Theoretical Study of Xenon-Noble Metal Interaction in MXeM' and XeMM' Molecular Species (M & M' = Cu, Ag, Au)

Devendra Kumar Mahawar
Assistant Professor,
Deptt. of Chemistry,
University of Rajasthan,
Jaipur, Rajasthan
India

Manu Sikarwar
Associate Professor,
Deptt. of Chemistry,
Govt. P.G. College,
Tonk, Rajasthan
India

R.K. Gunsaria
Associate Professor,
Deptt. of Chemistry,
University of Rajasthan,
Jaipur, Rajasthan
India

Ammilal Rao
Assistant Professor,
Deptt. of Chemistry,
University of Rajasthan,
Jaipur, Rajasthan
India

Abstract

In the present work, *ab initio* quantum chemical methods within the framework of density functional theory and second order Møller-Plessset perturbation theory (MP2) have been used for theoretical calculations to investigate the structure and stability of noble gas inserted molecules of type MXeM' and XeMM' (M & M' = Cu, Ag, Au). The structure of all the species are found to be linear having Xenon-Noble metal bond. Energy values for the XeMM´ (M and M´= Cu, Ag, Au), indicates that maximum stability is shown by XeCuAu molecular system (Energy= -277.9 kJ mol^{-1}) with smallest Xe-M bond length 2.485 Å .All the six predicted species of the type MXeM' are found to be metastable in their respective potential energy surface, however they are found to be kinetically stable as evident from the barrier height (ranging 38.9-86.1 kJ mol^{-1}) corresponding to the bent transition state involving the local minima. The present paper support the possibility of experimental synthesis of these xenon inserted compounds containing xenon-noble metal bond.

Keywords: Xenon-Noble Metal Interaction, Ab Initio Methods, Insertion Compounds.

Introduction

In recent years there is much interest shown in the field of chemical compounds formed by rare-gas elements. Rare gas compounds has been investigated[1] more than five decades ago, subsequently there has not been much progress along these lines due to the deficiency in the level of sophistication involved experimentally and also to the inadequacy in the computational power for carrying out theoretical investigations. Last decade was important due to the study of a large number of noble-gas compounds that have been reported in the literature [2-7], and thus opening a new study area in the field of rare gas chemistry. Theoretical studies[8-21] has been done on the nature of bonding in these compounds and on comparison some metastable states were detected to their corresponding dissociated products. Seidel and Seppelt reported[22] the existence of first bulk compound containing a noble-gas–noble-metal bond AuXe$_4$ $^{2+}$[Sb$_2$F$_{11}$]$_2$. It is in contrast with the conventional behavior of noble-gas and noble-metal atoms that have nearly covalent bonds between gold and Xenon although the stability of XeAuXe$^+$ species had already been reported[23] earlier. Consideration of gold as truly noble metal and Xenon as true noble gas will decline the possibility of Au-Xe bond. However, in actual fact, noble metal, such as gold has a very rich and unusual chemistry[24] with varying physicochemical properties, for which, the strong relativistic effect, which considerably decreases the size of the valence 6*s* orbital and leads to the expansion of the 5*d* orbital is responsible. After the study done by Seidel and Seppelt, there has been lot of interest in the search of compounds containing noble-gas–noble-metal bond. Since the polarizabilities increase in the order of He < Ne < Ar < Kr < Xe [25], so there is a greater possibility of binding of Xenon with noble metals. For the last few years there are numerous investigations on the compounds containing noble gas noble atom bond. Other compounds of gold with xenon viz. AuXe$^+$ and XeAuXe$^+$ had been observed[26] experimentally by mass spectroscopy. In all these compounds the noble-gas–noble-metal bonding has been found to be partially covalent in nature and strong interactions are involved between closed-shell fragments noble-gas and noble-metal in this class of systems. Recently, many noble gas- inserted compounds have been reported[27-31] and receiving extensive attention.

Aim of the Study

Owing to an unusually high relativistic effect[32-34], gold evidently tends to be strongly bonded to the noble gas atoms in comparison with silver and copper. The motivation behind this investigation has been the behavior of gold as hydrogen in various gold compounds as reported in the recent years. In this work our objective is to find out whether this class of compounds MXeM′ (M and M′=Cu, Ag, Au) where xenon would confine only to gold atom or this kind of compounds is possible with other coinage metal atoms such as Cu and Ag. Therefore, it would be interesting to investigate the structure and properties of the MXeM′ compounds (M and M′=Cu, Ag, Au) with the aid of quantum chemical calculations and thus to explore whether they are stable or not with respect to their corresponding metastable products on the respective potential energy surface. To the best of our knowledge, there is no such report on these species in the literature. Therefore in this paper we report XeMM′ and MXeM′ molecular species (M and M′=Cu, Ag, Au). Theoretical methods such as density functional theory (DFT) and second order Moller Plesset perturbation theory (MP2) have been used to predict the structure and stability of these species as these methods are often employed to predict analogous species.

Computational Methods

Electronic structures have been investigated using the GAMESS[35] and ORCA[36] package codes. MP2, DFT along with hybrid exchange correlation energy functional B3LYP method are employed to investigate the geometrical structures of XeMM′ and MXeM′ (M and M′= Cu, Ag, Au) molecular species in their minima and transition states (T.S.). Energy adjusted Stuttgart effective core potentials basis sets have been employed for all the MP2 and DFT calculations. The stability of the species is determined by computing the energy differences between the predicted species.

Results and Discussions

Structure

The MP2 calculated geometrical parameters corresponding to the optimized structures of the XeMM′ species are reported in Table I. The MP2 calculated Xe-Ag bond lengths in XeAgAu, XeAgCu and XeAgAg computed here have been found to be 2.819, 2.960, and 2.969 Å respectively , and Ag-M (M=Au, Cu, Ag) bond lengths have been found to be 2.513, 2.365 and 2.527 Å respectively . Therefore the shorter bond length of Xe-Ag bond in XeAgAu in comparison to XeAgCu indicates stronger binding between Xe-Ag bond in XeAgAu. The calculated **Xe-Au** bond lengths in the XeAuCu, XeAuAg and XeAuAu compounds have been found to be 2.983, 2.992, and 2.758 Å respectively and for Au-M (M=Cu, Ag, Au) bond lengths have been found to be 2.332, 2.516 to 2.499 Å respectively. Therefore the shorter bond length of Xe-Au bond in XeAuCu in comparison to XeAuAg indicates stronger binding between Xe-Au bond in XeAuCu. In the XeCuAu, XeCuAg and XeCuCu compounds , the calculated bond lengths for Xe-Cu have been found to be 2.485, 2.588 and 2.595 Å respectively and Cu-M (M=Au, Ag, Cu) bond lengths have been found to be 2.326, 2.364 and 2.203 Å respectively. Therefore the shorter bond length of Xe-Cu bond in XeCuAu in comparison to XeCuAg indicates stronger binding between Xe-Cu bond in XeCuAu. In the T.S., the bond length for Xe-Ag in XeAgAu, XeAgCu and XeAgAg molecular species have been calculated 2.941, 3.179 and 3.146 Å respectively. For XeAuCu, XeAuAg and XeAuAu molecular species, the bond lengths in the T.S. for Xe-Au bond have been calculated 3.156, 3.128 and 3.016 Å respectively. In the T.S., the bond lengths for Xe-Cu in XeCuAu, XeCuAg and XeCuCu molecular species have been calculated 2.568, 2.816 and 2.879 Å respectively. The structure of the T.S. has been found to be bent in all the cases, where the MXeM′ bending mode is involved in going from the minimum energy structure to the saddle point. An increase in almost all Xe-M bond distances has been observed at the T.S. The MP2 calculated bond angle is 180° for all the XeMM′ species. The bond angle also changes from minima position to the T.S. This is the result of transformation of linear structure at the minima to the nonlinear structure at the T.S. The bond angle has also been found to be changed from the equilibrium value of 180° to 103.3°, 104.3° and 100.7° in T.S. for XeAgCu, XeAuCu and XeAgAu.

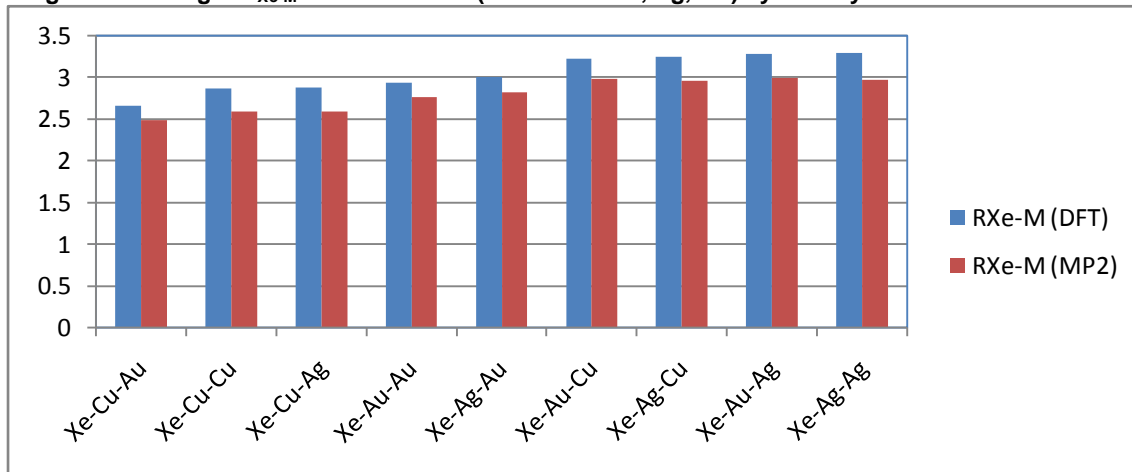**Fig 1: Bond length R_{Xe-M} in Å for XeMM′ (M and M′= Cu, Ag, Au) system by DFT and MP2 Methods**

Table I. Optimized geometrical parameters (bond length R in Å and bond angle θ in degrees: TS-Transition state) of XeMM´ (M and M´= Cu, Ag, Au) system by MP2 and DFT methods.

Bond	Methods	Xe-Ag-Cu Minima	Ag-Xe-Cu Minima	TS	Bond	Methods	Xe-Ag-Cu Minima	Xe-Cu-Ag Minima
R (Xe-Ag)	DFT	3.249	3.068	3.447	R (Ag-Cu)	DFT	2.412	2.419
	MP2	2.960	2.959	3.179		MP2	2.365	2.364
Angle	DFT	180	180	107.4	Angle	DFT	180	180
	MP2	180	180	103.3		MP2	180	180

Bond	Methods	Xe-Cu-Ag Minima	Ag-Xe-Cu Minima	TS	Bond	Methods	Xe-Ag-Au Minima	Ag-Xe-Au Minima	TS
R (Xe-Cu)	DFT	2.881	2.770	3.081	R (Xe-Ag)	DFT	3.000	2.994	
	MP2	2.588	2.668	2.816		MP2	2.819	2.857	2.941
Angle	MP2	180	180		Angle	DFT	180	180	104.5
	DFT	180	180			MP2	180	180	100.7

Bond	Methods	Xe-Ag-Au Minima	Xe-Au-Ag Minima	Bond	Methods	Xe-Au-Ag Minima	Ag-Xe-Au Minima	TS
R(Ag-Au)	DFT	2.570	2.575	R(Xe-Au)	DFT	3.279	2.989	
	MP2	2.513	2.516		MP2	2.992	2.828	3.128
Angle	MP2	180	180	Angle	DFT	180	180	
	DFT	180	180		MP2	180	180	

Bond	Methods	Xe-Au-Cu Minima	Au-Xe-Cu Minima	TS	Bond	Methods	Xe-Au-Cu Minima	Xe-Cu-Au Minima
R (Xe-Au)	DFT	3.226	2.966	3.385	R (Au-Cu)	DFT	2.384	2.382
	MP2	2.983	2.835	3.156		MP2	2.332	2.326
Angle	DFT	180	180	108.5	Angle	DFT	180	180
	MP2	180	180	104.3		MP2	180	180

Bond	Methods	Xe-Cu-Au Minima	Au-Xe-Cu Minima	TS	Bond	Methods	Xe-Ag-Ag Minima	Ag- Xe-Ag Minima	TS
R (Xe-Cu)	DFT	2.664	2.653	2.632	R (Xe-Ag)	DFT	3.291	3.108	3.420
	MP2	2.485	2.559	2.568		MP2	2.969	2.982	3.146
Angle	DFT	180	180		Angle	DFT	180	180	111
	MP2	180	180			MP2	180	180	104.8

Bond	Methods	Xe-Au-Au Minima	Au-Xe-Au Minima	TS	Bond	Methods	Xe-Ag-Ag Minima
R (Xe-Au)	DFT	2.934	2.868	3.255	R (Ag-Ag)	DFT	2.586
	MP2	2.758	2.736	3.016		MP2	2.527
Angle	DFT	180	180	100.7	Angle	DFT	180
	MP2	180	180			MP2	180

Bond	Methods	Xe-Cu-Cu Minima	Cu-Xe-Cu Minima	TS	Bond	Methods	Xe-Au-Au Minima
R (Xe-Cu)	DFT	2.863	2.794	3.140	R (Au-Au)	DFT	2.560
	MP2	2.595	2.690	2.879		MP2	2.499
Angle	DFT	180	180	105.2	Angle	DFT	180
	MP2	180	180	101.5		MP2	180

Bond	Methods	Xe-Cu-Cu Minima
R (Cu-Cu)	DFT	2.248
	MP2	2.203
	Angle	180

Energies and Stabilities

We have used two different theoretical methods, namely, MP2 and DFT in order to estimate the accurate energy diagram for the present system of rare gas –noble metal. It has been observed that the two methods provides similar energy diagram. Since the predicted molecular species MXeM´ (M and M´= Cu, Ag, Au) is metastable in nature, it changes to different molecular structure depending on its energetic stability. Table II lists the relevant computed energies in kJ mol^{-1} for different molecular species. It is clear from the energy table that the MXeM´ molecular species is metastable with respect to the global minimum XeMM´ and is higher in energy. It is clear from the tabulated energy values of MP2 methods that AgXeCu is 231.3 kJ mol^{-1} higher in energy than XeAgCu and 242.7 kJ mol^{-1} higher in energy than XeCuAg. The energy values calculated

using DFT, have been found to be -199.4, -201.6 and 30.7 kJ mol^{-1} respectively for XeAgCu, XeCuAg and AgXeCu [T.S]. The energy values calculated using MP2 method for AgXeAu suggests that it is 245.2 kJ mol^{-1} higher in energy than XeAgAu and 230.3 kJ mol^{-1} higher in energy than XeAuAg. The energy values calculated using DFT are -204.9, - 194.8 and 34.0 kJ mol^{-1} respectively for XeAgAu, XeAuAg and AgXeAu [T.S.]. Similarly using MP2 method, energy values for AuXeCu are higher in energy by 242.6 kJ mol^{-1} than XeAuCu and 277.9 kJ mol^{-1} from XeCuAu. The energy values calculated using DFT, have been found to be -209.5, -227.3 and 42.9 kJ mol^{-1} respectively for XeAuCu, XeCuAu and AuXeCu [T.S.]. The saddle

point energy calculated using MP2 method for AgXeCu, AgXeAu and AuXeCu are 48.1, 53.8 and 62.3 kJ mol^{-1} respectively. Comparison of saddle point energies indicate that the saddle point for the AuXeCu takes more time to reach than AgXeAu and AgXeCu. The barrier heights are crucial for storing and measuring properties of XeMM´ molecular species. Comparison of the energy values for the XeMM´ (M and M´= Cu, Ag, Au), indicates that maximum stability is shown by XeCuAu molecular system. Similarly comparing the energy values for XeAgAg, XeAuAu and XeCuCu molecular species, maximum stability is shown by XeCuCu system.

TABLE II. Energies (in kJ mol^{-1}) of the various molecular species relative to XeMM´ (M and M´=Cu, Ag, Au) calculated using MP2 and DFT methods.

Ag-Xe-Cu		Xe-Ag-Cu		Xe-Cu-Ag		T.S .	
MP2	DFT	MP2	DFT	MP2	DFT	MP2	DFT
0.0	0.0	-231.3	-199.4	-242.7	-201.6	48.1	30.7
Au-Xe-Cu		**Xe-Au-Cu**		**Xe-Cu-Au**		**T.S.**	
MP2	DFT	MP2	DFT	MP2	DFT	MP2	DFT
0.0	0.0	-242.6	-209.5	-277.9	-227.3	62.3	42.9
Ag-Xe-Au		**Xe-Ag-Au**		**Xe-Au-Ag**		**(T.S.)**	
MP2	DFT	MP2	DFT	MP2	DFT	MP2	DFT
0.0	0.0	-245.2	-204.9	-230.3	-194.8	53.8	34.0
Ag-Xe-Ag		**Xe-Ag-Ag**		**(T.S.)**			
MP2	DFT	MP2	DFT	MP2	DFT		
0.0	0.0	-221.1	-187.6	38.9	14.2		
Cu-Xe-Cu		**Xe-Cu-Cu**		**(T.S.)**			
MP2	DFT	MP2	DFT	MP2	DFT		
0.0	0.0	-258.8	-212.9	59.4	40.3		
Au-Xe-Au		**Xe-Au-Au**		**(T.S.)**			
MP2	DFT	MP2	DFT	MP2	DFT		
0.0	0.0	-231.4	-200.8	86.1	57.2		

Fig 2: Energies (in kJ mol^{-1}) Comparison of the Various Molecular Species of Type XeMM´ (M and M´=Cu, Ag, Au) Calculated Using MP2 and DFT Methods
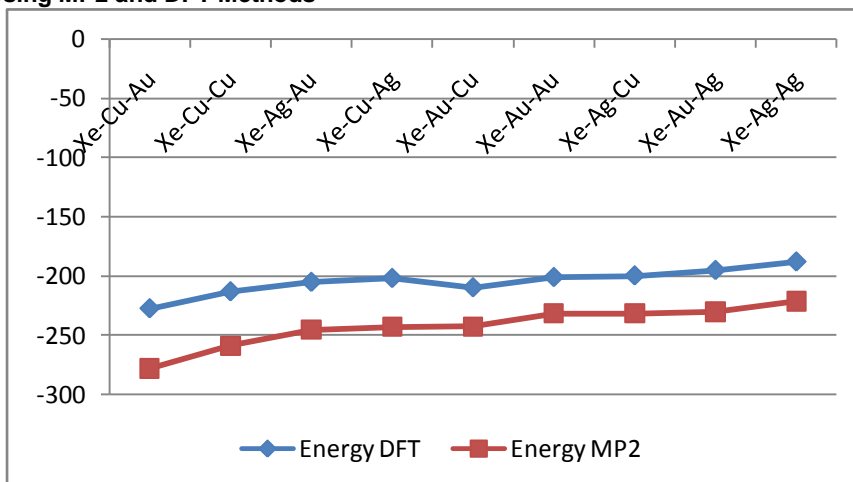
Conclusion

In the present work we have investigated the ground as well as transition states of rare gas inserted molecules of the general formula XeMM´ (M and M´=

Cu, Ag, Au) using *ab initio* quantum chemical methods within the framework of the DFT and second order Møller-Plessset MP2 perturbation theory . The structure and the stability XeMM´ species are

explored. Energy values for the XeMM´ (M and M´= Cu, Ag, Au), indicates that maximum stability is shown by XeCuAu molecular system (Energy= -277.9 kJ mol^{-1}) with smallest Xe-M bond length (2.485 Å) as calculated by MP2 method and it is very much close to the Xe-Cu bond lengths reported by J.M. Michaud[15] et al. in XeCuF and XeCuCl molecules. All the six predicted species of the type MXeM´ are found to be metastable in nature as compared to their corresponding global minimum structures of the type XeMM´. However, they are found to be kinetically stable as evident from the barrier height (ranging 38.9 - 86.1 kJ mol^{-1}) corresponding to the bent transition state involving the local minima. The predicted species widen the field of rare gas chemistry containing noble metal atoms–rare gas bonding. These species might be the next generation candidates for gas phase or matrix isolation experiments. Further, it would be interesting to perform CCSD (T), ZPE correction, IR studies, and harmonic vibrational analysis on these species, which will be considered later. We further believe that the present calculated values might not change significantly with the higher level of theory as is evident from the recently reported results of the molecule at MP4 levels of theories.

Acknowledgements

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