

Supporting Information:
Tuning the magnetic properties of beryllium chains

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Computational Details

In order to perform the CASSCF and NEVPT2 calculations we have used the RIJCOSX approximation implemented in the ORCA program. This approximation requires the choice of three integration grids. During the CASSCF procedure, a first grid is used for the initial iterations, which is followed by a second grid that is kept for all remaining iterations but the last one, for which a third grid is used. In all calculations we set the same grid for all three steps in order to avoid ending in local minima, which was otherwise the case for a number of systems when adopting the default settings. The parameter “gridx” was set to “3,3,3”, while the parameter “intaccx” was set to “4.34,4.34,4.34”, both of which appear in the “%method” block. Note that also the option “nofinalgridx” was necessary. On the other hand, in the “casscf” block, the “resetfreq” option was set to “1”. To ensure convergence, the option “tightSCF” was used.