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| Filename | Structure | Energy (eV) |
| POSCAR\_N\_H2O | N…H2O | -490.28 eV |
| POSCAR\_OH\_NH | OH&N-H | -488.98 eV |
| POSCAR\_NOH\_NH | N-OH&N-H | -487.67 eV |
| POSCAR\_NOH | N-OH | -483.86 eV |
| POSCAR\_COH\_NH | C-OH&N-H | -489.38 eV |
| POSCAR\_COH | C-OH | -484.33 eV |
| POSCAR\_NO\_2NH | N=O&2N-H | -487.67 eV |
| POSCAR\_NO\_NH | N=O&N-H | -484.04 eV |
| POSCAR\_NO | N=O | -480.28 eV |
| POSCAR\_CO\_2NH | C=O&2N-H | -489.23 eV |
| POSCAR\_CO\_NH | C=O&N-H | -484.76 eV |
| POSCAR\_CO | C=O | -478.93 eV |
| POSCAR\_CO\_H2O | C=O&H2O | -493.76 eV |
| POSCAR\_COOH\_NH | C-OOH&N-H | -494.30 eV |
| POSCAR\_COOH | C-OOH | -488.42 eV |
| POSCAR\_HO2 | HO2 | -489.45 eV |
| POSCAR\_H2O2 | H2O2 | -494.29 eV |
| POSCAR\_O2\_NH | O2&N-H | -489.03 eV |
| POSCAR\_COH\_H2O | C-OH&H2O | -499.09 eV |
| POSCAR\_CO\_H2O\_NH | CO&H2O&N-H | -489.39 eV |
| POSCAR\_CON | C-O-N | -479.16 eV |
| POSCAR\_NO\_H2O | N=O2+&H2O | -483.75 eV |
| POSCAR\_NOOH\_NH | N-OOH2+&N-H | -483.54 eV |
| POSCAR\_OH\_NH\_1H2O | OH&N-H1.13&1H2Oa | -503.91 eV |
| POSCAR\_OH\_NH\_2H2O | OH&N-H1.13&2H2Oa | -518.78 eV |
| POSCAR\_OH\_NH\_2HF | OH&N-H1.13&2HF | -506.70 eV |
| POSCAR\_OH\_NH\_2CH4 | OH&N-H1.13&2CH4 | -537.52 eV |