SUPPORTING INFORMATION

Strong Be-Be Bond in Double-Aromatic Bridged $Be_2(\mu$-SO) Molecule

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Table S1. Evaluated NBO charges (q), charge separation in SO (Δq) and Wiberg (W) and Mayer (M) bond indices of the SO, Be-S and Be-Be bond.

Table S2. Free energies (G) and electronic energies (E) of all dissociation products by different methods.

Table S3. Structures and coordinates of dissociation products at CCSD(T)/cc-pVTZ level of theory.

Fig. S1. Total NICS values and their zz components at a) center of the ring, b) 0.5Å and c) 1.0Å above the ring center at the MP2/cc-pVTZ level of theory.

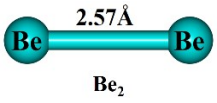
Table S1. Evaluated NBO charges (q), charge separation in SO (Δq) and Wiberg (W) and Mayer (M) bond indices of the SO, Be-S and Be-Be bond.

Moiety	**q(S)**	**q(O)**	**q(SO)**	**Δq(SO)s**	$\mathbf{W_{S-O}}$	$\mathbf{M_{S-O}}$	$\mathbf{W_{Be-S}}$	$\mathbf{M_{Be-S}}$	$\mathbf{W_{Be-Be}}$	$\mathbf{M_{Be-Be}}$
SO	+0.634	-0.634	0	1.268	1.247	0.264				
Be_2(μ-SO)	+0.279	-0.880	-0.601	1.159	1.035	1.435	0.855	1.015	0.837	1.091

Table S2. Free energies (G) and electronic energies (E) of all dissociation products by different methods. All values are in kcal.mol^{-1}.

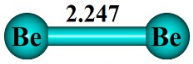
Dissociation product	G			E		
	ωB97X-D	**MP2**	**CCSD(T)**	**ωB97X-D**	**MP2**	**CCSD(T)**
Be	-14.679273	-14.614148	-14.631529	-14.6661701	-14.6010452	-14.618427
O	-74.978502	-74.862698	-74.906510	-74. 964587	-74.8487835	-74.8925947
S	-398.068133	-397.573598	-397.618715	-398.0532375	-397.5587018	-397.6038195
Be_2	-29.355042	-29.223349	-29.257615	-29.3356631	-29.2035378	-29.2386696
Be_2^+	-29.101001	-28.966076	-28.986324	-29.08266	-28.9477825	-28.9680192
BeSO	-488.065047	-487.413265	-487.460474	-488.0442933	-487.3930663	-487.439163
SO^-	-473.423961	-472.810047	-472.847527	-473.4044642	-472.791462	-472.8279566
SO(singlet)	-473.349838	-472.760023	-472.791090	-473.331752	-472.7414606	-472.7726904
SO(triplet)	-473.396265	-472.797657	-472.828867	-473.3771377	-472.7783666	-472.8095875

Table S3. Structures and coordinates of dissociation products at CCSD(T)/cc-pVTZ level of theory.



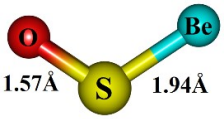
Be_2

```
0 1
Be 0.00000000 0.00000000  1.26791300
Be 0.00000000 0.00000000 -1.26791300
```



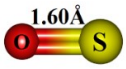
Be_2^+

```
1 2
Be 0.00000000 0.00000000  1.12318700
Be 0.00000000 0.00000000 -1.12318700
```



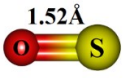
BeSO

```
0 1
Be 1.88066800 -0.05060100 0.00000000
S  0.00000000  0.42763500 0.00000000
O -0.94033400 -0.82997000 0.00000000
```



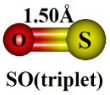
SO^-

```
-1 2
S 0.00000000 0.00000000 0.53306100
O 0.00000000 0.00000000 -1.06612200
```



SO(singlet)

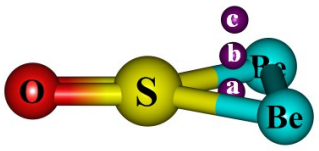
```
0 1
S 0.00000000 0.00000000 0.50478800
O 0.00000000 0.00000000 -1.00957600
```



SO(triplet)

```
0 3
S 0.00000000 0.00000000 0.50022900
O 0.00000000 0.00000000 -1.00045800
```

Fig. S1. Total NICS values and their zz components at a) center of the ring, b) 0.5Å and c) 1.0Å above the ring center at the MP2/cc-pVTZ level of theory.



	NICS	$NICS_{zz}$
a	-37.57	-30.20
b	-30.31	-25.05
c	-14.98	-16.47