

**Supplementary Information for:**

**“Investigation of the interaction of CO, NO, and HCN gases with  
Transition Metal-doped Ca<sub>12</sub>O<sub>12</sub> nanocages: Theoretical Study”**

**H. O. Taha <sup>1,\*</sup>, A. M. El Mahdy <sup>1</sup>**

<sup>1</sup> *Department of Physics, Faculty of Education, Ain Shams University, Roxy, 11575, Cairo, Egypt*

*\*Corresponding author. Emails: [hyamosman@edu.asu.edu.eg](mailto:hyamosman@edu.asu.edu.eg); [drhotaha@hotmail.com](mailto:drhotaha@hotmail.com)*

**Table S1**

Adsorption energies of CO, NO and HCN molecules on the  $\text{Ca}_{12}\text{O}_{12}$  nanocage. Calculated at B3LYP/6-31+G(d), B3LYP/6-311+G(d), and PBEPBE/6-311+G(d).

|                   | CO/ $\text{Ca}_{12}\text{O}_{12}$ | NO/ $\text{Ca}_{12}\text{O}_{12}$ | HCN/ $\text{Ca}_{12}\text{O}_{12}$ |
|-------------------|-----------------------------------|-----------------------------------|------------------------------------|
| B3LYP/6-31+G(d)   | -0.282                            | -0.894                            | -0.456                             |
| B3LYP/6-311+G(d)  | -0.404                            | -0.671                            | -0.423                             |
| PBEPBE/6-311+G(d) | -0.286                            | -0.985                            | -0.425                             |

**Table S2:**

The obtained xyz coordinates for all studied systems, including  $\text{Ca}_{12}\text{O}_{12}$  cluster CO, NO, and HCN, gases as well as CO/ $\text{Ca}_{12}\text{O}_{12}$ , NO/ $\text{Ca}_{12}\text{O}_{12}$ , HCN/ $\text{Ca}_{12}\text{O}_{12}$ , as well as TM/ $\text{Ca}_{11}\text{O}_{12}$  (TM=Sc-Zn), CO/TM $\text{Ca}_{11}\text{O}_{12}$ , NO/TM $\text{Ca}_{11}\text{O}_{12}$ , and HCN/TM $\text{Ca}_{11}\text{O}_{12}$  (TM=Sc-Zn) complex structures which have been calculated by DFT method and B3LYP/6-311+G(D)D3 level of theory.

**CO**

|   |          |          |           |
|---|----------|----------|-----------|
| 6 | 0.000000 | 0.000000 | -0.644394 |
| 8 | 0.000000 | 0.000000 | 0.483296  |

**NO**

|   |          |          |           |
|---|----------|----------|-----------|
| 7 | 0.000000 | 0.000000 | -0.612239 |
| 8 | 0.000000 | 0.000000 | 0.535709  |

**HCN**

|   |          |          |           |
|---|----------|----------|-----------|
| 1 | 0.000000 | 0.000000 | 0.650946  |
| 6 | 0.000000 | 0.000000 | -0.498276 |
| 7 | 0.000000 | 0.000000 | -1.566969 |

**CO/ $\text{Ca}_{12}\text{O}_{12}$** 

|    |           |           |           |
|----|-----------|-----------|-----------|
| 8  | 3.217817  | 0.530189  | 0.19975   |
| 8  | 0.739952  | 3.165709  | -0.956993 |
| 8  | -2.414750 | 1.515323  | -2.157595 |
| 8  | 0.711143  | 2.014760  | 2.603964  |
| 8  | -2.091440 | 2.518212  | 1.441678  |
| 8  | 1.932771  | -1.501940 | 2.141257  |
| 8  | -1.22571  | -3.165028 | 0.963179  |
| 8  | -3.63184  | -0.508917 | -0.190209 |
| 8  | 1.600133  | -2.506277 | -1.433316 |
| 8  | -1.19256  | -2.014311 | -2.619344 |
| 8  | 1.183245  | 0.888676  | -2.959131 |
| 8  | -1.65495  | -0.886107 | 2.977335  |
| 20 | -0.02207  | -2.317128 | 2.600848  |
| 20 | -3.30119  | 1.669339  | -0.145978 |
| 20 | -1.30793  | 1.250415  | 3.066573  |
| 20 | 2.347671  | 0.645077  | 2.251319  |
| 20 | -0.08967  | 3.344423  | 1.040738  |
| 20 | 2.407199  | 1.805101  | -1.388681 |
| 20 | -0.45825  | 2.319381  | -2.606009 |

**NO/ $\text{Ca}_{12}\text{O}_{12}$** 

|    |           |           |          |
|----|-----------|-----------|----------|
| 8  | -4.155800 | -2.596710 | -0.04843 |
| 8  | 1.367392  | -3.036710 | 1.522345 |
| 8  | 3.787655  | -0.392070 | -0.03076 |
| 8  | -1.26945  | -0.629730 | 3.160429 |
| 8  | 1.723256  | 0.478281  | 3.161613 |
| 8  | -3.17065  | 0.444831  | 0.027249 |
| 8  | -0.86583  | 3.073571  | -1.51856 |
| 8  | 2.687396  | 2.598456  | 0.049935 |
| 8  | -1.30248  | -0.483860 | -3.17005 |
| 8  | 1.689602  | 0.629160  | -3.15374 |
| 8  | 1.35133   | -2.960880 | -1.66879 |
| 8  | -0.85071  | 2.999889  | 1.663771 |
| 20 | -2.35946  | 2.531526  | 0.068125 |
| 20 | 3.212526  | 1.051429  | 1.618273 |
| 20 | -0.32694  | 1.437045  | 3.162416 |
| 20 | -2.75704  | -1.191950 | 1.61245  |
| 20 | 0.788451  | -1.583890 | 3.101079 |
| 20 | -0.152200 | -3.543650 | -0.08001 |
| 20 | 2.857115  | -2.408190 | -0.06803 |

|    |          |           |           |
|----|----------|-----------|-----------|
| 20 | 2.850004 | -1.694156 | 0.140858  |
| 20 | 0.825764 | -1.251291 | -3.067615 |
| 20 | -2.83351 | -0.648796 | -2.240903 |
| 20 | -0.40236 | -3.332068 | -1.036875 |
| 20 | -2.8921  | -1.789241 | 1.393102  |
| 8  | 6.072486 | 0.312024  | -0.045471 |
| 6  | 5.259731 | -0.486609 | 0.021938  |

|    |          |           |          |
|----|----------|-----------|----------|
| 20 | -2.77436 | -1.122980 | -1.63778 |
| 20 | 0.758948 | -1.436490 | -3.16968 |
| 20 | 3.193366 | 1.126903  | -1.59903 |
| 20 | -0.36123 | 1.580129  | -3.08973 |
| 20 | 0.683728 | 3.543082  | 0.07727  |
| 7  | -4.78346 | -0.453710 | 0.050279 |
| 8  | -5.71345 | 0.315358  | -0.02743 |

### HCN/Ca<sub>12</sub>O<sub>12</sub>

|    |           |           |           |
|----|-----------|-----------|-----------|
| 8  | -2.670590 | -1.949720 | 0.561662  |
| 8  | 0.8998180 | -3.504160 | 0.136212  |
| 8  | 3.1933050 | -1.003770 | -1.781640 |
| 8  | 0.1010450 | -1.359010 | 3.283487  |
| 8  | 3.0283600 | -0.887450 | 2.110359  |
| 8  | -2.642140 | 1.0015760 | 1.776060  |
| 8  | -0.330260 | 3.5245480 | -0.141970 |
| 8  | 3.2219430 | 1.9461010 | -0.567880 |
| 8  | -2.458100 | 0.8794040 | -2.086440 |
| 8  | 0.4673390 | 1.3565420 | -3.276310 |
| 8  | -0.372370 | -2.395770 | -2.569900 |
| 8  | 0.9327150 | 2.378406  | 2.552131  |
| 20 | -1.181050 | 2.668605  | 1.778306  |
| 20 | 3.8285230 | -0.097420 | 0.195021  |
| 20 | 1.5578830 | 0.378334  | 3.281547  |
| 20 | -1.952110 | -1.025200 | 2.496273  |
| 20 | 1.5457420 | -2.600370 | 2.057561  |
| 20 | -1.215160 | -3.146890 | -0.605670 |
| 20 | 1.7401620 | -2.685580 | -1.803770 |
| 20 | -3.360430 | 0.099644  | -0.193710 |
| 20 | -0.994380 | -0.380220 | -3.262920 |
| 20 | 2.5293190 | 1.0325130 | -2.524800 |
| 20 | -0.984290 | 2.5925670 | -2.050140 |
| 20 | 1.7777070 | 3.1681570 | 0.601352  |
| 1  | -8.124620 | -0.230740 | 0.469780  |
| 6  | -7.105350 | -0.072690 | 0.182355  |
| 7  | -6.007170 | 0.0986260 | -0.130170 |

### Sc/Ca<sub>11</sub>O<sub>12</sub>

|    |          |          |           |
|----|----------|----------|-----------|
| 8  | 1.50817  | -2.85813 | 0.000000  |
| 8  | 2.93772  | -0.22135 | 1.426390  |
| 8  | 1.63786  | 2.97977  | 0.000000  |
| 8  | -0.07497 | -1.53178 | 3.118640  |
| 8  | -1.55877 | -3.0186  | 0.000000  |
| 8  | -3.05231 | 0.06753  | -1.535620 |
| 8  | -1.43634 | 3.09413  | 0.000000  |
| 8  | -0.07497 | -1.53178 | -3.118640 |
| 8  | 0.05422  | 1.51788  | -3.072840 |
| 8  | 2.93772  | -0.22135 | -1.426390 |
| 8  | -3.05231 | 0.06753  | 1.535620  |
| 8  | 0.05422  | 1.51788  | 3.072840  |
| 20 | -3.12678 | -1.50674 | 0.000000  |
| 20 | -1.60228 | 0.05727  | 3.140550  |
| 20 | -0.05973 | -3.05038 | 1.597950  |
| 20 | 1.5495   | -0.07528 | 3.134590  |
| 20 | 3.17667  | 1.50024  | 0.000000  |

### Ti/Ca<sub>11</sub>O<sub>12</sub>

|    |          |          |           |
|----|----------|----------|-----------|
| 8  | -0.69566 | -3.14557 | 0.000000  |
| 8  | 2.02078  | -2.16979 | 1.419630  |
| 8  | 3.37384  | 1.16381  | 0.000000  |
| 8  | -1.14798 | -1.13994 | 3.317110  |
| 8  | -3.27895 | -1.32173 | 0.000000  |
| 8  | -2.32309 | 2.12572  | -1.595630 |
| 8  | 1.02796  | 3.3419   | 0.000000  |
| 8  | -1.14798 | -1.13994 | -3.317110 |
| 8  | 1.09804  | 1.11387  | -3.219540 |
| 8  | 2.02078  | -2.16979 | -1.419630 |
| 8  | -2.32309 | 2.12572  | 1.595630  |
| 8  | 1.09804  | 1.11387  | 3.219540  |
| 20 | -1.18319 | 1.13116  | 3.218520  |
| 20 | -2.07629 | -2.25149 | 1.655880  |
| 20 | 1.09279  | -1.13216 | 3.219800  |
| 20 | 3.5167   | -1.02375 | 0.000000  |
| 20 | -2.07629 | -2.25149 | -1.655880 |

|    |          |          |           |
|----|----------|----------|-----------|
| 20 | -0.05973 | -3.05038 | -1.597950 |
| 20 | 1.5495   | -0.07528 | -3.134590 |
| 20 | 0.09503  | 3.09041  | -1.579120 |
| 20 | -1.60228 | 0.05727  | -3.140550 |
| 20 | -3.05177 | 1.64769  | 0.000000  |
| 20 | 0.09503  | 3.09041  | 1.579120  |
| 21 | 2.93784  | -1.55233 | 0.000000  |

|    |          |          |           |
|----|----------|----------|-----------|
| 20 | 1.09279  | -1.13216 | -3.219800 |
| 20 | 2.15769  | 2.22453  | -1.608590 |
| 20 | -1.18319 | 1.13116  | -3.218520 |
| 20 | -1.19291 | 3.2735   | 0.000000  |
| 20 | 2.15769  | 2.22453  | 1.608590  |
| 20 | -3.38345 | 0.91553  | 0.000000  |
| 22 | 1.08054  | -2.78965 | 0.000000  |

### V/Ca<sub>11</sub>O<sub>12</sub>

|    |          |          |           |
|----|----------|----------|-----------|
| 8  | -1.29417 | -2.98131 | 0.000000  |
| 8  | 1.58549  | -2.4123  | 1.377520  |
| 8  | 3.3566   | 0.50709  | 0.000000  |
| 8  | -1.25907 | -0.88083 | 3.117080  |
| 8  | -3.31237 | -0.67076 | 0.000000  |
| 8  | -1.8282  | 2.43688  | -1.534990 |
| 8  | 1.55976  | 3.0068   | 0.000000  |
| 8  | -1.25907 | -0.88083 | -3.117080 |
| 8  | 1.21897  | 0.89642  | -3.085300 |
| 8  | 1.58549  | -2.4123  | -1.377520 |
| 8  | -1.8282  | 2.43688  | 1.534990  |
| 8  | 1.21897  | 0.89642  | 3.085300  |
| 20 | -0.94844 | 1.31225  | 3.154260  |
| 20 | -2.45088 | -1.84056 | 1.626930  |
| 20 | 0.89303  | -1.24887 | 3.143270  |
| 20 | 3.22031  | -1.60847 | 0.000000  |
| 20 | -2.45088 | -1.84056 | -1.626930 |
| 20 | 0.89303  | -1.24887 | -3.143270 |
| 20 | 2.50052  | 1.79951  | -1.581000 |
| 20 | -0.94844 | 1.31225  | -3.154260 |
| 20 | -0.56988 | 3.40505  | 0.000000  |
| 20 | 2.50052  | 1.79951  | 1.581000  |
| 20 | -3.09792 | 1.5115   | 0.000000  |
| 23 | 0.48813  | -2.8953  | 0.000000  |

### Cr /Ca<sub>11</sub>O<sub>12</sub>

|    |          |          |           |
|----|----------|----------|-----------|
| 8  | -1.69145 | -2.90619 | 0.000000  |
| 8  | 1.31606  | -2.56833 | 1.353790  |
| 8  | 3.47019  | 0.09425  | 0.000000  |
| 8  | -1.39498 | -0.68642 | 3.177690  |
| 8  | -3.35928 | -0.25922 | 0.000000  |
| 8  | -1.51117 | 2.64908  | -1.540980 |
| 8  | 1.92249  | 2.78158  | 0.000000  |
| 8  | -1.39498 | -0.68642 | -3.177690 |
| 8  | 1.32608  | 0.74326  | -3.078740 |
| 8  | 1.31606  | -2.56833 | -1.353790 |
| 8  | -1.51117 | 2.64908  | 1.540980  |
| 8  | 1.32608  | 0.74326  | 3.078740  |
| 20 | -0.77776 | 1.43039  | 3.172420  |
| 20 | -2.57896 | -1.52718 | 1.599450  |
| 20 | 0.68928  | -1.34799 | 3.062890  |
| 20 | 2.94869  | -1.99394 | 0.000000  |
| 20 | -2.57896 | -1.52718 | -1.599450 |
| 20 | 0.68928  | -1.34799 | -3.062890 |
| 20 | 2.70797  | 1.46435  | -1.573040 |
| 20 | -0.77776 | 1.43039  | -3.172420 |
| 20 | -0.14591 | 3.43885  | 0.000000  |
| 20 | 2.70797  | 1.46435  | 1.573040  |
| 20 | -2.87849 | 1.87009  | 0.000000  |
| 24 | 0.05756  | -2.79029 | 0.000000  |

### Mn /Ca<sub>11</sub>O<sub>12</sub>

|    |           |           |           |
|----|-----------|-----------|-----------|
| 8  | -1.278510 | -3.002700 | 0.000000  |
| 8  | 1.703460  | -2.322610 | 1.376420  |
| 8  | 3.418790  | 0.609110  | 0.000000  |
| 8  | -1.263670 | -0.899050 | 3.132790  |
| 8  | -3.340580 | -0.705320 | 0.000000  |
| 8  | -1.876860 | 2.412310  | -1.538490 |
| 8  | 1.497300  | 3.032790  | 0.000000  |
| 8  | -1.263670 | -0.899050 | -3.132790 |
| 8  | 1.205280  | 0.922690  | -3.090100 |
| 8  | 1.703460  | -2.322610 | -1.376420 |
| 8  | -1.876860 | 2.412310  | 1.538490  |
| 8  | 1.205280  | 0.922690  | 3.090100  |
| 20 | -0.977510 | 1.289790  | 3.152550  |
| 20 | -2.402010 | -1.884300 | 1.593470  |
| 20 | 0.890550  | -1.238830 | 3.106060  |
| 20 | 3.230850  | -1.528420 | 0.000000  |
| 20 | -2.402010 | -1.884300 | -1.593470 |

### Fe /Ca<sub>11</sub>O<sub>12</sub>

|    |          |          |           |
|----|----------|----------|-----------|
| 8  | 2.54335  | -1.78218 | 0.000000  |
| 8  | 2.67498  | 1.1031   | 1.415530  |
| 8  | 0.08243  | 3.4241   | 0.000000  |
| 8  | 0.56008  | -1.42403 | 3.152990  |
| 8  | -0.05001 | -3.39352 | 0.000000  |
| 8  | -2.78854 | -1.30646 | -1.539630 |
| 8  | -2.70629 | 2.11997  | 0.000000  |
| 8  | 0.56008  | -1.42403 | -3.152990 |
| 8  | -0.66361 | 1.38239  | -3.065650 |
| 8  | 2.67498  | 1.1031   | -1.415530 |
| 8  | -2.78854 | -1.30646 | 1.539630  |
| 8  | -0.66361 | 1.38239  | 3.065650  |
| 20 | -1.50172 | -0.65964 | 3.159310  |
| 20 | 1.29814  | -2.69973 | 1.590020  |
| 20 | 1.39373  | 0.59858  | 3.091810  |
| 20 | 2.11097  | 2.67209  | 0.000000  |
| 20 | 1.29814  | -2.69973 | -1.590020 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| 20 | 0.890550  | -1.238830 | -3.106060 |
| 20 | 2.462700  | 1.842940  | -1.576960 |
| 20 | -0.977510 | 1.289790  | -3.152550 |
| 20 | -0.641120 | 3.394590  | 0.000000  |
| 20 | 2.462700  | 1.842940  | 1.576960  |
| 20 | -3.139060 | 1.465230  | 0.000000  |
| 25 | 0.534790  | -2.731870 | 0.000000  |

|    |          |          |           |
|----|----------|----------|-----------|
| 20 | 1.39373  | 0.59858  | -3.091810 |
| 20 | -1.3316  | 2.80802  | -1.577220 |
| 20 | -1.50172 | -0.65964 | -3.159310 |
| 20 | -3.49779 | 0.10203  | 0.000000  |
| 20 | -1.3316  | 2.80802  | 1.577220  |
| 20 | -2.12765 | -2.73917 | 0.000000  |
| 26 | 3.09481  | -0.06212 | 0.000000  |

### Co /Ca<sub>11</sub>O<sub>12</sub>

|    |          |          |           |
|----|----------|----------|-----------|
| 8  | 0.70319  | -3.12496 | 0.000000  |
| 8  | 2.76829  | -0.86438 | 1.426350  |
| 8  | 2.34494  | 2.52715  | 0.000000  |
| 8  | -0.50431 | -1.44998 | 3.132750  |
| 8  | -2.3005  | -2.52118 | 0.000000  |
| 8  | -2.95981 | 0.85211  | -1.537910 |
| 8  | -0.6215  | 3.36615  | 0.000000  |
| 8  | -0.50431 | -1.44998 | -3.132750 |
| 8  | 0.40563  | 1.47703  | -3.072370 |
| 8  | 2.76829  | -0.86438 | -1.426350 |
| 8  | -2.95981 | 0.85211  | 1.537910  |
| 8  | 0.40563  | 1.47703  | 3.072370  |
| 20 | -1.56265 | 0.47862  | 3.151040  |
| 20 | -0.82862 | -2.91477 | 1.585840  |
| 20 | 1.44691  | -0.45734 | 3.099200  |
| 20 | 3.42002  | 0.64781  | 0.000000  |
| 20 | -0.82862 | -2.91477 | -1.585840 |
| 20 | 1.44691  | -0.45734 | -3.099200 |
| 20 | 0.86554  | 2.97923  | -1.576190 |
| 20 | -1.56265 | 0.47862  | -3.151040 |
| 20 | -2.55025 | 2.37589  | 0.000000  |
| 20 | 0.86554  | 2.97923  | 1.576190  |
| 20 | -3.42427 | -0.65637 | 0.000000  |
| 27 | 2.14358  | -1.96258 | 0.000000  |

### Ni /Ca<sub>11</sub>O<sub>12</sub>

|    |           |           |           |
|----|-----------|-----------|-----------|
| 8  | -1.227570 | -2.975320 | 0.000000  |
| 8  | 1.776790  | -2.244460 | 1.366850  |
| 8  | 3.413210  | 0.714910  | 0.000000  |
| 8  | -1.258940 | -0.900180 | 3.120190  |
| 8  | -3.345670 | -0.754110 | 0.000000  |
| 8  | -1.931530 | 2.393190  | -1.538140 |
| 8  | 1.431830  | 3.085840  | 0.000000  |
| 8  | -1.258940 | -0.900180 | -3.120190 |
| 8  | 1.175000  | 0.969710  | -3.078250 |
| 8  | 1.776790  | -2.244460 | -1.366850 |
| 8  | -1.931530 | 2.393190  | 1.538140  |
| 8  | 1.175000  | 0.969710  | 3.078250  |
| 20 | -1.010810 | 1.287700  | 3.155010  |
| 20 | -2.370830 | -1.926700 | 1.582940  |
| 20 | 0.905490  | -1.206480 | 3.067540  |
| 20 | 3.252250  | -1.445060 | 0.000000  |
| 20 | -2.370830 | -1.926700 | -1.582940 |
| 20 | 0.905490  | -1.206480 | -3.067540 |
| 20 | 2.426270  | 1.915380  | -1.575450 |
| 20 | -1.010810 | 1.287700  | -3.155010 |
| 20 | -0.714190 | 3.397500  | 0.000000  |
| 20 | 2.426270  | 1.915380  | 1.575450  |
| 20 | -3.172890 | 1.416280  | 0.000000  |
| 28 | 0.583450  | -2.651180 | 0.000000  |

### Cu /Ca<sub>11</sub>O<sub>12</sub>

|    |           |           |           |
|----|-----------|-----------|-----------|
| 8  | -0.665340 | -3.141420 | 0.000000  |
| 8  | 2.182540  | -1.865300 | 1.435220  |
| 8  | 3.200330  | 1.344150  | 0.000000  |
| 8  | -1.067390 | -1.107980 | 3.121600  |
| 8  | -3.142550 | -1.351360 | 0.000000  |
| 8  | -2.353760 | 2.001780  | -1.537460 |
| 8  | 0.819120  | 3.306890  | 0.000000  |
| 8  | -1.067390 | -1.107980 | -3.121600 |
| 8  | 0.967280  | 1.191720  | -3.088990 |
| 8  | 2.182540  | -1.865300 | -1.435220 |
| 8  | -2.353760 | 2.001780  | 1.537460  |
| 8  | 0.967280  | 1.191720  | 3.088990  |
| 20 | -1.240170 | 1.085740  | 3.151560  |
| 20 | -1.972270 | -2.326060 | 1.588360  |
| 20 | 1.123490  | -0.997360 | 3.114770  |
| 20 | 3.433770  | -0.809020 | 0.000000  |
| 20 | -1.972270 | -2.326060 | -1.588360 |
| 20 | 1.123490  | -0.997360 | -3.114770 |

### Zn /Ca<sub>11</sub>O<sub>12</sub>

|    |           |           |           |
|----|-----------|-----------|-----------|
| 8  | 0.663240  | -3.119730 | 0.000000  |
| 8  | 2.753270  | -0.807680 | 1.488670  |
| 8  | 2.356700  | 2.514710  | 0.000000  |
| 8  | -0.529000 | -1.433880 | 3.128710  |
| 8  | -2.320170 | -2.502130 | 0.000000  |
| 8  | -2.979830 | 0.875180  | -1.537440 |
| 8  | -0.612870 | 3.349470  | 0.000000  |
| 8  | -0.529000 | -1.433880 | -3.128710 |
| 8  | 0.379070  | 1.497580  | -3.103640 |
| 8  | 2.753270  | -0.807680 | -1.488670 |
| 8  | -2.979830 | 0.875180  | 1.537440  |
| 8  | 0.379070  | 1.497580  | 3.103640  |
| 20 | -1.586850 | 0.497190  | 3.152260  |
| 20 | -0.856900 | -2.913010 | 1.593560  |
| 20 | 1.426470  | -0.435660 | 3.155270  |
| 20 | 3.444340  | 0.645020  | 0.000000  |
| 20 | -0.856900 | -2.913010 | -1.593560 |
| 20 | 1.426470  | -0.435660 | -3.155270 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| 20 | 2.015990  | 2.346230  | -1.577480 |
| 20 | -1.240170 | 1.085740  | -3.151560 |
| 20 | -1.347950 | 3.217250  | 0.000000  |
| 20 | 2.015990  | 2.346230  | 1.577480  |
| 20 | -3.393260 | 0.809990  | 0.000000  |
| 29 | 1.093650  | -2.534330 | 0.000000  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| 20 | 0.872760  | 2.960380  | -1.577610 |
| 20 | -1.586850 | 0.497190  | -3.152260 |
| 20 | -2.558910 | 2.396360  | 0.000000  |
| 20 | 0.872760  | 2.960380  | 1.577610  |
| 20 | -3.440540 | -0.636390 | 0.000000  |
| 30 | 2.073710  | -1.883110 | 0.000000  |

### CO/ScCa<sub>11</sub>O<sub>12</sub>

|    |           |           |           |
|----|-----------|-----------|-----------|
| 8  | -2.438914 | -0.093182 | -1.655197 |
| 8  | -2.410121 | 1.313755  | 1.345555  |
| 8  | 0.388271  | -0.038407 | 3.428485  |
| 8  | -0.560814 | 3.099149  | -1.335495 |
| 8  | 0.072070  | 0.033598  | -3.393968 |
| 8  | 2.981262  | -1.424891 | -1.499420 |
| 8  | 3.070535  | 0.080741  | 1.936463  |
| 8  | -0.329778 | -3.124512 | -1.404323 |
| 8  | 1.074462  | -3.035658 | 1.311332  |
| 8  | -2.348263 | -1.535471 | 1.310306  |
| 8  | 2.872123  | 1.647796  | -1.464234 |
| 8  | 0.859972  | 3.076817  | 1.371248  |
| 20 | 1.549994  | 3.195925  | -0.727000 |
| 20 | -1.309835 | 1.561779  | -2.634475 |
| 20 | -1.245328 | 3.062355  | 0.743260  |
| 20 | -1.680198 | -0.111123 | 2.857985  |
| 20 | -1.183019 | -1.619577 | -2.678337 |
| 20 | -1.023790 | -3.154140 | 0.671345  |
| 20 | 1.818644  | -1.556269 | 2.707912  |
| 20 | 1.779798  | -3.078472 | -0.785685 |
| 20 | 3.734363  | 0.125592  | -0.127602 |
| 20 | 1.691383  | 1.602635  | 2.725754  |
| 20 | 2.185500  | 0.101822  | -2.877849 |
| 21 | -3.170214 | -0.109908 | 0.152176  |
| 8  | -6.619030 | -0.016891 | -0.053067 |
| 6  | -5.444986 | -0.027537 | 0.019438  |

### CO/TiCa<sub>11</sub>O<sub>12</sub>

|    |           |           |           |
|----|-----------|-----------|-----------|
| 8  | -2.428357 | 0.640724  | -1.474228 |
| 8  | -2.161019 | 1.253959  | 1.601388  |
| 8  | 0.385054  | -0.816686 | 3.325725  |
| 8  | -0.120126 | 3.410665  | -0.610635 |
| 8  | 0.007217  | 0.809468  | -3.292589 |
| 8  | 2.714833  | -1.395810 | -1.877759 |
| 8  | 3.046264  | -0.738157 | 1.786198  |
| 8  | -0.795024 | -2.623794 | -2.011146 |
| 8  | 0.634494  | -3.352104 | 0.585397  |
| 8  | -2.519361 | -1.429630 | 1.041400  |
| 8  | 3.047728  | 1.571376  | -1.161220 |
| 8  | 1.264466  | 2.583735  | 1.983571  |
| 20 | 1.981589  | 3.091733  | -0.046707 |
| 20 | -1.105468 | 2.333720  | -2.168989 |
| 20 | -0.817978 | 2.969117  | 1.414124  |
| 20 | -1.676212 | -0.488764 | 2.854041  |
| 20 | -1.431321 | -0.786948 | -2.907957 |
| 20 | -1.458580 | -3.067923 | 0.025173  |
| 20 | 1.587059  | -2.319101 | 2.241842  |
| 20 | 1.313902  | -2.994382 | -1.489354 |
| 20 | 3.708544  | -0.313283 | -0.233239 |
| 20 | 1.900818  | 0.746227  | 2.941670  |
| 20 | 2.121687  | 0.493926  | -2.841797 |
| 22 | -3.031718 | 0.222041  | 0.204674  |
| 8  | -6.245780 | 0.185257  | 0.019487  |
| 6  | -5.071021 | 0.172773  | 0.066056  |

### CO/VCa<sub>11</sub>O<sub>12</sub>

|    |           |           |           |
|----|-----------|-----------|-----------|
| 8  | 2.368547  | -0.008630 | -1.718934 |
| 8  | 2.469986  | -1.373799 | 1.032128  |
| 8  | -0.152475 | 0.014415  | 3.327476  |
| 8  | 0.401760  | -3.151533 | -1.356485 |
| 8  | -0.197355 | -0.014786 | -3.373724 |
| 8  | -2.958760 | 1.527915  | -1.372326 |
| 8  | -2.939538 | 0.008161  | 2.074858  |
| 8  | 0.399996  | 3.140015  | -1.382995 |
| 8  | -0.904562 | 3.081735  | 1.351584  |
| 8  | 2.468694  | 1.384302  | 1.017570  |
| 8  | -2.957984 | -1.541298 | -1.359636 |
| 8  | -0.902775 | -3.070219 | 1.377722  |
| 20 | -1.704088 | -3.162672 | -0.669616 |
| 20 | 1.097815  | -1.626276 | -2.678730 |
| 20 | 1.150755  | -3.154845 | 0.688433  |
| 20 | 1.890324  | 0.014170  | 2.823401  |
| 20 | 1.097184  | 1.602189  | -2.690177 |

### CO/CrCa<sub>11</sub>O<sub>12</sub>

|    |           |           |           |
|----|-----------|-----------|-----------|
| 8  | 1.668819  | 2.336999  | 0.000000  |
| 8  | -1.162539 | 2.403231  | 1.408634  |
| 8  | -3.432833 | -0.218446 | 0.000000  |
| 8  | 1.401588  | 0.397029  | 3.149185  |
| 8  | 3.395690  | -0.173439 | 0.000000  |
| 8  | 1.382704  | -2.958228 | -1.538515 |
| 8  | -2.034090 | -2.960557 | 0.000000  |
| 8  | 1.401588  | 0.397029  | -3.149185 |
| 8  | -1.367987 | -0.899112 | -3.067155 |
| 8  | -1.162539 | 2.403231  | -1.408634 |
| 8  | 1.382704  | -2.958228 | 1.538515  |
| 8  | -1.367987 | -0.899112 | 3.067155  |
| 20 | 0.700011  | -1.688412 | 3.153514  |
| 20 | 2.674913  | 1.158686  | 1.590874  |
| 20 | -0.639843 | 1.170598  | 3.129255  |
| 20 | -2.766392 | 1.821234  | 0.000000  |
| 20 | 2.674913  | 1.158686  | -1.590874 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| 20 | 1.148986  | 3.162590  | 0.661827  |
| 20 | -1.585707 | 1.594893  | 2.779560  |
| 20 | -1.705843 | 3.156063  | -0.696513 |
| 20 | -3.690701 | -0.000945 | 0.045606  |
| 20 | -1.584694 | -1.571483 | 2.793140  |
| 20 | -2.311981 | -0.012432 | -2.790706 |
| 23 | 2.986017  | 0.000111  | -0.013813 |
| 8  | 6.102135  | 0.000171  | -0.161879 |
| 6  | 4.949877  | 0.000138  | -0.108278 |

**CO/MnCa<sub>11</sub>O<sub>12</sub>**

|    |           |           |           |
|----|-----------|-----------|-----------|
| 8  | 1.858463  | 2.336895  | 0.000000  |
| 8  | -1.102857 | 2.396100  | 1.386621  |
| 8  | -3.450544 | -0.086904 | 0.000000  |
| 8  | 1.424680  | 0.347633  | 3.128081  |
| 8  | 3.390027  | -0.300910 | 0.000000  |
| 8  | 1.279700  | -3.020652 | -1.537443 |
| 8  | -2.137422 | -2.874980 | 0.000000  |
| 8  | 1.424680  | 0.347633  | -3.128081 |
| 8  | -1.388207 | -0.863887 | -3.075620 |
| 8  | -1.102857 | 2.396100  | -1.386621 |
| 8  | 1.279700  | -3.020652 | 1.537443  |
| 8  | -1.388207 | -0.863887 | 3.075620  |
| 20 | 0.651533  | -1.713960 | 3.145207  |
| 20 | 2.746018  | 1.068525  | 1.591014  |
| 20 | -0.595003 | 1.181070  | 3.114692  |
| 20 | -2.727723 | 1.944404  | 0.000000  |
| 20 | 2.746018  | 1.068525  | -1.591014 |
| 20 | -0.595003 | 1.181070  | -3.114692 |
| 20 | -2.820511 | -1.502231 | -1.577248 |
| 20 | 0.651533  | -1.713960 | -3.145207 |
| 20 | -0.137729 | -3.712801 | 0.000000  |
| 20 | -2.820511 | -1.502231 | 1.577248  |
| 20 | 2.720968  | -2.374153 | 0.000000  |
| 25 | 0.089263  | 2.911732  | 0.000000  |
| 8  | 0.021097  | 5.814644  | 0.000000  |
| 6  | 0.085103  | 4.644075  | 0.000000  |

**CO/CoCa<sub>11</sub>O<sub>12</sub>**

|    |           |           |           |
|----|-----------|-----------|-----------|
| 8  | 2.462933  | -0.131995 | -1.651219 |
| 8  | 2.290266  | -1.469517 | 1.355158  |
| 8  | -0.389489 | 0.102608  | 3.409208  |
| 8  | 0.332311  | -3.203783 | -1.280453 |
| 8  | -0.052206 | -0.108439 | -3.373492 |
| 8  | -2.889127 | 1.569389  | -1.545031 |
| 8  | -3.084037 | 0.140893  | 1.922309  |
| 8  | 0.516897  | 3.077230  | -1.460150 |
| 8  | -0.925799 | 3.143149  | 1.240764  |
| 8  | 2.375158  | 1.422992  | 1.301074  |
| 8  | -2.978198 | -1.505192 | -1.452590 |
| 8  | -1.098459 | -3.015030 | 1.421604  |
| 20 | -1.781315 | -3.136373 | -0.675469 |
| 20 | 1.207410  | -1.715305 | -2.561597 |
| 20 | 1.010552  | -3.125211 | 0.801233  |
| 20 | 1.693382  | 0.025981  | 2.824704  |
| 20 | 1.297653  | 1.466763  | -2.653139 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| 20 | -0.639843 | 1.170598  | -3.129255 |
| 20 | -2.770304 | -1.618915 | -1.580330 |
| 20 | 0.700011  | -1.688412 | -3.153514 |
| 20 | -0.000747 | -3.715071 | 0.000000  |
| 20 | -2.770304 | -1.618915 | 1.580330  |
| 20 | 2.805135  | -2.268613 | 0.000000  |
| 24 | -0.059244 | 2.979672  | 0.000000  |
| 8  | 0.121724  | 5.926200  | 0.000000  |
| 6  | 0.042686  | 4.747644  | 0.000000  |

**CO/FeCa<sub>11</sub>O<sub>12</sub>**

|    |          |          |           |
|----|----------|----------|-----------|
| 8  | 1.934713 | 2.289938 | 0.000000  |
| 8  | -1.07025 | 2.412849 | 1.382393  |
| 8  | -3.45967 | -0.01615 | 0.000000  |
| 8  | 1.43824  | 0.314377 | 3.123182  |
| 8  | 3.398615 | -0.38298 | 0.000000  |
| 8  | 1.217681 | -3.0452  | -1.538579 |
| 8  | -2.19985 | -2.83044 | 0.000000  |
| 8  | 1.43824  | 0.314377 | -3.123182 |
| 8  | -1.40487 | -0.83663 | -3.074322 |
| 8  | -1.07025 | 2.412849 | -1.382393 |
| 8  | 1.217681 | -3.0452  | 1.538579  |
| 8  | 2.673444 | -2.4394  | 0.000000  |
| 20 | 0.613204 | -1.72928 | 3.148498  |
| 20 | 2.784875 | 0.994687 | 1.596399  |
| 20 | -0.56907 | 1.195456 | 3.098473  |
| 20 | -2.68944 | 2.009246 | 0.000000  |
| 20 | 2.784875 | 0.994687 | -1.596399 |
| 20 | -0.56907 | 1.195456 | -3.098473 |
| 20 | -2.85519 | -1.4386  | -1.576847 |
| 20 | 0.613204 | -1.72928 | -3.148498 |
| 20 | -0.21864 | -3.70429 | 0.000000  |
| 20 | -2.85519 | -1.4386  | 1.576847  |
| 20 | -1.40487 | -0.83663 | 3.074322  |
| 26 | 0.191584 | 2.866544 | 0.000000  |
| 8  | -0.03278 | 5.726031 | 0.000000  |
| 6  | 0.12292  | 4.575151 | 0.000000  |

**CO/NiCa<sub>11</sub>O<sub>12</sub>**

|    |          |          |           |
|----|----------|----------|-----------|
| 8  | 1.590538 | 3.148908 | 0.000000  |
| 8  | -1.92307 | 2.031071 | 1.531643  |
| 8  | -3.37607 | -1.00042 | 0.000000  |
| 8  | 1.267122 | 0.72238  | 3.100136  |
| 8  | 3.25383  | 0.608064 | 0.000000  |
| 8  | 1.982953 | -2.58274 | -1.535705 |
| 8  | -1.35019 | -3.32229 | 0.000000  |
| 8  | 1.267122 | 0.72238  | -3.100136 |
| 8  | -1.13607 | -1.20272 | -3.084293 |
| 8  | -1.92307 | 2.031071 | -1.531643 |
| 8  | 1.982953 | -2.58274 | 1.535705  |
| 8  | -1.13607 | -1.20272 | 3.084293  |
| 20 | 1.043796 | -1.4765  | 3.142548  |
| 20 | 2.411538 | 1.762918 | 1.642192  |
| 20 | -0.93121 | 0.988692 | 3.130155  |
| 20 | -3.31015 | 1.145358 | 0.000000  |
| 20 | 2.411538 | 1.762918 | -1.642192 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| 20 | 1.186629  | 3.101405  | 0.626573  |
| 20 | -1.712680 | 1.699668  | 2.655316  |
| 20 | -1.598271 | 3.171366  | -0.863347 |
| 20 | -3.739871 | 0.096267  | -0.143751 |
| 20 | -1.805591 | -1.452279 | 2.749048  |
| 20 | -2.171221 | -0.031424 | -2.878946 |
| 27 | 2.957968  | -0.065686 | 0.152837  |
| 8  | 4.771759  | -0.036324 | 0.007216  |
| 6  | 5.911101  | -0.025518 | -0.109988 |

### CO/CuCa<sub>11</sub>O<sub>12</sub>

|    |           |           |           |
|----|-----------|-----------|-----------|
| 8  | 1.544519  | 3.155035  | 0.000000  |
| 8  | -2.084000 | 1.959821  | 1.517402  |
| 8  | -3.347561 | -1.184439 | 0.000000  |
| 8  | 1.226872  | 0.765135  | 3.042198  |
| 8  | 3.296008  | 0.687019  | 0.000000  |
| 8  | 2.071916  | -2.532236 | -1.534803 |
| 8  | -1.234743 | -3.412969 | 0.000000  |
| 8  | 1.226872  | 0.765135  | -3.042198 |
| 8  | -1.107787 | -1.249103 | -3.056059 |
| 8  | -2.084000 | 1.959821  | -1.517402 |
| 8  | 2.071916  | -2.532236 | 1.534803  |
| 8  | -1.107787 | -1.249103 | 3.056059  |
| 20 | 1.073554  | -1.442702 | 3.119166  |
| 20 | 2.435666  | 1.812559  | 1.651587  |
| 20 | -0.992640 | 0.953805  | 3.065550  |
| 20 | -3.342737 | 0.980832  | 0.000000  |
| 20 | 2.435666  | 1.812559  | -1.651587 |
| 20 | -0.992640 | 0.953805  | -3.065550 |
| 20 | -2.304706 | -2.306261 | -1.580528 |
| 20 | 1.073554  | -1.442702 | -3.119166 |
| 20 | 0.914271  | -3.623059 | 0.000000  |
| 20 | -2.304706 | -2.306261 | 1.580528  |
| 20 | 3.250289  | -1.507842 | 0.000000  |
| 29 | -1.190531 | 2.797111  | 0.000000  |
| 8  | 0.430426  | 3.887914  | 0.000000  |
| 6  | 0.406694  | 5.100820  | 0.000000  |

### NO/ScCa<sub>11</sub>O<sub>12</sub>

|    |           |           |           |
|----|-----------|-----------|-----------|
| 8  | -2.417607 | -0.236312 | -1.625542 |
| 8  | -2.421283 | 1.374175  | 1.288764  |
| 8  | 0.421449  | 0.170704  | 3.422244  |
| 8  | -0.596025 | 3.008768  | -1.507899 |
| 8  | 0.065058  | -0.176007 | -3.405750 |
| 8  | 2.983043  | -1.480799 | -1.429714 |
| 8  | 3.092221  | 0.229570  | 1.912916  |
| 8  | -0.297475 | -3.230112 | -1.207478 |
| 8  | 1.117767  | -2.939276 | 1.486070  |
| 8  | -2.316520 | -1.475899 | 1.411180  |
| 8  | 2.847582  | 1.584770  | -1.578443 |
| 8  | 0.839225  | 3.154796  | 1.185300  |
| 20 | 1.516544  | 3.161516  | -0.918702 |
| 20 | -1.321132 | 1.374491  | -2.705848 |
| 20 | -1.267851 | 3.087064  | 0.571783  |
| 20 | -1.649268 | 0.041018  | 2.860222  |
| 20 | -1.151965 | -1.799004 | -2.566153 |

|    |          |          |           |
|----|----------|----------|-----------|
| 20 | -0.93121 | 0.988692 | -3.130155 |
| 20 | -2.36566 | -2.17415 | -1.580646 |
| 20 | 1.043796 | -1.4765  | -3.142548 |
| 20 | 0.790428 | -3.62825 | 0.000000  |
| 20 | -2.36566 | -2.17415 | 1.580646  |
| 20 | 3.184231 | -1.58056 | 0.000000  |
| 28 | -1.02902 | 2.684419 | 0.000000  |
| 8  | 0.420308 | 3.8136   | 0.000000  |
| 6  | 0.332769 | 5.027904 | 0.000000  |

### CO/ZnCa<sub>11</sub>O<sub>12</sub>

|    |           |           |           |
|----|-----------|-----------|-----------|
| 8  | 0.712681  | 2.898938  | 0.000000  |
| 8  | -2.147127 | 1.653077  | 1.490331  |
| 8  | -3.195770 | -1.525149 | 0.000000  |
| 8  | 1.078798  | 0.838685  | 3.132072  |
| 8  | 3.145915  | 1.055931  | 0.000000  |
| 8  | 2.322579  | -2.287097 | -1.536505 |
| 8  | -0.863647 | -3.539262 | 0.000000  |
| 8  | 1.078798  | 0.838685  | -3.132072 |
| 8  | -0.980957 | -1.439467 | -3.109140 |
| 8  | -2.147127 | 1.653077  | -1.490331 |
| 8  | 2.322579  | -2.287097 | 1.536505  |
| 8  | -0.980957 | -1.439467 | 3.109140  |
| 20 | 1.225061  | -1.358394 | 3.155268  |
| 20 | 1.997778  | 2.040798  | 1.596310  |
| 20 | -1.117269 | 0.753235  | 3.161850  |
| 20 | -3.389772 | 0.628794  | 0.000000  |
| 20 | 1.997778  | 2.040798  | -1.596310 |
| 20 | -1.117269 | 0.753235  | -3.161850 |
| 20 | -2.042686 | -2.557827 | -1.579061 |
| 20 | 1.225061  | -1.358394 | -3.155268 |
| 20 | 1.303748  | -3.493570 | 0.000000  |
| 20 | -2.042686 | -2.557827 | 1.579061  |
| 20 | 3.374730  | -1.109133 | 0.000000  |
| 30 | -1.089888 | 2.350156  | 0.000000  |
| 8  | 0.512933  | 6.172940  | 0.000000  |
| 6  | -0.410408 | 5.518441  | 0.000000  |

### NO/TiCa<sub>11</sub>O<sub>12</sub>

|    |           |           |           |
|----|-----------|-----------|-----------|
| 8  | -2.368830 | -0.010820 | -1.646920 |
| 8  | -2.453540 | 1.365670  | 1.036210  |
| 8  | 0.208040  | 0.015240  | 3.318860  |
| 8  | -0.396280 | 3.131430  | -1.382350 |
| 8  | 0.164670  | -0.016130 | -3.356260 |
| 8  | 2.966030  | -1.542350 | -1.391590 |
| 8  | 2.987870  | 0.010330  | 2.042400  |
| 8  | -0.394570 | -3.144520 | -1.353600 |
| 8  | 0.936880  | -3.056000 | 1.365210  |
| 8  | -2.454990 | -1.357600 | 1.051970  |
| 8  | 2.965170  | 1.530680  | -1.405730 |
| 8  | 0.935660  | 3.069170  | 1.336670  |
| 20 | 1.719910  | 3.157510  | -0.720840 |
| 20 | -1.124470 | 1.605670  | -2.677260 |
| 20 | -1.123040 | 3.144650  | 0.670250  |
| 20 | -1.839020 | 0.014140  | 2.851760  |
| 20 | -1.123360 | -1.633600 | -2.665150 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| 20 | -0.982192 | -3.121746 | 0.868221  |
| 20 | 1.860630  | -1.371519 | 2.786848  |
| 20 | 1.813089  | -3.107016 | -0.604681 |
| 20 | 3.732037  | 0.154404  | -0.158575 |
| 20 | 1.703385  | 1.779559  | 2.622900  |
| 20 | 2.178879  | -0.047824 | -2.896786 |
| 21 | -3.169481 | -0.122880 | 0.176341  |
| 7  | -5.267209 | 0.029654  | -0.007681 |
| 8  | -6.469125 | -0.065126 | -0.055895 |

#### NO/VCa<sub>11</sub>O<sub>12</sub>

|    |          |          |          |
|----|----------|----------|----------|
| 8  | -2.27038 | 0.014937 | -1.70158 |
| 8  | -2.40196 | 1.381334 | 1.136246 |
| 8  | 0.160227 | -0.03683 | 3.435223 |
| 8  | -0.37402 | 3.162981 | -1.37684 |
| 8  | 0.242921 | 0.035489 | -3.40468 |
| 8  | 2.985884 | -1.51697 | -1.34661 |
| 8  | 2.921931 | -0.01706 | 2.087086 |
| 8  | -0.36327 | -3.13576 | -1.43992 |
| 8  | 0.87946  | -3.08045 | 1.347954 |
| 8  | -2.40172 | -1.41401 | 1.104954 |
| 8  | 2.981248 | 1.553488 | -1.31653 |
| 8  | 0.870321 | 3.055028 | 1.408954 |
| 20 | 1.697996 | 3.160648 | -0.64038 |
| 20 | -1.09602 | 1.619829 | -2.68898 |
| 20 | -1.18223 | 3.130278 | 0.646107 |
| 20 | -1.86746 | -0.0336  | 2.747756 |
| 20 | -1.09019 | -1.56674 | -2.71911 |
| 20 | -1.17226 | -3.14691 | 0.582553 |
| 20 | 1.572413 | -1.60645 | 2.779286 |
| 20 | 1.708457 | -3.14203 | -0.70301 |
| 20 | 3.711736 | 0.005597 | 0.065983 |
| 20 | 1.564993 | 1.552444 | 2.809732 |
| 20 | 2.328335 | 0.031518 | -2.76925 |
| 23 | -3.0155  | -0.00403 | 0.001577 |
| 7  | -4.67918 | -0.00216 | -0.08306 |
| 8  | -5.90624 | -0.00018 | -0.14285 |

#### NO/MnCa<sub>11</sub>O<sub>12</sub>

|    |           |           |           |
|----|-----------|-----------|-----------|
| 8  | 1.898230  | 2.248976  | 0.000000  |
| 8  | -0.974733 | 2.402323  | 1.366624  |
| 8  | -3.425113 | 0.017329  | 0.000000  |
| 8  | 1.443903  | 0.271549  | 3.135717  |
| 8  | 3.378563  | -0.409305 | 0.000000  |
| 8  | 1.184212  | -3.068529 | -1.537517 |
| 8  | -2.230321 | -2.821995 | 0.000000  |
| 8  | 1.443903  | 0.271549  | -3.135717 |
| 8  | -1.408808 | -0.838709 | -3.080561 |
| 8  | -0.974733 | 2.402323  | -1.366624 |
| 8  | 1.184212  | -3.068529 | 1.537517  |
| 8  | -1.408808 | -0.838709 | 3.080561  |
| 20 | 0.594082  | -1.760141 | 3.159507  |
| 20 | 2.769655  | 0.956080  | 1.602291  |
| 20 | -0.548109 | 1.182058  | 3.100589  |
| 20 | -2.618102 | 2.024565  | 0.000000  |
| 20 | 2.769655  | 0.956080  | -1.602291 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| 20 | -1.121610 | -3.137130 | 0.698880  |
| 20 | 1.643570  | -1.571120 | 2.780110  |
| 20 | 1.721550  | -3.163130 | -0.691290 |
| 20 | 3.716000  | 0.000930  | 0.005390  |
| 20 | 1.642480  | 1.597820  | 2.765250  |
| 20 | 2.289340  | -0.012520 | -2.811280 |
| 22 | -3.072150 | -0.001370 | 0.025980  |
| 7  | -5.038020 | -0.000880 | -0.084050 |
| 8  | -6.242800 | 0.001430  | -0.127320 |

#### NO/CrCa<sub>11</sub>O<sub>12</sub>

|    |           |           |           |
|----|-----------|-----------|-----------|
| 8  | 1.837446  | 2.284943  | 0.000000  |
| 8  | -1.072402 | 2.389987  | 1.373097  |
| 8  | -3.442855 | -0.073773 | 0.000000  |
| 8  | 1.428237  | 0.318004  | 3.129453  |
| 8  | 3.396515  | -0.330758 | 0.000000  |
| 8  | 1.262434  | -3.036295 | -1.536997 |
| 8  | -2.157688 | -2.873980 | 0.000000  |
| 8  | 1.428237  | 0.318004  | -3.129453 |
| 8  | -1.392017 | -0.867995 | -3.073136 |
| 8  | -1.072402 | 2.389987  | -1.373097 |
| 8  | 1.262434  | -3.036295 | 1.536997  |
| 8  | -1.392017 | -0.867995 | 3.073136  |
| 20 | 0.638852  | -1.737112 | 3.151839  |
| 20 | 2.751189  | 1.030875  | 1.594954  |
| 20 | -0.583341 | 1.169483  | 3.107023  |
| 20 | -2.714040 | 1.953026  | 0.000000  |
| 20 | 2.751189  | 1.030875  | -1.594954 |
| 20 | -0.583341 | 1.169483  | -3.107023 |
| 20 | -2.830787 | -1.496272 | -1.577005 |
| 20 | 0.638852  | -1.737112 | -3.151839 |
| 20 | -0.160807 | -3.718448 | 0.000000  |
| 20 | -2.830787 | -1.496272 | 1.577005  |
| 20 | 2.707183  | -2.399939 | 0.000000  |
| 24 | 0.114715  | 2.987698  | 0.000000  |
| 7  | 0.129378  | 4.691111  | 0.000000  |
| 8  | -0.003684 | 5.896882  | 0.000000  |

#### NO/FeCa<sub>11</sub>O<sub>12</sub>

|    |          |          |            |
|----|----------|----------|------------|
| 8  | 1.493231 | 2.429489 | 0.000000   |
| 8  | -1.3622  | 2.290604 | 1.4333680  |
| 8  | -3.40218 | -0.48869 | 0.000000   |
| 8  | 1.359815 | 0.441888 | 3.1508300  |
| 8  | 3.371573 | 0.031    | 0.000000   |
| 8  | 1.567316 | -2.90016 | -1.5377130 |
| 8  | -1.84844 | -3.14339 | 0.000000   |
| 8  | 1.359815 | 0.441888 | -3.1508300 |
| 8  | -1.31071 | -1.04707 | -3.0716870 |
| 8  | -1.3622  | 2.290604 | -1.4333680 |
| 8  | 1.567316 | -2.90016 | 1.5377130  |
| 8  | -1.31071 | -1.04707 | 3.0716870  |
| 20 | 0.804908 | -1.68533 | 3.1602960  |
| 20 | 2.560576 | 1.305925 | 1.5927600  |
| 20 | -0.73463 | 1.072039 | 3.1206410  |
| 20 | -2.87322 | 1.599183 | 0.000000   |
| 20 | 2.560576 | 1.305925 | -1.5927600 |

|                                       |           |           |           |                                       |           |           |            |
|---------------------------------------|-----------|-----------|-----------|---------------------------------------|-----------|-----------|------------|
| 20                                    | -0.548109 | 1.182058  | -3.100589 | 20                                    | -0.73463  | 1.072039  | -3.1206410 |
| 20                                    | -2.861081 | -1.419248 | -1.576155 | 20                                    | -2.66428  | -1.84517  | -1.5788180 |
| 20                                    | 0.594082  | -1.760141 | -3.159507 | 20                                    | 0.804908  | -1.68533  | -3.1602960 |
| 20                                    | -0.257764 | -3.715860 | 0.000000  | 20                                    | 0.235434  | -3.74519  | 0.0000000  |
| 20                                    | -2.861081 | -1.419248 | 1.576155  | 20                                    | -2.66428  | -1.84517  | 1.5788180  |
| 20                                    | 2.638862  | -2.465407 | 0.000000  | 20                                    | 2.930227  | -2.10204  | 0.0000000  |
| 25                                    | 0.251173  | 2.976680  | 0.000000  | 26                                    | -0.27126  | 3.028814  | 0.0000000  |
| 7                                     | 0.177610  | 4.586794  | 0.000000  | 7                                     | -0.24381  | 4.871881  | 0.0000000  |
| 8                                     | -0.231059 | 5.714172  | 0.000000  | 8                                     | 0.408322  | 5.877289  | 0.0000000  |
| NO/CoCa <sub>11</sub> O <sub>12</sub> |           |           |           | NO/NiCa <sub>11</sub> O <sub>12</sub> |           |           |            |
| 8                                     | 2.426429  | 1.922224  | 0.000000  | 8                                     | 2.117994  | 0.000000  | -2.107650  |
| 8                                     | -0.336492 | 2.449974  | 1.390509  | 8                                     | 2.515330  | -1.444436 | 0.936767   |
| 8                                     | -3.264727 | 0.746544  | 0.000000  | 8                                     | 0.203231  | 0.000000  | 3.421776   |
| 8                                     | 1.529671  | -0.052903 | 3.175294  | 8                                     | 0.189143  | -3.125898 | -1.465596  |
| 8                                     | 3.216814  | -1.053519 | 0.000000  | 8                                     | -0.649417 | 0.000000  | -3.387725  |
| 8                                     | 0.583332  | -3.261336 | -1.536363 | 8                                     | -3.149026 | 1.538519  | -1.019091  |
| 8                                     | -2.696652 | -2.293033 | 0.000000  | 8                                     | -2.699527 | 0.000000  | 2.379252   |
| 8                                     | 1.529671  | -0.052903 | -3.175294 | 8                                     | 0.189143  | 3.125898  | -1.465596  |
| 8                                     | -1.492100 | -0.566663 | -3.110698 | 8                                     | -0.772143 | 3.082444  | 1.445389   |
| 8                                     | -0.336492 | 2.449974  | -1.390509 | 8                                     | 2.515330  | 1.444436  | 0.936767   |
| 8                                     | 0.583332  | -3.261336 | 1.536363  | 8                                     | -3.149026 | -1.538519 | -1.019091  |
| 8                                     | -1.492100 | -0.566663 | 3.110698  | 8                                     | -0.772143 | -3.082444 | 1.445389   |
| 20                                    | 0.291737  | -1.876351 | 3.171173  | 20                                    | -1.792914 | -3.150458 | -0.511491  |
| 20                                    | 2.907340  | 0.428437  | 1.584568  | 20                                    | 0.775996  | -1.587605 | -2.854006  |
| 20                                    | -0.232856 | 1.220602  | 3.162414  | 20                                    | 1.201764  | -3.106996 | 0.478895   |
| 20                                    | -2.041768 | 2.535637  | 0.000000  | 20                                    | 2.178143  | 0.000000  | 2.530746   |
| 20                                    | 2.907340  | 0.428437  | -1.584568 | 20                                    | 0.775996  | 1.587605  | -2.854006  |
| 20                                    | -0.232856 | 1.220602  | -3.162414 | 20                                    | 1.201764  | 3.106996  | 0.478895   |
| 20                                    | -3.012428 | -0.789182 | -1.573934 | 20                                    | -1.261637 | 1.575578  | 2.927280   |
| 20                                    | 0.291737  | -1.876351 | -3.171173 | 20                                    | -1.792914 | 3.150458  | -0.511491  |
| 20                                    | -0.960207 | -3.592724 | 0.000000  | 20                                    | -3.703626 | 0.000000  | 0.457476   |
| 20                                    | -3.012428 | -0.789182 | 1.573934  | 20                                    | -1.261637 | -1.575578 | 2.927280   |
| 20                                    | 2.129832  | -2.939865 | 0.000000  | 20                                    | -2.643521 | 0.000000  | -2.515022  |
| 27                                    | 0.818879  | 2.883055  | 0.000000  | 28                                    | 2.797540  | 0.000000  | -0.349634  |
| 7                                     | 0.291024  | 4.546953  | 0.000000  | 7                                     | 4.651231  | 0.000000  | -0.611244  |
| 8                                     | -0.857660 | 4.905591  | 0.000000  | 8                                     | 5.406359  | 0.000000  | 0.271575   |
| NO/CuCa <sub>11</sub> O <sub>12</sub> |           |           |           | NO/ZnCa <sub>11</sub> O <sub>12</sub> |           |           |            |
| 8                                     | 2.117994  | 0.000000  | -2.107650 | 8                                     | 3.072804  | 0.572398  | 0.000000   |
| 8                                     | 2.515330  | -1.444436 | 0.936767  | 8                                     | 0.640271  | 2.523438  | 1.489428   |
| 8                                     | 0.203231  | 0.000000  | 3.421776  | 8                                     | -2.657700 | 1.932427  | 0.000000   |
| 8                                     | 0.189143  | -3.125898 | -1.465596 | 8                                     | 1.461888  | -0.711280 | 3.131422   |
| 8                                     | -0.649417 | 0.000000  | -3.387725 | 8                                     | 2.641701  | -2.442952 | 0.000000   |
| 8                                     | -3.149026 | 1.538519  | -1.019091 | 8                                     | -0.690960 | -3.297348 | -1.536845  |
| 8                                     | -2.699527 | 0.000000  | 2.379252  | 8                                     | -3.305546 | -1.082869 | 0.000000   |
| 8                                     | 0.189143  | 3.125898  | -1.465596 | 8                                     | 1.461888  | -0.711280 | -3.131422  |
| 8                                     | -0.772143 | 3.082444  | 1.445389  | 8                                     | -1.519506 | 0.016212  | -3.106783  |
| 8                                     | 2.515330  | 1.444436  | 0.936767  | 8                                     | 0.640271  | 2.523438  | -1.489428  |
| 8                                     | -3.149026 | -1.538519 | -1.019091 | 8                                     | -0.690960 | -3.297348 | 1.536845   |
| 8                                     | -0.772143 | -3.082444 | 1.445389  | 8                                     | -1.519506 | 0.016212  | 3.106783   |
| 20                                    | -1.792914 | -3.150458 | -0.511491 | 20                                    | -0.401064 | -1.884692 | 3.153433   |
| 20                                    | 0.775996  | -1.587605 | -2.854006 | 20                                    | 2.954852  | -0.956126 | 1.593868   |
| 20                                    | 1.201764  | -3.106996 | 0.478895  | 20                                    | 0.346474  | 1.180149  | 3.157965   |
| 20                                    | 2.178143  | 0.000000  | 2.530746  | 20                                    | -0.854983 | 3.136792  | 0.000000   |
| 20                                    | 0.775996  | 1.587605  | -2.854006 | 20                                    | 2.954852  | -0.956126 | -1.593868  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| 20 | 1.201764  | 3.106996  | 0.478895  |
| 20 | -1.261637 | 1.575578  | 2.927280  |
| 20 | -1.792914 | 3.150458  | -0.511491 |
| 20 | -3.703626 | 0.000000  | 0.457476  |
| 20 | -1.261637 | -1.575578 | 2.927280  |
| 20 | -2.643521 | 0.000000  | -2.515022 |
| 29 | 2.797540  | 0.000000  | -0.349634 |
| 7  | 4.651231  | 0.000000  | -0.611244 |
| 8  | 5.406359  | 0.000000  | 0.271575  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| 20 | 0.346474  | 1.180149  | -3.157965 |
| 20 | -3.006733 | 0.424069  | -1.577268 |
| 20 | -0.401064 | -1.884692 | -3.153433 |
| 20 | -2.234907 | -2.967304 | 0.000000  |
| 20 | -3.006733 | 0.424069  | 1.577268  |
| 20 | 0.843926  | -3.670884 | 0.000000  |
| 30 | 1.746514  | 1.900949  | 0.000000  |
| 7  | 0.393376  | 6.772617  | 0.000000  |
| 8  | -0.281019 | 5.840846  | 0.000000  |

#### HCN/ScCa<sub>11</sub>O<sub>12</sub>

|    |           |           |           |
|----|-----------|-----------|-----------|
| 8  | 2.388101  | -0.007894 | -1.754796 |
| 8  | 2.424872  | -1.499219 | 1.185958  |
| 8  | -0.243758 | -0.072674 | 3.415767  |
| 8  | 0.350377  | -3.097834 | -1.452924 |
| 8  | -0.194908 | 0.068605  | -3.397762 |
| 8  | -2.955150 | 1.607513  | -1.349097 |
| 8  | -2.991040 | 0.002931  | 2.039960  |
| 8  | 0.447454  | 3.134228  | -1.330536 |
| 8  | -0.870802 | 3.044893  | 1.426548  |
| 8  | 2.444274  | 1.352892  | 1.234858  |
| 8  | -3.002119 | -1.465747 | -1.409700 |
| 8  | -0.965995 | -3.074445 | 1.306723  |
| 20 | -1.740662 | -3.102715 | -0.765175 |
| 20 | 1.125387  | -1.555200 | -2.735798 |
| 20 | 1.109519  | -3.144591 | 0.595432  |
| 20 | 1.805360  | -0.091101 | 2.774632  |
| 20 | 1.177542  | 1.620551  | -2.670503 |
| 20 | 1.207568  | 3.079711  | 0.718216  |
| 20 | -1.618131 | 1.544981  | 2.799508  |
| 20 | -1.642148 | 3.177323  | -0.641917 |
| 20 | -3.737052 | 0.055595  | 0.003881  |
| 20 | -1.673780 | -1.613452 | 2.740864  |
| 20 | -2.288406 | 0.088972  | -2.801021 |
| 21 | 3.195892  | -0.056969 | 0.030492  |
| 7  | 5.326935  | -0.070038 | -0.034900 |
| 6  | 6.516236  | 0.183146  | 0.010214  |
| 1  | 7.345920  | -0.559758 | -0.139701 |

#### HCN/VCa<sub>11</sub>O<sub>12</sub>

|    |           |           |           |
|----|-----------|-----------|-----------|
| 8  | -2.403174 | 0.005410  | -1.731036 |
| 8  | -2.469361 | 1.386967  | 1.068269  |
| 8  | 0.175983  | -0.004639 | 3.340049  |
| 8  | -0.404072 | 3.141542  | -1.373054 |
| 8  | 0.185836  | 0.005157  | -3.373259 |
| 8  | 2.965104  | -1.538730 | -1.382404 |
| 8  | 2.963595  | -0.004800 | 2.063957  |
| 8  | -0.407975 | -3.136212 | -1.381647 |
| 8  | 0.914404  | -3.068813 | 1.356528  |
| 8  | -2.468629 | -1.384559 | 1.063407  |
| 8  | 2.966834  | 1.538358  | -1.377978 |
| 8  | 0.917589  | 3.064038  | 1.365083  |
| 20 | 1.704701  | 3.155166  | -0.692138 |
| 20 | -1.122960 | 1.615478  | -2.684488 |
| 20 | -1.145418 | 3.137887  | 0.681462  |
| 20 | -1.873015 | -0.002394 | 2.825677  |

#### HCN/TiCa<sub>11</sub>O<sub>12</sub>

|    |           |           |           |
|----|-----------|-----------|-----------|
| 8  | -2.308077 | -0.219097 | -1.730104 |
| 8  | -2.474803 | 1.182916  | 1.068034  |
| 8  | 0.130473  | 0.022255  | 3.424153  |
| 8  | -0.594817 | 3.059941  | -1.443886 |
| 8  | 0.234181  | -0.034500 | -3.394807 |
| 8  | 3.080082  | -1.344303 | -1.300481 |
| 8  | 2.896544  | 0.220582  | 2.097189  |
| 8  | -0.143686 | -3.179634 | -1.375343 |
| 8  | 1.074052  | -2.997167 | 1.417249  |
| 8  | -2.345225 | -1.565488 | 1.128308  |
| 8  | 2.867413  | 1.719489  | -1.337278 |
| 8  | 0.640678  | 3.124126  | 1.344436  |
| 20 | 1.470159  | 3.243498  | -0.700680 |
| 20 | -1.210659 | 1.470902  | -2.736623 |
| 20 | -1.410681 | 3.036651  | 0.582424  |
| 20 | -1.891871 | -0.117953 | 2.752015  |
| 20 | -0.970169 | -1.735054 | -2.719408 |
| 20 | -0.962531 | -3.206018 | 0.645779  |
| 20 | 1.661367  | -1.449451 | 2.819048  |
| 20 | 1.923844  | -3.042223 | -0.625671 |
| 20 | 3.698864  | 0.256226  | 0.083723  |
| 20 | 1.423771  | 1.702772  | 2.782369  |
| 20 | 2.316340  | 0.125436  | -2.751598 |
| 22 | -3.060854 | -0.239794 | -0.051851 |
| 7  | -4.930575 | -0.161696 | -0.095511 |
| 6  | -6.113286 | 0.230011  | 0.001281  |
| 1  | -6.890629 | -0.581392 | -0.005703 |

#### HCN/CrCa<sub>11</sub>O<sub>12</sub>

|    |           |           |           |
|----|-----------|-----------|-----------|
| 8  | -2.391089 | -0.358103 | 1.434000  |
| 8  | -2.268109 | -1.237508 | -1.553268 |
| 8  | 0.447856  | 0.546223  | -3.392477 |
| 8  | -0.357757 | -3.351780 | 0.861556  |
| 8  | -0.052318 | -0.550556 | 3.360936  |
| 8  | 2.796706  | 1.378017  | 1.794164  |
| 8  | 3.093274  | 0.409720  | -1.817356 |
| 8  | -0.614050 | 2.846279  | 1.822808  |
| 8  | 0.862829  | 3.262747  | -0.822009 |
| 8  | -2.398969 | 1.514873  | -1.176933 |
| 8  | 2.918772  | -1.655283 | 1.307885  |
| 8  | 1.097660  | -2.781668 | -1.766047 |
| 20 | 1.762225  | -3.186778 | 0.307657  |
| 20 | -1.270391 | -2.051023 | 2.312135  |
| 20 | -1.006516 | -2.985521 | -1.189436 |
| 20 | -1.636279 | 0.387720  | -2.906561 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| 20 | -1.125101 | -1.604733 | -2.687890 |
| 20 | -1.148838 | -3.137358 | 0.673073  |
| 20 | 1.607987  | -1.588347 | 2.781922  |
| 20 | 1.700937  | -3.155830 | -0.701120 |
| 20 | 3.701571  | -0.002616 | 0.029514  |
| 20 | 1.609799  | 1.578589  | 2.786027  |
| 20 | 2.298407  | 0.002294  | -2.799580 |
| 23 | -2.994686 | 0.002841  | 0.001025  |
| 7  | -4.969310 | -0.002829 | -0.087845 |
| 6  | -6.131626 | -0.004709 | -0.111117 |
| 1  | -7.197735 | -0.009790 | -0.094427 |

|    |           |           |           |
|----|-----------|-----------|-----------|
| 20 | -1.397005 | 1.089749  | 2.786979  |
| 20 | -1.249806 | 3.122759  | -0.248941 |
| 20 | 1.733048  | 2.041221  | -2.387228 |
| 20 | 1.506751  | 3.040468  | 1.285580  |
| 20 | 3.703027  | 0.104334  | 0.243601  |
| 20 | 1.857064  | -1.076237 | -2.869061 |
| 20 | 2.068498  | -0.386462 | 2.901302  |
| 24 | -2.970432 | -0.048521 | -0.282537 |
| 7  | -4.740449 | -0.073209 | -0.069072 |
| 6  | -5.867974 | -0.116474 | 0.368735  |
| 1  | -6.809407 | 0.187505  | -0.094620 |

#### HCN/MnCa<sub>11</sub>O<sub>12</sub>

|    |           |           |           |
|----|-----------|-----------|-----------|
| 8  | -2.403298 | 0.001829  | 1.777205  |
| 8  | -2.381620 | -1.396696 | -1.239024 |
| 8  | 0.235175  | 0.006373  | -3.452533 |
| 8  | -0.407130 | -3.124800 | 1.393248  |
| 8  | 0.180301  | -0.006154 | 3.409727  |
| 8  | 2.974950  | 1.531559  | 1.393157  |
| 8  | 2.970644  | -0.001201 | -2.035051 |
| 8  | -0.396471 | 3.122076  | 1.404249  |
| 8  | 0.933444  | 3.078537  | -1.358702 |
| 8  | -2.378584 | 1.411282  | -1.235133 |
| 8  | 2.969899  | -1.546280 | 1.387738  |
| 8  | 0.922959  | -3.076538 | -1.369550 |
| 20 | 1.682096  | -3.149773 | 0.705165  |
| 20 | -1.172132 | -1.587846 | 2.695152  |
| 20 | -1.160301 | -3.092484 | -0.662871 |
| 20 | -1.830219 | 0.008862  | -2.809134 |
| 20 | -1.166225 | 1.583247  | 2.701228  |
| 20 | -1.149699 | 3.099314  | -0.652005 |
| 20 | 1.623718  | 1.579557  | -2.766022 |
| 20 | 1.692862  | 3.141999  | 0.716235  |
| 20 | 3.716471  | -0.006164 | 0.000566  |
| 20 | 1.617944  | -1.574476 | -2.771419 |
| 20 | 2.271332  | -0.008744 | 2.806544  |
| 25 | -2.919463 | 0.005834  | -0.033221 |
| 7  | -4.717104 | 0.001093  | 0.044086  |
| 6  | -5.887284 | -0.004850 | 0.103024  |
| 1  | -6.949054 | 0.005913  | 0.032351  |

#### HCN/CoCa<sub>11</sub>O<sub>12</sub>

|   |           |           |           |
|---|-----------|-----------|-----------|
| 8 | -2.377870 | -1.366807 | -1.140733 |
| 8 | -2.658618 | 1.474299  | 0.924145  |
| 8 | 0.426988  | 1.623197  | 3.027195  |
| 8 | -1.175566 | 1.940151  | -2.495019 |
| 8 | 0.043772  | -1.620855 | -2.998798 |
| 8 | 3.222805  | -1.481091 | -0.946914 |
| 8 | 3.027489  | 1.478758  | 1.382695  |
| 8 | 0.340022  | -3.511293 | 0.231984  |
| 8 | 1.708320  | -1.881447 | 2.442230  |
| 8 | -1.909896 | -1.092820 | 2.018146  |
| 8 | 2.470134  | 1.169492  | -2.321534 |
| 8 | 0.291984  | 3.452345  | -0.266226 |

#### HCN/FeCa<sub>11</sub>O<sub>12</sub>

|    |           |           |           |
|----|-----------|-----------|-----------|
| 8  | 1.916674  | 2.315037  | 0.000000  |
| 8  | -1.164556 | 2.418821  | 1.397869  |
| 8  | -3.474812 | -0.071858 | 0.000000  |
| 8  | 1.431015  | 0.336770  | 3.117031  |
| 8  | 3.420546  | -0.339258 | 0.000000  |
| 8  | 1.266718  | -3.032270 | -1.539068 |
| 8  | -2.161555 | -2.863856 | 0.000000  |
| 8  | 1.431015  | 0.336770  | -3.117031 |
| 8  | -1.393146 | -0.868177 | -3.075120 |
| 8  | -1.164556 | 2.418821  | -1.397869 |
| 8  | 1.266718  | -3.032270 | 1.539068  |
| 8  | -1.393146 | -0.868177 | 3.075120  |
| 20 | 0.641141  | -1.717141 | 3.144652  |
| 20 | 2.773378  | 1.037287  | 1.589686  |
| 20 | -0.596633 | 1.183656  | 3.075381  |
| 20 | -2.753966 | 1.980595  | 0.000000  |
| 20 | 2.773378  | 1.037287  | -1.589686 |
| 20 | -0.596633 | 1.183656  | -3.075381 |
| 20 | -2.836824 | -1.478326 | -1.574437 |
| 20 | 0.641141  | -1.717141 | -3.144652 |
| 20 | -0.163157 | -3.701093 | 0.000000  |
| 20 | -2.836824 | -1.478326 | 1.574437  |
| 20 | 2.711589  | -2.399428 | 0.000000  |
| 26 | 0.123779  | 2.831289  | 0.000000  |
| 7  | 0.155342  | 4.612730  | 0.000000  |
| 6  | 0.107581  | 5.772986  | 0.000000  |
| 1  | 0.069745  | 6.836105  | 0.000000  |

#### HCN/NiCa<sub>11</sub>O<sub>12</sub>

|   |           |           |           |
|---|-----------|-----------|-----------|
| 8 | -3.074464 | 0.119152  | -0.286734 |
| 8 | -1.240047 | 2.055143  | 1.898829  |
| 8 | 1.977217  | 0.665214  | 2.938219  |
| 8 | -0.783000 | 2.825908  | -1.685925 |
| 8 | -1.474335 | -0.648938 | -2.834773 |
| 8 | 1.851900  | -2.263000 | -2.054817 |
| 8 | 3.633765  | -0.114172 | 0.451029  |
| 8 | -1.176422 | -3.164862 | -0.117453 |
| 8 | 1.336420  | -2.848676 | 1.609883  |
| 8 | -1.409682 | -0.588757 | 2.517667  |
| 8 | 2.043659  | 0.697175  | -2.846141 |
| 8 | 1.751529  | 3.101897  | 0.020815  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| 20 | 0.889250  | 2.649439  | -2.233550 |
| 20 | -1.588822 | -0.155404 | -2.810162 |
| 20 | -1.788825 | 2.783299  | -0.561076 |
| 20 | -1.617184 | 0.943391  | 2.744862  |
| 20 | -0.857845 | -2.917332 | -1.461435 |
| 20 | -0.349952 | -2.586601 | 2.094602  |
| 20 | 2.104730  | 0.196703  | 2.920405  |
| 20 | 2.393946  | -2.804805 | 0.556726  |
| 20 | 3.631995  | 0.641263  | -0.524006 |
| 20 | 1.383052  | 2.937559  | 1.536651  |
| 20 | 2.100818  | -0.956385 | -2.773986 |
| 27 | -2.859606 | -0.440219 | 0.451386  |
| 7  | -4.791462 | -0.324095 | 0.043402  |
| 6  | -5.927722 | -0.281437 | -0.139970 |
| 1  | -6.983833 | -0.250803 | -0.289394 |

#### HCN/CuCa11O12

|    |           |           |           |
|----|-----------|-----------|-----------|
| 8  | -3.073906 | 0.010928  | -0.205124 |
| 8  | -1.272540 | 1.520095  | 2.341319  |
| 8  | 2.023617  | 0.078146  | 2.958601  |
| 8  | -0.968246 | 3.080635  | -0.982937 |
| 8  | -1.510344 | -0.078018 | -2.860841 |
| 8  | 1.910877  | -1.628571 | -2.554442 |
| 8  | 3.651288  | -0.012016 | 0.340181  |
| 8  | -0.999990 | -3.127110 | -0.791526 |
| 8  | 1.561085  | -3.076688 | 0.889292  |
| 8  | -1.301391 | -1.336587 | 2.418666  |
| 8  | 1.931042  | 1.440376  | -2.650330 |
| 8  | 1.597783  | 3.115243  | 0.692362  |
| 20 | 1.182913  | 3.094780  | -1.475900 |
| 20 | -2.325475 | 1.564204  | -1.667250 |
| 20 | -0.541646 | 3.187961  | 1.159804  |
| 20 | -0.069063 | 0.110614  | 3.490917  |
| 20 | -2.336449 | -1.635993 | -1.565658 |
| 20 | -0.580264 | -3.085514 | 1.353935  |
| 20 | 2.863622  | -1.543042 | 1.709505  |
| 20 | 1.150882  | -3.199098 | -1.276740 |
| 20 | 3.278886  | -0.077622 | -1.793585 |
| 20 | 2.872099  | 1.610367  | 1.606376  |
| 20 | 0.589961  | -0.111726 | -3.447149 |
| 29 | -2.114888 | 0.075708  | 1.422736  |
| 7  | -6.997778 | -0.041115 | -0.028400 |
| 6  | -5.845825 | -0.016753 | 0.041108  |
| 1  | -4.712357 | 0.002662  | 0.045959  |

|    |           |           |           |
|----|-----------|-----------|-----------|
| 20 | 1.375660  | 2.613550  | -2.100948 |
| 20 | -2.204033 | 1.254607  | -2.046531 |
| 20 | -0.387212 | 3.375392  | 0.389864  |
| 20 | -0.118248 | 0.934943  | 3.375662  |
| 20 | -2.413672 | -1.821389 | -1.244573 |
| 20 | -0.810538 | -2.603421 | 1.957005  |
| 20 | 2.717651  | -1.244683 | 2.101058  |
| 20 | 0.976721  | -3.461971 | -0.483004 |
| 20 | 3.285949  | -0.647430 | -1.620654 |
| 20 | 2.935048  | 1.794405  | 1.291119  |
| 20 | 0.635214  | -0.928058 | -3.312289 |
| 28 | -2.097554 | 0.551982  | 1.245423  |
| 7  | -6.984389 | -0.017678 | 0.171457  |
| 6  | -5.835143 | 0.084640  | 0.141796  |
| 1  | -4.710008 | 0.152822  | 0.058226  |

#### HCN/ZnCa11O12

|    |           |           |           |
|----|-----------|-----------|-----------|
| 8  | 2.353679  | -0.019433 | -1.845786 |
| 8  | 2.322040  | -1.538718 | 1.252461  |
| 8  | -0.227556 | -0.024763 | 3.441263  |
| 8  | 0.284514  | -3.138450 | -1.429243 |
| 8  | -0.270077 | 0.025304  | -3.405005 |
| 8  | -3.023971 | 1.585315  | -1.352553 |
| 8  | -2.985065 | 0.022343  | 2.062313  |
| 8  | 0.367183  | 3.144555  | -1.385637 |
| 8  | -0.950385 | 3.103321  | 1.390337  |
| 8  | 2.360775  | 1.453941  | 1.273744  |
| 8  | -3.063623 | -1.492684 | -1.373736 |
| 8  | -1.031517 | -3.101554 | 1.347628  |
| 20 | -1.798805 | -3.128629 | -0.721374 |
| 20 | 1.064938  | -1.585547 | -2.710960 |
| 20 | 1.051784  | -3.164670 | 0.630333  |
| 20 | 1.838782  | -0.046589 | 2.775451  |
| 20 | 1.106238  | 1.590634  | -2.689971 |
| 20 | 1.134200  | 3.122078  | 0.674244  |
| 20 | -1.601200 | 1.575365  | 2.786143  |
| 20 | -1.716156 | 3.177631  | -0.677881 |
| 20 | -3.764039 | 0.045943  | 0.039884  |
| 20 | -1.643422 | -1.577636 | 2.764815  |
| 20 | -2.354390 | 0.047220  | -2.783630 |
| 30 | 2.679436  | -0.038359 | 0.018779  |
| 7  | 5.372207  | -0.040277 | -0.039354 |
| 6  | 6.502044  | 0.015721  | -0.235646 |
| 1  | 7.552636  | 0.068940  | -0.421372 |

**Table S3.**

The electronic configuration, orbital diagram, spin multiplicity and total electronic energy of free TM in the low-spin state and  $\text{TMCa}_{11}\text{O}_{12}$  at B3LYP/6-311+G(D)D3 level of theory

| Electronic configuration                              |                                  |                   | Orbital diagram | Spin multiplicity | Energy (E <sub>h</sub> )                                                                      | TMCa <sub>11</sub> O <sub>12</sub> |
|-------------------------------------------------------|----------------------------------|-------------------|-----------------|-------------------|-----------------------------------------------------------------------------------------------|------------------------------------|
| <sup>21</sup> Sc[Ar] 3d <sup>1</sup> 4s <sup>2</sup>  | 3d <sup>3</sup>                  | ↓↑ ↑              | doublet         | -760.620460       | [core]4S <sup>( 0.46)</sup> 3d <sup>( 1.09)</sup> 4p <sup>( 0.25)</sup> 4d <sup>( 0.04)</sup> |                                    |
| <sup>22</sup> Ti[Ar] 3d <sup>2</sup> 4s <sup>2</sup>  | 3d <sup>4</sup>                  | ↓↑ ↓↑             | singlet         | -849.290003       | [core]4S <sup>(0.63)</sup> 3d <sup>(2.26)</sup> 4p <sup>(0.26)</sup> 4d <sup>(0.04)</sup>     |                                    |
| <sup>23</sup> V[Ar] 3d <sup>3</sup> 4s <sup>2</sup>   | 3d <sup>5</sup>                  | ↓↑ ↓↑ ↑           | doublet         | -943.828778       | [core]4S <sup>(0.17)</sup> 3d <sup>(2.53)</sup> 4p <sup>(0.15)</sup> 4d <sup>(0.02)</sup>     |                                    |
| <sup>24</sup> Cr[Ar] 3d <sup>5</sup> 4s <sup>1</sup>  | 3d <sup>6</sup>                  | ↓↑ ↑↑↑↑           | triplet         | -1044.223886      | [core]4S <sup>(0.50)</sup> 3d <sup>(4.59)</sup> 4p <sup>(0.30)</sup> 4d <sup>(0.02)</sup>     |                                    |
| <sup>25</sup> Mn[Ar] 3d <sup>5</sup> 4s <sup>2</sup>  | 3d <sup>7</sup>                  | ↓↑ ↓↑ ↑↑↑         | doublet         | -1150.827718      | [core]4S <sup>(0.15)</sup> 3d <sup>(4.22)</sup> 4p <sup>(0.16)</sup> 4d <sup>(0.01)</sup>     |                                    |
| <sup>26</sup> Fe[Ar] 3d <sup>6</sup> 4s <sup>2</sup>  | 3d <sup>8</sup>                  | ↓↑ ↓↑ ↓↑ ↑↑       | triplet         | -1263.521952      | [core]4S <sup>(0.30)</sup> 3d <sup>(6.57)</sup> 4p <sup>(0.29)</sup>                          |                                    |
| <sup>27</sup> Co[Ar] 3d <sup>7</sup> 4s <sup>2</sup>  | 3d <sup>9</sup>                  | ↓↑ ↓↑ ↓↑ ↓↑ ↑     | doublet         | -1382.693183      | [core]4S <sup>(0.29)</sup> 3d <sup>(7.45)</sup> 4p <sup>(0.30)</sup> 4d <sup>(0.01)</sup>     |                                    |
| <sup>28</sup> Ni[Ar] 3d <sup>8</sup> 4s <sup>2</sup>  | 3d <sup>10</sup>                 | ↓↑ ↓↑ ↓↑ ↓↑ ↓↑    | singlet         | -1508.200249      | [core]4S <sup>(0.30)</sup> 3d <sup>(8.54)</sup> 4p <sup>(0.30)</sup>                          |                                    |
| <sup>29</sup> Cu[Ar] 3d <sup>10</sup> 4s <sup>1</sup> | 3d <sup>10</sup> 4s <sup>1</sup> | ↓↑ ↓↑ ↓↑ ↓↑ ↓↑ ↑  | doublet         | -1640.472257      | [core]4S <sup>(0.28)</sup> 3d <sup>(9.32)</sup> 4p <sup>(0.32)</sup>                          |                                    |
| <sup>30</sup> Zn[Ar] 3d <sup>10</sup> 4s <sup>2</sup> | 3d <sup>10</sup> 4s <sup>2</sup> | ↓↑ ↓↑ ↓↑ ↓↑ ↓↑ ↓↑ | singlet         | -1779.353534      | [core]4S <sup>(0.33)</sup> 3d <sup>(9.96)</sup> 4p <sup>(0.37)</sup>                          |                                    |

**Table S4.**

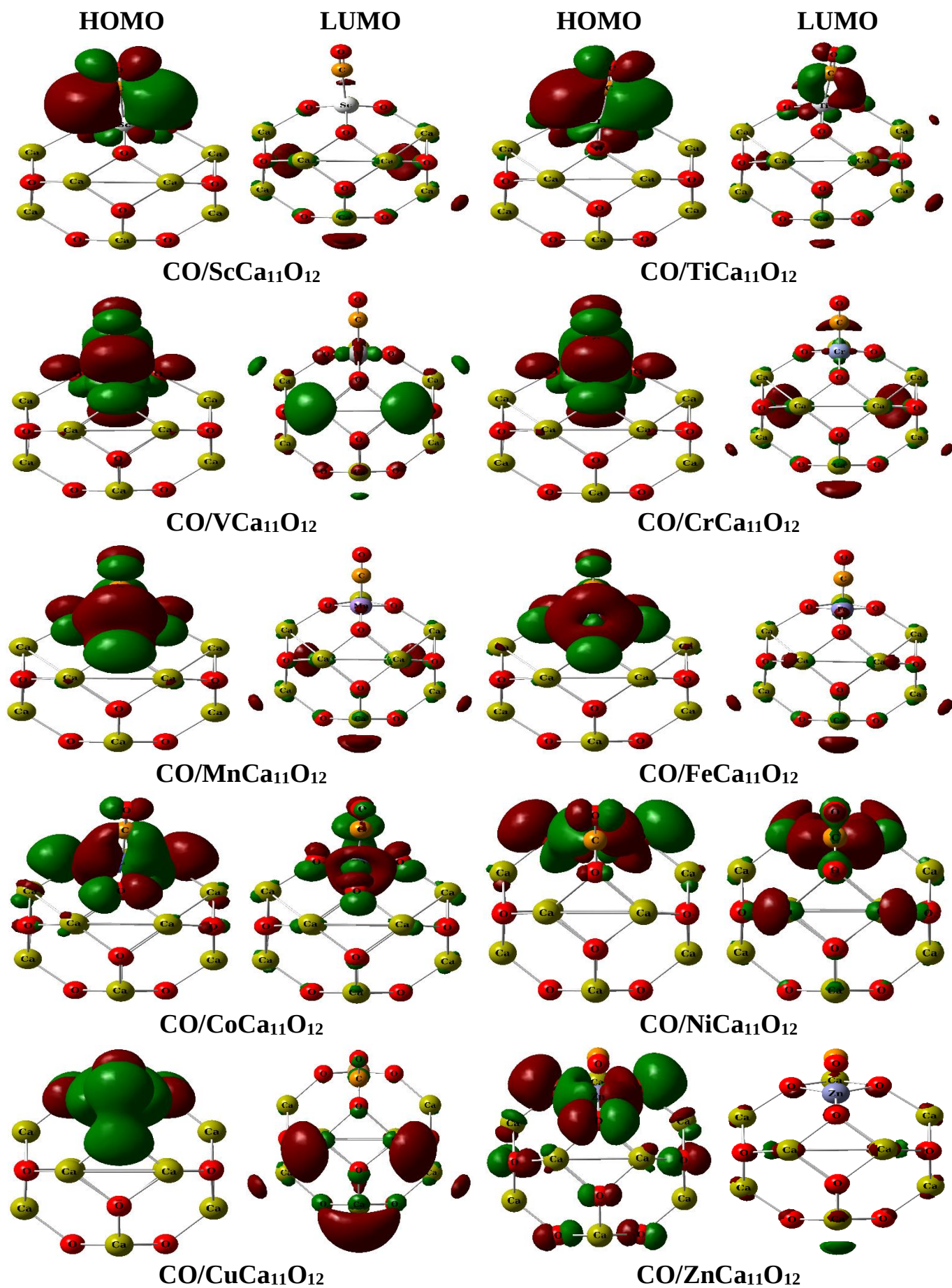
NBO charges ( $Q$ ,  $|e|$ ), for (CO, NO, HCN), gas/  $\text{Ca}_{12}\text{O}_{12}$  and gas/TM $\text{Ca}_{11}\text{O}_{12}$  systems at B3LYP/6-311+G(D)D3 level of theory.

| System                                 | Q <sub>site</sub> | Q <sub>C</sub> | Q <sub>O</sub> | Q <sub>CO</sub> |                  |
|----------------------------------------|-------------------|----------------|----------------|-----------------|------------------|
| CO                                     | ---               | 0.478          | -0.478         | 0.000           |                  |
| CO/Ca <sub>12</sub> O <sub>12</sub>    | 0.316             | 0.217          | -0.533         | -0.316          |                  |
| CO/ScCa <sub>11</sub> O <sub>12</sub>  | 0.162             | 0.372          | -0.534         | -0.162          |                  |
| CO/TiCa <sub>11</sub> O <sub>12</sub>  | -0.139            | 0.601          | -0.462         | 0.139           |                  |
| CO/VCa <sub>11</sub> O <sub>12</sub>   | -0.015            | 0.605          | -0.590         | 0.015           |                  |
| CO/CrCa <sub>11</sub> O <sub>12</sub>  | -0.119            | 0.680          | -0.561         | 0.119           |                  |
| CO/MnCa <sub>11</sub> O <sub>12</sub>  | -0.204            | 0.736          | -0.532         | 0.204           |                  |
| CO/FeCa <sub>11</sub> O <sub>12</sub>  | -0.168            | 0.644          | -0.476         | 0.168           |                  |
| CO/CoCa <sub>11</sub> O <sub>12</sub>  | -0.038            | 0.664          | -0.626         | 0.038           |                  |
| CO/NiCa <sub>11</sub> O <sub>12</sub>  | 0.048             | 0.561          | -0.609         | -0.048          |                  |
| CO/CuCa <sub>11</sub> O <sub>12</sub>  | -0.002            | 0.510          | -0.508         | 0.002           |                  |
| CO/ZnCa <sub>11</sub> O <sub>12</sub>  | 0.316             | 0.217          | -0.533         | -0.316          |                  |
| System                                 | Q <sub>site</sub> | Q <sub>N</sub> | Q <sub>O</sub> | Q <sub>NO</sub> |                  |
| NO                                     | ---               | 0.186          | -0.186         | 0.000           |                  |
| NO/Ca <sub>12</sub> O <sub>12</sub>    | 0.461             | -0.150         | -0.311         | -0.461          |                  |
| NO/ScCa <sub>11</sub> O <sub>12</sub>  | 0.319             | -0.055         | -0.264         | -0.319          |                  |
| NO/TiCa <sub>11</sub> O <sub>12</sub>  | 0.404             | 0.102          | -0.506         | -0.404          |                  |
| NO/VCa <sub>11</sub> O <sub>12</sub>   | 0.253             | 0.164          | -0.417         | -0.253          |                  |
| NO/CrCa <sub>11</sub> O <sub>12</sub>  | 0.113             | 0.282          | -0.395         | -0.113          |                  |
| NO/MnCa <sub>11</sub> O <sub>12</sub>  | 0.203             | 0.105          | -0.308         | -0.203          |                  |
| NO/FeCa <sub>11</sub> O <sub>12</sub>  | 0.211             | 0.154          | -0.365         | -0.211          |                  |
| NO/CoCa <sub>11</sub> O <sub>12</sub>  | -0.022            | 0.202          | -0.180         | 0.022           |                  |
| NO/NiCa <sub>11</sub> O <sub>12</sub>  | -0.099            | 0.253          | -0.154         | 0.099           |                  |
| NO/CuCa <sub>11</sub> O <sub>12</sub>  | -0.026            | 0.250          | -0.224         | 0.026           |                  |
| NO/ZnCa <sub>11</sub> O <sub>12</sub>  | 0.460             | -0.150         | -0.310         | -0.460          |                  |
| System                                 | Q <sub>site</sub> | Q <sub>H</sub> | Q <sub>C</sub> | Q <sub>N</sub>  | Q <sub>HCN</sub> |
| HCN                                    | ----              | 0.217          | 0.095          | -0.312          | 0.000            |
| HCN/Ca <sub>12</sub> O <sub>12</sub>   | 0.639             | -0.722         | -0.020         | 0.103           | -0.639           |
| HCN/ScCa <sub>11</sub> O <sub>12</sub> | 0.509             | -0.612         | -0.015         | 0.118           | -0.509           |
| HCN/TiCa <sub>11</sub> O <sub>12</sub> | -0.024            | -0.343         | 0.140          | 0.227           | 0.024            |
| HCN/VCa <sub>11</sub> O <sub>12</sub>  | 0.361             | -0.367         | -0.157         | 0.163           | -0.361           |
| HCN/CrCa <sub>11</sub> O <sub>12</sub> | 0.083             | -0.273         | -0.022         | 0.212           | -0.083           |
| HCN/MnCa <sub>11</sub> O <sub>12</sub> | -0.036            | -0.226         | 0.044          | 0.217           | 0.036            |
| HCN/FeCa <sub>11</sub> O <sub>12</sub> | -0.064            | -0.287         | 0.133          | 0.218           | 0.064            |
| HCN/CoCa <sub>11</sub> O <sub>12</sub> | 0.085             | -0.416         | 0.061          | 0.270           | -0.085           |
| HCN/NiCa <sub>11</sub> O <sub>12</sub> | 0.086             | -0.416         | 0.060          | 0.270           | -0.086           |
| HCN/CuCa <sub>11</sub> O <sub>12</sub> | -0.038            | -0.302         | 0.125          | 0.215           | 0.038            |
| HCN/ZnCa <sub>11</sub> O <sub>12</sub> | 0.639             | -0.722         | -0.020         | 0.103           | -0.639           |

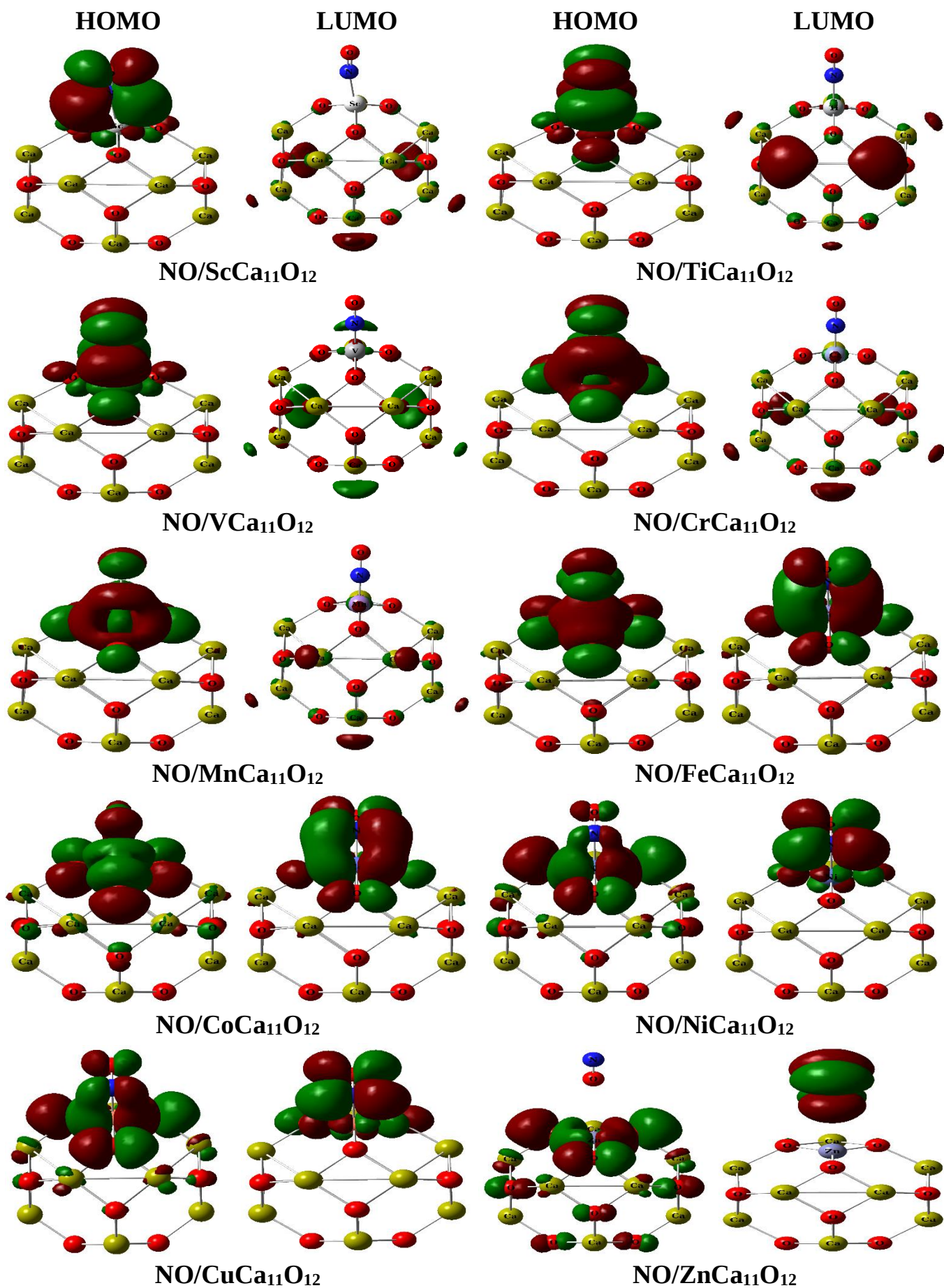
**Table S5.**

The electronic configuration of TM, TMCa<sub>11</sub>O<sub>12</sub>, NO/TMCa<sub>11</sub>O<sub>12</sub>, TMCO/Ca<sub>11</sub>O<sub>12</sub> and HCN/TMCa<sub>11</sub>O<sub>12</sub> nanocages obtained from the natural bond orbital analysis (NBO) at B3LYP/6-311+G(D)D3 level of theory.

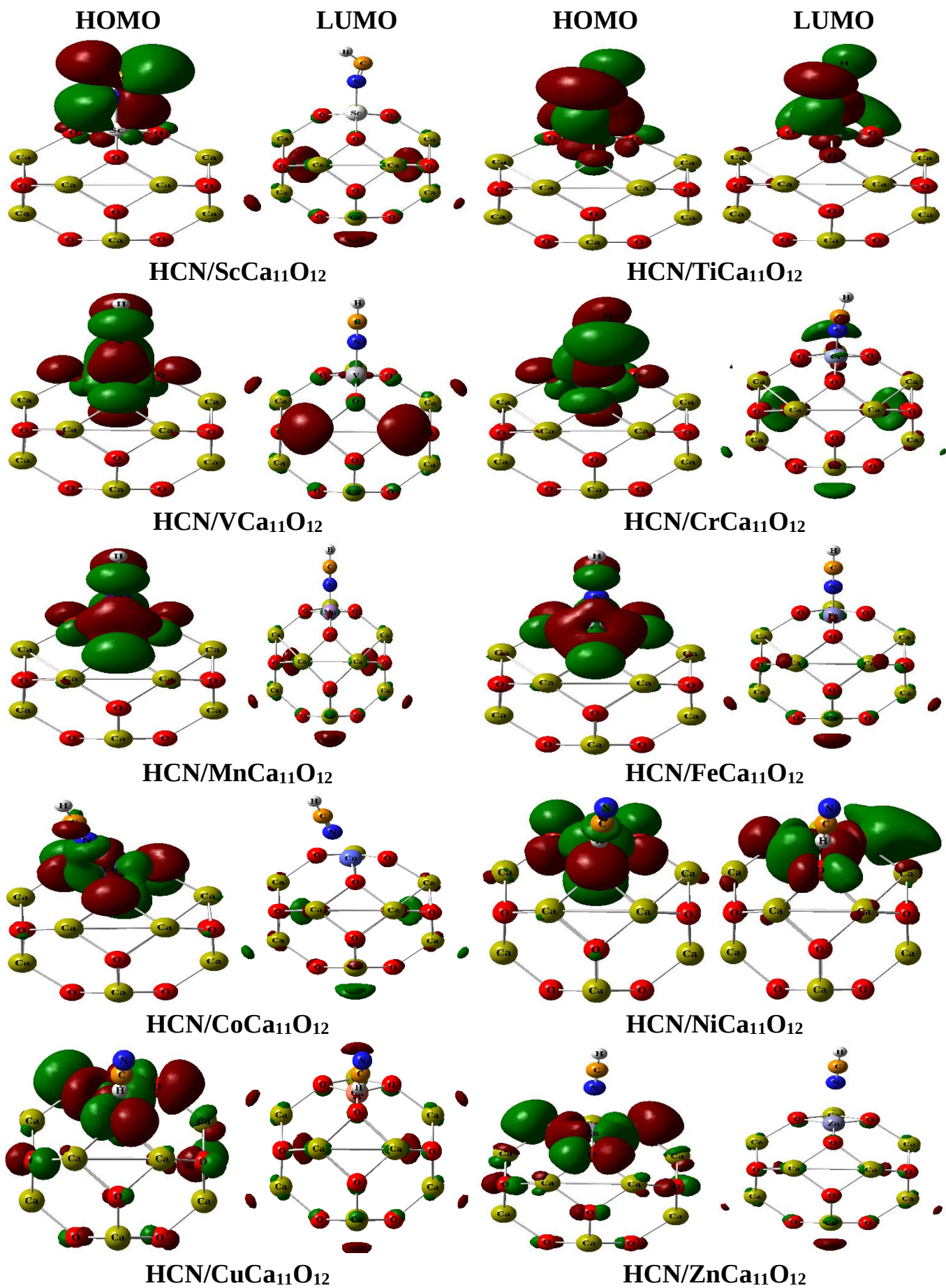
| Electronic Configuration |                                      |                                                                                                                |                                                                                           |                                                                                                                                     |
|--------------------------|--------------------------------------|----------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------|
| TM                       |                                      | NO/TMCa <sub>11</sub> O <sub>12</sub>                                                                          | CO/TMCa <sub>11</sub> O <sub>12</sub>                                                     | HCN/TMCa <sub>11</sub> O <sub>12</sub>                                                                                              |
| Sc                       | [Ar]3d <sup>1</sup> 4s <sup>2</sup>  | [core]3d <sup>(1.23)</sup> 4p <sup>(0.37)</sup> 5S <sup>(0.12)</sup> 4d <sup>(0.05)</sup>                      | [core]4S <sup>(0.15)</sup> 3d <sup>(1.27)</sup> 4p <sup>(0.44)</sup> 4d <sup>(0.05)</sup> | [core]4S <sup>(0.12)</sup> 3d <sup>(1.10)</sup> 4p <sup>(0.32)</sup> 4d <sup>(0.05)</sup>                                           |
| Ti                       | [Ar]3d <sup>2</sup> 4s <sup>2</sup>  | [core]4S <sup>(0.16)</sup> 3d <sup>(2.31)</sup> 4p <sup>(0.46)</sup> 4d <sup>(0.05)</sup> 5p <sup>(0.01)</sup> | [core]3d <sup>(1.27)</sup> 4p <sup>(0.26)</sup> 5S <sup>(0.10)</sup> 4d <sup>(0.02)</sup> | [core]4S <sup>(0.17)</sup> 3d <sup>(2.24)</sup> 4p <sup>(0.41)</sup> 4d <sup>(0.05)</sup>                                           |
| V                        | [Ar]3d <sup>3</sup> 4s <sup>2</sup>  | [core]4S <sup>(0.17)</sup> 3d <sup>(3.61)</sup> 4p <sup>(0.49)</sup> 4d <sup>(0.03)</sup>                      | [core]3d <sup>(2.44)</sup> 4p <sup>(0.29)</sup> 5S <sup>(0.10)</sup> 4d <sup>(0.03)</sup> | [core]4S <sup>(0.16)</sup> 3d <sup>(3.37)</sup> 4p <sup>(0.43)</sup> 4d <sup>(0.06)</sup> 5p <sup>(0.01)</sup>                      |
| Cr                       | [Ar]3d <sup>5</sup> 4s <sup>1</sup>  | [core]3d <sup>(2.44)</sup> 4p <sup>(0.27)</sup> 5S <sup>(0.10)</sup> 4d <sup>(0.02)</sup>                      | [core]4S <sup>(0.23)</sup> 3d <sup>(4.84)</sup> 4p <sup>(0.54)</sup> 4d <sup>(0.02)</sup> | [core]3d <sup>(4.55)</sup> 4p <sup>(0.43)</sup> 5S <sup>(0.18)</sup> 4d <sup>(0.02)</sup> 5p <sup>(0.01)</sup> 6S <sup>(0.01)</sup> |
| Mn                       | [Ar]3d <sup>5</sup> 4s <sup>2</sup>  | [core]4S <sup>(0.22)</sup> 3d <sup>(5.69)</sup> 4p <sup>(0.54)</sup> 4d <sup>(0.02)</sup>                      | [core]4S <sup>(0.25)</sup> 3d <sup>(5.78)</sup> 4p <sup>(0.56)</sup> 4d <sup>(0.02)</sup> | [core]4S <sup>(0.19)</sup> 3d <sup>(5.57)</sup> 4p <sup>(0.43)</sup> 4d <sup>(0.01)</sup>                                           |
| Fe                       | [Ar]3d <sup>6</sup> 4s <sup>2</sup>  | [core]3d <sup>(3.92)</sup> 4p <sup>(0.26)</sup> 5S <sup>(0.10)</sup>                                           | [core]4S <sup>(0.27)</sup> 3d <sup>(6.78)</sup> 4p <sup>(0.57)</sup> 4d <sup>(0.01)</sup> | [core]3d <sup>(6.58)</sup> 4p <sup>(0.46)</sup> 5S <sup>(0.20)</sup> 4d <sup>(0.01)</sup> 5p <sup>(0.01)</sup>                      |
| Co                       | [Ar]3d <sup>7</sup> 4s <sup>2</sup>  | [core]3d <sup>(7.49)</sup> 4p <sup>(0.50)</sup> 5S <sup>(0.22)</sup> 4d <sup>(0.01)</sup>                      | [core]4S <sup>(0.26)</sup> 3d <sup>(7.50)</sup> 4p <sup>(0.60)</sup> 4d <sup>(0.01)</sup> | [core]4S <sup>(0.21)</sup> 3d <sup>(7.52)</sup> 4p <sup>(0.43)</sup> 4d <sup>(0.01)</sup>                                           |
| Ni                       | [Ar]3d <sup>8</sup> 4s <sup>2</sup>  | [core]4S <sup>(0.25)</sup> 3d <sup>(8.32)</sup> 4p <sup>(0.52)</sup> 4d <sup>(0.01)</sup>                      | [core]4S <sup>(0.36)</sup> 3d <sup>(8.79)</sup> 4p <sup>(0.36)</sup> 4d <sup>(0.01)</sup> | [core]4S <sup>(0.29)</sup> 3d <sup>(8.54)</sup> 4p <sup>(0.29)</sup>                                                                |
| Cu                       | [Ar]3d <sup>10</sup> 4s <sup>1</sup> | [core]3d <sup>(9.36)</sup> 4p <sup>(0.53)</sup> 5S <sup>(0.27)</sup> 4d <sup>(0.01)</sup>                      | [core]4S <sup>(0.38)</sup> 3d <sup>(9.54)</sup> 4p <sup>(0.36)</sup>                      | [core]4S <sup>(0.13)</sup> 3d <sup>(4.96)</sup> 4p <sup>(0.15)</sup>                                                                |
| Zn                       | [Ar]3d <sup>10</sup> 4s <sup>2</sup> | [core]4S <sup>(0.32)</sup> 3d <sup>(9.96)</sup> 4p <sup>(0.37)</sup>                                           | [core]4S <sup>(0.32)</sup> 3d <sup>(9.96)</sup> 4p <sup>(0.38)</sup> 6p <sup>(0.01)</sup> | [core]4S <sup>(0.30)</sup> 3d <sup>(9.97)</sup> 4p <sup>(0.39)</sup> 5p <sup>(0.01)</sup>                                           |



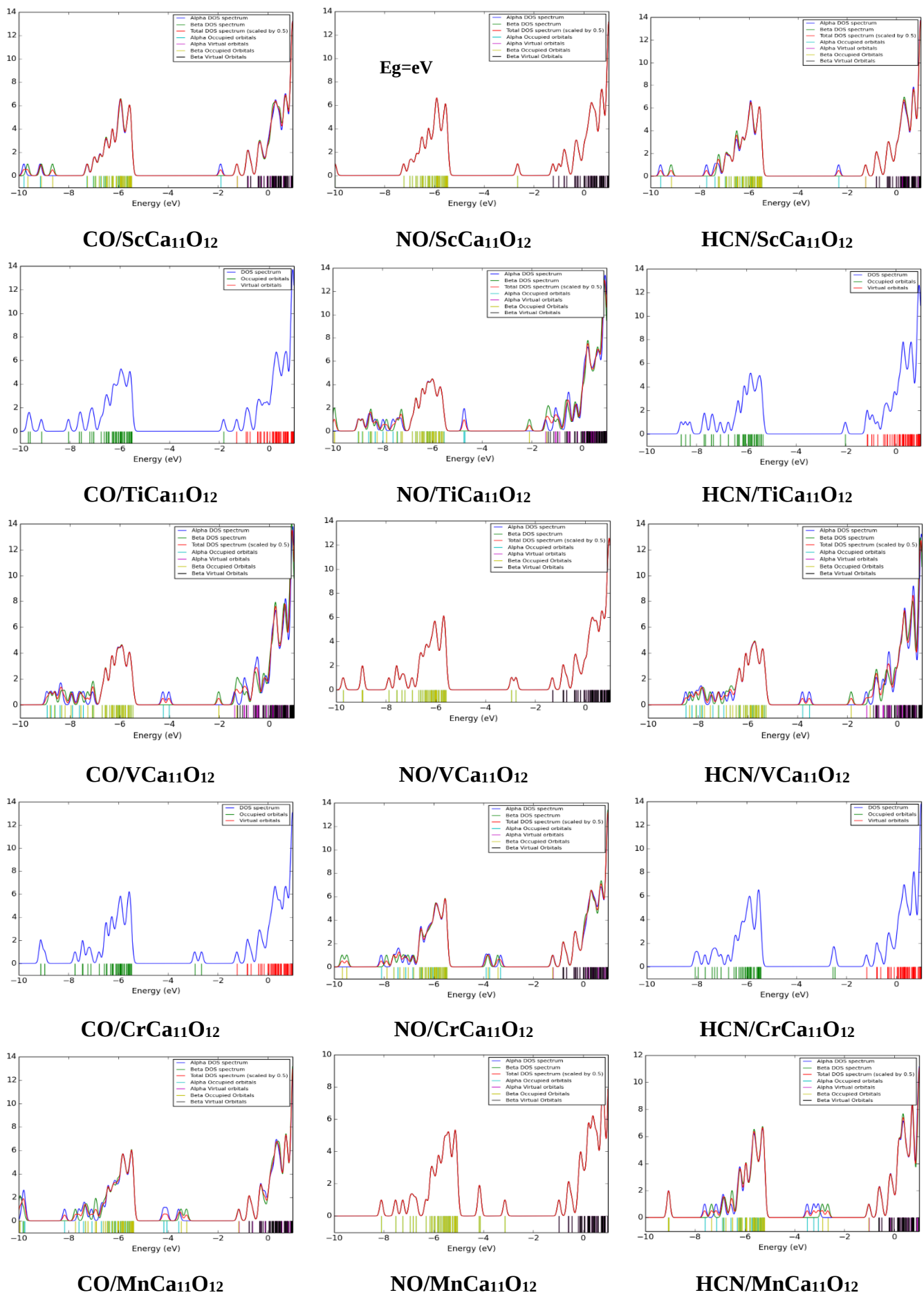
**Fig. S1** HOMO-LUMO plot (isodensity contours = 0.2 a.u) of CO/TM<sub>11</sub>Ca<sub>11</sub>O<sub>12</sub> (TM = Sc to Zn).



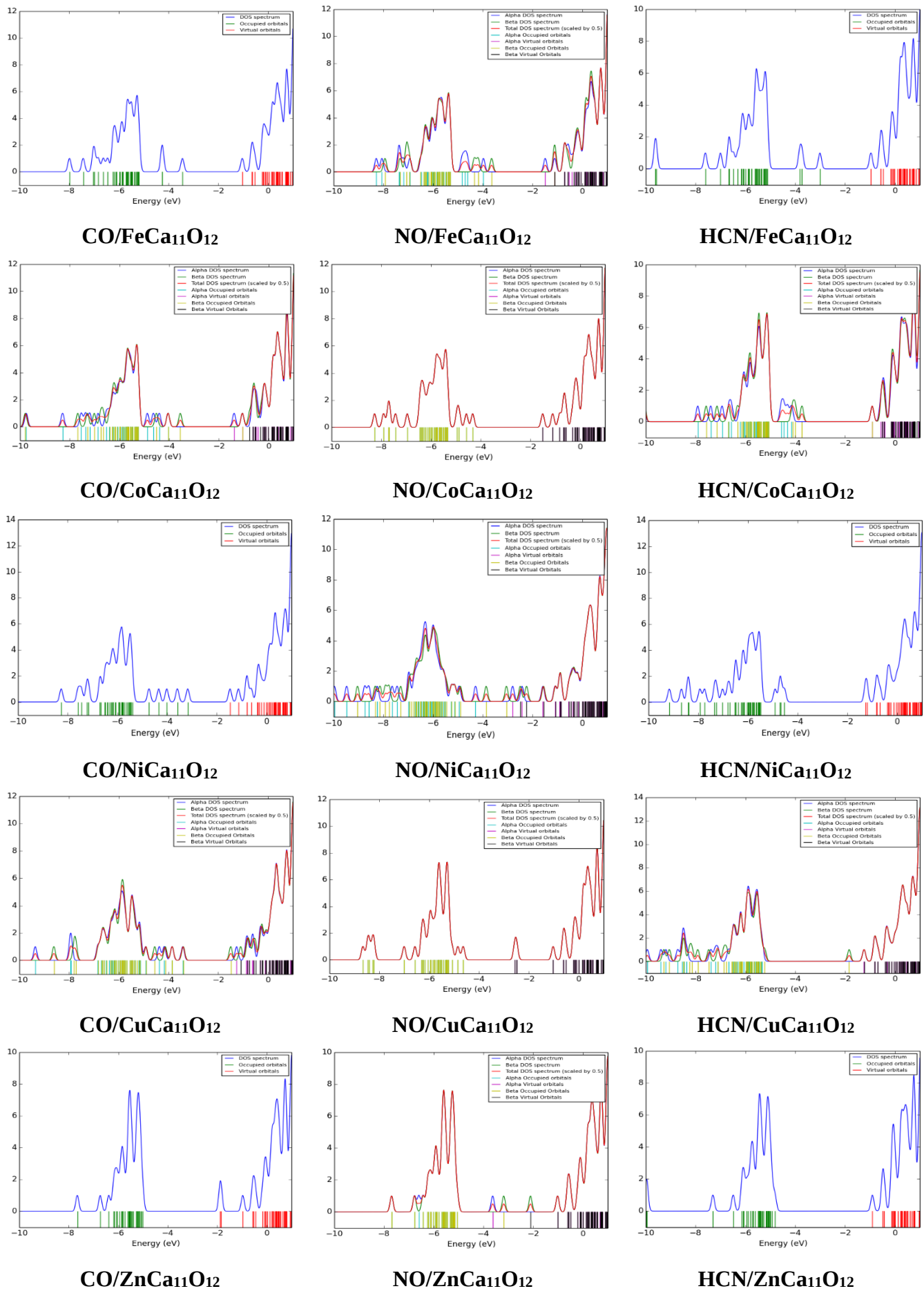
**Fig. S2** HOMO-LUMO plot (isodensity contours = 0.2 a.u) of NO-TMCa<sub>11</sub>O<sub>12</sub> (TM = Sc to Zn).



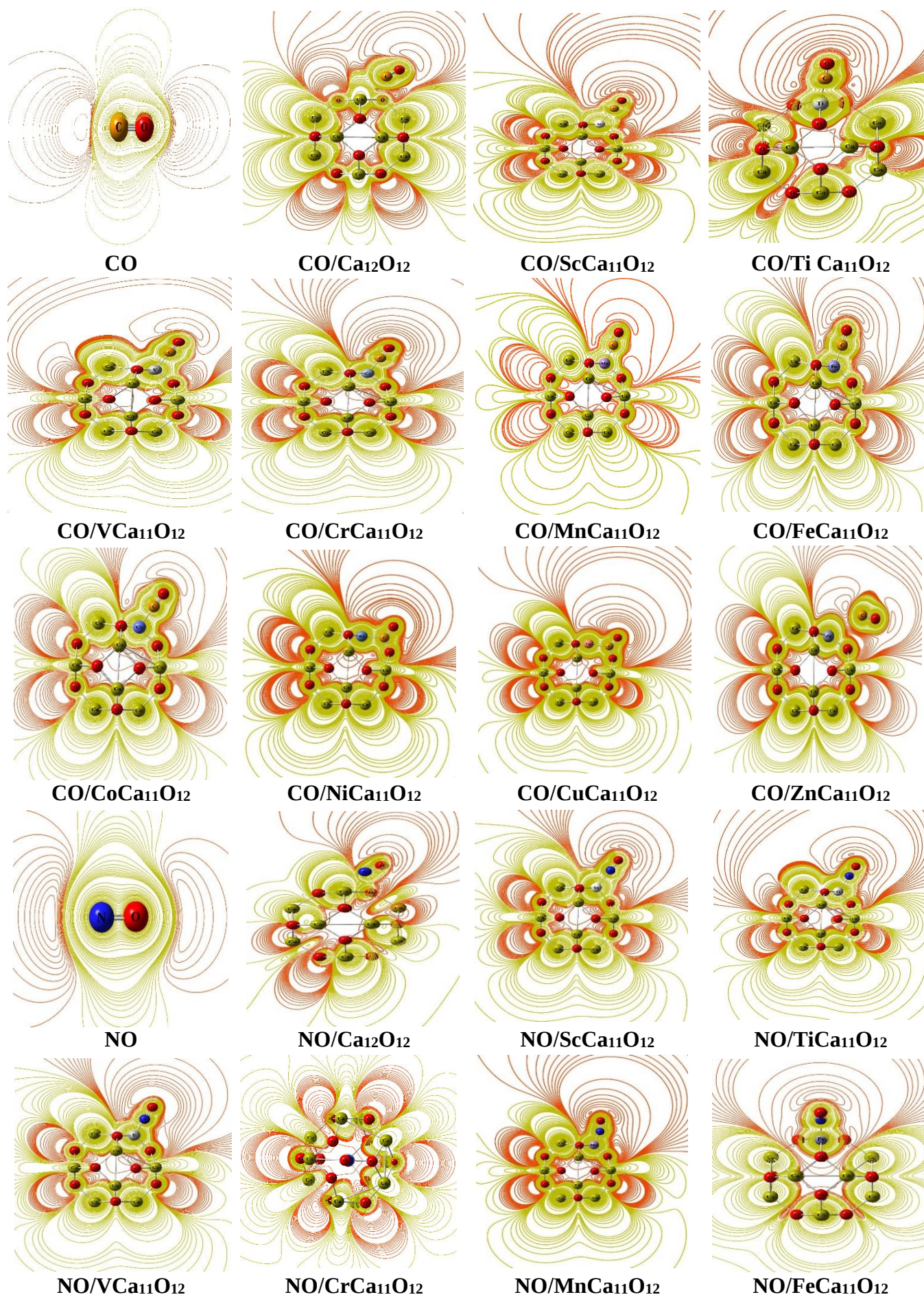
**Fig. S3.** HOMO-LUMO plot (isodensity contours = 0.2 a.u) of HCN/TMCA<sub>11</sub>O<sub>12</sub> (TM = Sc-Zn).



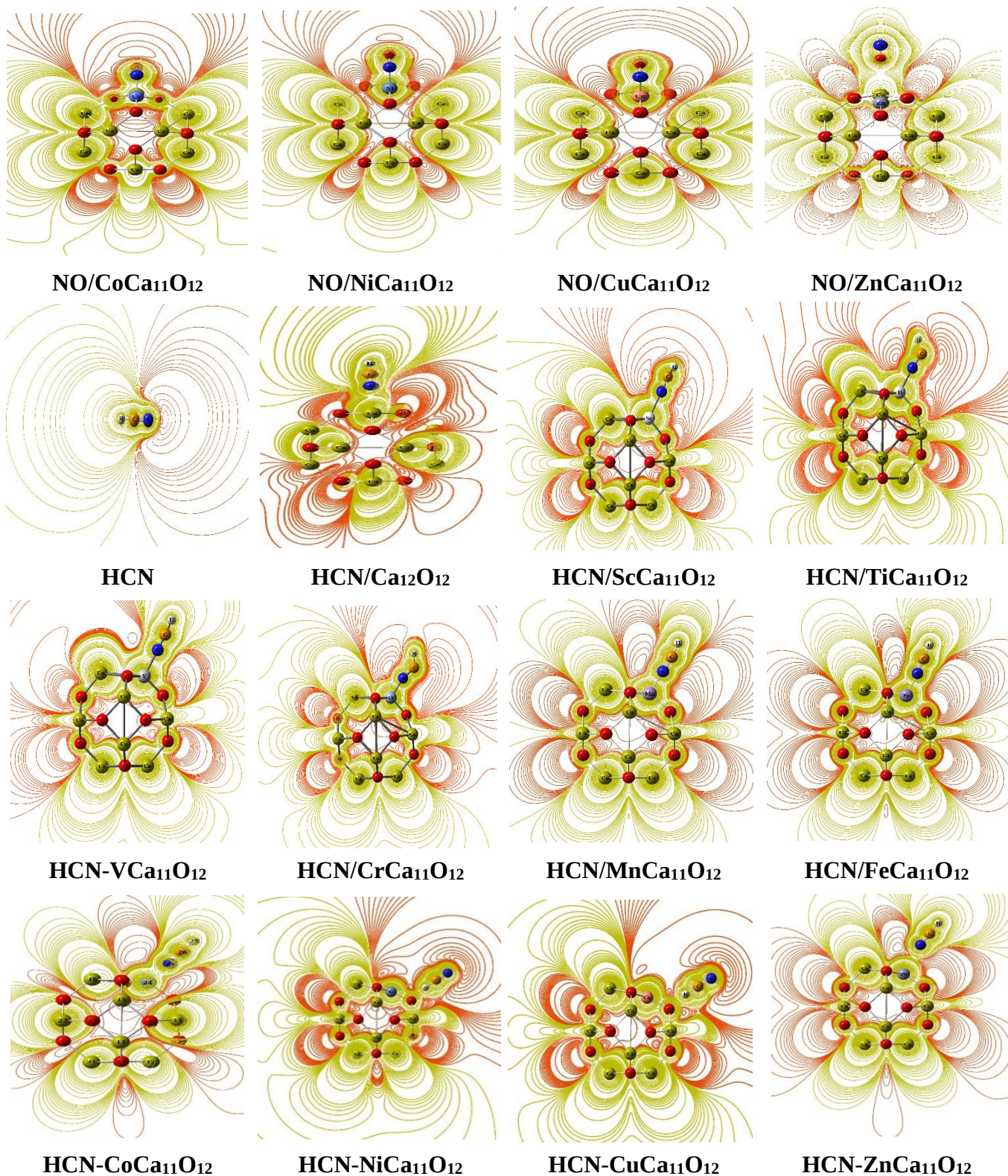
**Fig. S4** Density of states (DOS) of NO/TMCA<sub>11</sub>O<sub>12</sub>, CO/TMCA<sub>11</sub>O<sub>12</sub> and HCN/TMCA<sub>11</sub>O<sub>12</sub> (TM = Sc, V, Ti, Cr, Mn).



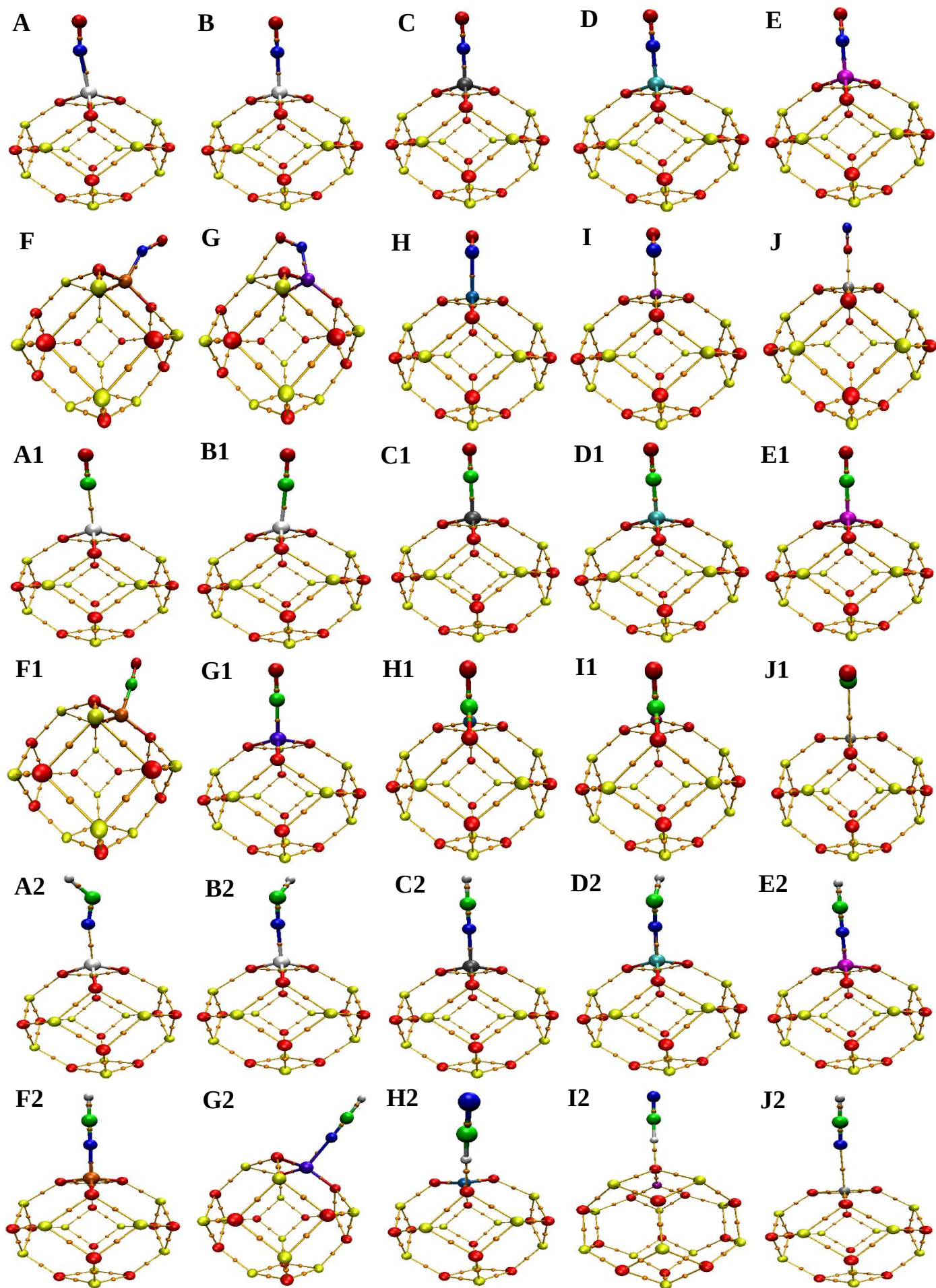
**Fig. S5** Density of states (DOS) of NO/TMCA<sub>11</sub>O<sub>12</sub>, CO/TMCA<sub>11</sub>O<sub>12</sub> and HCN/TMCA<sub>11</sub>O<sub>12</sub> (TM = Fe, Co, Ni, Cu, Zn).



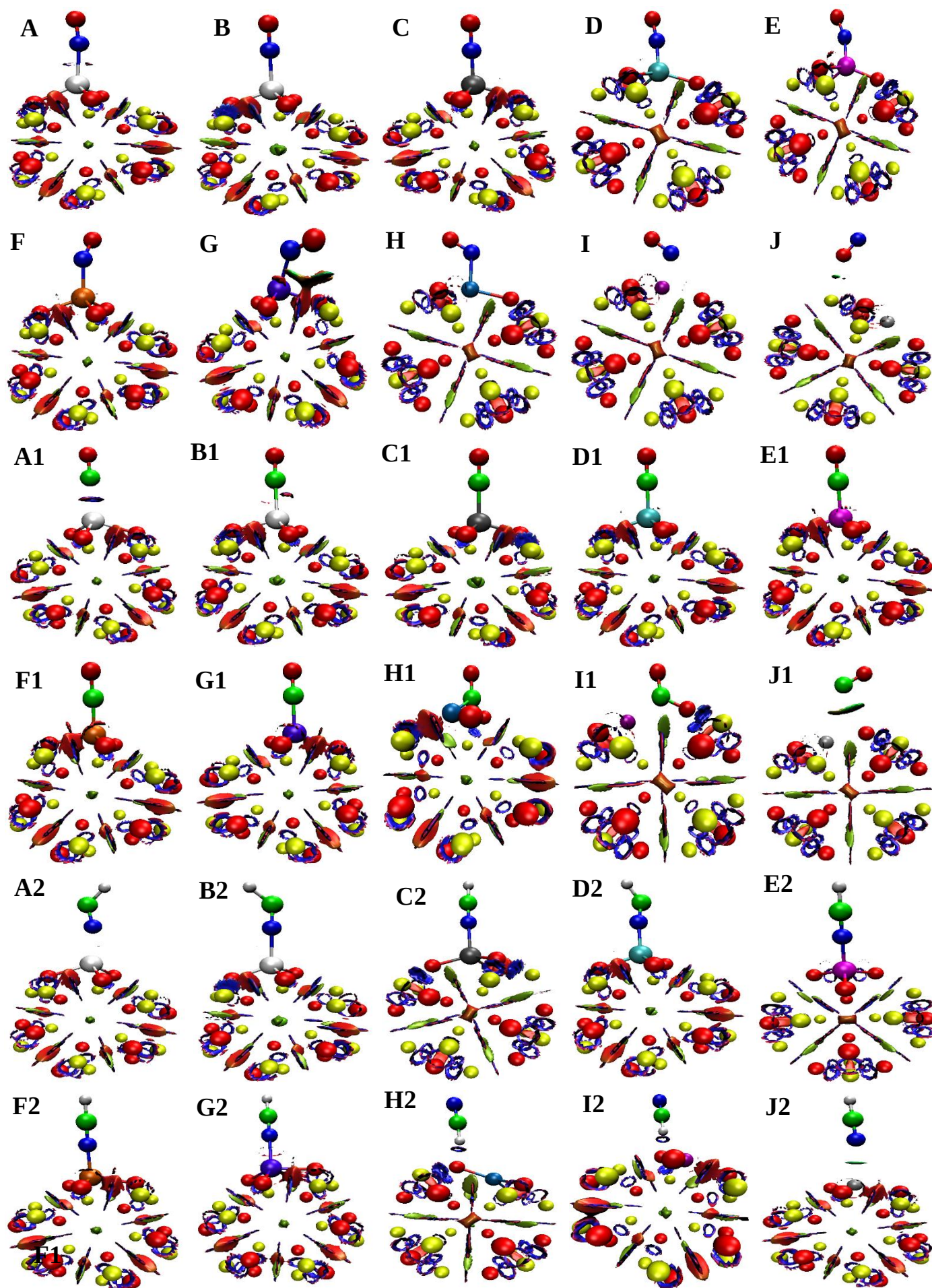
**Fig. S6** Molecular electrostatic potential (MEP) contours of CO, CO/Ca<sub>12</sub>O<sub>12</sub>, CO/TM<sub>Ca<sub>11</sub>O<sub>12</sub></sub> (TM= Sc to Zn), NO, NO/Ca<sub>12</sub>O<sub>12</sub>, NO/TM<sub>Ca<sub>11</sub>O<sub>12</sub></sub>, (TM= Sc to Fe).



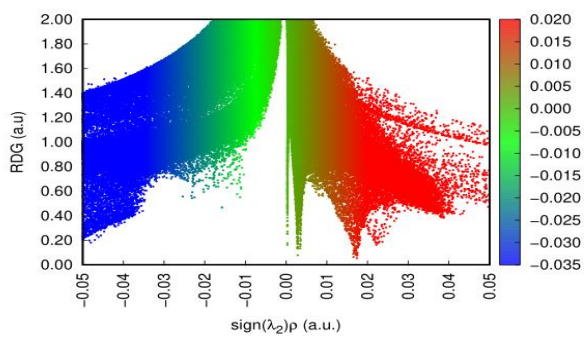
**Fig. S7** Molecular electrostatic potential (MEP) contours of NO/TMCa<sub>11</sub>O<sub>12</sub>, (TM= Co to Zn), HCN, HCN/Ca<sub>12</sub>O<sub>12</sub>, and HCN/TMCa<sub>11</sub>O<sub>12</sub> (TM= Sc to Zn).



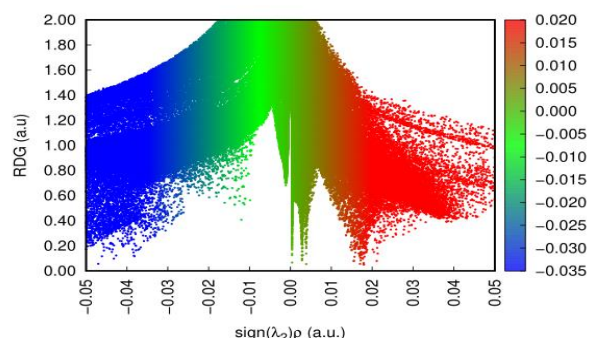
**Fig. S8** QTAIM molecular graphs (A-J) for NO/TMCA<sub>11</sub>O<sub>12</sub>, (A1-J1) for CO/TMCA<sub>11</sub>O<sub>12</sub>, and (A<sub>2</sub>-J<sub>2</sub>) for HCN/TMCA<sub>11</sub>O<sub>12</sub> complexes. The orange dots represent the BCPs.



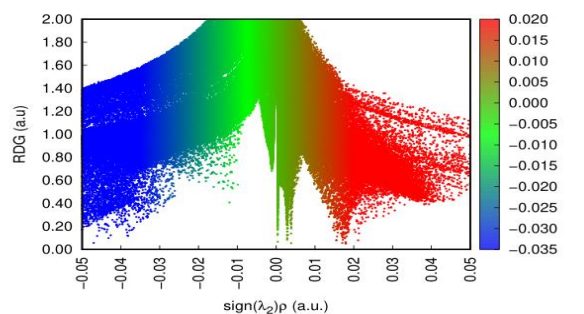
**Fig. S9** NCI molecular graphs (A-J) for NO/TM $\text{Ca}_{11}\text{O}_{12}$ , (A1-J1) for CO/TM $\text{Ca}_{11}\text{O}_{12}$ , and (A2-J2) for HCN/TM $\text{Ca}_{11}\text{O}_{12}$  complexes.



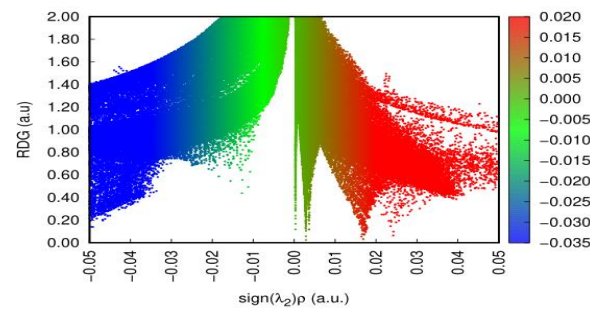
**NO-Sc-Ca<sub>11</sub>O<sub>12</sub>**



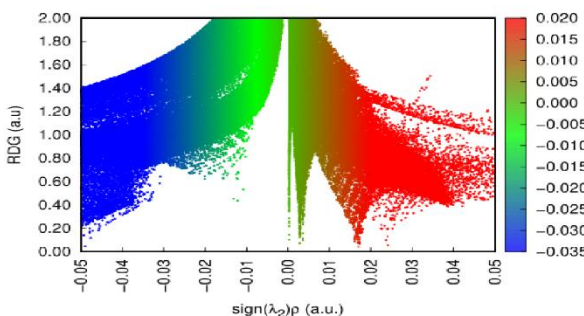
**NO-Ti-Ca<sub>11</sub>O<sub>12</sub>**



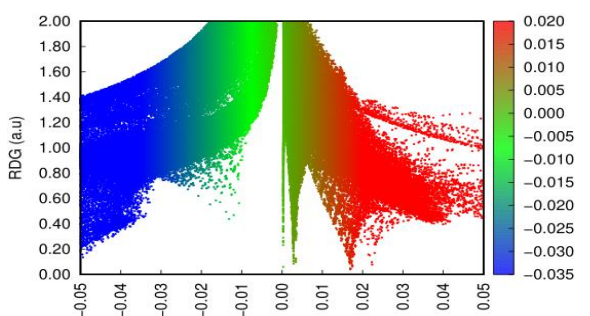
**NO-V-Ca<sub>11</sub>O<sub>12</sub>**



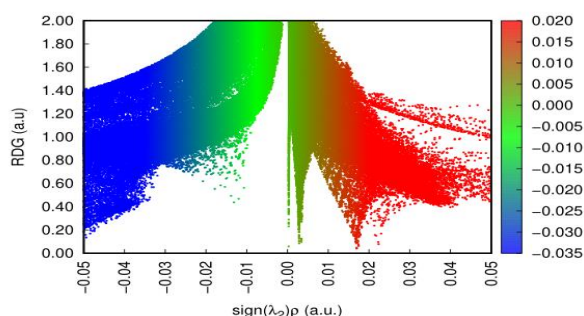
**NO-Cr-Ca<sub>11</sub>O<sub>12</sub>**



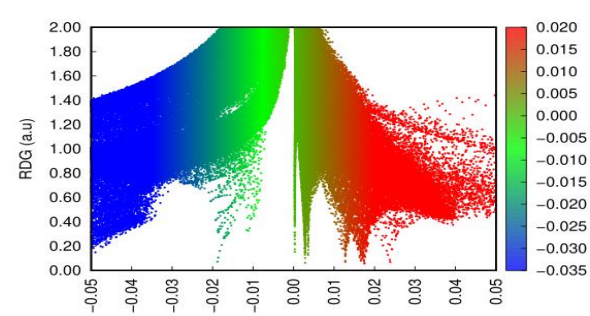
**NO-Mn-Ca<sub>11</sub>O<sub>12</sub>**



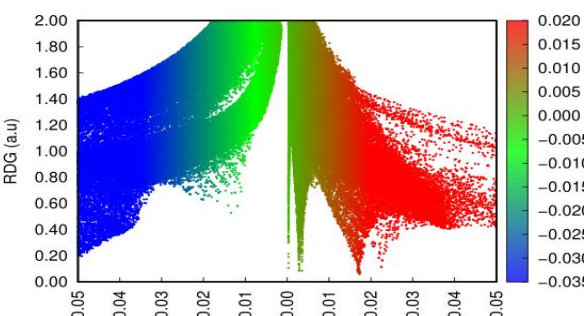
**NO-Fe-Ca<sub>11</sub>O<sub>12</sub>**



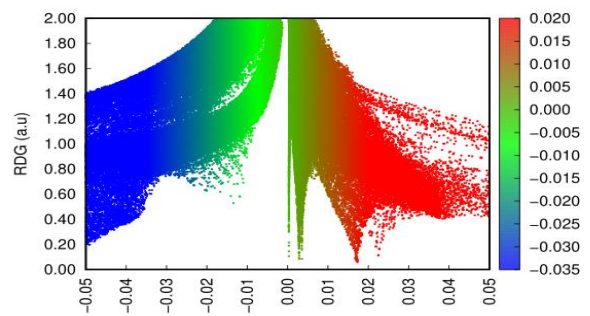
**NO-Co-Ca<sub>11</sub>O<sub>12</sub>**



**NO-Ni-Ca<sub>11</sub>O<sub>12</sub>**

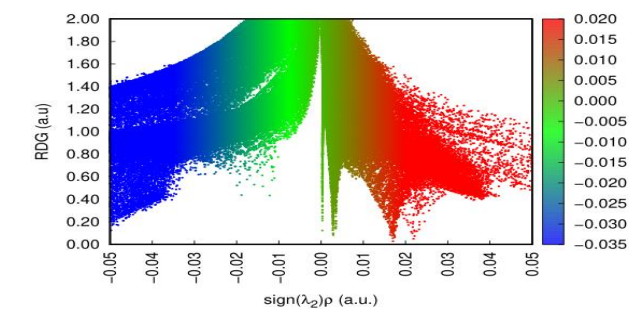


**NO-Cu-Ca<sub>11</sub>O<sub>12</sub>**

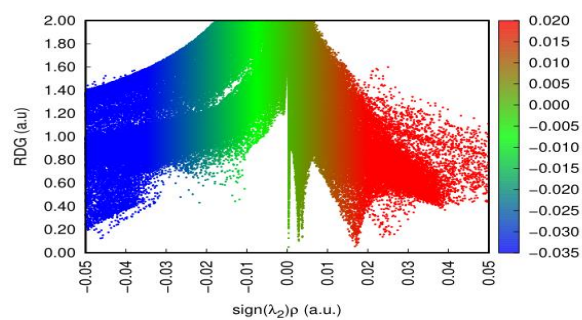


**NO-Zn-Ca<sub>11</sub>O<sub>12</sub>**

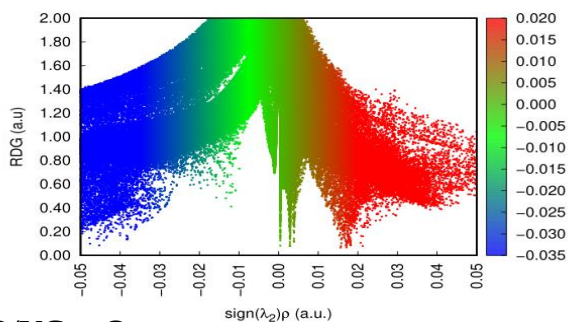
**Fig. S10** Reduced density gradient scatter maps for NO/TMCA<sub>11</sub>O<sub>12</sub>



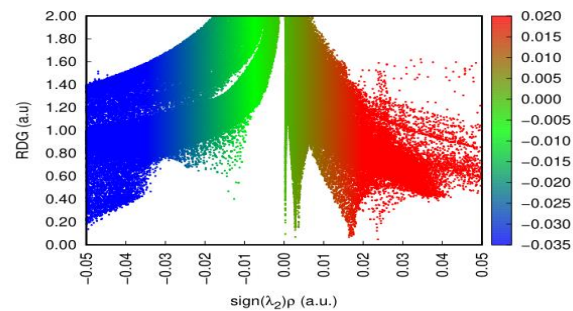
CO/ScCa<sub>11</sub>O<sub>12</sub>



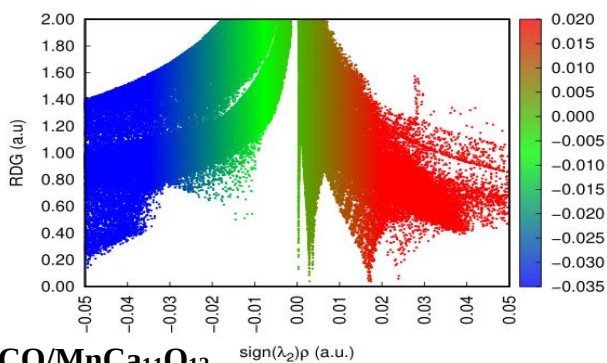
CO/TiCa<sub>11</sub>O<sub>12</sub>



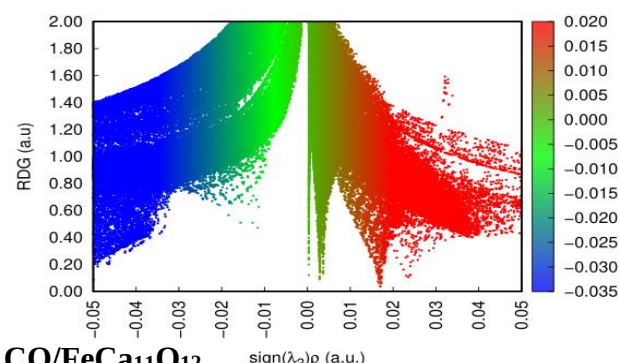
CO/VCa<sub>11</sub>O<sub>12</sub>



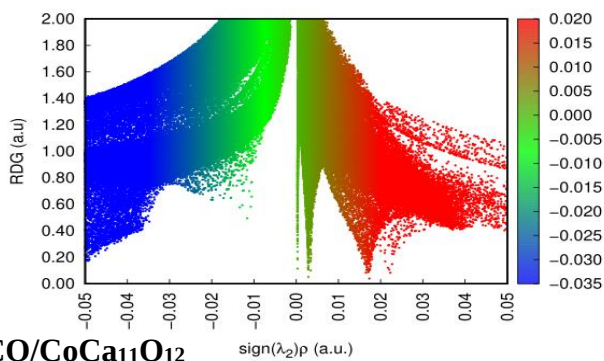
CO/CrCa<sub>11</sub>O<sub>12</sub>



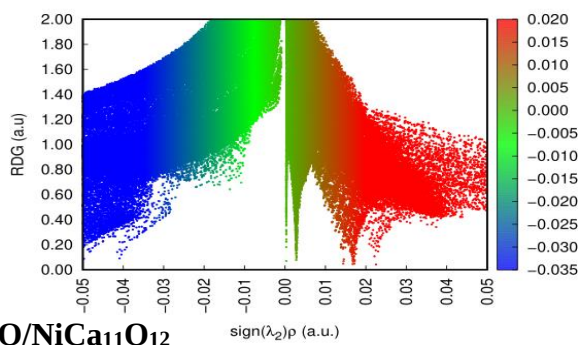
CO/MnCa<sub>11</sub>O<sub>12</sub>



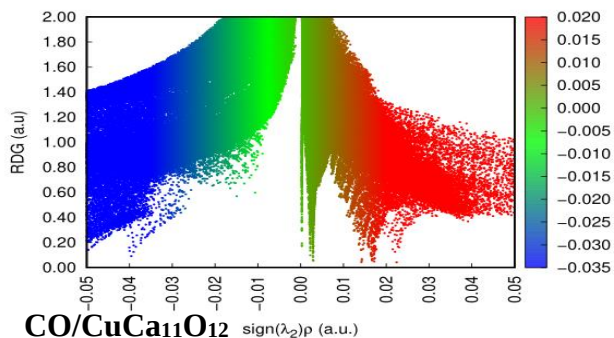
CO/FeCa<sub>11</sub>O<sub>12</sub>



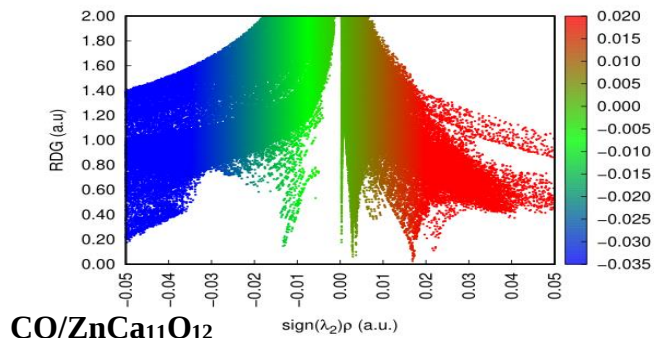
CO/CoCa<sub>11</sub>O<sub>12</sub>



CO/NiCa<sub>11</sub>O<sub>12</sub>

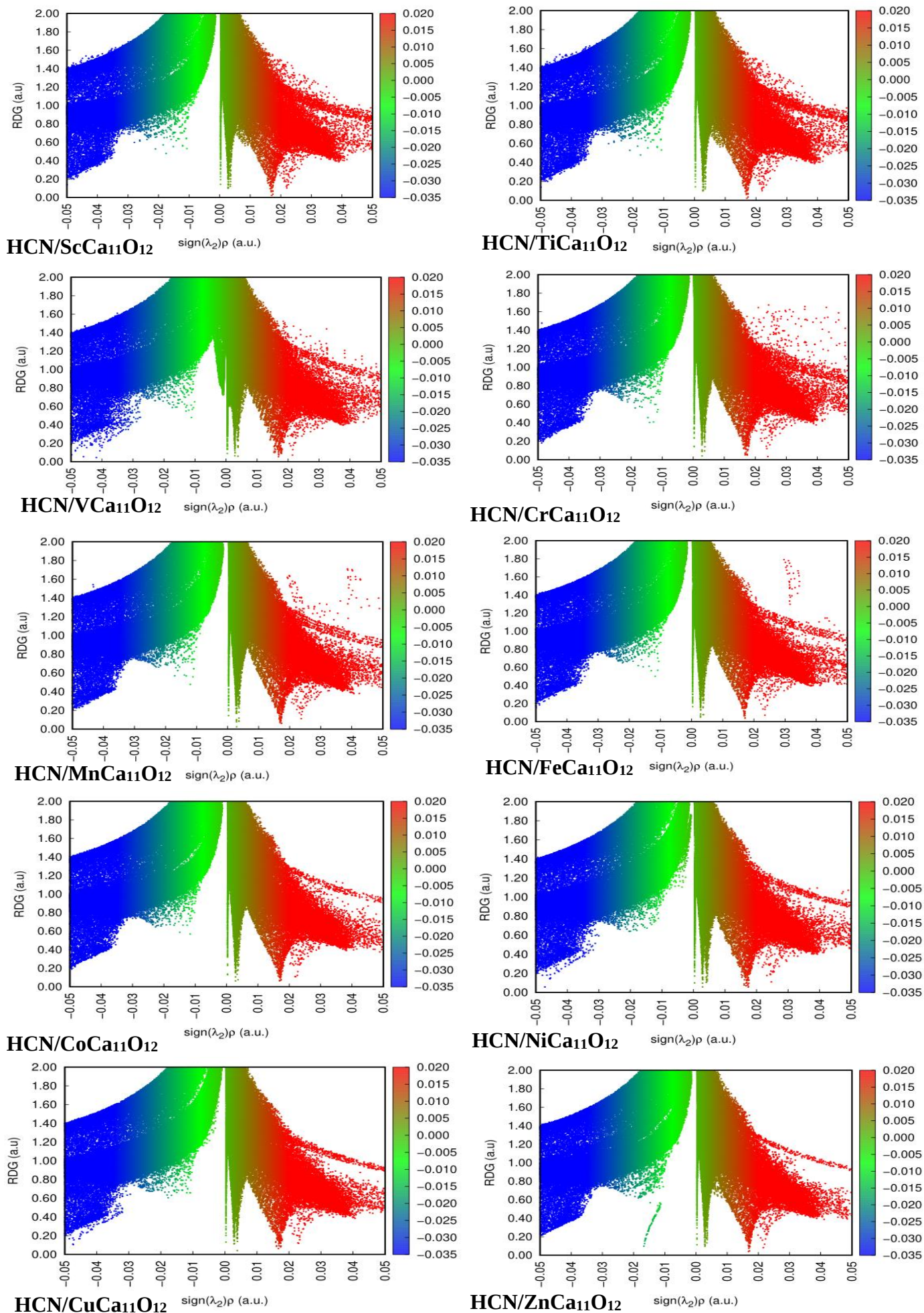


CO/CuCa<sub>11</sub>O<sub>12</sub>



CO/ZnCa<sub>11</sub>O<sub>12</sub>

**Fig. S11** Reduced density gradient scatter maps for CO/TMCA<sub>11</sub>O<sub>12</sub>



**Fig. S12** Reduced density gradient scatter maps for HCN/TMCA<sub>11</sub>O<sub>12</sub>