Supporting Information

O_2 Activation by Core-shell $Ru_{13}@Pt_{42}$ Particle in Comparison with Pt_{55} Particle: DFT Study

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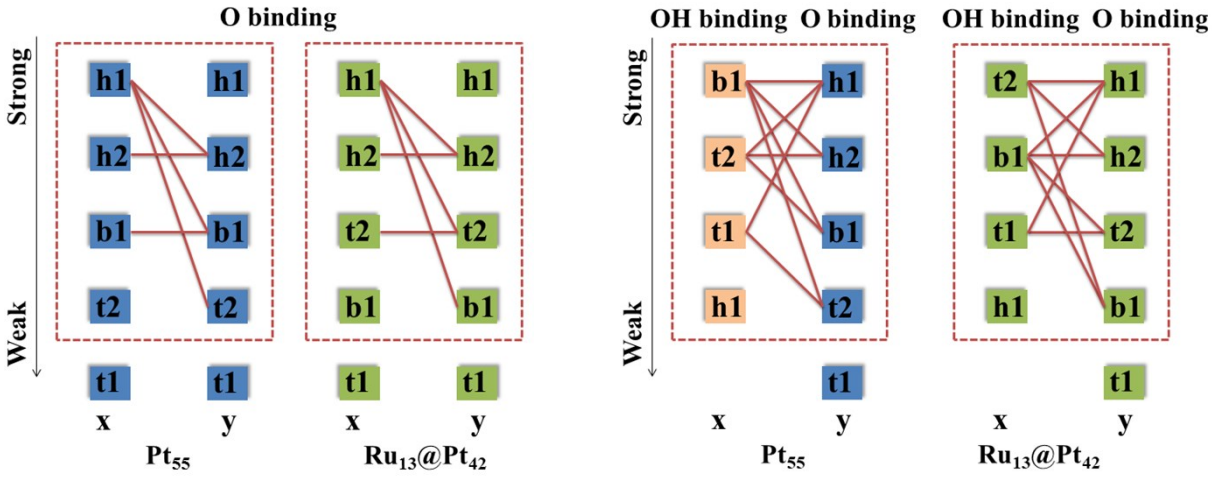
Scheme S1. (a) Possible adsorption structures of 2(O) species and (b) (O)(OH) species.



(a) 2(O) adsorption structure. **(b) (O)(OH) adsorption structure**

(O_2)-Binding

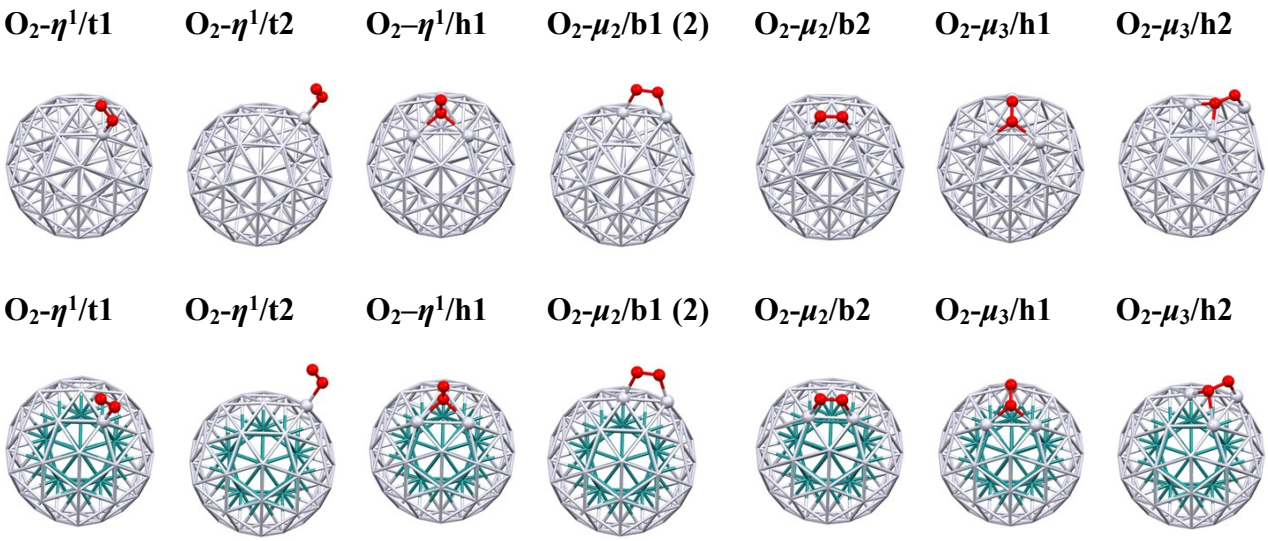
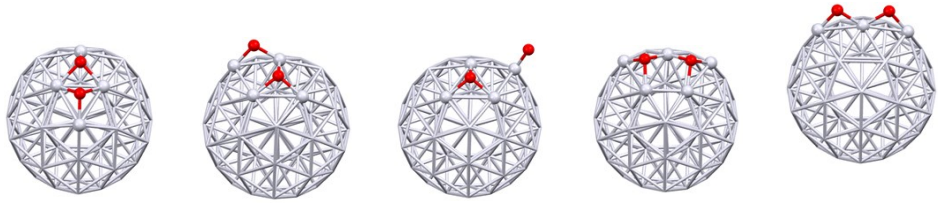


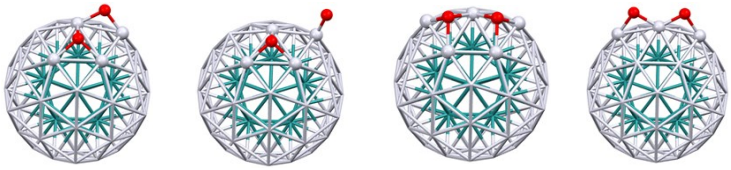
Figure S1. Optimized structures of (O_2)-binding species at different sites.

2O-Binding



-10.95 (13et) -26.08 (11et) -19.70 (15et) -23.19 (11et) -17.22(11et)

Change to 2O/h1b1



-19.85 (7et) -20.26 (7et) -22.62 (7et) -18.89 (9et)

2O/h1h2 **2O/h1b1** **2O/h1t2** **2O/h2h2** **2O/b1b1**

Figure S2. Optimized structures and relative energies (in kcal/mol) for 2O-binding species.
Note: $\Delta E = E_t(2O/xy) - E_t(O_2\text{-}\mu_2/b1)$.
In $Ru_{13}@Pt_{42}$, the 2O migrates from h1h2 sites to h1b1 sites.

Adsorption Sites of two O atoms. Because the direct O-O bond cleavage of dioxygen (O_2) molecule affords two O atoms bound on the Pt_{42} surface, we investigated Pt_{55} and $Ru_{13}@Pt_{42}$ clusters bound with two O atoms as finial state (**FS**) of the direct O-O bond cleavage of O_2 molecule ($O_2 \rightarrow 2O$), as will be discussed below. Because the $(O)_2$-binding energy becomes more negative following the order t1 < t2 < b1 < h2 < h1 for Pt_{55} and t1 < b1 < t2 < h2 < h1 for $Ru_{13}@Pt_{42}$, as shown in Table S3, several typical binding positions including 2O/h1h2, 2O/h1b1, 2O/h1t2, 2O/h2h2, and 2O/b1b1 were investigated, as shown in Scheme S1, where 2O/h1h2 etc represents two O atoms adsorbed at h1 and h2 sites. The optimized structures and relative energies to the O_2-μ_2/b1-binding species are shown in Figures S1 and S2 and Table S3. For Pt_{55}, 2O/h1b1-adsorption species is the most stable and the 2O/h2h2-adsorption species is the next. For $Ru_{13}@Pt_{42}$, 2O/h2h2 is the most stable combination and 2O/h1t2 is the next.

OOH-Binding

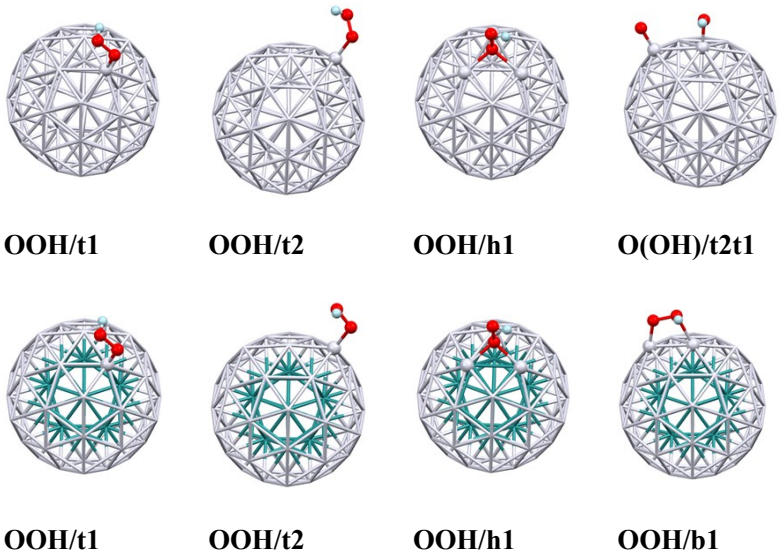
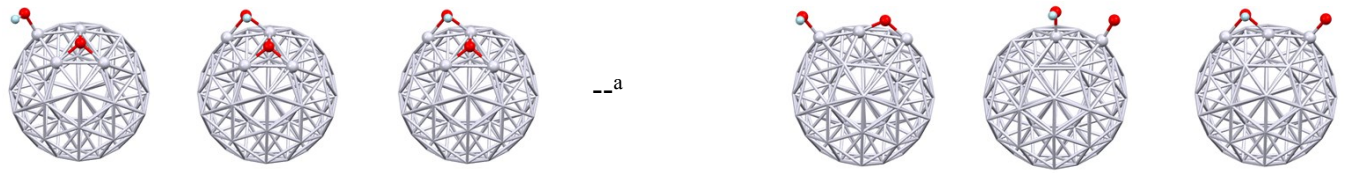


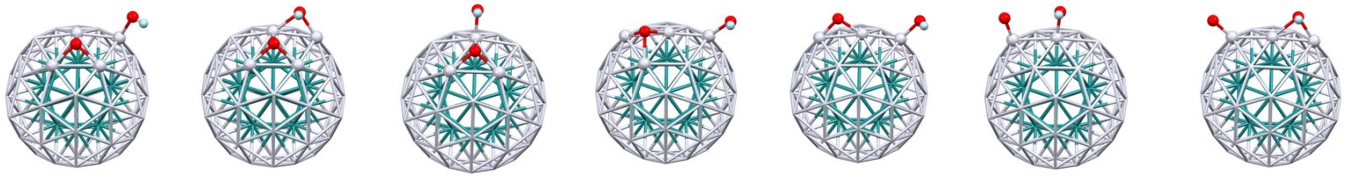
Figure S3. Optimized structures of OOH-binding species at different sites.

OOH-Adsorption Site. The OOH-binding species is one of the important intermediates for ORR. As listed in Table S2, the OOH binding energy increases (more negative) in the order of η^1/h1 < η^1/t1 < η^1/t2 for Pt_{55} and μ_2/h1 < η^1/t1 < η^1/b1 < η^1/t2 for $Ru_{13}@Pt_{42}$; the optimized structures are shown in Figure S3 in the Supporting Information. We tried to optimize the OOH binding at the h2 and b2 sites but the OOH group changed its binding position to the t2 and t1 sites, respectively, during the optimization. This means that the OOH/h2 and OOH/b2 species are not stable. In the case of Pt_{55}, the OOH-binding at the b1 site in μ_2-side-on structure is not stable but the O-OH bond cleavage occurs to afford O and OH species without energy barrier, where O and OH are located at the t2 and t1 sites, respectively. Also, we found that the OOH binding energy with $Ru_{13}@Pt_{42}$ is smaller (less negative) than that with Pt_{55} at the same adsorption site (Table S2).

(O)(OH)-Binding



-44.65 (14et) -43.76 (12et) O(OH)/h1b1 --[a] -43.93 (12et) -31.10 (14et) -35.95 (14et)



-35.86 (6et) -31.58 (8et) -19.80 (8et) -35.24 (8et) -33.52 (8et) -23.03 (2et) -30.50 (6et)

O(OH)/h1t2 O(OH)/h1b1 O(OH)/h1t1 O(OH)/h2t2 O(OH)/b1t2 O(OH)/t2t1 O(OH)/t2b1

Figure S4. Optimized structures and relative energies (in kcal/mol) for O(OH)-binding species.

Note: $\Delta E = E_t\{O(OH)/xy\} - E_t(OOH/t2)$;
O(OH)/h2b1 migrates to O(OH)/h2t2 after optimization; O(OH)/b1b1 migrates to O(OH)/b1t2 after optimization. [a] Icosahedron-like structure completely lost.

(O)(OH)-Adsorption Site. In this species, many possible adsorption structures should be investigated. As was discussed above, the O atom tends to interact with Pt_{55} and $Ru_{13}@Pt_{42}$ at the h1 and h2 sites and the next is b1 or t2. The OH group tends to interact with Pt_{55} and $Ru_{13}@Pt_{42}$ at the t2 and b1 sites. Considering these favorable adsorption structures, we investigated (O)(OH)/h1t2, (O)(OH)/h1b1, (O)(OH)/h2t2, (O)(OH)/h2b1, (O)(OH)/b1t2, (O)(OH)/b1b1, (O)(OH)/t2t1, and (O)(OH)/t2b1-adsorption structures; their optimized structures and relative energies are shown in Figure S4. Among them, the (O)(OH)/h1t2-adsorption species is the most stable in both Pt_{55} and $Ru_{13}@Pt_{42}$. The (O)(OH)/b1t2 is the next stable, while the energy difference from the most stable species is not large.

Stability of $Ru_{13}@Pt_{42}$

Previously, we have investigated the stability of the icosahedron-like $Pt_{42}Ru_{13}$ clusters at the PBE-D2 theoretical level, among which the core-shell $Ru_{13}@Pt_{42}$ is the most stable isomer.[92] In this study, PBE-D3 method was adopted to calculate the total energies for Pt_{55} and $Pt_{42}Ru_{13}$ in different possible spin states (see Table S1). Core-shell structure ($Ru_{13}@Pt_{42}$) in the septet state is much more stable than these non-core-shell structures ($Pt^{core\text{-}1}Ru_{12}@Pt_{41}Ru^{edge}$ and $Pt^{core\text{-}1}Ru_{12}@Pt_{41}Ru^{vertex}$) and the corresponding energy difference between $Ru_{13}@Pt_{42}$ and $Pt^{core\text{-}1}Ru_{12}@Pt_{41}Ru^{edge}$ ($Pt^{core\text{-}1}Ru_{12}@Pt_{41}Ru^{vertex}$) is 49.03 kcal/mol (43.27 kcal/mol).

Table S1. Total energies (in eV) for Pt_{55} and $Pt_{42}Ru_{13}$ in different possible spin states using PBE-D3 method.

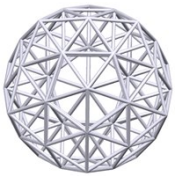
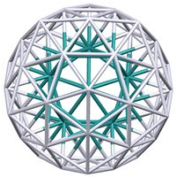
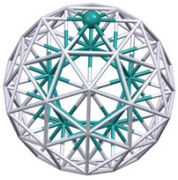
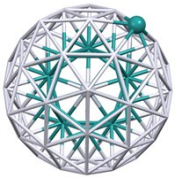
	Pure cluster	**Core-shell structure**	**Non-core-shell structure**	
				
	Pt_{55} (1)	**$Ru_{13}@Pt_{42}$ (1)**	**$Pt^{core\text{-}1}Ru_{12}@Pt_{41}Ru^{edge}$**	**$Pt^{core\text{-}1}Ru_{12}@Pt_{41}Ru^{vertex}$**
5et	-296.41180390	-346.70813144	-344.61750489	-344.84553235
7et	-296.51106938	**-346.87191611**	**-344.74563887**	**-344.99539856**
9et	-296.64541681	-346.51349432	-344.52195304	-344.67233624
11et	-296.80830127			
13et	-296.97450017			
15et	**-296.99019548**			
17et	-296.75368939			

Table S2. Binding energies (E_b, in eV) for O_2 and OOH species.[a]

Site x	Pt_{55}	$Ru_{13}@Pt_{42}$	Pt_{55}	$Ru_{13}@Pt_{42}$
	O_2		**4** (OOH-adsorbed species)	
η^1/t1	-1.05 (11et) [a]	-0.37 (9et)	-4.18 (10et)	-3.57 (6et)
η^1/t2	-1.13 (13et)	-0.72 (7et)	**-4.30 (14et)**	**-3.98 (6et)**
η^1/h1	-0.25 (13et)	0.42 (7et)	-3.75 (14et)	-3.15 (8et)
η^1/h2	To η^1-t2 [b]	To η^1-t2 [b]	To η^1-t2 [b]	To η^1-t2 [b]
μ_2/b1	-1.70 (11et)	-0.95 (7et)	- [c]	-3.89 (6et)
μ_2/b2	-1.41 (11et)	-0.19 (9et)	To *t1*-η^1	To *t1*-η^1

[a] The most stable spin state is given in parentheses.
[b] The η^1/h2 adsorption structure was converted to the η^1-t2 structure during the geometry optimization.
[c] OOH decomposes into O and OH at the top sites, where O is connected at t2 site and OH is connected at t1 site.

Table S3. Binding energies (E_b, in eV) for O, OH, and H/x-binding species.

Site x	Pt_{55}	$Ru_{13}@Pt_{42}$	Pt_{55}	$Ru_{13}@Pt_{42}$	Pt_{55}	$Ru_{13}@Pt_{42}$
	O [a]		**OH** [b]		**H** [c]	
t1	-4.14 (15et)	-3.30 (9et)	-3.19 (12et)	-2.59 (6et)	-2.95 (12et)	-2.45 (8et)
t2	-4.46 (15et)	-4.25 (7et)	**-3.35 (12et)**	**-3.06 (6et)**	-2.77 (14et)	-2.55 (6et)
h1	**-5.01 (11et)**	**-4.41 (7et)**	-2.94 (14et)	-2.35 (8et)	-2.76 (14et)	-2.60 (8et)
h2	-4.91 (11et)	-4.33 (7et)	t2	t2	-3.00 (12et)	-2.63 (8et)
b1	-4.84 (13et)	-4.22 (9et)	**-3.38 (10et)**	-2.86 (8et)	**-3.07 (12et)**	**-2.70 (8et)**

[a] O migrates from b2 to *hcp*-like h2.
[b] OH migrates from b2 to *fcc*-like h1.
[c] H migrates from b2 to *hcp*-like h2.

O-Adsorption site. Single O atom is preferentially adsorbed at the *fcc*-like h1 site with E_b(O/h1) of -5.01 eV and -4.41 eV for Pt_{55} and $Ru_{13}@Pt_{42}$, respectively, as listed in Table 2. For Pt_{55}, the E_b(O) increases (becomes more negative) following the order t1 > t2 > b1 > h2 > h1. The adsorbed O atom at the b2 site easily moves to *hcp*-like h2 site during geometry optimization. For $Ru_{13}@Pt_{42}$, the E_b(O) increases (becomes more negative) following the order t1 > b1 > t2 > h2 > h1. The O atom easily migrates from the b2 to the h2 site during geometry optimization, similar to the Pt_{55} case discussed above. The binding energy of single O at the same adsorption site of $Ru_{13}@Pt_{42}$ is found to be larger (less negative) than that of Pt_{55}.

OH-Adsorption Site. The binding energy increases (becomes more negative) following the order h1 < t1 < t2 ≈ b1 for Pt_{55} and h1 < t1 < b1 < t2 for $Ru_{13}@Pt_{42}$, as listed in Table S3. Both the t2 and b1 sites on the Pt_{55} surface are preferable for OH-binding, where E_b(OH/t2) is -3.35 eV and E_b(OH/b1) -3.38 eV. In $Ru_{13}@Pt_{42}$, on the other hand, t2 is the most favorable for OH-bonding, where E_b(OH/t2) is -3.06 eV. The OH-binding energy with $Ru_{13}@Pt_{42}$ is less negative than that with Pt_{55}.

H-Adsorption site. In the ORR catalytic cycle, the reaction of hydrogen atom (or proton) with oxygen-containing species is involved. We investigated that H was bound with metal cluster and then reacted with oxygen-containing species on the surface, as was discussed in recent works.[45-46] This is reasonable because a lot of protons exist around the electrode, its adsorption to the electrode surface occurs easily, and one-electron reduction of proton to hydrogen occurs easily at the cathode which is negatively charged. As shown in Table S3, the H-binding energy increases (becomes more negative) following the order of h1 ≈ t2 < t1 < h2 < b1 for Pt_{55} and t1 < t2 < h1 < h2 < b1 for $Ru_{13}@Pt_{42}$. The best binding site is b1 for both Pt_{55} and $Ru_{13}@Pt_{42}$, where E_b(H/b1) is -3.07 eV and -2.70 eV, respectively.

The dependence of DOS on the box size in periodic DFT calculations

We checked the dependence of the Fermi level on the box size of periodic calculation.

Table S4. The Fermi level ($\varepsilon_{F,\,eV}$) and the d-valence band top ($\varepsilon_{VB\_top,\,eV}$) energies

Box size	Before correction		After correction	
	ε_F	ε_{VB_top}	ε_F	ε_{VB_top}
		Pt_{55}		
25x25x25	-4.53	-4.57	-5.40	-5.44
35x35x35	-5.09	-5.13	-5.41	-5.45
		$Ru_{13}@Pt_{42}$		
25x25x25	-4.51	-5.06	-5.38	-5.93
35x35x35	-5.09	-5.67	-5.40	-5.98

As shown in Table S4, the direct computational results of the Fermi level (ε_F) and d-valence band top ($\varepsilon_{VB\text{-}top}$) without correction depend on the box size. However, the Fermi level (ε_F) and d-valence band top ($\varepsilon_{VB\text{-}top}$) little differ between two box sizes after the correction of vacuum level by the Baldereschi procedure.[1]

DOSs of Pt_{55} and $Ru_{13}@Pt_{42}$ calculated by the B3LYP and the PBE functionals.

The DOS and PDOS were calculated using the B3LYP,[2] B3PW91[2a,3] and PBE[4] functionals with LANL2DZ[5] in our previous work,[6] using the conventional DFT method. In this work, we performed periodic DFT calculations employing the PBE functional with plane wave basis sets.

We compared the Fermi level and the d-valence band top in Table S5. In our previous work,[6] the B3LYP, B3PW91 and PBE functionals provided the lower energy of d-valence band-top in Pt_{55} than in $Ru_{13}@Pt_{42}$. Though the absolute values depend on the functional, the difference in the d-valence band-top energy between Pt_{55} and $Ru_{13}@Pt_{42}$ is similar in these three cases. On the basis of these results, it is likely concluded that the trend of the d-valence band-top energy is calculated well using these three functionals.

In this work, the PBE functional with plane-wave basis set provided the higher energy of d-valence band-top of Pt_{55} than that of $Ru_{13}@Pt_{42}$; this is different trend from the results of the B3LYP, B3PW91 and PBE calculations with LANL2DZ basis set. It is likely that the difference in basis set is the origin of the difference in computational result, because these three functionals provided the same trend when LANL2DZ was used and the LANL2DZ is small, and that the results calculated by the PBE/plane-wave basis set seem better than the B3LYP or PBE/LANL2DZ calculation.

Table S5. d-Valence band top energy (in eV) calculated using several different functionals and basis sets

Functional/Basis sets	Pt_{55}	$Ru_{13}@Pt_{42}$
PBE/plane-wave basis set[a]	-4.57	-5.06
PBE0/plane-wave basis set[a]		
HSE06/plane-wave basis set[a]		
B3LYP/LAN2DZ[b]	-5.87	-5.78
B3PW91/LAN2DZ[b]	-5.93	-5.84
PBE/LAN2DZ[b]	-5.42	-5.36

a) This work. b) Ref. 6.

The d-valence band-top energy of the Pt_{42} shell in $Ru_{13}@Pt_{42}$ and Pt_{55}

Because Ru metal is more easily oxidized than Pt metal, it is likely that the fused alloy metal consisting of Ru and Pt is more easily oxidized than pure Pt metal. However, in the core-shell particle $Ru_{13}@Pt_{42}$, the Ru_{13} core influences the electronic structure of the Pt_{42} shell through charge-transfer (CT) from the higher energy 4d orbital of Ru_{13} core to Pt_{42} shell and exchange repulsion between Ru_{13} core and Pt_{42} shell. The CT raises the d-valence band top energy of the Pt_{42} shell because the CT enhances electron density on the Pt_{42} shell. However, the exchange repulsion between the Ru 4d of the Ru_{13} core and the Pt 5d of the Pt_{13} shell in $Ru_{13}@Pt_{42}$ is smaller than that between the Pt 5d of the Pt_{13} core and the Pt 5d of the Pt_{42} shell in Pt_{55}. Because the smaller exchange repulsion raises less the d-valence band-top energy of the Pt_{42} shell in $Ru_{13}@Pt_{42}$ than in Pt_{55}, it is likely that the smaller exchange repulsion between the Pt_{42} shell and the Ru_{13} core is one reason to lower the d-valence band-top energy of $Ru_{13}@Pt_{42}$ compared to that in Pt_{55}. In other words, the CT and the exchange repulsion provide the reverse effect on the d-valence band-top energy.

The larger O_2 adsorption energy, longer O-O bond distance, shorter Pt-O bond distance, and the smaller activation energy for O-O bond cleavage in Pt_{55} than in $Ru_{13}@Pt_{42}$ are good measures relating to the d orbital energy of the Pt_{42} shell. All these results suggest strongly that the d valence band-top exists at higher energy in Pt_{55} than in $Ru_{13}@Pt_{42}$. Considering these results, it likely concluded that the computational results by the PBE/plane-wave basis set are reasonable and the exchange repulsion between the Ru_{13} core and the Pt_{42} shell is more important than the CT for determining the d-valence band-top energy.

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Cartesian coordinates

Pt_{55}

Pt	11.786936	11.261912	16.858248
Pt	12.924528	13.634377	17.477797
Pt	14.564960	11.711991	16.518789
Pt	10.441153	13.716669	16.413576
Pt	10.720446	9.012858	15.804358
Pt	14.935944	14.444880	15.864313
Pt	12.387311	15.683885	15.799268
Pt	13.405090	9.280103	15.638195
Pt	9.281341	11.284796	15.533033
Pt	15.999579	9.868165	15.159313
Pt	8.162965	13.677834	14.959374
Pt	12.714821	13.073933	15.018514
Pt	16.554153	12.463060	14.644329
Pt	9.881757	15.706725	14.474013
Pt	11.599621	10.735681	14.171861
Pt	16.704706	15.061666	13.915673
Pt	14.376548	16.434965	13.924835
Pt	11.861381	17.416115	13.792029
Pt	14.270584	11.168326	13.845433
Pt	10.305687	13.095966	13.744344
Pt	11.899621	8.078079	13.558936
Pt	9.350997	9.317006	13.493864
Pt	14.627451	13.795964	13.216281
Pt	14.677511	8.528119	13.219539
Pt	12.177021	14.987280	13.153786
Pt	8.005122	11.771774	13.049206
Pt	16.623787	10.495264	12.605195
Pt	12.500013	12.500018	12.499990
Pt	8.376215	14.504721	12.394819
Pt	16.994879	13.228244	11.950760
Pt	12.822993	10.012704	11.846196
Pt	10.322436	16.471886	11.780494
Pt	10.372545	11.204035	11.783691
Pt	15.649022	15.683018	11.506128
Pt	13.100390	16.921947	11.441080
Pt	14.694321	11.904001	11.255653
Pt	10.729427	13.831708	11.154559
Pt	13.138596	7.583858	11.208008
Pt	10.623446	8.565020	11.075215
Pt	8.295279	9.938377	11.084338
Pt	13.400401	14.264337	10.828139
Pt	15.118247	9.293230	10.525981
Pt	8.445861	12.536976	10.355646
Pt	12.285172	11.926036	9.981466

Pt	16.837025	11.322135	10.040618
Pt	9.000399	15.131861	9.840707
Pt	15.718642	13.715172	9.466960
Pt	14.279570	15.987143	9.195605
Pt	10.064036	10.555077	9.135685
Pt	11.594914	15.719934	9.361821
Pt	12.612703	9.316092	9.200728
Pt	14.558861	11.283331	8.586398
Pt	10.435057	13.288010	8.481236
Pt	12.075499	11.365641	7.522194
Pt	13.213031	13.738096	8.141778

2^{Pt}

Pt	11.863721	10.908550	16.869352
Pt	13.008038	13.205125	17.607679
Pt	14.602067	11.350469	16.536644
Pt	10.494046	13.384746	16.563457
Pt	10.751261	8.757957	15.633574
Pt	15.024126	14.115951	16.012064
Pt	12.460213	15.482519	16.126377
Pt	13.426598	8.960753	15.417063
Pt	9.309429	11.059669	15.525551
Pt	16.005186	9.606226	14.994095
Pt	8.229704	13.483774	15.107266
Pt	12.709954	13.158438	15.109541
Pt	16.594652	12.235866	14.638747
Pt	9.940936	15.523887	14.720591
Pt	11.635711	10.713131	14.294201
Pt	16.739145	14.857689	14.071430
Pt	14.438883	16.250319	14.172318
Pt	11.912032	17.371555	14.132767
Pt	14.270226	11.139297	13.974859
Pt	10.324730	13.028399	13.754813
Pt	11.838227	7.923348	13.327411
Pt	9.340295	9.204644	13.387654
Pt	14.631417	13.726005	13.233119
Pt	14.723839	8.388376	12.976782
Pt	12.187907	14.947937	13.200667
Pt	8.030191	11.700067	13.093930
Pt	16.641434	10.383022	12.498959
Pt	12.521446	12.418695	12.571913
Pt	8.414929	14.481345	12.587393
Pt	17.005262	13.149630	12.001595
Pt	12.857115	9.894794	11.964555
Pt	10.374110	16.450027	12.085386

Pt	10.431089	11.080578	11.876897
Pt	15.669720	15.651995	11.703959
Pt	13.135955	16.895412	11.749393
Pt	14.702251	11.772572	11.359098
Pt	10.763831	13.739650	11.173668
Pt	13.101662	7.601089	10.943552
Pt	10.601961	8.601477	10.854164
Pt	8.298161	10.001727	11.018125
Pt	13.404097	14.166906	10.854362
Pt	15.073435	9.324046	10.310041
Pt	8.455602	12.628816	10.478475
Pt	12.315221	11.796689	10.040861
Pt	16.800011	11.374591	9.983494
Pt	9.021182	15.248166	10.076897
Pt	15.713017	13.800263	9.594679
Pt	14.285563	16.097794	9.436193
Pt	10.025090	10.743479	9.101114
Pt	11.605762	15.873760	9.631303
Pt	12.576474	9.415419	9.037956
Pt	14.530725	11.470531	8.552756
Pt	10.442001	13.491570	8.582716
Pt	12.038427	11.610806	7.529745
Pt	13.171783	13.932241	8.251434
O	12.264100	17.304644	16.918764
O	11.995081	18.213469	15.910289

TS2/3a^{Pt}

Pt	11.986125	11.347818	16.861744
Pt	13.068570	13.752468	17.409582
Pt	14.688828	11.790941	16.447113
Pt	10.548772	13.851826	16.399775
Pt	10.907782	8.861829	15.945538
Pt	15.033998	14.519067	15.739851
Pt	12.461267	15.753110	15.710087
Pt	13.514158	9.323018	15.578997
Pt	9.214372	11.441001	15.660713
Pt	16.096134	9.920745	15.082006
Pt	8.184574	13.843651	14.973629
Pt	16.594740	12.516122	14.527878
Pt	9.943951	15.772358	14.388429
Pt	16.752781	15.095494	13.755234
Pt	14.430523	16.464516	13.799642
Pt	11.917795	17.457169	13.679636
Pt	11.984739	8.144513	13.600445
Pt	9.411750	9.299600	13.563681
Pt	14.736694	8.532761	13.180367

Pt	8.028019	11.800313	13.133517
Pt	16.613800	10.514410	12.510956
Pt	8.416524	14.539962	12.400806
Pt	16.989088	13.231050	11.820700
Pt	10.339977	16.496029	11.706265
Pt	15.649011	15.673380	11.354959
Pt	13.105555	16.921135	11.324677
Pt	13.152710	7.566337	11.196356
Pt	10.623675	8.553282	11.141690
Pt	8.293001	9.925797	11.185968
Pt	15.087713	9.296047	10.499701
Pt	8.419809	12.516418	10.437642
Pt	16.786198	11.305124	9.938107
Pt	8.968509	15.104980	9.834084
Pt	15.666477	13.685575	9.351000
Pt	14.225004	15.958227	9.065772
Pt	10.007730	10.518952	9.188043
Pt	11.545782	15.679463	9.292475
Pt	12.541401	9.297126	9.220554
Pt	14.479345	11.241887	8.537389
Pt	10.362308	13.226427	8.491720
Pt	11.980962	11.304838	7.518236
Pt	13.142684	13.681979	8.079606
Pt	12.189066	14.999480	13.104527
Pt	12.785038	13.109505	14.974345
Pt	10.315070	13.041453	13.841133
Pt	10.708559	13.834049	11.176847
Pt	13.363485	14.280624	10.752512
Pt	14.640048	13.817735	13.119991
Pt	12.823680	10.018773	11.860029
Pt	11.525412	10.744237	14.277519
Pt	12.234515	11.918682	9.978065
Pt	10.379787	11.203504	11.823351
Pt	14.276274	11.178972	13.800037
Pt	14.660679	11.921381	11.189229
Pt	12.487294	12.508292	12.493458
O	8.641129	10.470038	17.112967
O	9.662180	8.904431	17.269732

3a^{Pt}

Pt	11.905089	11.218673	16.821877
Pt	12.942627	13.621964	17.384348
Pt	14.546774	11.717269	16.414354
Pt	10.467925	13.868380	16.365381
Pt	10.743770	8.936489	15.758989

Pt	14.897214	14.407331	15.769802
Pt	12.392863	15.631779	15.705826
Pt	13.416810	9.355161	15.535754
Pt	9.244100	11.242673	15.414330
Pt	15.973478	9.913620	15.076134
Pt	8.229700	13.664825	14.891561
Pt	16.485361	12.478954	14.578848
Pt	9.955021	15.653980	14.416400
Pt	16.658691	15.039806	13.872663
Pt	14.352118	16.363594	13.881794
Pt	11.885908	17.361826	13.744646
Pt	11.932992	8.192380	13.498018
Pt	9.430360	9.391187	13.427078
Pt	14.656761	8.603471	13.166416
Pt	8.101721	11.775753	13.005320
Pt	16.551146	10.552306	12.555819
Pt	8.475459	14.465674	12.373109
Pt	16.909334	13.229299	11.934749
Pt	10.370498	16.399784	11.775833
Pt	15.593517	15.634900	11.504938
Pt	13.102711	16.837734	11.434964
Pt	13.154893	7.663760	11.178918
Pt	10.680350	8.639473	11.063064
Pt	8.379458	9.982399	11.059352
Pt	15.085515	9.382372	10.535658
Pt	8.538874	12.551093	10.375631
Pt	16.792551	11.366808	10.032197
Pt	9.061371	15.108906	9.854094
Pt	15.670243	13.713596	9.505953
Pt	14.265758	15.946598	9.220908
Pt	10.146724	10.610374	9.168151
Pt	11.626281	15.671044	9.406462
Pt	12.624722	9.404688	9.233962
Pt	14.532667	11.334629	8.637070
Pt	10.496478	13.287512	8.542692
Pt	12.108465	11.409257	7.554399
Pt	13.208164	13.736021	8.203560
Pt	12.195257	14.870972	13.116825
Pt	12.698802	13.026905	14.895922
Pt	10.415154	13.047693	13.687940
Pt	10.814343	13.772840	11.212269
Pt	13.365677	14.193699	10.892380
Pt	14.530842	13.739011	13.178189
Pt	12.814069	10.135110	11.865518
Pt	11.632170	10.779964	14.110972
Pt	12.303684	11.960567	10.084105
Pt	10.488627	11.262719	11.807073
Pt	14.186714	11.229083	13.763289

Pt	14.599591	11.939709	11.298573
Pt	12.526562	12.539188	12.450306
O	10.019164	12.018782	17.181459
O	10.012427	8.056726	17.129309

3b^{Pt}

Pt	11.850120	11.166642	16.885086
Pt	12.953308	13.531457	17.498835
Pt	14.555171	11.601137	16.542591
Pt	10.412922	13.562729	16.426071
Pt	10.733375	8.954552	15.724914
Pt	15.048560	14.302452	15.854198
Pt	12.370704	15.854460	15.928981
Pt	13.405543	9.161498	15.528388
Pt	9.269942	11.223202	15.491157
Pt	15.981606	9.785122	15.076901
Pt	8.175602	13.622149	14.931391
Pt	12.697278	13.467166	15.006001
Pt	16.582253	12.383132	14.591771
Pt	9.866365	15.680112	14.447795
Pt	11.621682	10.886896	14.336326
Pt	16.736706	14.983529	13.872560
Pt	14.425076	16.382385	13.912155
Pt	11.869522	17.459742	13.812537
Pt	14.234036	11.281184	13.998826
Pt	10.339936	13.186842	13.690959
Pt	11.848874	8.003039	13.493548
Pt	9.342917	9.278761	13.454874
Pt	14.643805	13.792862	13.092632
Pt	14.703122	8.480262	13.127403
Pt	12.220994	15.066349	12.955239
Pt	8.026666	11.739852	13.022661
Pt	16.641417	10.443870	12.560892
Pt	12.514925	12.492952	12.524499
Pt	8.389932	14.479239	12.360977
Pt	17.001715	13.159707	11.906537
Pt	12.808670	9.921139	12.040188
Pt	10.335898	16.451622	11.770771
Pt	10.411262	11.136338	11.897254
Pt	15.656190	15.659417	11.471291
Pt	13.133420	16.924616	11.409225
Pt	14.681869	11.725513	11.342094
Pt	10.768294	13.732128	11.066839
Pt	13.119986	7.563519	11.136260
Pt	10.629860	8.560715	10.986681
Pt	8.323064	9.938822	11.044609

Pt	13.426086	14.098976	10.679884
Pt	15.084052	9.251294	10.431656
Pt	8.478380	12.528798	10.356394
Pt	12.297174	11.717072	10.015811
Pt	16.803278	11.286089	9.994894
Pt	9.018226	15.124419	9.820864
Pt	15.729743	13.687953	9.466635
Pt	14.290874	15.968897	9.171620
Pt	10.061531	10.572128	9.109363
Pt	11.611455	15.731888	9.366571
Pt	12.609750	9.279521	9.135566
Pt	14.543037	11.298899	8.559218
Pt	10.466467	13.293132	8.462152
Pt	12.072765	11.375708	7.499719
Pt	13.198191	13.733162	8.096962
O	11.885620	18.564241	15.465596
O	12.126347	17.771706	16.559542
H	12.652670	15.283026	17.549553

TS3/4b^{Pt}

Pt	11.787927	11.346121	16.847166
Pt	12.939083	13.705820	17.465418
Pt	14.584069	11.760825	16.530926
Pt	10.451964	13.803954	16.449400
Pt	10.735834	9.089578	15.833881
Pt	14.950956	14.525827	15.853411
Pt	12.397935	15.760767	15.862637
Pt	13.407935	9.354227	15.683688
Pt	9.311542	11.341434	15.536642
Pt	15.990257	9.916395	15.184472
Pt	8.192249	13.726049	14.944283
Pt	12.867424	13.009171	15.028191
Pt	16.555971	12.483939	14.684404
Pt	9.890747	15.751368	14.433092
Pt	11.651013	10.692882	14.076365
Pt	16.714825	15.051983	13.885514
Pt	14.436002	16.447582	13.886915
Pt	11.900366	17.495041	13.795328
Pt	14.293493	11.022629	13.661782
Pt	10.432841	13.145245	13.905069
Pt	11.914993	8.094579	13.609411
Pt	9.360628	9.362670	13.524339
Pt	14.718780	13.654390	13.187303
Pt	14.664206	8.498996	13.270350
Pt	12.298478	15.050861	13.276493

Pt	8.013247	11.816827	13.071297
Pt	16.655720	10.525274	12.623724
Pt	12.513569	12.520947	12.497499
Pt	8.379130	14.513567	12.384050
Pt	16.992071	13.215141	11.918138
Pt	12.663373	10.019176	11.635822
Pt	10.364405	16.525496	11.760379
Pt	10.294592	11.371947	11.834880
Pt	15.660074	15.674752	11.481575
Pt	13.098585	16.929413	11.414947
Pt	14.580242	11.857020	11.100087
Pt	10.729785	13.999018	11.311826
Pt	13.144386	7.564381	11.268215
Pt	10.594272	8.530364	11.137439
Pt	8.317211	9.956653	11.117396
Pt	13.409657	14.320013	10.902574
Pt	15.133736	9.249165	10.597064
Pt	8.457737	12.540839	10.323782
Pt	12.129242	12.089444	9.954207
Pt	16.813375	11.286394	10.054639
Pt	9.022207	15.121262	9.822013
Pt	15.711761	13.683990	9.462943
Pt	14.282720	15.951168	9.166506
Pt	10.085895	10.494298	9.174100
Pt	11.608558	15.681473	9.314978
Pt	12.640476	9.255589	9.172121
Pt	14.543303	11.225174	8.563599
Pt	10.400735	13.281046	8.448930
Pt	12.068160	11.314794	7.546282
Pt	13.230352	13.698819	8.140217
O	11.784534	19.070745	15.018636
O	11.957804	18.840200	16.305573
H	12.212134	17.301168	16.409611

4b^{Pt}

Pt	11.838165	10.982711	16.768078
Pt	12.995492	13.288309	17.501873
Pt	14.588494	11.411941	16.440996
Pt	10.494220	13.465649	16.484970
Pt	10.725403	8.821754	15.587814
Pt	15.000004	14.168778	15.931848
Pt	12.458200	15.480850	15.974633
Pt	13.406101	9.036336	15.383966
Pt	9.314486	11.136187	15.454324
Pt	15.990546	9.645132	14.941510

Pt	8.224113	13.568068	15.039195
Pt	12.689299	13.059446	14.998275
Pt	16.580429	12.276704	14.566575
Pt	9.959180	15.595344	14.672777
Pt	11.635270	10.690677	14.129827
Pt	16.724958	14.907396	14.001218
Pt	14.403826	16.311924	14.122545
Pt	11.901335	17.401209	14.052417
Pt	14.289230	11.161213	13.835576
Pt	10.315175	13.051968	13.698967
Pt	11.839208	7.980888	13.283268
Pt	9.337430	9.271571	13.327233
Pt	14.588484	13.808806	13.211729
Pt	14.676285	8.397877	12.955381
Pt	12.144556	15.050533	13.174852
Pt	8.022335	11.773881	13.029149
Pt	16.591806	10.392473	12.429760
Pt	12.508307	12.476517	12.481882
Pt	8.404835	14.554034	12.527273
Pt	16.993225	13.180592	11.944258
Pt	12.896505	9.936027	11.818151
Pt	10.330442	16.520880	11.969377
Pt	10.426412	11.140460	11.749184
Pt	15.677971	15.676275	11.625392
Pt	13.165431	16.958544	11.633017
Pt	14.703943	11.915563	11.259048
Pt	10.733169	13.806046	11.142269
Pt	13.073671	7.600094	10.893099
Pt	10.576816	8.636034	10.833428
Pt	8.269557	10.054263	10.968902
Pt	13.365149	14.268621	10.835251
Pt	15.056777	9.344648	10.280525
Pt	8.434859	12.670957	10.398557
Pt	12.321761	11.886677	9.967552
Pt	16.796337	11.383124	9.926424
Pt	9.015331	15.276997	10.000435
Pt	15.702873	13.806828	9.503232
Pt	14.296730	16.100864	9.351008
Pt	10.011278	10.765467	9.041392
Pt	11.605274	15.895025	9.535569
Pt	12.541911	9.445594	8.998899
Pt	14.519295	11.454464	8.490484
Pt	10.430124	13.507968	8.528551
Pt	12.022623	11.620873	7.463726
Pt	13.185163	13.932734	8.192552
O	11.672803	19.496107	15.938406
O	11.636453	19.268227	14.503399
H	10.714019	19.598013	16.133303

TS4/5b^{Pt}

Pt	11.838086	11.047694	16.805220
Pt	12.989952	13.366725	17.464109
Pt	14.578760	11.466240	16.475286
Pt	10.477383	13.518108	16.443823
Pt	10.734491	8.885697	15.599707
Pt	15.012253	14.213101	15.900076
Pt	12.462032	15.592480	15.964584
Pt	13.399722	9.070767	15.373895
Pt	9.297100	11.187501	15.439446
Pt	15.967573	9.694405	14.951088
Pt	8.223087	13.607824	14.982984
Pt	12.645228	13.250847	14.964149
Pt	16.588774	12.315116	14.548509
Pt	9.951835	15.626680	14.615268
Pt	11.634895	10.824163	14.225984
Pt	16.711506	14.926661	13.954745
Pt	14.420779	16.357460	14.069387
Pt	11.930559	17.378786	14.014438
Pt	14.276801	11.278087	13.920786
Pt	10.279675	13.107475	13.584910
Pt	11.811033	7.996099	13.304790
Pt	9.327124	9.293101	13.357292
Pt	14.541142	13.892782	13.164167
Pt	14.726916	8.385655	12.972614
Pt	12.066076	15.087596	12.996747
Pt	8.025404	11.777395	13.007225
Pt	16.606289	10.409353	12.452522
Pt	12.496214	12.508602	12.465765
Pt	8.386832	14.586501	12.465258
Pt	16.979671	13.188749	11.924777
Pt	12.950225	9.913560	11.978850
Pt	10.289737	16.575628	11.906165
Pt	10.483596	11.048328	11.787601
Pt	15.672927	15.675772	11.568578
Pt	13.188269	16.985512	11.592405
Pt	14.700827	11.883396	11.319812
Pt	10.703710	13.706376	10.998527
Pt	13.072366	7.617356	10.916764
Pt	10.580567	8.612418	10.829761
Pt	8.293103	10.051306	10.967962
Pt	13.323063	14.224826	10.737608
Pt	15.051163	9.346215	10.298682
Pt	8.406239	12.659958	10.382865
Pt	12.353849	11.774381	9.978210
Pt	16.779051	11.373542	9.938249

Pt	9.024527	15.274527	9.950213
Pt	15.686706	13.786851	9.493713
Pt	14.281507	16.085966	9.310040
Pt	10.004926	10.773269	9.044815
Pt	11.599920	15.905197	9.494266
Pt	12.546459	9.401189	9.004217
Pt	14.522243	11.440926	8.492167
Pt	10.430038	13.504929	8.441566
Pt	12.021895	11.586989	7.471801
Pt	13.185413	13.904715	8.140101
O	11.980372	18.548588	16.530476
O	11.662377	18.946508	15.155548
H	11.074439	18.443581	16.901791

5b^{Pt}

Pt	11.854931	10.939198	16.755157
Pt	13.014065	13.226685	17.550636
Pt	14.589284	11.364412	16.441525
Pt	10.465759	13.412865	16.516672
Pt	10.727764	8.793203	15.563414
Pt	15.046728	14.112502	15.963167
Pt	12.439164	15.524136	16.017941
Pt	13.413097	9.005161	15.356623
Pt	9.319391	11.110925	15.463765
Pt	16.000427	9.626694	14.917202
Pt	8.199420	13.539785	15.052451
Pt	12.677622	13.087191	15.076884
Pt	16.588991	12.258337	14.558485
Pt	9.876604	15.607130	14.641923
Pt	11.635942	10.679926	14.121511
Pt	16.745817	14.902004	14.011806
Pt	14.438081	16.357180	14.065291
Pt	11.837111	17.541853	13.927471
Pt	14.276592	11.153949	13.847174
Pt	10.303534	13.040750	13.739570
Pt	11.845892	7.990427	13.249842
Pt	9.335767	9.279862	13.309314
Pt	14.589866	13.817833	13.289781
Pt	14.671405	8.411839	12.922443
Pt	12.156507	15.074982	13.397567
Pt	8.022412	11.759122	13.033436
Pt	16.592724	10.404447	12.410967
Pt	12.510499	12.516869	12.549038
Pt	8.382584	14.543562	12.532815
Pt	16.993118	13.182998	11.944428

Pt	12.896712	9.978867	11.792735
Pt	10.347999	16.478580	11.948476
Pt	10.438309	11.175178	11.746180
Pt	15.693016	15.681541	11.630614
Pt	13.126272	16.924847	11.624775
Pt	14.705411	11.956063	11.290338
Pt	10.751647	13.870255	11.225215
Pt	13.068181	7.630402	10.869507
Pt	10.573209	8.660993	10.824421
Pt	8.272099	10.065075	10.965782
Pt	13.376410	14.327711	10.934467
Pt	15.046793	9.370741	10.263783
Pt	8.448231	12.682943	10.429597
Pt	12.328759	11.984761	10.000085
Pt	16.783680	11.402151	9.919815
Pt	8.996950	15.275255	9.992458
Pt	15.692644	13.827872	9.528472
Pt	14.296903	16.117935	9.351203
Pt	10.021468	10.789607	9.057043
Pt	11.598932	15.882958	9.517142
Pt	12.529556	9.497366	9.004934
Pt	14.502098	11.477867	8.506757
Pt	10.433920	13.513165	8.567280
Pt	12.017777	11.653230	7.477702
Pt	13.178873	13.950506	8.230371
O	12.484087	16.771349	17.516336
O	11.622215	19.190565	14.569485
H	11.562155	16.917961	17.813406

5^{Pt}

Pt	11.772223	11.286767	16.813820
Pt	12.948863	13.570378	17.571774
Pt	14.626211	11.661180	16.496311
Pt	10.415701	13.745412	16.387058
Pt	10.711137	9.029821	15.780219
Pt	15.103112	14.364502	15.923015
Pt	12.235984	15.715443	15.863556
Pt	13.407606	9.270306	15.643665
Pt	9.258087	11.268039	15.493952
Pt	15.993071	9.840198	15.108339
Pt	8.157253	13.662388	14.884658
Pt	12.872437	13.090192	15.108374
Pt	16.572153	12.435798	14.649751
Pt	9.850065	15.694245	14.413494
Pt	11.734385	10.719328	14.174329

Pt	16.736992	15.033669	13.858003
Pt	14.437981	16.557653	13.755915
Pt	11.826701	17.420765	13.714992
Pt	14.365396	11.184220	13.712214
Pt	10.386810	13.055685	13.858485
Pt	11.896243	8.098240	13.530888
Pt	9.360734	9.340271	13.471003
Pt	14.645203	13.816507	13.170674
Pt	14.638283	8.525211	13.193403
Pt	12.228444	14.976758	13.268227
Pt	8.003751	11.776773	12.980411
Pt	16.631897	10.475621	12.553616
Pt	12.517826	12.530902	12.508800
Pt	8.347326	14.488396	12.332946
Pt	16.961353	13.185741	11.909971
Pt	12.810884	10.062597	11.765538
Pt	10.334912	16.437996	11.715681
Pt	10.371099	11.220604	11.850984
Pt	15.628487	15.660526	11.440908
Pt	13.101896	16.905489	11.382940
Pt	14.614527	11.957778	11.085699
Pt	10.659869	13.845735	11.255542
Pt	13.119350	7.587972	11.191149
Pt	10.627549	8.572834	11.055549
Pt	8.314811	9.923150	11.052987
Pt	13.294540	14.309388	10.821031
Pt	15.102442	9.275509	10.522520
Pt	8.470878	12.494600	10.297471
Pt	12.151106	11.985385	9.921968
Pt	16.817232	11.287183	10.004802
Pt	9.006407	15.084642	9.774632
Pt	15.724723	13.691039	9.413697
Pt	14.259473	15.937406	9.137232
Pt	10.063046	10.517339	9.107988
Pt	11.573732	15.667240	9.278864
Pt	12.621686	9.301469	9.179482
Pt	14.541666	11.234466	8.535492
Pt	10.425322	13.258219	8.404941
Pt	12.067091	11.309205	7.480124
Pt	13.221593	13.673110	8.095119
O	14.242436	16.245848	15.793703
O	13.206640	14.149427	19.408442
H	14.067406	13.821836	19.740652

$Ru_{13@}Pt_{42}$

Pt	11.800611	11.285624	16.775110
Pt	12.918086	13.617216	17.402222
Pt	14.525551	11.727075	16.442154
Pt	10.480458	13.693535	16.338856
Pt	10.747552	9.065827	15.754241
Pt	14.889524	14.407799	15.800142
Pt	12.389524	15.623183	15.736353
Pt	13.387897	9.341546	15.578307
Pt	9.342814	11.307976	15.475139
Pt	15.946452	9.908091	15.118948
Pt	8.228866	13.659911	14.922033
Pt	16.476866	12.463820	14.603353
Pt	9.931745	15.645565	14.436403
Pt	16.640800	15.022798	13.894121
Pt	14.340724	16.359802	13.897649
Pt	11.871159	17.341475	13.772406
Pt	11.911068	8.162424	13.538795
Pt	9.411124	9.377774	13.474944
Pt	14.635984	8.603902	13.205725
Pt	8.090947	11.785674	13.038681
Pt	16.545078	10.533567	12.603176
Pt	8.454929	14.466436	12.396821
Pt	16.909061	13.214331	11.961214
Pt	10.363924	16.396103	11.794271
Pt	15.588884	15.622230	11.525051
Pt	13.088940	16.837580	11.461301
Pt	13.128848	7.658431	11.227590
Pt	10.659184	8.640103	11.102347
Pt	8.359107	9.977206	11.105874
Pt	15.068264	9.354439	10.563593
Pt	8.523244	12.536284	10.396643
Pt	16.771143	11.340094	10.077963
Pt	9.053556	15.091914	9.881148
Pt	15.657194	13.692029	9.524857
Pt	14.252456	15.934176	9.245755
Pt	10.110485	10.592206	9.199853
Pt	11.612110	15.658458	9.421688
Pt	12.610483	9.376821	9.263642
Pt	14.519550	11.306468	8.661039
Pt	10.474458	13.272929	8.557941
Pt	12.081923	11.382789	7.597775
Pt	13.199396	13.714380	8.224886
Ru	12.191883	14.871851	13.123362
Ru	12.704778	13.047335	14.901608
Ru	10.407529	13.068233	13.686522

Ru	10.811600	13.769765	11.216955
Ru	13.358545	14.182398	10.905766
Ru	14.528630	13.735904	13.183006
Ru	12.808125	10.128153	11.876635
Ru	11.641462	10.817605	14.094229
Ru	12.295230	11.952669	10.098388
Ru	10.471377	11.264100	11.816989
Ru	14.188409	11.230239	13.783041
Ru	14.592479	11.931771	11.313475
Ru	12.500005	12.500002	12.499998

2^{RuPt}

Pt	11.809970	11.306595	16.775135
Pt	12.932801	13.649814	17.379589
Pt	14.549726	11.744758	16.420254
Pt	10.478045	13.723280	16.315327
Pt	10.720995	9.014142	15.784359
Pt	14.894583	14.427831	15.763953
Pt	12.400819	15.639630	15.699670
Pt	13.412282	9.347318	15.521334
Pt	9.333212	11.329687	15.416784
Pt	15.962203	9.927511	15.082825
Pt	8.234195	13.683455	14.883555
Pt	16.480574	12.482424	14.572380
Pt	9.943340	15.659574	14.403650
Pt	16.654194	15.042132	13.868019
Pt	14.348060	16.375341	13.864305
Pt	11.877344	17.363852	13.744861
Pt	11.904187	8.210365	13.521464
Pt	9.453680	9.401814	13.458803
Pt	14.647503	8.615669	13.167596
Pt	8.094203	11.800723	12.998754
Pt	16.559517	10.546630	12.567022
Pt	8.456926	14.484626	12.357977
Pt	16.913744	13.225823	11.932272
Pt	10.370563	16.405954	11.763434
Pt	15.597563	15.631313	11.499192
Pt	13.091109	16.849508	11.434565
Pt	13.136056	7.658012	11.194491
Pt	10.665860	8.651837	11.080904
Pt	8.355997	9.981035	11.071267
Pt	15.079662	9.368277	10.546813
Pt	8.528369	12.552465	10.377791
Pt	16.784515	11.354097	10.045488
Pt	9.058031	15.109411	9.846049

Pt	15.664617	13.707699	9.495966
Pt	14.263029	15.954061	9.225433
Pt	10.121709	10.602503	9.173555
Pt	11.621608	15.672891	9.391607
Pt	12.614264	9.390969	9.237766
Pt	14.527988	11.326053	8.638305
Pt	10.486983	13.290328	8.533982
Pt	12.091803	11.399254	7.572351
Pt	13.210243	13.733567	8.200662
Ru	12.202370	14.882207	13.105260
Ru	12.687402	13.014483	14.914309
Ru	10.410449	13.077003	13.656812
Ru	10.818143	13.786225	11.193910
Ru	13.365772	14.196129	10.882941
Ru	14.530057	13.750916	13.165268
Ru	12.818111	10.138620	11.837750
Ru	11.647177	10.828068	14.047286
Ru	12.304106	11.968694	10.072814
Ru	10.475079	11.277280	11.777322
Ru	14.193839	11.238279	13.754492
Ru	14.602481	11.946956	11.291593
Ru	12.508297	12.516525	12.476521
O	11.187967	10.092398	18.335291
O	10.654066	8.964758	17.759340

TS2/3a^{RuPt}

Pt	11.916963	11.374783	16.755222
Pt	13.044259	13.713943	17.338766
Pt	14.616014	11.790124	16.377886
Pt	10.575033	13.779394	16.325325
Pt	10.873919	8.983727	15.845987
Pt	14.977675	14.476622	15.680665
Pt	12.458288	15.680526	15.651117
Pt	13.470127	9.387730	15.536037
Pt	9.231292	11.346899	15.554951
Pt	16.018753	9.953500	15.055503
Pt	8.270391	13.749163	14.940073
Pt	16.521948	12.514935	14.505993
Pt	9.980409	15.694700	14.376534
Pt	16.684469	15.059786	13.734521
Pt	14.384866	16.393442	13.775054
Pt	11.911285	17.383894	13.676786
Pt	11.965524	8.222709	13.576649
Pt	9.459567	9.396000	13.563214
Pt	14.672979	8.623115	13.169004

Pt	8.118350	11.802627	13.124910
Pt	16.557583	10.546224	12.517206
Pt	8.468479	14.488798	12.400949
Pt	16.908695	13.217677	11.831543
Pt	10.367957	16.408249	11.740310
Pt	15.580113	15.616085	11.377598
Pt	13.086088	16.835693	11.355552
Pt	13.127881	7.634992	11.223446
Pt	10.649633	8.629582	11.170080
Pt	8.355968	9.970562	11.202793
Pt	15.042443	9.348866	10.522729
Pt	8.496142	12.521209	10.457620
Pt	16.728968	11.320702	9.977390
Pt	9.008732	15.074785	9.876431
Pt	15.602785	13.667618	9.416965
Pt	14.188607	15.907490	9.127835
Pt	10.057266	10.564790	9.247383
Pt	11.558804	15.618942	9.365235
Pt	12.548290	9.357832	9.278560
Pt	14.453466	11.271622	8.605160
Pt	10.407521	13.228316	8.566120
Pt	11.995400	11.333984	7.590240
Pt	13.126625	13.671578	8.167800
Ru	12.238005	14.900634	13.068059
Ru	12.753523	13.079494	14.862945
Ru	10.430049	13.093456	13.718869
Ru	10.793630	13.766543	11.218681
Ru	13.338486	14.165367	10.840572
Ru	14.556496	13.751100	13.102794
Ru	12.805859	10.126969	11.880322
Ru	11.670988	10.829412	14.128798
Ru	12.252334	11.927977	10.087659
Ru	10.470487	11.262821	11.857629
Ru	14.226357	11.256311	13.737908
Ru	14.577888	11.922990	11.254913
Ru	12.511060	12.525087	12.464300
O	8.775576	10.592615	17.178341
O	9.752322	8.920286	17.279560

3a^{RuPt}

Pt	11.905089	11.218673	16.821877
Pt	12.942627	13.621964	17.384348
Pt	14.546774	11.717269	16.414354
Pt	10.467925	13.868380	16.365381
Pt	10.743770	8.936489	15.758989

Pt	14.897214	14.407331	15.769802
Pt	12.392863	15.631779	15.705826
Pt	13.416810	9.355161	15.535754
Pt	9.244100	11.242673	15.414330
Pt	15.973478	9.913620	15.076134
Pt	8.229700	13.664825	14.891561
Pt	16.485361	12.478954	14.578848
Pt	9.955021	15.653980	14.416400
Pt	16.658691	15.039806	13.872663
Pt	14.352118	16.363594	13.881794
Pt	11.885908	17.361826	13.744646
Pt	11.932992	8.192380	13.498018
Pt	9.430360	9.391187	13.427078
Pt	14.656761	8.603471	13.166416
Pt	8.101721	11.775753	13.005320
Pt	16.551146	10.552306	12.555819
Pt	8.475459	14.465674	12.373109
Pt	16.909334	13.229299	11.934749
Pt	10.370498	16.399784	11.775833
Pt	15.593517	15.634900	11.504938
Pt	13.102711	16.837734	11.434964
Pt	13.154893	7.663760	11.178918
Pt	10.680350	8.639473	11.063064
Pt	8.379458	9.982399	11.059352
Pt	15.085515	9.382372	10.535658
Pt	8.538874	12.551093	10.375631
Pt	16.792551	11.366808	10.032197
Pt	9.061371	15.108906	9.854094
Pt	15.670243	13.713596	9.505953
Pt	14.265758	15.946598	9.220908
Pt	10.146724	10.610374	9.168151
Pt	11.626281	15.671044	9.406462
Pt	12.624722	9.404688	9.233962
Pt	14.532667	11.334629	8.637070
Pt	10.496478	13.287512	8.542692
Pt	12.108465	11.409257	7.554399
Pt	13.208164	13.736021	8.203560
Ru	12.195257	14.870972	13.116825
Ru	12.698802	13.026905	14.895922
Ru	10.415154	13.047693	13.687940
Ru	10.814343	13.772840	11.212269
Ru	13.365677	14.193699	10.892380
Ru	14.530842	13.739011	13.178189
Ru	12.814069	10.135110	11.865518
Ru	11.632170	10.779964	14.110972
Ru	12.303684	11.960567	10.084105
Ru	10.488627	11.262719	11.807073
Ru	14.186714	11.229083	13.763289

Ru	14.599591	11.939709	11.298573
Ru	12.526562	12.539188	12.450306
O	10.019164	12.018782	17.181459
O	10.012427	8.056726	17.129309

3b^{RuPt}

Pt	11.783286	11.261843	16.849066
Pt	12.918101	13.630131	17.440676
Pt	14.551161	11.721518	16.387354
Pt	10.455818	13.711076	16.279160
Pt	10.733758	9.040042	15.700830
Pt	14.854404	14.396018	15.760122
Pt	12.396667	15.589743	15.695104
Pt	13.413030	9.310802	15.510201
Pt	9.301589	11.308543	15.401381
Pt	15.961462	9.906128	15.059288
Pt	8.216131	13.669438	14.854087
Pt	16.482330	12.470133	14.559646
Pt	9.930408	15.653311	14.386090
Pt	16.652866	15.037487	13.869917
Pt	14.338781	16.359735	13.870428
Pt	11.871731	17.360167	13.743363
Pt	11.894605	8.164008	13.472565
Pt	9.424561	9.364256	13.407180
Pt	14.628455	8.606554	13.152377
Pt	8.099126	11.779097	12.979357
Pt	16.553741	10.534675	12.549078
Pt	8.451812	14.471110	12.334574
Pt	16.906336	13.219304	11.932171
Pt	10.369797	16.395008	11.759186
Pt	15.589352	15.632047	11.497023
Pt	13.096839	16.842995	11.431067
Pt	13.135815	7.656929	11.162001
Pt	10.666708	8.648088	11.043819
Pt	8.359264	9.977930	11.035466
Pt	15.081779	9.365705	10.529673
Pt	8.528245	12.549973	10.356053
Pt	16.781399	11.349086	10.032992
Pt	9.059058	15.101128	9.828710
Pt	15.656881	13.695918	9.490730
Pt	14.258554	15.941016	9.214522
Pt	10.120650	10.607121	9.155703
Pt	11.619963	15.657348	9.383906
Pt	12.623769	9.390790	9.222001

Pt	14.523193	11.318624	8.622029
Pt	10.488941	13.278852	8.515224
Pt	12.088470	11.384382	7.557931
Pt	13.206333	13.719481	8.190519
Ru	12.194880	14.885600	13.077959
Ru	12.713124	13.068102	14.864170
Ru	10.413156	13.080634	13.655123
Ru	10.811160	13.768845	11.183281
Ru	13.360908	14.183702	10.870421
Ru	14.537644	13.747538	13.140059
Ru	12.800996	10.129059	11.860178
Ru	11.658639	10.858531	14.141178
Ru	12.297099	11.950511	10.069468
Ru	10.478445	11.257783	11.798697
Ru	14.194320	11.243423	13.755422
Ru	14.595406	11.930248	11.283269
Ru	12.499321	12.496717	12.461719
O	12.450700	12.755610	19.151316
O	11.866115	11.541634	18.958191
H	11.011506	9.694831	17.267447

TS3/4b^{RuPt}

Pt	11.777221	11.205987	16.756907
Pt	12.920173	13.581703	17.444641
Pt	14.505694	11.651539	16.376177
Pt	10.464281	13.622477	16.283463
Pt	10.734734	9.016473	15.658906
Pt	14.857284	14.337543	15.763803
Pt	12.386238	15.542553	15.706963
Pt	13.367563	9.284039	15.489424
Pt	9.332338	11.251810	15.396749
Pt	15.928581	9.849978	15.034426
Pt	8.219905	13.609329	14.857364
Pt	16.461081	12.412577	14.567943
Pt	9.927976	15.598652	14.417808
Pt	16.641825	14.980226	13.887546
Pt	14.340202	16.326403	13.891565
Pt	11.864460	17.310041	13.777526
Pt	11.893949	8.133944	13.423864
Pt	9.409654	9.345417	13.366787
Pt	14.616167	8.577356	13.107122
Pt	8.096243	11.756879	12.957297
Pt	16.537004	10.511641	12.531477
Pt	8.459631	14.450741	12.345758

Pt	16.905190	13.190353	11.931196
Pt	10.365268	16.379694	11.780665
Pt	15.589380	15.611471	11.524192
Pt	13.096692	16.827070	11.466747
Pt	13.122076	7.647868	11.107593
Pt	10.659807	8.642402	10.981807
Pt	8.357354	9.971354	10.998114
Pt	15.066436	9.360992	10.476642
Pt	8.534184	12.546462	10.326327
Pt	16.782475	11.345922	10.015013
Pt	9.059311	15.112220	9.837264
Pt	15.662157	13.704567	9.494843
Pt	14.267579	15.957895	9.237608
Pt	10.117774	10.618919	9.105960
Pt	11.625428	15.673251	9.401831
Pt	12.619599	9.398860	9.163490
Pt	14.528993	11.335919	8.595222
Pt	10.490211	13.305624	8.502170
Pt	12.096474	11.425190	7.522872
Pt	13.214454	13.748943	8.187228
Ru	12.192599	14.846292	13.101186
Ru	12.693794	12.997903	14.894485
Ru	10.409337	13.031787	13.638249
Ru	10.815656	13.777489	11.177761
Ru	13.366194	14.187477	10.878761
Ru	14.524426	13.709222	13.154795
Ru	12.815873	10.118751	11.773708
Ru	11.619850	10.753126	13.990762
Ru	12.304849	11.971056	10.031450
Ru	10.466908	11.264272	11.719666
Ru	14.172167	11.196792	13.724764
Ru	14.600984	11.931543	11.264814
Ru	12.495060	12.474031	12.427863
O	12.723764	13.265191	19.362099
O	12.197132	12.209202	19.900921
H	11.673575	11.068027	18.336069

4b^{RuPt}

Pt	11.782660	11.258322	16.740294
Pt	12.908525	13.613369	17.424437
Pt	14.515808	11.716439	16.403706
Pt	10.481410	13.684945	16.300983
Pt	10.733594	9.045677	15.697007
Pt	14.887828	14.409344	15.765985

Pt	12.381845	15.623312	15.699320
Pt	13.376154	9.327977	15.542846
Pt	9.331716	11.294565	15.434032
Pt	15.934581	9.907118	15.083771
Pt	8.229295	13.654979	14.882077
Pt	16.475374	12.462334	14.573728
Pt	9.923255	15.647008	14.401615
Pt	16.634829	15.017964	13.852594
Pt	14.335355	16.361069	13.858414
Pt	11.860536	17.335991	13.724325
Pt	11.907517	8.157418	13.489071
Pt	9.406281	9.373619	13.423057
Pt	14.628902	8.604154	13.169831
Pt	8.090384	11.779716	12.998058
Pt	16.536848	10.532124	12.571645
Pt	8.453139	14.462113	12.356733
Pt	16.901011	13.208081	11.926332
Pt	10.356912	16.387531	11.750460
Pt	15.579140	15.614614	11.487702
Pt	13.084563	16.828033	11.420107
Pt	13.127552	7.651876	11.182577
Pt	10.660226	8.641218	11.057487
Pt	8.353596	9.969432	11.055925
Pt	15.063068	9.356252	10.533243
Pt	8.525914	12.530674	10.358714
Pt	16.769815	11.335555	10.042841
Pt	9.048726	15.085751	9.835624
Pt	15.649218	13.684271	9.493103
Pt	14.251928	15.928852	9.198905
Pt	10.111918	10.590916	9.160284
Pt	11.611423	15.647001	9.384855
Pt	12.611429	9.376569	9.226670
Pt	14.517413	11.301860	8.629064
Pt	10.474081	13.266804	8.520740
Pt	12.082928	11.378865	7.563231
Pt	13.196413	13.706246	8.190786
Ru	12.189754	14.862294	13.108626
Ru	12.696449	13.061995	14.925819
Ru	10.414112	13.066682	13.665615
Ru	10.806998	13.771141	11.193048
Ru	13.355968	14.184576	10.883900
Ru	14.511485	13.733520	13.174109
Ru	12.804930	10.126001	11.856538
Ru	11.641879	10.831291	14.077647
Ru	12.293398	11.949396	10.066356
Ru	10.466216	11.262431	11.793364
Ru	14.172610	11.242512	13.769693
Ru	14.591925	11.932460	11.295083

Ru	12.491040	12.485560	12.418409
O	13.314411	13.884362	19.319443
O	12.677905	12.882312	20.161850
H	13.465325	12.380652	20.470154

TS4/5b^{RuPt}

Pt	11.814309	11.287491	16.748960
Pt	12.954680	13.606149	17.364969
Pt	14.539104	11.703585	16.401192
Pt	10.503713	13.705964	16.325968
Pt	10.739207	9.069982	15.744787
Pt	14.934385	14.379385	15.759240
Pt	12.436542	15.613919	15.702684
Pt	13.376504	9.330730	15.550145
Pt	9.351359	11.323198	15.460396
Pt	15.938348	9.861588	15.083140
Pt	8.255732	13.677734	14.905861
Pt	16.488068	12.412075	14.551869
Pt	9.954550	15.648185	14.408686
Pt	16.669651	14.963714	13.832848
Pt	14.396551	16.331745	13.845036
Pt	11.913051	17.394451	13.755967
Pt	11.882691	8.158398	13.523346
Pt	9.398993	9.392444	13.470379
Pt	14.606324	8.575617	13.175461
Pt	8.090308	11.800987	13.033623
Pt	16.524197	10.481821	12.562431
Pt	8.463600	14.481017	12.379133
Pt	16.917997	13.151966	11.908356
Pt	10.400502	16.396139	11.775743
Pt	15.620528	15.579263	11.469563
Pt	13.113514	16.804693	11.441871
Pt	13.085554	7.632143	11.212997
Pt	10.626986	8.636885	11.094772
Pt	8.333258	9.981300	11.105779
Pt	15.031642	9.311387	10.533117
Pt	8.516611	12.544497	10.391452
Pt	16.754583	11.273134	10.031572
Pt	9.063883	15.099174	9.866017
Pt	15.656228	13.640544	9.482448
Pt	14.270447	15.901883	9.203015
Pt	10.084292	10.586155	9.195147
Pt	11.624696	15.645939	9.388230
Pt	12.571795	9.349664	9.248980

Pt	14.491497	11.262092	8.632154
Pt	10.465924	13.263774	8.539844
Pt	12.051714	11.351823	7.574271
Pt	13.189940	13.683043	8.193604
Ru	12.214671	14.892654	13.080497
Ru	12.715446	13.088361	14.862879
Ru	10.423298	13.092158	13.663361
Ru	10.819849	13.776655	11.191736
Ru	13.363974	14.165014	10.865088
Ru	14.537891	13.722136	13.137081
Ru	12.788233	10.111970	11.857989
Ru	11.640391	10.831975	14.082805
Ru	12.280889	11.939206	10.069963
Ru	10.456701	11.273993	11.802981
Ru	14.182957	11.222381	13.759008
Ru	14.585735	11.906507	11.276329
Ru	12.505087	12.459096	12.463537
O	11.705073	18.789295	15.128897
O	12.046630	18.252798	16.458242
H	11.148829	18.183575	16.855585

5b^{RuPt}

Pt	11.827703	11.237808	16.742805
Pt	12.966335	13.551819	17.376040
Pt	14.541841	11.655682	16.396812
Pt	10.498796	13.650088	16.349514
Pt	10.736930	9.035149	15.731454
Pt	14.956034	14.337918	15.780219
Pt	12.431754	15.601651	15.735202
Pt	13.380411	9.297332	15.529563
Pt	9.361633	11.306276	15.462012
Pt	15.949039	9.836153	15.069549
Pt	8.257725	13.667643	14.919515
Pt	16.483730	12.400673	14.551011
Pt	9.956984	15.645096	14.426771
Pt	16.668097	14.965240	13.847661
Pt	14.391379	16.329620	13.860148
Pt	11.901128	17.465324	13.678301
Pt	11.881167	8.150404	13.502153
Pt	9.398717	9.390366	13.455879
Pt	14.607830	8.570423	13.155768
Pt	8.096731	11.800610	13.032414
Pt	16.521858	10.485212	12.548548
Pt	8.470707	14.492011	12.399796

Pt	16.909023	13.157390	11.908874
Pt	10.403577	16.382555	11.771649
Pt	15.615002	15.586130	11.485616
Pt	13.114466	16.796095	11.428801
Pt	13.083334	7.642147	11.191061
Pt	10.624932	8.642994	11.078506
Pt	8.328838	9.988477	11.100331
Pt	15.028480	9.319750	10.516710
Pt	8.516737	12.552661	10.407495
Pt	16.755150	11.283753	10.024954
Pt	9.059963	15.108885	9.878746
Pt	15.653302	13.649194	9.496732
Pt	14.269742	15.911612	9.211169
Pt	10.082618	10.601802	9.195440
Pt	11.621906	15.652506	9.385625
Pt	12.568058	9.366788	9.240330
Pt	14.487168	11.278223	8.632089
Pt	10.467489	13.278815	8.553493
Pt	12.047806	11.370678	7.574024
Pt	13.182698	13.696355	8.207667
Ru	12.213205	14.944096	13.138305
Ru	12.718431	13.083135	14.887296
Ru	10.434450	13.102274	13.681367
Ru	10.825043	13.784888	11.212340
Ru	13.360257	14.171691	10.888191
Ru	14.528205	13.727713	13.160281
Ru	12.786448	10.118653	11.856176
Ru	11.637518	10.820745	14.083590
Ru	12.278890	11.951923	10.081697
Ru	10.454938	11.284093	11.815465
Ru	14.185508	11.211936	13.759401
Ru	14.586401	11.916627	11.288730
Ru	12.507593	12.446291	12.468896
O	11.664961	19.003763	14.536407
O	12.456574	16.819841	17.303217
H	11.527919	16.957298	17.580219

5^{RuPt}

Pt	11.811465	11.174047	16.724855
Pt	12.993017	13.493210	17.444523
Pt	14.547194	11.637355	16.363176
Pt	10.466950	13.525287	16.431192
Pt	10.749600	8.994186	15.658337
Pt	14.952358	14.329122	15.755378

Pt	12.573941	15.637012	15.785223
Pt	13.393763	9.259818	15.490040
Pt	9.363778	11.252289	15.447571
Pt	15.949737	9.825145	15.016079
Pt	8.259255	13.632007	14.930386
Pt	16.507431	12.379195	14.537890
Pt	9.867256	15.711109	14.378315
Pt	16.688486	14.938487	13.837284
Pt	14.406122	16.300611	13.895197
Pt	11.936817	17.316133	13.791530
Pt	11.895485	8.134966	13.420107
Pt	9.395396	9.368196	13.403795
Pt	14.609818	8.562485	13.092312
Pt	8.105771	11.795928	13.019209
Pt	16.529207	10.482385	12.502421
Pt	8.484217	14.485110	12.406566
Pt	16.909428	13.150960	11.881364
Pt	10.393015	16.394053	11.815590
Pt	15.611246	15.587852	11.493943
Pt	13.124834	16.814327	11.472281
Pt	13.090796	7.648735	11.098824
Pt	10.629427	8.662508	11.019109
Pt	8.331576	10.008554	11.053689
Pt	15.029976	9.342793	10.462707
Pt	8.513840	12.575704	10.393119
Pt	16.745058	11.306236	9.976296
Pt	9.062635	15.131770	9.889850
Pt	15.642081	13.677594	9.478205
Pt	14.263166	15.941744	9.225630
Pt	10.080880	10.642580	9.154577
Pt	11.626099	15.685800	9.431972
Pt	12.563740	9.402328	9.182156
Pt	14.484451	11.323311	8.591041
Pt	10.468203	13.312645	8.547638
Pt	12.047832	11.425783	7.550103
Pt	13.180325	13.738950	8.200759
Ru	12.223191	14.846174	13.159840
Ru	12.735842	13.012799	14.941382
Ru	10.438523	13.058886	13.707091
Ru	10.818390	13.789621	11.228106
Ru	13.365655	14.188036	10.905632
Ru	14.542227	13.688627	13.170807
Ru	12.791297	10.120896	11.818851
Ru	11.651552	10.796041	14.056468
Ru	12.278130	11.972453	10.062696
Ru	10.458466	11.280105	11.797488
Ru	14.182409	11.194242	13.737336
Ru	14.585036	11.917038	11.268856

Ru	12.500447	12.473464	12.421041
O	10.566468	15.604130	16.329758
O	12.882750	14.005916	19.332605
H	12.366433	13.340621	19.830925