Electronic supplementary materials *Mendeleev Commun.*, 2024, **34**, 798–801

BeO analogues of annulated cyclooctatetraene and cyclodecapentaene as new inorganic species with unusual multiple hypervalent O···O interactions

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Atomic coordinates of optimized structures **11** and **12** calculated by the B3LYP/6-311+G(df,p) and wB97XD/6-311+G(df,p) methods:

11 [B3LYP/6-311+G(df,p)]
C_{4h}

O	-0.038433000000	1.976500000000	0.000000000000
Be	1.418249000000	1.418249000000	0.000000000000
O	2.080421000000	2.845233000000	0.000000000000
Be	0.594136000000	3.417737000000	0.000000000000
Be	-1.418249000000	1.418249000000	0.000000000000
O	-1.976500000000	-0.038433000000	0.000000000000
Be	-3.417737000000	0.594136000000	0.000000000000
O	-2.845233000000	2.080421000000	0.000000000000
O	1.976500000000	0.038433000000	0.000000000000
Be	1.418249000000	-1.418249000000	0.000000000000
O	2.845233000000	-2.080421000000	0.000000000000
Be	3.417737000000	-0.594136000000	0.000000000000
O	-2.080421000000	-2.845233000000	0.000000000000
Be	-0.594136000000	-3.417737000000	0.000000000000
Be	-1.418249000000	-1.418249000000	0.000000000000
O	0.038433000000	-1.976500000000	0.000000000000
H	3.205453000000	-2.963514000000	0.000000000000
H	-4.663173000000	0.084144000000	0.000000000000
H	0.084144000000	4.663173000000	0.000000000000
H	2.963514000000	3.205453000000	0.000000000000
H	4.663173000000	-0.084144000000	0.000000000000
H	-2.963514000000	-3.205453000000	0.000000000000
H	-0.084144000000	-4.663173000000	0.000000000000
H	-3.205453000000	2.963514000000	0.000000000000

11 [wB97XD/6-311+G(df,p)]
C_{4h}

O	-0.037375000000	1.976324000000	0.000000000000
Be	1.417826000000	1.417826000000	0.000000000000
O	2.083699000000	2.847864000000	0.000000000000
Be	0.590302000000	3.423008000000	0.000000000000
Be	-1.417826000000	1.417826000000	0.000000000000
O	-1.976324000000	-0.037375000000	0.000000000000
Be	-3.423008000000	0.590302000000	0.000000000000
O	-2.847864000000	2.083699000000	0.000000000000
O	1.976324000000	0.037375000000	0.000000000000
Be	1.417826000000	-1.417826000000	0.000000000000
O	2.847864000000	-2.083699000000	0.000000000000
Be	3.423008000000	-0.590302000000	0.000000000000
O	-2.083699000000	-2.847864000000	0.000000000000
Be	-0.590302000000	-3.423008000000	0.000000000000
Be	-1.417826000000	-1.417826000000	0.000000000000
O	0.037375000000	-1.976324000000	0.000000000000
H	3.204495000000	-2.964042000000	0.000000000000
H	-4.673773000000	0.071059000000	0.000000000000
H	0.071059000000	4.673773000000	0.000000000000
H	2.964042000000	3.204495000000	0.000000000000
H	4.673773000000	-0.071059000000	0.000000000000
H	-2.964042000000	-3.204495000000	0.000000000000
H	-0.071059000000	-4.673773000000	0.000000000000
H	-3.204495000000	2.964042000000	0.000000000000

12 [B3LYP/6-311+G(df,p)]
C_{5h}

O	0.444066000000	2.378868000000	0.000000000000
O	-2.125214000000	1.157443000000	0.000000000000
O	-1.757521000000	-1.663529000000	0.000000000000
O	1.039006000000	-2.185560000000	0.000000000000
Be	-2.481121000000	-0.289070000000	0.000000000000
Be	-0.491787000000	-2.449014000000	0.000000000000
Be	2.177180000000	-1.224504000000	0.000000000000
Be	1.837358000000	1.692229000000	0.000000000000
Be	-1.041630000000	2.270359000000	0.000000000000
O	2.399662000000	0.312779000000	0.000000000000
Be	1.221544000000	3.759526000000	0.000000000000
Be	-3.198044000000	2.323515000000	0.000000000000
Be	-3.198044000000	-2.323515000000	0.000000000000
Be	1.221544000000	-3.759526000000	0.000000000000
O	-3.927140000000	-0.926372000000	0.000000000000
O	-0.332521000000	-4.021197000000	0.000000000000
O	3.721630000000	-1.558865000000	0.000000000000
O	2.632615000000	3.057765000000	0.000000000000
O	-2.094585000000	3.448667000000	0.000000000000
Be	3.952999000000	0.000000000000	0.000000000000
H	0.791551000000	5.038123000000	0.000000000000
H	-4.546937000000	2.309676000000	0.000000000000
H	-3.601713000000	-3.610665000000	0.000000000000
H	2.320956000000	-4.541189000000	0.000000000000
H	-4.814531000000	-0.575113000000	0.000000000000
H	-0.940807000000	-4.756610000000	0.000000000000
H	4.233080000000	-2.364634000000	0.000000000000
H	3.556994000000	3.295186000000	0.000000000000
H	-2.034737000000	4.401171000000	0.000000000000
H	5.036143000000	0.804056000000	0.000000000000

12 [wB97XD/6-311+G(df,p)]
C_{5h}

O	2.400086000000	0.308758000000	0.000000000000
O	0.448021000000	2.378029000000	0.000000000000
O	-2.123194000000	1.160945000000	0.000000000000
O	-1.760227000000	-1.660526000000	0.000000000000
Be	-1.038103000000	2.271763000000	0.000000000000
Be	-2.481366000000	-0.285282000000	0.000000000000
Be	-0.495465000000	-2.448076000000	0.000000000000
Be	2.175152000000	-1.227713000000	0.000000000000
Be	1.839783000000	1.689308000000	0.000000000000
O	1.035314000000	-2.187206000000	0.000000000000
Be	3.956524000000	0.000000000000	0.000000000000
Be	1.222633000000	3.762878000000	0.000000000000
Be	-3.200895000000	2.325587000000	0.000000000000
Be	-3.200895000000	-2.325587000000	0.000000000000
O	-2.091166000000	3.455368000000	0.000000000000
O	-3.932456000000	-0.921050000000	0.000000000000
O	-0.339225000000	-4.024608000000	0.000000000000
O	3.722803000000	-1.566294000000	0.000000000000
O	2.640044000000	3.056584000000	0.000000000000
Be	1.222633000000	-3.762878000000	0.000000000000
H	5.038634000000	0.818473000000	0.000000000000
H	0.778609000000	5.044947000000	0.000000000000
H	-4.557427000000	2.299476000000	0.000000000000
H	-3.595254000000	-3.623793000000	0.000000000000
H	-2.022694000000	4.403572000000	0.000000000000
H	-4.813092000000	-0.562917000000	0.000000000000
H	-0.951961000000	-4.751474000000	0.000000000000
H	4.224748000000	-2.373655000000	0.000000000000
H	3.562999000000	3.284474000000	0.000000000000
H	2.335438000000	-4.539103000000	0.000000000000