An alternative way for hydrogen storage? Complexes between oxyacid beryllium salts and dihydrogen

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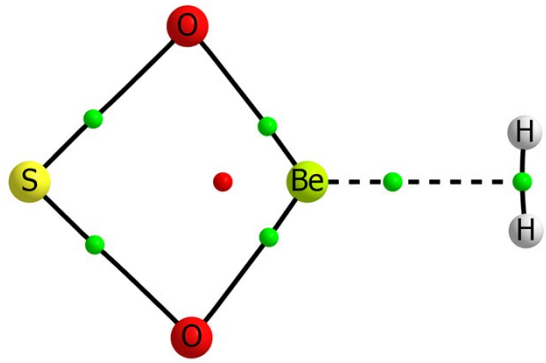
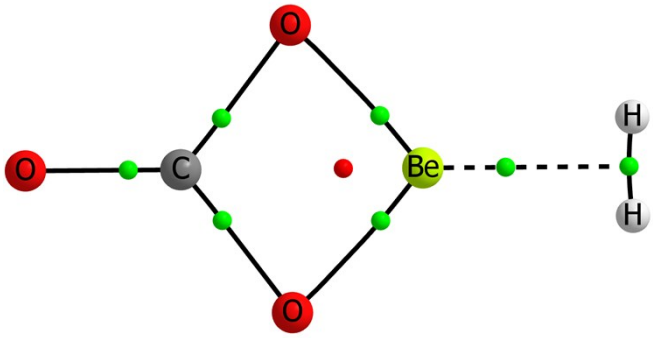
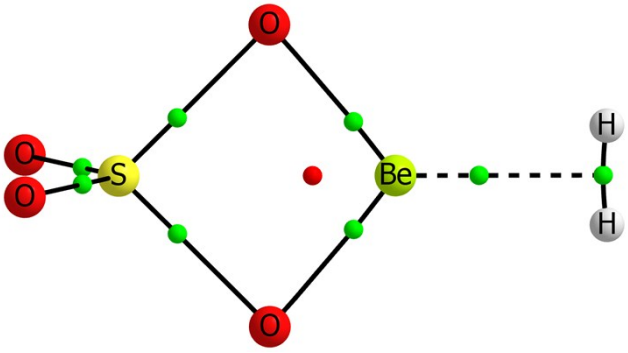
Supporting Information (A total of 9 pages)

Table S1. Molecular graph, electronic energy (Hartree) and geometry of the 1:1 complexes of **1-3** optimized at MP2/aug-cc-pVTZ computational level.

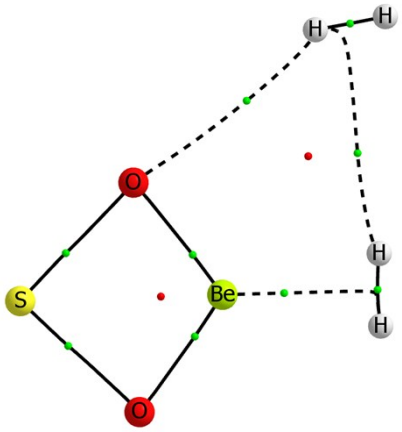
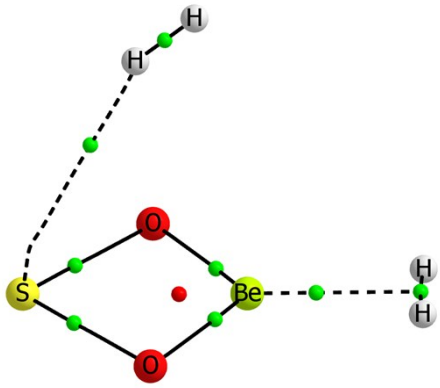
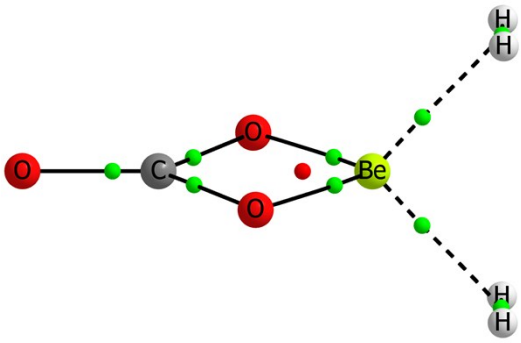
	$SO_2Be:H_2$ MP2= -563.84959638 NIMAG= 0 Be X,1,1. X,1,1.,2,90. O,1,r1,2,a1,3,90.,0 O,1,r1,2,a1,3,-90.,0 S,1,r2,3,90.,2,0.,0 X,1,r3,3,90.,2,180.,0 H,7,r4,1,90.,3,90.,0 H,7,r4,1,90.,3,-90.,0 r1=1.49258782 a1=53.27513526 r2=2.10495525 r3=1.65258664 r4=0.37764536
	$CO_3Be:H_2$ MP2= -279.34313020 NIMAG= 0 Be X,1,1. X,1,1.,2,90. O,1,r1,2,a1,3,90.,0 O,1,r1,2,a1,3,-90.,0 C,1,r2,3,90.,2,0.,0 O,1,r21,3,90.,2,0.,0 X,1,r3,3,90.,2,180.,0 H,8,r4,1,90.,3,90.,0 H,8,r4,1,90.,3,-90.,0 r1=1.49427611 a1=47.59059905 r2=1.85544422 r21=3.04680454 r3=1.60876866 r4=0.37955738

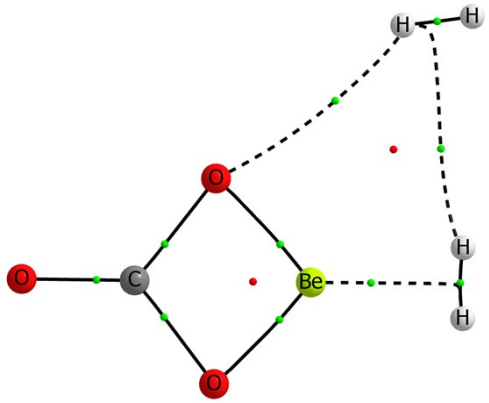
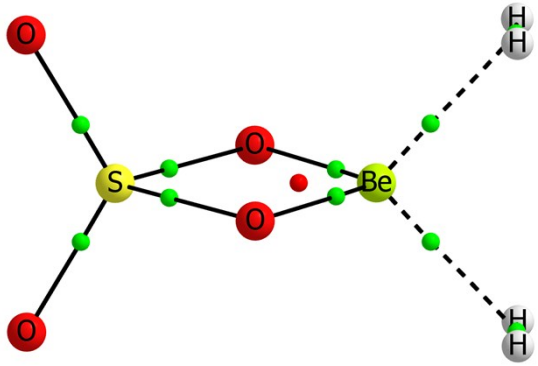


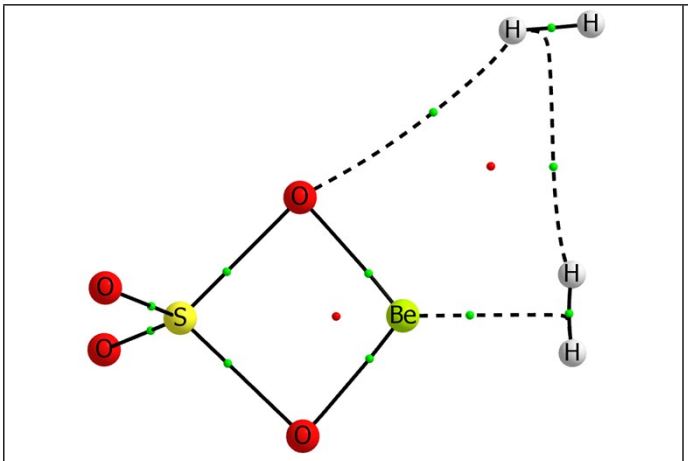
$SO_4Be:H_2$
MP2= -714.14816524 NIMAG= 0
Be
X,1,1.
X,1,1.,2,90.
O,1,r1,2,a1,3,90.,0
O,1,r1,2,a1,3,-90.,0
S,1,r2,3,90.,2,0.,0
O,6,r11,1,a11,3,0.,0
O,6,r11,1,a11,3,180.,0
X,1,r3,3,90.,2,180.,0
H,9,r4,1,90.,3,90.,0
H,9,r4,1,90.,3,-90.,0

r1=1.49989161
a1=50.47635495
r11=1.43729219
a11=119.66241088
r2=2.09881849
r3=1.6033096
r4=0.37989483

Table S2. Molecular graph, electronic energy (Hartree) and geometry of the 1:2 complexes of **1-3** optimized at MP2/aug-cc-pVTZ computational level.

	$SO_2Be:2H_2$ (A) MP2= -565.01727420 NIMAG= 0 Be,0.,-0.0576050337,-0.0510172525 O,0.,-1.2706265143,0.8219323145 O,0.,1.1208509286,0.8662306503 S,0.,-0.0955086654,2.0565391883 H,0.,-0.407268475,-1.7037326794 H,0.,0.3488329716,-1.685741617 H,0.,-2.7686826411,-1.1451446258 H,0.,-2.8699925708,-1.8794027402
	$SO_2Be:2H_2$ (B) MP2= -565.01705474 NIMAG= 0 Be,-0.6444732922,0.0379588867,-1.0476958572 O,-0.0696208149,1.1698896127,-0.2607816083 O,-0.2300889251,-1.2137292895,-0.345923521 S,0.5471911538,-0.1040561799,0.68136201 H,-1.5380065157,0.5248628125,-2.4003649116 H,-1.5884637929,-0.2283953142,-2.4270811398 H,2.0899391805,-0.1172872782,-1.696595476 H,2.1735240065,-0.10424325,-2.432590496
	$CO_3Be:2H_2$ (A) MP2= -280.51487969 NIMAG= 0 Be X,1,1. X,1,1.,2,90. O,1,r1,2,a1,3,90.,0 O,1,r1,2,a1,3,-90.,0 C,1,r2,3,90.,2,0.,0 O,1,r21,3,90.,2,0.,0 X,1,r3,3,90.,2,180.,0 X,8,r31,1,90.,3,0.,0 X,8,r31,1,90.,3,180.,0 H,10,r4,8,90.,1,90.,0 H,10,r4,8,90.,1,-90.,0 H,9,r4,8,90.,1,90.,0 H,9,r4,8,90.,1,-90.,0 r1=1.50929033 a1=46.7291445

	r2=1.87699118 r21=3.07104419 r3=1.1452973 r31=1.27043769 r4=0.37667349
	$CO_3Be:2H_2$ (B) MP2= -280.51070539 NIMAG= 0 Be,0.0071532629,-0.3729763831,0.3024079591 O,-0.0120738283,-1.0621986673,1.6293671137 O,0.0114244247,1.0091183295,0.8737712387 C,-0.0064888738,0.2654104917,2.0476424666 O,-0.0151418316,0.6732041854,3.1671520226 H,0.0155433134,-1.2903130061,-1.0683104595 H,0.0236916819,-0.5772762895,-1.3309947734 H,-0.0142907693,-3.2972508245,0.3660426017 H,-0.0098173799,-3.6477178363,-0.2868167546
	$SO_4Be:2H_2$ (A) MP2= -715.32067256 NIMAG= 0 Be X,1,1. X,1,1.,2,90. O,1,r1,2,a1,3,90.,0 O,1,r1,2,a1,3,-90.,0 S,1,r2,3,90.,2,0.,0 O,6,r11,1,a11,3,0.,0 O,6,r11,1,a11,3,180.,0 X,1,r3,3,90.,2,180.,0 X,9,r31,1,90.,3,0.,0 X,9,r31,1,90.,3,180.,0 H,10,r4,9,90.,1,90.,0 H,10,r4,9,90.,1,-90.,0 H,11,r4,9,90.,1,90.,0 H,11,r4,9,90.,1,-90.,0 r1=1.51663168 a1=49.55587702 r11=1.43914406 a11=119.9460698 r2=2.11680764 r3=1.14296524 r31=1.26972525 r4=0.37678666



$SO_4Be:2H_2$ (B)
MP2= -715.31578831 NIMAG= 0
Be,0.,-0.0439667064,-0.035781325
O,0.,-1.2004193824,0.9211661991
O,0.,1.1125365697,0.920906412
S,0.,-0.0422323724,2.0651871126
O,1.2489773823,-0.0429384998,2.7765530622
O,-1.2489773823,-0.0429384998,2.7765530622
H,0.,-0.426949931,-1.6348321911
H,0.,0.3337624625,-1.631817147
H,0.,-2.7960404545,-1.1021359992
H,0.,-2.8508131865,-1.8409309601

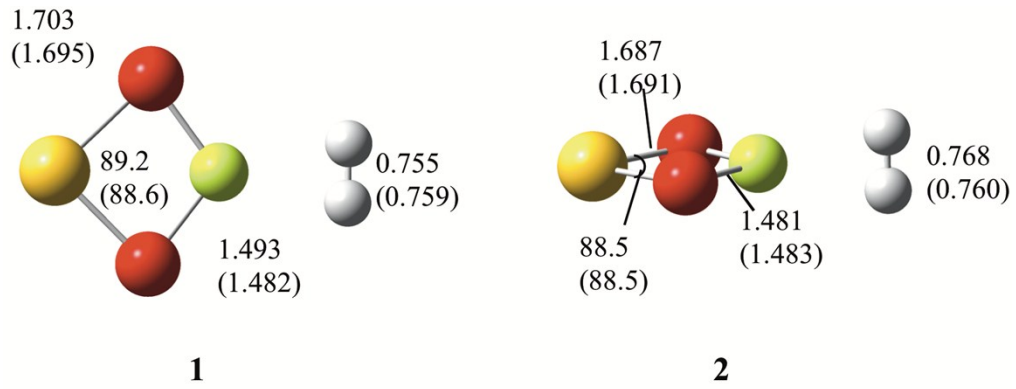


Figure S1. Structures **1** and **2** obtained by MP2/aug-cc-pVTZ and B3LYP/6-31G(2df,p) geometry optimizations, respectively. The latter is the one used by default in the G4 calculations. When these two structures are optimized at the CCSD/aug-cc-pVTZ, structure **1** is found to be the most stable, though the energy gap with respect to structure **2** is less than 2 kJ.mol^{-1}. Geometrical parameters within parenthesis are those obtained at the CCSD level.

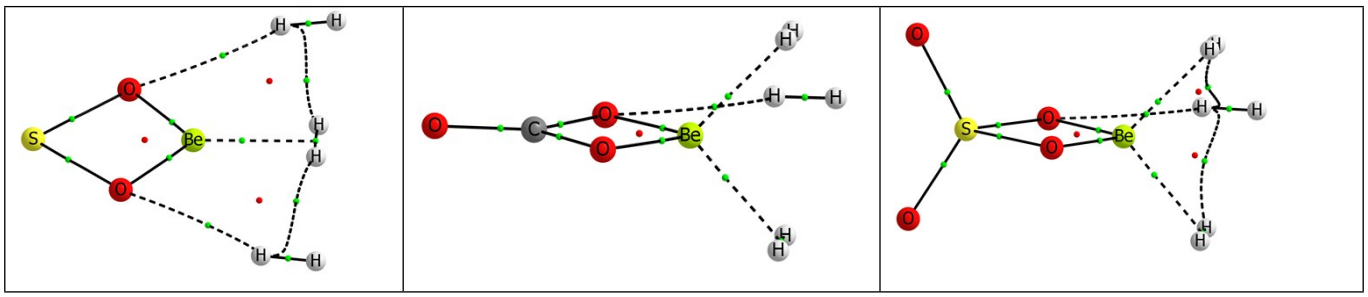


Figure S2. Molecular graphs of the most stable 1:3 complexes of **1-3**

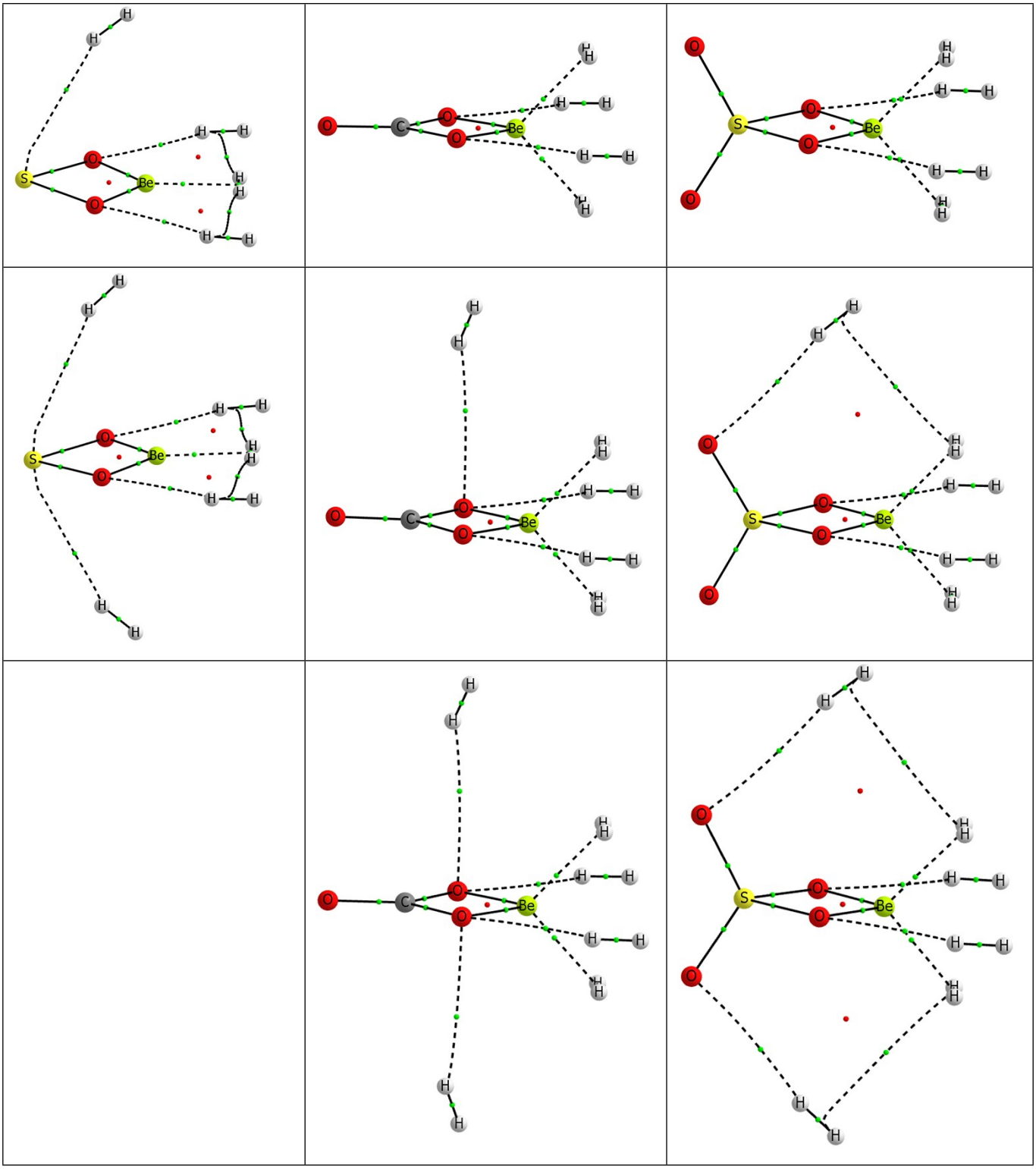


Figure S3. Molecular graphs of the most stable 1:n (n = 4,5,6) complexes of **1-3**