Supporting Information

Reply to the 'Comment on "Strong Be–Be bonds in double-aromatic bridged $Be_2(\mu$-SO) molecules" by F. Rezaie and S. Noorizadeh, Dalton Trans., 2022, 51, 12596.

F. Rezaie and S. Noorizadeh*

Output file of bridged Be2(μ-SO) molecule

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Summary of Natural Population Analysis:

			Natural Population			
		Natural	----------			
Atom	No	Charge	Core	Valence	Rydberg	Total
Be	1	0.37729	1.99694	1.61287	0.01290	3.62271
Be	2	0.37695	1.99694	1.61319	0.01291	3.62305
S	3	0.24499	9.99819	5.60294	0.15388	15.75501
O	4	-0.99923	1.99990	6.95852	0.04082	8.99923
* Total *		0.00000	15.99197	15.78752	0.22051	32.00000

Natural Population	
Core	15.99197 (99.9498% of 16)
Valence	15.78752 (98.6720% of 16)
Natural Minimal Basis	31.77949 (99.3109% of 32)
Natural Rydberg Basis	0.22051 (0.6891% of 32)

Atom	No	Natural Electron Configuration
Be	1	[core]2S(0.86)2p(0.76)3p(0.01)
Be	2	[core]2S(0.86)2p(0.76)3p(0.01)
S	3	[core]3S(1.51)3p(4.09)4S(0.02)3d(0.11)4p(0.01)
O	4	[core]2S(1.82)2p(5.14)3p(0.01)3d(0.03)

Wiberg bond index matrix in the NAO basis:

Atom	1	2	3	4
1. Be	0.0000	0.9693	0.9370	0.1708
2. Be	0.9693	0.0000	0.9381	0.1709
3. S	0.9370	0.9381	0.0000	1.1039
4. O	0.1708	0.1709	1.1039	0.0000

Wiberg bond index, Totals by atom:

Atom	1

1.	Be	2.0772
2.	Be	2.0783
3.	S	2.9791
4.	O	1.4456

Atom-atom overlap-weighted NAO bond order:

	Atom	1	2	3	4
1.	Be	0.0000	0.9687	0.9279	-0.0333
2.	Be	0.9687	0.0000	0.9287	-0.0334
3.	S	0.9279	0.9287	0.0000	0.9554
4.	O	-0.0333	-0.0334	0.9554	0.0000

Atom-atom overlap-weighted NAO bond order, Totals by atom:

	Atom	1
1.	Be	1.8632
2.	Be	1.8640
3.	S	2.8121
4.	O	0.8887

MO bond order:

	Atom	1	2	3	4
1.	Be	0.0000	1.5658	0.4598	0.1595
2.	Be	1.5658	0.0000	0.5079	-0.3309
3.	S	0.4598	0.5079	0.0000	-0.7540
4.	O	0.1595	-0.3309	-0.7540	0.0000

MO atomic valencies:

	Atom	1
1.	Be	2.1851
2.	Be	1.7428
3.	S	0.2137
4.	O	-0.9253

NATURAL BOND ORBITAL ANALYSIS:

		Occupancies		Lewis Structure				Low	High	
Cycle	Occ. Thresh.	Lewis	Non-Lewis	CR	BD	3C	LP	occ (L)	occ (NL)	Dev
1(1)	1.90	30.43505	1.56495	8	7	0	1	4	4	0.17
2(2)	1.90	30.97164	1.02836	8	6	0	2	3	3	0.17
3(3)	1.90	30.97156	1.02844	8	6	0	2	3	3	0.17
4(1)	1.80	31.26818	0.73182	8	5	0	3	0	1	0.17
5(2)	1.80	31.26818	0.73182	8	5	0	3	0	1	0.17
6(1)	1.70	31.26818	0.73182	8	5	0	3	0	1	0.17
7(2)	1.70	31.26818	0.73182	8	5	0	3	0	1	0.17
8(1)	1.60	30.67506	1.32494	8	3	0	5	0	4	0.94
9(2)	1.60	30.67421	1.32579	8	3	0	5	0	4	0.94
10(3)	1.60	30.67506	1.32494	8	3	0	5	0	4	0.94
11(1)	1.50	30.50365	1.49635	8	2	0	6	0	4	0.94
12(2)	1.50	30.50365	1.49635	8	2	0	6	0	4	0.94
13(1)	1.80	31.26818	0.73182	8	5	0	3	0	1	0.17

Structure accepted: RESONANCE keyword permits strongly delocalized structure

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1\1\GINC-PSM09\SP\RCCSD-FC\CC-pVTZ\Be2O1S1\REZAIE\06-Jul-2023\0\\# ccs
d/cc-pvtz pop=nboread\\Title Card Required\\0,1\Be,0,1.652798,-0.98853
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000174\O,0,-1.557461,-0.000112,0.000184\\Version=ES64L-G09RevD.01\Stat
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38\MP4DQ=-502.0850024\MP4SDQ=-502.0973795\CCSD=-502.0931293\RMSD=5.430
e-09\PG=C01 [X(Be2O1S1)]\\@

ADAM SMITH SAID, "THE REAL PRICE OF ANYTHING IS THE TOIL AND TROUBLE OF ACQUIRING IT." BUT IN ALL UNDERTAKINGS WITH NATURE WE SHOULD FIRST READ CAREFULLY THE SMALL PRINT IN THE CONTRACT. THIS MIGHT DISCLOSE THAT THE REAL PRICE IS TO BE PAID BY THOSE WHO INHERIT THE DEPLETION AND DESPOILATION THAT FOLLOWS.

-- E. R. HARRISON IN "COSMOLOGY" (1980)

Job cpu time: 0 days 0 hours 23 minutes 37.2 seconds.
File lengths (MBytes): RWF= 620 Int= 0 D2E= 0 Chk= 2 Scr= 1
Normal termination of Gaussian 09 at Thu Jul 6 17:39:26 2023.

Output file of bridged Be2SO molecule

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Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
Be	1	0.42742	1.99785	1.56128	0.01344	3.57258
Be	2	0.74313	1.99773	1.23895	0.02018	3.25687
S	3	-0.06827	9.99885	6.00241	0.06701	16.06827
O	4	-1.10228	1.99979	7.09068	0.01181	9.10228
* Total *		0.00000	15.99422	15.89333	0.11245	32.00000

Natural Population

Core	15.99422 (99.9639% of 16)
Valence	15.89333 (99.3333% of 16)
Natural Minimal Basis	31.88755 (99.6486% of 32)
Natural Rydberg Basis	0.11245 (0.3514% of 32)

Atom	No	Natural Electron Configuration
Be	1	[core]2S(0.84)2p(0.72)3p(0.01)
Be	2	[core]2S(0.76)2p(0.48)4p(0.01)4d(0.01)
S	3	[core]3S(1.77)3p(4.23)3d(0.05)4p(0.01)
O	4	[core]2S(1.82)2p(5.27)3d(0.01)

Wiberg bond index matrix in the NAO basis:

Atom	1	2	3	4

1.	Be	0.0000	0.9826	0.8734	0.0545
2.	Be	0.9826	0.0000	0.0843	0.4744
3.	S	0.8734	0.0843	0.0000	0.8402
4.	O	0.0545	0.4744	0.8402	0.0000

Wiberg bond index, Totals by atom:

	Atom	1
1.	Be	1.9104
2.	Be	1.5413
3.	S	1.7979
4.	O	1.3690

Atom-atom overlap-weighted NAO bond order:

	Atom	1	2	3	4
1.	Be	0.0000	0.8330	0.8039	0.0179
2.	Be	0.8330	0.0000	0.0869	0.5802
3.	S	0.8039	0.0869	0.0000	0.5354
4.	O	0.0179	0.5802	0.5354	0.0000

Atom-atom overlap-weighted NAO bond order, Totals by atom:

	Atom	1
1.	Be	1.6548
2.	Be	1.5002
3.	S	1.4263
4.	O	1.1335

MO bond order:

	Atom	1	2	3	4
1.	Be	0.0000	1.9426	-0.2178	-0.1960
2.	Be	1.9426	0.0000	-0.3653	-0.3193
3.	S	-0.2178	-0.3653	0.0000	-0.2655
4.	O	-0.1960	-0.3193	-0.2655	0.0000

MO atomic valencies:

	Atom	1
1.	Be	1.5288
2.	Be	1.2579
3.	S	-0.8486
4.	O	-0.7809

NATURAL BOND ORBITAL ANALYSIS:

	Occupancies		Lewis Structure				Low	High	
Occ. Cycle	Thresh.	Lewis	Non-Lewis	CR	BD	3C	LP	occ (L)	occ (NL)	Dev
1(1)	1.90	31.77182	0.22818	8	5	0	3	0	0	0.08

Structure accepted: No low occupancy Lewis orbitals

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1\1\GINC-PSM09\SP\RCCSD-FC\CC-pVTZ\Be2O1S1\REZAIE\06-Jul-2023\0\\# ccs
d/cc-pvtz pop=nboread\\Title Card Required\\0,1\Be,0,-0.09722,1.623937
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8\MP4DQ=-502.1805161\MP4SDQ=-502.1875057\CCSD=-502.1855755\RMSD=6.761e
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You don't have to suffer to be a poet.
Adolescence is enough suffering for anyone.
-- John Ciardi

Job cpu time: 0 days 0 hours 17 minutes 30.4 seconds.
File lengths (MBytes): RWF= 620 Int= 0 D2E= 0 Chk= 2 Scr= 1
Normal termination of Gaussian 09 at Thu Jul 6 17:43:24 2023.

Output file of bridged SBe2O molecule

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Summary of Natural Population Analysis:

			Natural Population			
		Natural	----------			
Atom	No	Charge	Core	Valence	Rydberg	Total
Be	1	1.12881	1.99665	0.85172	0.02282	2.87119
Be	2	1.12878	1.99665	0.85175	0.02282	2.87122
O	3	-1.34715	1.99987	7.30939	0.03789	9.34715
S	4	-0.91044	9.99916	6.85461	0.05667	16.91044
* Total *		0.00000	15.99234	15.86747	0.14019	32.00000

Natural Population		
Core	15.99234	(99.9521% of 16)
Valence	15.86747	(99.1717% of 16)
Natural Minimal Basis	31.85981	(99.5619% of 32)
Natural Rydberg Basis	0.14019	(0.4381% of 32)

Atom	No	Natural Electron Configuration
Be	1	[core]2S(0.28)2p(0.58)3p(0.01)4p(0.01)
Be	2	[core]2S(0.28)2p(0.58)3p(0.01)4p(0.01)
O	3	[core]2S(1.78)2p(5.52)3d(0.03)
S	4	[core]3S(1.80)3p(5.05)3d(0.05)

Wiberg bond index matrix in the NAO basis:

Atom	1	2	3	4
1. Be	0.0000	0.1061	0.5668	0.8459
2. Be	0.1061	0.0000	0.5667	0.8461
3. O	0.5668	0.5667	0.0000	0.0441
4. S	0.8459	0.8461	0.0441	0.0000

Wiberg bond index, Totals by atom:

	Atom	1
1.	Be	1.5188
2.	Be	1.5189
3.	O	1.1777
4.	S	1.7361

Atom-atom overlap-weighted NAO bond order:

	Atom	1	2	3	4
1.	Be	0.0000	0.3123	0.6228	0.8248
2.	Be	0.3123	0.0000	0.6227	0.8249
3.	O	0.6228	0.6227	0.0000	-0.0381
4.	S	0.8248	0.8249	-0.0381	0.0000

Atom-atom overlap-weighted NAO bond order, Totals by atom:

	Atom	1
1.	Be	1.7599
2.	Be	1.7599
3.	O	1.2074
4.	S	1.6116

MO bond order:

	Atom	1	2	3	4
1.	Be	0.0000	0.1579	0.0446	0.7720
2.	Be	0.1579	0.0000	1.4396	0.2835
3.	O	0.0446	1.4396	0.0000	-0.0505
4.	S	0.7720	0.2835	-0.0505	0.0000

MO atomic valencies:

	Atom	1
1.	Be	0.9745
2.	Be	1.8810
3.	O	1.4337

4. S 1.0049

NATURAL BOND ORBITAL ANALYSIS:

	Occupancies		Lewis Structure				Low	High	
Occ.							occ	occ	
Cycle	Thresh.	Lewis	Non-Lewis	CR	BD	3C	LP	(L)	(NL)	Dev
1(1)	1.90	31.51355	0.48645	8	6	0	2	0	2	0.11
2(2)	1.90	31.51348	0.48652	8	6	0	2	0	2	0.11
3(1)	1.80	31.16775	0.83225	8	3	0	5	0	5	0.57
4(2)	1.80	31.16773	0.83227	8	3	0	5	0	5	0.57
5(3)	1.80	31.16775	0.83225	8	3	0	5	0	5	0.57
6(4)	1.80	31.16773	0.83227	8	3	0	5	0	5	0.57
7(1)	1.70	31.02813	0.97187	8	2	0	6	0	6	0.57
8(2)	1.70	31.02813	0.97187	8	2	0	6	0	6	0.57
9(1)	1.60	30.69183	1.30817	8	2	0	6	0	6	0.85
10(2)	1.60	30.69178	1.30822	8	2	0	6	0	6	0.85
11(3)	1.60	30.69183	1.30817	8	2	0	6	0	6	0.85
12(1)	1.50	30.53603	1.46397	8	1	0	7	0	8	0.85
13(2)	1.50	30.53607	1.46393	8	1	0	7	0	8	0.85
14(3)	1.50	30.53603	1.46397	8	1	0	7	0	8	0.85
15(1)	1.90	31.51355	0.48645	8	6	0	2	0	2	0.11

Structure accepted: RESONANCE keyword permits strongly delocalized structure

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1\1\GINC-PSM11\SP\RCCSD-FC\CC-pVTZ\Be2O1S1\REZAIE\06-Jul-2023\0\\# ccs
d/cc-pvtz pop=nboread\\Title Card Required\\0,1\Be,0,-0.579972,0.92645
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00012\S,0,1.145564,0.000017,-0.000004\\Version=ES64L-G09RevD.01\State=
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TELEVISION IS CALLED A MEDIUM BECAUSE IT ISN'T
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Job cpu time: 0 days 0 hours 12 minutes 4.9 seconds.

File lengths (MBytes): RWF=   620 Int=   0 D2E=   0 Chk=   2 Scr=   1
Normal termination of Gaussian 09 at Thu Jul 6 17:43:45 2023.