10)	1.97810	51.14% C9 ($sp^{1.73}$), 48.86% C10 ($sp^{1.81}$)
σ (C14-C13)	1.97563	50.64% C14 ($sp^{1.82}$), 49.36% C13 ($sp^{1.82}$)
σ (C14-H19)	1.97641	61.69% C14 ($sp^{2.46}$), 38.31% H19 (s)
σ (C10-C11)	1.97641	50.56% C10 ($sp^{1.82}$), 49.44% C11 ($sp^{1.82}$)
π (C10-C11)	1.63983	49.35% C10 (p), 50.65% C11 (p)
σ (C10-H15)	1.97629	62.01% C10 ($sp^{2.45}$), 37.99% H15 (s)
σ (C13-C12)	1.98162	50.10% C13 ($sp^{1.83}$), 49.90% C12 ($sp^{1.83}$)
π (C13-C12)	1.64475	50.67% C13 (p), 49.33% C12 (p)
σ (C13-H18)	1.97670	61.38% C13 ($sp^{2.44}$), 38.62% H18 (s)
σ (C11-C12)	1.98159	49.99% C11 ($sp^{1.84}$), 50.01% C12 ($sp^{1.83}$)
σ (C11-H16)	1.97654	61.61% C11 ($sp^{2.42}$), 38.39% H16 (s)
σ (C12-H17)	1.97745	61.39% C12 ($sp^{2.42}$), 38.61% H17 (s)
σ (N3-C7)	1.99257	62.29% N3 ($sp^{1.78}$), 37.71% C7 ($sp^{2.29}$)
σ (N3-N4)	1.98219	54.57% N3 ($sp^{2.93}$), 45.43% N4 ($sp^{3.68}$)
σ (C7-H8)	1.97697	60.84% C7 ($sp^{1.67}$), 39.16% H8 (s)
σ (C7-N6)	1.98555	41.66% C7 ($sp^{2.09}$), 58.34% N6 ($sp^{2.09}$)
π (C7-N6)	1.82782	41.72% C7 (p), 58.28% N6 (p)
σ (N6-N5)	1.97724	50.37% N6 ($sp^{3.42}$), 49.63% N5 ($sp^{3.35}$)
σ (N5-N4)	1.98435	49.02% N5 ($sp^{3.01}$), 50.98% N4 ($sp^{2.82}$)
π (N5-N4)	1.90680	48.94% N5 (p), 51.06% N4 (p)

Table 4. Second-order Interaction Energy between Donor-acceptor Orbitals of (5H-Tetrazol-1-yl)(triphenylphosphine)gold

Donor \rightarrow acceptor	E^2	$E(j)-E(i)$	F (i,j)
σ (Au-P) \rightarrow σ^* (P-C9)	3.14	0.68	0.041
σ (Au-P) \rightarrow σ^* (P-C20)	3.08	0.68	0.041
σ (Au-P) \rightarrow σ^* (P-C31)	3.11	0.68	0.041
σ (Au-P) \rightarrow σ^* (C9-C14)	3.02	0.95	0.048
σ (Au-P) \rightarrow π^* (C9-C14)	1.02	0.44	0.021
σ (Au-P) \rightarrow σ^* (C20-C21)	2.80	0.95	0.046
σ (Au-P) \rightarrow π^* (C20-C21)	1.33	0.44	0.024
σ (Au-P) \rightarrow σ^* (C31-C36)	2.94	0.95	0.048
σ (Au-P) \rightarrow π^* (C31-C36)	1.10	0.44	0.021
σ (P-C9) \rightarrow σ^* (C13-C14)	4.37	1.09	0.062
σ (P-C9) \rightarrow σ^* (C10-C11)	4.64	1.09	0.064
σ (P-C9) \rightarrow σ^* (C20-C21)	0.57	1.07	0.022
σ (P-C9) \rightarrow π^* (C20-C21)	1.41	0.56	0.027
σ (P-C9) \rightarrow σ^* (C31-C32)	1.77	1.08	0.039
σ (C9-C14) \rightarrow σ^* (P-C9)	1.00	0.97	0.028
σ (C9-C14) \rightarrow σ^* (C9-C10)	2.68	1.25	0.052
σ (C9-C14) \rightarrow σ^* (Au-P)	0.92	0.31	0.015
σ (C9-C14) \rightarrow σ^* (P-C31)	2.81	0.52	0.036
σ (C9-C14) \rightarrow π^* (C10-C11)	20.77	0.30	0.070
σ (C9-C14) \rightarrow π^* (C13-C14)	18.14	0.30	0.066
σ (C10-C11) \rightarrow π^* (C9-C14)	21.78	0.26	0.068
σ (C10-C11) \rightarrow π^* (C12-C13)	21.73	0.28	0.070
σ (C12-C13) \rightarrow π^* (C9-C14)	24.62	0.26	0.073
σ (C12-C13) \rightarrow π^* (C10-C11)	20.14	0.28	0.068
LP (3) Au \rightarrow σ^* (Au-P)	2.74	0.36	0.030
LP (3) Au \rightarrow σ^* (P-C9)	0.59	0.57	0.017
LP (3) Au \rightarrow σ^* (P-C20)	0.74	0.57	0.019

Table 4. Continued

LP (3) Au \rightarrow σ^* (P-C31)	0.69	0.57	0.018
LP (4) Au \rightarrow σ^* (P-C9)	2.12	0.57	0.031
LP (4) Au \rightarrow σ^* (P-C20)	1.25	0.57	0.024
LP (5) Au \rightarrow σ^* (P-C20)	0.90	0.57	0.020
LP (5) Au \rightarrow σ^* (P-C31)	2.24	0.57	0.032
π^* (C9-C14) \rightarrow π^* (C10-C11)	154.09	0.02	0.080
π^* (C9-C14) \rightarrow π^* (C12-C13)	196.30	0.02	0.084
σ (Au-P) \rightarrow σ^* (N3-C7)	0.84	0.89	0.024
σ (Au-P) \rightarrow σ^* (N3-N4)	0.36	0.75	0.015
LP (3) Au \rightarrow σ^* (N3-C7)	0.20	0.77	0.011
LP (3) Au \rightarrow σ^* (N3-N4)	0.15	0.64	0.009
LP (4) Au \rightarrow σ^* (N3-C7)	1.22	0.78	0.028
LP (4) Au \rightarrow σ^* (N3-N4)	1.92	0.64	0.032
LP (5) Au \rightarrow LP (2) N3	7.75	0.10	0.046
σ (N3-C7) \rightarrow σ^* (Au-P)	3.67	0.85	0.054
σ (N3-N4) \rightarrow σ^* (Au-P)	2.27	0.82	0.041
LP (1) N3 \rightarrow σ^* (Au-P)	103.57	0.50	0.203
σ (N3-N4) \rightarrow σ^* (C7-H8)	3.47	1.31	0.060
σ (N6-C7) \rightarrow LP (2) N3	57.92	0.05	0.081
σ (N6-C7) \rightarrow σ^* (N4-N5)	22.57	0.26	0.073
π (N4-N5) \rightarrow LP (2) N3	32.58	0.08	0.079
π (N4-N5) \rightarrow π^* (C7-N6)	11.00	0.32	0.057
LP (2) N6 \rightarrow π^* (C7-N6)	54.16	0.24	0.107
LP (2) N6 \rightarrow π^* (N4-N5)	42.70	0.21	0.086
π (N4-N5) \rightarrow π^* (C7-N6)	44.10	0.04	0.056

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