

Structural characteristics of small magnesium dichloride clusters: A systematic theoretical study.

Supporting information

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The isomers of $(\text{MgCl}_2)_n$ clusters were systematically constructed up to $n = 3$. We started from atoms, and combined the atoms to compounds in all possible ways. In order to take control of the large number of combinations, rising rapidly as a function of the cluster size, two building mechanisms were considered separately. In the first mechanism, forming only structures called **singles**, atoms and smaller **single** substructures were connected to each other via bridging units. Consequently, these **single** structures do not contain any terminal (1-coordinated) atoms, excluding atoms and linear chains, which are considered as **single** structures for simplicity. The second building mechanism combines these **single** structures via bonds. The resulting structures are denoted as **doubles**, **triples**, **quadruples** and so on, depending on the number of **single** structures, which they are constructed of. All combinations were considered for both construction mechanisms.

In the tables below, all structures required for all-inclusive consideration of the isomers of magnesium dichloride clusters are listed. Since the contents of the tables can be utilized also for studies on other compounds than $(\text{MgCl}_2)_n$, explanation of the applied terms is necessary. The tables are arranged as follows: The left column (Group) contains information on the composition of atoms in the compound. The first number describes how many atoms the molecule has. It is followed by a superscript with a number and a minus sign in brackets. This gives the numeric relationship between the more electropositive (Mg) and more electronegative (Cl) atom in the compound. In the case of magnesium dichlorides, a group symbol of $9^{(3-)}$, for example, tells us that the molecule contains 9 atoms, 3 magnesiums and 6 chlorines. The substructures with a plus sign also need to be, and have been, considered, even though they are not listed separately to save space. The middle column (Fragment) contains a sketchy drawing of the molecule in question. The role of the right column (Type) is to identify the structural characteristics of the compound: Group, number of bonds and highest coordination numbers ($\alpha = 1$, $\beta = 2$, etc.) for both electropositive and electronegative atoms.

Group	Fragment	Type
1 ⁽⁻⁾		1 ⁽⁻⁾

Group	Fragment	Type
2		2-1- $\alpha\alpha$

Group	Fragment	Type
3 ⁽⁻⁾		3 ⁽⁻⁾ -2- $\beta\alpha$

Group	Fragment	Type
4		4-3- $\beta\beta$

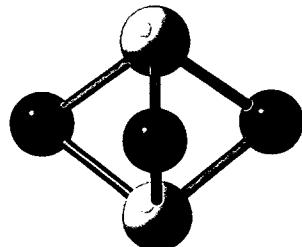
Group	Fragment	Type
4		4-4- $\beta\beta$

Group	Fragment	Type



$5^{(-)}$

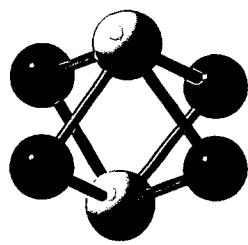
$5^{(+)}\text{-}6\text{-}\gamma\beta$

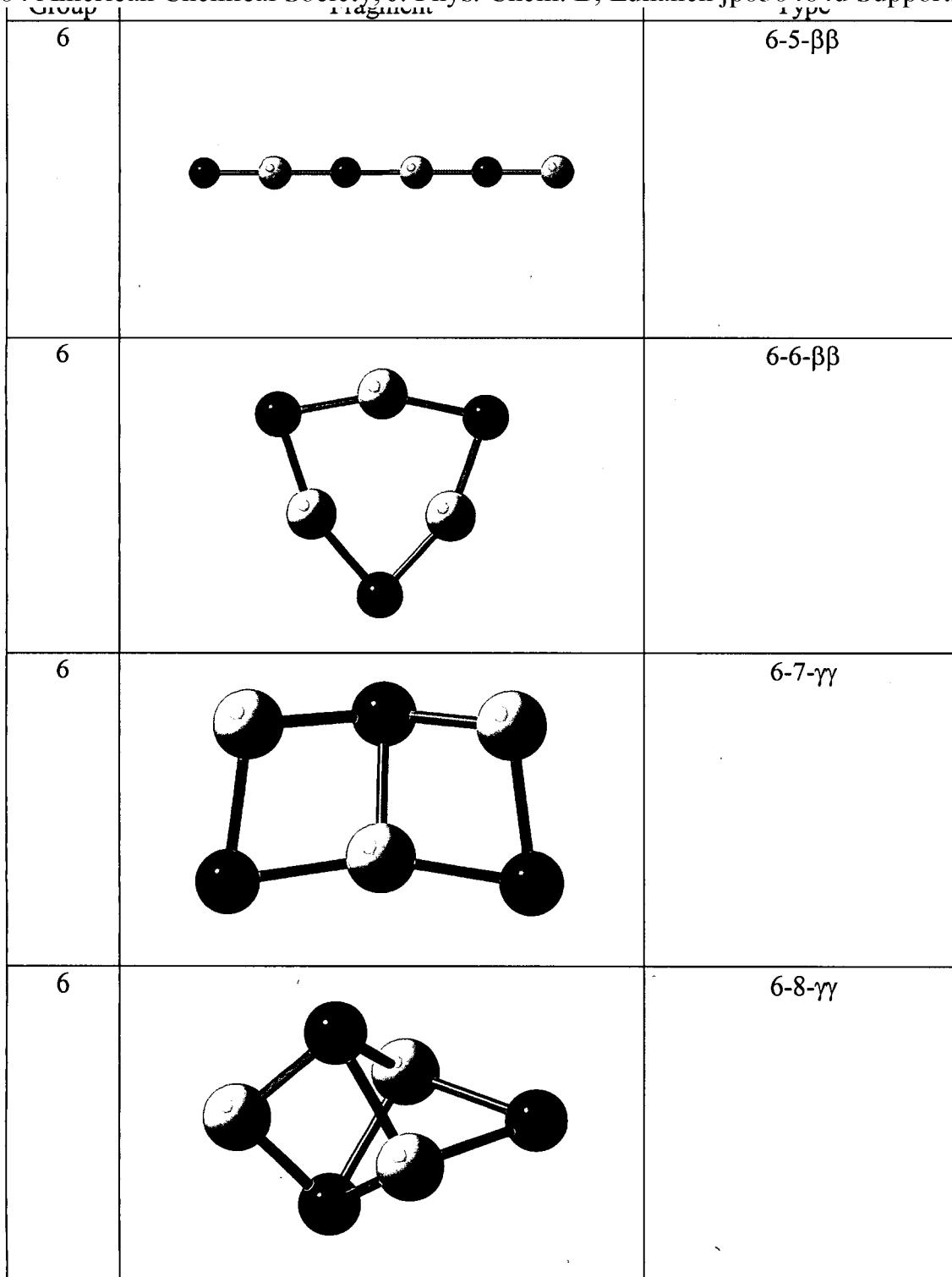


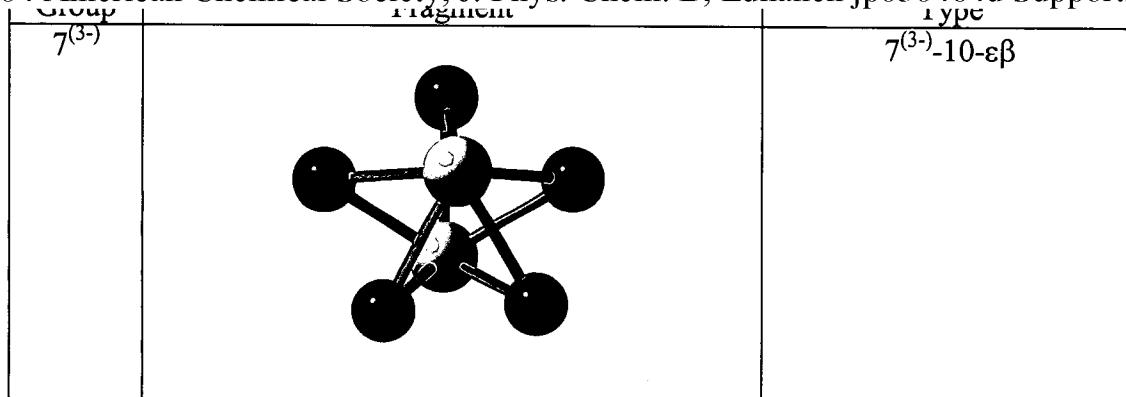
Group
 $6^{(2-)}$

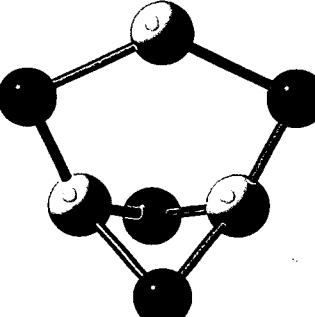
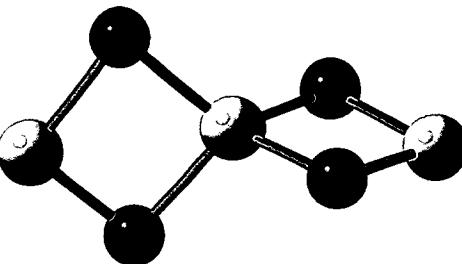
Fragment

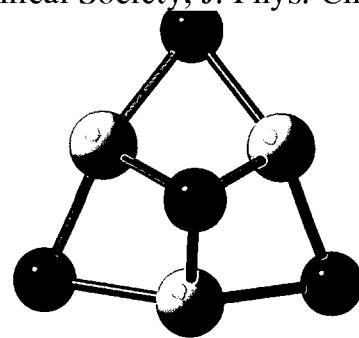
Type
 $6^{(2-)}\text{-}8\text{-}\delta\beta$





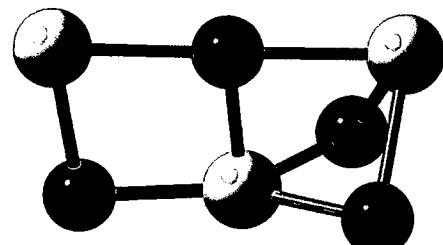


Group $7^{(-)}$	Fragment	Type $7^{(-)}\text{-}6\text{-}\beta\beta$
		
		Fragment $7^{(-)}\text{-}8\text{-}\gamma\beta$
		Fragment $7^{(-)}\text{-}8\text{-}\delta\beta$



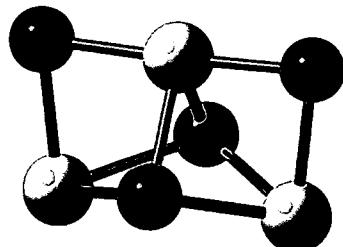
7⁽⁺⁾

7⁽⁺⁾-9- $\delta\gamma$



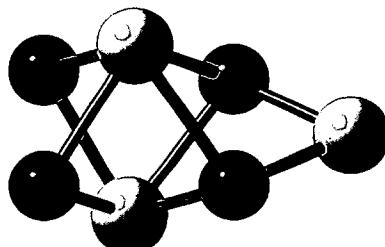
7⁽⁺⁾

7⁽⁺⁾-10- $\delta\gamma$ 1



7⁽⁺⁾

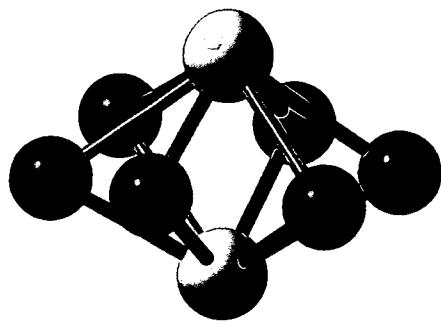
7⁽⁺⁾-10- $\delta\gamma$ 2



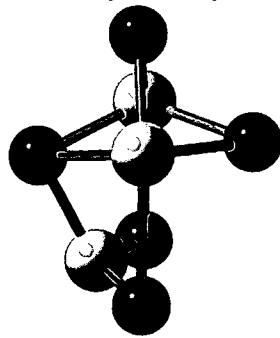
Group

Fragment

Type

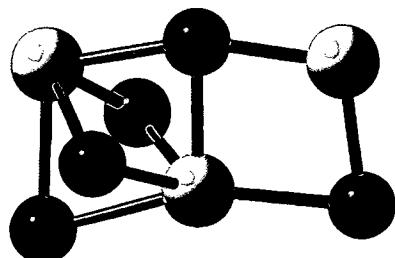


Group	Fragment	Type
$8^{(2)}$		$8^{(2)}\text{-}10\text{-}\delta\beta 1$
$8^{(2)}$		$8^{(2)}\text{-}10\text{-}\delta\beta 2$
$8^{(2)}$		$8^{(2)}\text{-}10\text{-}\varepsilon\beta$



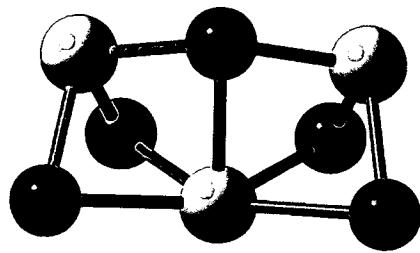
$8^{(2-)}$

$8^{(2-)}-11-\varepsilon\gamma 1$



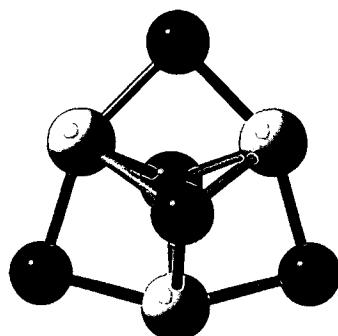
$8^{(2-)}$

$8^{(2-)}-11-\varepsilon\gamma 2$



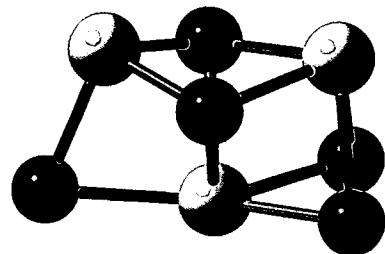
$8^{(2-)}$

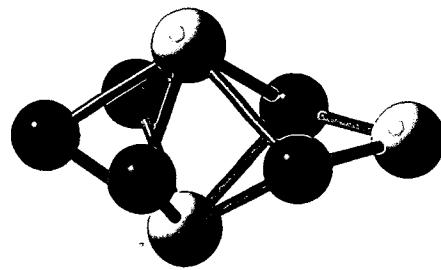
$8^{(2-)}-12-\delta\gamma$



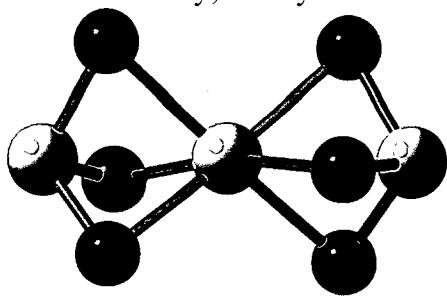
$8^{(2-)}$

$8^{(2-)}-12-\varepsilon\gamma 1$



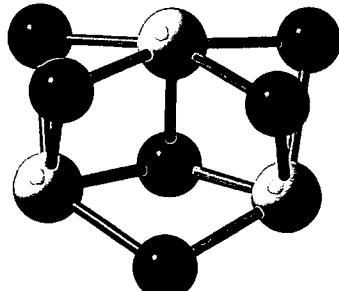


Group	Fragment	Type
$9^{(3)}$		$9^{(3)}\text{-}12\text{-}\delta\beta$
$9^{(3)}$		$9^{(3)}\text{-}12\text{-}\epsilon\beta 1$
$9^{(3)}$		$9^{(3)}\text{-}12\text{-}\epsilon\beta 2$
$9^{(3)}$		$9^{(3)}\text{-}12\text{-}\phi\beta 1$



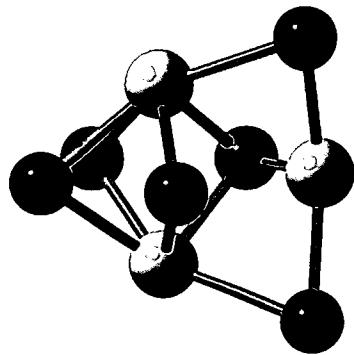
$9^{(3)}$

$9^{(3)}\text{-}13\text{-}\varepsilon\gamma 1$



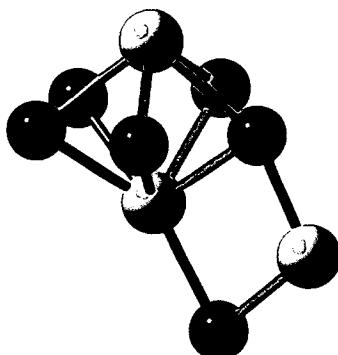
$9^{(3)}$

$9^{(3)}\text{-}13\text{-}\varepsilon\gamma 2$



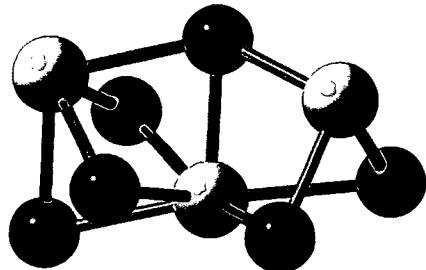
$9^{(3)}$

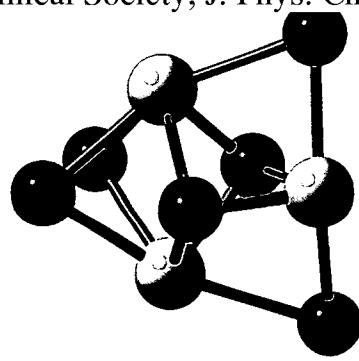
$9^{(3)}\text{-}13\text{-}\phi\gamma 1$



$9^{(3)}$

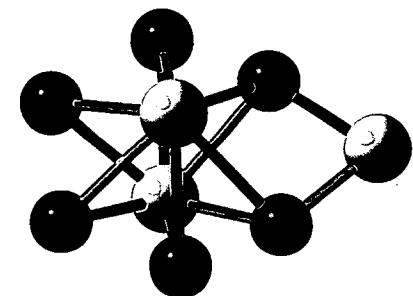
$9^{(3)}\text{-}13\text{-}\phi\gamma 2$





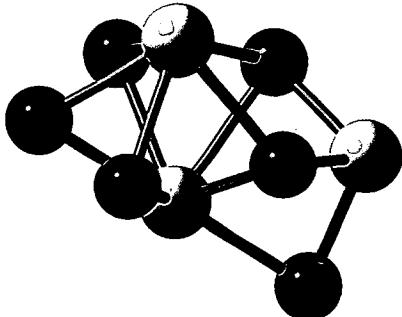
$9^{(3)}$

$9^{(3)}\text{-}14\text{-}\phi\gamma 1$



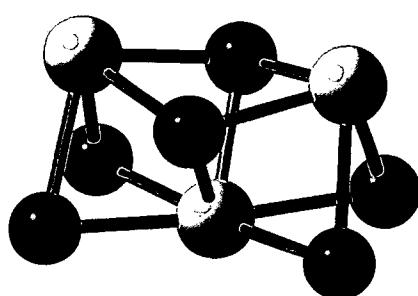
$9^{(3)}$

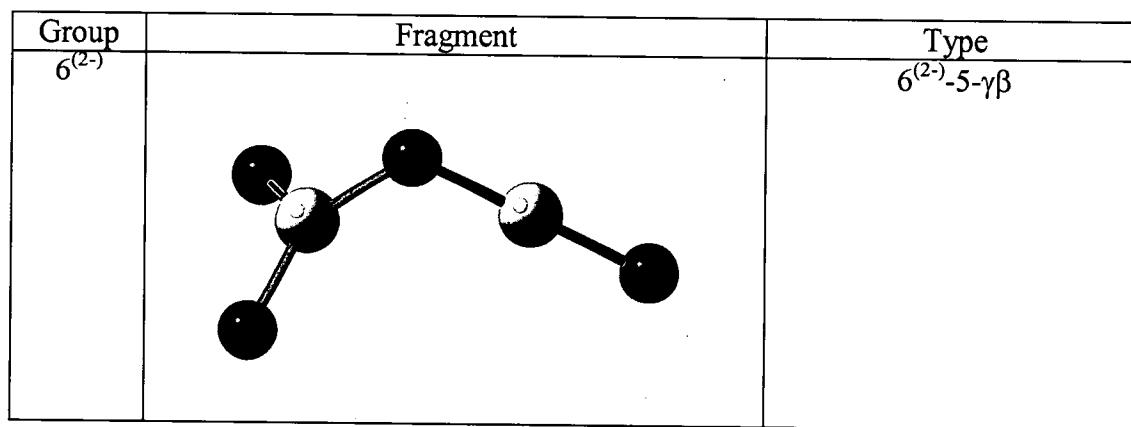
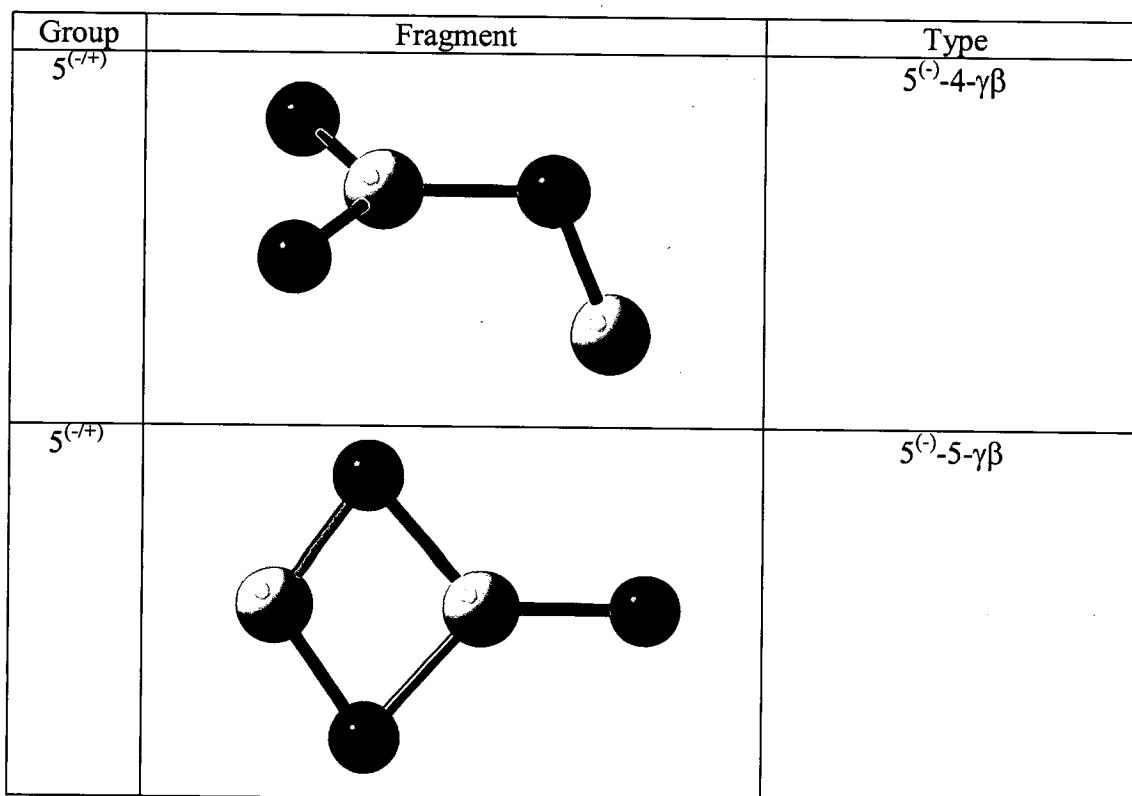
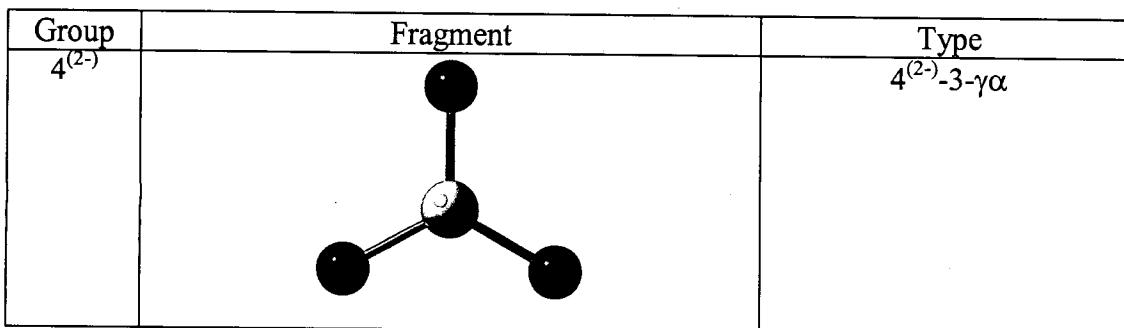
$9^{(3)}\text{-}14\text{-}\phi\gamma 2$

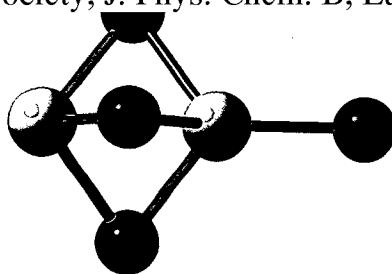


$9^{(3)}$

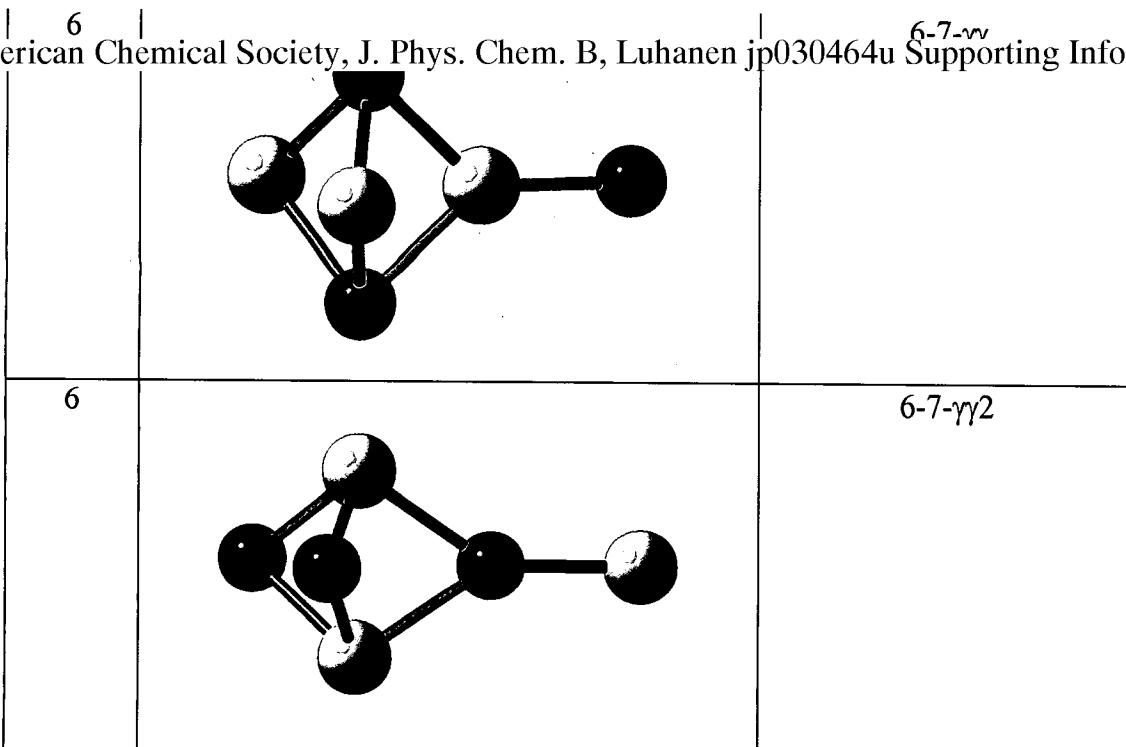
$9^{(3)}\text{-}14\text{-}\phi\gamma 3$

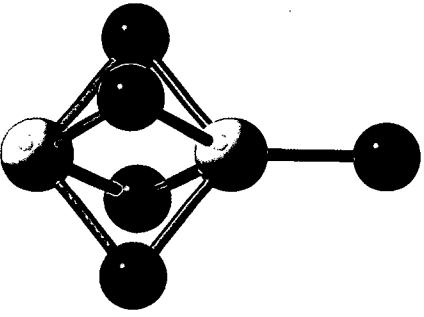


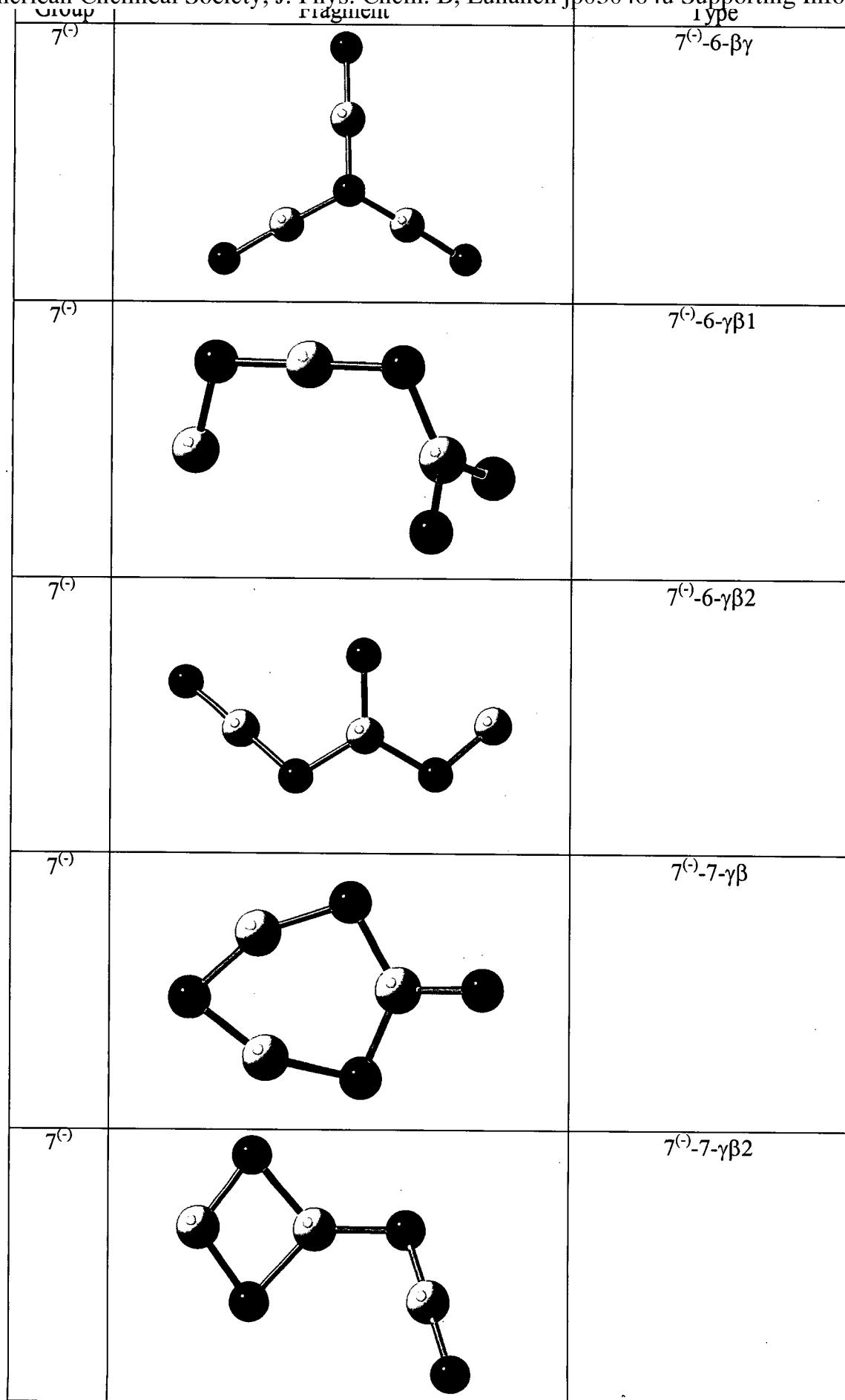


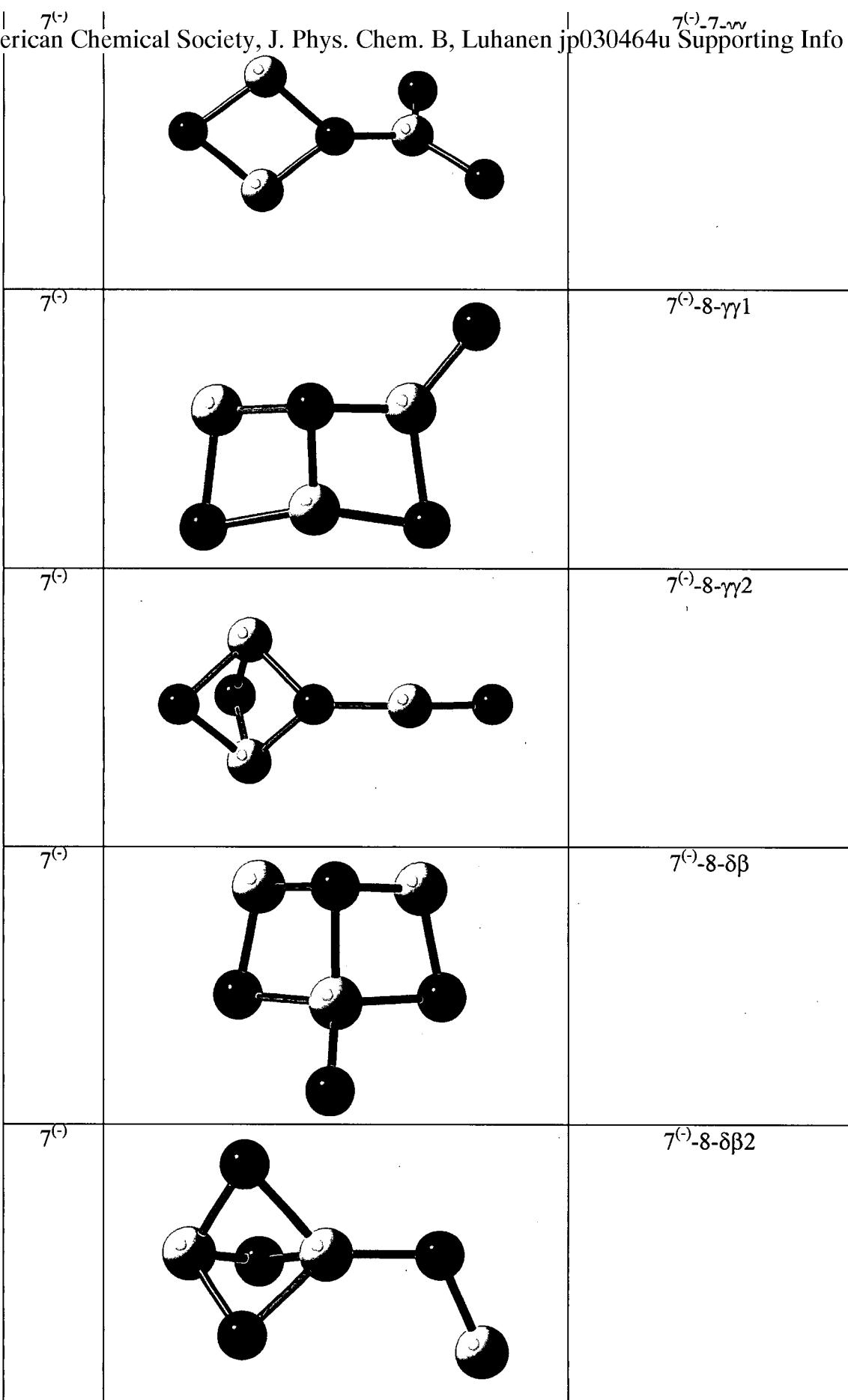


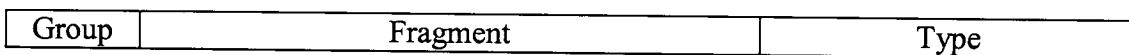
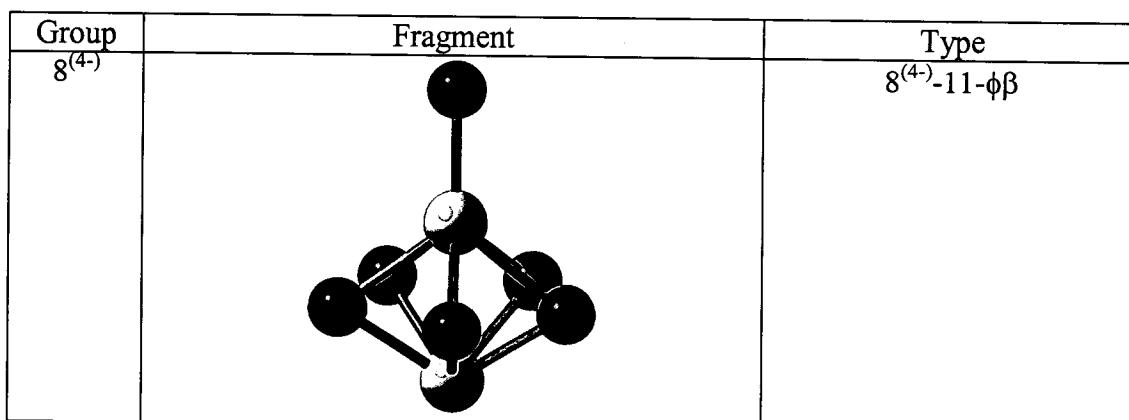
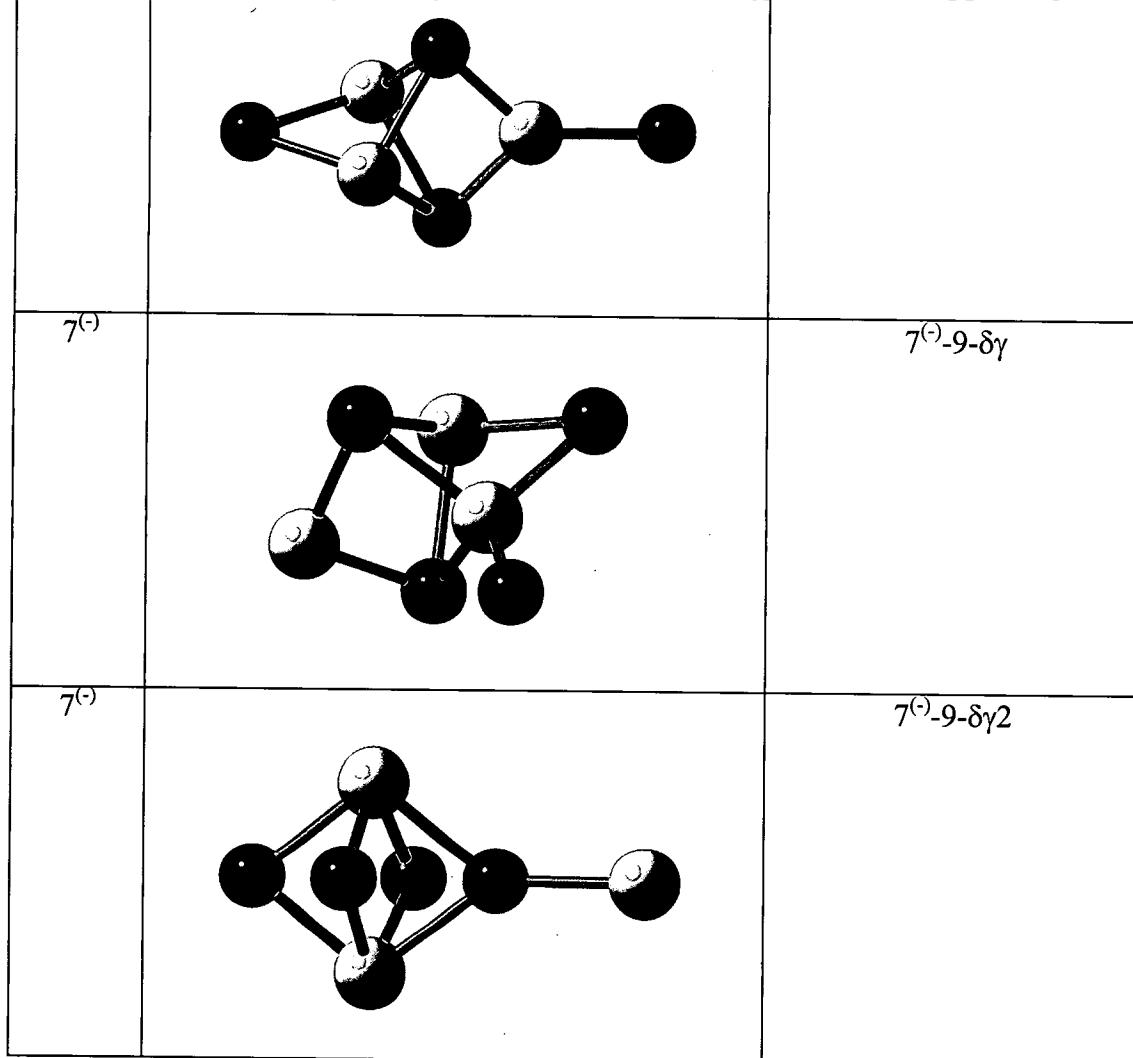
Group	Fragment	Type
6		6-5- $\beta\gamma$
6		6-5- $\gamma\beta$
6		6-6- $\beta\gamma$
6		6-6- $\gamma\beta$

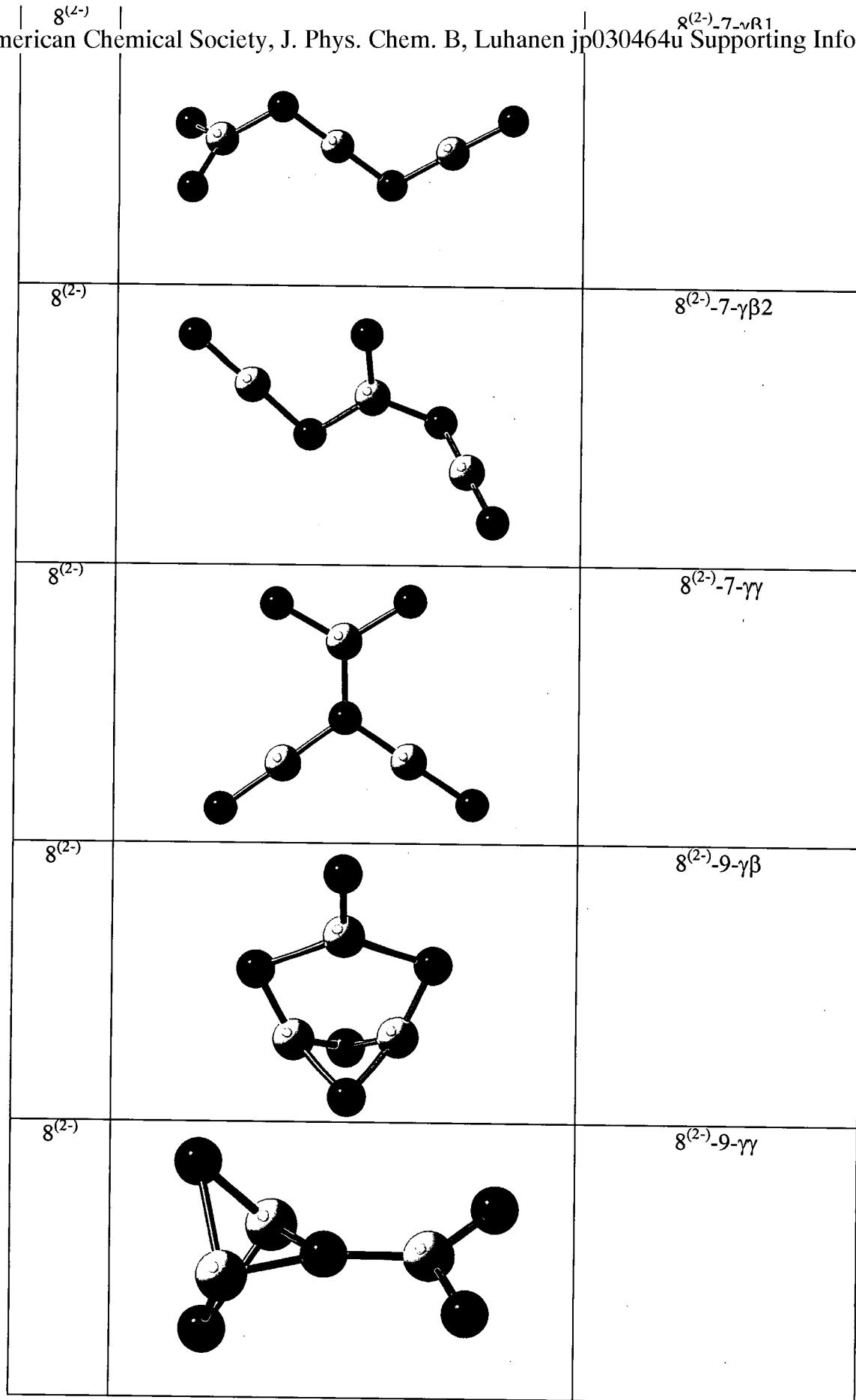


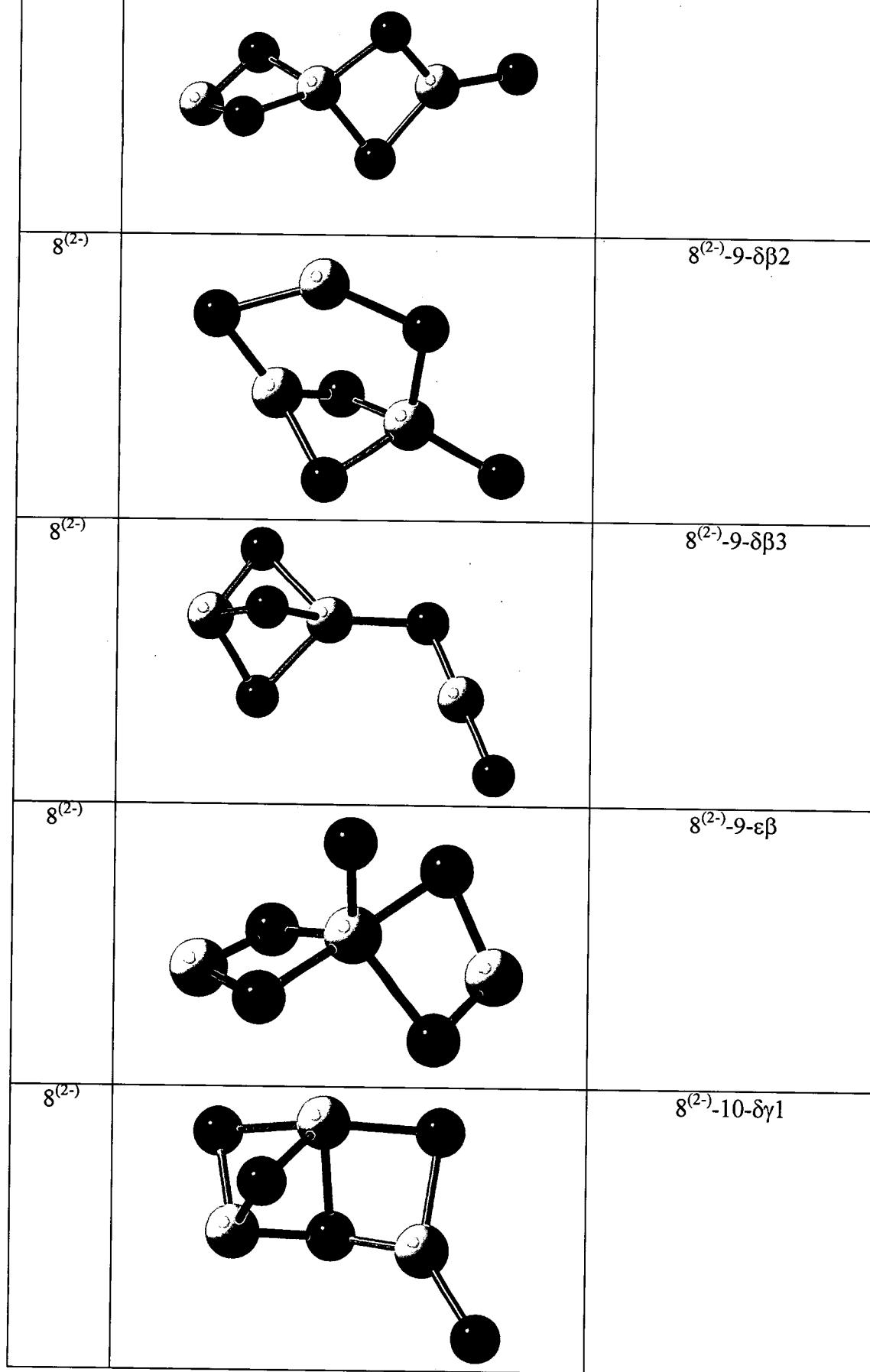
Group	Fragment	Type
$7^{(3)}$		$7^{(3)}\text{-}9\text{-}\epsilon\beta$

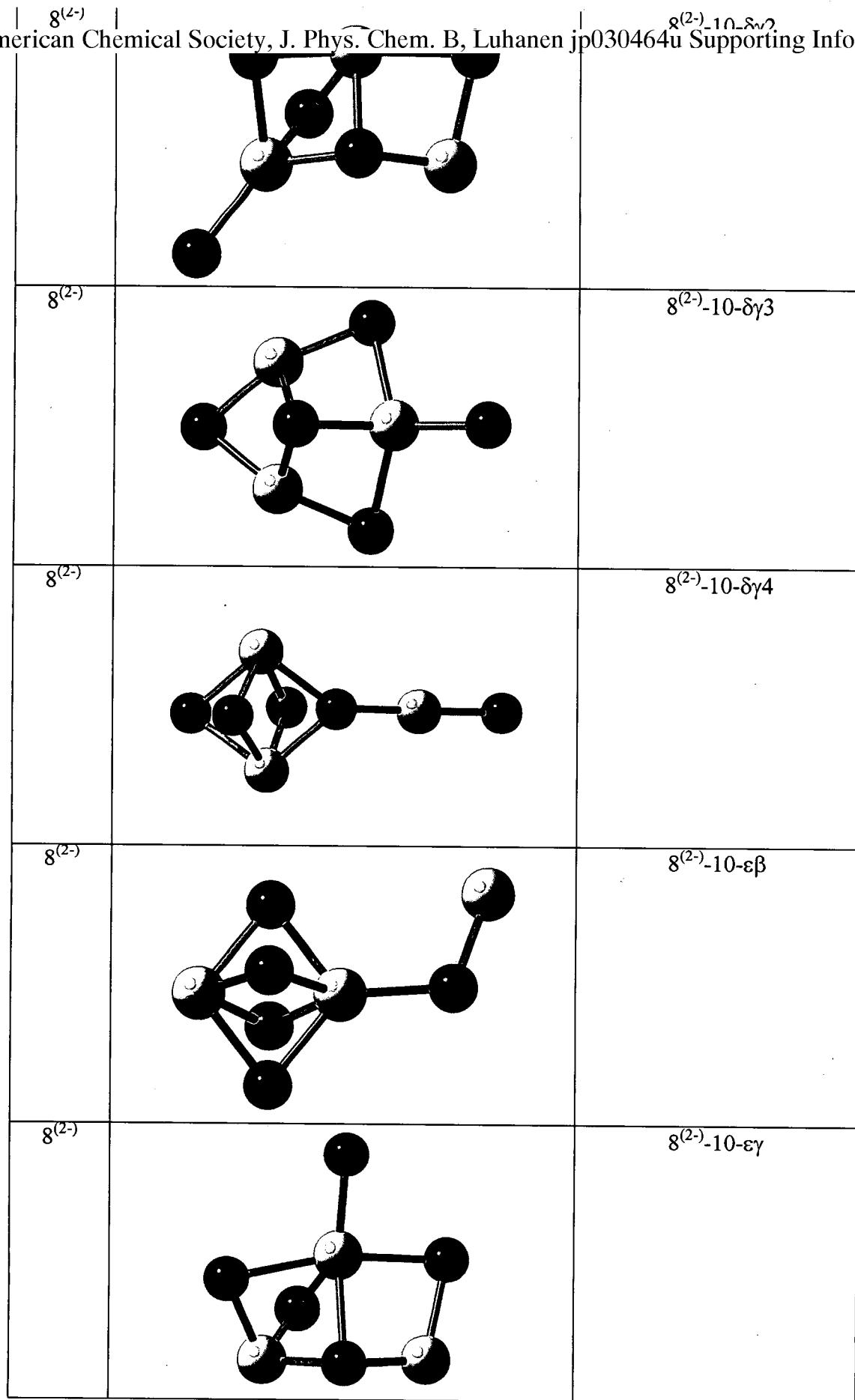


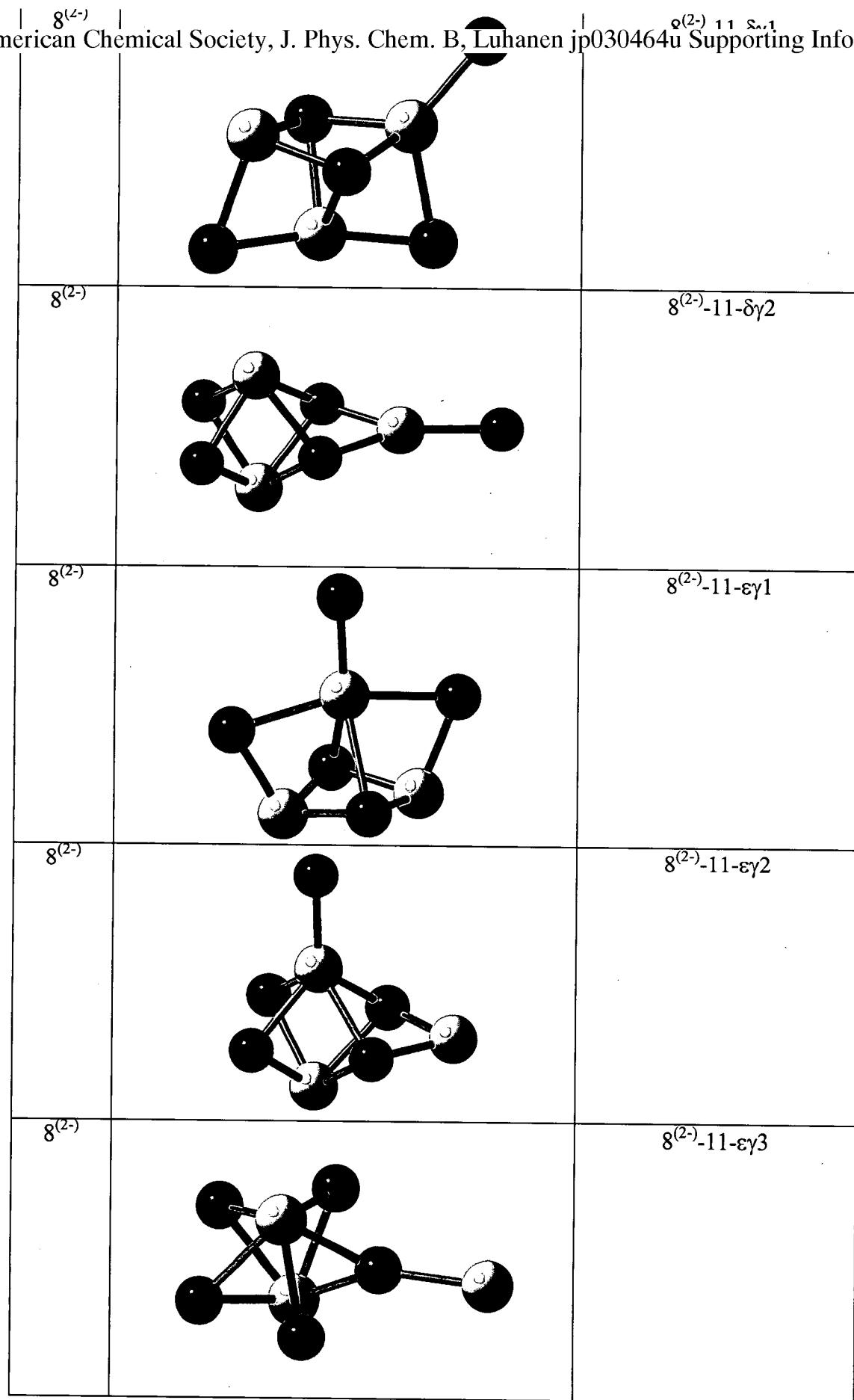




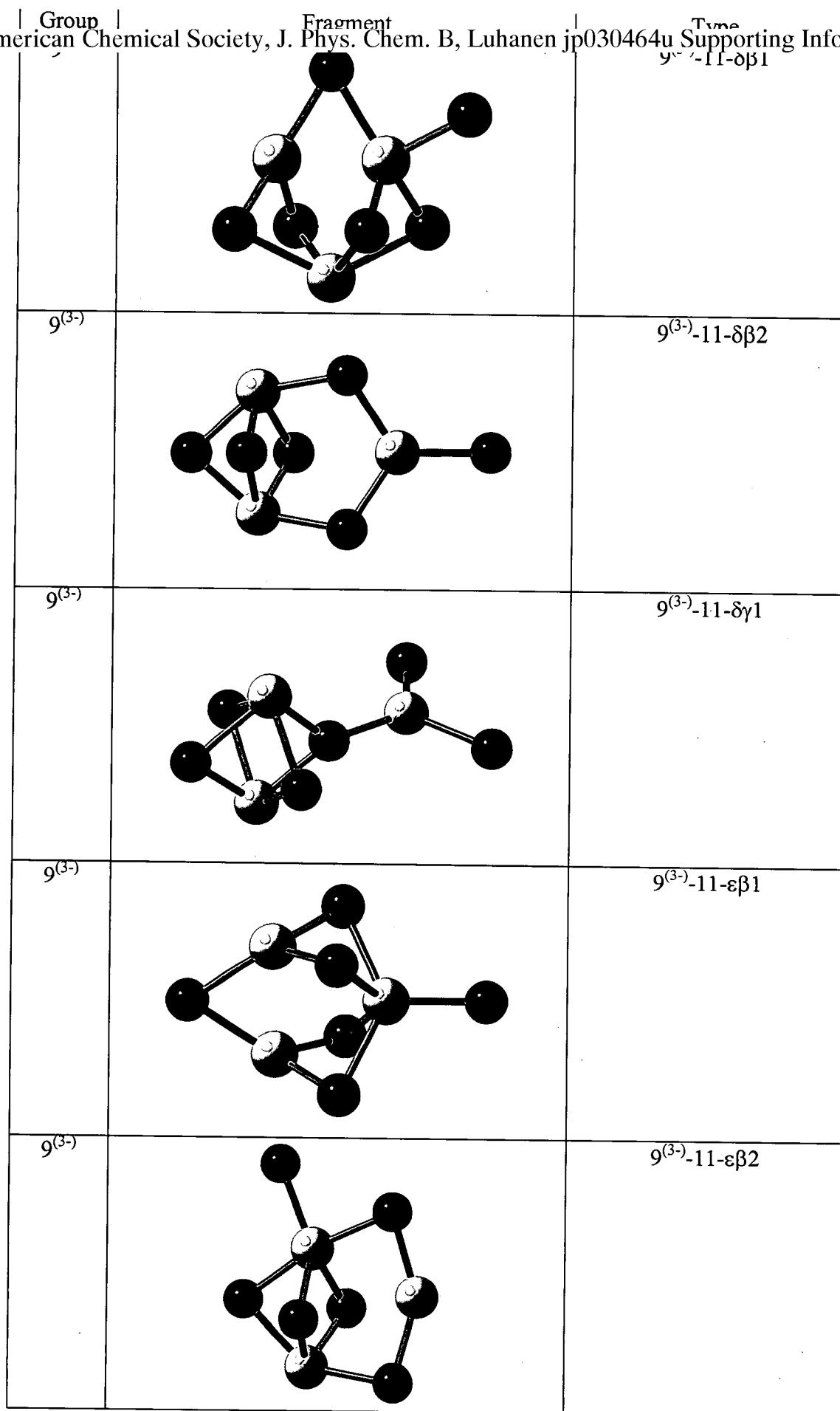


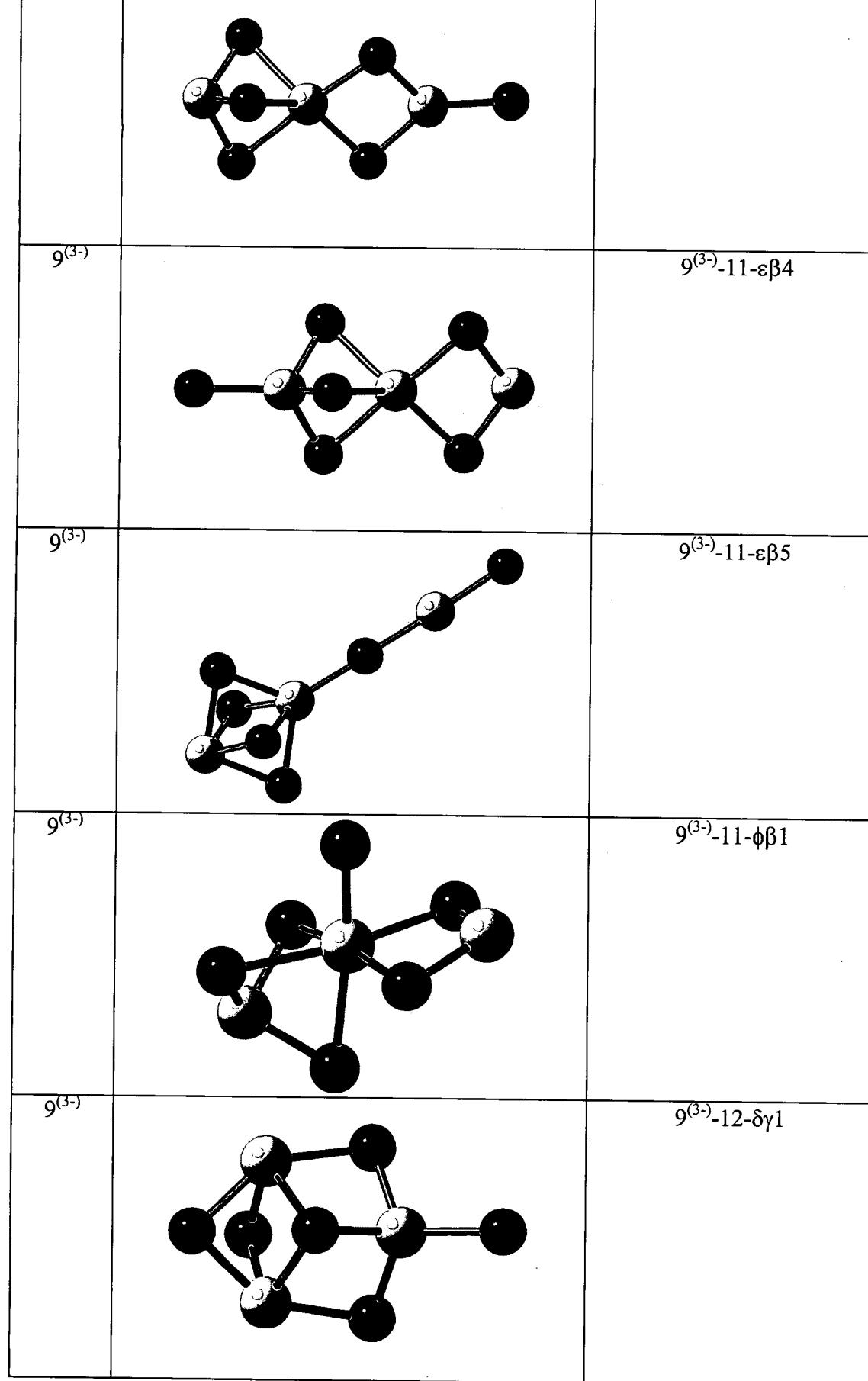


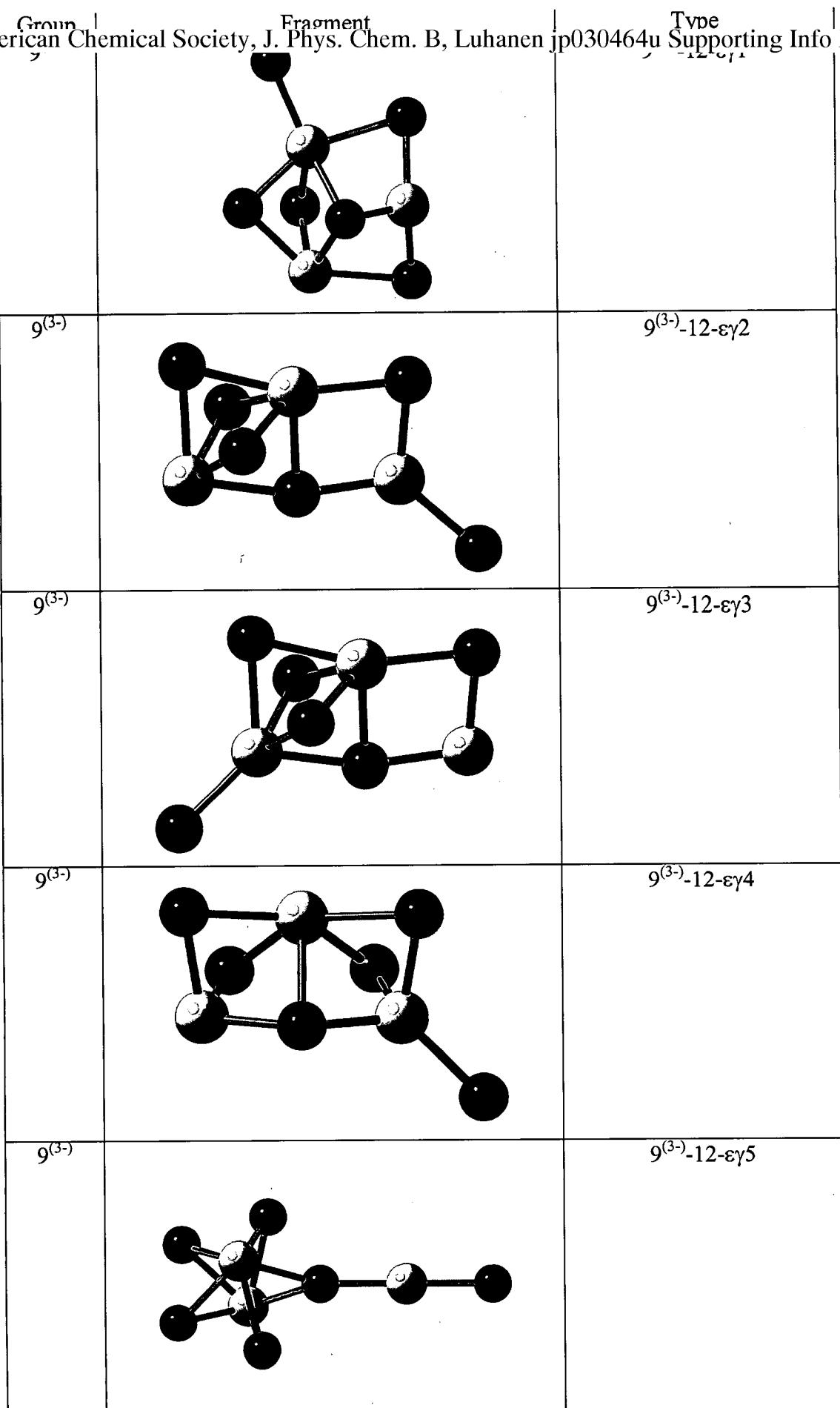


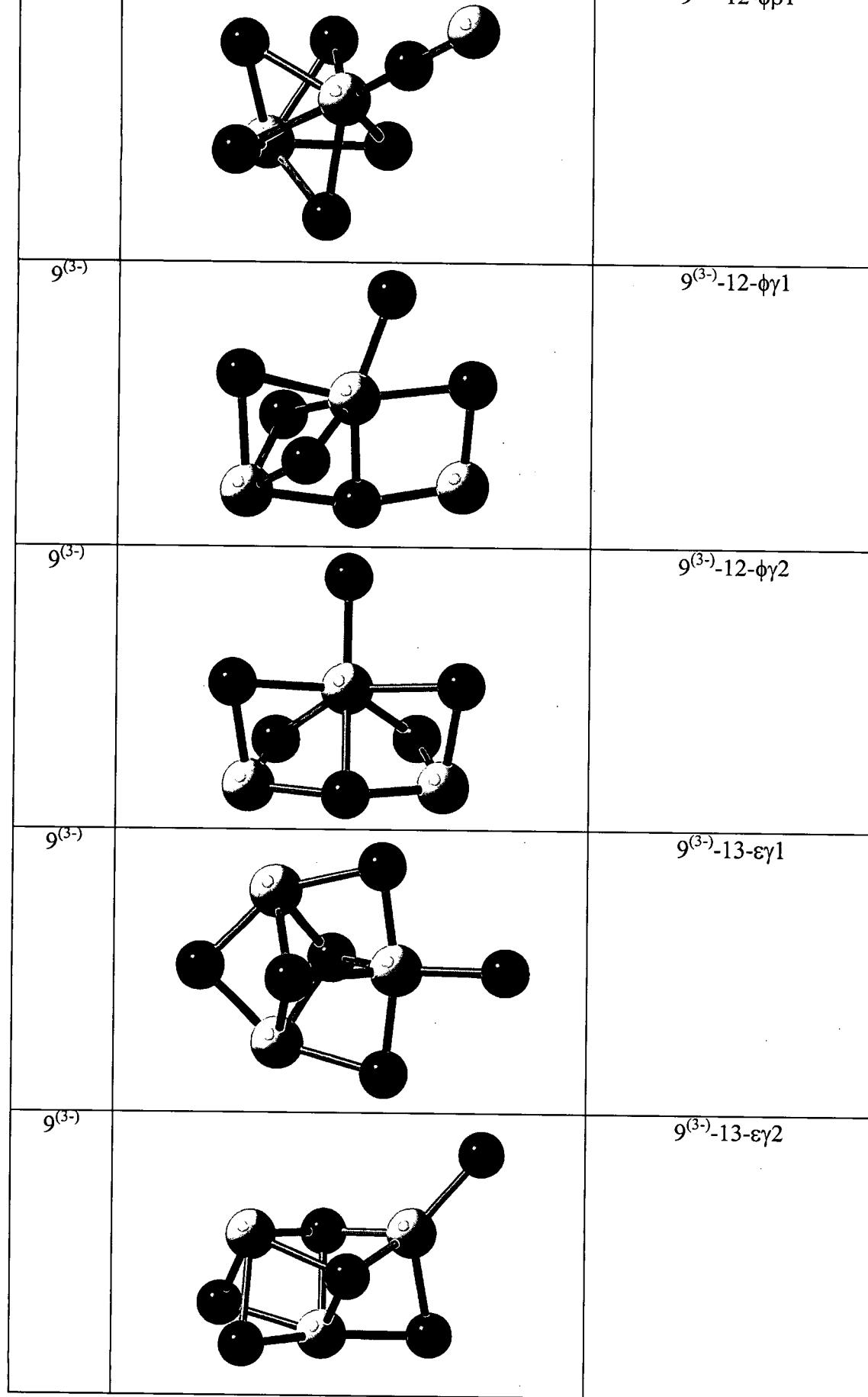


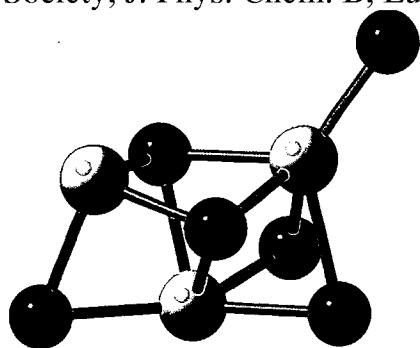
Group	Fragment	Type
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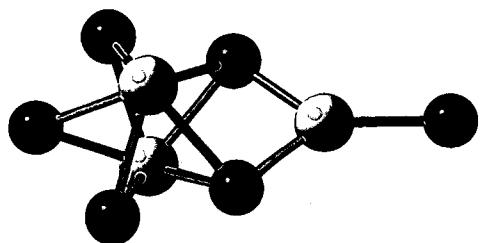






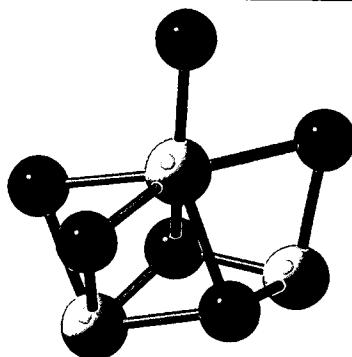
$9^{(3)}$

$9^{(3)}-13-\epsilon\gamma 3$



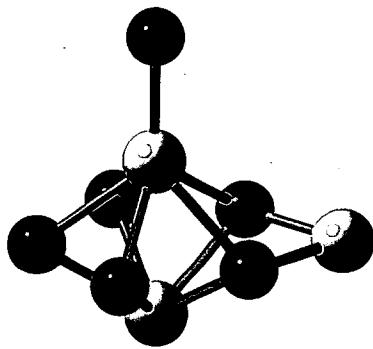
$9^{(3)}$

$9^{(3)}-13-\phi\gamma 1$



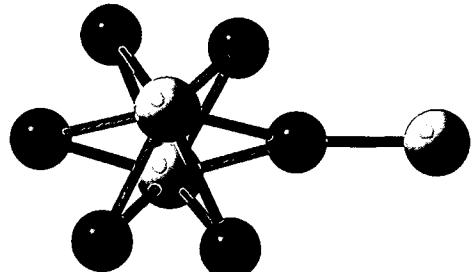
$9^{(3)}$

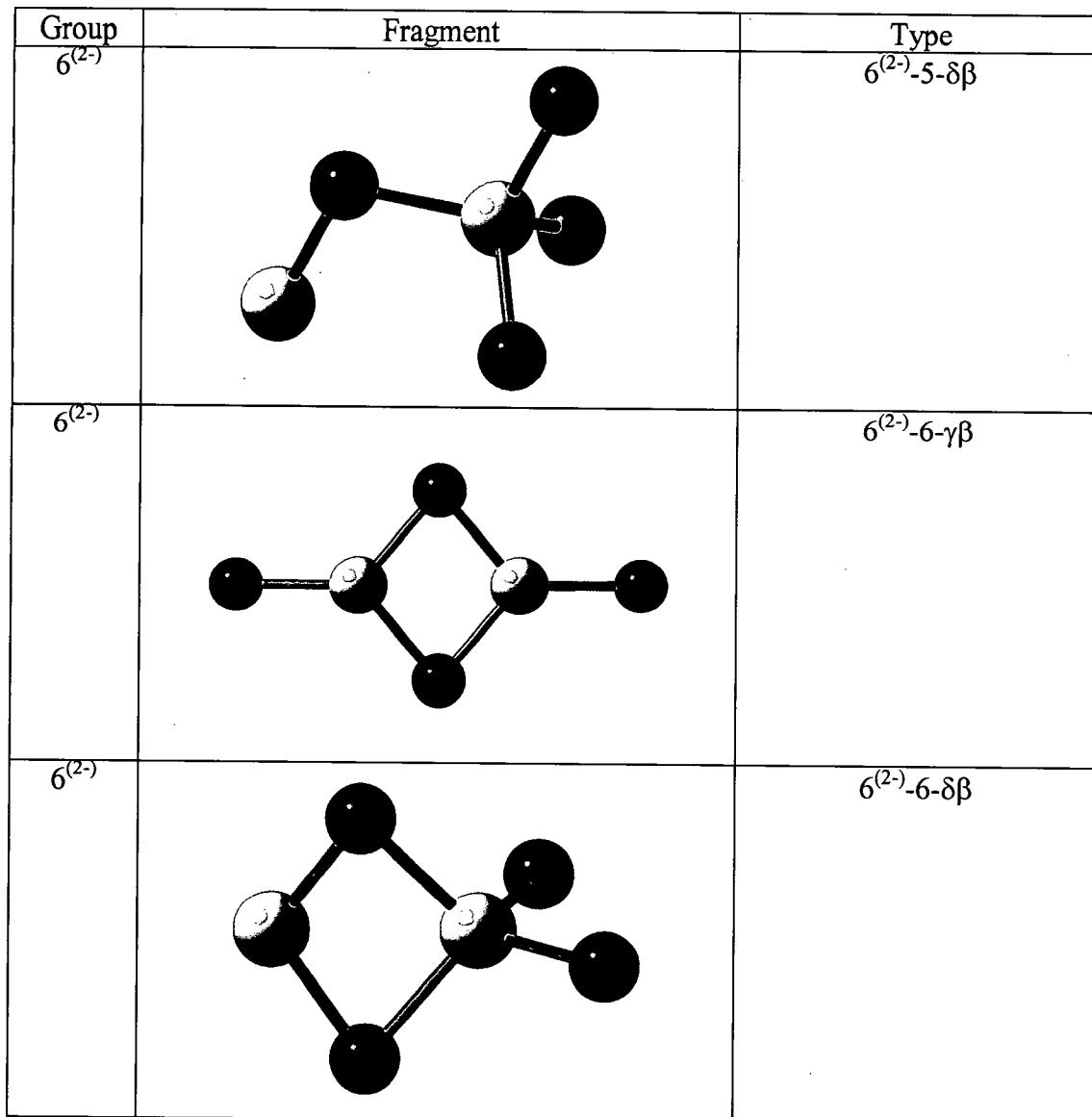
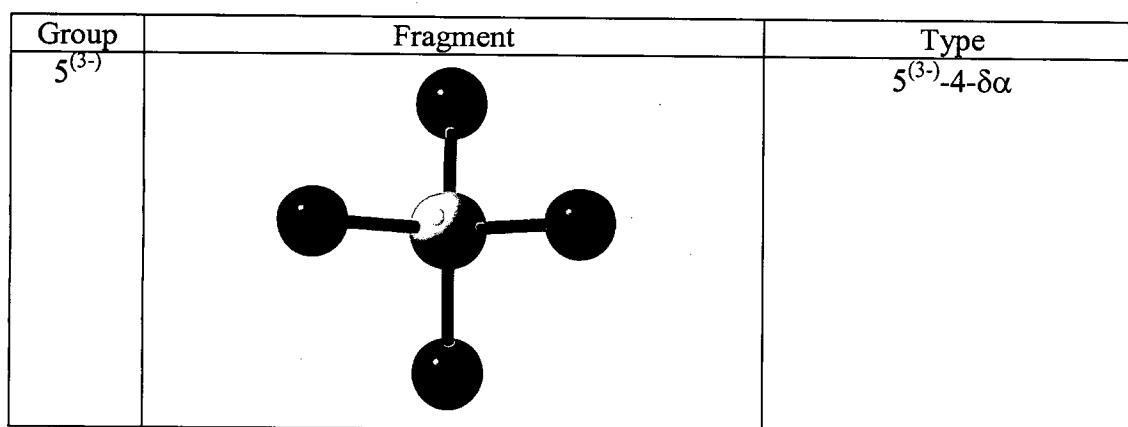
$9^{(3)}-13-\phi\gamma 2$

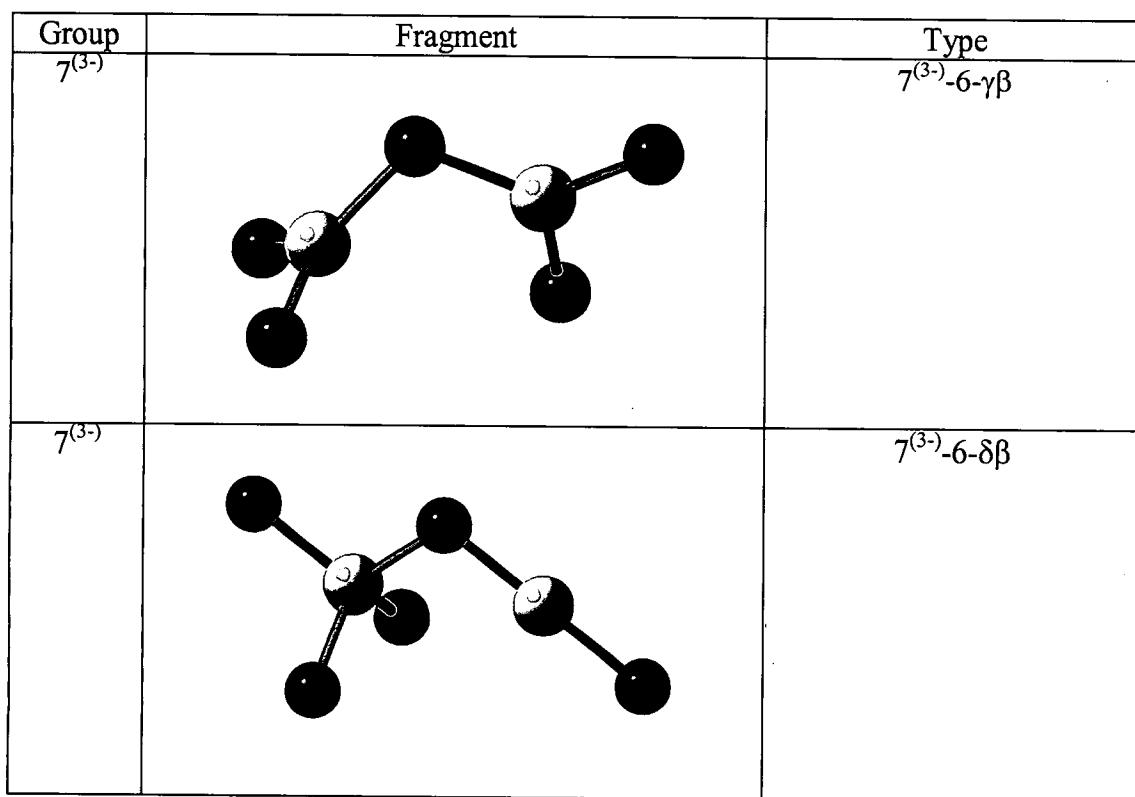
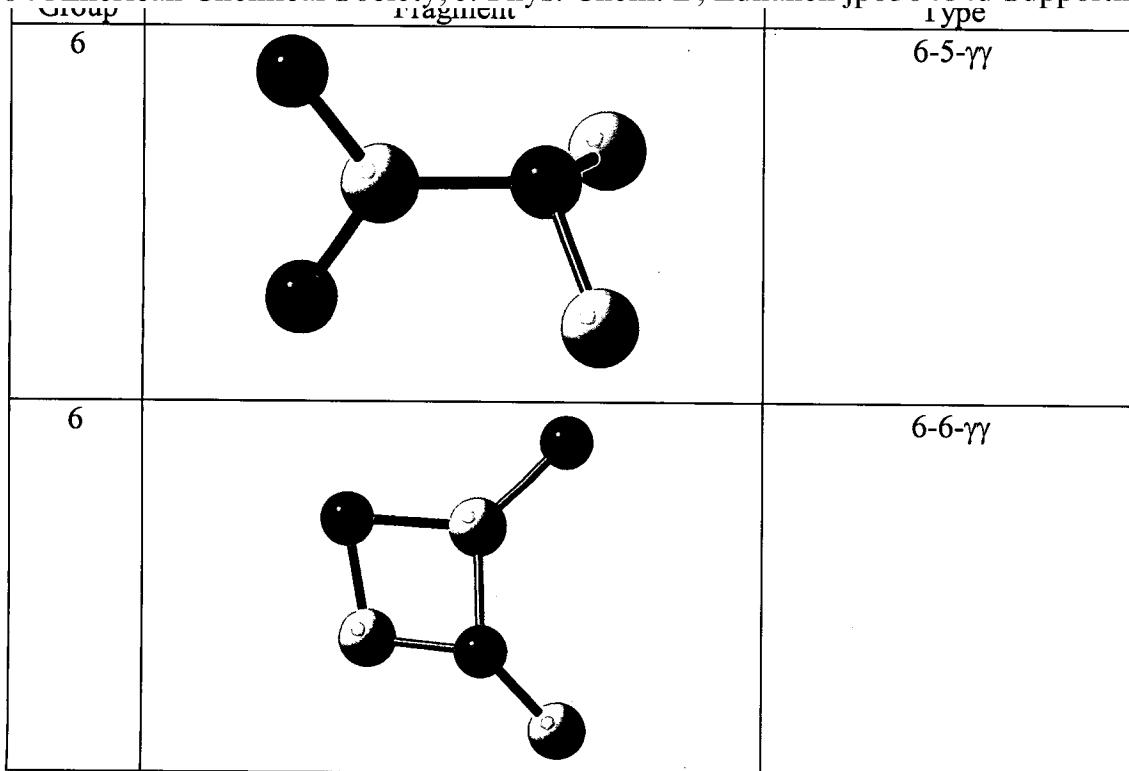


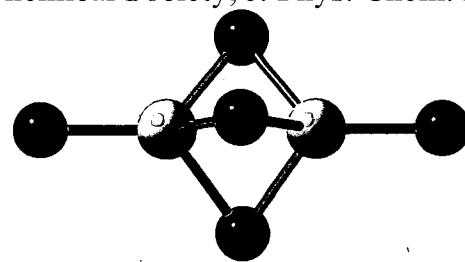
$9^{(3)}$

$9^{(3)}-13-\phi\gamma 3$



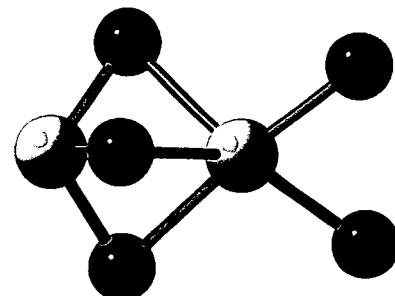






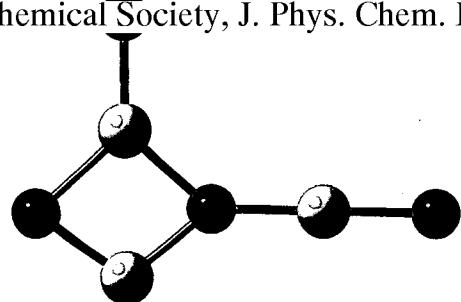
$7^{(3-)}-8-\delta\beta$

$7^{(3-)}$



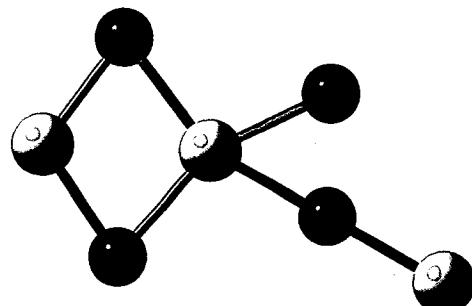
$7^{(3-)}-8-\epsilon\beta$

Group	Fragment	Type
$7^{(-)}$	<p>A ball-and-stick model of a fragment labeled $7^{(-)}$. It features a central three-membered ring of black spheres. One single bond extends from one of the ring vertices, ending in a small circle with a dot.</p>	$7^{(-)}-6-\gamma\gamma$
$7^{(-)}$	<p>A ball-and-stick model of a fragment labeled $7^{(-)}$. It features a central three-membered ring of black spheres. One single bond extends from one of the ring vertices, ending in a small circle with a dot.</p>	$7^{(-)}-6-\delta\beta$
$7^{(-)}$	<p>A ball-and-stick model of a fragment labeled $7^{(-)}$. It features a central four-membered ring of black spheres. One single bond extends from one of the ring vertices, ending in a small circle with a dot.</p>	$7^{(-)}-7-\gamma\beta$



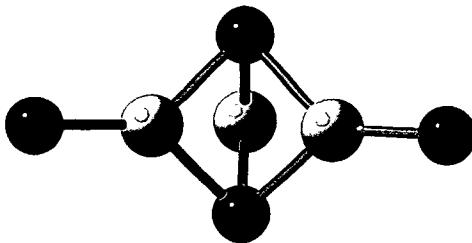
7⁽⁺⁾

7⁽⁺⁾-7- $\delta\beta$



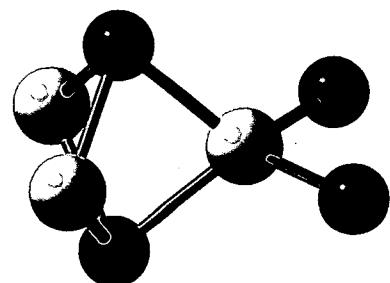
7⁽⁻⁾

7⁽⁻⁾-8- $\gamma\gamma$



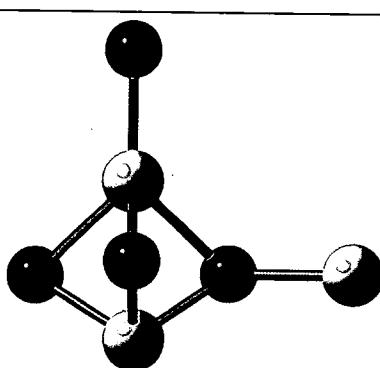
7⁽⁻⁾

7⁽⁻⁾-8- $\delta\gamma 1$

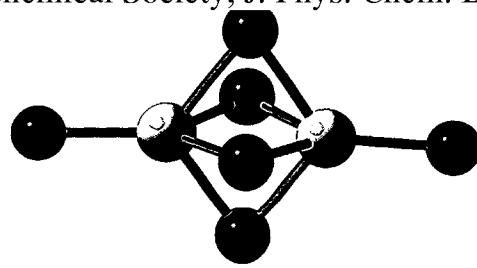


7⁽⁻⁾

7⁽⁻⁾-8- $\delta\gamma 2$

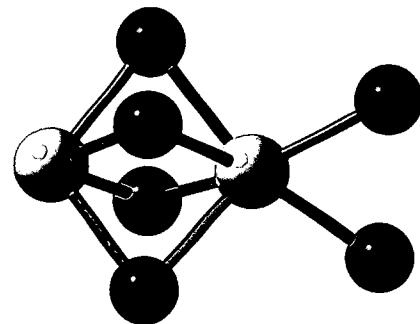


Group	Fragment	Type
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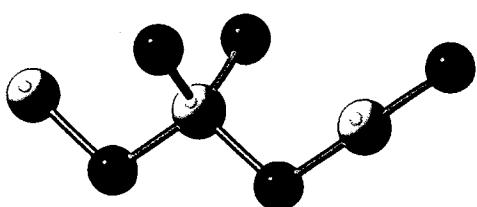


$g^{(4-)}$

$g^{(4-)}\text{-}10\text{-}\phi\beta$

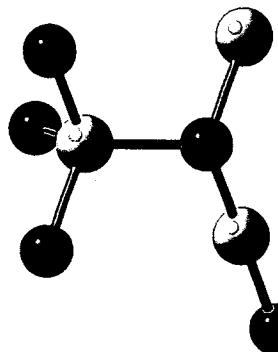


Group	Fragment	Type
$g^{(2-)}$	<p>A ball-and-stick model of a fragment with a $g^{(2-)}$ charge. It consists of a linear chain of four black spheres connected by sticks.</p>	$g^{(2-)}\text{-}7\text{-}\gamma\beta 1$
$g^{(2-)}$	<p>A ball-and-stick model of a fragment with a $g^{(2-)}$ charge. It features a branched structure with three rings and several atoms.</p>	$g^{(2-)}\text{-}7\text{-}\gamma\gamma 1$
$g^{(2-)}$	<p>A ball-and-stick model of a fragment with a $g^{(2-)}$ charge. It consists of a linear chain of five black spheres connected by sticks.</p>	$g^{(2-)}\text{-}7\text{-}\delta\beta 1$



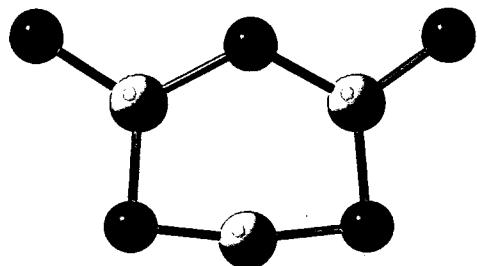
$g^{(2)}$

$g^{(2)}-7-\delta\beta 1$



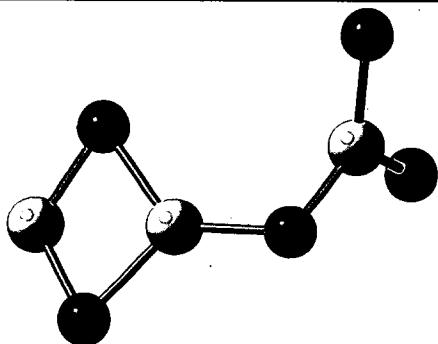
$g^{(2)}$

$g^{(2)}-8-\gamma\beta 1$



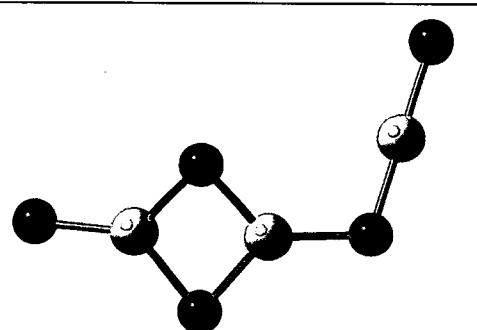
$g^{(2)}$

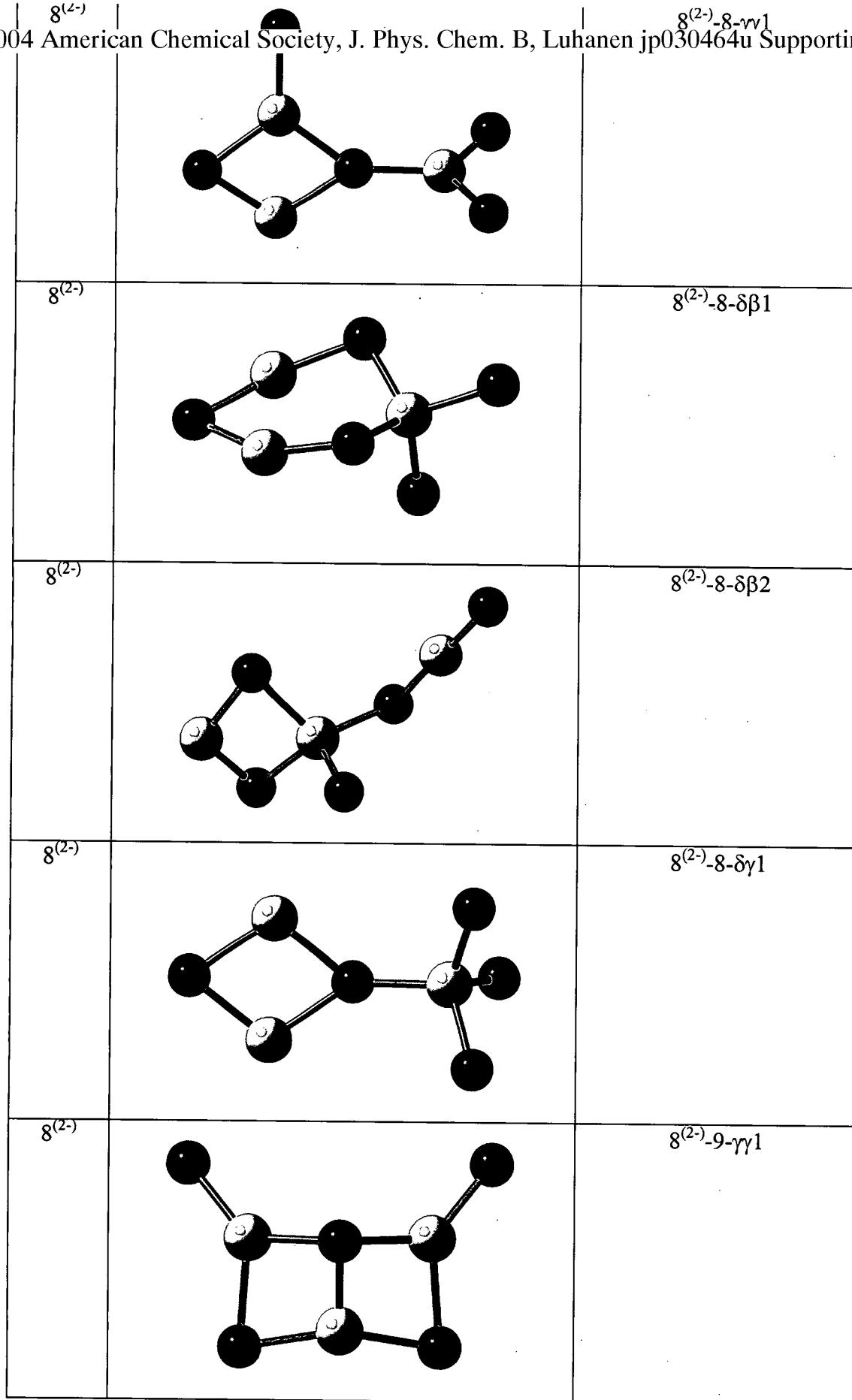
$g^{(2)}-8-\gamma\beta 2$

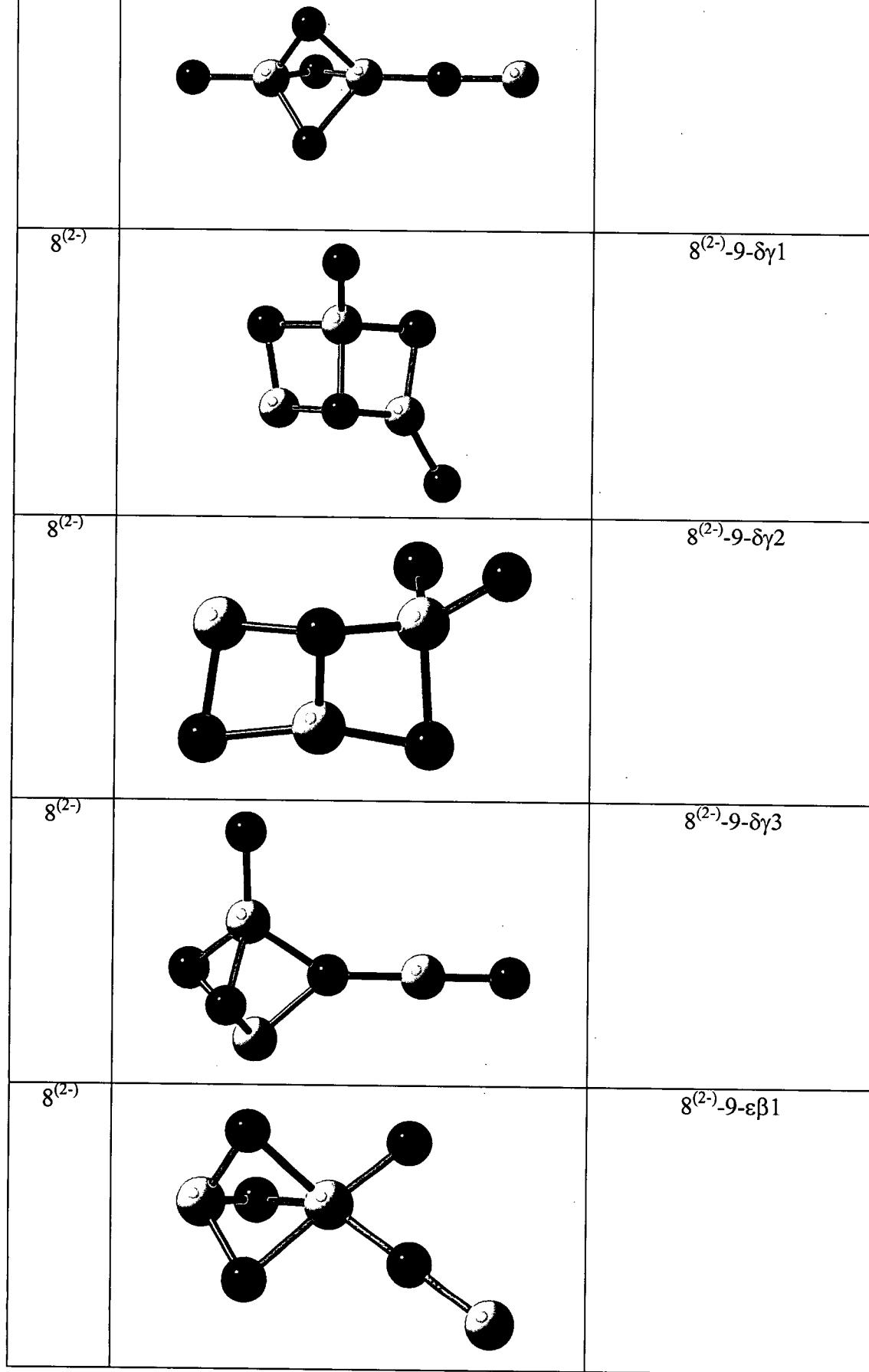


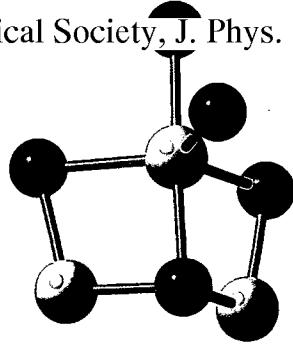
$g^{(2)}$

$g^{(2)}-8-\gamma\beta 3$



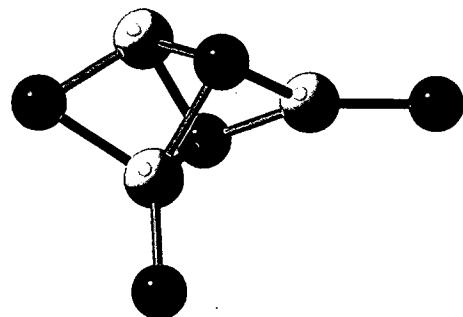






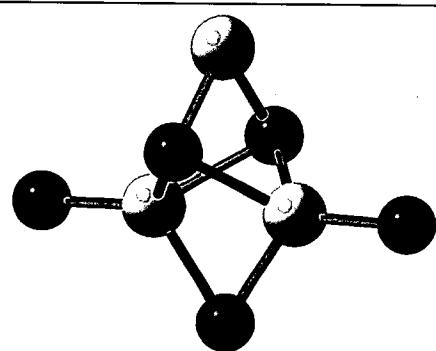
$8^{(2)}$

$8^{(2)}\text{-}10\text{-}\delta\gamma 1$



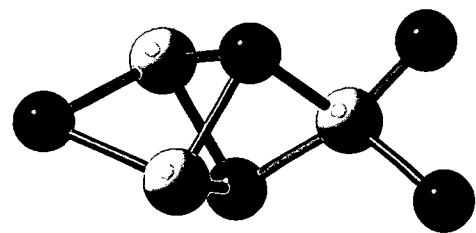
$8^{(2)}$

$8^{(2)}\text{-}10\text{-}\delta\gamma 2$



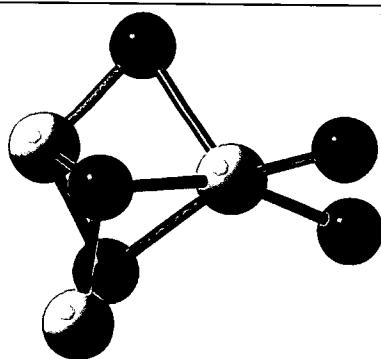
$8^{(2)}$

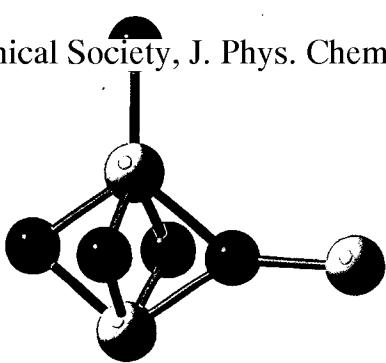
$8^{(2)}\text{-}10\text{-}\delta\gamma 3$



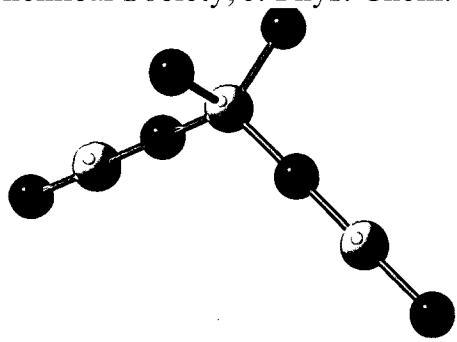
$8^{(2)}$

$8^{(2)}\text{-}10\text{-}\varepsilon\gamma 1$





Group	Fragment	Type
$9^{(3)}$		$9^{(3)}\text{-}8\text{-}\gamma\beta 1$
$9^{(3)}$		$9^{(3)}\text{-}8\text{-}\gamma\beta 2$
$9^{(3)}$		$9^{(3)}\text{-}8\text{-}\gamma\gamma 1$
$9^{(3)}$		$9^{(3)}\text{-}8\text{-}\delta\beta 1$



$9^{(3)}$

$9^{(3)}\text{-}8\text{-}\delta\gamma 1$

$9^{(3)}$

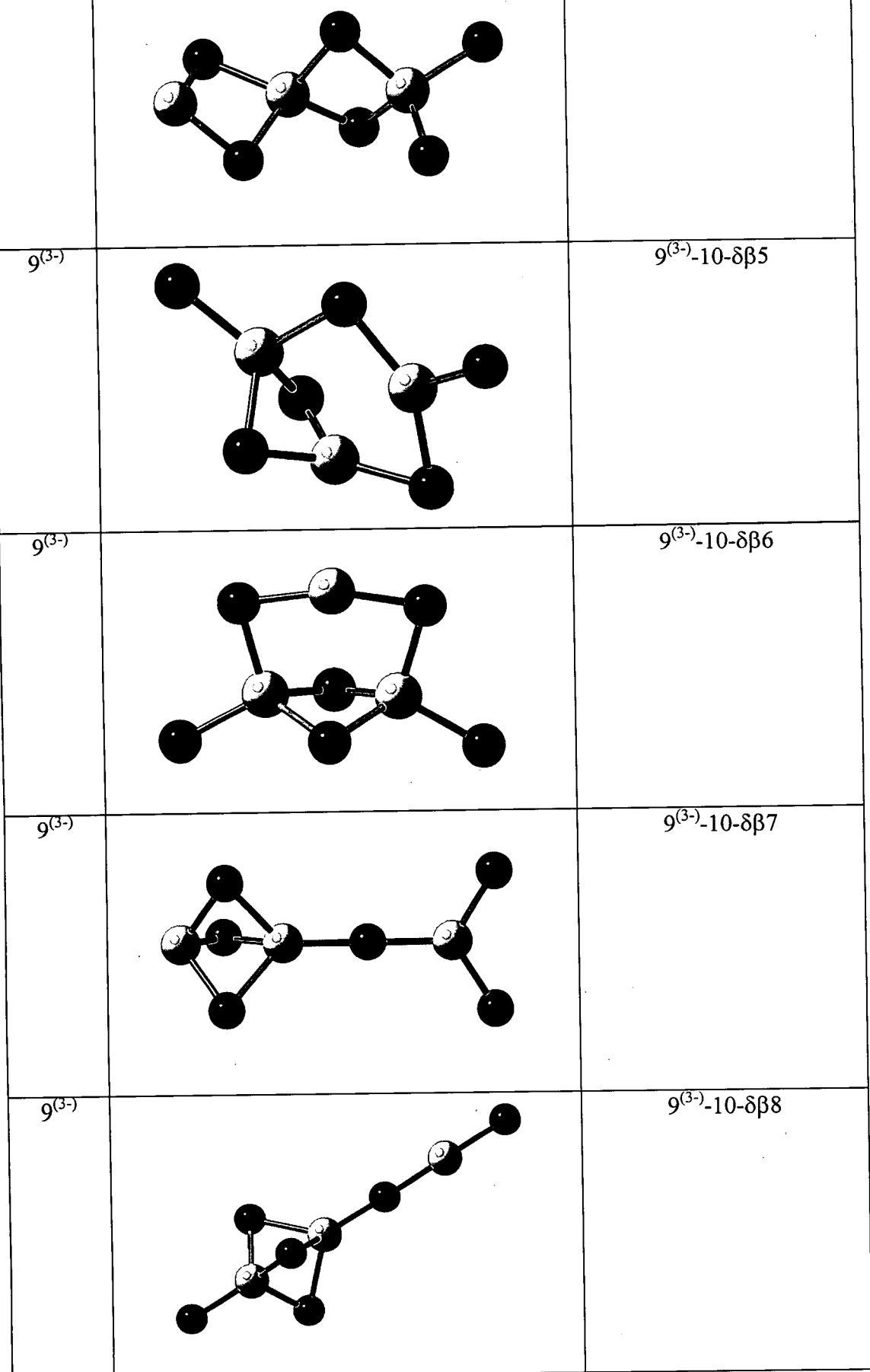
$9^{(3)}\text{-}10\text{-}\delta\beta 1$

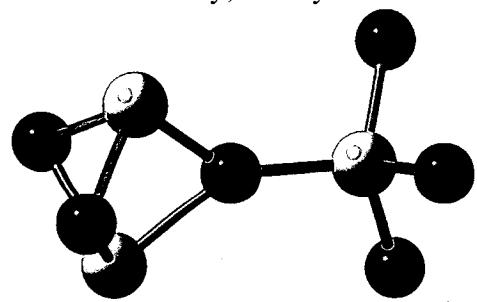
$9^{(3)}$

$9^{(3)}\text{-}10\text{-}\delta\beta 2$

$9^{(3)}$

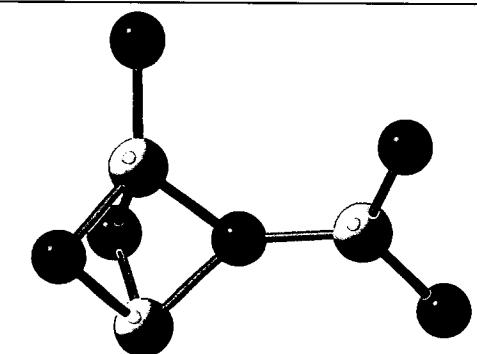
$9^{(3)}\text{-}10\text{-}\delta\beta 3$





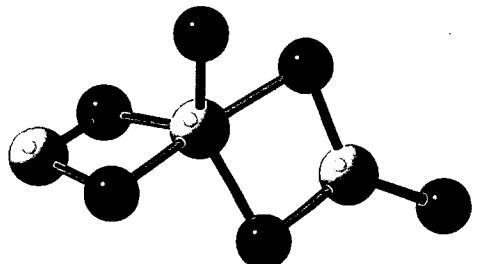
$9^{(3)}$

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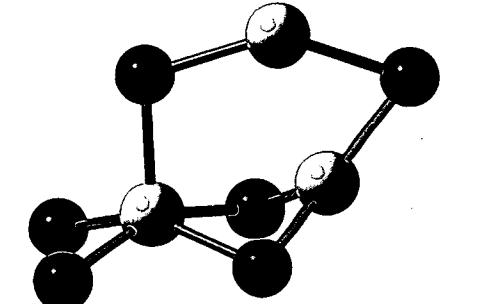
$9^{(3)}$

$9^{(3)}\text{-}10\text{-}\epsilon\beta 1$



$9^{(3)}$

$9^{(3)}\text{-}10\text{-}\epsilon\beta 2$



$9^{(3)}$

$9^{(3)}\text{-}10\text{-}\epsilon\beta 3$

