$_{60}S_8$ 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)[2-3].

However, in high-pressure Raman studies of $C_{60}S_{16}$ [4], 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 $C_{120}OS$ [5]. A plausible synthesis for $C_{60}S$, however, has yet to be determined [6]. 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 [6] and AM1 [7] levels. A mechanism for the rearrangch i-empirica

ec.94

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_{60}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 o

[6,6]$C_{60}S$, however, is 38.48 kcal mol^{-1} 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 (°)
$C_{60}S^{2-}$				
	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]$C_{60}S$				
	C-C	1.387 - 1.592	C-S-C	51.1
	C-C (bound to S)	1.592		
	C-S	1.846		
[6,6]$C_{60}S$				
	C-C	1.387 - 1.541	C-S-C	49.6
	C-C (bound to S)	1.541		
	C-S	1.836		
[5,6]$C_{60}S^{1-}$				
	C-C	In Progress	C-S-C	In Progress
	C-C (bound to S)	In Progress		
	C-S	In Progress		
[6,6]$C_{60}S^{1-}$				
	C-C	1.390 – 1.532	C-S-C	48.9
	C-C (bound to S)	1.532		
	C-S	1.850		
$C_{60}SH^{1-}$(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
$C_{60}SH^{1-}$(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
$C_{60}S^{2-}$ 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]$C_{60}S$ 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]$C_{60}S$ 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 $C_{60}S$.

It is also worthwhile to

It should be noted that these calculations were preformed 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]C60S.

Table 4: Vertical Electron Affinities (Coarse Grid)

Compound	Electron Affinity (eV)
[5,6]C_{60}S	3.797
[6,6]C_{60}S	2.477
C_{60}	2.683 [11]
Br^-	3.363 [12]
I^-	3.063 [12]
S^-	2.07 [12]

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

$C_{60}S^{2-}$ B3LYP/DH(d)+S(d,p)

C	-0.0085200297	-0.7159922782	-3.4780183383
C	-0.0085200297	-0.7159922782	3.4780183383
C	-0.0106389959	0.6886085927	-3.4715691038
C	-0.0106389959	0.6886085927	3.4715691038
C	-1.1849674677	-1.4592191866	-3.0586793318
C	-1.1849674677	-1.4592191866	3.0586793318
C	1.1781948384	-1.4396616353	-3.0369074367
C	1.1781948384	-1.4396616353	3.0369074367
C	-1.1970252874	1.4203696247	-3.0173549831
C	-1.1970252874	1.4203696247	3.0173549831
C	1.1583854820	1.4189497884	-3.0287079357
C	1.1583854820	1.4189497884	3.0287079357
C	-2.3166667187	-0.7457713197	-2.6041691254
C	-2.3166667187	-0.7457713197	2.6041691254
C	2.3135754042	-0.7281526952	-2.6100268871
C	2.3135754042	-0.7281526952	2.6100268871
C	-2.3495156403	0.6968311859	-2.6176439520
C	-2.3495156403	0.6968311859	2.6176439520
C	2.3128563953	0.7217881981	-2.6147227527
C	2.3128563953	0.7217881981	2.6147227527
C	-0.7217883062	-2.6143412195	-2.3085625615
C	-0.7217883062	-2.6143412195	2.3085625615
C	0.7391374917	-2.6207500204	-2.3153001073
C	0.7391374917	-2.6207500204	2.3153001073
C	-0.7681153571	2.6009234473	-2.3261252535
C	-0.7681153571	2.6009234473	2.3261252535
C	0.7005349674	2.5936062987	-2.3053555360
C	0.7005349674	2.5936062987	2.3053555360
C	-3.0461290151	-1.2111445090	-1.4292222333
C	-3.0461290151	-1.2111445090	1.4292222333
C	3.0407673542	-1.1792986563	-1.4270798808
C	3.0407673542	-1.1792986563	1.4270798808
C	-3.0681148687	1.1397222768	-1.4306020829
C	-3.0681148687	1.1397222768	1.4306020829
C	3.0238393355	1.1744585223	-1.4378875701
C	3.0238393355	1.1744585223	1.4378875701
C	-1.4183459830	-3.0658606152	-1.1777177254
C	-1.4183459830	-3.0658606152	1.1777177254
C	1.4394961538	-3.0518505135	-1.1757418565
C	1.4394961538	-3.0518505135	1.1757418565
C	-1.4484175365	3.0139165090	-1.1506331610
C	-1.4484175365	3.0139165090	1.1506331610
C	1.3890698397	3.0317820050	-1.1770415195
C	1.3890698397	3.0317820050	1.1770415195
C	-2.6028542721	-2.3399494873	-0.7271250415
C	-2.6028542721	-2.3399494873	0.7271250415
C	2.6154240369	-2.3192681411	-0.7284696198
C	2.6154240369	-2.3192681411	0.7284696198
C	-2.6398710549	2.2691457943	-0.7248929343
C	-2.6398710549	2.2691457943	0.7248929343
C	2.5399636990	2.2895692512	-0.7283666498
C	2.5399636990	2.2895692512	0.7283666498
C	-3.5130094489	-0.0402604581	-0.7004708754
C	-3.5130094489	-0.0402604581	0.7004708754
C	3.4806816254	0.0001372376	-0.6997674900
C	3.4806816254	0.0001372376	0.6997674900
C	-0.6860436086	-3.5003735131	0.0000000000
C	0.7227211988	-3.5190289542	0.0000000000
C	-0.7606732546	3.4916493684	0.0000000000
C	0.7332360420	3.7537063264	0.0000000000
S	1.2539950002	5.5450295139	0.0000000000

[5,6]-closed $C_{60}S$ B3LYP/DH(d)+S(d,p)

C	-0.0102791633	-0.7097525383	-3.4980829198
C	-0.0102791633	-0.7097525383	3.4980829198
C	-0.0089072880	0.6916132562	-3.4856378776
C	-0.0089072880	0.6916132562	3.4856378776
C	-1.1886458401	-1.4371615313	-3.0432373775
C	-1.1886458401	-1.4371615313	3.0432373775
C	1.1674473659	-1.4341838165	-3.0497331856
C	1.1674473659	-1.4341838165	3.0497331856
C	-1.1857818406	1.4156248256	-3.0309387421
C	-1.1857818406	1.4156248256	3.0309387421
C	1.1668797281	1.4180853512	-3.0350803012
C	1.1668797281	1.4180853512	3.0350803012
C	-2.3194767034	-0.7398357981	-2.6093780761
C	-2.3194767034	-0.7398357981	2.6093780761
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	-0.7338641715	-2.6146369411	-2.3143491863
C	-0.7338641715	-2.6146369411	2.3143491863
C	0.7227833457	-2.6074277455	-2.3186181120
C	0.7227833457	-2.6074277455	2.3186181120
C	-0.7372491403	2.5889301397	6420

[6,6]-closed C_{60}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 (illegible)	

[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	