

# Supporting Information: Cage Doping of Ti, Zr, and Hf-based 13-atom Nanoclusters: Two Sides of the Same Coin

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# 1 Convergence Tests

The main parameters used in our calculations and mentioned in methodology section from main manuscript are obtained by performing some convergence tests. To exemplify, in Tables S1, S2, S3, and S4 we show some properties for two illustrative cases: Hf<sub>13</sub> (named A) and Hg@Hf<sub>12</sub> (named B) as a function of the parameters. The properties considered are the relative total energy ( $\Delta E_{\text{tot}} = E_{\text{tot}}^{\text{B}} - E_{\text{tot}}^{\text{A}}$ ), average bond length ( $d_{\text{av}}^{\text{A}}$  and  $d_{\text{av}}^{\text{B}}$ ), effective coordination number (ECN<sup>A</sup> and ECN<sup>B</sup>), and total magnetic moment ( $m_{\text{T}}^{\text{A}}$  and  $m_{\text{T}}^{\text{B}}$ ).

Table S1: Convergence tests for Hf<sub>13</sub> (A) and Hg@Hf<sub>12</sub> (B) with regard to the box size (*Box Size*): the relative total energy ( $\Delta E_{\text{tot}}$ ), average bond length ( $d_{\text{av}}^{\text{A}}$  and  $d_{\text{av}}^{\text{B}}$ ), effective coordination number (ECN<sup>A</sup> and ECN<sup>B</sup>), and total magnetic moment ( $m_{\text{T}}^{\text{A}}$  and  $m_{\text{T}}^{\text{B}}$ ).

<i>Box Size</i> (Å)	$\Delta E_{\text{tot}}$ (eV)	ECN <sup>A</sup>	ECN <sup>B</sup>	$d_{\text{av}}^{\text{A}}$ (Å)	$d_{\text{av}}^{\text{B}}$ (Å)	$m_{\text{T}}^{\text{A}}$ ( $\mu_{\text{B}}$ )	$m_{\text{T}}^{\text{B}}$ ( $\mu_{\text{B}}$ )
12	-12.4168	6.3730	6.3914	2.2093	2.9398	6.0000	2.0000
14	-12.4939	6.3722	6.3941	2.9461	2.9382	6.0000	2.0000
16	-12.4236	6.3730	6.3913	2.9457	2.9389	6.0000	2.0000
18	-12.4608	6.3731	6.3945	2.9457	2.9396	6.0000	2.0000
20	-12.4599	6.3729	6.3945	2.9450	2.9398	6.0000	2.0000
22	-12.4337	6.3702	6.3946	2.9441	2.9398	6.0000	2.0000
24	-12.4271	6.3724	6.3913	2.9456	2.9389	6.0000	2.0000

Table S2: Convergence tests for Hf<sub>13</sub> (A) and Hg@Hf<sub>12</sub> (B) with regard to the cutoff energy (*ENCUT*): the relative total energy ( $\Delta E_{\text{tot}}$ ), average bond length ( $d_{\text{av}}^{\text{A}}$  and  $d_{\text{av}}^{\text{B}}$ ), effective coordination number (ECN<sup>A</sup> and ECN<sup>B</sup>), and total magnetic moment ( $m_{\text{T}}^{\text{A}}$  and  $m_{\text{T}}^{\text{B}}$ ).

<i>ENCUT</i> (eV)	$\Delta E_{\text{tot}}$ (eV)	ECN <sup>A</sup>	ECN <sup>B</sup>	$d_{\text{av}}^{\text{A}}$ (Å)	$d_{\text{av}}^{\text{B}}$ (Å)	$m_{\text{T}}^{\text{A}}$ ( $\mu_{\text{B}}$ )	$m_{\text{T}}^{\text{B}}$ ( $\mu_{\text{B}}$ )
141.4820	-10.4053	6.1700	6.3569	2.8254	2.7650	6.0000	2.0000
212.2230	-12.3137	6.3542	6.3587	2.9876	2.9451	6.0000	2.0000
282.9640	-12.3937	6.3776	6.3901	2.9423	2.9341	6.0000	2.0000
318.3345	-12.4290	6.3733	6.3923	2.9461	2.9402	6.0000	2.0000
353.7050	-12.4594	6.3731	6.3945	2.9459	2.9398	6.0000	2.0000
424.4460	-12.4279	6.3730	6.3920	2.9456	2.9388	6.0000	2.0000
565.9280	-12.4362	6.3729	6.3913	2.9450	2.9383	6.0000	2.0000

Table S3: Convergence tests for Hf<sub>13</sub> (A) and Hg@Hf<sub>12</sub> (B) with regard to the energy criterion (electronic convergence, *EDIFF*): the relative total energy ( $\Delta E_{\text{tot}}$ ), average bond length ( $d_{\text{av}}^{\text{A}}$  and  $d_{\text{av}}^{\text{B}}$ ), effective coordination number (ECN<sup>A</sup> and ECN<sup>B</sup>), and total magnetic moment ( $m_{\text{T}}^{\text{A}}$  and  $m_{\text{T}}^{\text{B}}$ ).

<i>EDIFF</i> (eV)	$\Delta E_{\text{tot}}$ (eV)	ECN <sup>A</sup>	ECN <sup>B</sup>	$d_{\text{av}}^{\text{A}}$ (Å)	$d_{\text{av}}^{\text{B}}$ (Å)	$m_{\text{T}}^{\text{A}}$ ( $\mu_{\text{B}}$ )	$m_{\text{T}}^{\text{B}}$ ( $\mu_{\text{B}}$ )
10 <sup>-2</sup>	-12.4600	6.3729	6.3946	2.9454	2.9386	6.0000	2.0000
10 <sup>-3</sup>	-12.4598	6.3740	6.3943	2.9457	2.9385	6.0000	2.0000
10 <sup>-4</sup>	-12.4600	6.3726	6.3939	2.9459	2.9394	6.0000	2.0000
10 <sup>-5</sup>	-12.4600	6.3731	6.3946	2.9457	2.9391	6.0000	2.0000
10 <sup>-6</sup>	-12.4599	6.3729	6.3945	2.9450	2.9398	6.0000	2.0000
10 <sup>-7</sup>	-12.4600	6.3731	6.3947	2.9456	2.9398	6.0000	2.0000
10 <sup>-8</sup>	-12.4599	6.3729	6.3946	2.9450	2.9398	6.0000	2.0000

Table S4: Convergence tests for Hf<sub>13</sub> (A) and Hg@Hf<sub>12</sub> (B) with regard to the force criterion (ionic convergence, *EDIFFG*): the relative total energy ( $\Delta E_{\text{tot}}$ ), average bond length ( $d_{\text{av}}^{\text{A}}$  and  $d_{\text{av}}^{\text{B}}$ ), effective coordination number (ECN<sup>A</sup> and ECN<sup>B</sup>), and total magnetic moment ( $m_{\text{T}}^{\text{A}}$  and  $m_{\text{T}}^{\text{B}}$ ).

<i>EDIFFG</i> (eV/Å)	$\Delta E_{\text{tot}}$ (eV)	ECN <sup>A</sup>	ECN <sup>B</sup>	$d_{\text{av}}^{\text{A}}$ (Å)	$d_{\text{av}}^{\text{B}}$ (Å)	$m_{\text{T}}^{\text{A}}$ ( $\mu_{\text{B}}$ )	$m_{\text{T}}^{\text{B}}$ ( $\mu_{\text{B}}$ )
-0.100	-12.4265	6.3729	6.3918	2.9450	2.9389	6.0000	2.0000
-0.050	-12.4265	6.3729	6.3918	2.9450	2.9389	6.0000	2.0000
-0.025	-12.4265	6.3729	6.3918	2.9450	2.9389	6.0000	2.0000
-0.020	-12.4265	6.3729	6.3918	2.9450	2.9389	6.0000	2.0000
-0.015	-12.4266	6.3731	6.3918	2.9457	2.9389	6.0000	2.0000
-0.010	-12.4266	6.3732	6.3918	2.9461	2.9389	6.0000	2.0000
-0.005	-12.4265	6.3731	6.3913	2.9460	2.9389	6.0000	2.0000

## 2 Methodological Tests

As reported in main manuscript, our first-principles calculations were performed considering spin-polarized density functional theory (DFT) within projector augmented wave (PAW) method, considering the PBE exchange-correlation (xc) functional. This xc functional choice is justified since, among all xc functionals, we have tested some specific types in previous study<sup>1</sup> and PBE approach appears to be more reliable for predicting the TM bulk and nanocluster properties. However, it is known that plain DFT calculations can suffer some drawbacks in the description of weakly interacting systems or those composed by heavy chemical species. In the first case, due to the deficiency in the long-range interaction description, i.e., failure in the van der Waals (vdW) interactions description and; in the second case, due to the fact that our PAW calculations are performed within the scalar-relativistic approximation, not being accounted for hence spin-orbit coupling (SOC). Consequently, to verify the correct description of the nonlocal long-range vdW interactions,<sup>2</sup> we have performed some methodological tests considering the vdW D3 correction proposed by Grimme,<sup>3,4</sup> as well as SOC corrections for the valence states, as implemented by Bucko *et al.*<sup>5</sup> in VASP.<sup>5,6</sup> In Figure S1 we show the methodological tests carried out for two illustrative cases: the energetic property of the TM@Ti<sub>12</sub> nanoclusters and the structural properties of the TM<sub>13</sub> nanoclusters in ICO configuration. Basically, we have obtained practically the same trend for PBE and PBE+D3+SOC approaches in the energetic and structural properties, such as: relative total energy ( $\Delta E_{\text{tot}} = E_{\text{tot}}^{\text{TM@Ti}_{12}} - E_{\text{tot}}^{\text{Ti}_{13}}$ ), average bond lengths ( $d_{\text{av}}$ ), atomic radius ( $R$ ), and effective coordination number (ECN).

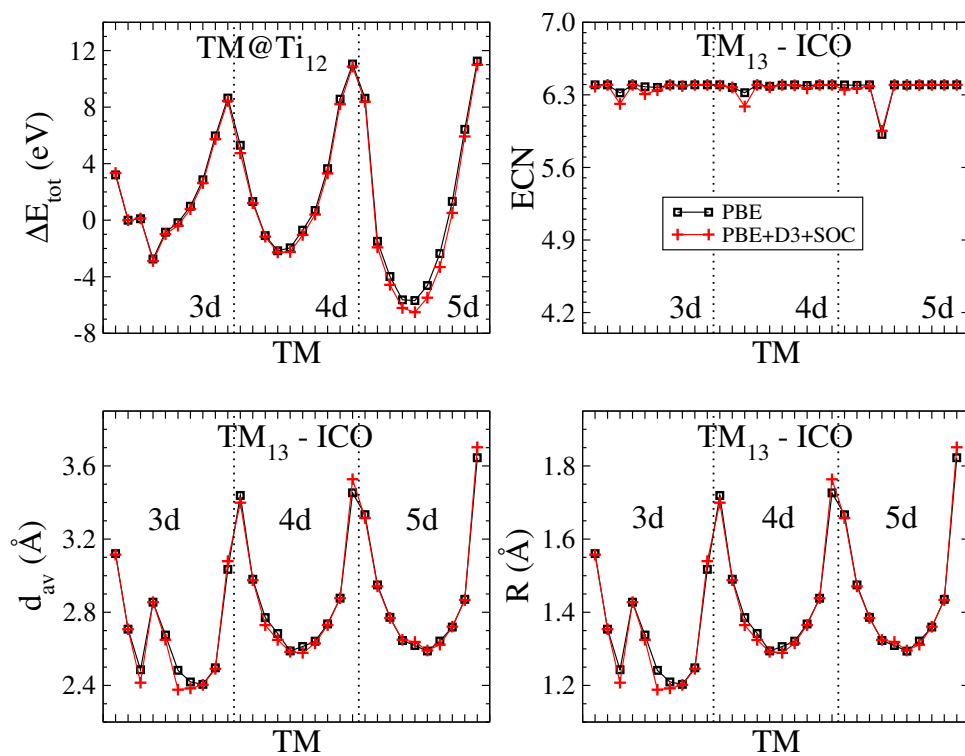


Figure S1: The relative total energy ( $\Delta E_{\text{tot}}$ ) for TM@Ti<sub>12</sub> and average bond length ( $d_{\text{av}}$ ), atomic radius ( $R$ ), and effective coordination number (ECN), for TM<sub>13</sub> nanoclusters *versus* the atomic number, for PBE and PBE+D3+SOC approaches.

### 3 Study Systems Choice

As discussed in the main manuscript, we have chosen the transition-metal 13-atom nanoclusters (TM<sub>13</sub>) since this amount is the magic number that reflects the smallest possible geometry to form a closed shell (core-shell configuration), thus combining low dimensionality and high stability in bimetallic systems. To justify the chemical species choice, which implicitly ends up determining the nanocluster geometry, we have carried out the verification through the energetic stability of the different magnetic configurations considering the prediction given by the Hund's rule through the total magnetic moment ( $m_T^H$  values). Thus, we have performed calculations for the icosahedral (ICO) and lowest-energy (LOW) configurations<sup>7</sup> for all TM<sub>13</sub> nanoclusters relaxing and fixing the total magnetic moment values. The atomic configurations for the ICO and LOW nanoclusters are shown in Figure S2, while the relative total energy values,  $\Delta E_{tot}^{ICO/LOW} = E_{tot}^{ICO/LOW}(m_T^H) - E_{tot}^{ICO/LOW}(m_T^{ICO/LOW})$ , are shown in Table 1, where it is possible to notice that the configurations with  $m_T^H$  are less stable than the relaxed systems ( $m_T^{ICO/LOW}$ ), except some cases where  $\Delta E_{tot}^{ICO/LOW}$  is equal to 0.00 eV, for which  $m_T^{ICO/LOW} = m_T^H$ .

Thus, we have two main choices (highlighted in red in the Table 1): group 4 (Ti / Zr / Hf) and group 12 (Zn / Cd / Hg), where  $\Delta E_{tot}^{ICO/LOW} = 0.00$  eV and  $m_T^{ICO/LOW} = m_T^H$ . However, only one of these groups presents the high-symmetry ICO geometry as the most stable fundamental structure (LOW = ICO), i.e., group 4, with  $m_T^{ICO/LOW} = m_T^H = 6\mu_B$ . On the other hand, for group 12, we have LOW  $\neq$  ICO to Zn<sub>13</sub> and Cd<sub>13</sub>, while LOW = ICO to Hg<sub>13</sub>,<sup>7,8</sup> with  $m_T^{ICO} = m_T^{LOW} = m_T^H = 0\mu_B$ , i.e, we observe a non-magnetic behaviour, since there are 156 valence electrons distributed in 1S<sup>2</sup> 1P<sup>6</sup> 1D<sup>10</sup> 2S<sup>2</sup> 1F<sup>14</sup> 2P<sup>6</sup> 1G<sup>18</sup> 2D<sup>10</sup> 3S<sup>2</sup> 1H<sup>22</sup> 2F<sup>14</sup> 3P<sup>6</sup> 1I<sup>26</sup> 2G<sup>18</sup> closed-shell electronic configuration, leaving non-unpaired electrons (similar to the elements from s-block, e.g., alkaline earth metals).

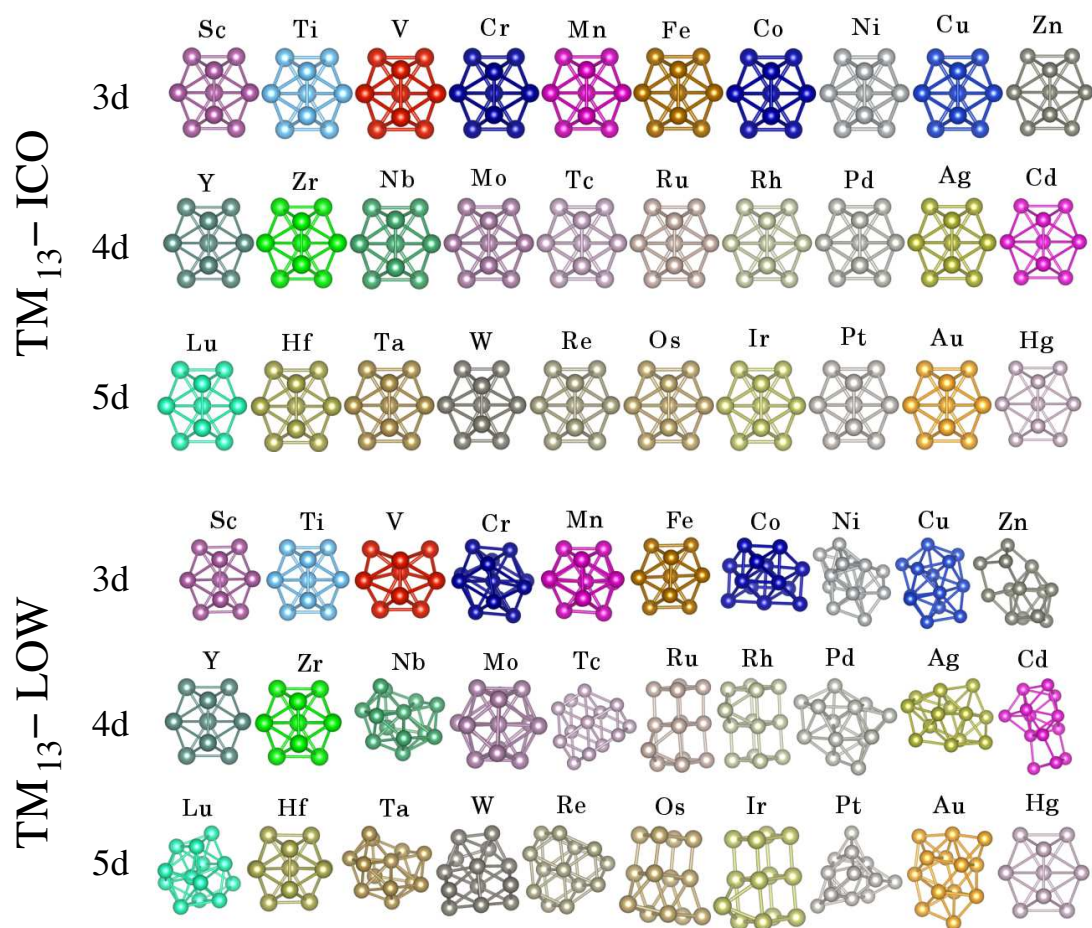


Figure S2: The atomic configurations for the icosahedral (ICO) and the lowest energy (LOW) structures of the  $\text{TM}_{13}$  nanoclusters, where TM is equal to all 3d, 4d, and 5d transition metals from periodic table.



## 4 Vibrational Frequencies

We performed harmonic vibrational frequency calculations after each geometry optimization to determine the vibrational frequencies for the unary and binary TM@Ti<sub>12</sub>, TM@Zr<sub>12</sub>, and TM@Hf<sub>12</sub> configurations. The resulting  $3N - 6$  (33) vibrational frequencies for each nanocluster were found to be real and positive, confirming the stationary nature of the obtained states and indicating the presence of local minimum configurations on the potential energy surface. Table S5 presents the lowest vibrational frequency (in cm<sup>-1</sup>) for each cluster with numerical accuracy. It is noteworthy that vibrational frequencies obtained from VASP may vary depending on factors such as the convergence criteria, choice and size of the basis set, and the specific system under investigation. While the numerical accuracy of the lowest frequencies typically falls within a few percent of experimental values for most systems, we assessed the root mean squared shifts (RMSS) in frequency for our nanoclusters. We compared the frequencies of all (33) modes calculated with ENCUT = 500 eV to those obtained with a larger cutoff (ENCUT = 800 eV). This comparison allowed us to estimate the maximum absolute error in RMSS frequency as 0.14 cm<sup>-1</sup>.

Table S5: The lowest vibrational frequencies,  $\nu_{low}$  (in cm<sup>-1</sup>), for the unary and binary TM@Ti<sub>12</sub>, TM@Zr<sub>12</sub>, and TM@Hf<sub>12</sub> systems. We estimate the numerical accuracy of these frequencies to be within the range of 1 cm<sup>-1</sup> based on ENCUT convergence tests.

TM@Ti <sub>12</sub>	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn
$\nu_{low}$ (cm <sup>-1</sup> )	5.99	13.88	3.75	48.06	6.06	3.02	0.22	108.52	24.90	80.32
TM@Ti <sub>12</sub>	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd
$\nu_{low}$ (cm <sup>-1</sup> )	3.53	11.99	7.23	16.11	3.12	6.04	9.75	97.74	12.22	49.88
TM@Ti <sub>12</sub>	Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg
$\nu_{low}$ (cm <sup>-1</sup> )	12.73	79.05	14.38	2.75	19.76	74.32	107.16	112.43	10.06	81.59
TM@Zr <sub>12</sub>	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn
$\nu_{low}$ (cm <sup>-1</sup> )	11.05	2.53	103.35	9.62	42.92	9.12	10.21	102.87	1.47	50.05
TM@Zr <sub>12</sub>	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd
$\nu_{low}$ (cm <sup>-1</sup> )	19.77	61.57	20.60	6.66	24.57	4.54	0.54	94.10	0.66	58.19
TM@Zr <sub>12</sub>	Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg
$\nu_{low}$ (cm <sup>-1</sup> )	13.67	9.20	3.21	21.66	38.55	9.45	6.19	13.71	31.56	62.97
TM@Hf <sub>12</sub>	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn
$\nu_{low}$ (cm <sup>-1</sup> )	4.33	10.14	4.09	7.12	10.82	8.12	6.00	82.76	2.67	3.31
TM@Hf <sub>12</sub>	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd
$\nu_{low}$ (cm <sup>-1</sup> )	3.68	11.62	3.46	1.28	4.99	1.35	7.42	68.11	17.88	17.40
TM@Hf <sub>12</sub>	Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg
$\nu_{low}$ (cm <sup>-1</sup> )	8.30	2.70	17.08	3.10	3.13	2.22	36.47	84.87	17.91	6.94

## 5 AIMD Calculations

In order to explore the thermal stability, *ab-initio* molecular dynamic (AIMD) simulations were performed to ensure that the proposed ICO structures were the lowest energy configurations (LOW = ICO) for  $\text{Ti}_{13}$ ,  $\text{Zr}_{13}$ , and  $\text{Hf}_{13}$  nanoclusters. After AIMD simulations, conventional total energy calculations were performed. For those AIMD simulations (Nosé thermostat), a time step of 4 fs was used, with AIMD runs being about 30 ps long at 300 K, to check the stability of the geometric structures, as well as to certify the magnetic moment configurations. Performing an AIMD at approximately room temperature is similar to a thermalization process, which aims to elucidate the thermodynamic stability of the studied systems. We performed the AIMD calculations also for the  $\text{TM@Ti}_{12}$ ,  $\text{TM@Zr}_{12}$ , and  $\text{TM@Hf}_{12}$  configurations considering the same parameters, except the fact that these AIMD runs were about 20 ps long. In Figure S3 are shown the AIMD simulations, temperature in relation to the simulation time step for  $\text{Ti}_{13}$ ,  $\text{Zr}_{13}$ , and  $\text{Hf}_{13}$  as well as for an illustrative case, i.e.,  $\text{Ni@Ti}_{12}$ ,  $\text{Ni@Zr}_{12}$ , and  $\text{Ni@Hf}_{12}$  nanoclusters.

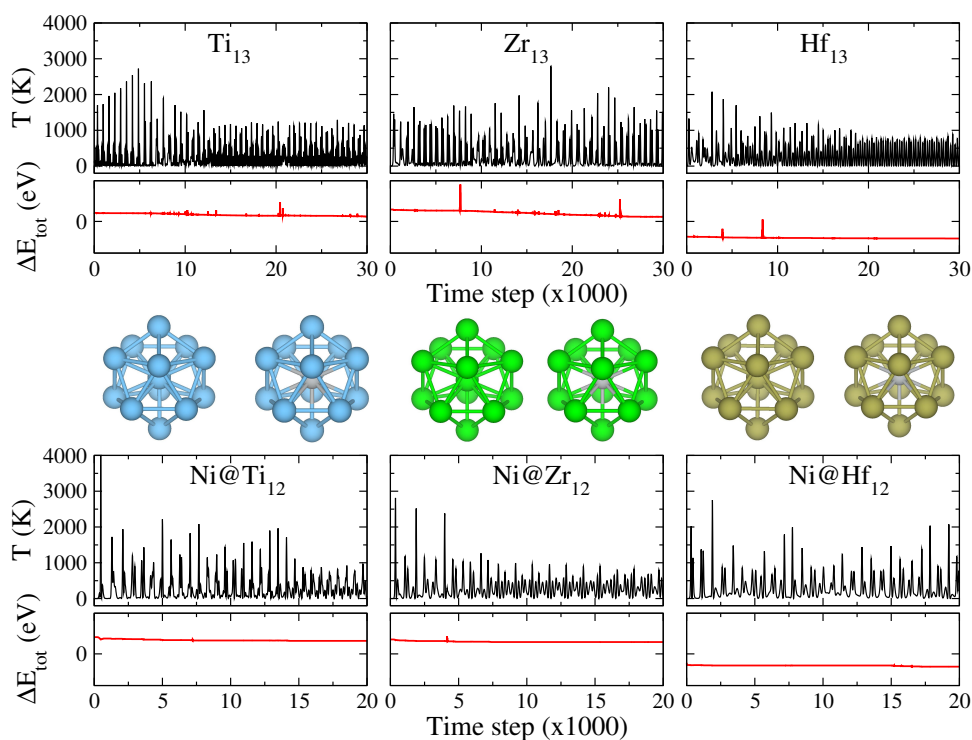


Figure S3: AIMD simulations, temperature *versus* time step, for  $\text{Ti}_{13}$ ,  $\text{Zr}_{13}$ , and  $\text{Hf}_{13}$  as well as for  $\text{Ni@Ti}_{12}$ ,  $\text{Ni@Zr}_{12}$ , and  $\text{Ni@Hf}_{12}$  nanoclusters.

## 6 Total Magnetic Moment Tests

Although we have carried out structural optimization calculations without symmetry constraints and without specified magnetic configurations, which enables the free local exploration of the structural and magnetic potential energy surfaces, we have also been concerned with testing different total magnetic moment values for the nanoclusters of group 4. In Table S6 (S7) we show the  $\text{Ti}_{13}$ ,  $\text{Zr}_{13}$ , and  $\text{Hf}_{13}$  (e.g.,  $\text{TM@Ti}_{12}$ ,  $\text{TM@Zr}_{12}$ , and  $\text{TM@Hf}_{12}$ , where  $\text{TM} = \text{Ni}$ ,  $\text{Pd}$ , and  $\text{Pt}$ ) relative total energies,  $\Delta E_{tot}$ , in relation to the most stable configuration for  $m_T^{\text{ICO}} = m_T^{\text{H}} = 6\mu_{\text{B}}$  ( $m_T^{\text{ICO}} = m_T^{\text{H}} = 0$ ) for different fixed total magnetic moment values.

Table S6: The relative total energy ( $\Delta E_{tot}$ ) between the lowest energy configurations ( $m_T^{\text{ICO}} = m_T^{\text{H}} = 6\mu_{\text{B}}$ ) and the configurations considering different fixed total magnet moment values for  $\text{Ti}_{13}$ ,  $\text{Zr}_{13}$ , and  $\text{Hf}_{13}$  nanoclusters in ICO configuration.

	$\text{Ti}_{13}$	$\text{Zr}_{13}$	$\text{Hf}_{13}$
$m_T$ ( $\mu_{\text{B}}$ )	$\Delta E_{tot}$ (eV)	$\Delta E_{tot}$ (eV)	$\Delta E_{tot}$ (eV)
0	0.177	0.347	0.251
1	0.182	0.433	0.273
2	0.218	0.426	0.262
3	0.259	0.405	0.298
4	0.166	0.295	0.218
5	0.093	0.170	0.117
6	0.000	0.000	0.000
7	0.380	0.447	0.473
8	0.623	0.950	0.660
9	1.000	1.357	1.261

Table S7: Illustrative cases: The relative total energy ( $\Delta E_{tot}$ ) between the lowest energy configurations ( $m_T^{\text{ICO}} = m_T^{\text{H}} = 0$ ) and the configurations considering different fixed total magnet moment values for  $\text{TM@Ti}_{12}$ ,  $\text{TM@Zr}_{12}$ , and  $\text{TM@Hf}_{12}$ , where  $\text{TM} = \text{Ni}$ ,  $\text{Pd}$ , and  $\text{Pt}$ , nanoclusters in ICO configuration.

	$\text{Ni@Ti}_{12}$	$\text{Pd@Ti}_{12}$	$\text{Pt@Ti}_{12}$	$\text{Ni@Zr}_{12}$	$\text{Pd@Zr}_{12}$	$\text{Pt@Zr}_{12}$	$\text{Ni@Hf}_{12}$	$\text{Pd@Hf}_{12}$	$\text{Pt@Hf}_{12}$
$m_T$ ( $\mu_{\text{B}}$ )	$\Delta E_{tot}$ (eV)	$\Delta E_{tot}$ (eV)	$\Delta E_{tot}$ (eV)	$\Delta E_{tot}$ (eV)	$\Delta E_{tot}$ (eV)	$\Delta E_{tot}$ (eV)	$\Delta E_{tot}$ (eV)	$\Delta E_{tot}$ (eV)	$\Delta E_{tot}$ (eV)
0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
1	0.214	0.249	0.311	0.259	0.306	0.328	0.247	0.312	0.384
2	0.360	0.517	0.598	0.459	0.588	0.677	0.425	0.608	0.743
3	0.597	0.731	0.874	0.660	0.847	0.967	0.616	0.889	1.104
4	0.752	0.972	1.099	0.838	1.087	1.224	0.746	1.140	1.416
5	0.839	1.095	1.369	0.956	1.297	1.445	0.907	1.358	1.709
6	0.899	1.264	1.608	1.085	1.459	1.632	0.994	1.543	1.982
7	1.022	1.470	1.801	1.265	1.810	1.917	1.121	1.742	2.302
8	1.064	1.682	2.128	1.292	1.849	2.160	1.187	1.901	2.537
9	1.099	1.701	2.259	1.429	2.031	2.317	1.339	2.074	2.772

## 7 Electron Localization Function

In Figure S4 we show the electron localization function (ELF) for  $\text{Ti}_{13}$ ,  $\text{Zr}_{13}$ , and  $\text{Hf}_{13}$  nanoclusters, as well as for some illustrative cases with Ni, Pd, and Pt inside them, i.e.,  $\text{Ni@Ti}_{12}$ ,  $\text{Pd@Ti}_{12}$ ,  $\text{Pt@Ti}_{12}$ ,  $\text{Ni@Zr}_{12}$ ,  $\text{Pd@Zr}_{12}$ ,  $\text{Pt@Zr}_{12}$ ,  $\text{Ni@Hf}_{12}$ ,  $\text{Pd@Hf}_{12}$ , and  $\text{Pt@Hf}_{12}$ .

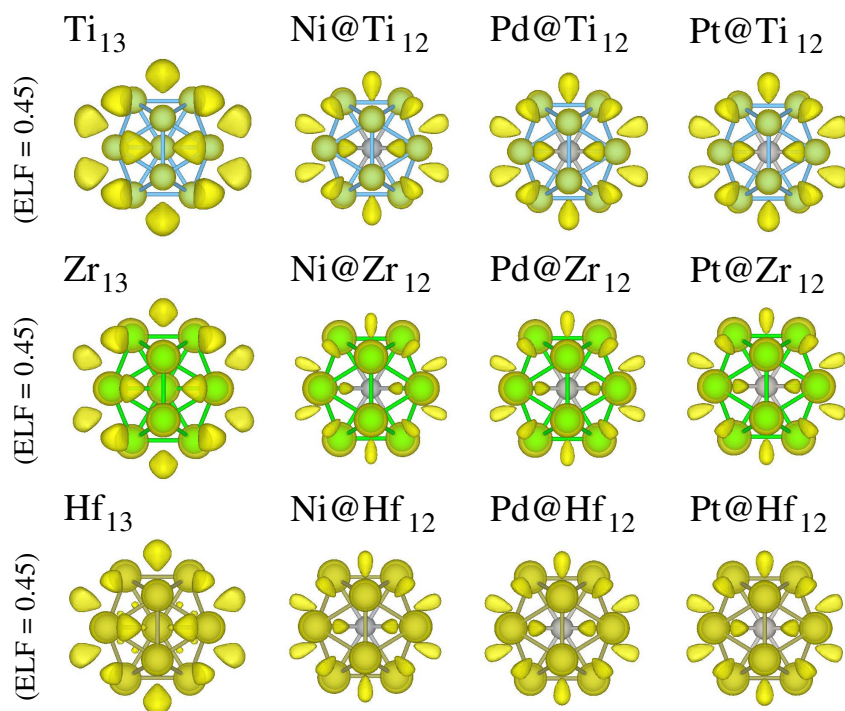


Figure S4: The electron localization function (ELF) of the  $\text{Ti}_{13}$ ,  $\text{Zr}_{13}$ , and  $\text{Hf}_{13}$  lowest energy nanoclusters and some illustrative configurations:  $\text{Ni@Ti}_{12}$ ,  $\text{Pd@Ti}_{12}$ ,  $\text{Pt@Ti}_{12}$ ,  $\text{Ni@Zr}_{12}$ ,  $\text{Pd@Zr}_{12}$ ,  $\text{Pt@Zr}_{12}$ ,  $\text{Ni@Hf}_{12}$ ,  $\text{Pd@Hf}_{12}$ , and  $\text{Pt@Hf}_{12}$ . For all cases the ELF isosurface is equal to 0.45, represented by the color yellow.

## 8 Cage Doping Configurations

As ICO has higher degeneracy level in the electronic orbitals and only two non-equivalent substitutional sites, to tune the magnetic properties of the  $\text{Ti}_{13}$ ,  $\text{Zr}_{13}$ , and  $\text{Hf}_{13}$  nanoclusters by performing modifications in the electron count, we have performed simple substitutions of the internal (central) atom from  $\text{TM}_{13}$  by foreign TM species, more specifically, all TM species from periodic table, resulting in the complete set of  $\text{TM}@\text{Ti}_{12}$ ,  $\text{TM}@\text{Zr}_{12}$ , and  $\text{TM}@\text{Hf}_{12}$  systems.

## 9 Energy Equations

Here, we perform a deeper detailing of the mathematical expression used for the atomization energy ( $\Delta E_a$ ) of the TM@Ti<sub>12</sub>, TM@Zr<sub>12</sub>, and TM@Hf<sub>12</sub> systems, providing the expressions for the interaction and distortion energies. The usual  $\Delta E_a$  expression is given by:

$$\Delta E_a = \frac{12E_{\text{tot}}^{\text{Ti/Zr/Hf free-atom}} + E_{\text{tot}}^{\text{TM free-atom}} - E_{\text{tot}}^{\text{TM@Ti}_{12}/\text{TM@Zr}_{12}/\text{TM@Hf}_{12}}}{13}, \quad (1)$$

where  $E_{\text{tot}}^{\text{Ti/Zr/Hf free-atom}}$  and  $E_{\text{tot}}^{\text{TM free-atom}}$  are the total energies of the free-atoms, while  $E_{\text{tot}}^{\text{TM@Ti}_{12}/\text{TM@Zr}_{12}/\text{TM@Hf}_{12}}$  is the total energy of the TM@Ti<sub>12</sub>/TM@Zr<sub>12</sub>/TM@Hf<sub>12</sub> systems.

On the other hand, the alternative  $\Delta E_a$  expression is given by:

$$\Delta E_a = \frac{12\Delta E_a^{\text{Ti}_{12}/\text{Zr}_{12}/\text{Hf}_{12}} + \Delta E_{\text{int}} + 12\Delta E_{\text{dis}}}{13}, \quad (2)$$

where the cage atomization energy ( $\Delta E_a^{\text{Ti}_{12}/\text{Zr}_{12}/\text{Hf}_{12}}$ ), the interaction energy between the cage and the internal TM atom ( $\Delta E_{\text{int}}$ ), and the distortion energy caused by the presence of a TM atom inside the Ti<sub>12</sub>/Zr<sub>12</sub>/Hf<sub>12</sub> system ( $\Delta E_{\text{dis}}$ ) are given respectively by:

$$\Delta E_a^{\text{Ti}_{12}/\text{Zr}_{12}/\text{Hf}_{12}} = \frac{12E_{\text{tot}}^{\text{Ti/Zr/Hf free-atom}} - E_{\text{tot}}^{\text{Ti}_{12}/\text{Zr}_{12}/\text{Hf}_{12}}}{12}, \quad (3)$$

where  $E_{\text{tot}}^{\text{Ti}_{12}/\text{Zr}_{12}/\text{Hf}_{12}}$  is the total energy of the cage systems;

$$\Delta E_{\text{int}} = E_{\text{tot}}^{\text{Ti}_{12}/\text{Zr}_{12}/\text{Hf}_{12} \text{ frozen}} + E_{\text{tot}}^{\text{TM free-atom}} - E_{\text{tot}}^{\text{TM@Ti}_{12}/\text{TM@Zr}_{12}/\text{TM@Hf}_{12}}, \quad (4)$$

where  $E_{\text{tot}}^{\text{Ti}_{12}/\text{Zr}_{12}/\text{Hf}_{12} \text{ frozen}}$  is the total energy of the frozen cage clusters at their original positions obtained from the TM@Ti<sub>12</sub>/TM@Zr<sub>12</sub>/TM@Hf<sub>12</sub> systems;

$$\Delta E_{\text{dis}} = \frac{E_{\text{tot}}^{\text{Ti}_{12}/\text{Zr}_{12}/\text{Hf}_{12}} - E_{\text{tot}}^{\text{Ti}_{12}/\text{Zr}_{12}/\text{Hf}_{12} \text{ frozen}}}{12}, \quad (5)$$

where the energy demanded to distort the configurations from its initial to the final stage is given by the difference per atom between the frozen and relaxed cage systems.

## 10 Stability

The stability of the  $B_{13}$  and  $A@B_{12}$  nanoclusters is the central pivot of our work. We elucidate and bring to light a new family of nanoclusters with peculiar properties of atomic and electronic shell closure that fit into the superatom behavior trend. Various aspects of cluster stability were addressed:

- The cluster geometries reported are stable with respect to distortion, they are minima of the potential energy surface as shown by the absence of imaginary frequency.
- The 300 K AIMD simulations further show stability at room temperature.
- Extra calculations were done for many fixed magnetic moments and we report results for the lowest energy magnetic state in every case.
- We characterize the stability of clusters with energy decomposition into cage binding, dopant-cage interaction, and energy distortion terms.
- We got only positive values for the atomization energy of all studied systems, ensuring the stability of the nanoclusters compared to their individual atomic constituents.
- We characterize the stability of clusters relative to one another with a linear fit of atomization energies: a cluster with atomization energy bigger than what is predicted by the fit function is stable relative to the set of 89 other clusters.
- The energy for B-to-TM central atom substitution in one cluster:  $B_{13} + TM \rightarrow TM@B_{12} + B$ ; see Table S8.
- The energy for mixing elements B and TM in 14 clusters according to the scheme:  $13 B_{13} + TM_{13} \rightarrow 13 TM@B_{12} + B_{13}$ , reporting one-fourteenth of the energy difference associated with the chemical equation; see Table S9.

Table S8: The energy for B-to-TM central atom substitution in one cluster:  $B_{13} + TM \rightarrow TM@B_{12} + B$ , where the respective energies are shown for  $\Delta E_1 = (B_{13} + TM)$  and  $\Delta E_1 = (TM@B_{12} + B)$ , and  $B = Ti, Zr, Hf$ , while  $TM = \text{all } 3d, 4d, 5d$ .

TM	$\Delta E_1$ (B = Ti) (eV)	$\Delta E_2$ (B = Ti) (eV)	$\Delta E_1$ (B = Zr) (eV)	$\Delta E_2$ (B = Zr) (eV)	$\Delta E_1$ (B = Hf) (eV)	$\Delta E_2$ (B = Hf) (eV)
Sc	-113.85	-110.84	-116.74	-114.10	-146.63	-143.64
Ti	-114.04	-114.04	-116.93	-117.02	-146.82	-146.68
V	-112.57	-113.94	-115.45	-116.49	-145.35	-146.45
Cr	-116.48	-116.79	-119.36	-118.81	-149.26	-149.11
Mn	-114.38	-114.89	-117.27	-116.78	-147.16	-147.28
Fe	-112.64	-114.22	-115.53	-115.87	-145.42	-146.62
Co	-111.33	-113.05	-114.22	-114.60	-144.11	-145.42
Ni	-110.00	-111.18	-112.89	-113.00	-142.78	-143.64
Cu	-109.52	-108.08	-112.41	-110.25	-142.30	-140.62
Zn	-109.28	-105.40	-112.17	-107.99	-142.06	-138.01
Y	-113.66	-108.74	-116.54	-112.42	-146.44	-141.78
Zr	-113.24	-112.72	-116.12	-116.12	-146.02	-145.70
Nb	-113.77	-115.13	-116.66	-118.12	-146.55	-148.05
Mo	-114.69	-116.21	-117.58	-118.97	-147.47	-148.98
Tc	-112.90	-116.00	-115.78	-118.60	-145.67	-148.79
Ru	-111.31	-114.75	-114.20	-117.03	-144.09	-147.57
Rh	-110.80	-113.35	-113.68	-115.53	-143.58	-146.19
Pd	-110.75	-110.39	-113.64	-112.87	-143.53	-143.38
Ag	-109.48	-105.48	-112.36	-108.36	-142.26	-138.59
Cd	-109.29	-102.99	-112.18	-106.33	-142.07	-136.22
Lu	-109.63	-105.41	-112.51	-108.95	-142.41	-138.36
Hf	-115.62	-115.53	-118.50	-118.80	-148.40	-148.40
Ta	-115.35	-118.02	-118.23	-121.37	-148.13	-151.02
W	-115.91	-119.67	-118.80	-122.54	-148.69	-152.51
Re	-115.52	-119.73	-118.41	-122.47	-148.30	-152.63
Os	-113.27	-118.66	-116.15	-121.08	-146.05	-151.54
Ir	-111.34	-116.40	-114.23	-118.67	-144.12	-149.29
Pt	-109.95	-112.71	-112.84	-115.18	-142.73	-145.70
Au	-109.46	-107.61	-112.35	-110.41	-142.24	-140.67
Hg	-109.40	-102.79	-112.29	-106.08	-142.18	-135.96



Table S9: The energy for mixing elements B and TM in 14 clusters according to the scheme:  $13 B_{13} + TM_{13} \rightarrow 13 TM@B_{12} + B_{13}$ . The respective energies are shown for  $\Delta E_3 = (1/14)(13B_{13} + TM_{13})$  and  $\Delta E_4 = (1/14)(13TM@B_{12} + B_{13})$ , and B = Ti, Zr, Hf, while TM = all  $3d$ ,  $4d$ ,  $5d$ .

TM	$\Delta E_3$ (B = Ti) (eV)	$\Delta E_4$ (B = Ti) (eV)	$\Delta E_3$ (B = Zr) (eV)	$\Delta E_4$ (B = Zr) (eV)	$\Delta E_3$ (B = Hf) (eV)	$\Delta E_4$ (B = Hf) (eV)
Sc	-108.27	-106.30	-110.95	-110.28	-138.69	-137.64
Ti	-109.28	-109.28	-111.96	-112.99	-139.70	-140.46
V	-107.99	-109.18	-110.67	-112.50	-138.42	-140.25
Cr	-109.71	-111.83	-112.39	-114.65	-140.13	-142.72
Mn	-108.10	-110.06	-110.78	-112.77	-138.52	-141.01
Fe	-107.59	-109.44	-110.27	-111.93	-138.01	-140.40
Co	-106.31	-108.36	-108.99	-110.75	-136.73	-139.29
Ni	-105.04	-106.62	-107.72	-109.26	-135.46	-137.64
Cu	-103.80	-103.74	-106.48	-106.71	-134.22	-134.83
Zn	-101.75	-101.25	-104.43	-104.61	-132.17	-132.41
Y	-108.14	-104.35	-110.82	-108.72	-138.57	-135.91
Zr	-109.48	-108.05	-112.16	-112.16	-139.90	-139.55
Nb	-110.15	-110.29	-112.83	-114.01	-140.57	-141.73
Mo	-109.89	-111.29	-112.57	-114.80	-140.31	-142.59
Tc	-109.00	-111.09	-111.68	-114.46	-139.42	-142.42
Ru	-107.37	-109.93	-110.04	-113.01	-137.79	-141.28
Rh	-106.34	-108.64	-109.02	-111.61	-136.76	-140.01
Pd	-105.02	-105.89	-107.69	-109.14	-135.44	-137.40
Ag	-103.12	-101.33	-105.80	-104.95	-133.54	-132.95
Cd	-101.69	-99.02	-104.37	-103.07	-132.11	-130.75
Lu	-104.31	-101.26	-106.99	-105.50	-134.73	-132.73
Hf	-111.62	-110.66	-114.30	-114.65	-142.04	-142.06
Ta	-112.59	-112.97	-115.26	-117.03	-143.01	-144.49
W	-112.47	-114.51	-115.15	-118.12	-142.89	-145.87
Re	-111.56	-114.56	-114.24	-118.05	-141.98	-145.98
Os	-109.91	-113.57	-112.59	-116.76	-140.33	-144.97
Ir	-107.68	-111.47	-110.36	-114.53	-138.10	-142.88
Pt	-105.33	-108.04	-108.00	-111.29	-135.75	-139.55
Au	-103.42	-103.31	-106.10	-106.86	-133.85	-134.88
Hg	-101.57	-98.83	-104.24	-102.84	-131.99	-130.51

# 11 Bulk TM

For the bulk systems, stress tensor and atomic forces optimizations were performed considering an increased cutoff energy (two times larger than the recommended PAW cutoff energy) and a  $\mathbf{k}$ -point density of  $50 \text{ \AA}^{-3}$ . We have considered the most stable crystalline structures for each TM element in bulk configuration, within the face-centered cubic (fcc), body-centered cubic (bcc), and hexagonal close-packed (hcp). The properties of interest shown in Figure S5 are the cohesive energy ( $E_{\text{coh}}$ ) and the atomic radius ( $R_{\text{TM}}$ ), the first being obtained by subtracting the bulk total energy (per atom) from the free-atom total energy, while the second property results from  $R_{\text{TM}} = \frac{d_{\text{av}}}{2}$  (where  $d_{\text{av}}$  is the average weighted nearest-neighbor distance) which comes from the combination of the effective coordination concept<sup>9</sup> and the hard-sphere model.<sup>10</sup> These properties are compared with the literature (Exp.),<sup>11</sup> throughout the main text other bulk properties were also needed in a comparative character, as well as some atomic properties, such as electronegativity, being also obtained from the literature.<sup>12</sup>

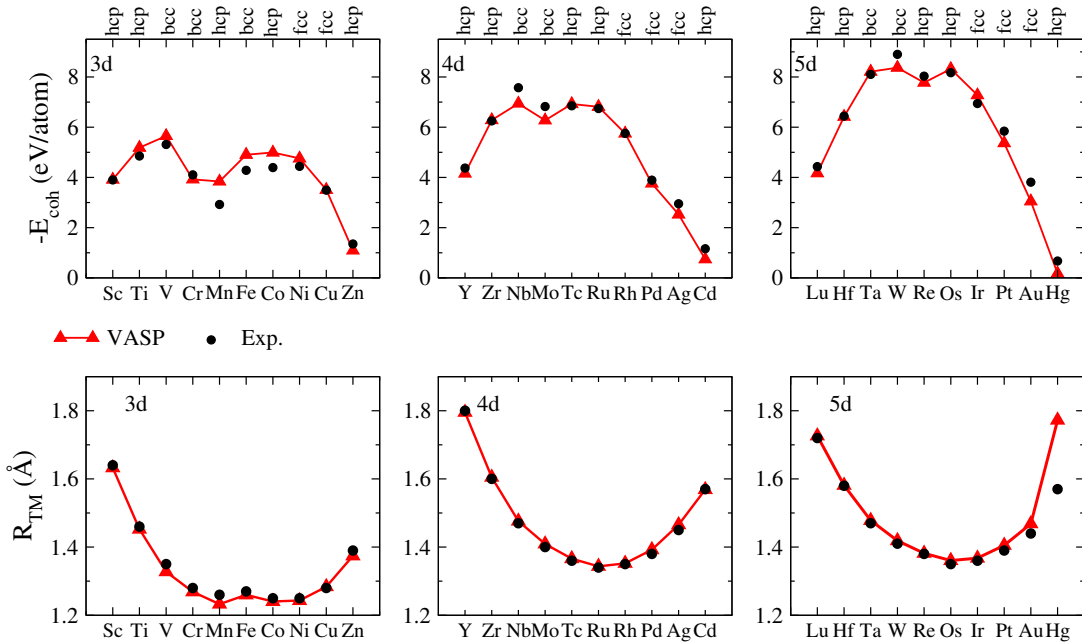


Figure S5: The cohesive energy ( $E_{\text{coh}}$ ) and the atomic radius ( $R_{\text{TM}}$ ) versus atomic number of the most stable TM crystalline structures in face-centered cubic (fcc), body-centered cubic (bcc), or hexagonal close-packed (hcp) configurations. Our  $E_{\text{coh}}$  and  $R_{\text{TM}}$  values (VASP) are compared to experimental (Exp.) ones.<sup>11</sup>

## 12 Statistical Analysis

The quality of  $\Delta E_a$  (atomization energy) fits for TM@Ti<sub>12</sub>, TM@Zr<sub>12</sub>, and TM@Hf<sub>12</sub> systems is assessed by the fraction of variance unexplained (FVU) by the model, the  $R^2$ , correlation coefficient (c.c.), mean absolute error (MAE), and root-mean square error (RMSE).

System / FVU /  $R^2$  / c.c. / MAE / RMSE

TM@Ti<sub>12</sub> / 0.04199947 / 0.95800053 / 0.97877502 / 0.52817D+00 / 0.66190D+00

TM@Zr<sub>12</sub> / 0.04170369 / 0.95829631 / 0.97892610 / 0.47518D+00 / 0.60925D+00

TM@Hf<sub>12</sub> / 0.05628804 / 0.94371196 / 0.97144838 / 0.56307D+00 / 0.74963D+00

The intercepts and slopes of the 3 fits:

System /  $b_0$  /  $b_1$  /  $b_2$  /  $b_3$

TM@Ti<sub>12</sub> / 60.2242 / 1.13944 / -1.00437 / 0.56236

TM@Zr<sub>12</sub> / 67.0683 / 1.18011 / -0.59078 / 0.48868

TM@Hf<sub>12</sub> / 71.9577 / 1.14568 / -0.86461 / 0.55488

For which,  $b_0$  divided by 12 times the cohesive energy gives numbers close to 1 as expected;  $b_1$  is close to 1 as expected, since the contribution of the central atom (TM) to the nanocluster  $\Delta E_a$  is roughly the cohesive energy of TM;  $b_2$  is a negative contribution to  $\Delta E_a$ , since the surface energy is a destabilizing factor, as expected; and  $b_3$  is larger than zero, since the ionic contribution to  $\Delta E_a$  is stabilizing, as expected. Part of the surface energy may be embedded in  $b_0$ , but the variation in surface energy for Ti<sub>12</sub>/Zr<sub>12</sub>/Hf<sub>12</sub> should depend on the radius of the nanocluster which depends on the radius of the central atom.

The  $\Delta\Delta E_a$  values are the differences between  $\Delta E_a$  - model and  $\Delta E_a$  - DFT, which are shown below for TM@Ti<sub>12</sub>, TM@Zr<sub>12</sub>, and TM@Hf<sub>12</sub> systems. Thus,  $\Delta\Delta E_a < 0$  means the nanocluster's DFT ('true') energy is lower (more stable) than the values predicted by the model. These  $\Delta\Delta E_a$  values are the part of  $\Delta E_a$  unexplained by the model. They can be explained by invoking physical effects other than adding cohesive energies, estimating surface energies, and correcting for ionic bonding. In particular,  $\Delta\Delta E_a$  could be caused by electronic shell filling at certain electron counts ( $N_e$ ): 2, 8, 18, 20, 34, 40, 58, 68, 70, ...

Table S10: The  $\Delta E_a$  - DFT,  $\Delta E_a$  - model, and  $\Delta\Delta E_a$  (difference between  $\Delta E_a$  - model and - DFT) values for TM@Ti<sub>12</sub>, TM@Zr<sub>12</sub>, and TM@Hf<sub>12</sub> systems, as well as the chemical species (TM) and electron count ( $N_e$ ) values.

TM@Ti <sub>12</sub>			TM@Zr <sub>12</sub>			TM@Hf <sub>12</sub>			TM	$N_e$
$\Delta E_a$ - DFT (eV)	$\Delta E_a$ - model (eV)	$\Delta\Delta E_a$ (eV)	$\Delta E_a$ - DFT (eV)	$\Delta E_a$ - model (eV)	$\Delta\Delta E_a$ (eV)	$\Delta E_a$ - DFT (eV)	$\Delta E_a$ - model (eV)	$\Delta\Delta E_a$ (eV)		
44.322216	44.054364	-0.267802	58.025244	57.978419	-0.04674748	56.634296	57.872462	0.184851	Sc	51
47.337713	47.044816	-0.292849	60.752046	60.430749	-0.32123247	59.481834	59.780045	0.192330	Ti	52
48.705432	48.742388	0.037002	61.703225	61.590396	-0.11277104	60.721834	60.100216	0.390456	V	53
47.648963	47.336937	-0.311978	60.108196	59.882642	-0.22548899	59.474283	58.302822	0.044473	Cr	54
47.840754	47.542976	-0.297730	60.171500	59.974448	-0.19698831	59.732781	55.736943	-0.034399	Mn	55
48.913202	48.721331	-0.191826	61.007848	61.254069	0.24628072	60.817745	58.512223	-0.006309	Fe	56
49.057214	49.124675	0.067505	61.044266	61.581779	0.53757086	60.924925	58.788774	0.301978	Co	57
48.515212	48.888149	0.372981	60.777368	61.337540	0.56023128	60.480729	58.881705	0.481839	Ni	58
45.891717	47.168861	1.277190	58.508683	59.688316	1.17969945	57.940636	57.945494	1.323900	Cu	59
43.454305	43.631190	0.176934	56.489023	56.337456	-0.15148541	55.566712	55.587526	0.211991	Zn	60
42.419339	42.908762	0.489473	56.539453	57.392427	0.85305628	54.964041	56.835579	0.847371	Y	51
46.820969	47.049779	0.228856	60.664505	60.783729	0.11928887	59.298882	60.874050	0.295967	Zr	52
48.698599	49.155333	0.456777	62.123909	62.461432	0.33757986	61.120138	63.003249	0.300894	Nb	53
48.849741	48.922056	0.072359	62.052153	61.991382	-0.06071340	61.124871	62.024330	0.007679	Mo	54
50.437695	51.722918	1.285254	63.482773	64.646142	1.16342227	62.732789	63.286868	1.538086	Tc	55
50.775475	50.435070	-0.340364	63.501319	63.275284	-0.22598167	63.095991	62.013808	-0.500574	Ru	56
49.894538	49.044149	-0.850346	62.514500	61.881182	-0.63325990	62.238345	60.855104	-1.033007	Rh	57
46.977528	46.513861	-0.463621	59.891570	59.385957	-0.50554345	59.465693	58.722426	-0.774075	Pd	58
43.340942	44.460062	1.119167	56.663243	57.521553	0.85838823	55.952351	57.604649	0.734766	Ag	59
41.041819	41.451355	0.409586	54.819046	54.788310	-0.03064567	53.768030	55.339294	-0.018161	Cd	60
43.120879	43.452270	0.331442	57.098214	57.661513	0.56337905	55.568910	57.451474	0.672717	Lu	51
47.252726	47.512756	0.260076	60.960416	61.159795	0.19944312	59.619640	61.111294	0.240726	Hf	52
50.015005	50.648952	0.633989	63.798329	64.005216	0.20693804	62.517124	63.673358	0.406206	Ta	53
51.097585	51.507008	0.409463	64.403393	64.656967	0.25362205	63.435956	64.695542	0.298542	W	54
51.542977	50.934276	-0.608659	64.728055	63.969482	-0.75852277	63.945031	63.529433	-0.812298	Re	55
52.733435	52.239163	-0.494235	65.588296	65.161764	-0.42648544	65.106940	63.920747	-0.689070	Os	56
52.393814	51.262150	-1.131628	65.104034	64.130828	-0.97315452	64.782511	62.642491	-1.345902	Ir	57
50.099195	48.880396	-1.218761	63.010683	61.774776	-1.23584542	62.585044	61.460728	-1.515580	Pt	58
45.491167	45.786365	0.295239	58.728072	58.777645	0.04964826	58.051539	59.086230	-0.043251	Au	59
40.722053	39.269841	-1.452162	54.458546	53.236711	-1.22173372	53.403072	54.913808	-1.672751	Hg	60

Very similar pattern for TM@Ti<sub>12</sub>, TM@Zr<sub>12</sub>, and TM@Hf<sub>12</sub> systems are found, where the TM dopants that give extra stability are: Ru, Rh, Pd, Re, Os, Ir, Pt, and Hg. Among the  $N_e = 58$  cases, all Pt and Pd containing nanoclusters are 'extra stable' (significant negative  $\Delta\Delta E_a$ ), however Ni does not bring any stability. There must be other factors at play, for example, the overlap of the  $d$  orbitals of the central atom with the  $d$  orbitals of the Ti<sub>12</sub>/Zr<sub>12</sub>/Hf<sub>12</sub> shell, since TM species from the 3rd row have very small  $3d$  orbitals.

## 13 Atomic Positions

Below, we provide the atomic coordinates (*xyz* positions) for the lowest energy (LOW) and icosahedral (ICO) configurations of the  $\text{TM}_{13}$  nanoclusters (for all *3d*, *4d*, and *5d* elements).

### LOW $\text{TM}_{13}$

#### $\text{Sc}_{13}$

Sc -0.0000387127018371 0.0000018622190812 -0.0005048496125060  
Sc 2.5941950889363756 0.7129546418268031 1.3443364164021698  
Sc -2.5936233875090231 -0.7126527899063397 -1.3446095069018220  
Sc -1.8467340969440968 2.2813256355782254 -0.6542426837575590  
Sc -1.2950556177782158 -2.5758874190555350 0.8556864231084749  
Sc 0.0862890480741978 -2.2689299485724153 -1.9717153817529365  
Sc 1.2951171999472368 2.5760290790203300 -0.8552842144902311  
Sc 1.8472480406245513 -2.2815378908300161 0.6543467056810677  
Sc 2.4895887566377866 -0.2366547815385669 -1.6702269471233659  
Sc 0.2549230800393456 -0.7330276577411343 2.9052496920133422  
Sc -0.0864819444185745 2.2686971522272827 1.9723315270790387  
Sc -2.4903370793385946 0.2366910266282662 1.6699237505004234  
Sc -0.2550903755691625 0.7329910901440169 -2.9052909311460962

#### $\text{Ti}_{13}$

Ti 0.0007128099818896 -0.0022643005664786 0.0084565756716977  
Ti 2.2904418622151343 0.6525976125886359 1.1076087255400378  
Ti -2.2865179936490634 -0.6494522766287201 -1.1103278961095668  
Ti -1.6275014005510045 1.9969931917926438 -0.4993980488708107  
Ti -1.1526089223461771 -2.2596666661007250 0.6760572793521273  
Ti 0.0836754903922277 -2.0294721776527993 -1.6632892009482578  
Ti 1.1533648204535272 2.2587687601816260 -0.6754525468674899  
Ti 1.6281363500627783 -1.9989968569035241 0.4969618698098817  
Ti 2.2073685306176802 -0.2278620094558370 -1.3983558951491251

Ti 0.2208224792336164 -0.6334411471546755 2.5115334920151806  
Ti -0.0836917625399813 2.0274069820486922 1.6646235567267116  
Ti -2.2134006736134895 0.2311551233417291 1.3948369609250282  
Ti -0.2208015902571177 0.6342337645094140 -2.5132548720954038

V<sub>13</sub>

V -0.0006452183576400 0.6353509391391654 -0.2619215509980251  
V -0.0213901162306289 1.3180834279935674 1.9748090413357051  
V -0.0125249446379279 -0.9352911907385515 1.9596905545213676  
V 0.0157875894875712 0.5636371299088694 -2.6670019474555025  
V 0.0251140617831513 -1.2604687912286590 -2.2699473274912814  
V 2.0947119948600665 1.7425146596507837 0.4899850809285429  
V 1.3195142148237924 -1.7282088473809214 -0.1206979408483964  
V -2.1152462255632489 1.7233302298951294 0.4458970142881569  
V -1.2996263432795381 -1.7415274863694066 -0.1395136346970567  
V 2.1264901459214069 0.0354056813658783 1.4529750727244473  
V 2.1339184539798151 -0.1734022275905218 -1.1221250072812943  
V -2.1510028910787957 0.0195816450976452 1.4157526110376715  
V -2.1151007217080071 -0.1990051697429642 -1.1579019660643421

Cr<sub>13</sub>

Cr -0.0001254253143053 -0.0003215919718436 0.0004031620518905  
Cr -0.3290784926583559 1.1413106830384301 2.0768112167871688  
Cr 0.0357531006210152 -1.3635143724528493 2.2703806315088038  
Cr -0.0369206922144514 1.3618749090362581 -2.2709591406571077  
Cr 0.3279343084059967 -1.1407089783307693 -2.0763433795626192  
Cr 1.1663487626746001 2.0454788458301856 -0.4221518502372152  
Cr 1.3215210279757876 -2.2946879678084997 -0.0416175899755817  
Cr -1.3205654424653428 2.2954883992115072 0.0421048318108994

Cr -1.1665868154161760 -2.0462342280205643 0.4211983193466544  
Cr 2.0863014314711350 -0.4320575807853597 1.0899336739820029  
Cr 2.2419809075861252 -0.0278147756090927 -1.4112649840047968  
Cr -2.2411089070930483 0.0285144206561245 1.4118278936356834  
Cr -2.0854537635729837 0.4326722372064662 -1.0903227846857941

### Mn<sub>13</sub>

Mn 0.1917351805380925 -0.0401226099306644 0.1619060842488356  
Mn 2.1891064668720723 0.6015906049002009 1.1774312364013291  
Mn -2.1624562993816712 -0.5532000801484607 -1.0069919139201904  
Mn -1.4674037855496831 1.8079807233887788 -0.6490782551105987  
Mn -1.0048359242593836 -2.0290511321923113 0.6647824443982362  
Mn -0.0154443219424820 -1.7231760463832018 -1.7000835421241955  
Mn 1.1161674811416518 2.0647687856238583 -0.7059511287559914  
Mn 1.5803638321425506 -1.9580427347929614 0.5043991381753639  
Mn 1.9456349479238817 -0.2815523870597669 -1.3246133425404540  
Mn 0.2017675024252092 -0.5691246822013110 2.4564268244231631  
Mn -0.1821320869035645 1.7858189100915549 1.5001644048572924  
Mn -2.1525303371783284 0.2315013672010782 1.4202928120445719  
Mn -0.2399726558283497 0.6626092815031797 -2.4986847620973620

### Fe<sub>13</sub>

Fe -0.5499095497171016 -1.9656423312307219 1.0968512862100237  
Fe 2.3630722609528565 0.3339230709709629 -0.3571035554882425  
Fe -1.5640902839233615 0.6726667251428431 -1.7093593657818911  
Fe -2.3637035794188481 -0.3336260691058719 0.3544686618827342  
Fe 1.3944697088507887 -1.8907512016790307 -0.5517875295756038  
Fe 1.0343491622037249 1.6787327914524255 1.3906243119456878  
Fe -0.0002067524118257 0.0001843845326839 0.0000750029307550

Fe 0.7585560962875650 -0.2890937081939811 -2.2716085558107268  
Fe -1.0318288362444168 -1.6809349304127341 -1.3896754458450982  
Fe 1.5631506538530644 -0.6733632441219335 1.7108031723365809  
Fe -1.3923193605930884 1.8918809636939855 0.5533022576201425  
Fe 0.5486093916665755 1.9658887049125600 -1.0978094809029280  
Fe -0.7601489115059419 0.2901348440388123 2.2712192404785796

### Co<sub>13</sub>

Co -0.9537095176637091 2.2938577402367812 0.4901541397683893  
Co -0.7084035435552511 -0.0828350292781757 0.6110040526297240  
Co 1.3490139264887979 -1.0411516604415976 -0.1045127419755065  
Co -1.7973103744939092 -1.4751865920659419 -1.0017257648426519  
Co 0.8636944302851184 -1.0421066996114519 2.1400340330365246  
Co 0.5674297464604372 1.2731438122404288 2.1130830627564183  
Co -0.1466462170379810 -0.0383243757539642 -1.6999073204735478  
Co -0.4325369270103590 2.3040684128501052 -1.7050003790962354  
Co -0.3456464334777323 -2.4479842223832664 0.5458831205205747  
Co 1.0436011364363633 1.3455527799036719 -0.1323851380000907  
Co -2.1082782908760667 0.9510426892271315 -1.0314085882660358  
Co 0.1676092791062693 -2.3762941071356716 -1.6506044093232237  
Co 2.5011827853380115 0.3362172522119682 1.4253859332656642

### Ni<sub>13</sub>

Ni -0.0100095819097312 2.5019700856375984 -0.8517417300358687  
Ni 0.6328069531954554 1.2848449058599094 -2.7370326389570891  
Ni 1.6379441838239650 0.7256742780224776 -0.7309739438939822  
Ni -0.8146582753667975 -2.5619721380420026 1.5231004729562745  
Ni -1.1232617312408344 -1.9562858874135980 -0.8165793379148187  
Ni -1.5980875984223477 -0.4523288703083530 0.9909018591002638



Ni 0.6961324754994536 -1.0488595563682122 -2.0417727297657189  
Ni 2.2171394344067394 0.1343629347053721 1.4740489958093050  
Ni 0.7075345433056413 -1.2009899566015836 0.3274892608264253  
Ni -0.8247157232530782 0.3813120780801427 -1.1079344097007429  
Ni 0.2593442923394438 -0.7461100681124542 2.5224596371554622  
Ni -1.9434849061001955 1.7896040169341596 0.3554017090174515  
Ni 0.1633159337222789 1.1487781776065589 1.0926328554030302

### Cu<sub>13</sub>

Cu -0.8051129437054971 -2.4296106301746327 -1.4018451893701300  
Cu -2.7306774166640375 0.1318810110688311 1.0258975043550596  
Cu 0.2411341549774324 -0.7821668449875361 -2.8912916646790716  
Cu 0.8647167618798317 1.8682795231404334 2.4129835901316721  
Cu 1.0488683435257347 -0.4303154815803349 1.8049381209968125  
Cu -1.0441801806421065 0.2567897249679358 2.8056771504506006  
Cu 2.3951610402803638 0.2527583448177211 -2.0658767278495693  
Cu 0.2922928340372959 1.3015327711352338 -1.6616341697065380  
Cu 1.9084308277343567 1.2413392048749277 0.2035361966100595  
Cu 0.8868749117221650 -0.8820877777894136 -0.5829737848570122  
Cu -0.5374663835860272 1.1083330918369061 0.6203066530620589  
Cu -0.9628160892138471 -1.4457290105973328 0.9026914981233229  
Cu -1.5572258603456461 -0.1910039267127459 -1.1724091772672569

### Zn<sub>13</sub>

Zn -1.8398428799943538 0.1705557742520298 -1.6770431534616552  
Zn -1.9804303877569467 2.2458934312850065 1.9098560819196493  
Zn 0.2912915764559028 -1.2228362157360646 -1.9231902687493676  
Zn -0.8003029075004502 -0.8975826183330362 0.5396858242009390  
Zn 0.3516726153991474 1.3415366114790430 -1.0348714508913410

Zn 2.3914335650115088 0.3636257955437969 -2.3552679700170156  
Zn 0.4543284257058691 1.3258203328971945 1.5791364372994252  
Zn 2.7385489013609803 -1.5920403350034960 -0.7127116267461755  
Zn 0.7118478795181673 -2.9332136341439448 0.0622204656806620  
Zn -3.4667856277392382 1.4908251679379383 -0.1183091517207338  
Zn 1.5576047706996334 -1.0054278515940247 1.6540110714666234  
Zn -3.0796316292076877 -0.2342551486804005 1.8738251941694770  
Zn 2.6702656980474675 0.9470986900959453 0.2026585468495199

Y<sub>13</sub>

Y -0.0000026153846342 -0.0000026153846342 -0.0000026153846342  
Y -0.0000026153846342 1.7417733821675760 2.8179972144867307  
Y -0.0000026153846342 -1.7417616129367204 2.8179972144867307  
Y -0.0000026153846342 1.7417733821675760 -2.8180024452560000  
Y -0.0000026153846342 -1.7417616129367204 -2.8180024452560000  
Y 1.7417733821675760 2.8179972144867307 -0.0000026153846342  
Y 1.7417733821675760 -2.8180024452559991 -0.0000026153846342  
Y -1.7417616129367204 2.8179972144867307 -0.0000026153846342  
Y -1.7417616129367204 -2.8180024452559991 -0.0000026153846342  
Y 2.8179972144867307 -0.0000026153846342 1.7417733821675743  
Y 2.8179972144867307 -0.0000026153846342 -1.7417616129367204  
Y -2.8180024452559991 -0.0000026153846342 1.7417733821675743  
Y -2.8180024452559991 -0.0000026153846342 -1.7417616129367204

Zr<sub>13</sub>

Zr 0.0000691884991522 -0.0001030684634973 -0.0004825465930853  
Zr -0.0212869707271874 1.5423221813348569 2.4248530107110291  
Zr 0.0466507965573992 -1.4975814938330938 2.4528105344659821  
Zr -0.0468144931208982 1.4969223497432633 -2.4527594170641063

Zr 0.0219946780646119 -1.5428377217011597 -2.4244505303446680  
Zr 1.5389169576888904 2.4268399076124005 -0.0305907477617726  
Zr 1.5003754027942815 -2.4501358322306093 -0.0410693746538424  
Zr -1.5000578822943389 2.4506527386361014 0.0418264435971487  
Zr -1.5399273545392038 -2.4265138383143512 0.0303527020935750  
Zr 2.4290256641404859 -0.0229408055049198 1.5354229765330949  
Zr 2.4482333105104246 0.0418062863502691 -1.5048594226605605  
Zr -2.4483017136306193 -0.0405755047473093 1.5042174971628235  
Zr -2.4288775839430050 0.0221448011180705 -1.5352711254856324

### Nb<sub>13</sub>

Nb 2.6185249004120674 -1.2829413768122357 0.6426137570328709  
Nb 0.3426789438335476 0.5335323959872404 0.4466906551667407  
Nb 0.2723916188155471 -2.4805446428831566 -0.1021522322878976  
Nb -1.3645888846598275 2.4210519795192820 1.2151151866455674  
Nb -1.0369973331588991 2.1531031192718473 -1.3906334473525650  
Nb 1.2541945989909404 1.3308040343273611 -2.1977845851423830  
Nb -0.8865798460533991 -0.6014978999860467 -1.8226025840293012  
Nb -1.9145495339734566 -1.6335092896968781 0.6615464756177154  
Nb -2.7022873351762531 0.6622347554298855 -0.1717355494507533  
Nb 1.9269996889078573 -1.0274034976219486 -1.7604346411236271  
Nb -1.6631601297742051 0.2500662095745909 2.4420866080362664  
Nb 2.8041446002296411 1.0624957936025510 -0.2310545204007504  
Nb 0.3492287116064432 -1.3873915807124781 2.2683448772881150

### Mo<sub>13</sub>

Mo 0.0001181225595897 0.0001237262120508 0.0002188042360611  
Mo -0.4728464047777745 1.1847558165507319 2.2290100893730767  
Mo 0.0466698992794985 -1.3667900611938908 2.3038087257930897

Mo -0.0474856271942610 1.3656449882287323 -2.3042255666792730  
Mo 0.4729148666882139 -1.1848337324030158 -2.2288036740989190  
Mo 1.2017590454797560 2.1965601323099353 -0.5735806404583492  
Mo 1.3242359794841878 -2.3284565299048534 -0.0488592735458901  
Mo -1.3235355652866776 2.3287223989777832 0.0493723721691648  
Mo -1.2019158493307174 -2.1963468992649275 0.5726093576691369  
Mo 2.2340051110309673 -0.5848367941127375 1.1244630087814382  
Mo 2.2722303627442901 -0.0223175245189502 -1.4178393357276349  
Mo -2.2721845505525309 0.0224412982045639 1.4181136248532837  
Mo -2.2339653901245402 0.5853331809145885 -1.1242874923651840

### Tc<sub>13</sub>

Tc -0.3706291049450918 2.7045924443765887 0.0277502049903511  
Tc -0.1419610220886707 0.2813050555185210 0.9145203493770726  
Tc 0.9761685955240580 -1.4984188490577655 -0.4857484149870945  
Tc -2.2402155044501075 -1.1870862455253999 0.9941447298557549  
Tc 2.1789609535141317 -0.7073903637201582 1.4777991524045131  
Tc 2.0792205609443126 1.6056426572490352 0.7417476925120390  
Tc -1.3673885667033314 -0.4478687149797587 -1.1689760980613837  
Tc -1.4073303584476093 1.9477030611602668 -1.9757380209082207  
Tc -0.0318009914106359 -2.1737533069328236 1.6384988788159394  
Tc 0.8391225933275592 1.0290091858643837 -1.2972237002643414  
Tc -2.3727571068527187 1.3354374917588157 0.1490854347129158  
Tc -1.1767840109429084 -2.8451936154105608 -0.3366333470576439  
Tc 3.0353939625310016 -0.0439788003011490 -0.6792268613899104

### Ru<sub>13</sub>

Ru -1.3839493422002942 -1.1612177281343907 -2.3340277660871696  
Ru -1.3219087143332313 -1.1377699345089223 0.1199609942240905

Ru -1.4275625066848754 -1.1648760573051717 2.5247339593936111  
Ru 0.9112752409756091 -1.1991256436687276 -2.4044068696098400  
Ru 0.9525888425431557 -1.1621812346033238 0.1781584160426704  
Ru 0.8995467984887657 -1.1658375218031942 2.5553326188136776  
Ru -1.3852674136913574 1.1639764059956459 -2.3324182854571500  
Ru -1.3236975459427853 1.1350453377201131 0.1211670035066312  
Ru -1.4297343655618668 1.1587011511864507 2.5259005530620211  
Ru 0.9098125217765123 1.2042369564401607 -2.4018287938153904  
Ru 0.9507396295906076 1.1628066812058275 0.1795236159076516  
Ru 0.8975075217775021 1.1643228488428310 2.5564494092242462  
Ru 2.7506493332622579 0.0019187386326980 -1.2885448552050214

### Rh<sub>13</sub>

Rh -1.5888693846358333 -1.2092673263933200 -2.3958917156594701  
Rh -1.4353322269031921 -1.1813438049295968 -0.0196660399858679  
Rh -1.3203066617710668 -1.2015733473763355 2.3661247365893274  
Rh 0.8123669386944794 -1.2091224652296226 -2.5326344675387347  
Rh 0.9521250949665507 -1.1762400851846095 -0.1757996094908378  
Rh 1.0965253439858795 -1.2192468264694316 2.2699698825342924  
Rh -1.5879692306503834 1.2078674012130932 -2.3976176934144640  
Rh -1.4341496466357917 1.1828545256524396 -0.0213820082742551  
Rh -1.3187122461008762 1.2063299411039878 2.3644588295883917  
Rh 0.8132111533165478 1.2055269401499586 -2.5341588465641385  
Rh 0.9531437341446036 1.1741626282444422 -0.1774588866247448  
Rh 1.0979173740072206 1.2214285195863877 2.2679896676427980  
Rh 2.9600497575818707 -0.0013761003673967 0.9860661511977060

### Pd<sub>13</sub>

Pd -0.4937589282135146 -0.2807630344681691 -1.9212905722298288

Pd 2.2263330033493354 0.1307136751917337 -1.9200169388975716  
Pd 0.8833697257614244 1.4962897199850964 -0.0811474807894808  
Pd -1.4446448250571642 0.1346029201466692 3.2722864299144661  
Pd -0.9350521045792028 -2.5026838561721823 -0.4995226462125402  
Pd -0.3016806003120553 -1.9975013119656779 2.1132996599490923  
Pd 1.1705645332726640 -2.2851894081580078 -2.1662423577121306  
Pd 1.2828824113392230 -1.1578336315668043 0.2027716894638232  
Pd 0.5193013693261221 2.0280184483769013 -2.6271274462812197  
Pd -1.6093963908791196 1.9584833870974094 -0.9784917408709664  
Pd -0.9352887989601335 2.2162590457572975 1.6600244058413143  
Pd 0.9849050718293491 0.3977227974727562 2.3344581676994434  
Pd -1.3475344668769456 -0.1381187516970162 0.6109988301256077

Ag<sub>13</sub>

Ag -0.9234715159940414 -2.9728534466452317 1.2932873940259721  
Ag -1.3033824367424867 0.5694761175771177 -1.9921442457917422  
Ag 0.2022221364699242 -1.4180677985303731 -0.7477967956212304  
Ag -2.4836701100783651 2.4161575885567643 -0.2550523990795774  
Ag 0.0837460292678678 1.5686383996110997 0.3834897766741090  
Ag 1.5306930938140066 0.7970217465274168 -1.9464419579643337  
Ag 2.8476521823175318 -1.7388332029404587 -1.4703052872723532  
Ag -0.2030248194924162 3.1145738162894396 -1.8827719125815943  
Ag 1.8604167291304599 -2.7369035902516803 1.0513572459541294  
Ag -2.1515472626796690 -0.4822413044209171 0.4246031974921198  
Ag -1.9311738132873515 1.4804832758822606 2.3306677677475136  
Ag 0.1123574316455702 -0.5829132579212253 2.1634278550818760  
Ag 2.3591823556289793 -0.0145383437342197 0.6476793613351113

Cd<sub>13</sub>

Cd 1.5994997784099514 2.6791958262543307 1.3050429305433120  
Cd 1.9141029495153834 -0.4181904621093668 1.6562312653126696  
Cd -2.8573592622800810 -0.9835496879702763 0.1725783711894575  
Cd -1.8017602720819372 1.3812346448588055 -1.3720200698729723  
Cd -1.9310790158380762 -3.5935843419804243 1.4199257877577018  
Cd 0.1017293291504711 -1.0530601635036678 -0.9674537878882035  
Cd 0.7054932543848409 3.2944349960237478 -1.6630812774619859  
Cd 0.3104483842785868 -4.1534123741453026 -0.6745635653608133  
Cd 2.5531743406090062 0.7968799887663014 -1.0204665605239303  
Cd 0.9678192472788485 -3.2259050679627785 2.2921301385441737  
Cd -1.2353074711345133 3.7066358845869978 0.6434638752111521  
Cd -0.8759866365477809 0.7830860088360243 1.5756655754830327  
Cd 0.5492253742553146 0.7862347483455974 -3.3674526829335951

Lu<sub>13</sub>

Lu -0.5199685944143546 -0.3206433858566040 0.3466637420812759  
Lu 2.3823060827712901 0.8642190948022321 0.5139419818247362  
Lu -2.7893366456851885 -0.7770463328540576 -1.4200422657849874  
Lu -1.8369887071472242 2.3884595041200232 -0.6653759969167545  
Lu -1.4708016136695150 -2.9051789620419317 0.9797911416766265  
Lu 0.1652298500708262 -2.3279379438882586 -2.0219187022351859  
Lu 1.2402339118661274 3.5424398959688599 -0.8218141057264248  
Lu 1.9242622660776121 -2.3354325702452954 0.6059504184876996  
Lu 3.1096759591179826 -0.8617949690101625 -2.0852217050867070  
Lu 0.2538122098658970 -0.7856554006139280 3.1156197575517908  
Lu -0.0780814263565972 2.3824727720084393 1.9612954947891499  
Lu -2.8152153094219816 0.2641591319815770 1.8878517898160787  
Lu 0.4348720169251443 0.8719391656290920 -2.3967415504773211

Hf<sub>13</sub>

Hf 0.0311028134630718 0.0578588311051256 0.0453088685376422  
Hf 0.0025815238035918 1.4618453378718321 2.4518421005090794  
Hf -0.0008664842069521 -1.4845097627734720 2.5034121556123079  
Hf -0.0205686888665184 1.4129840032582059 -2.3667039773665310  
Hf -0.0222569936325847 -1.5089347569091114 -2.4443248469921031  
Hf 1.5512466609863118 2.4109796911074266 -0.0309238368008291  
Hf 1.4236931143911278 -2.3665830903638820 -0.0280446257972784  
Hf -1.5438302778763386 2.4540924356630818 -0.0055451285558412  
Hf -1.5153230406033718 -2.4267371615600730 -0.0155550688277177  
Hf 2.4271477713158696 -0.0336485817344574 1.4725762289281974  
Hf 2.4850970875103187 0.0466077259040141 -1.5001549888122891  
Hf -2.3679177653826198 -0.0248073464304195 1.4263192331495045  
Hf -2.4501057209018935 0.0008526748617257 -1.5082061135841478

Ta<sub>13</sub>

Ta 2.5623185956253458 -1.2406130472100436 0.8287956416930982  
Ta 0.3380993308860809 0.5278324022585146 0.4354783373964342  
Ta 0.3990190731657641 -2.5106175440880518 -0.1998664258230693  
Ta -1.2846542520647315 2.5387404804017883 1.2078539568612054  
Ta -1.0612450552810522 2.1804970069788929 -1.3714332366462418  
Ta 1.1584956553001202 1.2807268762684902 -2.2762789741456846  
Ta -0.8844637449482438 -0.5985550150085768 -1.8085187826722890  
Ta -1.8561409707746250 -1.6798975768860380 0.6170080230979309  
Ta -2.7254706945387390 0.7073749364746327 -0.0677728162971167  
Ta 1.9645678362498753 -1.0543198618413889 -1.7283503066459733  
Ta -1.7044872805108859 0.2876920855003426 2.3931592135333997  
Ta 2.8016266970574755 1.0649836499641872 -0.2900219441641081



Ta 0.2923348098336227 -1.5038443928127414 2.2599473138124235

W<sub>13</sub>

W -1.2756867990008800 2.5174526717496288 -0.4020420536131990

W -2.2615402062338807 0.1112645798787053 -0.1056891483232008

W -1.9304009784403586 -2.3561043766968588 0.0294638894980430

W -1.4720970434269169 1.0336165083221367 -2.3595274033977880

W 0.0370319390191476 -0.8597896760394761 -1.0494371583781223

W 0.2573542816388041 -2.1473022683034211 1.2880597265649545

W 1.0141671151518317 2.7875521001903412 0.0674715528316572

W 0.0037626414195184 0.5181510986666691 1.2544912095836622

W -1.9506008608685192 -1.1242482532968374 2.0663669080282876

W 0.7680953250982085 1.7197282567711856 -2.1397861085599867

W 2.1836487321816467 0.5374909578121496 -0.2832477223542007

W 2.3041670035922568 -0.7622465550817967 1.8410009249119845

W 2.3220988498691586 -1.9755650439724288 -0.2071246167920808

Re<sub>13</sub>

Re -1.0374728001696187 2.5153615742640945 0.5223287484921091

Re -0.7257024731482140 -0.0857937373591184 0.6262670287142225

Re 1.4725761988453936 -1.1800568795791886 -0.0767270237913369

Re -1.9552230633555485 -1.6210041825092940 -1.1074643118639340

Re 0.9608265279090613 -1.1343792297085624 2.3380937265762149

Re 0.6372962272176252 1.3916178595854021 2.3094794662540394

Re -0.2135317868012638 -0.0486127923585720 -1.8758462812221506

Re -0.4749696926292799 2.4963102319782671 -1.8406349312136037

Re -0.3721532526306728 -2.6832582792674025 0.5815422428583528

Re 1.1283149486338235 1.5108895092939534 -0.1071512381038495

Re -2.2969788322352791 1.0514484734841290 -1.1379829836299020

Re 0.1736139402719079 -2.5761101681105778 -1.7829051069406283

Re 2.7034040580920493 0.3635876202868626 1.5510006638704752

### Os<sub>13</sub>

Os -1.7022640364956683 -1.1929683872710513 -2.4545382440163372

Os -1.0402246866891893 -1.1747000377187771 -0.0937679387037367

Os -1.4655629460445532 -1.1992494455545213 2.2515783048097919

Os 0.6449071280801419 -1.1966315797074607 -2.1160982246736015

Os 1.4004086643906337 -1.2112856625246593 0.4019426223212292

Os 0.8701733722476241 -1.2031353632314730 2.6791366469438156

Os -1.7183678126512092 1.1800257953448323 -2.4496503394579321

Os -1.0559890834788419 1.1610261620489251 -0.0888905171982373

Os -1.4811237960188688 1.1702603634518507 2.2566021523863284

Os 0.6284367794558836 1.2139386350130206 -2.1112866434683131

Os 1.3838594647692197 1.2285151520653610 0.4071403302508827

Os 0.8543799586782779 1.2028269995303376 2.6843282066435208

Os 2.6813669937565603 0.0213773685535887 -1.3664963558374019

### Ir<sub>13</sub>

Ir -1.4549832239127998 -1.2245712487516531 -2.3251023867254279

Ir -1.4324174443839173 -1.2017961902959975 0.1138018894066004

Ir -1.4393326245936748 -1.1993276520671721 2.5215558534218214

Ir 0.9398702825729526 -1.2100230668918304 -2.3528519991003805

Ir 0.9898932419112114 -1.1939926198185908 0.1306567312314773

Ir 0.9516186454155964 -1.1995134896139898 2.5197724564639667

Ir -1.4579193642919570 1.2196707368485598 -2.3260457129948460

Ir -1.4351424192257678 1.1987764172385269 0.1129683110209854

Ir -1.4418485569991688 1.1976314091538391 2.5207553099696636

Ir 0.9370162373009077 1.2103561400400924 -2.3538111993359241

Ir 0.9871260656673222 1.1963491352537687 0.1299825912492754  
Ir 0.9489998765250700 1.2029059314435457 2.5189904377311212  
Ir 2.9071192840142057 0.0035344974608833 -1.2106722823383471

Pt<sub>13</sub>

Pt 2.9316738734128158 1.2337364360880478 0.8288133288244453  
Pt -1.6320264175437948 0.7083693742005686 0.8084884120050866  
Pt 2.7687570662256018 -0.6459493118801447 -0.8891649970873612  
Pt -1.6313029022741148 -1.7957342040892783 1.0120654301196570  
Pt 1.0706119732604069 -2.2655583632605634 -2.1245044904656183  
Pt -1.9495358977014465 0.7053998895483318 -1.6946729155083382  
Pt 0.5107510281984986 0.2554519758646059 -1.5341469923452937  
Pt 0.7887122135246329 -1.5333592552445694 0.3892573442530107  
Pt -1.4770355048182484 -1.8262141152788764 -1.5502027915662850  
Pt 0.7152373400004528 2.2087023962173866 0.0273635538577643  
Pt -1.3058041012021775 -0.3623345898522903 3.1346705549741003  
Pt -1.6598288344457330 2.9522375352810677 -0.4603545758185028  
Pt 0.8697901633630991 0.3652522324057337 2.0523881387573368

Au<sub>13</sub>

Au -1.3168344010157806 -1.1537245643546790 -2.9502654231317109  
Au -1.8198466257781085 -1.6429719176696782 2.3721873371232522  
Au 0.6820030475932661 0.6228726028264617 -3.3003509984229566  
Au 0.2215045818192642 0.1849395866066761 2.1589918616458679  
Au 2.5659587060690470 -0.6264158657190713 0.8136487708405333  
Au 0.5379076700158816 -2.4429991386277070 1.1722932727270656  
Au 1.5616677131047414 1.4037890391459928 -0.8923032527715815  
Au -0.3343775037079197 2.6143407155174678 0.8356904579073241  
Au 2.2331511742865668 1.9884803858153131 1.6543202602981850

Au 1.0011935647288350 -1.3957683723555636 -1.3747245610506393  
Au -2.3616761429426285 0.7960374156522594 1.1903210279386940  
Au -1.6897463593734141 -1.5102795854615092 -0.3197590592580806  
Au -1.2809054247997427 1.1616996986240089 -1.3600496938459532

Hg<sub>13</sub>

Hg -0.0000000000000213 -0.000000000000195 -0.000000000000195  
Hg -0.0000000000000213 1.8399065899347828 2.9728550621494936  
Hg -0.0000000000000213 -1.8399065899348273 2.9728550621494936  
Hg -0.0000000000000213 1.8399065899347828 -2.9728550621493950  
Hg -0.0000000000000213 -1.8399065899348273 -2.9728550621493950  
Hg 1.8399065899347811 2.9728550621494936 -0.000000000000195  
Hg 1.8399065899347811 -2.9728550621493950 -0.000000000000195  
Hg -1.8399065899348290 2.9728550621494936 -0.000000000000195  
Hg -1.8399065899348290 -2.9728550621493950 -0.000000000000195  
Hg 2.9728550621494918 -0.000000000000195 1.8399065899347828  
Hg 2.9728550621494918 -0.000000000000195 -1.8399065899348273  
Hg -2.9728550621493968 -0.000000000000195 1.8399065899347828  
Hg -2.9728550621493968 -0.000000000000195 -1.8399065899348273

**ICO TM<sub>13</sub>**

Sc<sub>13</sub>

Sc 0.000000000000018 0.000000000000000 0.000000000000000  
Sc 0.000000000000018 1.5811900052775982 2.5584450130230092  
Sc 0.000000000000018 1.5811900052775982 -2.5584450130230119  
Sc 0.000000000000018 -1.5811900052776000 2.5584450130230092  
Sc 0.000000000000018 -1.5811900052776000 -2.5584450130230119  
Sc 1.5811900052776000 2.5584450130230110 0.000000000000000  
Sc -1.5811900052776000 2.5584450130230110 0.000000000000000

Sc 1.5811900052776000 -2.5584450130230110 0.0000000000000000  
Sc -1.5811900052776000 -2.5584450130230110 0.0000000000000000  
Sc 2.5584450130230110 0.0000000000000000 1.5811900052775982  
Sc 2.5584450130230110 0.0000000000000000 -1.5811900052776018  
Sc -2.5584450130230101 0.0000000000000000 1.5811900052775982  
Sc -2.5584450130230101 0.0000000000000000 -1.5811900052776018

Ti<sub>13</sub>

Ti 0.0000000000000000 0.0000000000000000 0.0000000000000000  
Ti 0.0000000000000000 1.3719275217307914 2.2198006497774543  
Ti 0.0000000000000000 1.3719275217307914 -2.2198006497774525  
Ti 0.0000000000000000 -1.3719275217307914 2.2198006497774543  
Ti 0.0000000000000000 -1.3719275217307914 -2.2198006497774525  
Ti 1.3719275217307914 2.2198006497774543 0.0000000000000000  
Ti -1.3719275217307914 2.2198006497774543 0.0000000000000000  
Ti 1.3719275217307914 -2.2198006497774525 0.0000000000000000  
Ti -1.3719275217307914 -2.2198006497774525 0.0000000000000000  
Ti 2.2198006497774543 0.0000000000000000 1.3719275217307914  
Ti 2.2198006497774543 0.0000000000000000 -1.3719275217307914  
Ti -2.2198006497774525 0.0000000000000000 1.3719275217307914  
Ti -2.2198006497774525 0.0000000000000000 -1.3719275217307914

V<sub>13</sub>

V 0.0000000000000000 0.0000000000000000 0.0000000000000000  
V 0.0000000000000000 1.3219372070960169 2.0044903385589929  
V 0.0000000000000000 1.3219372070960169 -2.0044903385589929  
V 0.0000000000000000 -1.3219372070960169 2.0044903385589929  
V 0.0000000000000000 -1.3219372070960169 -2.0044903385589929  
V 1.3219372070960169 2.0044903385589929 0.0000000000000000

V -1.3219372070960169 2.0044903385589929 0.0000000000000000  
V 1.3219372070960169 -2.0044903385589929 0.0000000000000000  
V -1.3219372070960169 -2.0044903385589929 0.0000000000000000  
V 2.0044903385589929 0.0000000000000000 1.3219372070960169  
V 2.0044903385589929 0.0000000000000000 -1.3219372070960169  
V -2.0044903385589929 0.0000000000000000 1.3219372070960169  
V -2.0044903385589929 0.0000000000000000 -1.3219372070960169

Cr<sub>13</sub>

Cr -0.000000000000000018 0.0000000000000000 0.0000000000000000  
Cr -0.000000000000000018 1.2054212267970303 2.0128021754595782  
Cr -0.000000000000000018 1.2054212267970303 -2.0128021754595782  
Cr -0.000000000000000018 -1.2054212267970321 2.0128021754595800  
Cr -0.000000000000000018 -1.2054212267970321 -2.0128021754595782  
Cr 1.2054212267970286 2.0128021754595782 0.0000000000000000  
Cr -1.2054212267970339 2.0128021754595800 0.0000000000000000  
Cr 1.2054212267970286 -2.0128021754595782 0.0000000000000000  
Cr -1.2054212267970339 -2.0128021754595782 0.0000000000000000  
Cr 2.0128021754595782 0.0000000000000000 1.2054212267970303  
Cr 2.0128021754595782 0.0000000000000000 -1.2054212267970321  
Cr -2.0128021754595800 0.0000000000000000 1.2054212267970303  
Cr -2.0128021754595800 0.0000000000000000 -1.2054212267970321

Mn<sub>13</sub>

Mn 0.0000000000000000 0.0000000000000000 0.0000000000000000  
Mn 0.0000000000000000 1.3870061983045119 2.1755151797349921  
Mn 0.0000000000000000 1.3870061983045119 -2.1755151797349903  
Mn 0.0000000000000000 -1.3870061983045101 2.1755151797349921  
Mn 0.0000000000000000 -1.3870061983045101 -2.1755151797349903

Mn 1.3870061983045119 2.1755151797349921 0.0000000000000000  
Mn -1.3870061983045101 2.1755151797349921 0.0000000000000000  
Mn 1.3870061983045119 -2.1755151797349903 0.0000000000000000  
Mn -1.3870061983045101 -2.1755151797349903 0.0000000000000000  
Mn 2.1755151797349921 0.0000000000000000 1.3870061983045119  
Mn 2.1755151797349921 0.0000000000000000 -1.3870061983045101  
Mn -2.1755151797349903 0.0000000000000000 1.3870061983045119  
Mn -2.1755151797349903 0.0000000000000000 -1.3870061983045101

Fe<sub>13</sub>

Fe 0.0000000000000000 0.0000000000000000 0.0000000000000000  
Fe 0.0000000000000000 1.2918631355798045 2.0160473319233638  
Fe 0.0000000000000000 1.2918631355798045 -2.0160473319233629  
Fe 0.0000000000000000 -1.2918631355798027 2.0160473319233638  
Fe 0.0000000000000000 -1.2918631355798027 -2.0160473319233629  
Fe 1.2918631355798045 2.0160473319233638 0.0000000000000000  
Fe -1.2918631355798027 2.0160473319233638 0.0000000000000000  
Fe 1.2918631355798045 -2.0160473319233629 0.0000000000000000  
Fe -1.2918631355798027 -2.0160473319233629 0.0000000000000000  
Fe 2.0160473319233638 0.0000000000000000 1.2918631355798045  
Fe 2.0160473319233638 0.0000000000000000 -1.2918631355798027  
Fe -2.0160473319233629 0.0000000000000000 1.2918631355798045  
Fe -2.0160473319233629 0.0000000000000000 -1.2918631355798027

Co<sub>13</sub>

Co 0.0000000000000000 0.0000000000000000 0.0000000000000000  
Co 0.0000000000000000 1.2291701524827285 1.9813122707945130  
Co 0.0000000000000000 1.2291701524827285 -1.9813122707945130  
Co 0.0000000000000000 -1.2291701524827268 1.9813122707945130

Co 0.0000000000000000 -1.2291701524827268 -1.9813122707945130  
Co 1.2291701524827285 1.9813122707945130 0.0000000000000000  
Co -1.2291701524827268 1.9813122707945130 0.0000000000000000  
Co 1.2291701524827285 -1.9813122707945130 0.0000000000000000  
Co -1.2291701524827268 -1.9813122707945130 0.0000000000000000  
Co 1.9813122707945130 0.0000000000000000 1.2291701524827285  
Co 1.9813122707945130 0.0000000000000000 -1.2291701524827268  
Co -1.9813122707945130 0.0000000000000000 1.2291701524827285  
Co -1.9813122707945130 0.0000000000000000 -1.2291701524827268

Ni<sub>13</sub>

Ni -0.0000000000000000 0.0000000000000000 0.0000000000000000  
Ni -0.0000000000000000 1.2072275410410160 1.9798941366478502  
Ni -0.0000000000000000 1.2072275410410160 -1.9798941366478484  
Ni -0.0000000000000000 -1.2072275410410160 1.9798941366478502  
Ni -0.0000000000000000 -1.2072275410410160 -1.9798941366478484  
Ni 1.2072275410410143 1.9798941366478502 0.0000000000000000  
Ni -1.2072275410410178 1.9798941366478502 0.0000000000000000  
Ni 1.2072275410410143 -1.9798941366478484 0.0000000000000000  
Ni -1.2072275410410178 -1.9798941366478484 0.0000000000000000  
Ni 1.9798941366478484 0.0000000000000000 1.2072275410410160  
Ni 1.9798941366478484 0.0000000000000000 -1.2072275410410160  
Ni -1.9798941366478502 0.0000000000000000 1.2072275410410160  
Ni -1.9798941366478502 0.0000000000000000 -1.2072275410410160

Cu<sub>13</sub>

Cu 0.0000000000000000 0.0000000000000000 0.0000000000000000  
Cu 0.0000000000000000 1.2653843607548065 2.0462836135514006  
Cu 0.0000000000000000 1.2653843607548065 -2.0462836135514006



Cu 0.0000000000000000 -1.2653843607548065 2.0462836135514006  
Cu 0.0000000000000000 -1.2653843607548065 -2.0462836135514006  
Cu 1.2653843607548065 2.0462836135514006 0.0000000000000000  
Cu -1.2653843607548065 2.0462836135514006 0.0000000000000000  
Cu 1.2653843607548065 -2.0462836135514006 0.0000000000000000  
Cu -1.2653843607548065 -2.0462836135514006 0.0000000000000000  
Cu 2.0462836135514006 0.0000000000000000 1.2653843607548065  
Cu 2.0462836135514006 0.0000000000000000 -1.2653843607548065  
Cu -2.0462836135514006 0.0000000000000000 1.2653843607548065  
Cu -2.0462836135514006 0.0000000000000000 -1.2653843607548065

Zn<sub>13</sub>

Zn 0.0000000000000000 0.0000000000000000 0.0000000000000000  
Zn 0.0000000000000000 1.5377458152765033 2.4877128510266822  
Zn 0.0000000000000000 1.5377458152765033 -2.4877128510266822  
Zn 0.0000000000000000 -1.5377458152765033 2.4877128510266822  
Zn 0.0000000000000000 -1.5377458152765033 -2.4877128510266822  
Zn 1.5377458152765033 2.4877128510266822 0.0000000000000000  
Zn -1.5377458152765033 2.4877128510266822 0.0000000000000000  
Zn 1.5377458152765033 -2.4877128510266822 0.0000000000000000  
Zn -1.5377458152765033 -2.4877128510266822 0.0000000000000000  
Zn 2.4877128510266822 0.0000000000000000 1.5377458152765033  
Zn 2.4877128510266822 0.0000000000000000 -1.5377458152765033  
Zn -2.4877128510266822 0.0000000000000000 1.5377458152765033  
Zn -2.4877128510266822 0.0000000000000000 -1.5377458152765033

Y<sub>13</sub>

Y 0.000000000000000018 0.0000000000000000 0.0000000000000000  
Y 0.000000000000000018 1.7444744569767892 2.8179146762943663

Y 0.00000000000000018 1.7444744569767892 -2.8179146762943699  
Y 0.00000000000000018 -1.7444744569767892 2.8179146762943663  
Y 0.00000000000000018 -1.7444744569767892 -2.8179146762943699  
Y 1.7444744569767892 2.8179146762943663 0.0000000000000000  
Y -1.7444744569767874 2.8179146762943663 0.0000000000000000  
Y 1.7444744569767892 -2.8179146762943699 0.0000000000000000  
Y -1.7444744569767874 -2.8179146762943699 0.0000000000000000  
Y 2.8179146762943681 0.0000000000000000 1.7444744569767892  
Y 2.8179146762943681 0.0000000000000000 -1.7444744569767892  
Y -2.8179146762943681 0.0000000000000000 1.7444744569767892  
Y -2.8179146762943681 0.0000000000000000 -1.7444744569767892

Zr<sub>13</sub>

Zr -0.00000000000000018 0.0000000000000000 0.0000000000000000  
Zr -0.00000000000000018 1.4736438065015989 2.4682286828536455  
Zr -0.00000000000000018 1.4736438065015989 -2.4682286828536437  
Zr -0.00000000000000018 -1.4736438065015989 2.4682286828536455  
Zr -0.00000000000000018 -1.4736438065015989 -2.4682286828536437  
Zr 1.4736438065015971 2.4682286828536455 0.0000000000000000  
Zr -1.4736438065016007 2.4682286828536455 0.0000000000000000  
Zr 1.4736438065015971 -2.4682286828536437 0.0000000000000000  
Zr -1.4736438065016007 -2.4682286828536437 0.0000000000000000  
Zr 2.4682286828536437 0.0000000000000000 1.4736438065015989  
Zr 2.4682286828536437 0.0000000000000000 -1.4736438065015989  
Zr -2.4682286828536455 0.0000000000000000 1.4736438065015989  
Zr -2.4682286828536455 0.0000000000000000 -1.4736438065015989

Nb<sub>13</sub>

Nb 0.00000000000000000 0.0000000000000000 0.0000000000000000

Nb 0.0000000000000000 1.4727749137437307 2.2347366972833722  
Nb 0.0000000000000000 1.4727749137437307 -2.2347366972833704  
Nb 0.0000000000000000 -1.4727749137437307 2.2347366972833722  
Nb 0.0000000000000000 -1.4727749137437307 -2.2347366972833704  
Nb 1.4727749137437307 2.2347366972833722 0.0000000000000000  
Nb -1.4727749137437307 2.2347366972833722 0.0000000000000000  
Nb 1.4727749137437307 -2.2347366972833704 0.0000000000000000  
Nb -1.4727749137437307 -2.2347366972833704 0.0000000000000000  
Nb 2.2347366972833722 0.0000000000000000 1.4727749137437307  
Nb 2.2347366972833722 0.0000000000000000 -1.4727749137437307  
Nb -2.2347366972833704 0.0000000000000000 1.4727749137437307  
Nb -2.2347366972833704 0.0000000000000000 -1.4727749137437307

Mo<sub>13</sub>

Mo 0.0000000000000000 0.0000000000000000 0.0000000000000000  
Mo 0.0000000000000000 1.3600587756559079 2.2005757284365597  
Mo 0.0000000000000000 1.3600587756559079 -2.2005757284365579  
Mo 0.0000000000000000 -1.3600587756559079 2.2005757284365597  
Mo 0.0000000000000000 -1.3600587756559079 -2.2005757284365579  
Mo 1.3600587756559079 2.2005757284365597 0.0000000000000000  
Mo -1.3600587756559079 2.2005757284365597 0.0000000000000000  
Mo 1.3600587756559079 -2.2005757284365579 0.0000000000000000  
Mo -1.3600587756559079 -2.2005757284365579 0.0000000000000000  
Mo 2.2005757284365597 0.0000000000000000 1.3600587756559079  
Mo 2.2005757284365597 0.0000000000000000 -1.3600587756559079  
Mo -2.2005757284365579 0.0000000000000000 1.3600587756559079  
Mo -2.2005757284365579 0.0000000000000000 -1.3600587756559079

Tc<sub>13</sub>

Tc 0.0000000000000000 0.0000000000000000 0.0000000000000000  
 Tc 0.0000000000000000 1.3378507797589805 2.1070643992682676  
 Tc 0.0000000000000000 1.3378507797589805 -2.1070643992682658  
 Tc 0.0000000000000000 -1.3378507797589823 2.1070643992682676  
 Tc 0.0000000000000000 -1.3378507797589823 -2.1070643992682658  
 Tc 1.3378507797589805 2.1070643992682676 0.0000000000000000  
 Tc -1.3378507797589823 2.1070643992682676 0.0000000000000000  
 Tc 1.3378507797589805 -2.1070643992682658 0.0000000000000000  
 Tc -1.3378507797589823 -2.1070643992682658 0.0000000000000000  
 Tc 2.1070643992682676 0.0000000000000000 1.3378507797589805  
 Tc 2.1070643992682676 0.0000000000000000 -1.3378507797589823  
 Tc -2.1070643992682658 0.0000000000000000 1.3378507797589805  
 Tc -2.1070643992682658 0.0000000000000000 -1.3378507797589823

Ru<sub>13</sub>

Ru -0.0000000000000018 0.0000000000000000 0.0000000000000000  
 Ru -0.0000000000000018 1.3131971065647221 2.1487138265131556  
 Ru -0.0000000000000018 1.3131971065647221 -2.1487138265131556  
 Ru -0.0000000000000018 -1.3131971065647186 2.1487138265131556  
 Ru -0.0000000000000018 -1.3131971065647186 -2.1487138265131556  
 Ru 1.3131971065647203 2.1487138265131556 0.0000000000000000  
 Ru -1.3131971065647203 2.1487138265131556 0.0000000000000000  
 Ru 1.3131971065647203 -2.1487138265131556 0.0000000000000000  
 Ru -1.3131971065647203 -2.1487138265131556 0.0000000000000000  
 Ru 2.1487138265131538 0.0000000000000000 1.3131971065647221  
 Ru 2.1487138265131538 0.0000000000000000 -1.3131971065647186  
 Ru -2.1487138265131573 0.0000000000000000 1.3131971065647221  
 Ru -2.1487138265131573 0.0000000000000000 -1.3131971065647186

Rh<sub>13</sub>

Rh 0.0000000000000000 0.0000000000000000 0.0000000000000000  
Rh 0.0000000000000000 1.3387257944734756 2.1659629708727550  
Rh 0.0000000000000000 1.3387257944734756 -2.1659629708727568  
Rh 0.0000000000000000 -1.3387257944734756 2.1659629708727550  
Rh 0.0000000000000000 -1.3387257944734756 -2.1659629708727568  
Rh 1.3387257944734756 2.1659629708727550 0.0000000000000000  
Rh -1.3387257944734756 2.1659629708727550 0.0000000000000000  
Rh 1.3387257944734756 -2.1659629708727568 0.0000000000000000  
Rh -1.3387257944734756 -2.1659629708727568 0.0000000000000000  
Rh 2.1659629708727550 0.0000000000000000 1.3387257944734756  
Rh 2.1659629708727550 0.0000000000000000 -1.3387257944734756  
Rh -2.1659629708727568 0.0000000000000000 1.3387257944734756  
Rh -2.1659629708727568 0.0000000000000000 -1.3387257944734756

Pd<sub>13</sub>

Pd 0.0000000000000000 0.0000000000000000 0.0000000000000000  
Pd 0.0000000000000000 1.4046731683050240 2.2324424890406043  
Pd 0.0000000000000000 1.4046731683050240 -2.2324424890406069  
Pd 0.0000000000000000 -1.4046731683050222 2.2324424890406043  
Pd 0.0000000000000000 -1.4046731683050222 -2.2324424890406069  
Pd 1.4046731683050240 2.2324424890406078 0.0000000000000000  
Pd -1.4046731683050240 2.2324424890406078 0.0000000000000000  
Pd 1.4046731683050240 -2.2324424890406060 0.0000000000000000  
Pd -1.4046731683050240 -2.2324424890406060 0.0000000000000000  
Pd 2.2324424890406043 0.0000000000000000 1.4046731683050240  
Pd 2.2324424890406043 0.0000000000000000 -1.4046731683050240  
Pd -2.2324424890406069 0.0000000000000000 1.4046731683050240

Pd -2.2324424890406069 0.0000000000000000 -1.4046731683050240

Ag<sub>13</sub>

Ag 0.0000000000000000 0.0000000000000000 0.0000000000000000

Ag 0.0000000000000000 1.4573245243633313 2.3590365498062305

Ag 0.0000000000000000 1.4573245243633313 -2.3590365498062305

Ag 0.0000000000000000 -1.4573245243633313 2.3590365498062305

Ag 0.0000000000000000 -1.4573245243633313 -2.3590365498062305

Ag 1.4573245243633330 2.3590365498062305 0.0000000000000000

Ag -1.4573245243633295 2.3590365498062305 0.0000000000000000

Ag 1.4573245243633330 -2.3590365498062305 0.0000000000000000

Ag -1.4573245243633295 -2.3590365498062305 0.0000000000000000

Ag 2.3590365498062305 0.0000000000000000 1.4573245243633330

Ag 2.3590365498062305 0.0000000000000000 -1.4573245243633295

Ag -2.3590365498062305 0.0000000000000000 1.4573245243633330

Ag -2.3590365498062305 0.0000000000000000 -1.4573245243633295

Cd<sub>13</sub>

Cd 0.0000000000000000 0.0000000000000000 0.0000000000000000

Cd 0.0000000000000000 1.7493708655969993 2.8309546242054040

Cd 0.0000000000000000 1.7493708655969993 -2.8309546242054040

Cd 0.0000000000000000 -1.7493708655970011 2.8309546242054022

Cd 0.0000000000000000 -1.7493708655970011 -2.8309546242054040

Cd 1.7493708655969993 2.8309546242054022 0.0000000000000000

Cd -1.7493708655970011 2.8309546242054022 0.0000000000000000

Cd 1.7493708655969993 -2.8309546242054040 0.0000000000000000

Cd -1.7493708655970011 -2.8309546242054040 0.0000000000000000

Cd 2.8309546242054022 0.0000000000000000 1.7493708655969993

Cd 2.8309546242054022 0.0000000000000000 -1.7493708655970011

Cd -2.8309546242054040 0.0000000000000000 1.7493708655969993  
Cd -2.8309546242054040 0.0000000000000000 -1.7493708655970011

Lu<sub>13</sub>

Lu 0.0000000000000000 0.0000000000000000 0.0000000000000000  
Lu 0.0000000000000000 1.6830476056966681 2.7366551346220227  
Lu 0.0000000000000000 1.6830476056966663 -2.7366551346220271  
Lu 0.0000000000000000 -1.6830476056966681 2.7366551346220227  
Lu 0.0000000000000000 -1.6830476056966681 -2.7366551346220271  
Lu 1.6830476056966663 2.7366551346220209 0.0000000000000000  
Lu -1.6830476056966681 2.7366551346220209 0.0000000000000000  
Lu 1.6830476056966663 -2.7366551346220280 0.0000000000000000  
Lu -1.6830476056966681 -2.7366551346220280 0.0000000000000000  
Lu 2.7366551346220209 0.0000000000000000 1.6830476056966681  
Lu 2.7366551346220209 0.0000000000000000 -1.6830476056966663  
Lu -2.7366551346220280 0.0000000000000000 1.6830476056966681  
Lu -2.7366551346220280 0.0000000000000000 -1.6830476056966663

Hf<sub>13</sub>

Hf 0.0000000000000018 0.0000000000000000 0.0000000000000000  
Hf 0.0000000000000018 1.5100245741611360 2.4086761573632600  
Hf 0.0000000000000018 1.5100245741611360 -2.4086761573632653  
Hf 0.0000000000000018 -1.5100245741611342 2.4086761573632600  
Hf 0.0000000000000018 -1.5100245741611342 -2.4086761573632653  
Hf 1.5100245741611378 2.4086761573632618 0.0000000000000000  
Hf -1.5100245741611324 2.4086761573632618 0.0000000000000000  
Hf 1.5100245741611378 -2.4086761573632653 0.0000000000000000  
Hf -1.5100245741611324 -2.4086761573632653 0.0000000000000000  
Hf 2.4086761573632636 0.0000000000000000 1.5100245741611360

Hf 2.4086761573632636 0.0000000000000000 -1.5100245741611360  
Hf -2.4086761573632636 0.0000000000000000 1.5100245741611360  
Hf -2.4086761573632636 0.0000000000000000 -1.5100245741611360

Ta<sub>13</sub>

Ta 0.0000000000000000 0.0000000000000000 0.0000000000000000  
Ta 0.0000000000000000 1.4046929123880165 2.2727698449377662  
Ta 0.0000000000000000 1.4046929123880165 -2.2727698449377698  
Ta 0.0000000000000000 -1.4046929123880147 2.2727698449377662  
Ta 0.0000000000000000 -1.4046929123880147 -2.2727698449377698  
Ta 1.4046929123880165 2.2727698449377662 0.0000000000000000  
Ta -1.4046929123880147 2.2727698449377662 0.0000000000000000  
Ta 1.4046929123880165 -2.2727698449377698 0.0000000000000000  
Ta -1.4046929123880147 -2.2727698449377698 0.0000000000000000  
Ta 2.2727698449377662 0.0000000000000000 1.4046929123880165  
Ta 2.2727698449377662 0.0000000000000000 -1.4046929123880147  
Ta -2.2727698449377698 0.0000000000000000 1.4046929123880165  
Ta -2.2727698449377698 0.0000000000000000 -1.4046929123880147

W<sub>13</sub>

W 0.0000000000000000 0.0000000000000000 0.0000000000000000  
W 0.0000000000000000 1.2193866439474910 2.2778491479785572  
W 0.0000000000000000 1.2193866439474910 -2.2778491479785590  
W 0.0000000000000000 -1.2193866439474910 2.2778491479785572  
W 0.0000000000000000 -1.2193866439474910 -2.2778491479785590  
W 1.2193866439474910 2.2778491479785572 0.0000000000000000  
W -1.2193866439474910 2.2778491479785572 0.0000000000000000  
W 1.2193866439474910 -2.2778491479785590 0.0000000000000000  
W -1.2193866439474910 -2.2778491479785590 0.0000000000000000



W 2.2778491479785572 0.0000000000000000 1.2193866439474910  
W 2.2778491479785572 0.0000000000000000 -1.2193866439474910  
W -2.2778491479785590 0.0000000000000000 1.2193866439474910  
W -2.2778491479785590 0.0000000000000000 -1.2193866439474910

Re<sub>13</sub>

Re 0.0000000000000000 0.0000000000000000 0.0000000000000000  
Re 0.0000000000000000 1.3227767597703597 2.1490919963820652  
Re 0.0000000000000000 1.3227767597703597 -2.1490919963820643  
Re 0.0000000000000000 -1.3227767597703615 2.1490919963820652  
Re 0.0000000000000000 -1.3227767597703615 -2.1490919963820643  
Re 1.3227767597703597 2.1490919963820652 0.0000000000000000  
Re -1.3227767597703632 2.1490919963820652 0.0000000000000000  
Re 1.3227767597703597 -2.1490919963820634 0.0000000000000000  
Re -1.3227767597703632 -2.1490919963820634 0.0000000000000000  
Re 2.1490919963820652 0.0000000000000000 1.3227767597703597  
Re 2.1490919963820652 0.0000000000000000 -1.3227767597703632  
Re -2.1490919963820643 0.0000000000000000 1.3227767597703597  
Re -2.1490919963820643 0.0000000000000000 -1.3227767597703632

Os<sub>13</sub>

Os 0.0000000000000000 0.0000000000000000 0.0000000000000000  
Os 0.0000000000000000 1.2995901112851005 2.1292383433219477  
Os 0.0000000000000000 1.2995901112851005 -2.1292383433219486  
Os 0.0000000000000000 -1.2995901112851005 2.1292383433219477  
Os 0.0000000000000000 -1.2995901112851005 -2.1292383433219486  
Os 1.2995901112851005 2.1292383433219477 0.0000000000000000  
Os -1.2995901112851005 2.1292383433219477 0.0000000000000000  
Os 1.2995901112851005 -2.1292383433219486 0.0000000000000000

Os -1.2995901112851005 -2.1292383433219486 0.0000000000000000  
Os 2.1292383433219477 0.0000000000000000 1.2995901112851005  
Os 2.1292383433219477 0.0000000000000000 -1.2995901112851005  
Os -2.1292383433219486 0.0000000000000000 1.2995901112851005  
Os -2.1292383433219486 0.0000000000000000 -1.2995901112851005

Ir<sub>13</sub>

Ir 0.0000000000000000 0.0000000000000000 0.0000000000000000  
Ir 0.0000000000000000 1.3166767310542848 2.1588607043426240  
Ir 0.0000000000000000 1.3166767310542848 -2.1588607043426222  
Ir 0.0000000000000000 -1.3166767310542848 2.1588607043426240  
Ir 0.0000000000000000 -1.3166767310542848 -2.1588607043426222  
Ir 1.3166767310542848 2.1588607043426240 0.0000000000000000  
Ir -1.3166767310542848 2.1588607043426240 0.0000000000000000  
Ir 1.3166767310542848 -2.1588607043426222 0.0000000000000000  
Ir -1.3166767310542848 -2.1588607043426222 0.0000000000000000  
Ir 2.1588607043426240 0.0000000000000000 1.3166767310542848  
Ir 2.1588607043426240 0.0000000000000000 -1.3166767310542848  
Ir -2.1588607043426222 0.0000000000000000 1.3166767310542848  
Ir -2.1588607043426222 0.0000000000000000 -1.3166767310542848

Pt<sub>13</sub>

Pt 0.0000000000000000 0.0000000000000000 0.0000000000000000  
Pt 0.0000000000000000 1.3776831778551841 2.2291190480631222  
Pt 0.0000000000000000 1.3776831778551841 -2.2291190480631240  
Pt 0.0000000000000000 -1.3776831778551824 2.2291190480631222  
Pt 0.0000000000000000 -1.3776831778551824 -2.2291190480631240  
Pt 1.3776831778551841 2.2291190480631222 0.0000000000000000  
Pt -1.3776831778551824 2.2291190480631222 0.0000000000000000

Pt 1.3776831778551841 -2.2291190480631240 0.0000000000000000  
Pt -1.3776831778551824 -2.2291190480631240 0.0000000000000000  
Pt 2.2291190480631222 0.0000000000000000 1.3776831778551841  
Pt 2.2291190480631222 0.0000000000000000 -1.3776831778551824  
Pt -2.2291190480631240 0.0000000000000000 1.3776831778551841  
Pt -2.2291190480631240 0.0000000000000000 -1.3776831778551824

Au<sub>13</sub>

Au 0.0000000000000000 0.0000000000000000 0.0000000000000000  
Au 0.0000000000000000 1.4546816699926506 2.3535337245366588  
Au 0.0000000000000000 1.4546816699926506 -2.3535337245366605  
Au 0.0000000000000000 -1.4546816699926524 2.3535337245366588  
Au 0.0000000000000000 -1.4546816699926524 -2.3535337245366605  
Au 1.4546816699926506 2.3535337245366588 0.0000000000000000  
Au -1.4546816699926524 2.3535337245366588 0.0000000000000000  
Au 1.4546816699926506 -2.3535337245366605 0.0000000000000000  
Au -1.4546816699926524 -2.3535337245366605 0.0000000000000000  
Au 2.3535337245366588 0.0000000000000000 1.4546816699926506  
Au 2.3535337245366588 0.0000000000000000 -1.4546816699926524  
Au -2.3535337245366605 0.0000000000000000 1.4546816699926506  
Au -2.3535337245366605 0.0000000000000000 -1.4546816699926524

Hg<sub>13</sub>

Hg 0.0000000000000000 0.0000000000000000 0.0000000000000000  
Hg 0.0000000000000000 1.8494749558787227 2.9862810281927601  
Hg 0.0000000000000000 1.8494749558787227 -2.9862810281927610  
Hg 0.0000000000000000 -1.8494749558787227 2.9862810281927601  
Hg 0.0000000000000000 -1.8494749558787227 -2.9862810281927610  
Hg 1.8494749558787227 2.9862810281927601 0.0000000000000000

Hg -1.8494749558787227 2.9862810281927601 0.0000000000000000  
 Hg 1.8494749558787227 -2.9862810281927610 0.0000000000000000  
 Hg -1.8494749558787227 -2.9862810281927610 0.0000000000000000  
 Hg 2.9862810281927601 0.0000000000000000 1.8494749558787227  
 Hg 2.9862810281927601 0.0000000000000000 -1.8494749558787227  
 Hg -2.9862810281927610 0.0000000000000000 1.8494749558787227  
 Hg -2.9862810281927610 0.0000000000000000 -1.8494749558787227

Below, we provide the atomic coordinates (*xyz* positions) for the lowest energy TM@Ti<sub>12</sub>, TM@Zr<sub>12</sub>, and TM@Hf<sub>12</sub> configurations (for all 3*d*, 4*d*, and 5*d* elements).

**TM@Ti<sub>12</sub>**

Sc

Ti 0.0000000000000000 1.3733100968202230 2.2581282814083856  
 Ti 0.0000000000000000 1.3733100968202230 -2.2581282814083847  
 Ti 0.0000000000000000 -1.3733100968202248 2.2581282814083856  
 Ti 0.0000000000000000 -1.3733100968202248 -2.2581282814083847  
 Ti 1.3733100968202212 2.2581282814083838 0.0000000000000000  
 Ti -1.3733100968202230 2.2581282814083838 0.0000000000000000  
 Ti 1.3733100968202212 -2.2581282814083856 0.0000000000000000  
 Ti -1.3733100968202230 -2.2581282814083856 0.0000000000000000  
 Ti 2.2581282814083856 0.0000000000000018 1.3733100968202230  
 Ti 2.2581282814083856 0.0000000000000018 -1.3733100968202230  
 Ti -2.2581282814083847 0.0000000000000018 1.3733100968202230  
 Ti -2.2581282814083847 0.0000000000000018 -1.3733100968202230  
 Sc 0.0000000000000000 0.0000000000000018 0.0000000000000000

Ti

Ti 0.0000000000000000 0.0000000000000000 0.0000000000000000  
 Ti 0.0000000000000000 1.3714488813592851 2.2190413449192654

Ti 0.0000000000000000 1.3714488813592851 -2.2190413449192681  
Ti 0.0000000000000000 -1.3714488813592833 2.2190413449192654  
Ti 0.0000000000000000 -1.3714488813592833 -2.2190413449192681  
Ti 1.3714488813592851 2.2190413449192690 0.0000000000000000  
Ti -1.3714488813592851 2.2190413449192690 0.0000000000000000  
Ti 1.3714488813592851 -2.2190413449192672 0.0000000000000000  
Ti -1.3714488813592851 -2.2190413449192672 0.0000000000000000  
Ti 2.2190413449192654 0.0000000000000000 1.3714488813592851  
Ti 2.2190413449192654 0.0000000000000000 -1.3714488813592851  
Ti -2.2190413449192681 0.0000000000000000 1.3714488813592851  
Ti -2.2190413449192681 0.0000000000000000 -1.3714488813592851

V

Ti 0.0000000000000000 1.3984962726027206 2.1699903018546358  
Ti 0.0000000000000000 1.3984962726027206 -2.1699903018546358  
Ti 0.0000000000000000 -1.3984962726027188 2.1699903018546358  
Ti 0.0000000000000000 -1.3984962726027188 -2.1699903018546358  
Ti 1.3984962726027224 2.1699903018546340 0.0000000000000000  
Ti -1.3984962726027206 2.1699903018546340 0.0000000000000000  
Ti 1.3984962726027224 -2.1699903018546376 0.0000000000000000  
Ti -1.3984962726027206 -2.1699903018546376 0.0000000000000000  
Ti 2.1699903018546358 0.0000000000000000 1.3984962726027224  
Ti 2.1699903018546358 0.0000000000000000 -1.3984962726027170  
Ti -2.1699903018546340 0.0000000000000000 1.3984962726027224  
Ti -2.1699903018546340 0.0000000000000000 -1.3984962726027170  
V 0.0000000000000000 0.0000000000000000 0.0000000000000000

Cr

Ti 0.0000000000000000 1.2904556563721101 2.2034653760477774

Ti 0.0000000000000000 1.2904556563721101 -2.2034653760477818  
Ti 0.0000000000000000 -1.2904556563721048 2.2034653760477774  
Ti 0.0000000000000000 -1.2904556563721048 -2.2034653760477818  
Ti 1.2904556563721101 2.2034653760477791 0.0000000000000000  
Ti -1.2904556563721048 2.2034653760477791 0.0000000000000000  
Ti 1.2904556563721101 -2.2034653760477818 0.0000000000000000  
Ti -1.2904556563721048 -2.2034653760477818 0.0000000000000000  
Ti 2.2034653760477774 0.0000000000000000 1.2904556563721066  
Ti 2.2034653760477774 0.0000000000000000 -1.2904556563721048  
Ti -2.2034653760477818 0.0000000000000000 1.2904556563721066  
Ti -2.2034653760477818 0.0000000000000000 -1.2904556563721048  
Cr 0.0000000000000000 0.0000000000000000 0.0000000000000000

Mn

Ti 0.0000000000000000 1.3725300122795225 2.1367735726567982  
Ti 0.0000000000000000 1.3725300122795225 -2.1367735726567973  
Ti 0.0000000000000000 -1.3725300122795225 2.1367735726567982  
Ti 0.0000000000000000 -1.3725300122795225 -2.1367735726567973  
Ti 1.3725300122795225 2.1367735726567982 0.0000000000000000  
Ti -1.3725300122795225 2.1367735726567982 0.0000000000000000  
Ti 1.3725300122795225 -2.1367735726567982 0.0000000000000000  
Ti -1.3725300122795225 -2.1367735726567982 0.0000000000000000  
Ti 2.1367735726567982 0.0000000000000000 1.3725300122795225  
Ti 2.1367735726567982 0.0000000000000000 -1.3725300122795208  
Ti -2.1367735726567982 0.0000000000000000 1.3725300122795225  
Ti -2.1367735726567982 0.0000000000000000 -1.3725300122795208  
Mn 0.0000000000000000 0.0000000000000000 0.0000000000000000

Fe

Ti 0.0000000000000000 1.3484676121466261 2.1560408364756896  
Ti 0.0000000000000000 1.3484676121466261 -2.1560408364756896  
Ti 0.0000000000000000 -1.3484676121466208 2.1560408364756896  
Ti 0.0000000000000000 -1.3484676121466208 -2.1560408364756896  
Ti 1.3484676121466261 2.1560408364756896 0.0000000000000000  
Ti -1.3484676121466244 2.1560408364756896 0.0000000000000000  
Ti 1.3484676121466261 -2.1560408364756896 0.0000000000000000  
Ti -1.3484676121466244 -2.1560408364756896 0.0000000000000000  
Ti 2.1560408364756896 0.0000000000000000 1.3484676121466261  
Ti 2.1560408364756896 0.0000000000000000 -1.3484676121466208  
Ti -2.1560408364756878 0.0000000000000000 1.3484676121466261  
Ti -2.1560408364756878 0.0000000000000000 -1.3484676121466208  
Fe 0.0000000000000000 0.0000000000000000 0.0000000000000000

Co

Ti 0.0000000000000000 1.3197314051781319 2.1762990328611878  
Ti 0.0000000000000000 1.3197314051781319 -2.1762990328611895  
Ti 0.0000000000000000 -1.3197314051781355 2.1762990328611878  
Ti 0.0000000000000000 -1.3197314051781355 -2.1762990328611895  
Ti 1.3197314051781355 2.1762990328611842 0.0000000000000000  
Ti -1.3197314051781373 2.1762990328611842 0.0000000000000000  
Ti 1.3197314051781355 -2.1762990328611878 0.0000000000000000  
Ti -1.3197314051781373 -2.1762990328611878 0.0000000000000000  
Ti 2.1762990328611878 -0.0000000000000018 1.3197314051781337  
Ti 2.1762990328611878 -0.0000000000000018 -1.3197314051781337  
Ti -2.1762990328611842 -0.0000000000000018 1.3197314051781337  
Ti -2.1762990328611842 -0.0000000000000018 -1.3197314051781337  
Co 0.0000000000000000 -0.0000000000000018 0.0000000000000000

Ni

Ti 0.00000000000000018 1.3424008603927220 2.1720106047117547  
Ti 0.00000000000000018 1.3424008603927220 -2.1720106047117547  
Ti 0.00000000000000018 -1.3424008603927238 2.1720106047117547  
Ti 0.00000000000000018 -1.3424008603927238 -2.1720106047117547  
Ti 1.3424008603927238 2.1720106047117529 0.00000000000000000  
Ti -1.3424008603927202 2.1720106047117529 0.00000000000000000  
Ti 1.3424008603927238 -2.1720106047117547 0.00000000000000000  
Ti -1.3424008603927202 -2.1720106047117547 0.00000000000000000  
Ti 2.1720106047117529 0.00000000000000000 1.3424008603927220  
Ti 2.1720106047117529 0.00000000000000000 -1.3424008603927238  
Ti -2.1720106047117520 0.00000000000000000 1.3424008603927220  
Ti -2.1720106047117520 0.00000000000000000 -1.3424008603927238  
Ni 0.00000000000000018 0.00000000000000000 0.00000000000000000

Cu

Ti 0.00000000000000000 1.3601106236321314 2.1807889930649385  
Ti 0.00000000000000000 1.3601106236321314 -2.1807889930649420  
Ti 0.00000000000000000 -1.3601106236321296 2.1807889930649385  
Ti 0.00000000000000000 -1.3601106236321296 -2.1807889930649420  
Ti 1.3601106236321332 2.1807889930649349 -0.00000000000000018  
Ti -1.3601106236321314 2.1807889930649349 -0.00000000000000018  
Ti 1.3601106236321332 -2.1807889930649429 -0.00000000000000018  
Ti -1.3601106236321314 -2.1807889930649429 -0.00000000000000018  
Ti 2.1807889930649367 -0.00000000000000018 1.3601106236321332  
Ti 2.1807889930649367 -0.00000000000000018 -1.3601106236321296  
Ti -2.1807889930649393 -0.00000000000000018 1.3601106236321332  
Ti -2.1807889930649393 -0.00000000000000018 -1.3601106236321296



Cu 0.0000000000000000 -0.0000000000000018 -0.0000000000000018

Zn

Ti 0.0000000000000000 1.3774125603582199 2.1892774121484511  
Ti 0.0000000000000000 1.3774125603582199 -2.1892774121484555  
Ti 0.0000000000000000 -1.3774125603582199 2.1892774121484511  
Ti 0.0000000000000000 -1.3774125603582199 -2.1892774121484555  
Ti 1.3774125603582199 2.1892774121484511 0.0000000000000000  
Ti -1.3774125603582199 2.1892774121484511 0.0000000000000000  
Ti 1.3774125603582199 -2.1892774121484537 0.0000000000000000  
Ti -1.3774125603582199 -2.1892774121484537 0.0000000000000000  
Ti 2.1892774121484511 0.0000000000000000 1.3774125603582217  
Ti 2.1892774121484511 0.0000000000000000 -1.3774125603582164  
Ti -2.1892774121484537 0.0000000000000000 1.3774125603582217  
Ti -2.1892774121484537 0.0000000000000000 -1.3774125603582164  
Zn 0.0000000000000000 0.0000000000000000 0.0000000000000000

Y

Ti 0.0000000000000000 1.4257272993583214 2.2840261651084290  
Ti 0.0000000000000000 1.4257272993583214 -2.2840261651084282  
Ti 0.0000000000000000 -1.4257272993583214 2.2840261651084290  
Ti 0.0000000000000000 -1.4257272993583214 -2.2840261651084282  
Ti 1.4257272993583214 2.2840261651084290 0.0000000000000000  
Ti -1.4257272993583214 2.2840261651084290 0.0000000000000000  
Ti 1.4257272993583214 -2.2840261651084282 0.0000000000000000  
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Ti 2.2840261651084290 0.0000000000000000 -1.4257272993583214  
Ti -2.2840261651084282 0.0000000000000000 1.4257272993583214

Ti -2.2840261651084282 0.0000000000000000 -1.4257272993583214  
Y 0.0000000000000000 0.0000000000000000 0.0000000000000000

Zr

Ti 0.0000000000000000 1.4199208714851270 2.2554441986747804  
Ti 0.0000000000000000 1.4199208714851270 -2.2554441986747804  
Ti 0.0000000000000000 -1.4199208714851270 2.2554441986747804  
Ti 0.0000000000000000 -1.4199208714851270 -2.2554441986747804  
Ti 1.4199208714851270 2.2554441986747804 0.0000000000000000  
Ti -1.4199208714851252 2.2554441986747804 0.0000000000000000  
Ti 1.4199208714851270 -2.2554441986747804 0.0000000000000000  
Ti -1.4199208714851252 -2.2554441986747804 0.0000000000000000  
Ti 2.2554441986747804 0.0000000000000000 1.4199208714851288  
Ti 2.2554441986747804 0.0000000000000000 -1.4199208714851270  
Ti -2.2554441986747786 0.0000000000000000 1.4199208714851288  
Ti -2.2554441986747786 0.0000000000000000 -1.4199208714851270  
Zr 0.0000000000000000 0.0000000000000000 0.0000000000000000

Mo

Ti -0.0000000000000018 1.3229482239953647 2.2576007040811525  
Ti -0.0000000000000018 1.3229482239953647 -2.2576007040811525  
Ti -0.0000000000000018 -1.3229482239953612 2.2576007040811525  
Ti -0.0000000000000018 -1.3229482239953612 -2.2576007040811525  
Ti 1.3229482239953594 2.2576007040811561 -0.0000000000000018  
Ti -1.3229482239953612 2.2576007040811561 -0.0000000000000018  
Ti 1.3229482239953594 -2.2576007040811517 -0.0000000000000018  
Ti -1.3229482239953612 -2.2576007040811517 -0.0000000000000018  
Ti 2.2576007040811525 0.0000000000000000 1.3229482239953594  
Ti 2.2576007040811525 0.0000000000000000 -1.3229482239953612

Ti -2.2576007040811525 0.0000000000000000 1.3229482239953594  
Ti -2.2576007040811525 0.0000000000000000 -1.3229482239953612  
Mo -0.00000000000000018 0.0000000000000000 -0.0000000000000018

Tc

Ti 0.0000000000000000 1.3748616787005101 2.2093034493243913  
Ti 0.0000000000000000 1.3748616787005101 -2.2093034493243913  
Ti 0.0000000000000000 -1.3748616787005066 2.2093034493243913  
Ti 0.0000000000000000 -1.3748616787005066 -2.2093034493243913  
Ti 1.3748616787005083 2.2093034493243895 0.0000000000000000  
Ti -1.3748616787005119 2.2093034493243895 0.0000000000000000  
Ti 1.3748616787005083 -2.2093034493243895 0.0000000000000000  
Ti -1.3748616787005119 -2.2093034493243895 0.0000000000000000  
Ti 2.2093034493243895 0.0000000000000018 1.3748616787005101  
Ti 2.2093034493243895 0.0000000000000018 -1.3748616787005083  
Ti -2.2093034493243913 0.0000000000000018 1.3748616787005101  
Ti -2.2093034493243913 0.0000000000000018 -1.3748616787005083  
Tc 0.0000000000000000 0.0000000000000018 0.0000000000000000

Ru

Ti 0.00000000000000018 1.3379228590219405 2.2161325295600065  
Ti 0.00000000000000018 1.3379228590219405 -2.2161325295600030  
Ti 0.00000000000000018 -1.3379228590219441 2.2161325295600065  
Ti 0.00000000000000018 -1.3379228590219441 -2.2161325295600030  
Ti 1.3379228590219441 2.2161325295600030 0.0000000000000000  
Ti -1.3379228590219387 2.2161325295600030 0.0000000000000000  
Ti 1.3379228590219441 -2.2161325295600056 0.0000000000000000  
Ti -1.3379228590219387 -2.2161325295600056 0.0000000000000000  
Ti 2.2161325295600065 0.0000000000000000 1.3379228590219441

Ti 2.2161325295600065 0.0000000000000000 -1.3379228590219423  
Ti -2.2161325295600047 0.0000000000000000 1.3379228590219441  
Ti -2.2161325295600047 0.0000000000000000 -1.3379228590219423  
Ru 0.00000000000000018 0.0000000000000000 0.0000000000000000

Rh

Ti 0.0000000000000000 1.3452810831404527 2.2132248997597426  
Ti 0.0000000000000000 1.3452810831404527 -2.2132248997597417  
Ti 0.0000000000000000 -1.3452810831404562 2.2132248997597426  
Ti 0.0000000000000000 -1.3452810831404562 -2.2132248997597417  
Ti 1.3452810831404545 2.2132248997597426 0.0000000000000000  
Ti -1.3452810831404527 2.2132248997597426 0.0000000000000000  
Ti 1.3452810831404545 -2.2132248997597417 0.0000000000000000  
Ti -1.3452810831404527 -2.2132248997597417 0.0000000000000000  
Ti 2.2132248997597426 0.0000000000000000 1.3452810831404562  
Ti 2.2132248997597426 0.0000000000000000 -1.3452810831404509  
Ti -2.2132248997597426 0.0000000000000000 1.3452810831404562  
Ti -2.2132248997597426 0.0000000000000000 -1.3452810831404509  
Rh 0.0000000000000000 0.0000000000000000 0.0000000000000000

Pd

Ti 0.0000000000000000 1.3669219999999882 2.2116789999999753  
Ti 0.0000000000000000 1.3669219999999882 -2.2116789999999753  
Ti 0.0000000000000000 -1.3669219999999882 2.2116789999999753  
Ti 0.0000000000000000 -1.3669219999999882 -2.2116789999999753  
Ti 1.3669219999999882 2.2116789999999753 -0.0000000000000018  
Ti -1.3669219999999882 2.2116789999999753 -0.0000000000000018  
Ti 1.3669219999999882 -2.2116789999999753 -0.0000000000000018  
Ti -1.3669219999999882 -2.2116789999999753 -0.0000000000000018

Ti 2.211678999999753 0.0000000000000000 1.3669219999999882  
Ti 2.211678999999753 0.0000000000000000 -1.3669219999999882  
Ti -2.211678999999753 0.0000000000000000 1.3669219999999882  
Ti -2.211678999999753 0.0000000000000000 -1.3669219999999882  
Pd 0.0000000000000000 0.0000000000000000 -0.0000000000000018

Ag

Ti 0.0000000000000018 1.3880617599822784 2.2260978643210869  
Ti 0.0000000000000018 1.3880617599822784 -2.2260978643210869  
Ti 0.0000000000000018 -1.3880617599822767 2.2260978643210869  
Ti 0.0000000000000018 -1.3880617599822767 -2.2260978643210869  
Ti 1.3880617599822820 2.2260978643210816 0.0000000000000000  
Ti -1.3880617599822767 2.2260978643210816 0.0000000000000000  
Ti 1.3880617599822820 -2.2260978643210851 0.0000000000000000  
Ti -1.3880617599822767 -2.2260978643210851 0.0000000000000000  
Ti 2.2260978643210851 -0.0000000000000018 1.3880617599822820  
Ti 2.2260978643210851 -0.0000000000000018 -1.3880617599822784  
Ti -2.2260978643210843 -0.0000000000000018 1.3880617599822820  
Ti -2.2260978643210843 -0.0000000000000018 -1.3880617599822784  
Ag 0.0000000000000018 -0.0000000000000018 0.0000000000000000

Cd

Ti 0.0000000000000000 1.4096685250238963 2.2398033254191905  
Ti 0.0000000000000000 1.4096685250238963 -2.2398033254191887  
Ti 0.0000000000000000 -1.4096685250238963 2.2398033254191905  
Ti 0.0000000000000000 -1.4096685250238963 -2.2398033254191887  
Ti 1.4096685250238963 2.2398033254191887 0.0000000000000018  
Ti -1.4096685250238963 2.2398033254191887 0.0000000000000018  
Ti 1.4096685250238963 -2.2398033254191896 0.0000000000000018

Ti -1.4096685250238963 -2.2398033254191896 0.0000000000000018  
Ti 2.2398033254191887 -0.0000000000000018 1.4096685250238981  
Ti 2.2398033254191887 -0.0000000000000018 -1.4096685250238963  
Ti -2.2398033254191851 -0.0000000000000018 1.4096685250238981  
Ti -2.2398033254191851 -0.0000000000000018 -1.4096685250238963  
Cd 0.0000000000000000 -0.0000000000000018 0.0000000000000018

Lu

Ti 0.0000000000000000 1.4211576337653771 2.2716905089838910  
Ti 0.0000000000000000 1.4211576337653771 -2.2716905089838866  
Ti 0.0000000000000000 -1.4211576337653771 2.2716905089838910  
Ti 0.0000000000000000 -1.4211576337653771 -2.2716905089838866  
Ti 1.4211576337653771 2.2716905089838875 0.0000000000000000  
Ti -1.4211576337653753 2.2716905089838875 0.0000000000000000  
Ti 1.4211576337653771 -2.2716905089838875 0.0000000000000000  
Ti -1.4211576337653753 -2.2716905089838875 0.0000000000000000  
Ti 2.2716905089838875 0.0000000000000000 1.4211576337653788  
Ti 2.2716905089838875 0.0000000000000000 -1.4211576337653771  
Ti -2.2716905089838857 0.0000000000000000 1.4211576337653788  
Ti -2.2716905089838857 0.0000000000000000 -1.4211576337653771  
Lu 0.0000000000000000 0.0000000000000000 0.0000000000000000

Hf

Ti 0.0000000000000000 1.3607351500242650 2.2842619049783295  
Ti 0.0000000000000000 1.3607351500242650 -2.2842619049783242  
Ti 0.0000000000000000 -1.3607351500242704 2.2842619049783295  
Ti 0.0000000000000000 -1.3607351500242704 -2.2842619049783242  
Ti 1.3607351500242668 2.2842619049783259 0.0000000000000000  
Ti -1.3607351500242704 2.2842619049783259 0.0000000000000000

Ti 1.3607351500242668 -2.2842619049783286 0.0000000000000000  
Ti -1.3607351500242704 -2.2842619049783286 0.0000000000000000  
Ti 2.2842619049783277 -0.00000000000000018 1.3607351500242686  
Ti 2.2842619049783277 -0.00000000000000018 -1.3607351500242650  
Ti -2.2842619049783242 -0.00000000000000018 1.3607351500242686  
Ti -2.2842619049783242 -0.00000000000000018 -1.3607351500242650  
Hf 0.0000000000000000 -0.00000000000000018 0.0000000000000000

### Ta

Ti 0.0000000000000000 1.4208578364814333 2.2215403808402598  
Ti 0.0000000000000000 1.4208578364814333 -2.2215403808402590  
Ti 0.0000000000000000 -1.4208578364814350 2.2215403808402598  
Ti 0.0000000000000000 -1.4208578364814350 -2.2215403808402590  
Ti 1.4208578364814350 2.2215403808402581 0.0000000000000000  
Ti -1.4208578364814350 2.2215403808402581 0.0000000000000000  
Ti 1.4208578364814350 -2.2215403808402598 0.0000000000000000  
Ti -1.4208578364814350 -2.2215403808402598 0.0000000000000000  
Ti 2.2215403808402598 -0.00000000000000018 1.4208578364814368  
Ti 2.2215403808402598 -0.00000000000000018 -1.4208578364814386  
Ti -2.2215403808402590 -0.00000000000000018 1.4208578364814368  
Ti -2.2215403808402590 -0.00000000000000018 -1.4208578364814386  
Ta 0.0000000000000000 -0.00000000000000018 0.0000000000000000

### W

Ti 0.0000000000000000 1.3253190771497412 2.2627317582480071  
Ti 0.0000000000000000 1.3253190771497412 -2.2627317582480018  
Ti 0.0000000000000000 -1.3253190771497465 2.2627317582480071  
Ti 0.0000000000000000 -1.3253190771497465 -2.2627317582480018  
Ti 1.3253190771497447 2.2627317582480071 0.0000000000000000

Ti -1.3253190771497447 2.2627317582480071 0.0000000000000000  
Ti 1.3253190771497447 -2.2627317582480062 0.0000000000000000  
Ti -1.3253190771497447 -2.2627317582480062 0.0000000000000000  
Ti 2.2627317582480071 0.0000000000000000 1.3253190771497447  
Ti 2.2627317582480071 0.0000000000000000 -1.3253190771497465  
Ti -2.2627317582480044 0.0000000000000000 1.3253190771497447  
Ti -2.2627317582480044 0.0000000000000000 -1.3253190771497465  
W 0.0000000000000000 0.0000000000000000 0.0000000000000000

Re

Ti 0.0000000000000000 1.3708538133378294 2.2171244996445161  
Ti 0.0000000000000000 1.3708538133378294 -2.2171244996445125  
Ti 0.0000000000000000 -1.3708538133378294 2.2171244996445161  
Ti 0.0000000000000000 -1.3708538133378294 -2.2171244996445125  
Ti 1.3708538133378294 2.2171244996445143 0.0000000000000000  
Ti -1.3708538133378312 2.2171244996445143 0.0000000000000000  
Ti 1.3708538133378294 -2.2171244996445143 0.0000000000000000  
Ti -1.3708538133378312 -2.2171244996445143 0.0000000000000000  
Ti 2.2171244996445143 0.0000000000000000 1.3708538133378294  
Ti 2.2171244996445143 0.0000000000000000 -1.3708538133378276  
Ti -2.2171244996445161 0.0000000000000000 1.3708538133378294  
Ti -2.2171244996445161 0.0000000000000000 -1.3708538133378276  
Re 0.0000000000000000 0.0000000000000000 0.0000000000000000

Os

Ti 0.0000000000000000 1.3391741825087795 2.2217292763212466  
Ti 0.0000000000000000 1.3391741825087795 -2.2217292763212431  
Ti 0.0000000000000000 -1.3391741825087831 2.2217292763212466  
Ti 0.0000000000000000 -1.3391741825087831 -2.2217292763212431



Ti 1.3391741825087795 2.2217292763212466 0.0000000000000000  
Ti -1.3391741825087813 2.2217292763212466 0.0000000000000000  
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Ti 2.2217292763212448 0.0000000000000000 1.3391741825087795  
Ti 2.2217292763212448 0.0000000000000000 -1.3391741825087795  
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Ti -2.2217292763212448 0.0000000000000000 -1.3391741825087795  
Os 0.0000000000000000 0.0000000000000000 0.0000000000000000

Ir

Ti 0.0000000000000000 1.3482681683191409 2.2169560329065554  
Ti 0.0000000000000000 1.3482681683191409 -2.2169560329065563  
Ti 0.0000000000000000 -1.3482681683191391 2.2169560329065554  
Ti 0.0000000000000000 -1.3482681683191391 -2.2169560329065563  
Ti 1.3482681683191409 2.2169560329065572 0.0000000000000000  
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Ti 2.2169560329065554 0.0000000000000000 -1.3482681683191409  
Ti -2.2169560329065563 0.0000000000000000 1.3482681683191409  
Ti -2.2169560329065563 0.0000000000000000 -1.3482681683191409  
Ir 0.0000000000000000 0.0000000000000000 0.0000000000000000

Pt

Ti 0.0000000000000000 1.3680725475748190 2.2135139438908027  
Ti 0.0000000000000000 1.3680725475748190 -2.2135139438908036  
Ti 0.0000000000000000 -1.3680725475748208 2.2135139438908027

Ti 0.0000000000000000 -1.3680725475748208 -2.2135139438908036  
Ti 1.3680725475748190 2.2135139438908027 0.0000000000000000  
Ti -1.3680725475748190 2.2135139438908027 0.0000000000000000  
Ti 1.3680725475748190 -2.2135139438908045 0.0000000000000000  
Ti -1.3680725475748190 -2.2135139438908045 0.0000000000000000  
Ti 2.2135139438908027 0.0000000000000000 1.3680725475748172  
Ti 2.2135139438908027 0.0000000000000000 -1.3680725475748190  
Ti -2.2135139438908036 0.0000000000000000 1.3680725475748172  
Ti -2.2135139438908036 0.0000000000000000 -1.3680725475748190  
Pt 0.0000000000000000 0.0000000000000000 0.0000000000000000

Au

Ti 0.0000000000000000 1.3695193142632380 2.2371366906466772  
Ti 0.0000000000000000 1.3695193142632380 -2.2371366906466763  
Ti 0.0000000000000000 -1.3695193142632380 2.2371366906466772  
Ti 0.0000000000000000 -1.3695193142632380 -2.2371366906466763  
Ti 1.3695193142632363 2.2371366906466807 0.0000000000000000  
Ti -1.3695193142632345 2.2371366906466807 0.0000000000000000  
Ti 1.3695193142632363 -2.2371366906466754 0.0000000000000000  
Ti -1.3695193142632345 -2.2371366906466754 0.0000000000000000  
Ti 2.2371366906466772 0.0000000000000000 1.3695193142632345  
Ti 2.2371366906466772 0.0000000000000000 -1.3695193142632327  
Ti -2.2371366906466772 0.0000000000000000 1.3695193142632345  
Ti -2.2371366906466772 0.0000000000000000 -1.3695193142632327  
Au 0.0000000000000000 0.0000000000000000 0.0000000000000000

Hg

Ti 0.0000000000000000 1.3698672518122965 2.2719898404870946  
Ti 0.0000000000000000 1.3698672518122965 -2.2719898404870946

Ti 0.0000000000000000 -1.3698672518122965 2.2719898404870946  
Ti 0.0000000000000000 -1.3698672518122965 -2.2719898404870946  
Ti 1.3698672518122983 2.2719898404870928 0.0000000000000000  
Ti -1.3698672518123001 2.2719898404870928 0.0000000000000000  
Ti 1.3698672518122983 -2.2719898404870937 0.0000000000000000  
Ti -1.3698672518123001 -2.2719898404870937 0.0000000000000000  
Ti 2.2719898404870946 0.0000000000000000 1.3698672518122983  
Ti 2.2719898404870946 0.0000000000000000 -1.3698672518122983  
Ti -2.2719898404870964 0.0000000000000000 1.3698672518122983  
Ti -2.2719898404870964 0.0000000000000000 -1.3698672518122983  
Hg 0.0000000000000000 0.0000000000000000 0.0000000000000000

**TM@Zr<sub>12</sub>**

Sc

Zr 0.0000000000000000 1.5063088590511029 2.4371887443616185  
Zr 0.0000000000000000 1.5063088590511029 -2.4371887443616176  
Zr 0.0000000000000000 -1.5063088590510993 2.4371887443616185  
Zr 0.0000000000000000 -1.5063088590510993 -2.4371887443616176  
Zr 1.5063088590510993 2.4371887443616203 0.0000000000000000  
Zr -1.5063088590510976 2.4371887443616203 0.0000000000000000  
Zr 1.5063088590510993 -2.4371887443616167 0.0000000000000000  
Zr -1.5063088590510976 -2.4371887443616167 0.0000000000000000  
Zr 2.4371887443616185 0.0000000000000000 1.5063088590511011  
Zr 2.4371887443616185 0.0000000000000000 -1.5063088590510993  
Zr -2.4371887443616203 0.0000000000000000 1.5063088590511011  
Zr -2.4371887443616203 0.0000000000000000 -1.5063088590510993  
Sc 0.0000000000000000 0.0000000000000000 0.0000000000000000

Ti

Zr 0.0000000000000000 1.4862959124711903 2.4048354056108590  
Zr 0.0000000000000000 1.4862959124711903 -2.4048354056108581  
Zr 0.0000000000000000 -1.4862959124711903 2.4048354056108590  
Zr 0.0000000000000000 -1.4862959124711903 -2.4048354056108581  
Zr 1.4862959124711921 2.4048354056108607 0.0000000000000000  
Zr -1.4862959124711939 2.4048354056108607 0.0000000000000000  
Zr 1.4862959124711921 -2.4048354056108607 0.0000000000000000  
Zr -1.4862959124711939 -2.4048354056108607 0.0000000000000000  
Zr 2.4048354056108590 0.0000000000000000 1.4862959124711921  
Zr 2.4048354056108590 0.0000000000000000 -1.4862959124711921  
Zr -2.4048354056108590 0.0000000000000000 1.4862959124711921  
Zr -2.4048354056108590 0.0000000000000000 -1.4862959124711921  
Ti 0.0000000000000000 0.0000000000000000 0.0000000000000000

V

Zr 0.0000000000000000 1.4676674614713381 2.3746958148335437  
Zr 0.0000000000000000 1.4676674614713381 -2.3746958148335429  
Zr 0.0000000000000000 -1.4676674614713399 2.3746958148335437  
Zr 0.0000000000000000 -1.4676674614713399 -2.3746958148335429  
Zr 1.4676674614713381 2.3746958148335437 -0.0000000000000018  
Zr -1.4676674614713381 2.3746958148335437 -0.0000000000000018  
Zr 1.4676674614713381 -2.3746958148335437 -0.0000000000000018  
Zr -1.4676674614713381 -2.3746958148335437 -0.0000000000000018  
Zr 2.3746958148335437 -0.0000000000000018 1.4676674614713381  
Zr 2.3746958148335437 -0.0000000000000018 -1.4676674614713381  
Zr -2.3746958148335429 -0.0000000000000018 1.4676674614713381  
Zr -2.3746958148335429 -0.0000000000000018 -1.4676674614713381  
V 0.0000000000000000 -0.0000000000000018 -0.0000000000000018

Cr

Zr 0.0000000000000018 1.4691294454804584 2.3526353270830835  
Zr 0.0000000000000018 1.4691294454804584 -2.3526353270830800  
Zr 0.0000000000000018 -1.4691294454804602 2.3526353270830835  
Zr 0.0000000000000018 -1.4691294454804602 -2.3526353270830800  
Zr 1.4691294454804584 2.3526353270830835 0.0000000000000000  
Zr -1.4691294454804567 2.3526353270830835 0.0000000000000000  
Zr 1.4691294454804584 -2.3526353270830800 0.0000000000000000  
Zr -1.4691294454804567 -2.3526353270830800 0.0000000000000000  
Zr 2.3526353270830835 0.0000000000000000 1.4691294454804584  
Zr 2.3526353270830835 0.0000000000000000 -1.4691294454804567  
Zr -2.3526353270830818 0.0000000000000000 1.4691294454804584  
Zr -2.3526353270830818 0.0000000000000000 -1.4691294454804567  
Cr 0.0000000000000018 0.0000000000000000 0.0000000000000000

Mn

Zr 0.0000000000000000 1.4226539988010707 2.3718046184511223  
Zr 0.0000000000000000 1.4226539988010707 -2.3718046184511223  
Zr 0.0000000000000000 -1.4226539988010671 2.3718046184511223  
Zr 0.0000000000000000 -1.4226539988010671 -2.3718046184511223  
Zr 1.4226539988010689 2.3718046184511259 0.0000000000000000  
Zr -1.4226539988010689 2.3718046184511259 0.0000000000000000  
Zr 1.4226539988010689 -2.3718046184511259 0.0000000000000000  
Zr -1.4226539988010689 -2.3718046184511259 0.0000000000000000  
Zr 2.3718046184511241 0.0000000000000000 1.4226539988010689  
Zr 2.3718046184511241 0.0000000000000000 -1.4226539988010671  
Zr -2.3718046184511277 0.0000000000000000 1.4226539988010689  
Zr -2.3718046184511277 0.0000000000000000 -1.4226539988010671

Mn 0.0000000000000000 0.0000000000000000 0.0000000000000000

Fe

Zr 0.0000000000000000 1.4350236928571256 2.3666507432422446  
Zr 0.0000000000000000 1.4350236928571256 -2.3666507432422437  
Zr 0.0000000000000000 -1.4350236928571256 2.3666507432422446  
Zr 0.0000000000000000 -1.4350236928571256 -2.3666507432422437  
Zr 1.4350236928571256 2.3666507432422446 0.0000000000000000  
Zr -1.4350236928571256 2.3666507432422446 0.0000000000000000  
Zr 1.4350236928571256 -2.3666507432422454 0.0000000000000000  
Zr -1.4350236928571256 -2.3666507432422454 0.0000000000000000  
Zr 2.3666507432422446 0.0000000000000000 1.4350236928571256  
Zr 2.3666507432422446 0.0000000000000000 -1.4350236928571238  
Zr -2.3666507432422446 0.0000000000000000 1.4350236928571256  
Zr -2.3666507432422446 0.0000000000000000 -1.4350236928571238  
Fe 0.0000000000000000 0.0000000000000000 0.0000000000000000

Co

Zr 0.0000000000000000 1.4729932891204989 2.3534214171846539  
Zr 0.0000000000000000 1.4729932891204989 -2.3534214171846486  
Zr 0.0000000000000000 -1.4729932891204989 2.3534214171846539  
Zr 0.0000000000000000 -1.4729932891204989 -2.3534214171846486  
Zr 1.4729932891204989 2.3534214171846539 0.0000000000000000  
Zr -1.4729932891204989 2.3534214171846539 0.0000000000000000  
Zr 1.4729932891204989 -2.3534214171846557 0.0000000000000000  
Zr -1.4729932891204989 -2.3534214171846557 0.0000000000000000  
Zr 2.3534214171846521 0.0000000000000000 1.4729932891204989  
Zr 2.3534214171846521 0.0000000000000000 -1.4729932891204971  
Zr -2.3534214171846557 0.0000000000000000 1.4729932891204989

Zr -2.3534214171846557 0.0000000000000000 -1.4729932891204971

Co 0.0000000000000000 0.0000000000000000 0.0000000000000000

Ni

Zr 0.0000000000000000 1.4689581612404599 2.3750210134332619

Zr 0.0000000000000000 1.4689581612404599 -2.3750210134332619

Zr 0.0000000000000000 -1.4689581612404652 2.3750210134332619

Zr 0.0000000000000000 -1.4689581612404652 -2.3750210134332619

Zr 1.4689581612404616 2.3750210134332637 0.0000000000000000

Zr -1.4689581612404634 2.3750210134332637 0.0000000000000000

Zr 1.4689581612404616 -2.3750210134332601 0.0000000000000000

Zr -1.4689581612404634 -2.3750210134332601 0.0000000000000000

Zr 2.3750210134332619 0.0000000000000000 1.4689581612404634

Zr 2.3750210134332619 0.0000000000000000 -1.4689581612404616

Zr -2.3750210134332628 0.0000000000000000 1.4689581612404634

Zr -2.3750210134332628 0.0000000000000000 -1.4689581612404616

Ni 0.0000000000000000 0.0000000000000000 0.0000000000000000

Cu

Zr 0.0000000000000000 1.4628740414613652 2.3933237326196775

Zr 0.0000000000000000 1.4628740414613652 -2.3933237326196810

Zr 0.0000000000000000 -1.4628740414613688 2.3933237326196775

Zr 0.0000000000000000 -1.4628740414613688 -2.3933237326196810

Zr 1.4628740414613688 2.3933237326196775 -0.0000000000000018

Zr -1.4628740414613706 2.3933237326196775 -0.0000000000000018

Zr 1.4628740414613688 -2.3933237326196801 -0.0000000000000018

Zr -1.4628740414613706 -2.3933237326196801 -0.0000000000000018

Zr 2.3933237326196792 -0.0000000000000018 1.4628740414613670

Zr 2.3933237326196792 -0.0000000000000018 -1.4628740414613706

Zr -2.3933237326196810 -0.0000000000000018 1.4628740414613670  
Zr -2.3933237326196810 -0.0000000000000018 -1.4628740414613706  
Cu 0.0000000000000000 -0.0000000000000018 -0.0000000000000018

Zn

Zr 0.0000000000000000 1.4554132346213713 2.4107323385070778  
Zr 0.0000000000000000 1.4554132346213713 -2.4107323385070778  
Zr 0.0000000000000000 -1.4554132346213748 2.4107323385070778  
Zr 0.0000000000000000 -1.4554132346213748 -2.4107323385070778  
Zr 1.4554132346213748 2.4107323385070778 -0.0000000000000018  
Zr -1.4554132346213766 2.4107323385070778 -0.0000000000000018  
Zr 1.4554132346213748 -2.4107323385070814 -0.0000000000000018  
Zr -1.4554132346213766 -2.4107323385070814 -0.0000000000000018  
Zr 2.4107323385070796 -0.0000000000000018 1.4554132346213713  
Zr 2.4107323385070796 -0.0000000000000018 -1.4554132346213766  
Zr -2.4107323385070778 -0.0000000000000018 1.4554132346213713  
Zr -2.4107323385070778 -0.0000000000000018 -1.4554132346213766  
Zn 0.0000000000000000 -0.0000000000000018 -0.0000000000000018

Y

Zr 0.0000000000000000 1.5079295062744755 2.4804023443110257  
Zr 0.0000000000000000 1.5079295062744755 -2.4804023443110248  
Zr 0.0000000000000000 -1.5079295062744755 2.4804023443110257  
Zr 0.0000000000000000 -1.5079295062744755 -2.4804023443110248  
Zr 1.5079295062744738 2.4804023443110275 -0.0000000000000018  
Zr -1.5079295062744755 2.4804023443110275 -0.0000000000000018  
Zr 1.5079295062744738 -2.4804023443110257 -0.0000000000000018  
Zr -1.5079295062744755 -2.4804023443110257 -0.0000000000000018  
Zr 2.4804023443110275 0.0000000000000000 1.5079295062744755



Zr 2.4804023443110275 0.0000000000000000 -1.5079295062744773  
Zr -2.4804023443110257 0.0000000000000000 1.5079295062744755  
Zr -2.4804023443110257 0.0000000000000000 -1.5079295062744773  
Y 0.0000000000000000 0.0000000000000000 -0.0000000000000018

Zr

Zr 0.0000000000000000 0.0000000000000000 0.0000000000000000  
Zr 0.0000000000000000 1.4737953769103012 2.4667700581228758  
Zr 0.0000000000000000 1.4737953769103012 -2.4667700581228758  
Zr 0.0000000000000000 -1.4737953769102994 2.4667700581228758  
Zr 0.0000000000000000 -1.4737953769102994 -2.4667700581228758  
Zr 1.4737953769103012 2.4667700581228758 0.0000000000000000  
Zr -1.4737953769102994 2.4667700581228758 0.0000000000000000  
Zr 1.4737953769103012 -2.4667700581228758 0.0000000000000000  
Zr -1.4737953769102994 -2.4667700581228758 0.0000000000000000  
Zr 2.4667700581228758 0.0000000000000000 1.4737953769103012  
Zr 2.4667700581228758 0.0000000000000000 -1.4737953769102994  
Zr -2.4667700581228758 0.0000000000000000 1.4737953769103012  
Zr -2.4667700581228758 0.0000000000000000 -1.4737953769102994

Nb

Zr 0.0000000000000000 1.4970636727811506 2.4226968783166960  
Zr 0.0000000000000000 1.4970636727811506 -2.4226968783166969  
Zr 0.0000000000000000 -1.4970636727811453 2.4226968783166960  
Zr 0.0000000000000000 -1.4970636727811453 -2.4226968783166969  
Zr 1.4970636727811470 2.4226968783166942 0.0000000000000000  
Zr -1.4970636727811470 2.4226968783166942 0.0000000000000000  
Zr 1.4970636727811470 -2.4226968783166951 0.0000000000000000  
Zr -1.4970636727811470 -2.4226968783166951 0.0000000000000000

Zr 2.4226968783166960 0.0000000000000000 1.4970636727811488  
Zr 2.4226968783166960 0.0000000000000000 -1.4970636727811524  
Zr -2.4226968783166969 0.0000000000000000 1.4970636727811488  
Zr -2.4226968783166969 0.0000000000000000 -1.4970636727811524  
Nb 0.0000000000000000 0.0000000000000000 0.0000000000000000

Mo

Zr 0.0000000000000018 1.4649989699860519 2.4082762720055566  
Zr 0.0000000000000018 1.4649989699860519 -2.4082762720055602  
Zr 0.0000000000000018 -1.4649989699860502 2.4082762720055566  
Zr 0.0000000000000018 -1.4649989699860502 -2.4082762720055602  
Zr 1.4649989699860537 2.4082762720055566 0.0000000000000000  
Zr -1.4649989699860502 2.4082762720055566 0.0000000000000000  
Zr 1.4649989699860537 -2.4082762720055584 0.0000000000000000  
Zr -1.4649989699860502 -2.4082762720055584 0.0000000000000000  
Zr 2.4082762720055584 0.0000000000000018 1.4649989699860502  
Zr 2.4082762720055584 0.0000000000000018 -1.4649989699860484  
Zr -2.4082762720055566 0.0000000000000018 1.4649989699860502  
Zr -2.4082762720055566 0.0000000000000018 -1.4649989699860484  
Mo 0.0000000000000018 0.0000000000000018 0.0000000000000000

Tc

Zr 0.0000000000000018 1.4400817039500442 2.4040780661377070  
Zr 0.0000000000000018 1.4400817039500442 -2.4040780661377079  
Zr 0.0000000000000018 -1.4400817039500478 2.4040780661377070  
Zr 0.0000000000000018 -1.4400817039500478 -2.4040780661377079  
Zr 1.4400817039500460 2.4040780661377052 0.0000000000000018  
Zr -1.4400817039500442 2.4040780661377052 0.0000000000000018  
Zr 1.4400817039500460 -2.4040780661377044 0.0000000000000018

Zr -1.4400817039500442 -2.4040780661377044 0.0000000000000018  
Zr 2.4040780661377070 0.0000000000000000 1.4400817039500460  
Zr 2.4040780661377070 0.0000000000000000 -1.4400817039500442  
Zr -2.4040780661377052 0.0000000000000000 1.4400817039500460  
Zr -2.4040780661377052 0.0000000000000000 -1.4400817039500442  
Tc 0.0000000000000018 0.0000000000000000 0.0000000000000018

Ru

Zr 0.0000000000000000 1.4505426241498665 2.3930121344503839  
Zr 0.0000000000000000 1.4505426241498665 -2.3930121344503830  
Zr 0.0000000000000000 -1.4505426241498647 2.3930121344503839  
Zr 0.0000000000000000 -1.4505426241498647 -2.3930121344503830  
Zr 1.4505426241498665 2.3930121344503874 -0.0000000000000018  
Zr -1.4505426241498665 2.3930121344503874 -0.0000000000000018  
Zr 1.4505426241498665 -2.3930121344503821 -0.0000000000000018  
Zr -1.4505426241498665 -2.3930121344503821 -0.0000000000000018  
Zr 2.3930121344503839 0.0000000000000000 1.4505426241498647  
Zr 2.3930121344503839 0.0000000000000000 -1.4505426241498665  
Zr -2.3930121344503830 0.0000000000000000 1.4505426241498647  
Zr -2.3930121344503830 0.0000000000000000 -1.4505426241498665  
Ru 0.0000000000000000 0.0000000000000000 -0.0000000000000018

Rh

Zr 0.0000000000000000 1.4887372017247102 2.3782317094413230  
Zr 0.0000000000000000 1.4887372017247102 -2.3782317094413266  
Zr 0.0000000000000000 -1.4887372017247138 2.3782317094413230  
Zr 0.0000000000000000 -1.4887372017247138 -2.3782317094413266  
Zr 1.4887372017247120 2.3782317094413230 0.0000000000000000  
Zr -1.4887372017247102 2.3782317094413230 0.0000000000000000

Zr 1.4887372017247120 -2.3782317094413266 0.0000000000000000  
Zr -1.4887372017247102 -2.3782317094413266 0.0000000000000000  
Zr 2.3782317094413230 -0.00000000000000018 1.4887372017247102  
Zr 2.3782317094413230 -0.00000000000000018 -1.4887372017247138  
Zr -2.3782317094413230 -0.00000000000000018 1.4887372017247102  
Zr -2.3782317094413230 -0.00000000000000018 -1.4887372017247138  
Rh 0.0000000000000000 -0.00000000000000018 0.0000000000000000

Pd

Zr 0.0000000000000000 1.4851980556503719 2.4030601364092430  
Zr 0.0000000000000000 1.4851980556503719 -2.4030601364092439  
Zr 0.0000000000000000 -1.4851980556503754 2.4030601364092430  
Zr 0.0000000000000000 -1.4851980556503754 -2.4030601364092439  
Zr 1.4851980556503737 2.4030601364092377 0.0000000000000000  
Zr -1.4851980556503719 2.4030601364092377 0.0000000000000000  
Zr 1.4851980556503737 -2.4030601364092421 0.0000000000000000  
Zr -1.4851980556503719 -2.4030601364092421 0.0000000000000000  
Zr 2.4030601364092430 -0.00000000000000018 1.4851980556503737  
Zr 2.4030601364092430 -0.00000000000000018 -1.4851980556503737  
Zr -2.4030601364092430 -0.00000000000000018 1.4851980556503737  
Zr -2.4030601364092430 -0.00000000000000018 -1.4851980556503737  
Pd 0.0000000000000000 -0.00000000000000018 0.0000000000000000

Ag

Zr 0.0000000000000000 1.4845068464795261 2.4268337459245295  
Zr 0.0000000000000000 1.4845068464795261 -2.4268337459245304  
Zr 0.0000000000000000 -1.4845068464795244 2.4268337459245295  
Zr 0.0000000000000000 -1.4845068464795244 -2.4268337459245304  
Zr 1.4845068464795261 2.4268337459245313 0.0000000000000000

Zr -1.4845068464795261 2.4268337459245313 0.0000000000000000  
Zr 1.4845068464795261 -2.4268337459245295 0.0000000000000000  
Zr -1.4845068464795261 -2.4268337459245295 0.0000000000000000  
Zr 2.4268337459245295 -0.00000000000000018 1.4845068464795261  
Zr 2.4268337459245295 -0.00000000000000018 -1.4845068464795261  
Zr -2.4268337459245304 -0.00000000000000018 1.4845068464795261  
Zr -2.4268337459245304 -0.00000000000000018 -1.4845068464795261  
Ag 0.0000000000000000 -0.00000000000000018 0.0000000000000000

Cd

Zr 0.0000000000000000 1.4787543716425624 2.4511039368422054  
Zr 0.0000000000000000 1.4787543716425624 -2.4511039368422054  
Zr 0.0000000000000000 -1.4787543716425624 2.4511039368422054  
Zr 0.0000000000000000 -1.4787543716425624 -2.4511039368422054  
Zr 1.4787543716425624 2.4511039368422054 -0.00000000000000018  
Zr -1.4787543716425642 2.4511039368422054 -0.00000000000000018  
Zr 1.4787543716425624 -2.4511039368422027 -0.00000000000000018  
Zr -1.4787543716425642 -2.4511039368422027 -0.00000000000000018  
Zr 2.4511039368422072 -0.00000000000000018 1.4787543716425624  
Zr 2.4511039368422072 -0.00000000000000018 -1.4787543716425660  
Zr -2.4511039368422036 -0.00000000000000018 1.4787543716425624  
Zr -2.4511039368422036 -0.00000000000000018 -1.4787543716425660  
Cd 0.0000000000000000 -0.00000000000000018 -0.00000000000000018

Lu

Zr -0.00000000000000018 1.5002679517681408 2.4716181062892773  
Zr -0.00000000000000018 1.5002679517681408 -2.4716181062892773  
Zr -0.00000000000000018 -1.5002679517681425 2.4716181062892773  
Zr -0.00000000000000018 -1.5002679517681425 -2.4716181062892773

Zr 1.5002679517681390 2.4716181062892790 -0.0000000000000018  
Zr -1.5002679517681390 2.4716181062892790 -0.0000000000000018  
Zr 1.5002679517681390 -2.4716181062892826 -0.0000000000000018  
Zr -1.5002679517681390 -2.4716181062892826 -0.0000000000000018  
Zr 2.4716181062892773 0.0000000000000000 1.5002679517681390  
Zr 2.4716181062892773 0.0000000000000000 -1.5002679517681408  
Zr -2.4716181062892790 0.0000000000000000 1.5002679517681390  
Zr -2.4716181062892790 0.0000000000000000 -1.5002679517681408  
Lu -0.0000000000000018 0.0000000000000000 -0.0000000000000018

Hf

Zr 0.0000000000000000 1.4722261023727867 2.4645000176325382  
Zr 0.0000000000000000 1.4722261023727850 -2.4645000176325382  
Zr 0.0000000000000000 -1.4722261023727867 2.4645000176325382  
Zr 0.0000000000000000 -1.4722261023727867 -2.4645000176325382  
Zr 1.4722261023727885 2.4645000176325365 0.0000000000000000  
Zr -1.4722261023727867 2.4645000176325365 0.0000000000000000  
Zr 1.4722261023727885 -2.4645000176325382 0.0000000000000000  
Zr -1.4722261023727867 -2.4645000176325382 0.0000000000000000  
Zr 2.4645000176325382 -0.0000000000000018 1.4722261023727885  
Zr 2.4645000176325382 -0.0000000000000018 -1.4722261023727867  
Zr -2.4645000176325382 -0.0000000000000018 1.4722261023727885  
Zr -2.4645000176325382 -0.0000000000000018 -1.4722261023727867  
Hf 0.0000000000000000 -0.0000000000000018 0.0000000000000000

Ta

Zr -0.0000000000000018 1.4975028847605643 2.4229690270094082  
Zr -0.0000000000000018 1.4975028847605643 -2.4229690270094038  
Zr -0.0000000000000018 -1.4975028847605678 2.4229690270094082

Zr -0.00000000000000018 -1.4975028847605678 -2.4229690270094038  
Zr 1.4975028847605643 2.4229690270094082 0.0000000000000000  
Zr -1.4975028847605660 2.4229690270094082 0.0000000000000000  
Zr 1.4975028847605643 -2.4229690270094064 0.0000000000000000  
Zr -1.4975028847605660 -2.4229690270094064 0.0000000000000000  
Zr 2.4229690270094029 -0.00000000000000018 1.4975028847605660  
Zr 2.4229690270094029 -0.00000000000000018 -1.4975028847605660  
Zr -2.4229690270094046 -0.00000000000000018 1.4975028847605660  
Zr -2.4229690270094046 -0.00000000000000018 -1.4975028847605660  
Ta -0.00000000000000018 -0.00000000000000018 0.0000000000000000

W

Zr 0.00000000000000000 1.4661193921668776 2.4120248398096429  
Zr 0.00000000000000000 1.4661193921668776 -2.4120248398096429  
Zr 0.00000000000000000 -1.4661193921668758 2.4120248398096429  
Zr 0.00000000000000000 -1.4661193921668758 -2.4120248398096429  
Zr 1.4661193921668758 2.4120248398096429 0.0000000000000000  
Zr -1.4661193921668758 2.4120248398096429 0.0000000000000000  
Zr 1.4661193921668758 -2.4120248398096402 0.0000000000000000  
Zr -1.4661193921668758 -2.4120248398096402 0.0000000000000000  
Zr 2.4120248398096429 0.00000000000000000 1.4661193921668758  
Zr 2.4120248398096429 0.00000000000000000 -1.4661193921668740  
Zr -2.4120248398096411 0.00000000000000000 1.4661193921668758  
Zr -2.4120248398096411 0.00000000000000000 -1.4661193921668740  
W 0.00000000000000000 0.00000000000000000 0.00000000000000000

Re

Zr 0.00000000000000000 1.4412649042261236 2.4082962773085228  
Zr 0.00000000000000000 1.4412649042261236 -2.4082962773085237

Zr 0.0000000000000000 -1.4412649042261148 2.4082962773085228  
Zr 0.0000000000000000 -1.4412649042261148 -2.4082962773085237  
Zr 1.4412649042261219 2.4082962773085228 0.0000000000000000  
Zr -1.4412649042261183 2.4082962773085228 0.0000000000000000  
Zr 1.4412649042261219 -2.4082962773085246 0.0000000000000000  
Zr -1.4412649042261183 -2.4082962773085246 0.0000000000000000  
Zr 2.4082962773085246 0.0000000000000000 1.4412649042261183  
Zr 2.4082962773085246 0.0000000000000000 -1.4412649042261183  
Zr -2.4082962773085281 0.0000000000000000 1.4412649042261183  
Zr -2.4082962773085281 0.0000000000000000 -1.4412649042261183  
Re 0.0000000000000000 0.0000000000000000 0.0000000000000000

Os

Zr 0.0000000000000000 1.4512597338957480 2.3955058989010922  
Zr 0.0000000000000000 1.4512597338957480 -2.3955058989010922  
Zr 0.0000000000000000 -1.4512597338957427 2.3955058989010922  
Zr 0.0000000000000000 -1.4512597338957427 -2.3955058989010922  
Zr 1.4512597338957463 2.3955058989010904 0.0000000000000000  
Zr -1.4512597338957445 2.3955058989010904 0.0000000000000000  
Zr 1.4512597338957463 -2.3955058989010940 0.0000000000000000  
Zr -1.4512597338957445 -2.3955058989010940 0.0000000000000000  
Zr 2.3955058989010887 0.0000000000000000 1.4512597338957445  
Zr 2.3955058989010887 0.0000000000000000 -1.4512597338957409  
Zr -2.3955058989010913 0.0000000000000000 1.4512597338957445  
Zr -2.3955058989010913 0.0000000000000000 -1.4512597338957409  
Os 0.0000000000000000 0.0000000000000000 0.0000000000000000

Ir

Zr 0.0000000000000000 1.4890881845726618 2.3779946938494092



Zr 0.0000000000000000 1.4890881845726618 -2.3779946938494092  
Zr 0.0000000000000000 -1.4890881845726600 2.3779946938494092  
Zr 0.0000000000000000 -1.4890881845726600 -2.3779946938494092  
Zr 1.4890881845726600 2.3779946938494110 0.0000000000000000  
Zr -1.4890881845726600 2.3779946938494110 0.0000000000000000  
Zr 1.4890881845726600 -2.3779946938494092 0.0000000000000000  
Zr -1.4890881845726600 -2.3779946938494092 0.0000000000000000  
Zr 2.3779946938494092 0.0000000000000000 1.4890881845726600  
Zr 2.3779946938494092 0.0000000000000000 -1.4890881845726636  
Zr -2.3779946938494101 0.0000000000000000 1.4890881845726600  
Zr -2.3779946938494101 0.0000000000000000 -1.4890881845726636  
Ir 0.0000000000000000 0.0000000000000000 0.0000000000000000

Pt

Zr 0.0000000000000000 1.4838798762421881 2.4009205464424763  
Zr 0.0000000000000000 1.4838798762421881 -2.4009205464424772  
Zr 0.0000000000000000 -1.4838798762421881 2.4009205464424763  
Zr 0.0000000000000000 -1.4838798762421881 -2.4009205464424817  
Zr 1.4838798762421881 2.4009205464424799 0.0000000000000000  
Zr -1.4838798762421881 2.4009205464424799 0.0000000000000000  
Zr 1.4838798762421881 -2.4009205464424790 0.0000000000000000  
Zr -1.4838798762421881 -2.4009205464424790 0.0000000000000000  
Zr 2.4009205464424781 0.0000000000000000 1.4838798762421899  
Zr 2.4009205464424781 0.0000000000000000 -1.4838798762421863  
Zr -2.4009205464424799 0.0000000000000000 1.4838798762421899  
Zr -2.4009205464424799 0.0000000000000000 -1.4838798762421863  
Pt 0.0000000000000000 0.0000000000000000 0.0000000000000000

Au

Zr 0.0000000000000000 1.5002036755490398 2.4134066500323392  
Zr 0.0000000000000000 1.5002036755490398 -2.4134066500323392  
Zr 0.0000000000000000 -1.5002036755490398 2.4134066500323392  
Zr 0.0000000000000000 -1.5002036755490398 -2.4134066500323392  
Zr 1.5002036755490415 2.4134066500323410 -0.0000000000000018  
Zr -1.5002036755490433 2.4134066500323410 -0.0000000000000018  
Zr 1.5002036755490415 -2.4134066500323410 -0.0000000000000018  
Zr -1.5002036755490433 -2.4134066500323410 -0.0000000000000018  
Zr 2.4134066500323392 0.0000000000000000 1.5002036755490415  
Zr 2.4134066500323392 0.0000000000000000 -1.5002036755490433  
Zr -2.4134066500323392 0.0000000000000000 1.5002036755490415  
Zr -2.4134066500323392 0.0000000000000000 -1.5002036755490433  
Au 0.0000000000000000 0.0000000000000000 -0.0000000000000018

Hg

Zr 0.0000000000000018 1.4814050319935248 2.4538142091229140  
Zr 0.0000000000000018 1.4814050319935248 -2.4538142091229131  
Zr 0.0000000000000018 -1.4814050319935266 2.4538142091229140  
Zr 0.0000000000000018 -1.4814050319935266 -2.4538142091229131  
Zr 1.4814050319935266 2.4538142091229123 -0.0000000000000018  
Zr -1.4814050319935230 2.4538142091229123 -0.0000000000000018  
Zr 1.4814050319935266 -2.4538142091229140 -0.0000000000000018  
Zr -1.4814050319935230 -2.4538142091229140 -0.0000000000000018  
Zr 2.4538142091229158 0.0000000000000000 1.4814050319935248  
Zr 2.4538142091229158 0.0000000000000000 -1.4814050319935248  
Zr -2.4538142091229158 0.0000000000000000 1.4814050319935248  
Zr -2.4538142091229158 0.0000000000000000 -1.4814050319935248  
Hg 0.0000000000000018 0.0000000000000000 -0.0000000000000018

**TM@Hf<sub>12</sub>**

Sc

Hf -0.0483632976751736 1.5080133090089021 2.4612107717831222  
Hf 0.0065244417418207 1.4729160957586469 -2.3657571381368525  
Hf -0.0065244417418207 -1.4729160957586451 2.3657571381368498  
Hf 0.0483632976751718 -1.5080133090089021 -2.4612107717831222  
Hf 1.5080133090089021 2.4612107717831222 -0.0483632976751736  
Hf -1.4729160957586469 2.3657571381368498 -0.0065244417418207  
Hf 1.4729160957586469 -2.3657571381368525 0.0065244417418207  
Hf -1.5080133090089038 -2.4612107717831222 0.0483632976751736  
Hf 2.4612107717831222 -0.0483632976751736 1.5080133090089021  
Hf 2.3657571381368498 -0.0065244417418207 -1.4729160957586451  
Hf -2.3657571381368525 0.0065244417418207 1.4729160957586487  
Hf -2.4612107717831222 0.0483632976751718 -1.5080133090089021  
Sc 0.0000000000000000 0.0000000000000000 0.0000000000000000

Ti

Hf 0.0039164189609515 1.4782363330414583 2.3885383456486426  
Hf -0.0593420508991720 1.4056982624110006 -2.4319623833229258  
Hf 0.0593420508991471 -1.4056982624110255 2.4319623833228992  
Hf -0.0039164189609746 -1.4782363330414778 -2.3885383456485236  
Hf 1.4782363330414583 2.3885383456486444 0.0039164189609497  
Hf -1.4056982624110219 2.4319623833229009 0.0593420508991471  
Hf 1.4056982624110042 -2.4319623833229196 -0.0593420508991720  
Hf -1.4782363330414778 -2.3885383456485219 -0.0039164189609746  
Hf 2.3885383456486426 0.0039164189609497 1.4782363330414583  
Hf 2.4319623833229009 0.0593420508991471 -1.4056982624110219  
Hf -2.4319623833229258 -0.0593420508991667 1.4056982624110042  
Hf -2.3885383456485236 -0.0039164189609728 -1.4782363330414778

Ti -0.0000000000000107 -0.0000000000000107 -0.0000000000000107

V

Hf 0.0077548187461893 1.4597282197485857 2.3605655078735488  
Hf -0.0179341732916374 1.4453798427293236 -2.3893556720022637  
Hf 0.0179341732916374 -1.4453798427293183 2.3893556720022602  
Hf -0.0077548187461876 -1.4597282197485857 -2.3605655078735479  
Hf 1.4597282197485857 2.3605655078735506 0.0077548187461893  
Hf -1.4453798427293219 2.3893556720022620 0.0179341732916356  
Hf 1.4453798427293219 -2.3893556720022620 -0.0179341732916374  
Hf -1.4597282197485875 -2.3605655078735461 -0.0077548187461876  
Hf 2.3605655078735506 0.0077548187461911 1.4597282197485857  
Hf 2.3893556720022620 0.0179341732916356 -1.4453798427293201  
Hf -2.3893556720022637 -0.0179341732916356 1.4453798427293219  
Hf -2.3605655078735488 -0.0077548187461858 -1.4597282197485875  
V 0.0000000000000000 0.0000000000000000 0.0000000000000000

Cr

Hf -0.0003900611832819 1.4541877765292099 2.3531659986616660  
Hf 0.0001257702918167 1.4552401289702743 -2.3544193912830735  
Hf -0.0001257702918167 -1.4552401289702743 2.3544193912830735  
Hf 0.0003900611832819 -1.4541877765292099 -2.3531659986616660  
Hf 1.4541877765292099 2.3531659986616660 -0.0003900611832819  
Hf -1.4552401289702743 2.3544193912830735 -0.0001257702918167  
Hf 1.4552401289702743 -2.3544193912830735 0.0001257702918167  
Hf -1.4541877765292099 -2.3531659986616660 0.0003900611832819  
Hf 2.3531659986616660 -0.0003900611832819 1.4541877765292099  
Hf 2.3544193912830735 -0.0001257702918167 -1.4552401289702743  
Hf -2.3544193912830735 0.0001257702918167 1.4552401289702743

Hf -2.3531659986616660 0.0003900611832819 -1.4541877765292099  
Cr 0.0000000000000000 0.0000000000000000 0.0000000000000000

Mn

Hf -0.0259102052669125 1.4549039301146429 2.3695178602403644  
Hf -0.0141353823257333 1.4175453160764953 -2.3305408446086062  
Hf 0.0141353823257351 -1.4175453160764953 2.3305408446086080  
Hf 0.0259102052669142 -1.4549039301146429 -2.3695178602403644  
Hf 1.4549039301146429 2.3695178602403644 -0.0259102052669125  
Hf -1.4175453160764953 2.3305408446086098 0.0141353823257351  
Hf 1.4175453160764953 -2.3305408446086098 -0.0141353823257351  
Hf -1.4549039301146429 -2.3695178602403635 0.0259102052669142  
Hf 2.3695178602403644 -0.0259102052669107 1.4549039301146429  
Hf 2.3305408446086080 0.0141353823257351 -1.4175453160764953  
Hf -2.3305408446086080 -0.0141353823257298 1.4175453160764953  
Hf -2.3695178602403644 0.0259102052669142 -1.4549039301146429  
Mn 0.0000000000000000 0.0000000000000000 0.0000000000000000

Fe

Hf 0.0016460644477689 1.4147467774065667 2.3573928869506808  
Hf -0.0000928380762399 1.4138988688245018 -2.3555830154363031  
Hf 0.0000928380762399 -1.4138988688244982 2.3555830154363022  
Hf -0.0016460644477672 -1.4147467774065650 -2.3573928869506764  
Hf 1.4147467774065667 2.3573928869506791 0.0016460644477689  
Hf -1.4138988688245000 2.3555830154363022 0.0000928380762399  
Hf 1.4138988688245036 -2.3555830154363058 -0.0000928380762364  
Hf -1.4147467774065614 -2.3573928869506791 -0.0016460644477672  
Hf 2.3573928869506808 0.0016460644477672 1.4147467774065667  
Hf 2.3555830154363022 0.0000928380762382 -1.4138988688245000

Hf -2.3555830154363022 -0.0000928380762346 1.4138988688245036  
Hf -2.3573928869506755 -0.0016460644477689 -1.4147467774065632  
Fe 0.0000000000000000 0.0000000000000000 0.0000000000000000

Co

Hf -0.0203834878800162 1.4334339925849413 2.3309810254050465  
Hf -0.0072688668465837 1.4451290399014933 -2.3563580843100436  
Hf 0.0072688668465819 -1.4451290399014951 2.3563580843100471  
Hf 0.0203834878800162 -1.4334339925849413 -2.3309810254050429  
Hf 1.4334339925849413 2.3309810254050483 -0.0203834878800144  
Hf -1.4451290399014951 2.3563580843100453 0.0072688668465819  
Hf 1.4451290399014933 -2.3563580843100462 -0.0072688668465837  
Hf -1.4334339925849413 -2.3309810254050456 0.0203834878800162  
Hf 2.3309810254050483 -0.0203834878800144 1.4334339925849395  
Hf 2.3563580843100453 0.0072688668465837 -1.4451290399014933  
Hf -2.3563580843100462 -0.0072688668465837 1.4451290399014933  
Hf -2.3309810254050456 0.0203834878800180 -1.4334339925849378  
Co 0.0000000000000000 0.0000000000000000 0.0000000000000000

Ni

Hf -0.0000068815367626 1.4493200688025354 2.3450063504979823  
Hf 0.0000015279475463 1.4493253694317332 -2.3450063840979851  
Hf -0.0000015279475463 -1.4493253694317332 2.3450063840979851  
Hf 0.0000068815367626 -1.4493200688025354 -2.3450063504979823  
Hf 1.4493200688025354 2.3450063504979823 -0.0000068815367626  
Hf -1.4493253694317332 2.3450063840979851 -0.0000015279475463  
Hf 1.4493253694317332 -2.3450063840979851 0.0000015279475463  
Hf -1.4493200688025354 -2.3450063504979823 0.0000068815367626  
Hf 2.3450063504979823 -0.0000068815367626 1.4493200688025354

Hf 2.3450063840979851 -0.0000015279475463 -1.4493253694317332  
Hf -2.3450063840979851 0.0000015279475463 1.4493253694317332  
Hf -2.3450063504979823 0.0000068815367626 -1.4493200688025354  
Ni 0.0000000000000000 0.0000000000000000 0.0000000000000000

Cu

Hf -0.0003602086570602 1.4477860132046612 2.3617592687827571  
Hf 0.0022649283050917 1.4498571270953438 -2.3588672672139301  
Hf -0.0022649283050917 -1.4498571270953438 2.3588672672139275  
Hf 0.0003602086570620 -1.4477860132046612 -2.3617592687827562  
Hf 1.4477860132046612 2.3617592687827571 -0.0003602086570602  
Hf -1.4498571270953438 2.3588672672139293 -0.0022649283050917  
Hf 1.4498571270953438 -2.3588672672139293 0.0022649283050882  
Hf -1.4477860132046612 -2.3617592687827553 0.0003602086570620  
Hf 2.3617592687827589 -0.0003602086570602 1.4477860132046629  
Hf 2.3588672672139293 -0.0022649283050917 -1.4498571270953402  
Hf -2.3588672672139293 0.0022649283050882 1.4498571270953438  
Hf -2.3617592687827553 0.0003602086570620 -1.4477860132046576  
Cu 0.0000000000000000 0.0000000000000000 0.0000000000000000

Zn

Hf -0.0122299353391249 1.4770818201252531 2.3588392366468707  
Hf -0.0179168764337803 1.4596333275530320 -2.3706292835047655  
Hf 0.0179168764337785 -1.4596333275530373 2.3706292835046234  
Hf 0.0122299353389845 -1.4770818201251146 -2.3588392366467286  
Hf 1.4770818201252549 2.3588392366468689 -0.0122299353391249  
Hf -1.4596333275530338 2.3706292835046217 0.0179168764337803  
Hf 1.4596333275530338 -2.3706292835047673 -0.0179168764337785  
Hf -1.4770818201251128 -2.3588392366467303 0.0122299353389863

Hf 2.3588392366468707 -0.0122299353391266 1.4770818201252549  
Hf 2.3706292835046252 0.0179168764337785 -1.4596333275530355  
Hf -2.3706292835047655 -0.0179168764337803 1.4596333275530338  
Hf -2.3588392366467277 0.0122299353389845 -1.4770818201251128  
Zn 0.0000000000000000 -0.0000000000000018 0.0000000000000000

Y

Hf -0.0497585497080877 1.5114811658306451 2.4755974771030225  
Hf 0.0129559764888718 1.5143404267541793 -2.4161040678669803  
Hf -0.0129559764888718 -1.5143404267541740 2.4161040678669803  
Hf 0.0497585497080895 -1.5114811658306451 -2.4755974771030225  
Hf 1.5114811658306451 2.4755974771030225 -0.0497585497080895  
Hf -1.5143404267541776 2.4161040678669803 -0.0129559764888683  
Hf 1.5143404267541793 -2.4161040678669776 0.0129559764888718  
Hf -1.5114811658306486 -2.4755974771030198 0.0497585497080895  
Hf 2.4755974771030225 -0.0497585497080877 1.5114811658306451  
Hf 2.4161040678669803 -0.0129559764888718 -1.5143404267541776  
Hf -2.4161040678669803 0.0129559764888718 1.5143404267541793  
Hf -2.4755974771030225 0.0497585497080895 -1.5114811658306486  
Y 0.0000000000000000 0.0000000000000000 0.0000000000000000

Zr

Hf 0.0000008620889957 1.5154688211725045 2.4110366816470581  
Hf -0.0000002534039822 1.5154686913105895 -2.4110372413336094  
Hf 0.0000002534039822 -1.5154686913105930 2.4110372413336130  
Hf -0.0000008620889957 -1.5154688211725098 -2.4110366816470545  
Hf 1.5154688211725045 2.4110366816470563 0.0000008620889957  
Hf -1.5154686913105930 2.4110372413336130 0.0000002534039822  
Hf 1.5154686913105877 -2.4110372413336112 -0.0000002534039805



Hf -1.5154688211725098 -2.4110366816470563 -0.0000008620889940  
Hf 2.4110366816470581 0.0000008620889957 1.5154688211725045  
Hf 2.4110372413336130 0.0000002534039805 -1.5154686913105913  
Hf -2.4110372413336112 -0.0000002534039822 1.5154686913105913  
Hf -2.4110366816470563 -0.0000008620889957 -1.5154688211725080  
Zr 0.0000000000000000 0.0000000000000000 0.0000000000000000

Nb

Hf 0.0235116102190052 1.4863085143098420 2.3904006817661028  
Hf 0.0157372051609546 1.5023673168300142 -2.3896890689953878  
Hf -0.0157372051609546 -1.5023673168300160 2.3896890689953878  
Hf -0.0235116102189998 -1.4863085143098456 -2.3904006817661019  
Hf 1.4863085143098438 2.3904006817661028 0.0235116102190034  
Hf -1.5023673168300160 2.3896890689953878 -0.0157372051609510  
Hf 1.5023673168300178 -2.3896890689953878 0.0157372051609528  
Hf -1.4863085143098438 -2.3904006817661019 -0.0235116102190016  
Hf 2.3904006817661045 0.0235116102190034 1.4863085143098438  
Hf 2.3896890689953878 -0.0157372051609510 -1.5023673168300160  
Hf -2.3896890689953860 0.0157372051609528 1.5023673168300178  
Hf -2.3904006817661045 -0.0235116102190052 -1.4863085143098456  
Nb 0.0000000000000000 -0.0000000000000018 0.0000000000000000

Mo

Hf 0.0513188134368860 1.5040300128724464 2.4012067775455552  
Hf 0.0103706317504280 1.4677862560124471 -2.3478701422107910  
Hf -0.0103706317504280 -1.4677862560124506 2.3478701422107910  
Hf -0.0513188134368878 -1.5040300128724464 -2.4012067775455552  
Hf 1.5040300128724464 2.4012067775455552 0.0513188134368860  
Hf -1.4677862560124488 2.3478701422107910 -0.0103706317504244

Hf 1.4677862560124488 -2.3478701422107902 0.0103706317504297  
Hf -1.5040300128724446 -2.4012067775455543 -0.0513188134368843  
Hf 2.4012067775455552 0.0513188134368843 1.5040300128724482  
Hf 2.3478701422107893 -0.0103706317504244 -1.4677862560124506  
Hf -2.3478701422107893 0.0103706317504297 1.4677862560124488  
Hf -2.4012067775455535 -0.0513188134368843 -1.5040300128724464  
Mo 0.0000000000000000 0.0000000000000000 0.0000000000000000

Tc

Hf 0.0323476719298341 1.4691241412769198 2.3621559601400914  
Hf -0.0015861767271215 1.4647238157008520 -2.3795243936064452  
Hf 0.0015861767271232 -1.4647238157008573 2.3795243936064470  
Hf -0.0323476719298306 -1.4691241412769234 -2.3621559601400914  
Hf 1.4691241412769163 2.3621559601400914 0.0323476719298341  
Hf -1.4647238157008555 2.3795243936064452 0.0015861767271232  
Hf 1.4647238157008537 -2.3795243936064452 -0.0015861767271215  
Hf -1.4691241412769216 -2.3621559601400914 -0.0323476719298306  
Hf 2.3621559601400897 0.0323476719298323 1.4691241412769180  
Hf 2.3795243936064470 0.0015861767271215 -1.4647238157008520  
Hf -2.3795243936064434 -0.0015861767271232 1.4647238157008537  
Hf -2.3621559601400897 -0.0323476719298323 -1.4691241412769180  
Tc 0.0000000000000000 -0.0000000000000018 0.0000000000000000

Ru

Hf -0.0220448063460310 1.4862312351625917 2.3522079485073277  
Hf -0.0318701828149415 1.4533163958758166 -2.3696466329630539  
Hf 0.0318701828149415 -1.4533163958758166 2.3696466329630539  
Hf 0.0220448063460310 -1.4862312351625917 -2.3522079485073277  
Hf 1.4862312351625917 2.3522079485073277 -0.0220448063460310

Hf -1.4533163958758166 2.3696466329630539 0.0318701828149415  
Hf 1.4533163958758166 -2.3696466329630539 -0.0318701828149415  
Hf -1.4862312351625917 -2.3522079485073277 0.0220448063460310  
Hf 2.3522079485073277 -0.0220448063460310 1.4862312351625917  
Hf 2.3696466329630539 0.0318701828149415 -1.4533163958758166  
Hf -2.3696466329630539 -0.0318701828149415 1.4533163958758166  
Hf -2.3522079485073277 0.0220448063460310 -1.4862312351625917  
Ru 0.0000000000000000 0.0000000000000000 0.0000000000000000

Rh

Hf -0.0293001422203076 1.4571797012254706 2.3802247365892981  
Hf 0.0013694231677164 1.4560215068749471 -2.3562545437071947  
Hf -0.0013694231677164 -1.4560215068749471 2.3562545437071947  
Hf 0.0293001422203076 -1.4571797012254706 -2.3802247365892981  
Hf 1.4571797012254706 2.3802247365892981 -0.0293001422203076  
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Hf 1.4560215068749471 -2.3562545437071947 0.0013694231677164  
Hf -1.4571797012254706 -2.3802247365892981 0.0293001422203076  
Hf 2.3802247365892981 -0.0293001422203076 1.4571797012254706  
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Hf -2.3802247365892981 0.0293001422203076 -1.4571797012254706  
Rh 0.0000000000000000 0.0000000000000000 0.0000000000000000

Pd

Hf -0.0000001520859882 1.4667244074384200 2.3731625322979255  
Hf 0.0000003154757167 1.4667237187836690 -2.3731628498214263  
Hf -0.0000003154757167 -1.4667237187836690 2.3731628498214263  
Hf 0.0000001520859882 -1.4667244074384200 -2.3731625322979255

Hf 1.4667244074384200 2.3731625322979255 -0.0000001520859882  
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Hf 1.4667237187836690 -2.3731628498214263 0.0000003154757167  
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Hf 2.3731628498214263 -0.0000003154757167 -1.4667237187836690  
Hf -2.3731628498214263 0.0000003154757167 1.4667237187836690  
Hf -2.3731625322979255 0.0000001520859882 -1.4667244074384200  
Pd 0.0000000000000000 0.0000000000000000 0.0000000000000000

Ag

Hf -0.0009179560293830 1.4687742625803466 2.3937094025498507  
Hf 0.0014804080548174 1.4711980573284258 -2.3931812201878779  
Hf -0.0014804080548227 -1.4711980573284276 2.3931812201878788  
Hf 0.0009179560293830 -1.4687742625803466 -2.3937094025498498  
Hf 1.4687742625803448 2.3937094025498507 -0.0009179560293830  
Hf -1.4711980573284293 2.3931812201878788 -0.0014804080548174  
Hf 1.4711980573284276 -2.3931812201878797 0.0014804080548210  
Hf -1.4687742625803502 -2.3937094025498515 0.0009179560293848  
Hf 2.3937094025498489 -0.0009179560293813 1.4687742625803484  
Hf 2.3931812201878770 -0.0014804080548245 -1.4711980573284293  
Hf -2.3931812201878806 0.0014804080548192 1.4711980573284311  
Hf -2.3937094025498524 0.0009179560293830 -1.4687742625803484  
Ag -0.0000000000000018 -0.0000000000000018 0.0000000000000000

Cd

Hf -0.0122824799277748 1.5025071042371891 2.3968426261583282  
Hf -0.0206887656024559 1.4811438043198528 -2.4086784806284705  
Hf 0.0206887656025874 -1.4811438043198741 2.4086784806284474

Hf 0.0122824799277357 -1.5025071042371980 -2.3968426261583549  
Hf 1.5025071042371874 2.3968426261583282 -0.0122824799277730  
Hf -1.4811438043198759 2.4086784806284509 0.0206887656025874  
Hf 1.4811438043198493 -2.4086784806284696 -0.0206887656024559  
Hf -1.5025071042372016 -2.3968426261583549 0.0122824799277339  
Hf 2.3968426261583300 -0.0122824799277712 1.5025071042371874  
Hf 2.4086784806284474 0.0206887656025874 -1.4811438043198759  
Hf -2.4086784806284696 -0.0206887656024541 1.4811438043198510  
Hf -2.3968426261583593 0.0122824799277339 -1.5025071042371980  
Cd -0.0000000000000124 -0.0000000000000107 -0.0000000000000107

Lu

Hf -0.0173997223535682 1.4624388919995202 2.3769455251930225  
Hf -0.0208653489227366 1.5074243610301430 -2.4933868290716088  
Hf 0.0208653489227384 -1.5074243610301448 2.4933868290716088  
Hf 0.0173997223535682 -1.4624388919995219 -2.3769455251930216  
Hf 1.4624388919995202 2.3769455251930225 -0.0173997223535682  
Hf -1.5074243610301430 2.4933868290716088 0.0208653489227384  
Hf 1.5074243610301430 -2.4933868290716097 -0.0208653489227366  
Hf -1.4624388919995202 -2.3769455251930225 0.0173997223535682  
Hf 2.3769455251930225 -0.0173997223535700 1.4624388919995202  
Hf 2.4933868290716088 0.0208653489227384 -1.5074243610301430  
Hf -2.4933868290716088 -0.0208653489227366 1.5074243610301430  
Hf -2.3769455251930216 0.0173997223535682 -1.4624388919995202  
Lu 0.0000000000000000 -0.0000000000000018 0.0000000000000000

Hf

Hf 0.0000000000000018 0.0000000000000000 0.0000000000000000  
Hf 0.0292141837949096 1.5028208105149368 2.4089017175927161

Hf 0.0296271431334301 1.5305986954094379 -2.3932940784266421  
Hf -0.0296271431334265 -1.5305986954094397 2.3932940784266439  
Hf -0.0292141837949060 -1.5028208105149421 -2.4089017175927196  
Hf 1.5028208105149385 2.4089017175927161 0.0292141837949078  
Hf -1.5305986954094379 2.3932940784266439 -0.0296271431334283  
Hf 1.5305986954094397 -2.3932940784266421 0.0296271431334283  
Hf -1.5028208105149403 -2.4089017175927196 -0.0292141837949078  
Hf 2.4089017175927179 0.0292141837949078 1.5028208105149368  
Hf 2.3932940784266457 -0.0296271431334283 -1.5305986954094397  
Hf -2.3932940784266403 0.0296271431334283 1.5305986954094379  
Hf -2.4089017175927179 -0.0292141837949078 -1.5028208105149421

Ta

Hf -0.0696226456518012 1.4543689688427168 2.4003666782805926  
Hf 0.0202473278950883 1.5229363222210939 -2.4164965637943441  
Hf -0.0202473278950865 -1.5229363222210885 2.4164965637943450  
Hf 0.0696226456517994 -1.4543689688427168 -2.4003666782805881  
Hf 1.4543689688427168 2.4003666782805926 -0.0696226456518048  
Hf -1.5229363222210885 2.4164965637943467 -0.0202473278950901  
Hf 1.5229363222210921 -2.4164965637943432 0.0202473278950865  
Hf -1.4543689688427168 -2.4003666782805873 0.0696226456517994  
Hf 2.4003666782805926 -0.0696226456518030 1.4543689688427168  
Hf 2.4164965637943467 -0.0202473278950883 -1.5229363222210903  
Hf -2.4164965637943432 0.0202473278950883 1.5229363222210921  
Hf -2.4003666782805899 0.0696226456518012 -1.4543689688427168  
Ta 0.0000000000000000 0.0000000000000000 -0.0000000000000018

W

Hf 0.0536129776337351 1.4934617904521907 2.3853871621872145

Hf -0.0133018859678220 1.4598643487678089 -2.3981356222192804  
Hf 0.0133018859678220 -1.4598643487678089 2.3981356222192787  
Hf -0.0536129776337351 -1.4934617904521943 -2.3853871621872100  
Hf 1.4934617904521925 2.3853871621872145 0.0536129776337351  
Hf -1.4598643487678071 2.3981356222192787 0.0133018859678220  
Hf 1.4598643487678089 -2.3981356222192831 -0.0133018859678220  
Hf -1.4934617904521925 -2.3853871621872127 -0.0536129776337333  
Hf 2.3853871621872109 0.0536129776337333 1.4934617904521925  
Hf 2.3981356222192769 0.0133018859678202 -1.4598643487678071  
Hf -2.3981356222192769 -0.0133018859678238 1.4598643487678089  
Hf -2.3853871621872109 -0.0536129776337351 -1.4934617904521925  
W 0.0000000000000000 0.0000000000000000 0.0000000000000000

Re

Hf 0.0308145535420579 1.4750291623101930 2.3628865524509024  
Hf -0.0046865612675617 1.4675484657547599 -2.3807515967872916  
Hf 0.0046865612675617 -1.4675484657547599 2.3807515967872916  
Hf -0.0308145535420579 -1.4750291623101930 -2.3628865524509024  
Hf 1.4750291623101930 2.3628865524509024 0.0308145535420579  
Hf -1.4675484657547599 2.3807515967872934 0.0046865612675617  
Hf 1.4675484657547599 -2.3807515967872916 -0.0046865612675617  
Hf -1.4750291623101930 -2.3628865524509024 -0.0308145535420579  
Hf 2.3628865524509024 0.0308145535420579 1.4750291623101930  
Hf 2.3807515967872916 0.0046865612675617 -1.4675484657547599  
Hf -2.3807515967872916 -0.0046865612675617 1.4675484657547599  
Hf -2.3628865524509024 -0.0308145535420579 -1.4750291623101930  
Re 0.0000000000000000 0.0000000000000000 0.0000000000000000

Os

Hf -0.0230747347363547 1.4579500339006302 2.3733863837477998  
Hf -0.0162491889798844 1.4405305643187205 -2.3734628625589949  
Hf 0.0162491889798844 -1.4405305643187205 2.3734628625589949  
Hf 0.0230747347363547 -1.4579500339006302 -2.3733863837477998  
Hf 1.4579500339006302 2.3733863837477998 -0.0230747347363547  
Hf -1.4405305643187205 2.3734628625589949 0.0162491889798844  
Hf 1.4405305643187205 -2.3734628625589949 -0.0162491889798844  
Hf -1.4579500339006302 -2.3733863837477998 0.0230747347363547  
Hf 2.3733863837477998 -0.0230747347363547 1.4579500339006302  
Hf 2.3734628625589949 0.0162491889798844 -1.4405305643187205  
Hf -2.3734628625589949 -0.0162491889798844 1.4405305643187205  
Hf -2.3733863837477998 0.0230747347363547 -1.4579500339006302  
Os 0.0000000000000000 0.0000000000000000 0.0000000000000000

Ir

Hf -0.0303928241322637 1.4585673711943059 2.3784075077550426  
Hf 0.0007599434071892 1.4585148124764657 -2.3562809412479169  
Hf -0.0007599434071892 -1.4585148124764657 2.3562809412479169  
Hf 0.0303928241322637 -1.4585673711943059 -2.3784075077550426  
Hf 1.4585673711943059 2.3784075077550426 -0.0303928241322637  
Hf -1.4585148124764657 2.3562809412479169 -0.0007599434071892  
Hf 1.4585148124764657 -2.3562809412479169 0.0007599434071892  
Hf -1.4585673711943059 -2.3784075077550426 0.0303928241322637  
Hf 2.3784075077550426 -0.0303928241322637 1.4585673711943059  
Hf 2.3562809412479169 -0.0007599434071892 -1.4585148124764657  
Hf -2.3562809412479169 0.0007599434071892 1.4585148124764657  
Hf -2.3784075077550426 0.0303928241322637 -1.4585673711943059  
Ir 0.0000000000000000 0.0000000000000000 0.0000000000000000



Pt

Hf -0.0000005617151544 1.4666183195829774 2.3729945959941290  
Hf 0.0000002144126654 1.4666183258347569 -2.3729941692707257  
Hf -0.0000002144126654 -1.4666183258347587 2.3729941692707257  
Hf 0.0000005617151544 -1.4666183195829774 -2.3729945959941290  
Hf 1.4666183195829774 2.3729945959941272 -0.0000005617151544  
Hf -1.4666183258347587 2.3729941692707257 -0.0000002144126654  
Hf 1.4666183258347587 -2.3729941692707257 0.0000002144126672  
Hf -1.4666183195829774 -2.3729945959941290 0.0000005617151544  
Hf 2.3729945959941290 -0.0000005617151544 1.4666183195829792  
Hf 2.3729941692707257 -0.0000002144126654 -1.4666183258347587  
Hf -2.3729941692707257 0.0000002144126654 1.4666183258347587  
Hf -2.3729945959941290 0.0000005617151544 -1.4666183195829774  
Pt 0.0000000000000000 0.0000000000000000 0.0000000000000000

Au

Hf -0.0045008153554367 1.4816733158434516 2.3847711318553078  
Hf -0.0084597443777756 1.4729380237246570 -2.3898722824356646  
Hf 0.0084597443777774 -1.4729380237246605 2.3898722824356646  
Hf 0.0045008153554367 -1.4816733158434552 -2.3847711318553069  
Hf 1.4816733158434552 2.3847711318553078 -0.0045008153554367  
Hf -1.4729380237246588 2.3898722824356646 0.0084597443777810  
Hf 1.4729380237246570 -2.3898722824356646 -0.0084597443777739  
Hf -1.4816733158434552 -2.3847711318553069 0.0045008153554367  
Hf 2.3847711318553095 -0.0045008153554384 1.4816733158434552  
Hf 2.3898722824356646 0.0084597443777774 -1.4729380237246552  
Hf -2.3898722824356629 -0.0084597443777774 1.4729380237246570  
Hf -2.3847711318553060 0.0045008153554349 -1.4816733158434552

Au 0.0000000000000000 0.0000000000000000 0.0000000000000000

Hg

Hf -0.0000286122208593 1.4720792602213528 2.4202903760890404

Hf -0.0000056202017618 1.4720774535163805 -2.4202862247635695

Hf 0.0000056202017618 -1.4720774535163805 2.4202862247635704

Hf 0.0000286122208593 -1.4720792602213528 -2.4202903760890395

Hf 1.4720792602213528 2.4202903760890404 -0.0000286122208575

Hf -1.4720774535163788 2.4202862247635704 0.0000056202017618

Hf 1.4720774535163805 -2.4202862247635704 -0.0000056202017600

Hf -1.4720792602213510 -2.4202903760890404 0.0000286122208610

Hf 2.4202903760890404 -0.0000286122208593 1.4720792602213528

Hf 2.4202862247635704 0.0000056202017618 -1.4720774535163788

Hf -2.4202862247635704 -0.0000056202017618 1.4720774535163805

Hf -2.4202903760890404 0.0000286122208610 -1.4720792602213510

Hg 0.0000000000000000 0.0000000000000000 0.0000000000000000

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