

Supporting Information for the paper entitled:

**Appraising spin-state energetics in transition metal complexes using double-hybrid models:
Accountability of SOS0-PBESCAN0-2(a) as a promising paradigm**

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An illustrative sample of the definition of SOS0-PBESCAN0-2(a) in ORCA:

```
%method
Exchange X_PBE
Correlation C_SCAN
ScalHFX=0.7937
ScalDFX=0.2063
ScalMP2C=1.0
ScalLDAC=0.50
ScalGGAC=0.50
end
%MP2
DoSCS true
PS 0.6667
PT 0.0000
end
```