Electronic Supplementary Material (ESI) for RSC Advances.

Hydrogen bonding capabilities of group 14 homologues of HCN and HNC

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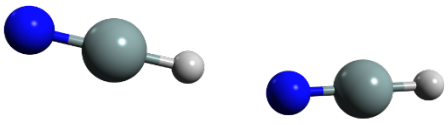
Energies and coordinates of the calculated dimers

$(HCN)_2$ dimmer

```
E(BSSE Corrected  MP2/aug-cc-pVDZ//CCSD(T)/aug-cc-pVQZ)= -186.6117560 Ha
H 0.0000000000 0.0000000000 -3.7949516300
C 0.0000000000 0.0000000000 -2.7180143800
N 0.0000000000 0.0000000000 -1.5386830800
H 0.0000000000 0.0000000000  0.6078420000
C 0.0000000000 0.0000000000  1.6916814900
N 0.0000000000 0.0000000000  2.8736983500
```

$(HSiN)_2$ dimmer



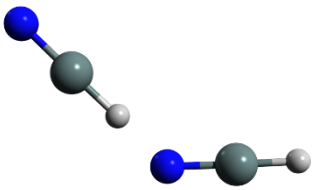
```
E(BSSE Corrected  MP2/aug-cc-pVDZ//CCSD(T)/aug-cc-pVQZ)= -688.4614417 Ha
Si -0.3510000000 -3.0730000000 0.0000000000
Si  0.2940000000  2.1770000000 0.0000000000
N  -0.4850000000 -1.4430000000 0.0000000000
N   0.6290000000  3.7850000000 0.0000000000
H  -0.2200000000 -4.5570000000 0.0000000000
H   0.0000000000  0.7090000000 0.0000000000
```

$(HGeN)_2$ dimmer

```
E(BSSE Corrected  MP2/aug-cc-pVDZ//CCSD(T)/aug-cc-pVQZ)= -4261.662058 Ha
H  0.0000000000 0.0000000000  4.4462977100
Ge 0.0000000000 0.0000000000  2.9214801200
N  0.0000000000 0.0000000000  1.2235170700
```

```
H  0.0000000000 0.0000000000 -0.8692058500
Ge 0.0000000000 0.0000000000 -2.4016481400
N  0.0000000000 0.0000000000 -4.1109049800
```

$(HSnN)_2$ dimmer



```
E(BSSE Corrected  MP2/aug-cc-pVDZ//CCSD(T)/aug-cc-pVQZ)= -537.4864554 Ha
Sn  1.1670000000  2.0560000000 0.0000000000
Sn -1.3010000000 -2.3960000000 0.0000000000
N   2.4900000000  3.4180000000 0.0000000000
N  -1.3590000000 -0.5300000000 0.0000000000
H   0.0000000000  0.8150000000 0.0000000000
H  -1.2150000000 -4.0630000000 0.0000000000
```

$(HNC)_2$ dimmer

```
E(BSSE Corrected  MP2/aug-cc-pVDZ//CCSD(T)/aug-cc-pVQZ)= -186.5695365 Ha
H 0.0000000000 0.0000000000  3.5618994900
N 0.0000000000 0.0000000000  2.5557680100
C 0.0000000000 0.0000000000  1.3698327800
H 0.0000000000 0.0000000000 -0.6594665500
N 0.0000000000 0.0000000000 -1.6823277500
C 0.0000000000 0.0000000000 -2.8725852400
```

$(HNSi)_2$ dimmer

```
E(BSSE Corrected  MP2/aug-cc-pVDZ//CCSD(T)/aug-cc-pVQZ)= -688.6733033 Ha
H  0.0000000000 0.0000000000 -4.6679536400
N  0.0000000000 0.0000000000 -3.6572584400
Si 0.0000000000 0.0000000000 -2.0691857000
H  0.0000000000 0.0000000000  0.7142637600
N  0.0000000000 0.0000000000  1.7260077000
Si 0.0000000000 0.0000000000  3.3172175000
```

$(HNGe)_2$ dimmer

```
E(BSSE Corrected  MP2/aug-cc-pVDZ//CCSD(T)/aug-cc-pVQZ)= -4261.8605290 Ha
H  0.0000000000 0.0000000000 -4.9943781800
N  0.0000000000 0.0000000000 -3.9804115500
```

```
Ge 0.0000000000 0.0000000000 -2.3017368100
H  0.0000000000 0.0000000000  0.3265298500
N  0.0000000000 0.0000000000  1.3417870800
Ge 0.0000000000 0.0000000000  3.0248061800
```

$(HNSn)_2$ dimmer

```
E(BSSE Corrected  MP2/aug-cc-pVDZ//CCSD(T)/aug-cc-pVQZ)= -537.6974426 Ha
H  0.0000000000 0.0000000000 -5.5081804700
N  0.0000000000 0.0000000000 -4.4891063400
Sn 0.0000000000 0.0000000000 -2.5971742100
H  0.0000000000 0.0000000000  0.2392024100
N  0.0000000000 0.0000000000  1.2584780000
Sn 0.0000000000 0.0000000000  3.1548417400
```

$(HNPb)_2$ dimmer

```
E(BSSE Corrected  MP2/aug-cc-pVDZ//CCSD(T)/aug-cc-pVQZ)= -494.8606690 Ha
H  0.0000000000 0.0000000000 -5.7554648500
N  0.0000000000 0.0000000000 -4.7316109000
Pb 0.0000000000 0.0000000000 -2.7409907800
H  0.0000000000 0.0000000000  0.0991947000
N  0.0000000000 0.0000000000  1.1222635600
Pb 0.0000000000 0.0000000000  3.1180847000
```