First principles study on structural and magnetic properties of small and pure carbon clusters (C_n, $n = 2 - 12$)

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Abstract

We have demonstrated the structural and magnetic properties of small carbon clusters (C_n, $n = 2-12$) in the framework of collinear approximation using density functional theory. The calculations were performed for amorphous, linear, and ring carbon clusters using full-potential local-orbital (FPLO) method. We have obtained stable structures, total energies, total magnetic moments, and HOMO-LUMO energy gap of these clusters. We have found that the amorphous carbon clusters with minimum energy are not magnetic clusters whereas their less-stable isomers with special configurations are ferromagnetic objects. Two robust magnetic moments were found for C_5 carbon ring ($6\mu_B$) and for pentagonal pyramid C_6 structure ($4\mu_B$).

Keywords

Carbon cluster; Density functional theory; Nanomagnetism

Introduction

The intriguing possibility of magnetism and structural properties of carbon clusters has triggered great research interests due to their potential applications in molecular magnetism and spin functional nanodevices. Especially, nanodiamond particles can be used as a potential candidate to increase wear resistance and microhardness, and decrease the coefficients of friction and corrosion in composite functional layers such as hard disks and magnetic heads [1]. In addition, nanoscale magnetic sensors have been developed on the bases of nanodiamonds including nitrogen-vacancy impurities [2]. It has been found that carbon atoms can be magnetized around a vacancy defect in graphene [3] and also those carbon atoms located at the edges of a graphene nanoribbon [4,5]. As a consequence, one can examine a magnetic feature for carbon clusters with some especial configurations. Therefore, it is prime important to know the magnetic properties of carbon structures and to know in which structure the carbon clusters are magnetized.

In the present work, our interest is concerned with the theoretical density functional theory (DFT) calculations to investigate the structures, electronic, and especially the magnetic properties of pure and

neutral small carbon clusters. In this context, many experimental and theoretical studies have been conducted on the pure carbon clusters [6-12]. Raghavachari and Binkley, using spin-unrestricted version of Hartree-Fock method, have obtained the structures and energies of small carbon clusters (C_n, $n = 2 - 10$) and revealed an odd-even pattern in the cluster geometries and that the odd-numbered clusters prefer linear structure and the even-numbered clusters prefer irregular cyclic structure [13]. Xu and co-workers have studied a number of annular carbon structures (C_n, $n = 3 - 31$) and linear carbon clusters (C_n, $n = 2 - 12$). They have found electronic properties of these carbon clusters such as total energies, energy gaps between highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO), and bond lengths at the level of DFT/B3LYP/6-31G* approach [14,15]. Zhang and co-workers have optimized the structure of C_n clusters ($n = 2 - 30$) and have calculated binding energy for these clusters using the genetic algorithm associated with simulated annealing method [16]. The electronic properties and relative energies of carbon clusters with $2n$ atoms ($2 \leq n \leq 16$) for stable isomers including chains, rings, cages, and graphitic (plate and bowl) structures have been found by R.O. Jones [17]. Also, López-Urías and co-workers, using single-band Hubbard model and pseudo-potential approach implemented in the SIESTA package, have studied the electronic and magnetic properties of sp^2 carbon isomers $C_n(n = 10,12,14)$ [18]. They have found a triplet state for some studied isomers in which this state strongly depends on the cluster geometry [18]. It has to be taken into account that carbon atoms are hybridized together in the form of sp, sp^2, and sp^3. Therefore, one can examine that there are many stable isomers for a typical pure carbon cluster including n atoms. To the best of our knowledge, there is no systematic study on magnetic and structural properties of all isomers of carbon clusters even for small structures.

In this paper we made an exhaustive search in carbon isomers to find out magnetic and stable objects with amorphous structure. In addition, the binding energies, HOMO-LUMO energy gaps and magnetic properties of sp, sp^2, and sp^3 carbon clusters (C_n, $n = 2 - 12$) were studied. These properties were investigated for carbon clusters in the form of amorphous wire and ring structures using full-potential local-orbital method which is developed on the basis of linear combination of atomic orbitals (LCAO) method. In Section 'Computational method,' the numerical approach is discussed. Section 'Results and discussion' presents the structural properties of different carbon isomers, calculated magnetic moments, binding energies, etc. Finally, the paper is summarized in Section 'Conclusions.'

Computational method

All magnetic calculations were performed using density functional theory [19] implemented within a self-consistent full-potential local-orbital basis band structure method, FPLO.9 package [20]. In this scheme, the scalar relativistic calculations were implemented within a spherical average on the spin-orbit interaction, using four-component Kohn-Sham-Dirac equation [21]. The generalized gradient approximation of (GGA) Perdew-Burke-Ernzerhof 96 was used for the exchange-correlation potential [22]. The valence basis set of carbon consisted of 1s, 2s, 2p, 3s, 3p, and 3d states so that for the sake of completeness, carbon core electrons and its polarization states were considered as valence electrons. For each size of studied clusters, several initial configurations were considered. In order to optimize atomic geometries, the position of all carbon atoms was fully relaxed. In the optimization process, the total energy and force converged to 0.001 meV and 0.001 eV/Å, respectively. The binding energy per atom (E_b) for all studied clusters was determined as $E_b = (nE_s - E_t)/n$, where n is the size of the cluster (number of carbon atoms), E_s is the energy of the single carbon atom and E_t is the total energy of the relaxed cluster.

Results and discussion

In order to obtain stable carbon clusters, all amorphous structures were taken with most possible symmetry as initial configurations. However, it has to be pointed out that after relaxation process, most of the selected structures were unstable and deformed. The relaxed isomers and related point group symmetries of amorphous carbon clusters are illustrated in Figure 1. The relaxed carbon rings and their related point groups are shown in Figure 2. Table 1 shows the total energies of the lowest amorphous, linear, and ring structures. In Figure 3, we have indicated the calculated binding energies, related HOMO-LUMO gaps, and second difference energies for linear, ring, and amorphous structures with minimum energy.

Figure 1 The relaxed amorphous carbon clusters ($C_n, n = 2 - 12$) and their related point group symmetries. The isomers with constant n are ordered with increasing energy. The corresponding magnetic moments (M_s) of magnetic carbon clusters are also presented. The magnetic moments are in Bohr magnetons. The magic icosahedron structure (12b) is not a stable isomer at ambient pressure and it relaxes to (12a) structure.

Figure 2 The relaxed ring carbon clusters ($C_n, n = 2 - 12$) and their related point group symmetries. The corresponding magnetic moments (M_s) of magnetic carbon rings are also presented. The magnetic moments are in Bohr magnetons.

Table 1 The total energies of lowest amorphous, linear, and ring structures

	Amorphous	Linear	Ring
C_2	-	$-2,064.6157$	-
C_3	-	$-3,101.6398$ a	$-3,101.6398$ b
C_4	$-4,135.9885$	$-4,136.4412$ a	$-4,135.9885$ b
C_5	$-5,169.8423$ b	$-5,173.2075$ a	$-5,168.9118$
C_6	$-6,204.1416$	$-6,208.2140$ b	$-6,208.5764$ a
C_7	$-7,244.0570$ b	-7244.7196 a	$-7,243.7094$
C_8	$-8,279.4919$	$-8,279.8854$ a	$-8,279.6294$ b
C_9	$-9,313.6903$	$-9,316.2462$ a	$-9,315.3016$ b
C_{10}	$-10,347.5800$	$-10,351.5172$ b	$-1,0354.1995$ a
C_{11}	$-11,382.8994$	$-11,387.7825$ b	$-11,388.7931$ a
C_{12}	$-12,417.3442$	$-12,423.1274$ b	$-12,423.6741$ a

All values are in electron volt units. With constant n, letters a and b have denoted the first and second minimum energies for carbon structures, respectively.

Figure 3 Binding energies, second difference energies, and HOMO-LUMO gaps. The binding energies (top panel), the second difference energies $\Delta_2 E(n)$ (middle panel), and the HOMO-LUMO gaps $\Delta_{\text{H-L}}$ (bottom panel) are shown for most stable (lowest amorphous, linear, and ring) structure of carbon clusters found with minimum energy. All values are presented in electron volts.

At first, the calculations were performed for carbon dimer. The optimized bond length is 1.316 Å, and its magnetic moment was obtained $2\mu_{\text{B}}$. The calculated C-C bond length at the DFT (GGA) level is larger than that in experimental value (1.243 Å) by about five percent [23]. Our calculated GGA bond length for C_2 dimer can be compared to the calculated bond length (1.315 Å) done by Congie Zhang [16].

For C_3 cluster, we considered linear and triangular structures. Linear isomer with $D_{\infty h}$ symmetry was found to be the most stable structure whose magnetic moment is zero. Triangular structure (D_{3h}) with

magnetic moment $2\mu_B$ lies 564 meV higher in total energy compared to its linear isomer. The calculated bond length for triangular structure is 1.377 Å, which is in agreement with the calculated bond length done by Martin and co-workers [24]. The calculated C-C bond length of the C_3 linear cluster is 1.304 Å, where it can be compared to the experimental value of 1.297 Å, determined by Hinkle et al. [25] and calculated bond length (1.305 Å) done by Hutter and co-workers [26].

We have studied square and tetrahedron structures for C_4 cluster but after relaxation due to Jahn-Teller effect, they distorted to Figure 1 (4a) and (4b) structures, respectively. The most stable structure is a rhombic structure (Figure 1 (4a)) with D_{2h} point group symmetry and zero magnetic moment. The Figure 1 (4b) structure with C_{2v} symmetry is a ferromagnetic object with magnetic moment $2\mu_B$ lying 807 meV higher in total energy compared to rhombic isomer (Figure 1 (4a)). For the C_5 cluster, we examined two different initial configurations: triangular bipyramid and squared pyramid. It is found that both isomers were deformed to the same structure after relaxation (see (5a) in Figure 1). The symmetry of C_5 structure is D_{3h}, and it was found to be a nonmagnetic object.

We have investigated three different geometries for C_6. A distorted trigonal prismatic (Figure 1 (6a), C_{2v}) was found to be the most stable structure and nonmagnetic cluster. The next two isomers are a pentagonal pyramid (6b, C_{5v}) and a distorted octahedron (6c, C_{2v}), which lie at 614 and 1041 meV higher than the structure with minimum energy whose magnetic moments are 4 and $2\mu_B$, respectively. Our findings show that the pentagonal pyramid structure has the largest magnetic moment among the tridimensional carbon structures investigated in this work. For C_7, we obtained two structures: hexagonal prism and plane-like structure. Our calculations have indicated that the planar C_{2v} isomer is the most stable structure with 4,386 meV energy below the hexagonal prism with C_{6v} point group symmetry. We have also studied five structures for C_8 cluster. Our calculations indicated that Figure 1 (8a) with D_{4d} symmetry is the most stable structure, and the planar D_{2h} isomer in Figure 1 (8b) with energy difference of 2,016 meV lies higher than the D_{4d} isomer. The next isomer with C_{2v} symmetry lies 2330 meV higher compare to D_{4d} structure. The Figure 1 (8d) structure has a cubic form with O_h symmetry and energy difference of 3950 meV higher than Figure 1 (8a) structure. The most nonstable isomer (Figure 1 (8e)) has also C_{2v} symmetry with 5.011 eV higher with respect to the most stable structure.

For C_9 cluster, two initial structures (capped tetragonal prism and tricapped trigonal prism) were deformed to Figure 1 (9a) and (9b) structures. The square pyramid structure was also stable (Figure 1 (9c), C_{4v}). The Figure 1 (9a) cluster with C_{2v} symmetry was found as the structure with minimum energy. The Figure 1 (9b) structure also with C_{2v} symmetry lies 4,489 meV higher in energy and square pyramid in Figure 1 (9c) is less stable with energy difference of 5,959 meV higher than the Figure 1 (9a) cluster. In the case of C_{10} cluster, we have studied three structures, but only the square dipyramid structure Figure 1 (10c) retained its initial geometric configuration. However, this structure is the most nonstable isomer in comparison to the other studied C_{10} clusters and lies 11,070 meV higher in energy with respect to the minimum energy structure (Figure 1 (10a), C_s). The (10b) carbon cluster in Figure 1 with C_s symmetry and energy difference of 502 meV lies higher than Figure 1 (10a) structure. For C_{11}, two stable structures were investigated. It was found that both relaxed configurations have amorphous feature with no symmetry. The most stable Figure 1 (11a) carbon structure lies below Figure 1 (11b) structure with energy difference of 715 meV. The last tridimensional cluster studied in this work is C_{12}. The initial structure for C_{12} was chosen as an icosahedron with I_h symmetry. The total energy calculated for structure Figure 1 (12b) was $-12,384.260$ eV, whereas after relaxation the initial structure was totally deformed (see (12a) structure in Figure 1). This structure has C_s symmetry and its total energy is $-12,417.34$ eV. However, we have found that the icosahedral C_{12} cluster is a magnetic object and its calculated magnetic moment is $2\mu_B$ whereas it is not a stable structure at room temperature and ambient pressure.

We have also studied the magnetic properties of ring and linear carbon clusters in which they are isoelectronics to the considered amorphous structures. It has to be pointed out that our calculated magnetic moments for even-numbered linear clusters are $2\mu_B$ and for odd-numbered linear structures have vanished. Li and co-workers have also shown the same magnetic pattern for finite-sized carbon wires [27]. It can be seen in Figure 2 that the magnetic properties of ring structures are completely dependent on the size and structure of the clusters. It has to be pointed out that C_3 (D_{3h}) with triangular structure, C_5 ring with pentagonal structure (D_{5h}), and C_7, C_9, and C_{12} with C_{2v} symmetry are magnetic rings. Among the studied carbon clusters with $n \leq 12$, the C_5 ring has the largest magnetic moment ($6\mu_B$). According to the data in Table 1, it can be argued that the carbon rings of C_6, C_{10}, C_{11}, and C_{12} are more stable than their linear isomers with 362 meV, 2682 meV, 1011 meV and 547 meV lower in total energy, respectively. Martin and co-workers have found that the carbon linear structures with $n \leq 10$ are more stable than their ring isomers [28,29]. Their findings are in contradiction with our results, since we have found that the ring structures of C_6 and C_{10} are more stable than their linear structures. We have also found that the C_5 with D_{3h} symmetry and C_7 with C_{2v} symmetry are more stable than the isoelectronic ring structures (see Table 1).

The behavior of binding energies (E_b), second difference energies $\Delta_2 E(n)$, and HOMO-LUMO gaps for the all studied carbon structures are depicted in Figure 3. It can be seen that the binding energies per carbon atom are increased with the increasing size of the cluster. For the amorphous carbon structures, it can be seen that there is a gradual increase in the binding energy in the range of $n = 3 - 6$ and $n = 7 - 12$ for tridimensional (amorphous) structure with minimum energy (see Figure 3). It has to be pointed out that also with increasing the number of carbon atoms in the clusters, the binding energies are merged to 6.5 eV. This value is very close to the binding energy of carbon macromolecules [16]. A better way to show the relative stability of a cluster is the second differences in energy $\Delta_2 E(n)$ defined by $\Delta_2 E(n) = E(n+1) + E(n-1) - 2E(n)$, where $E(n)$ is the total energy of C_n clusters. It was shown in the middle panel of Figure 3 that the C_3, C_7, and C_{11} amorphous structures are more stable than their neighbors. The same argument can be concluded for C_6 and C_{10} ring structures (see the middle panel of Figure 3). The $\Delta_2 E(n)$ for linear structures shows a systematic behavior whereas for amorphous and rings structures it behaves very irregular. It is obvious from $\Delta_2 E(n)$ in Figure 3 that the odd-numbered linear carbon structures are more stable than the even-numbered linear carbon structures. We have also investigated the behavior of HOMO-LUMO energy gaps (Δ_{H-L}) for the studied structures (see Figure 3). It can be pointed out that the HOMO-LUMO gap can give a criterion for chemical reactivity of a typical cluster, in which a larger HOMO-LUMO gap means less reactivity. In Figure 3 it can be seen that HOMO-LUMO gaps of the odd-numbered linear structures are larger than the even-numbered linear clusters. On the other hand, the behavior of HOMO-LUMO gaps for amorphous and rings clusters is completely irregular compared to their linear isomers. We have found that the C_6 carbon cluster with C_{5v} point group symmetry is the less reactive cluster compared to the other studied amorphous carbon clusters. We have also clarified that C_{10} carbon ring is less reactive object compared to the other studied carbon rings. It can be seen in Figure 3 that the $\Delta_2 E(n)$ and Δ_{H-L} have the same pattern for linear carbon structures, whereas this behavior cannot be seen for amorphous and linear structures.

Conclusions

In conclusion, we have studied the structures and magnetic properties of small carbon clusters ($C_n, n = 2 - 12$) using density functional theory method with generalized gradient approximation. The stable geometrical carbon structures are obtained after relaxation calculations. Then we have investigated the most stable structures, magnetic moments, binding energies, the second differences of energy, and the related HOMO-LUMO energy gaps. Furthermore, we have found that the magnetizations of amorphous and ring structures are completely dependent on the cluster size and configuration of the carbon atoms in the cluster. We have also shown that the lowest amorphous carbon structures with minimum energy when formed in a tridimensional structure have no net magnetic moments. According to our results for small

and amorphous carbon clusters, we may expect a nonmagnetic feature for larger carbon clusters formed at room temperature and ambient pressure. Finally, we have shown that some less stable carbon isomers are magnetic in which one can imagine that they are initial building blocks for magnetic nanodiamonds at high pressure.

Competing interests

The authors declare that they have no competing interests.

Authors' contributions

MA, MB, and AHK conceived of the study and participated in its design and coordination. All authors read and approved the final manuscript.

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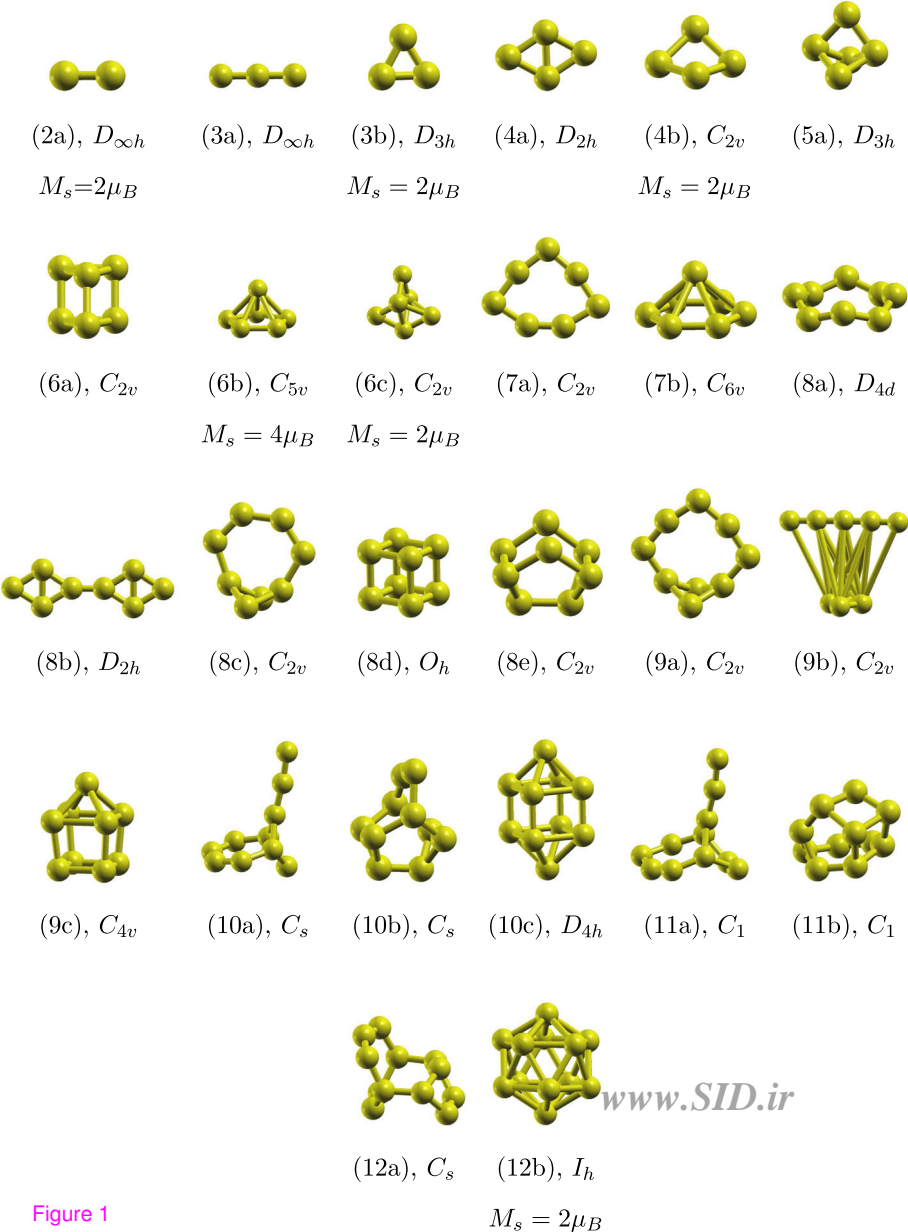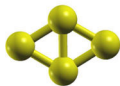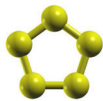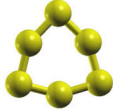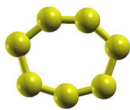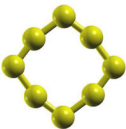
(2a), $D_{\infty h}$ (3a), $D_{\infty h}$ (3b), D_{3h} (4a), D_{2h} (4b), C_{2v} (5a), D_{3h}

$M_s=2\mu_B$ $M_s=2\mu_B$ $M_s=2\mu_B$

(6a), C_{2v} (6b), C_{5v} (6c), C_{2v} (7a), C_{2v} (7b), C_{6v} (8a), D_{4d}

$M_s=4\mu_B$ $M_s=2\mu_B$

(8b), D_{2h} (8c), C_{2v} (8d), O_h (8e), C_{2v} (9a), C_{2v} (9b), C_{2v}

(9c), C_{4v} (10a), C_s (10b), C_s (10c), D_{4h} (11a), C_1 (11b), C_1

(12a), C_s (12b), I_h

$M_s=2\mu_B$

Figure 1

C$_3$, D_{3h} C$_4$, D_{2h} C$_5$, D_{5h} C$_6$, D_{3h} C$_7$, C_{2v}

$M_s = 2\mu_B$ $M_s = 6\mu_B$ $M_s = 2\mu_B$

C$_8$, C_{4h} C$_9$, C_{2v} C$_{10}$, D_{5h} C$_{11}$, C_{2v} C$_{12}$, C_{2v}

Figure 2 $M_s = 2\mu_B$ $M_s = 4\mu_B$

Figure 3

Axis labels — left column (Amorphous), center column (Linear), right column (Ring):

- E_b (eV/atom)
- $\Delta_2 E$ (eV)
- Δ_{H-L} (eV)

Cluster Size (Amorphous)   Cluster Size (Linear)   Cluster Size (Ring)
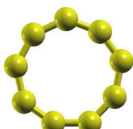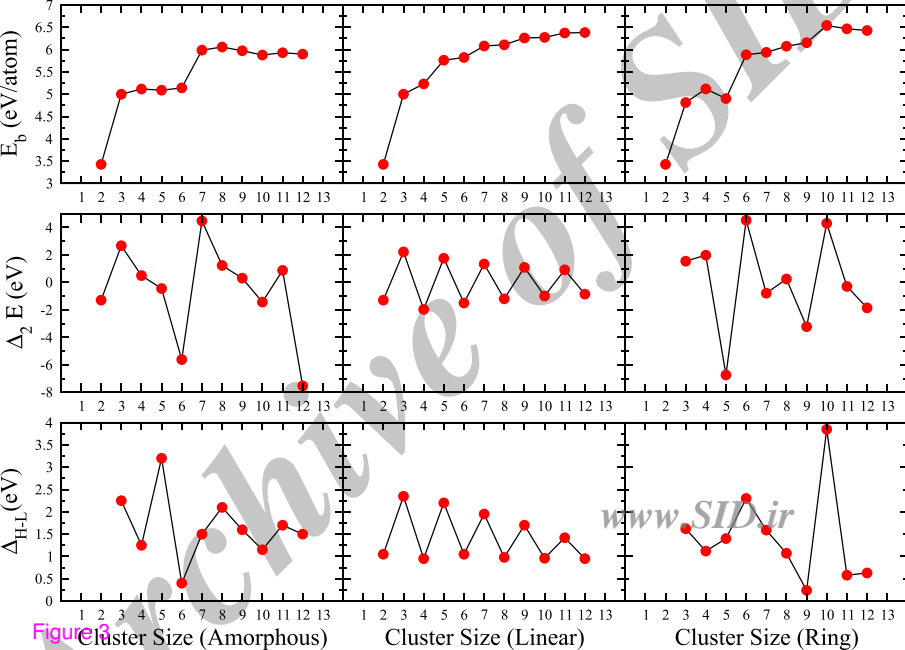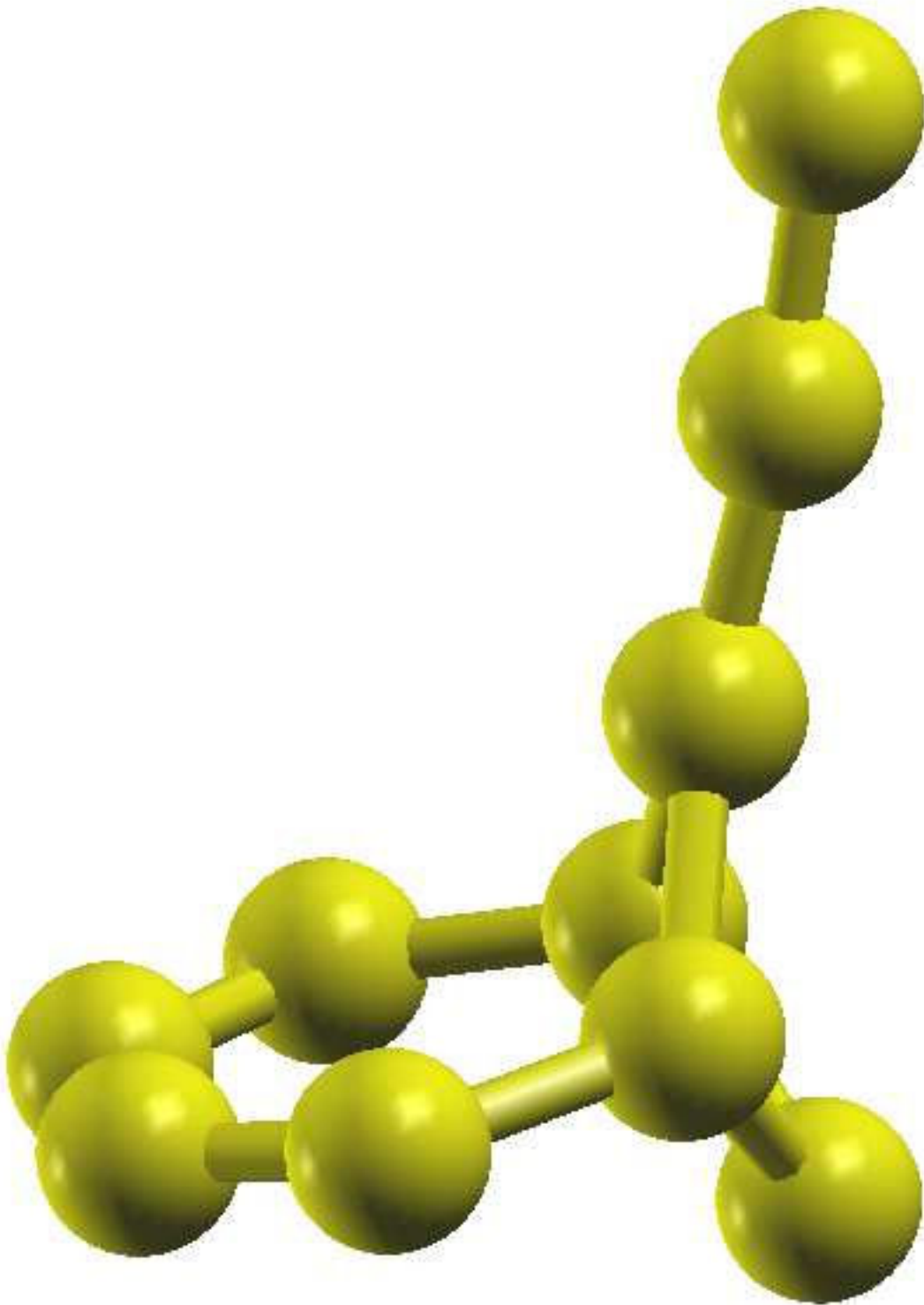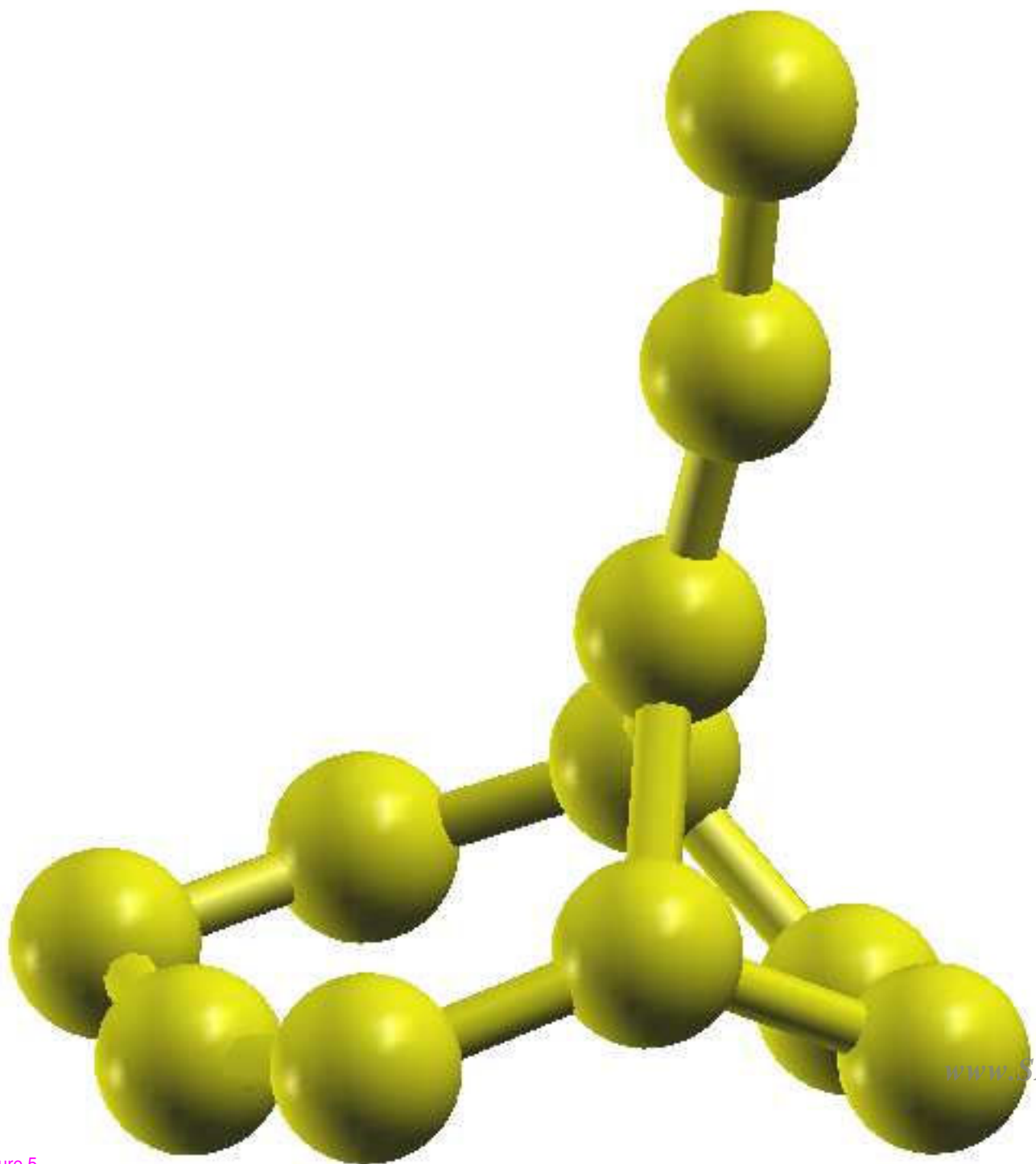
Figure 4

Figure 5

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Figure 6
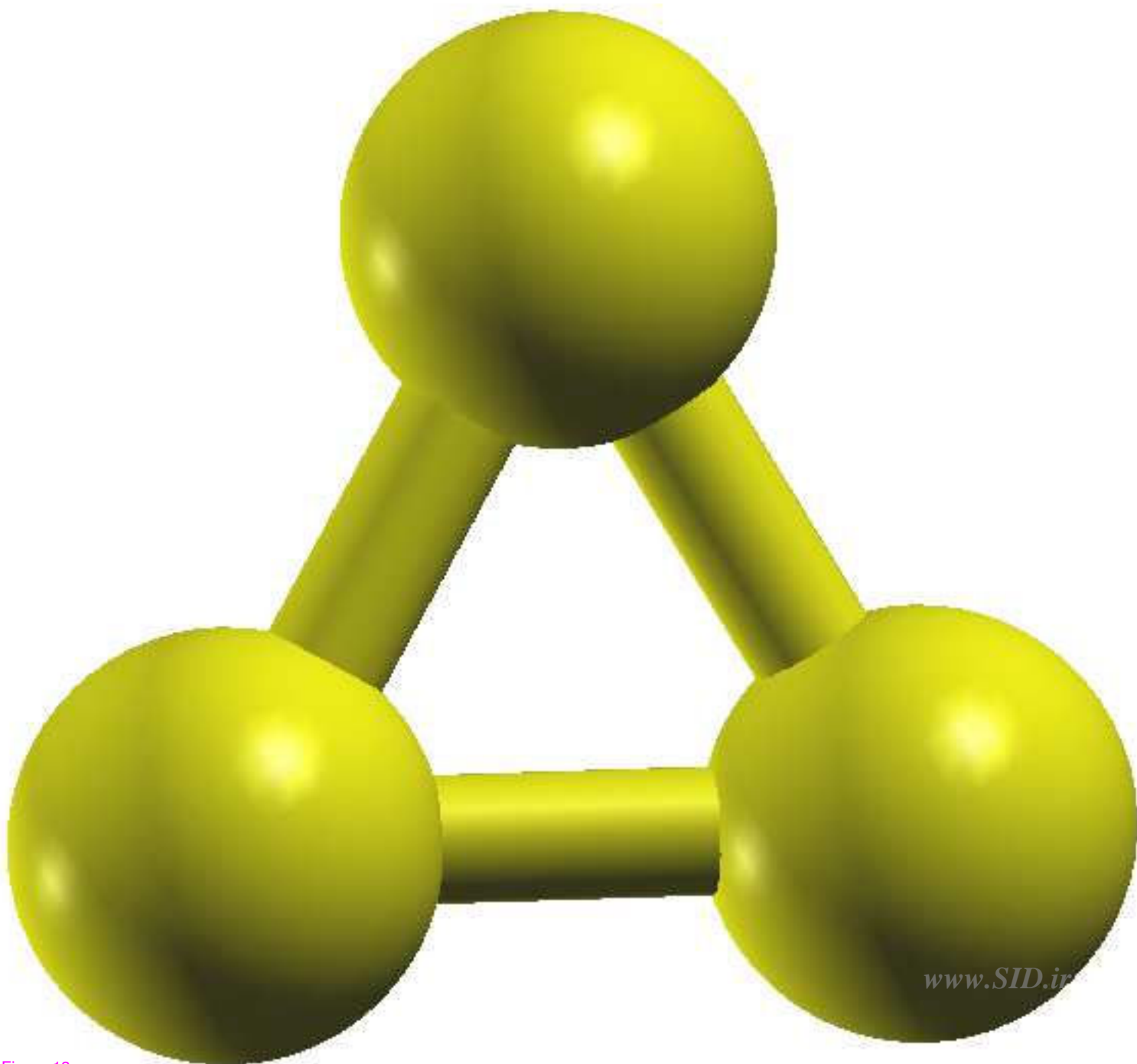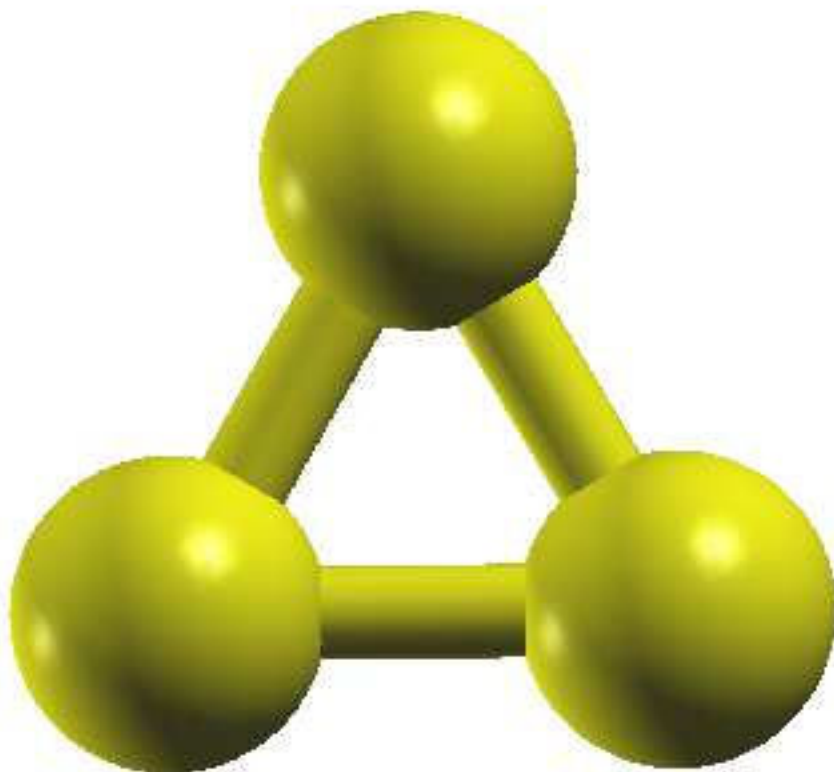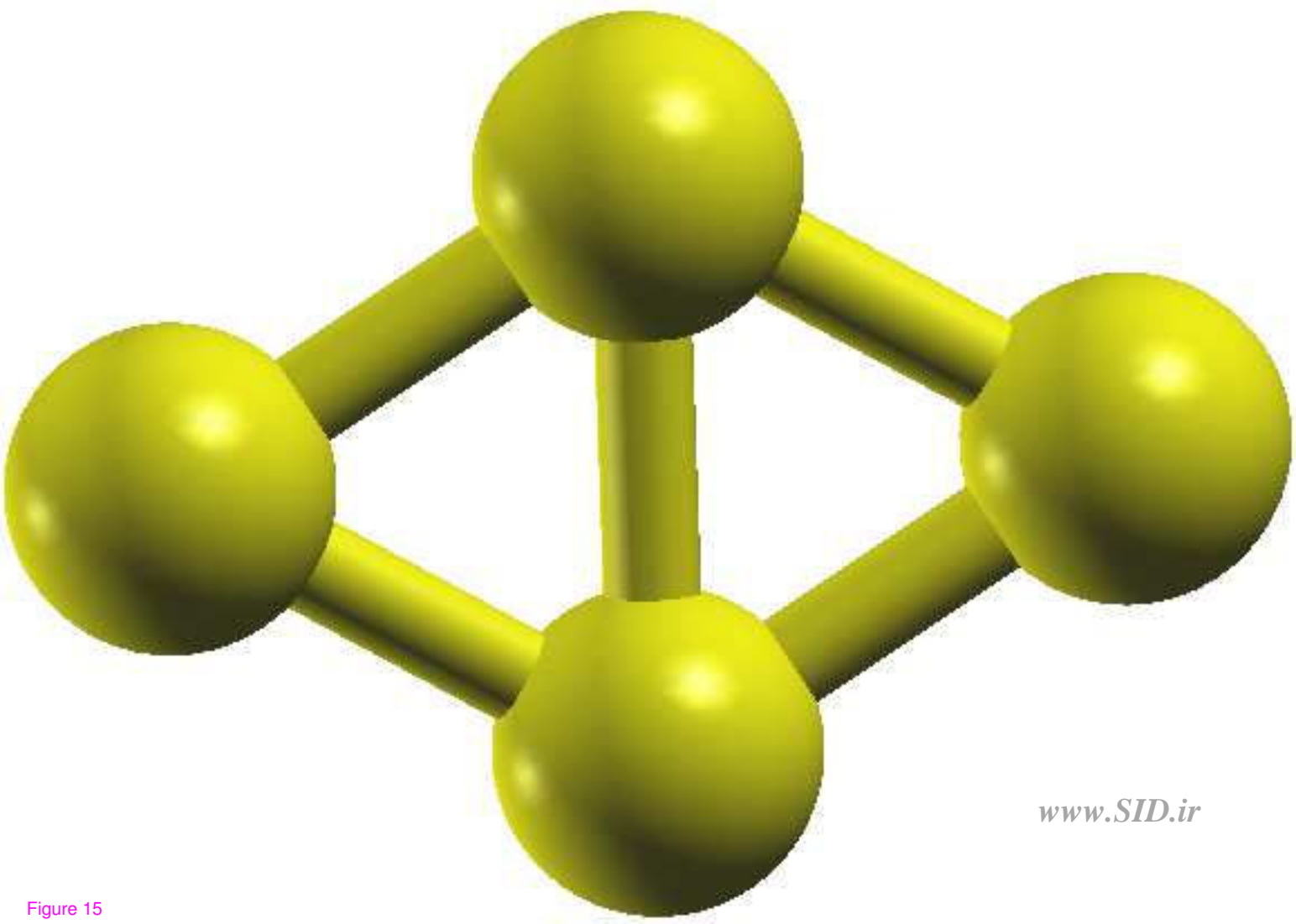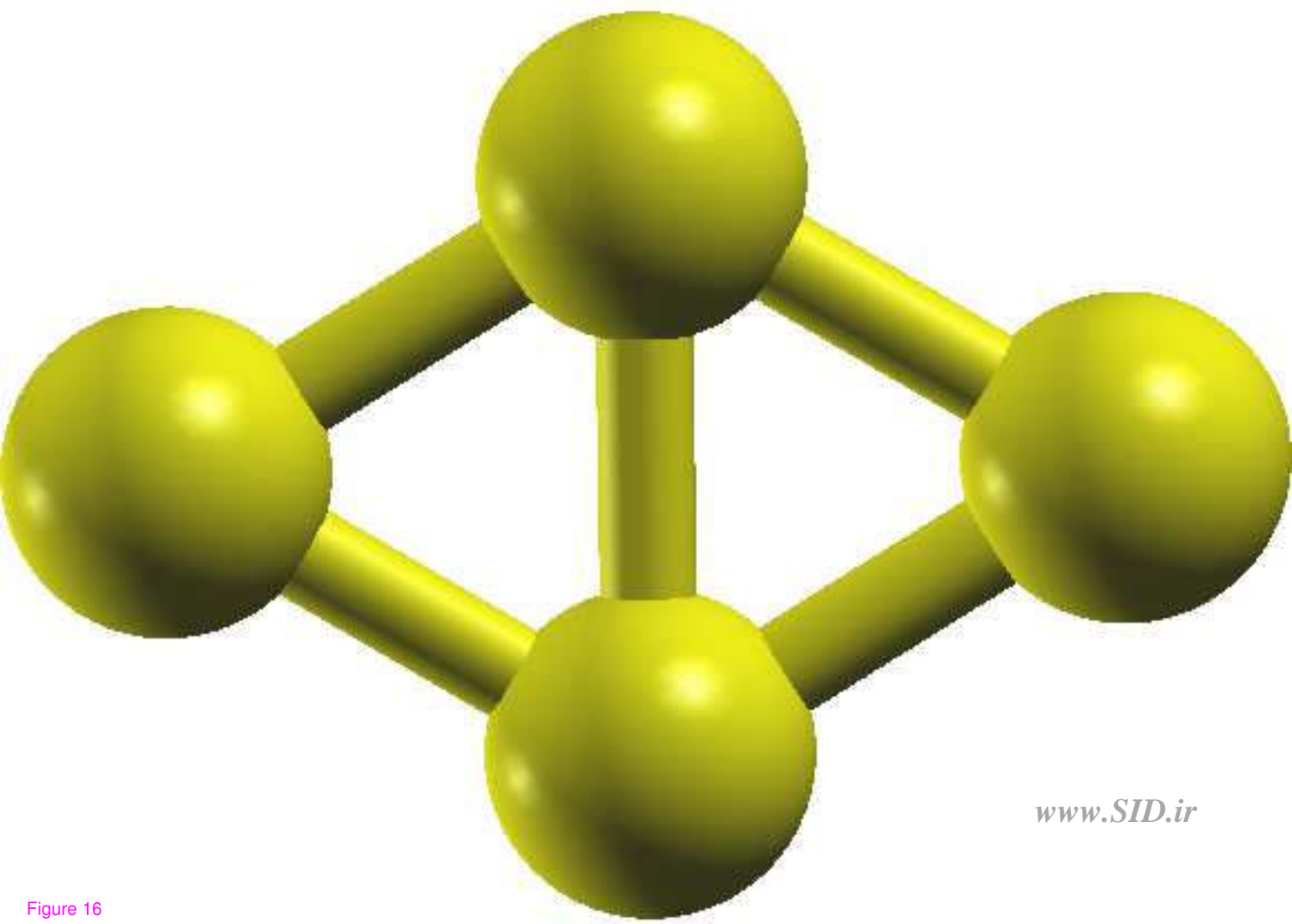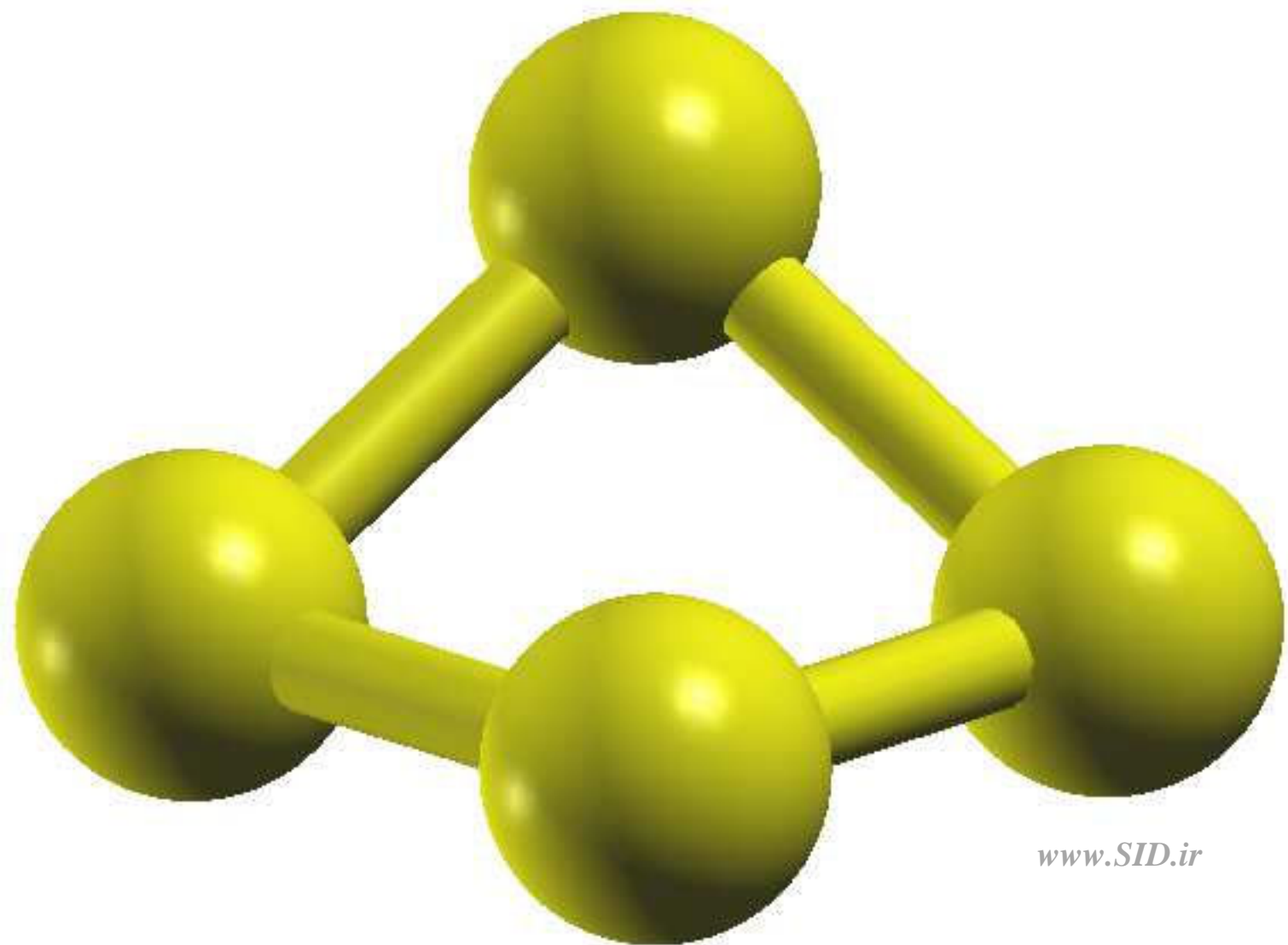
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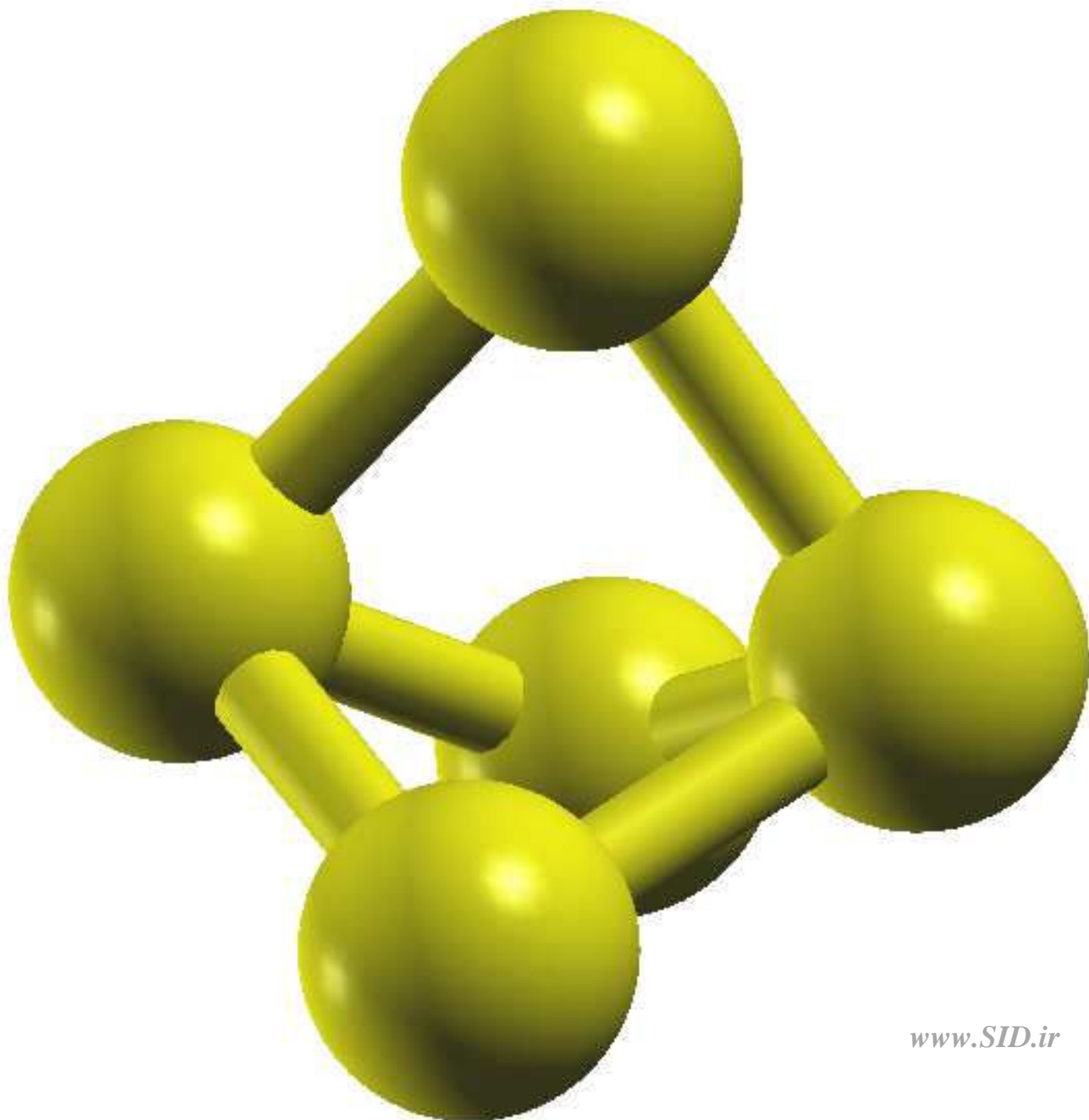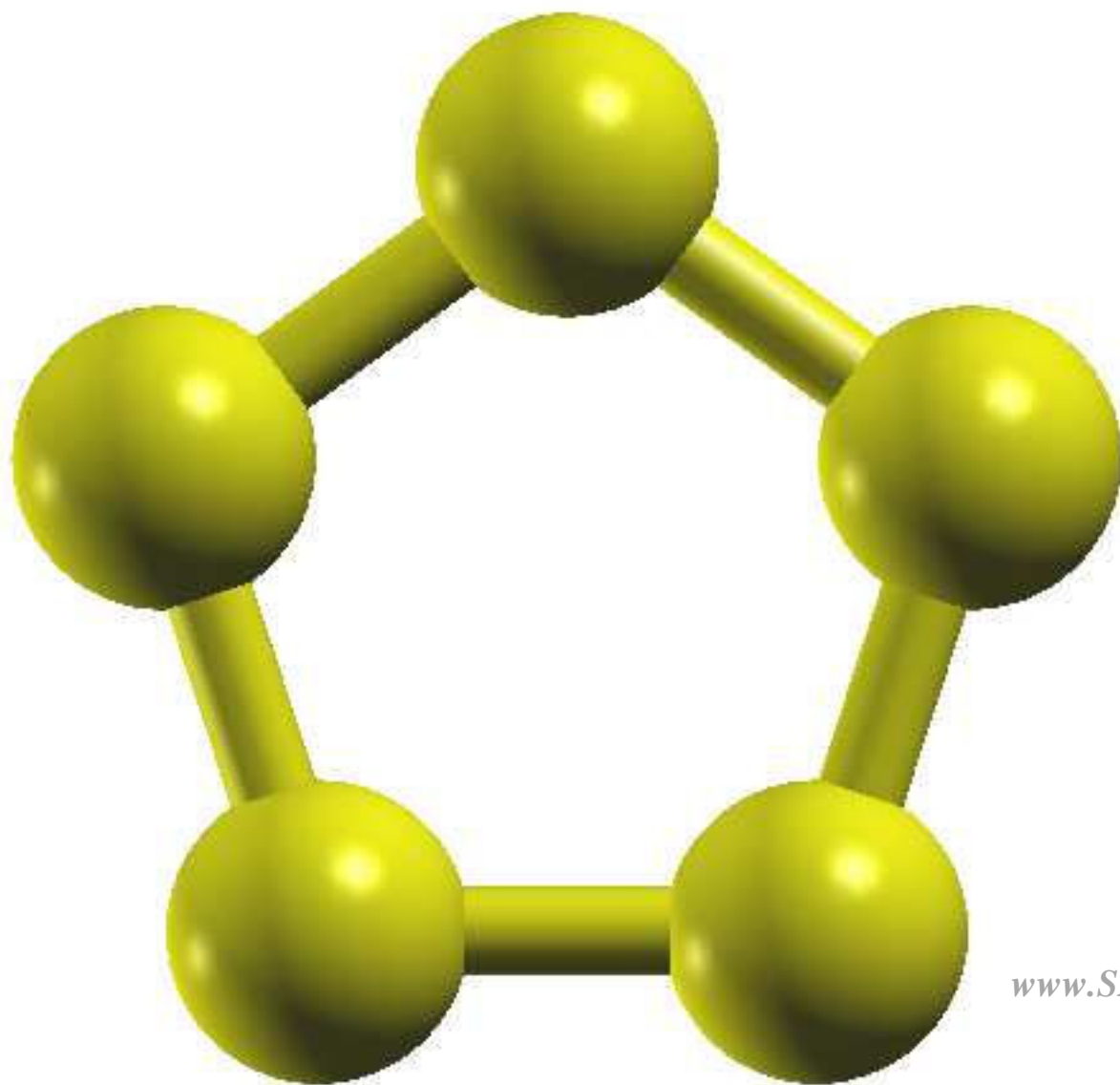
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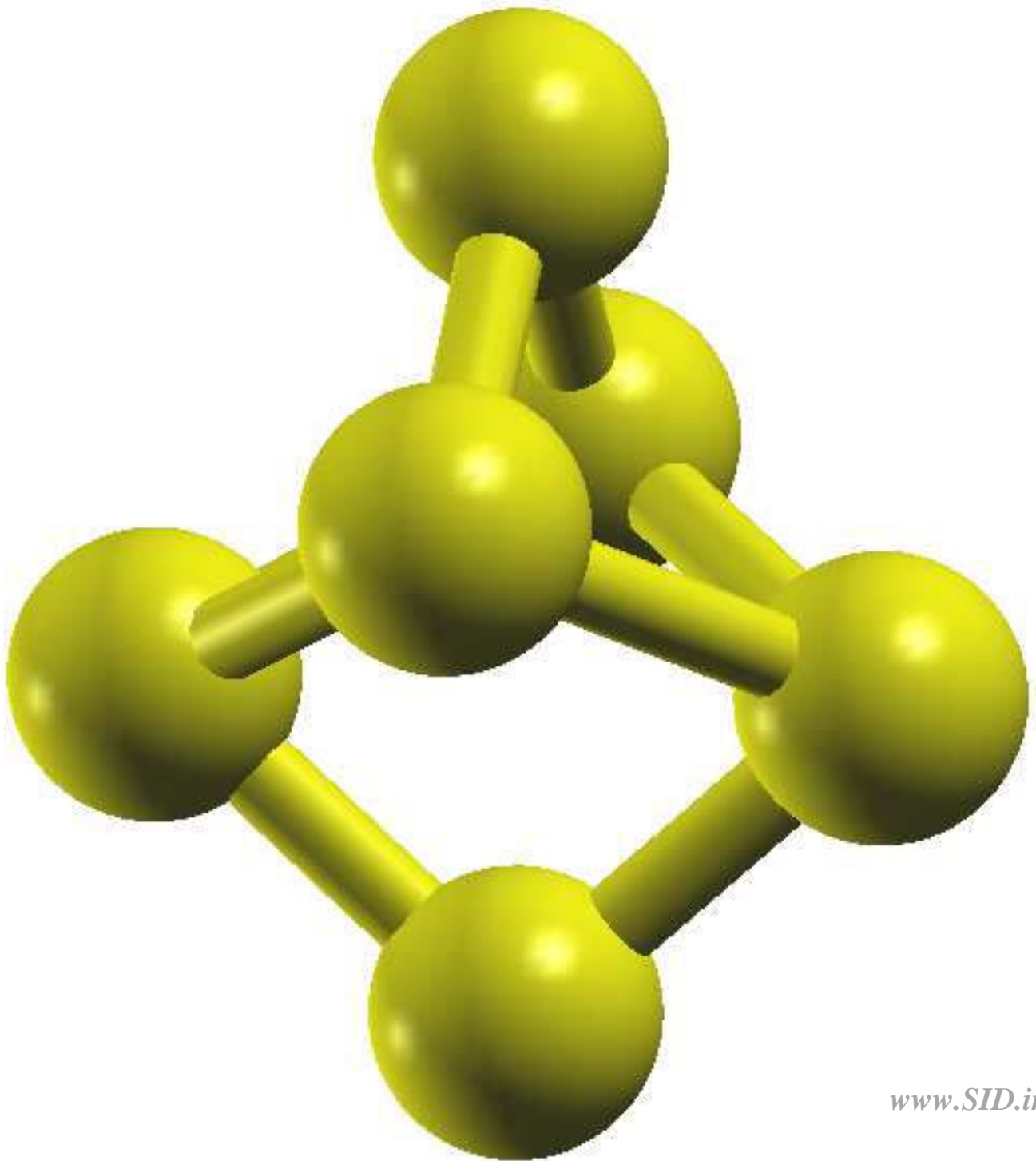
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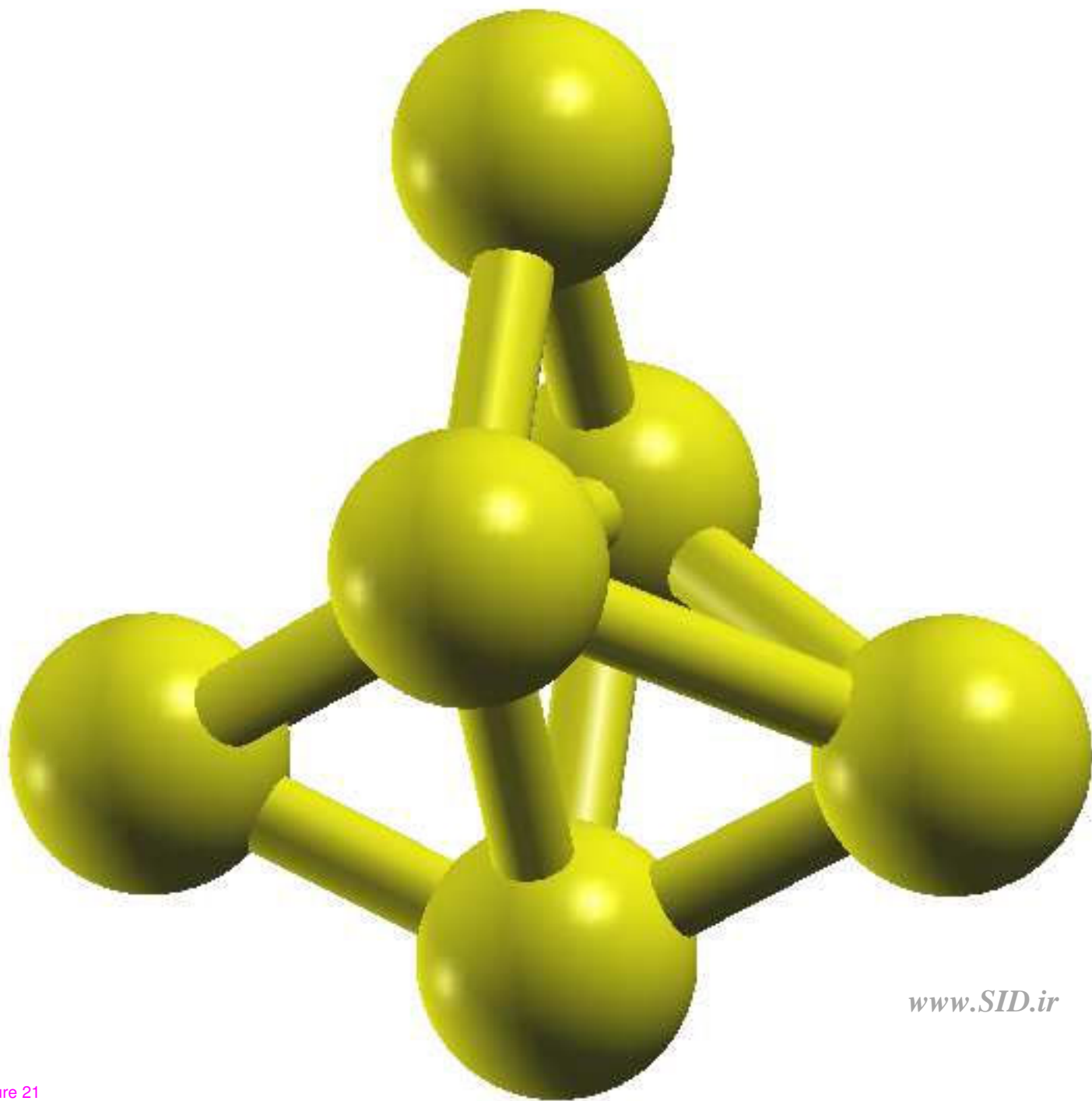
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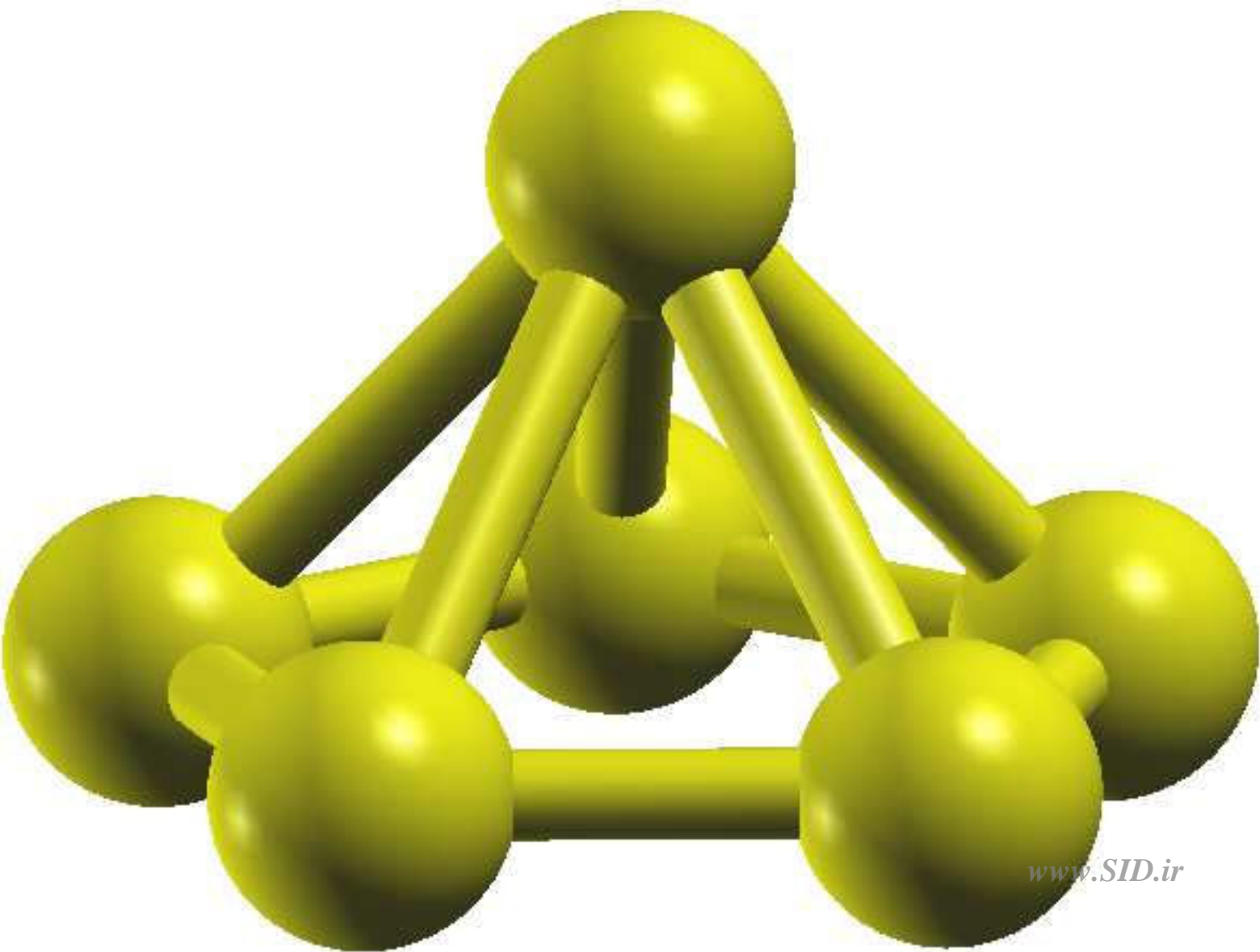
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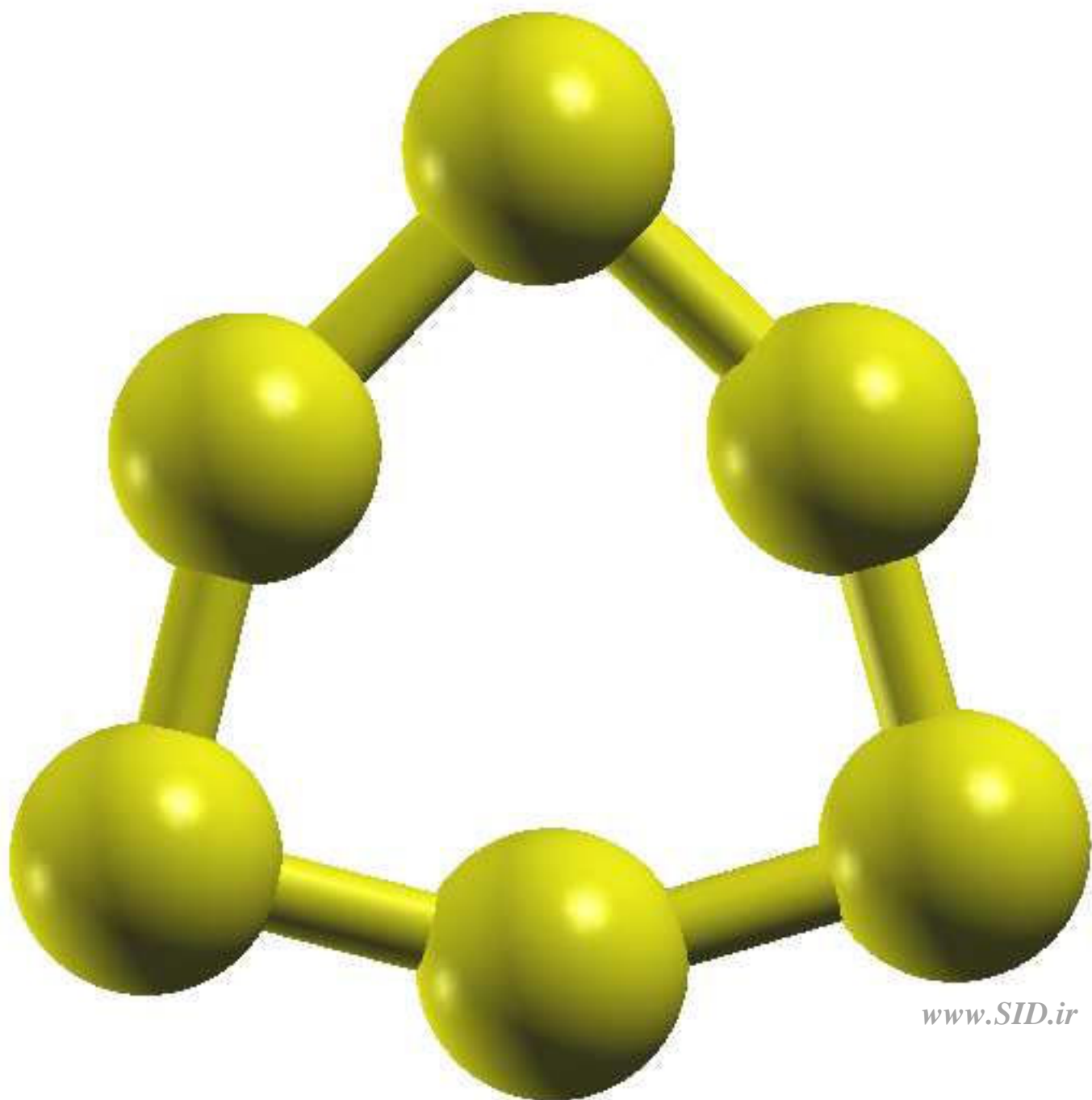
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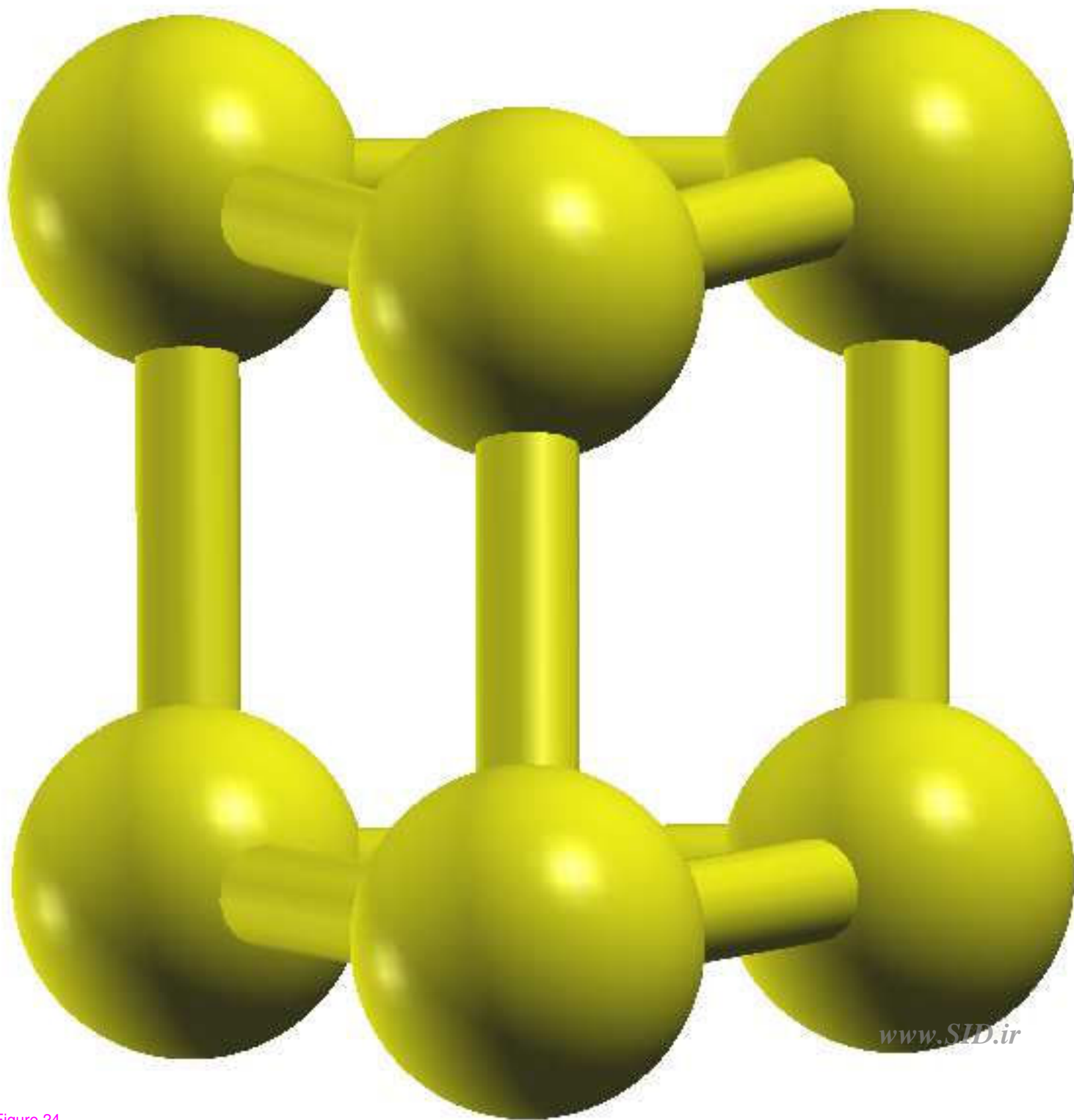
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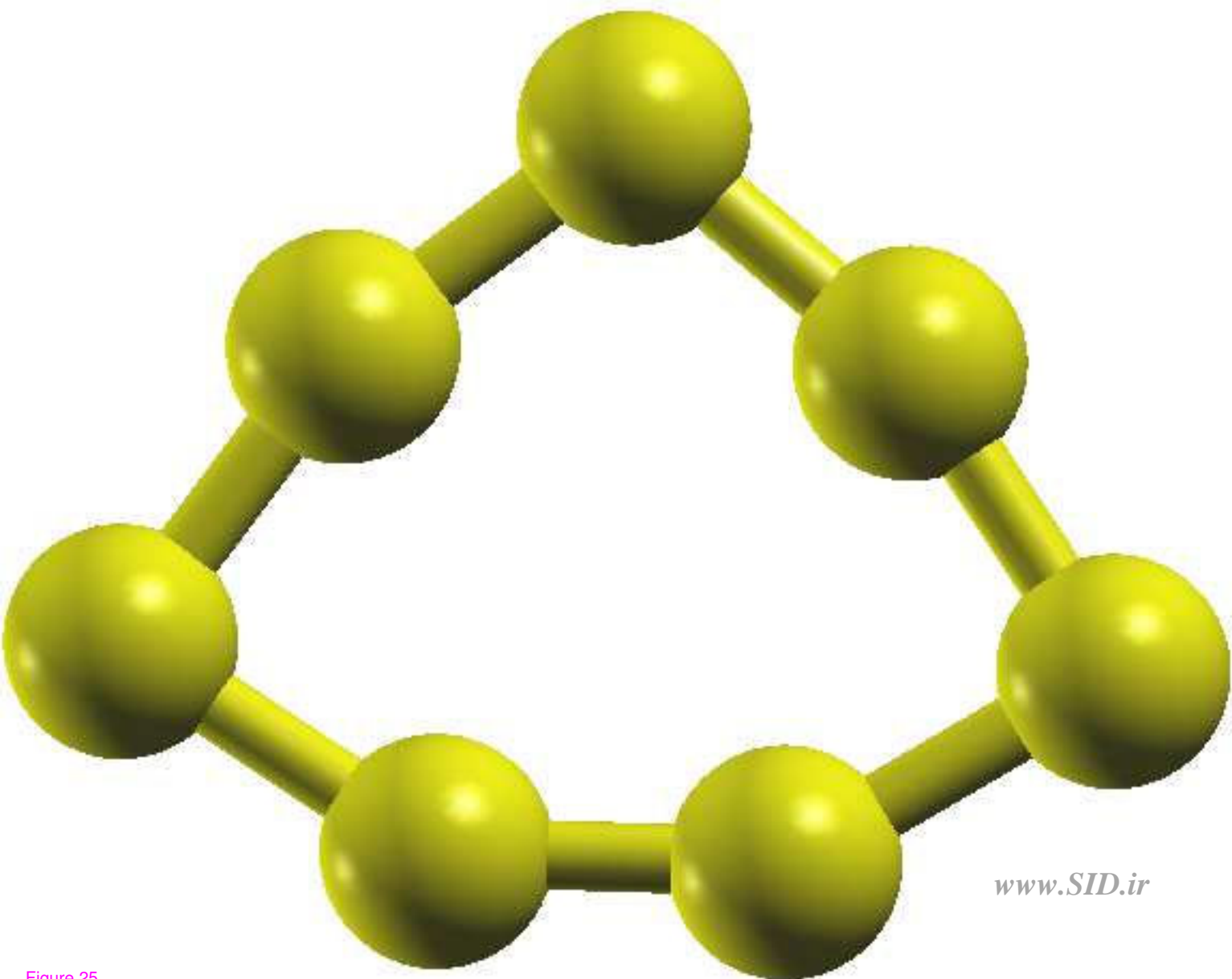
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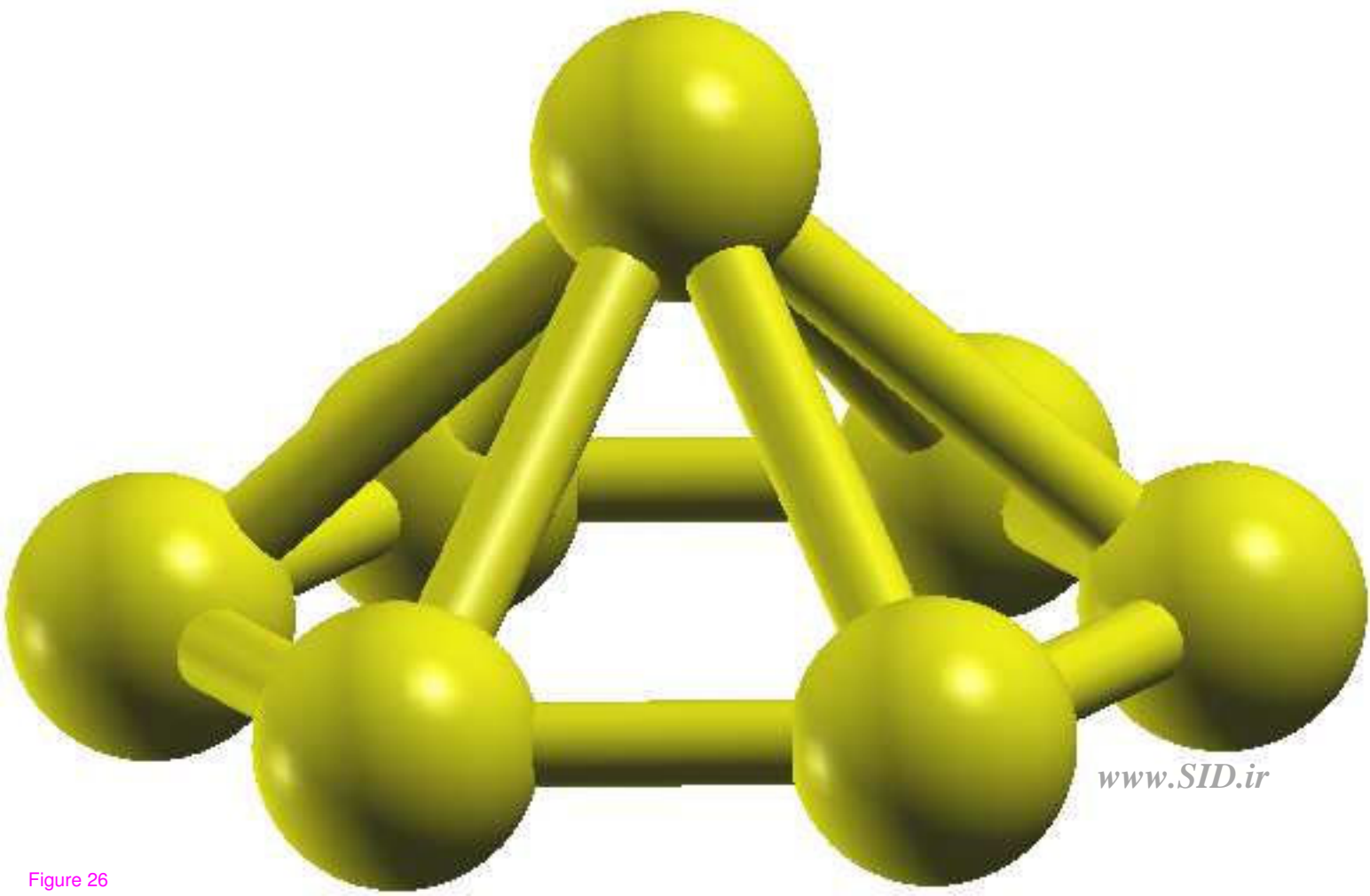
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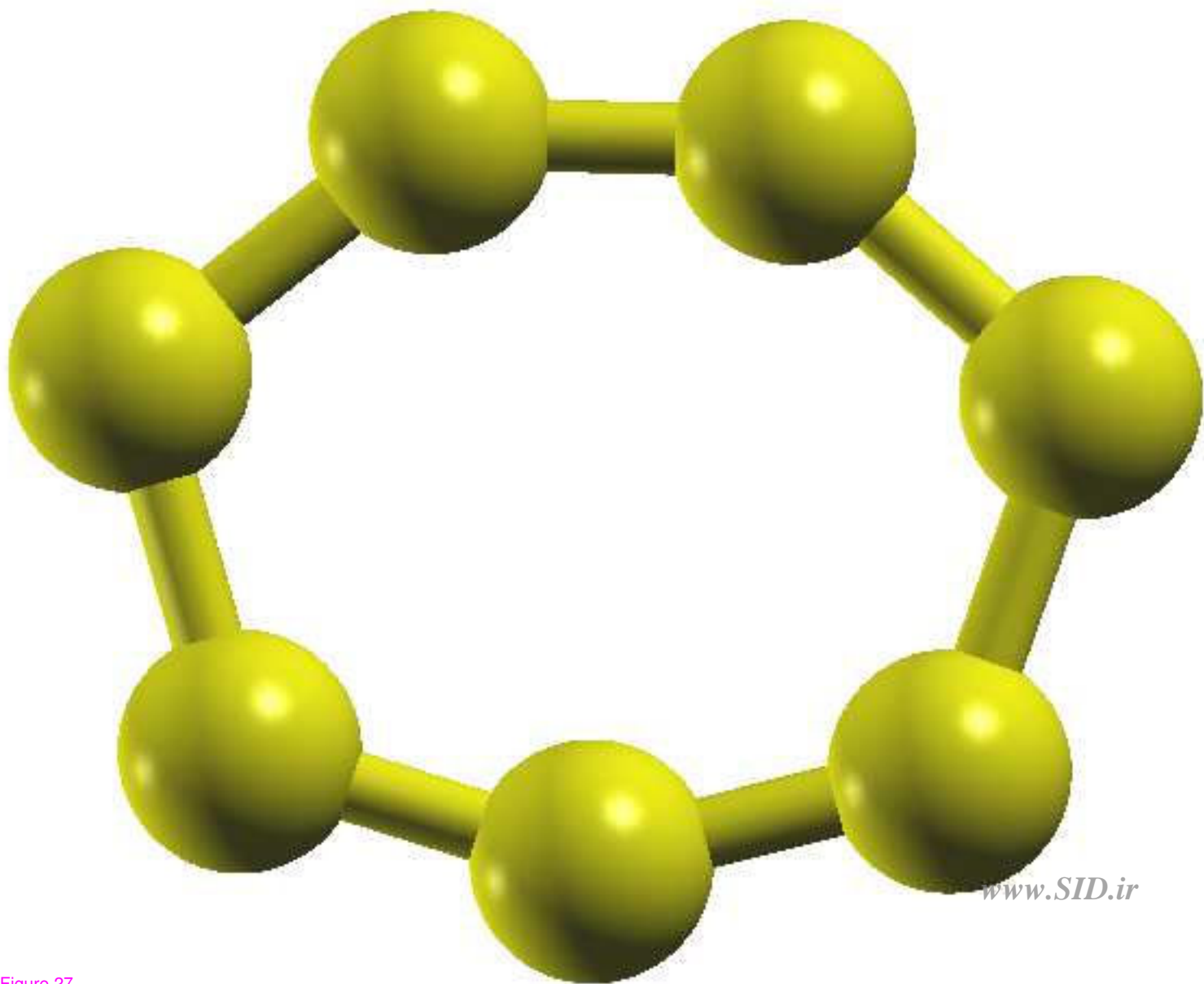
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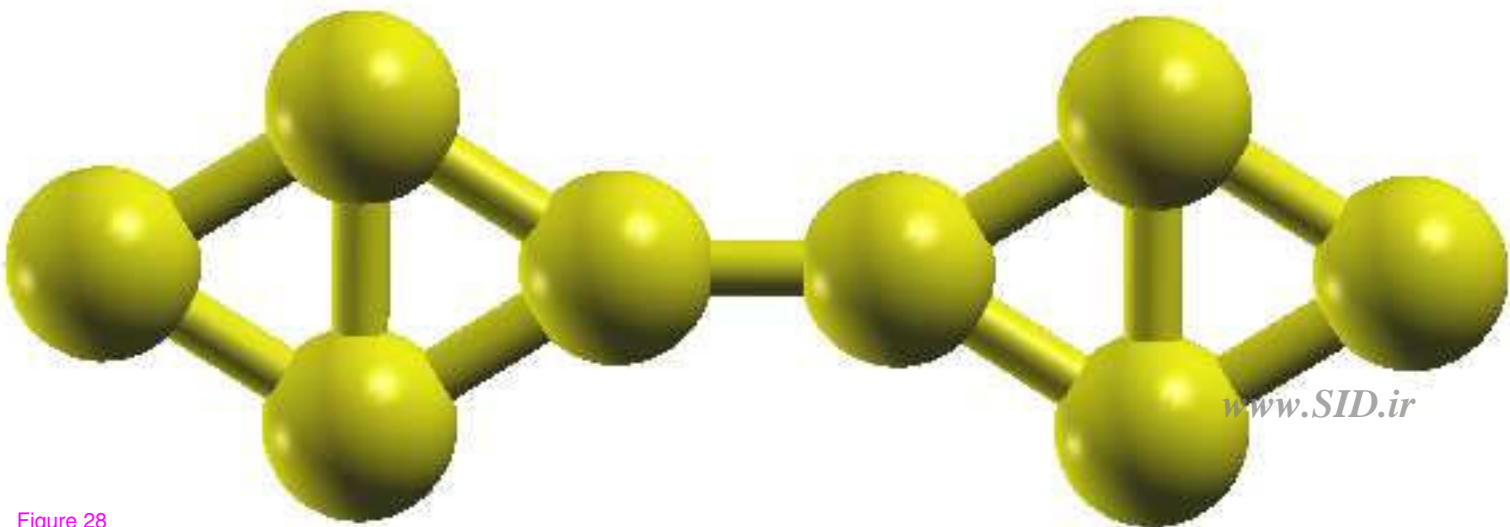
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Figure 25
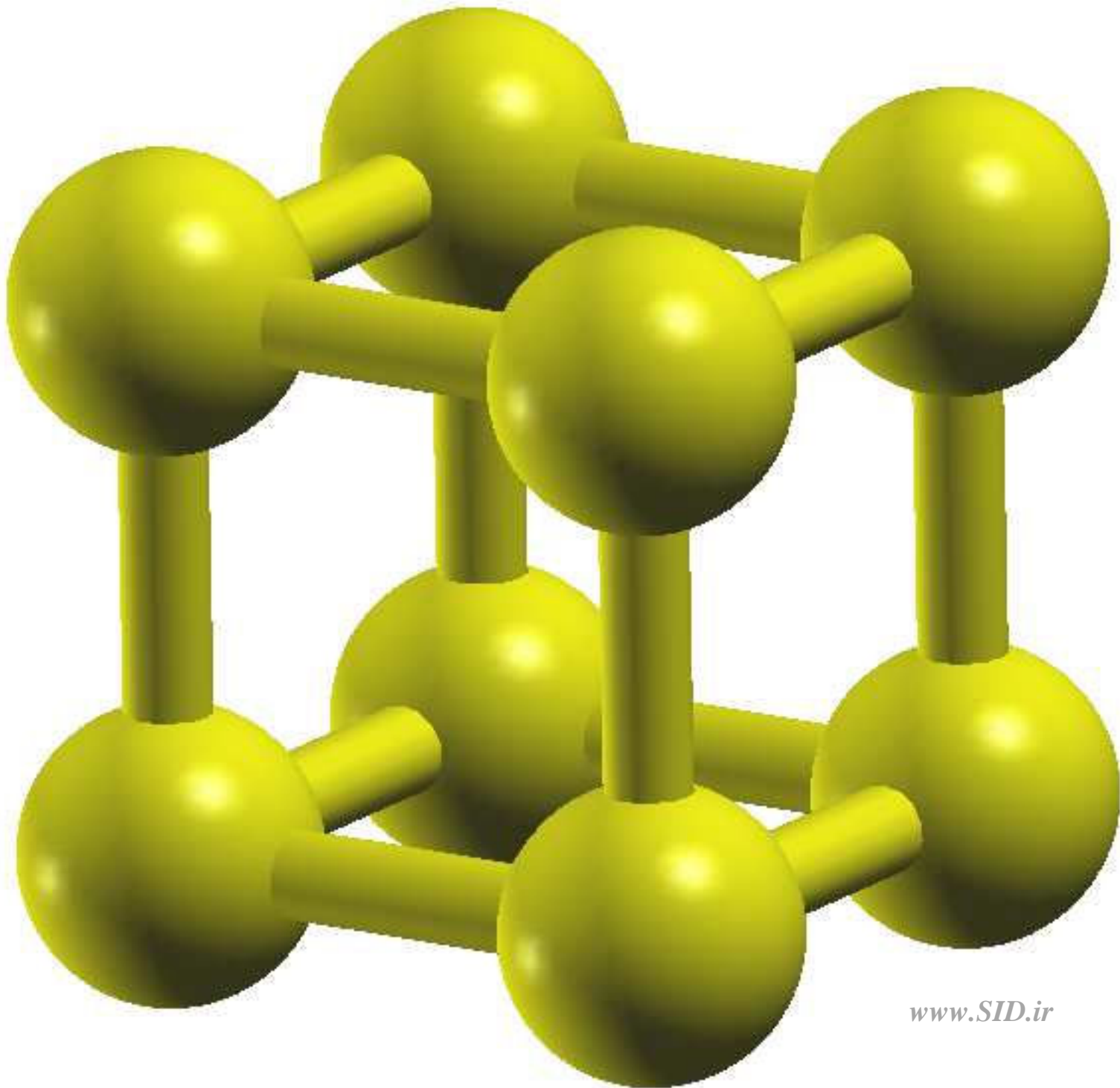
Figure 26

Figure 27

Figure 28

Figure 29

Figure 30

Figure 31

Figure 32

Figure 33

Figure 34

Figure 35

Figure 36

Figure 37

Figure 38

Additional files provided with this submission:

Additional file 1: Afshar-revised.tex, 32K
http://www.jtaphys.com/imedia/5079038102173051/supp1.tex
Additional file 2: Afshar-revised.dvi, 51K
http://www.jtaphys.com/imedia/1338321719102173/supp2.dvi
Additional file 3: Afshar-revised.pdf, 740K
http://www.jtaphys.com/imedia/2091235338102173/supp3.pdf