

${}_{60}S_8$  and  $C_{60}S_{16}$  were reported. It was determined that the interactions between the  $C_{60}$  and sulfur consisted mainly of weak van der Waals interactions—a structure in which the  $C_{60}$  cages were surrounded by unbound crown-shaped sulfur rings ( $S_8$ )<sup>[2-3]</sup>.

However, in high-pressure Raman studies of  $C_{60}S_{16}$ <sup>[4]</sup>, it has been proposed that the crown  $S_8$  rings break down and form covalent C-S bonds with the  $C_{60}$  cage. The covalent bonding of sulfur directly to  $C_{60}$  has been reported in the thermolysis preparation of  $C_{120}OS$ <sup>[5]</sup>. A plausible synthesis for  $C_{60}S$ , however, has yet to be determined<sup>[6]</sup>. While  $C_{60}S$  has yet to be synthesized, computational results for the [6,6] $C_{60}S$  and [5,6] $C_{60}S$  bridged systems have been

reported at the semi-empirical MNDO <sup>[6]</sup> and AM1 <sup>[7]</sup> levels. A mechanism for the rearrangch i-empirica



**Table 1:** This table is a summary of the calculated molecular energies for each of the compounds at different levels of theory. Only the initial singlet compounds were treated at the HF/DH(d)+S(d,p) level. Triplet states, protonated compounds and ionized compounds were built from B3LYP/DH(d)+S(d,p) geometries.

The geometry of the [6,6]C<sub>60</sub>S supports it as the most stable neutral isomer. The crucial C-C bond over which the sulfur atom is bridged was calculated to be 1.541 Å, while in the [5,6] isomer this C-C bond was 1.592 Å, as shown in Table 2. Since the difference in the le

[6,6]C<sub>60</sub>S, however, is 38.48 kcal mol<sup>-1</sup> higher in energy than the singlet state. Therefore, the singlet state is most likely preferred.

Table 2: Bond Distances and Angles at B3LYP/DH(d) + S(d,p) Fine Grid theory level

Compound	Bond	Distance (Å)	Bond	Angle (°)
C <sub>60</sub> S <sup>2-</sup>	C-C	1.393 - 1.529	S-C-C (to Hexagon)	116.2
	C-S	1.865	S-C-C (to Pentagon)	109.5
[5,6]C <sub>60</sub> S	C-C	1.387 - 1.592	C-S-C	51.1
	C-C (bound to S)	1.592		
	C-S	1.846		
[6,6]C <sub>60</sub> S	C-C	1.387 - 1.541	C-S-C	49.6
	C-C (bound to S)	1.541		
	C-S	1.836		
[5,6]C <sub>60</sub> S <sup>1-</sup>	C-C	In Progress	C-S-C	In Progress
	C-C (bound to S)	In Progress		
	C-S	In Progress		
[6,6]C <sub>60</sub> S <sup>1-</sup>	C-C	1.390 - 1.532	C-S-C	48.9
	C-C (bound to S)	1.532		
	C-S	1.850		
C <sub>60</sub> SH <sup>1-</sup> (on hexagon)	C-C	In Progress	S-C-C (to Hexagon)	In Progress
	C-S	In Progress	S-C-C (to Pentagon)	In Progress
	S-H	In Progress	C-S-H	In Progress
C <sub>60</sub> SH <sup>1-</sup> (in pentagon)	C-C	In Progress	S-C-C (to Hexagon)	In Progress
	C-S	In Progress	S-C-C (to Pentagon)	In Progress
	S-H	In Progress	C-S-H	In Progress
C <sub>60</sub> S <sup>2-</sup> Triplet	C-C	1.396 - 1.531	S-C-C (to Hexagon)	99.8
	C-S	1.863	S-C-C (to Pentagon)	116.8
[5,6]C <sub>60</sub> S Triplet	C-C	1.387 - 1.536	C-S-C	48.6
	C-C (bound to S)	1.536		
	C-S	1.867		
[6,6]C <sub>60</sub> S Triplet	C-C	1.395 - 1.530	C-S-C	49.2
	C-C (bound to S)	1.530		
	C-S	1.838		

Table 2: Unique bond lengths and angles for each of the three studied isomers of C<sub>60</sub>S.

It is also worthwhile to

It should be noted that these calculations were performed using the energies as calculated at the coarse grid B3LYP/DH(d)+S(d,p) level—fine grid energy is still being calculated for [5,6]C<sub>60</sub>S.

Table 4: Vertical Electron Affinities (Coarse Grid)

Compound	Electron Affinity (eV)
[5,6]C <sub>60</sub> S	3.797
[6,6]C <sub>60</sub> S	2.477
C <sub>60</sub>	2.683 <sup>[11]</sup>
Br <sup>-</sup>	3.363 <sup>[12]</sup>
I <sup>-</sup>	3.063 <sup>[12]</sup>
S <sup>-</sup>	2.07 <sup>[12]</sup>

Table 6: Proto



proton affinity for each of the closed isomers as well as calculating the frequency data for all the aforementioned forms of  $C_{60}S$ .

While this study brushes the surface of the characterization of  $C_{60}S$  at a decent theory level, there is still a need to computationally explore, at an electron correlated theory level, a plausible mechanism of isomer rearrangement as well

[6] D

### Appendix A: Cartesian Coordinates

C<sub>60</sub>S<sup>2-</sup> B3LYP/DH(d)+S(d,p)

[5,6]-closed C<sub>60</sub>S B3LYP/DH(d)+S(d,p)

C -0.0085200297 -0.7159922782 -3.4780183383  
 C -0.0085200297 -0.7159922782 3.4780183383  
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 C -0.0106389959 0.6886085927 3.4715691038  
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 C -1.1849674677 -1.4592191866 3.0586793318  
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 C -0.7372491403 2.5889301397 2.0439409000  
 C 2.2975216408 -0.7285947785 2.6152617319  
 C 2.2975216408 -0.7285947785 2.6152617319  
 C -2.3196743900 0.7170215928 -2.6048152534  
 C -2.3196743900 0.7170215928 2.6048152534  
 C 2.2916121954 0.7235250789 2.6033940155  
 C 2.2916121954 0.7235250789 2.6033940155  
 C -0.7338641715 -2.6146369411 -2.3143491863  
 C -0.7338641715 -2.6146369411 2.3143491863  
 C 0.722

[6,6]-closed C<sub>60</sub>S B3LYP/DH(d)+S(d,p)

C	0.0076383625	-0.7015876108	-3.4782106185
C	0.0076383625	-0.7015876108	3.4782106185
C	0.0202950203	0.6964112348	-3.4660658130
C	0.0202950203	0.6964112348	3.4660658130
C	-1.1781221259	-1.4228565406	-3.0338979572
C	-1.1781221259	-1.4228565406	3.0338979572
C	1.1801460427	-1.4442050632	-3.0338983597
C	1.1801460427	-1.4442050632	3.0338983597
C	-1.1522623000	1.4349459211	-3.0202553182
C	-1.1522623000	1.4349459211	3.0202553182
C	1.2060316368	1.4135976284	-3.0202567522
C	1.2060316368	1.4135976284	3.0202567522
C	-2.3073323269	-0.7160536141	-2.6046290159
C	-2.3073323269	-0.7160536141	2.6046290159
C	2.3219676950	-0.7579625855	-2.6046296631
C	2.3219676950	-0.7579625855	2.6046296631
C	-2.2966068097	0.7390620473	-2.6012235463
C	-2.2966068097	0.7390620473	2.6012235463
C	2.3375900965	0.6971087530	-2.6012241559
C	2.3375900965	0.6971087530	2.6012241559
C	-0.7386787490	-2.6033070947	-2.3091512963
C	-0.7386787490	-2.6033070947	2.3091512963
C	0.7193994622	-2.6165006422	-2.3091473201
C	0.7193994622	-2.6165006422	2.3091473201
C	-0.7017424744	2.6091503566	-2.2984941107
C	-0.7017424744	2.6091503566	2.2984941107
C	0.7768452044	2.5957666703	-2.2984958599
C	0.7768452044	2.5957666703	2.2984958599
C	-3.0407791727	-1.1639924336	-1.4284221165
C	-3.0407791727	-1.1639924336	1.4284221165
C	3.0471845750	-1.2191081953	-1.4284234227
C	3.0471845750	-1.2191081953	1.4284234227
C	-3.0158128351	1.1888744680	-1.4287956266
C	-3.0158128351	1.1888744680	1.4287956266
C	3.0648217143	1.1338248826	-1.4287956274
C	3.0648217143	1.1338248826	1.4287956274
C	-1.4423042514	-3.0336547323	-1.1777926644
C	-1.4423042514	-3.0336547323	1.1777926644
C	1.4151186888	-3.0595165961	-1.1777902951
C	1.4151186888	-3.0595165961	1.1777902951
C	-1.4048253342	3.0491960545	-1.1868513571
C	-1.4048253342	3.0491960545	1.1868513571
C	1.4877796810	3.0230	(+)



[6,6]-closed  $C_{60}S^{-1}$  B3LYP/DH(d)+S(d,p)

C	0.0075517316	-0.7111596146	-3.4891950699
C	0.0075517316	-0.7111596146	3.4891950699
C	0.0203649695	0.7041773394	-3.4783868314
C	0.0203649695	0.7041773394	3.4783868314
C	-1.1709844305	-1.4235134702	-3.0346485930
C	-1.1709844305	-1.4235134702	3.0346485930
C	1.1729968387	-1.4	