Supplementary Information (SI) for Physical Chemistry Chemical Physics.

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Correction to The *p*-block challenge: assessing quantum chemistry methods for inorganic heterocycle dimerizations

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S1 Computational Details for DFT Calculations

S1.1 ORCA Input for B2NC-PLYP

```
! RKS DEFGRID3 def2/J RIJCOSX def2-QZVPP def2-QZVPP/C TightSCF

%method
Exchange X_B88
Correlation C_LYP
LDAOpt C_VWN3
ScalHFX=0.81
ScalDFX=0.19
ScalMP2C=0.55
ScalLDAC=0.45
ScalGGAC=0.45
end

* xyzfile 0 1 mol.xyz
```

S1.2 ORCA Input for revDSD-PBEP86-D3(BJ)

```
! RKS D3BJ DEFGRID3 def2/J RIJCOSX def2-QZVPP def2-QZVPP/C TightSCF NOTRAH

%method
Exchange X_PBE
Correlation C_P86
ScalHFX 0.69
ScalDFX 0.31
ScalGGAC 0.4296
ScalLDAC 0.4296
ScalMP2C 1.0
D3S6 0.4377
D3A2 5.5
D3S8 0.0
D3A1 0.0
end
%mp2
DoSCS true
PS 0.5785
PT 0.0799
end

* xyzfile 0 1 mol.xyz
```