Supplementary material for:

σ-holes on Transition Metal Nanoclusters and their Influence on the Local Lewis Acidity

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Overview of content

S1. Spin-states and spin contamination corrections

Prior to the study of the electrostatic surface potentials and adsorption properties of the TM nanoclusters of the main article, an investigation of the favored spin-state for each system was performed. The identified ground-state (low-energy) spin-states of the TM_{13} clusters are summarized in **Table 1** of the main article, as well as in **Table S2**. **Table S1** reports the identified spin states for the smaller Pt_4, and TM_8 clusters.

For the smaller nanoclusters, the identified ground-states are in agreement with previously determined spin-states for the Pt_4 and Pt_8 clusters,[1,2] whereas both a singlet and a quintet spin-state has been reported for Ir_8 using GGA DFT.[2–4] The higher (tridecatet) spin-state identified in this study is not unexpected since it is well known that the hybrid DFT functional approach (here PBE0[5]) used herein has a larger preference for high-spin compared to GGA DFT functionals, see e.g. refs [6,7]. The expectation value of the $\hat{S}^2$ ($\langle\hat{S}^2\rangle$) spin operator is also reported in **Table S2** for the identified low-energy spin-states. This can be compared to the theoretical value of S(S+1). **Table S2** contains the ratio between the calculated $\langle\hat{S}^2\rangle$ and the theoretical S(S+1). The reported ratios show little indication of spin contamination, except for the Pt_4 cluster. As a rule of thumb, the ratio between $\langle\hat{S}^2\rangle$ and S(S+1) should not be larger than 1.1 for a spin-contaminated electronic configuration.[8] If the ratio is larger, it is an indication of a multi-reference character of the studied system, which is not well represented by the single-determinant KS-DFT method. An approach to overcome the above is to use correction schemes via spin projection as discussed below. For Pt_4 the $\langle\hat{S}^2\rangle$/S(S+1) ratio is 1.04 and thus within the acceptable range.

Table S1. Spin multiplicity (2S+1), S(S+1) and DFT $\langle S^2\rangle$ expectation value for the favored spin state of the TM nanoclusters of figure 1 and 3. The $[\langle S^2\rangle]/[S(S+1)]$ ratios are also reported.

	(2S+1)	S(S+1)	$\langle\hat{S}^2\rangle$	Ratio
Pt_4	3	2.00	2.07	1.04
Au_8-O_h	1	0.00	0.00	1.00
Au_8-T_d	1	0.00	0.00	1.00
Pt_8	9	20.00	20.08	1.00
Ir_8	13	42.00	42.17	1.00

The spin-states of the majority of the TM_{13} nanoclusters are in agreement with previous studies – including Au_{13}, Cu_{13}, Pt_{13}, Pt_7Cu_6, Co_{13}, and Ir_{13}.[3,9–14] For Ru_{13} a triplet and septet spin states have been reported previously using GGA-DFT, and for Pd_{13} a septet spin-state.[4,9,12] At the level of theory used herein, the tridecatet (Ru_{13}) and nonet (Pd_{13}) spin-states are, however, clearly lower in energy than the previously reported spin-states. For Rh_{13} the doublet spin-state was here identified as the lowest energy state, however, only by 0.01 eV compared to the decatet (2S+1=10) spin-state reported in other studies.[9,11,12,15] The relative energies for the spin-states of Rh_{13} are as follows – doublet: 0.00 eV; quartet: 0.06 eV; sextet: 0.06 eV; octet: 0.23 eV; decatet: 0.01 eV; dodecatet: 0.53 eV.

The $\langle\hat{S}^2\rangle$/S(S+1) ratios of **Table S2** for the TM_{13} nanoclusters suggests small to modest spin contamination for all but the Ir_{13}, Rh_{13}, and, possible, the Pt_{13} clusters. For Pt_{13} the ratio is 1.09, which is below 1.1 and considered acceptable. For Ir_{13} the ratio is 1.34. Therefore we tested whether the energies for the Ir_{13} structures had to be corrected or not using the spin projection correction schemes outlined below. The tests amounts to the quartet-sextet coupling and affects the H_2O adsorption leading to minor adjustments to the H_2O interaction energies for Ir_{13}. The primary result is overall slightly more favorable interactions (i.e. more negative ΔE_{in}) compared to the non-corrected case (see **Table S3**). We can also note that the amount of Hartree-Fock (HF) exchange in the PBE0 hybrid functional (25% HF admixture) affects the spin contamination; for Ir_{13} the $\langle\hat{S}^2\rangle$/S(S+1) ratio is decreased to 1.10 if the HF

admixture is reduced to 10%, and to 1.04 if no HF exchange is included (i.e. using the PBE GGA functional). For Rh_{13}, the $\langle\hat{S}^2\rangle$/S(S+1) ratio is large (7.55), which is reduced to 3.04 with 0% HF exchange (i.e PBE). The large spin contamination could be an indication that the Rh_{13} cluster is beyond reach for the employed DFT method, i.e. that the multi-reference character of the wave function is too pronounced. Nonetheless, Rh_{13}-H_2O adsorption energies were determined and the effect of using the same spin contamination correction scheme as for Ir_{13} was tested. For Rh_{13} both the doublet-quartet and doublet-decatet coupling were considered separately. The adjustments to the ΔE_{int} obtained for Rh_{13} are larger than for Ir_{13} (see **Table S3**). The spin contamination correction affects the site ranking and the 1(7) site is no longer the most favored. The average interaction energy is lowered by 0.12 eV for the quartet state, but increased by 0.15 eV (single point energies at the doublet geometries) for the decatet state. If the structures are relaxed, the interaction energy is favored by an average of 0.4 eV for the decatet state (see section S3)

Table S2. Spin multiplicity (2S+1), corresponding S(S+1) and DFT $\langle S^2\rangle$ expectation value for the favored spin state of the TM_{13} nanoclusters. The $[\langle S^2\rangle]/[S(S+1)]$ ratios are also reported.

	(2S+1)	S(S+1)	$\langle\hat{S}^2\rangle$	Ratio
Au_{13}	2	0.75	0.76	1.01
Cu_{13}	2	0.75	0.76	1.02
Pt_{13}	3	2.00	2.18	1.09
Pt_7Cu_6	3	2.00	2.04	1.02
Pd_{13}	9	20.00	20.15	1.01
Co_{13}	28	195.75	184.40	0.94
Rh_{13}	2	0.75	5.66	7.55 [1]
Ir_{13}	4	3.75	5.03	1.34 [1]
Ru_{13}	13	42.00	43.23	1.03

[1] The ratio suggests a broken symmetry UHF-DFT solution with a large contamination from higher spin states. Corrections according to the suggestions by Yamaguchi et al[16,17] to the reported H_2O interaction energies were therefore tested (see text).

The approximate spin-projection procedure (the AP procedure) of Yamaguchi et al.[16–18] were used to correct the ground-state energies of the Ir_{13} and Rh_{13} structures. These methods are primarily applied in the study of binuclear TM compounds and hence the results herein could be seen as experimental. The lowest energy state of the Ir_{13} and Rh_{13} compounds are found to be of broken symmetry character with a large amount of spin contamination from higher spin-states. The coupling between a low-spin state and a high-spin state (antiferromagnetic and ferromagnetic states) between two localized magnetic centers A and B can be expressed by the coupling constant J_{AB} via the Heisenberg Hamiltonian by[19,20]

$$\hat{H} = -2\sum_{A,B} J_{AB}\hat{S}_A \cdot \hat{S}_B, \tag{S1}$$

where $\hat{S}_A$ and $\hat{S}_B$ are the total spin operators of site A and B. Assuming that this approach – here using a single J_{AB} coupling – is valid in the cases of Rh_{13} and Ir_{13}, the coupling constant takes the form of eq. S2 in the AP approximation. Already this is a bold assumption since eq. S1 was originally formulated for the case of singlet-triplet coupling and since multiple spin sites (and centers) may be involved in the coupling in our systems.

$$J_{AB} = \frac{E_{BS}^{LS} - E^{HS}}{\left\langle \hat{S}^2 \right\rangle^{HS} - \left\langle \hat{S}^2 \right\rangle_{BS}^{LS}}. \tag{S2}$$

Eq. S2 thus includes the computation of the energies and $\langle \hat{S}^2 \rangle$ of the non-broken symmetry high-spin state (HS) and the broken symmetry (BS) low-spin state (LS). The relation is valid in the full range from weak to strong coupling. The final AP approximation energy is obtained by

$$E_{AP}^{LS} = \alpha E_{BS}^{LS} - \beta E^{HS}, \tag{S3}$$

with

$$\alpha = \frac{\left\langle \hat{S}^2 \right\rangle^{HS} - \left\langle \hat{S}^2 \right\rangle_{exact}^{LS}}{\left\langle \hat{S}^2 \right\rangle^{HS} - \left\langle \hat{S}^2 \right\rangle_{BS}^{LS}}, \text{ and } \beta = \alpha - 1, \tag{S4}$$

As indicated above, the H_2O interaction energies were not greatly altered by the spin projection corrections for Ir_{13}. Because of the small energy differences, and because of the various assumptions of the correction scheme, the main article contains the non-corrected interaction energies. For Rh_{13} we find slightly larger effects (see also section S3). Both the non-corrected and the corrected interaction energies are given in **Table S3** below. Also for Rh_{13}, the main article will only consider the uncorrected interaction energies for consistency.

Table S3. Spin projection corrected (ΔE_{int}-corr) and non-corrected (ΔE_{int}-non) H_2O interaction energies in eV for Ir_{13} and Ru_{13}.

Particle	**Site**[1]	**ΔE_{int}-corr**		**ΔE_{int}-non**
Ir_{13}	6	-1.08		-1.00
	5 [2-5]	-0.63		-0.58
	4 [13-4]	-0.52		-0.49
	12 [13-12]	-0.55		-0.50
	1(8) [10-1]	-0.52		-0.48
	11(2) [10-11]	-0.56		-0.52
	11(3) [7-11]	-0.66		-0.61
	7 [2-7]	-0.54		-0.51
	12 [8-12]	-0.70		-0.63
	11(3) [4-11]	-0.78		-0.77
	1(8) [12-1]	-0.66		-0.64
	1(8) [5-1]	-0.63		-0.65
	10(9) [5-10]	-0.53		-0.51
	5 [8-5]	-0.74		-0.72
	13 [9-13]	-0.47		-0.42
	10(9) [2-10]	-0.67		-0.62
	4 [3-4]	-0.46		-0.42
Rh_{13}	1(7) [1-7]	-0.62 [2]	-0.71 [3]	-0.81
	3(9) [3-9]	-0.49 [2]	-0.74 [3]	-0.62
	6(12) [6-12]	-0.65 [2]	-0.86 [3]	-0.71
	4(10) [4-10]	-0.39 [2]	-0.74 [3]	-0.47
	13 [11-13]	-0.57 [2]	-1.20 [3]	-0.70
	2(8) [2-8]	-0.37 [2]	-0.34 [3]	-0.50
	5(11) [5-11]	-0.47 [2]	-1.01 [3]	-0.65

[1] Symmetrically equivalent sites in parenthesis. $V_{S,max}$ positioned along the extension of the TMx-TMy bond in brackets (here only depicting one of the equivalent positions if multiple degenerate sites). [2] Doublet-quartet coupling. [3] Doublet-decatet coupling.

S2. Site resolved data – including H_2O interaction energies, $V_{S,max}$ and $E_{S,min}$

The **Table S4** below contains H_2O adsorption data for all TM_{13} clusters (sites, interaction energies and binding distances) as well as information on the $V_{S,max}$ (magnitude and character), $E_{S,min}$ and information on the position of σ-holes with respect to the closest TM atom and the optimized position of the O atom of H_2O upon adsorption.

Table S4. H_2O adsorption position with the corresponding $V_{S,max}$ (kcal/mol) and $E_{S,min}$ (eV) for all sites with identified $V_{S,max}$ of the TM_{13} nanocluster. Interaction energies (ΔE_{int} in eV) and distances (d_{TM-O} in Å) are also included, as are the σ-hole character of the $V_{S,max}$ (σ_{type}) and distance from the $V_{S,max}$ to the optimized position of the O-atom of H_2O upon adsorption ($d_{\sigma-O}$ in Å).

Particle	Site [1]	$V_{S,max}$	σ_{type}	$E_{S,min}$ [2]	ΔE_{int}	d_{TM-O}	$d_{TM-\sigma}$	$d_{\sigma-O}$
Au_{13}	13	16.80	σ_s	-8.88	-0.37	2.44	2.20	0.48
	11	15.26	σ_s	-8.30	-0.35	2.46	2.20	0.37
	9	12.02	σ_s	-7.68	-0.31	2.55	2.21	0.67
	10	8.89	σ_s	-6.55	-0.30	2.45	2.21	1.16
	4(1)	7.07	σ_s	-6.14	-0.29	2.55	2.21	0.53
	7	6.82	σ_s	-5.81	-0.26	2.64	2.24	1.47
	8	6.19	σ_s	-6.16	-0.24	2.53	2.21	0.36
	6(2)	5.75	σ_s	-6.07	-0.28	2.72	2.21	0.95
	3(5)	4.22	σ_s	-5.63	-0.27	2.57	2.20	0.87
	12	1.87	σ_s	(-4.87)	-0.18	2.80	2.24	1.48
Cu_{13}	1(2)	19.55	σ_s	-6.53	-0.54	2.14	2.02	0.56
	5(8)	18.9	σ_s	-6.38	-0.54	2.16	1.97	0.20
	7(4)	16.03	σ_s	-5.47	-0.48	2.16	2.04	0.49
	3(6)	14.68	σ_s	-5.18	-0.43	2.22	2.03	0.49
	12(13)	10.74	σ_s	-5.22	-0.42	2.24	2.03	0.35
	9	7.4	σ_s	-4.82	-0.41	2.19	2.09	0.52
Pt_{13}	12 [4-12]	20.12	σ_d	-11.93	-0.80	2.22	2.13	0.13
	11 [10-11]	17.29	σ_d	-11.05	-0.78	2.21	2.15	0.13
	10(4) [11-10]	16.14	σ_d	-10.47	-0.66	2.27	2.27	0.26
	8(13) [2-8]	16.03	σ_d	-8.85	-0.46	2.36	2.18	0.39
	12 [9-12]	15.08	σ_d	-9.40	-0.36	2.51	2.20	0.71
	8(13) [5-8]	14.72	σ_d	-9.22	-0.53	2.31	2.19	0.45
	4 [3-4]	13.81	σ_d	-8.93	-0.49	2.41	2.27	0.89
	10 [3-10]	11.65	σ_d	-8.16	-0.45	2.34	2.22	1.04
	1(5) [2-1]	9.08	σ_d	-7.62	-0.38	2.50	2.17	0.32
	1(5) [7-1]	8.59	σ_d	-7.63	-0.46	2.45	2.19	0.46
	6(9) [3-6]	7.09	σ_d	-7.48	-0.48	2.39	2.21	0.34
	11 [5-11]	6.84	σ_d	-7.77	-0.39	2.37	2.23	0.29
	2	2.07	σ_s	(-5.63)	-0.07	2.52	2.27	0.48
	8(13) [6-8]	14.31	σ_d	-9.00	-0.52	2.33	2.16	0.38
	6(9) [9-6]	4.27	σ_d	-4.99	-0.31	2.50	2.25	0.27
Pt_7Cu_6	1 – Cu	35.38	σ_s	-10.88	-0.73	2.09	1.91	0.23
	12 – Pt [9-12]	25.4	σ_d	-11.19	-0.64	2.25	2.12	0.82
	11 – Pt [10-11]	18.61	σ_d	-10.27	-0.60	2.29	2.14	0.25

	13 – Pt [9-13]	18.3	σ_d	-9.87	-0.44	2.37	2.19	0.69
	10 – Pt [7-10]	16.26	σ_d	-9.2	-0.53	2.35	2.15	0.22
	3 – Cu	13.79	σ_s	(-5.21)	-0.48	2.19	2.00	0.75
	4 – Cu	10.22	σ_s	(-4.77)	-0.42	2.24	2.01	0.37
	8 – Pt	7.66	σ_s	-5.6	-0.35	2.42	2.22	0.69
	5 – Cu	7.4	σ_s	(-4.15)	-0.38	2.32	2.03	0.69
	6 – Cu	6.67	σ_s	(-4.37)	-0.37	2.16	2.03	0.62
	2 – Cu	6.42	σ_s	(-3.98)	-0.40	2.31	2.03	1.05
	9 – Pt [7-9]	1.13	σ_d	-6.45	-0.30	2.57	2.20	0.46
Pd_{13}	13(10) [9-13]	16.22	σ_d	-7.32	-0.49	2.31	2.14	0.25
	13(10) [4-13]	16.07	σ_d	-6.97	-0.43	2.33	2.14	1.35
	5(4)	14.86	σ_s	-6.36	-0.49	2.31	2.14	0.79
	9(1)	14.3	σ_s	-6.95	-0.50	2.36	2.12	1.23
	8(11)	13.31	σ_s	-5.14	-0.59	2.28	2.16	1.35
	6(12)	5.23	σ_s	(-4.81)	-0.32	2.42	2.17	0.34
	3	-2.56	σ_s	(-4.09)	-0.33	2.36	2.19	0.42
Co_{13}	8(12,13)	21.65	σ_s	-5.64	-0.48	2.13	2.06	0.90
	1(4,5,6,9,11)	20.27	σ_s	(-5.76)	-0.46	2.11	2.08	0.35
	3(7,10)	6.65	σ_s	-5.11	-0.48	2.21	2.17	0.56
Rh_{13}	1(7) [1-7]	20.43	σ_d	-8.74	-0.81	2.23	2.13	0.27
	3(9) [3-9]	18.72	σ_d	-8.56	-0.62	2.28	2.13	0.28
	6(12) [6-12]	16.25	σ_d	-8.04	-0.71	2.27	2.10	0.51
	4(10) [4-10]	14.63	σ_d	-6.86	-0.47	2.29	2.20	0.41
	13 [11-13]	10.87	σ_d	-6.08	-0.70	2.24	2.18	0.59
	2(8) [2-8]	7.58	σ_d	-7.06	-0.50	2.35	2.19	0.30
	5(11) [5-11]	6.42	σ_d	-6.96	-0.65	2.36	2.17	0.19
Ir_{13}	6	33.75	σ_s	-12.86	-1.00	2.17	2.19	0.33
	5 [2-5]	15.81	σ_d	-10.64	-0.58	2.47	2.20	0.66
	4 [13-4]	14.54	σ_d	-9.05	-0.49	2.43	2.24	0.57
	12 [13-12]	13.06	σ_d	-9.5	-0.50	2.54	2.23	0.50
	1(8) [10-1]	12.37	σ_d	(-9.39)	-0.48	2.55	2.23	0.58
	11(2) [10-11]	12.16	σ_d	-8.85	-0.52	2.50	2.24	0.43
	11(3) [7-11]	11.95	σ_d	-8.48	-0.61	2.34	2.24	0.58
	7 [2-7]	9.79	σ_d	-9.15	-0.51	2.52	2.29	0.76
	12 [8-12]	8.61	σ_d	-7.24	-0.63	2.31	2.30	0.19
	11(3) [4-11]	6.88	σ_d	-6.25	-0.77	2.19	2.32	0.44
	1(8) [12-1]	5.89	σ_d	-6.88	-0.64	2.26	2.30	0.62
	1(8) [5-1]	5.06	σ_d	-6.55	-0.65	2.27	2.32	0.36
	10(9) [5-10]	4.74	σ_d	-6.9	-0.51	2.55	2.30	0.30
	5 [8-5]	3.15	σ_d	-6.32	-0.72	2.29	2.32	0.12
	13 [9-13]	2.46	σ_d	(-5.81)	-0.42	2.45	2.34	0.19
	10(9) [2-10]	-0.33	σ_d	-5.56	-0.62	2.43	2.48	0.49
	4 [3-4]	0.42	σ_d	-6.76	-0.42	2.63	2.26	1.81
Ru_{13}	9(10)	34.18	σ_s	-12.11	-0.92	2.22	2.07	0.96
	1(3)	29.16	σ_s	-12.78	-0.69	2.19	2.08	1.24
	13	19.54	σ_s	-12.11	-0.92	2.21	2.07	0.96

11(12) [12-11]	18.37	σ_d	-6.48	-0.50	2.22	2.24	0.96
6(8) [8-6]	7.05	$\sigma_{s/d}$	-8.54	-0.41	2.25	2.18	0.33
7(5)	3.07	σ_s	-7.09	-0.50	2.31	2.19	0.54

[1] Symmetrically equivalent sites in parenthesis, $V_{S,max}$ positioned along extension of TMx-TMy bond in brackets (here only depicting one of the equivalent positions if multiple degenerate sites). [2] Local $E_S(\mathbf{r})$ values are given in parenthesis in case of no corresponding minima in $E_S(\mathbf{r})$ in proximity to the $V_{S,max}$ site.

S3. Studies of Rh_{13} at the 2S+1=10 spin-state

The geometry of Rh_{13} does not change much compared to the doublet structure upon re-optimization at the decatet (2S+1=10) spin-state. The structural difference compared to the doublet state amounts to a RMSD of 0.046 Å for the atomic positions. Similarly, the electronic occupation of the *s*-, *d*- and *p*-orbitals is essentially unaltered going from the doublet to the decatet state (*cf.* **Table S5** and **Table 1** of the main article). As concerning the $V_S(\mathbf{r})$ profile (**Figure S1**), two additional σ-holes can be identified at the decatet compared to the doublet state. These appear below the cluster at the opposite side of the capping atom. On the whole, the surface electrostatic potential profiles are largely similar for the two spin states, with the magnitudes of the $V_{S,max}$ generally slightly decreased for the decatet state compared to the doublet. There is a larger tendency for σ_s-holes to be created on the decatet $V_S(\mathbf{r})$ profile; e.g. does the σ-holes at the 6(12) and 4(10) positions show clear σ_s-hole character. The $E_{S,min}$ positions are the same for the two considered spin states, although there values and mutual ranking are shifted (**Table S6**). Although there are a larger amount of $E_{S,min}$ compared to $V_{S,max}$, they tend to coincide at the same position. The exception is the σ_s-hole on site 6(12) where $E_{S,min}$ positions instead resembles σ_d-holes. A $\langle\hat{S}^2\rangle$ of 25.62 was, furthermore, obtained for the decatet state yielding a $\langle\hat{S}^2\rangle$/S(S+1) ratio of 1.03.

Table S5. TM_{13} nanocluster Schönflies symmetry group (Sym), ground-state spin multiplicity (2S+1), as well as the number of unique atom binding sites (AS), as well as unique $V_{S,max}$ sites (VS) and $E_{S,min}$ sites (ES) identified on each cluster. Included are also the atom average valence *s*-, *d*- and *p*-occupations (*s*-, *d*- and *p*-occ) as determined by NBO analysis.

	Sym	**(2S+1)**	**AS**	**VS**	**ES**	***s*-occ** [1]	***d*-occ** [1]	***p*-occ** [1]
Rh_{13}	C_s	10	7	9	13	0.44	8.29	0.28

[1] In case the total valence occupation does not fully amount to the total number of valence electrons, the remaining electron density is spread over the +1 super-valence *s*-, *p*-, *d*-, and *f*-orbitals.

At the decatet state, the favored adsorption position for H_2O (O-down) is toward the capping atom. For the doublet case the strongest adsorption was at the 1(7) position. The O-down adsorption to the capping atom takes place on the side and at a position along the extension of the 6-13 bond, whereas for the doublet state H_2O adsorbed toward the extension of the 5-13 bond. This is a refection of the shifted position of the $V_{S,max}$ on the capping atom going from one spin state to the other. The deviation from the σ-hole positions and the position of the O-atom of the adsorbed H_2O are small for the σ_d-holes, but larger for σ_s-holes. For the latter case the H_2O molecules tend to move toward extensions of Rh-Rh bonds, i.e. at typical σ_d-hole positions. No H_2O H-down adsorption mode could be established.

Table S6. H_2O adsorption position with the corresponding $V_{S,max}$ (kcal/mol) and $E_{S,min}$ (eV) for all sites with identified $V_{S,max}$ of the Rh_{13} nanocluster at the decatet (2S+1=10) spin-state. Interaction energies (ΔE_{int} in eV) and distances (d_{TM-O} in Å) are also included, as are the σ-hole character of the $V_{S,max}$ (σ_{type}) and distance from the $V_{S,max}$ to the optimized position of the O-atom of H_2O upon adsorption ($d_{\sigma-O}$ in Å).

Particle	Site [1]	$V_{S,max}$	σ_{type}	$E_{S,min}$ [2]	ΔE_{int}	d_{TM-O}	$d_{TM-\sigma}$	$d_{\sigma-O}$
Rh_{13}	1(7) [1-7]	17.56	σ_d	-8.00	-1.16	2.23	2.15	0.27
	3(9) [3-9]	17.58	σ_d	-8.51	-1.21	2.22	2.12	0.16
	6(12) [6-12]	6.61	σ_s	(-4.93)	-1.21	2.24	2.24	0.86
	4(10) [4-10]	15.96	σ_s	-7.20	-1.04	2.29	2.18	1.81
	13 [11-13]	19.32	$\sigma_{s/d}$	-6.83	-1.22	2.19	2.14	1.02
	2(8) [2-8]	7.17	σ_d	-7.55	-0.52	2.34	2.15	0.22
	5(11) [5-11]	2.19	σ_d	-6.40	-1.05	2.31	2.17	0.21
	1(7) [4-1]	16.87	σ_d	-7.77	-1.12	2.28	2.16	0.39
	2(8) [5-2]	-2.2	σ_d	-5.19	-0.91	2.43	2.25	0.23
Average					-1.05	2.28	2.17	0.57
R^2 vs $V_{S,max}$					0.23			
R^2 vs $E_{S,min}$					0.00			

[1] Symmetrically equivalent sites in parenthesis, $V_{S,max}$ positioned along extension of TMx-TMy bond in brackets (here only depicting one of the equivalent positions if multiple degenerate sites). [2] Local $E_S(\mathbf{r})$ values are given in parenthesis in case of no corresponding minima in $E_S(\mathbf{r})$ in proximity to the $V_{S,max}$ site.

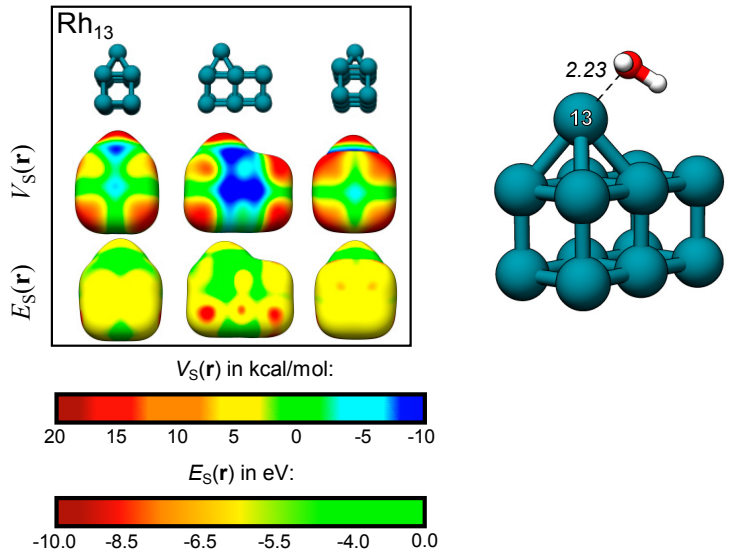

Figure S1. $V_S(\mathbf{r})$ and $E_S(\mathbf{r})$ maps at the 0.001 a.u. isodensity surface of the Rh_{13} nanoparticle at the 2S+1=10 spin-state. Shown is also the favored adsorption structure for H_2O at the same spin-state.

S4. Additional computational details (for the figures 1 and 3)

The HF and I_2 molecules and the small TM clusters Pt_4, Au_8, Pt_8 and Ir_8 of **Figure 1** and **3** in the main article were optimized at the PBE0/Def2-SV(P) level of theory[5,21] using the Turbomole 6.4 software package under symmetry constraints.[22] The structures correspond to local minima – verified by the lack of imaginary vibrational frequencies. The cubic O_h Au_8 structure is an exception and it relaxes to a T_d structure when the symmetry constraints are lifted. For the TM nanoclusters different spin-states where considered up to 2S+1=19. The lowest energy states are reported in the main article and in **Table S1**. The electrostatic surface potentials [V_S(**r**)] were determined at the 0.001 au isosurfaces and based on single-point calculations at the optimized geometries on the PBE0/Def2-TZVPP level of theory.

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S6. Appendix – xyz-coordinates

Below are the coordinates of all structures of this study included.

S5.1. Structures of Figure 1 and 3

HF

H	0.0000000	0.0000000	-0.4661949
F	0.0000000	0.0000000	0.4661949

I_2

I	0.0000000	0.0000000	1.3408296
I	0.0000000	0.0000000	-1.3408296

Pt_4

Pt	1.2542727	1.2542727	0.0000000
Pt	1.2542727	-1.2542727	0.0000000
Pt	-1.2542727	-1.2542727	0.0000000
Pt	-1.2542727	1.2542727	0.0000000

Au_8-O_h

Au	-1.3679380	-1.3679380	1.3679380
Au	-1.3679380	-1.3679380	-1.3679380
Au	1.3679380	-1.3679380	-1.3679380
Au	1.3679380	-1.3679380	1.3679380
Au	-1.3679380	1.3679380	1.3679380
Au	-1.3679380	1.3679380	-1.3679380
Au	1.3679380	1.3679380	-1.3679380
Au	1.3679380	1.3679380	1.3679380

Au_8-T_d

Au	1.0367956	-1.0367956	1.0367956
Au	1.6342282	1.6342282	1.6342282
Au	-1.0367956	1.0367956	1.0367956
Au	-1.6342282	-1.6342282	1.6342282
Au	1.6342282	-1.6342282	-1.6342282
Au	1.0367956	1.0367956	-1.0367956
Au	-1.6342282	1.6342282	-1.6342282
Au	-1.0367956	-1.0367956	-1.0367956

Pt_8

Pt	-1.2905373	-1.2905373	1.2905373
Pt	-1.2905373	-1.2905373	-1.2905373
Pt	1.2905373	-1.2905373	-1.2905373
Pt	1.2905373	-1.2905373	1.2905373
Pt	-1.2905373	1.2905373	1.2905373
Pt	-1.2905373	1.2905373	-1.2905373
Pt	1.2905373	1.2905373	-1.2905373
Pt	1.2905373	1.2905373	1.2905373

Ir_8

Ir	-1.2263598	-1.2263598	1.2263598
Ir	-1.2263598	-1.2263598	-1.2263598
Ir	1.2263598	-1.2263598	-1.2263598
Ir	1.2263598	-1.2263598	1.2263598
Ir	-1.2263598	1.2263598	1.2263598
Ir	-1.2263598	1.2263598	-1.2263598
Ir	1.2263598	1.2263598	-1.2263598
Ir	1.2263598	1.2263598	1.2263598

S5.2. TM_{13} structures

Au_{13}

Au	1.5226909	1.0068646	-1.4123336
Au	-1.2262195	0.6013521	-1.5180432
Au	0.4326622	-1.4812743	-1.5179738
Au	1.5226909	1.0068646	1.4123336
Au	0.4326622	-1.4812743	1.5179738
Au	-1.2262195	0.6013521	1.5180432
Au	-3.0961126	-0.7850983	0.0000000
Au	-1.4124540	-2.8985176	0.0000000
Au	1.2968916	-3.6384603	0.0000000
Au	2.7755879	-1.1956087	0.0000000
Au	-2.9767958	2.1489372	0.0000000
Au	-0.3436011	2.8490470	0.0000000
Au	2.2982168	3.2658156	0.0000000

Cu_{13}

Cu	1.7445824	-1.1430203	-2.1521696
Cu	-1.7445824	1.1430203	-2.1521696
Cu	3.0454250	0.2637936	-0.4969580
Cu	-2.5622179	0.2833367	1.9977170
Cu	-1.3408868	-1.5008157	0.8251607
Cu	-3.0454250	-0.2637936	-0.4969580
Cu	2.5622179	-0.2833367	1.9977170
Cu	1.3408868	1.5008157	0.8251607
Cu	0.0000000	0.0000000	2.3302492
Cu	1.0069719	-0.8849700	0.1993550
Cu	-1.0069719	0.8849700	0.1993550
Cu	-0.7721439	-1.0054350	-1.5382296
Cu	0.7721439	1.0054350	-1.5382296

Pt_{13}

Pt	-1.7177135	0.6388509	1.8135349
Pt	-1.6308684	-1.0676305	0.0000000
Pt	0.7226119	0.8355705	-1.2707853
Pt	2.9221750	1.0326664	0.0000000
Pt	-1.7177135	0.6388509	-1.8135349
Pt	0.8819984	-1.6806128	-1.3271164
Pt	0.7226119	0.8355705	1.2707853
Pt	-1.3907894	-1.8109358	-2.4772564
Pt	0.8819984	-1.6806128	1.3271164
Pt	0.5468157	3.0886633	0.0000000
Pt	-1.8991648	2.4484268	0.0000000
Pt	3.0688277	-1.4678719	0.0000000
Pt	-1.3907894	-1.8109358	2.4772564

Pt_7Cu_6

Cu	-0.0539685	1.0486796	2.6968248
Cu	0.9144388	-0.9328779	1.2858197
Cu	-1.6189239	-1.0776575	-1.0005329
Cu	-0.0261801	0.4725026	-2.2591378
Cu	-1.6123516	-0.4458239	1.3569079
Cu	0.7591239	-1.8339209	-1.1291965
Pt	0.0850047	1.3581862	0.1819134
Pt	-0.7395748	-2.7134691	0.6713623
Pt	2.2180553	0.2886537	-0.7445657
Pt	-2.1591666	1.3571572	-1.0790463
Pt	-2.0804264	2.0191153	1.4076021
Pt	2.0303548	-0.7572395	-2.9868955
Pt	2.2836144	1.2166943	1.5989443

Pd_{13}

Pd	-1.0089390	0.9366811	2.4942102
Pd	-0.8905614	-1.0607618	0.6059867
Pd	0.0000000	0.0000000	-1.9518656
Pd	2.6234956	0.5324958	-1.3304615
Pd	-2.6234956	-0.5324958	-1.3304615
Pd	1.4582731	-1.6983591	-0.2910091
Pd	0.8905614	1.0607618	0.6059867
Pd	-0.6964846	-2.4956173	-1.6184984
Pd	1.0089390	-0.9366811	2.4942102
Pd	-3.1531185	0.1898435	1.1157049
Pd	0.6964846	2.4956173	-1.6184984
Pd	-1.4582731	1.6983591	-0.2910091
Pd	3.1531185	-0.1898435	1.1157049

Co_{13}

Co	2.3602230	1.0552441	0.9334023
Co	0.0000000	0.0000000	0.8755261
Co	-0.8811135	-1.1754101	-1.0738875
Co	-2.0939797	1.5163910	0.9334023
Co	-0.2662433	-2.5716351	0.9334023
Co	2.0960473	-1.4612260	0.9384004
Co	-0.5773782	1.3507717	-1.0738875
Co	1.7372460	2.3426908	-1.0897573
Co	-2.3134825	-1.0846172	0.9384004
Co	1.4584918	-0.1753617	-1.0738875
Co	0.2174352	2.5458432	0.9384004
Co	-2.8974528	0.3331537	-1.0897573
Co	1.1602068	-2.6758446	-1.0897573

Rh_{13}

Rh	2.7245601	1.0038178	-1.1584368
Rh	0.3003280	1.4182007	-1.1765924
Rh	-2.1194656	1.8654503	-1.1665928
Rh	2.3631784	-1.3759702	-1.1706199
Rh	-0.0203744	-0.9497893	-1.1572097
Rh	-2.4480654	-0.5788628	-1.1657303
Rh	2.7245601	1.0038178	1.1584368
Rh	0.3003280	1.4182007	1.1765924
Rh	-2.1194656	1.8654503	1.1665928
Rh	2.3631784	-1.3759702	1.1706199
Rh	-0.0203744	-0.9497893	1.1572097
Rh	-2.4480654	-0.5788628	1.1657303
Rh	-1.6003221	-2.7656929	0.0000000

Ir_{13}

Ir	0.2061338	-2.5336905	-1.7093142
Ir	1.4879970	0.1164845	0.0000000
Ir	-0.7557351	2.2272315	1.7002959
Ir	-2.4173828	1.8530211	0.0000000
Ir	1.8427721	-2.2283461	0.0000000
Ir	3.1132193	1.8915253	0.0000000
Ir	0.8830721	2.6030051	0.0000000
Ir	0.2061338	-2.5336905	1.7093142
Ir	-0.2377705	-0.1533540	1.6717373
Ir	-0.2377705	-0.1533540	-1.6717373
Ir	-0.7557351	2.2272315	-1.7002959
Ir	-1.4382140	-2.8379346	0.0000000
Ir	-1.8967200	-0.4781292	0.0000000

Ru_{13}

Ru	2.0764332	-1.6246782	1.1569472
Ru	-0.1301770	-0.9261745	1.1065396
Ru	2.0764332	-1.6246782	-1.1569472
Ru	-0.1301770	-0.9261745	-1.1065396
Ru	2.7187745	0.5929945	1.1538669
Ru	0.5116677	1.3301617	1.1658228
Ru	2.7187745	0.5929945	-1.1538669
Ru	0.5116677	1.3301617	-1.1658228
Ru	-2.4820252	-1.6140446	1.1323631
Ru	-2.4820252	-1.6140446	-1.1323631
Ru	-2.1129699	0.8064100	-1.1698125
Ru	-2.1129699	0.8064100	1.1698125
Ru	-1.1634067	2.8706622	0.0000000

S5.3. H_2O adsorption structures

The below structures are sorted under subheadings corresponding to each TM13 nanocluster and given for each unique site (indicated above the xyz-coordinates) labeled according to the notation in **Table S4**.

S5.3.2. H_2O

O	0.098658	-0.002810	0.000000
H	-0.484227	0.760257	0.000000
H	-0.495313	-0.757447	0.000000

S5.3.2. Au_{13}

13

Au	0.00000	0.00000	2.31467
Au	2.02293	0.00000	0.40679
Au	0.31647	-2.03919	0.54508
Au	-1.77254	1.36659	0.59129
Au	-1.58847	-0.57051	-1.30703
Au	0.11812	1.46858	-1.44519
Au	2.15112	-0.18926	-2.36297
Au	0.41911	-2.25836	-2.22230
Au	-1.76700	-3.29252	-0.79388
Au	-2.31723	-1.40018	1.27262
Au	2.72460	2.32512	-0.95896
Au	0.92054	2.54536	1.07120
Au	-0.95376	2.51965	2.97858
O	-3.61657	-5.01861	-1.12721
H	-3.32106	-5.90356	-0.89365
H	-3.91292	-5.07034	-2.04053

11

Au	0.00000	0.00000	2.31467
Au	2.02293	0.00000	0.40679
Au	0.31647	-2.03919	0.54508
Au	-1.77254	1.36659	0.59129
Au	-1.58847	-0.57051	-1.30703
Au	0.11812	1.46858	-1.44519
Au	2.15112	-0.18926	-2.36297
Au	0.41911	-2.25836	-2.22230
Au	-1.76700	-3.29252	-0.79388
Au	-2.31723	-1.40018	1.27262
Au	2.72460	2.32512	-0.95896
Au	0.92054	2.54536	1.07120
Au	-0.95376	2.51965	2.97858
O	-3.61657	-5.01861	-1.12721
H	-3.32106	-5.90356	-0.89365
H	-3.91292	-5.07034	-2.04053

9

Au	0.00000	0.00000	2.31467
Au	2.02293	0.00000	0.40679
Au	0.31647	-2.03919	0.54508
Au	-1.77254	1.36659	0.59129

Au	-1.58847	-0.57051	-1.30703
Au	0.11812	1.46858	-1.44519
Au	2.15112	-0.18926	-2.36297
Au	0.41911	-2.25836	-2.22230
Au	-1.76700	-3.29252	-0.79388
Au	-2.31723	-1.40018	1.27262
Au	2.72460	2.32512	-0.95896
Au	0.92054	2.54536	1.07120
Au	-0.95376	2.51965	2.97858
O	-3.61657	-5.01861	-1.12721
H	-3.32106	-5.90356	-0.89365
H	-3.91292	-5.07034	-2.04053

10

Au	0.00000	0.00000	2.31467
Au	2.02293	0.00000	0.40679
Au	0.31647	-2.03919	0.54508
Au	-1.77254	1.36659	0.59129
Au	-1.58847	-0.57051	-1.30703
Au	0.11812	1.46858	-1.44519
Au	2.15112	-0.18926	-2.36297
Au	0.41911	-2.25836	-2.22230
Au	-1.76700	-3.29252	-0.79388
Au	-2.31723	-1.40018	1.27262
Au	2.72460	2.32512	-0.95896
Au	0.92054	2.54536	1.07120
Au	-0.95376	2.51965	2.97858
O	-3.61657	-5.01861	-1.12721
H	-3.32106	-5.90356	-0.89365
H	-3.91292	-5.07034	-2.04053

4(1)

Au	0.00003	0.00011	2.30180
Au	2.02717	0.00001	0.39837
Au	0.36603	-2.07278	0.58144
Au	-1.79815	1.28578	0.54307
Au	-1.56648	-0.69091	-1.30856
Au	0.09483	1.38179	-1.49152
Au	2.16636	-0.25162	-2.36591
Au	0.48034	-2.35482	-2.17976
Au	-1.68583	-3.40339	-0.73157
Au	-2.28301	-1.47555	1.28852
Au	2.68072	2.30711	-1.02030
Au	0.86645	2.53548	0.99987
Au	-1.01082	2.51257	2.90433
O	-4.03046	2.52295	0.53251
H	-3.89702	3.37724	0.95291
H	-4.21076	2.70893	-0.39353

7

Au	-0.00000	-0.00000	2.33623
Au	1.98404	0.00001	0.38792
Au	0.31237	-2.06229	0.59288
Au	-1.82764	1.31181	0.62790
Au	-1.65178	-0.65249	-1.24306
Au	0.02000	1.40971	-1.44789
Au	2.05953	-0.23171	-2.38055
Au	0.36288	-2.32424	-2.17223
Au	-1.77792	-3.36830	-0.68364
Au	-2.31576	-1.45160	1.36358
Au	2.62216	2.31326	-1.02819
Au	0.85598	2.53872	1.03444
Au	-0.97906	2.51526	2.97965
O	2.56994	0.15145	-4.94469
H	3.22081	-0.49439	-5.23490
H	1.73654	-0.14060	-5.32701

8

Au	0.000000	0.000000	2.336198
Au	1.999522	0.000000	0.403799
Au	0.302154	-2.044655	0.570425
Au	-1.798273	1.353890	0.629537
Au	-1.630442	-0.589635	-1.263716
Au	0.067054	1.454925	-1.430221
Au	2.094618	-0.199159	-2.366599
Au	0.371850	-2.273810	-2.197172
Au	-1.792991	-3.310320	-0.738385
Au	-2.324748	-1.412220	1.327675
Au	2.676185	2.322465	-0.978985
Au	0.896226	2.543923	1.072202
Au	-0.954588	2.518735	3.002383
O	0.990563	-3.993209	-3.940396
H	1.866437	-4.377758	-3.845266
H	0.950989	-3.659051	-4.841157

6(2)

Au	0.00000	0.00000	2.33060
Au	2.00495	0.00000	0.40384
Au	0.34844	-2.07448	0.60869
Au	-1.81990	1.28162	0.59138
Au	-1.60739	-0.69712	-1.26045
Au	0.04925	1.37726	-1.46517
Au	2.11240	-0.25483	-2.36154
Au	0.43109	-2.35974	-2.15333
Au	-1.71693	-3.40900	-0.67888
Au	-2.29289	-1.47939	1.34572
Au	2.63907	2.30632	-1.02535
Au	0.84884	2.53457	1.01612
Au	-1.00693	2.51234	2.94158
O	-0.24870	3.65861	-2.92146
H	-1.07651	3.54338	-3.39635
H	-0.46482	4.20039	-2.15694

3(5)

Au	0.000001	0.000000	2.305162
Au	1.996217	0.000000	0.369337
Au	0.296347	-2.042563	0.535981
Au	-1.799343	1.358738	0.603490
Au	-1.637394	-0.582342	-1.292788
Au	0.062589	1.460134	-1.459322
Au	2.086290	-0.195385	-2.401503
Au	0.360994	-2.267928	-2.232031
Au	-1.802763	-3.303546	-0.770988
Au	-2.328387	-1.407633	1.298642
Au	2.673677	2.323485	-1.011340
Au	0.897523	2.544489	1.043189
Au	-0.949996	2.519093	2.976520
O	1.674820	-4.204971	0.697997
H	2.104205	-4.167775	-0.162706
H	2.355523	-3.958598	1.331780

12

Au	0.000053	0.000018	2.296160
Au	1.995903	-0.000089	0.360274
Au	0.350805	-2.081607	0.583346
Au	-1.834388	1.263477	0.558959
Au	-1.620606	-0.723761	-1.283665
Au	0.024623	1.357824	-1.506879
Au	2.091797	-0.268622	-2.404451
Au	0.422014	-2.380809	-2.177486
Au	-1.713821	-3.433101	-0.687558
Au	-2.290004	-1.495913	1.329665
Au	2.611772	2.302039	-1.084022
Au	0.830101	2.531900	0.964569
Au	-1.016710	2.510429	2.898876
O	0.462857	5.308908	1.080153
H	1.243638	5.610496	1.566416
H	-0.236430	5.381704	1.744067

S5.3.3. Cu_{13}

1(2)

Cu	0.00000	0.00000	2.89337
Cu	2.99803	0.00000	-0.00675
Cu	-1.36421	1.90777	1.93932
Cu	0.25696	-1.12110	-3.14660
Cu	-0.37124	-1.95717	-0.92036
Cu	2.06075	-1.87116	-1.43189
Cu	-3.02920	1.21287	0.06814
Cu	-0.77068	2.02300	-0.47274
Cu	-1.61735	0.04954	-1.77827
Cu	-1.09133	-0.16237	0.67455
Cu	0.81955	0.21438	-1.16812
Cu	1.13064	-1.25724	0.92601
Cu	1.01365	1.27084	1.07805
O	-0.23513	-1.28747	4.59205
H	-1.11279	-1.68446	4.57520
H	0.38583	-2.02059	4.52261

5(8)

Cu	-0.00000	0.00000	3.02010
Cu	3.02348	-0.00000	0.14651
Cu	-1.32181	1.94887	2.08977
Cu	0.29140	-1.01445	-3.03715
Cu	-0.37136	-1.87995	-0.83228
Cu	2.06625	-1.82776	-1.32108
Cu	-2.98192	1.31810	0.19171
Cu	-0.70474	2.09781	-0.31453
Cu	-1.57424	0.16400	-1.66364
Cu	-1.07405	-0.10224	0.78929
Cu	0.85959	0.27432	-1.02949
Cu	1.12596	-1.24081	1.03965
Cu	1.05211	1.28573	1.23744
O	-1.46066	-3.72701	-1.11577
H	-1.16016	-4.08416	-1.95748
H	-2.39155	-3.51194	-1.23432

7(4)

Cu	0.00000	-0.00000	2.99553
Cu	3.09857	0.00000	0.20309
Cu	-1.36336	1.86346	1.95651
Cu	0.49112	-1.23181	-3.00828
Cu	-0.20064	-2.03653	-0.78934
Cu	2.24604	-1.91523	-1.21673
Cu	-2.94823	1.10202	0.04214
Cu	-0.68678	1.94340	-0.43503
Cu	-1.45119	-0.07010	-1.73011
Cu	-1.00883	-0.22515	0.74339
Cu	0.95919	0.15160	-1.03812
Cu	1.22202	-1.27356	1.09441
Cu	1.05456	1.25435	1.19210
O	-5.10153	1.07037	-0.05548
H	-5.50886	0.83676	0.78548
H	-5.39675	0.40993	-0.69122

3(6)

Cu	0.00000	-0.00002	2.92947
Cu	3.03676	-0.00000	0.06994
Cu	-1.41048	1.83016	1.89427
Cu	0.37672	-1.31232	-3.06553
Cu	-0.25566	-2.09374	-0.82066
Cu	2.17925	-1.94664	-1.30341
Cu	-3.02634	1.02034	0.02618
Cu	-0.78730	1.88424	-0.51247

Cu	-1.55267	-0.15771	-1.76167
Cu	-1.05462	-0.27102	0.70344
Cu	0.86904	0.10554	-1.12600
Cu	1.19729	-1.28492	1.02031
Cu	0.99812	1.24174	1.08563
O	-2.33303	3.66195	2.74601
H	-2.80687	3.52440	3.57267
H	-3.00186	3.89800	2.09428

12(13)

Cu	-0.00000	-0.00000	2.94827
Cu	2.95675	0.00000	0.00608
Cu	-1.35455	1.93521	2.03672
Cu	0.15859	-1.05031	-3.10779
Cu	-0.44822	-1.90600	-0.88307
Cu	1.97719	-1.84245	-1.42802
Cu	-3.05389	1.28289	0.18115
Cu	-0.79366	2.07286	-0.38197
Cu	-1.68216	0.12561	-1.69899
Cu	-1.12428	-0.12244	0.74337
Cu	0.76486	0.25421	-1.12159
Cu	1.08774	-1.24640	0.95008
Cu	1.00318	1.28082	1.13416
O	1.68001	-2.75957	2.49148
H	2.54605	-3.09800	2.24162
H	1.06620	-3.49121	2.36907

9

Cu	0.00000	0.00000	3.06651
Cu	3.05745	-0.00000	0.22911
Cu	-1.35835	1.88968	2.06912
Cu	0.39056	-1.16681	-2.95763
Cu	-0.27742	-1.99002	-0.73819
Cu	2.16395	-1.88947	-1.20000
Cu	-2.97894	1.16732	0.16957
Cu	-0.71582	1.99039	-0.33101
Cu	-1.52044	0.00027	-1.63782
Cu	-1.04383	-0.18826	0.82698
Cu	0.90199	0.18857	-0.97877
Cu	1.18056	-1.26407	1.13315
Cu	1.04156	1.26415	1.26236
O	-3.15404	-0.45074	-3.02035
H	-2.72871	-0.71953	-3.84283
H	-3.59037	-1.23927	-2.67952

S5.3.4. Pt_{13}

12 [4-12]

Pt	0.00000	0.00000	2.60027
Pt	1.76473	0.00000	0.84125
Pt	-0.62336	-1.08175	-1.13455
Pt	-2.54625	0.50155	-1.67010
Pt	1.20606	-2.30253	0.07009
Pt	1.08871	0.59329	-1.92350
Pt	-1.46841	0.53155	0.63826
Pt	2.96925	-0.98722	-1.23750
Pt	0.20622	2.27806	-0.07215
Pt	-2.54224	-1.82048	0.44491
Pt	-0.57369	-2.40888	1.91873
Pt	-0.85615	2.19699	-2.40737
Pt	1.32204	2.15750	2.21815
O	0.61749	3.73632	-3.03116
H	0.85476	3.64614	-3.96026
H	0.25499	4.62016	-2.90868

11 [10-11]

Pt	0.00000	-0.00000	2.55584
Pt	1.76277	0.00000	0.79486
Pt	-0.64709	-0.99924	-1.19788
Pt	-2.54035	0.62973	-1.70104
Pt	1.16017	-2.27668	-0.01880
Pt	1.09545	0.65790	-1.95735
Pt	-1.45999	0.59595	0.60608
Pt	2.94657	-0.97032	-1.30366
Pt	0.24654	2.32376	-0.07346
Pt	-2.57805	-1.73143	0.36987
Pt	-0.61954	-2.38440	1.82980
Pt	-0.81934	2.30671	-2.40842
Pt	1.36204	2.13910	2.21272
O	0.98045	-3.03176	3.20286
H	1.70855	-2.46700	2.89567
H	0.76295	-2.72242	4.09050

10(4) [11-10]

Pt	0.00000	0.00000	2.58483
Pt	1.78878	0.00000	0.85028
Pt	-0.58599	-1.02208	-1.17278
Pt	-2.47985	0.59441	-1.71262
Pt	1.21002	-2.28397	0.03976
Pt	1.15918	0.64012	-1.91498
Pt	-1.43381	0.57822	0.61046
Pt	3.00865	-0.97505	-1.22526
Pt	0.27380	2.31132	-0.05273
Pt	-2.53632	-1.75612	0.36992
Pt	-0.59646	-2.39132	1.86224
Pt	-0.75709	2.27659	-2.40317
Pt	1.35604	2.14433	2.25072
O	-4.47408	-1.39813	-0.76039
H	-4.79801	-0.50184	-0.60105
H	-4.37695	-1.49046	-1.71713

8(13) [2-8]

Pt	0.00000	-0.00001	2.59885
Pt	1.74771	0.00001	0.82292
Pt	-0.67570	-1.01344	-1.14603
Pt	-2.57846	0.60778	-1.63827
Pt	1.14566	-2.28123	0.02173
Pt	1.05492	0.64685	-1.92559
Pt	-1.47843	0.58494	0.65967
Pt	2.91682	-0.97327	-1.28245
Pt	0.21664	2.31604	-0.03989
Pt	-2.59089	-1.74678	0.44043
Pt	-0.61793	-2.38871	1.88573
Pt	-0.86899	2.28801	-2.36564
Pt	1.35211	2.14236	2.23730
O	3.93352	-2.32671	-2.93089
H	4.25768	-1.84117	-3.70148
H	3.12404	-2.77885	-3.20936

12 [9-12]

Pt	-0.00000	0.00000	2.60579
Pt	1.77860	0.00000	0.86079
Pt	-0.59569	-1.07391	-1.13581
Pt	-2.51146	0.51380	-1.68369
Pt	1.22197	-2.30013	0.08106
Pt	1.12555	0.59947	-1.90814
Pt	-1.45188	0.53771	0.63318
Pt	2.99779	-0.98564	-1.21014
Pt	0.23143	2.28249	-0.06078
Pt	-2.52833	-1.81204	0.42708
Pt	-0.57256	-2.40662	1.91536
Pt	-0.81256	2.20752	-2.40448
Pt	1.32886	2.15581	2.23806
O	-2.29368	2.57391	-4.40156
H	-1.96995	3.33309	-4.88246
H	-2.17921	1.82814	-4.99374

8(13) [5-8]

Pt	0.00000	0.00000	2.59646
Pt	1.74575	0.00000	0.81860
Pt	-0.67437	-1.03684	-1.14224
Pt	-2.58636	0.57151	-1.64089
Pt	1.15507	-2.28863	0.03013
Pt	1.04644	0.62858	-1.93251
Pt	-1.48369	0.56673	0.65590
Pt	2.91773	-0.97809	-1.28294
Pt	0.20127	2.30319	-0.05471
Pt	-2.58383	-1.77206	0.45023
Pt	-0.60586	-2.39574	1.89667
Pt	-0.88675	2.25703	-2.37905
Pt	1.34017	2.14765	2.22208
O	4.76195	0.03565	-2.24636
H	4.56211	0.43819	-3.09893
H	4.94941	0.76227	-1.64017

4 [3-4]

Pt	0.00000	0.00000	2.59752
Pt	1.78784	0.00000	0.86199
Pt	-0.57999	-1.05651	-1.15149
Pt	-2.48657	0.54094	-1.70311
Pt	1.22635	-2.29476	0.07003
Pt	1.15189	0.61317	-1.90792
Pt	-1.43925	0.55136	0.61943
Pt	3.01415	-0.98211	-1.20641
Pt	0.25456	2.29226	-0.05854
Pt	-2.52379	-1.79328	0.39813
Pt	-0.57832	-2.40154	1.89434
Pt	-0.77723	2.23083	-2.40803
Pt	1.33924	2.15202	2.24555
O	-4.47860	1.86696	-1.94126
H	-4.19068	2.74470	-1.66524
H	-5.04859	1.55412	-1.23127

10 [3-10]

Pt	-0.00000	-0.00000	2.57152
Pt	1.78892	0.00000	0.83710
Pt	-0.59010	-1.00257	-1.19070
Pt	-2.47686	0.62456	-1.72337
Pt	1.20025	-2.27776	0.01628
Pt	1.16236	0.65530	-1.92529
Pt	-1.43109	0.59336	0.59968
Pt	3.00470	-0.97101	-1.24272
Pt	0.28412	2.32195	-0.05559
Pt	-2.54377	-1.73504	0.34855
Pt	-0.60683	-2.38541	1.83813
Pt	-0.74670	2.30231	-2.40623
Pt	1.36542	2.13987	2.24716
O	-4.28753	-2.31039	1.80363
H	-4.62486	-1.48698	2.16040
H	-5.02617	-2.78643	1.42776

1(5) [2-1]

Pt	0.00000	0.00000	2.58288
Pt	1.76376	0.00000	0.82289
Pt	-0.64830	-0.98447	-1.17454
Pt	-2.53581	0.65252	-1.67328
Pt	1.15400	-2.27190	0.00126
Pt	1.10021	0.66936	-1.92747
Pt	-1.45687	0.60738	0.63432
Pt	2.94549	-0.96723	-1.27821
Pt	0.25582	2.33173	-0.03847
Pt	-2.58260	-1.71543	0.38967
Pt	-0.62711	-2.37986	1.84849
Pt	-0.80879	2.32608	-2.37407

Pt	1.36939	2.13566	2.24770
O	0.63184	-4.43477	-0.82253
H	1.07009	-4.85254	-1.56685
H	0.04531	-5.07383	-0.41212

1(5) [7-1]

Pt	0.00001	0.00001	2.54814
Pt	1.76134	-0.00000	0.78574
Pt	-0.64324	-1.02914	-1.19815
Pt	-2.54792	0.58348	-1.71080
Pt	1.17360	-2.28620	-0.01192
Pt	1.08740	0.63461	-1.97032
Pt	-1.46556	0.57271	0.59561
Pt	2.95006	-0.97650	-1.30712
Pt	0.22866	2.30744	-0.09710
Pt	-2.56794	-1.76374	0.37614
Pt	-0.60388	-2.39344	1.83885
Pt	-0.83892	2.26726	-2.43100
Pt	1.34719	2.14592	2.18936
O	1.71712	-0.66331	4.16537
H	2.47116	-0.80054	3.56839
H	1.69461	-1.47589	4.70460

6(9) [3-6]

Pt	0.00000	0.00000	2.59671
Pt	1.75528	0.00000	0.82826
Pt	-0.64777	-1.06385	-1.13910
Pt	-2.56697	0.52950	-1.65786
Pt	1.18303	-2.29704	0.05072
Pt	1.06693	0.60739	-1.93037
Pt	-1.47669	0.54561	0.64479
Pt	2.94460	-0.98360	-1.26093
Pt	0.20130	2.28816	-0.06745
Pt	-2.56120	-1.80119	0.44761
Pt	-0.58723	-2.40369	1.90843
Pt	-0.87387	2.22102	-2.39725
Pt	1.32884	2.15363	2.21632
O	2.76097	2.23885	-2.37990
H	3.38034	1.84971	-3.00565
H	3.19427	2.18762	-1.51837

11 [5-11]

Pt	-0.00001	0.00000	2.55214
Pt	1.77695	-0.00000	0.80548
Pt	-0.61502	-1.00669	-1.20498
Pt	-2.50691	0.61820	-1.72620
Pt	1.18476	-2.27908	-0.00914
Pt	1.13081	0.65210	-1.95316
Pt	-1.44517	0.59017	0.58963
Pt	2.97931	-0.97187	-1.28174
Pt	0.26389	2.31972	-0.07905
Pt	-2.55738	-1.73950	0.34836
Pt	-0.60964	-2.38667	1.82520
Pt	-0.78304	2.29689	-2.42252
Pt	1.36117	2.14082	2.21639
O	-2.18750	-2.46798	3.59727
H	-2.78611	-1.75760	3.33063
H	-1.72448	-2.13277	4.37322

2

Pt	0.00000	0.00000	2.56129
Pt	1.75325	-0.00000	0.79083
Pt	-0.66182	-1.02300	-1.18346
Pt	-2.56657	0.59299	-1.68513
Pt	1.15866	-2.28426	-0.00731
Pt	1.06760	0.63941	-1.96123
Pt	-1.47366	0.57751	0.61627
Pt	2.93101	-0.97524	-1.30880
Pt	0.21979	2.31082	-0.08176
Pt	-2.58033	-1.75711	0.39861
Pt	-0.61048	-2.39160	1.85143
Pt	-0.85852	2.27538	-2.41081
Pt	1.34854	2.14454	2.19932
O	3.35888	-1.29422	2.24043
H	4.11317	-1.12140	1.66319
H	3.49025	-0.73287	3.01231

8(13) [6-8]

Pt	0.000000	0.000000	2.583978
Pt	1.745754	0.000000	0.806127
Pt	-0.681223	-1.007644	-1.161453
Pt	-2.582368	0.616752	-1.649461
Pt	1.139749	-2.279370	0.002608
Pt	1.050744	0.651370	-1.940776
Pt	-1.479808	0.589436	0.647228
Pt	2.911191	-0.972064	-1.301837
Pt	0.216779	2.319205	-0.051965
Pt	-2.595610	-1.740511	0.426175
Pt	-0.621901	-2.386955	1.868439
Pt	-0.871470	2.295653	-2.376533
Pt	1.354553	2.141036	2.223726
O	4.706702	-2.442142	-1.104288
H	5.126506	-2.178467	-0.278029
H	4.302468	-3.300044	-0.933669

6(9) [9-6]

Pt	0.000000	0.000000	2.607271
Pt	1.760726	0.000000	0.844246
Pt	-0.642965	-1.035830	-1.137234
Pt	-2.550297	0.573085	-1.651670
Pt	1.176204	-2.288310	0.050278
Pt	1.084857	0.629375	-1.912543

Pt	-1.467092	0.567514	0.654367
Pt	2.950207	-0.977880	-1.247534
Pt	0.224218	2.303752	-0.041569
Pt	-2.565995	-1.770969	0.438856
Pt	-0.600472	-2.395434	1.901834
Pt	-0.844113	2.258373	-2.375035
Pt	1.343781	2.147428	2.244735
O	1.345631	-0.239248	-4.238630
H	1.691202	-1.097778	-3.967351
H	0.400908	-0.375090	-4.372445

S5.3.5. Pt_7Cu_6

1 – Cu

Cu	2.06747	1.46436	1.30471
Cu	0.69686	1.52363	-0.92533
Cu	0.53388	-1.85671	-1.39044
Cu	-1.66657	-1.51334	-0.13903
Cu	2.24125	-0.45483	-0.35219
Cu	-0.91975	-0.00739	-2.23380
Pt	0.00011	-0.00015	1.16008
Pt	1.53237	0.00006	-2.73209
Pt	-1.86499	1.19300	-0.12474
Pt	0.42293	-2.53457	1.00850
Pt	2.17984	-0.99954	2.09675
Pt	-3.30600	-0.24489	-1.54409
Pt	-0.25194	2.60714	1.20057
O	3.60383	2.77498	1.82550
H	4.41840	2.26633	1.87737
H	3.46110	3.11633	2.71208

12 – Pt [9-12]

Cu	2.14845	1.30612	1.54914
Cu	0.95570	1.52799	-0.77105
Cu	0.59142	-1.81706	-1.36056
Cu	-1.66677	-1.35130	-0.26102
Cu	2.31054	-0.57252	-0.15467
Cu	-0.66199	0.15595	-2.24408
Pt	0.00000	-0.00000	1.20572
Pt	1.81491	0.00001	-2.56301
Pt	-1.67567	1.36095	-0.16982
Pt	0.25444	-2.55315	0.99979
Pt	2.02841	-1.18093	2.26362
Pt	-3.10387	0.07210	-1.73757
Pt	-0.07100	2.61632	1.31581
O	-5.25224	-0.37679	-2.24844
H	-5.79025	0.34924	-1.91525
H	-5.52594	-1.16294	-1.76429

11 – Pt [10-11]

Cu	2.20877	1.23404	1.34280
Cu	0.85181	1.52698	-0.87711
Cu	0.33765	-1.79614	-1.47889
Cu	-1.81503	-1.27738	-0.20524
Cu	2.18174	-0.62321	-0.39169
Cu	-0.91544	0.22747	-2.23994
Pt	0.00000	0.00000	1.14737
Pt	1.52406	0.00000	-2.74808
Pt	-1.73060	1.43221	-0.07981
Pt	0.15669	-2.55643	0.89090
Pt	2.06388	-1.25846	2.03328
Pt	-3.31350	0.21141	-1.55045
Pt	0.02090	2.61535	1.29513
O	3.98608	-2.19950	2.86001
H	4.40715	-2.58411	2.08371
H	3.80756	-2.92880	3.46268

13 – Pt [9-13]

Cu	2.01409	1.53352	1.33035
Cu	0.70092	1.51856	-0.93471
Cu	0.66064	-1.87107	-1.35700
Cu	-1.58168	-1.58447	-0.16738
Cu	2.29364	-0.40015	-0.29485
Cu	-0.83012	-0.08180	-2.26285
Pt	0.00000	0.00000	1.15297
Pt	1.63256	0.00000	-2.69826
Pt	-1.86882	1.11395	-0.19564
Pt	0.50934	-2.52094	1.04747
Pt	2.18616	-0.91474	2.15904
Pt	-3.22455	-0.38909	-1.63146
Pt	-0.33801	2.59770	1.15088
O	0.97815	3.96992	2.57360
H	0.98234	4.90702	2.35231
H	0.67078	3.89961	3.48332

10 – Pt [7-10]

Cu	2.26078	1.11655	1.45526
Cu	0.98804	1.52170	-0.79666
Cu	0.32683	-1.75857	-1.48388
Cu	-1.83482	-1.15684	-0.26300
Cu	2.19348	-0.70224	-0.31844
Cu	-0.79988	0.34055	-2.23799
Pt	0.00000	0.00000	1.16904
Pt	1.63947	0.00000	-2.67927
Pt	-1.61885	1.54199	-0.07747
Pt	0.03637	-2.55551	0.86286
Pt	1.97059	-1.37861	2.08795
Pt	-3.21553	0.43223	-1.61946
Pt	0.14716	2.60750	1.37303
O	0.30815	-4.88963	0.75512
H	-0.41755	-5.24927	0.23470
H	1.09121	-5.01026	0.20653

3 – Cu

Cu	2.22831	1.18218	1.48173
Cu	0.94978	1.52518	-0.77723
Cu	0.38132	-1.78008	-1.42664
Cu	-1.79887	-1.22419	-0.21707
Cu	2.21538	-0.65861	-0.27037
Cu	-0.80151	0.27789	-2.20778
Pt	0.00000	-0.00000	1.20456
Pt	1.64731	0.00001	-2.64039
Pt	-1.65824	1.48161	-0.06321
Pt	0.10790	-2.55695	0.92884
Pt	2.00604	-1.31241	2.14348
Pt	-3.22013	0.30980	-1.59489
Pt	0.07434	2.61281	1.37783
O	-0.42319	-3.03691	-3.02916
H	-0.21974	-2.45318	-3.76929
H	-1.37870	-2.98194	-2.91649

4 – Cu

Cu	2.20266	1.21514	1.51034
Cu	0.98550	1.52642	-0.78678
Cu	0.48217	-1.79038	-1.43104
Cu	-1.73969	-1.25799	-0.28858
Cu	2.26616	-0.63621	-0.22948
Cu	-0.70605	0.24595	-2.25927
Pt	0.00000	0.00000	1.17652
Pt	1.75791	0.00000	-2.61914
Pt	-1.64126	1.45039	-0.14817
Pt	0.15143	-2.55680	0.92053
Pt	1.99605	-1.27829	2.18147
Pt	-3.14163	0.24744	-1.71677
Pt	0.03290	2.61459	1.33502
O	-3.20179	-2.81686	0.39074
H	-2.67175	-3.14742	1.12750
H	-3.20633	-3.52721	-0.25971

8 – Pt

Cu	2.13043	1.36788	1.38999
Cu	0.76821	1.52740	-0.84028
Cu	0.45566	-1.83361	-1.36510
Cu	-1.72971	-1.41465	-0.11051
Cu	2.22177	-0.52766	-0.30031
Cu	-0.91243	0.09330	-2.17739
Pt	0.00000	0.00000	1.21706
Pt	1.53850	-0.00001	-2.67272
Pt	-1.80744	1.29733	-0.04873
Pt	0.30988	-2.54782	1.02139
Pt	2.13129	-1.11202	2.13859
Pt	-3.30829	-0.04977	-1.49495
Pt	-0.13564	2.61467	1.30320
O	3.66113	0.95877	-3.31601
H	4.26745	0.21901	-3.40059
H	3.84325	1.35100	-2.45391

5 – Cu

Cu	2.17811	1.29008	1.36149
Cu	0.80800	1.52790	-0.85694
Cu	0.37450	-1.81255	-1.42519
Cu	-1.78672	-1.33486	-0.14994
Cu	2.19209	-0.58396	-0.35501
Cu	-0.93044	0.17203	-2.20174
Pt	0.00000	0.00000	1.18473
Pt	1.51247	0.00000	-2.71524
Pt	-1.76899	1.37708	-0.05078
Pt	0.21916	-2.55414	0.95232
Pt	2.09691	-1.19845	2.07630
Pt	-3.32540	0.10336	-1.50474
Pt	-0.04339	2.61637	1.30733
O	4.10012	-1.70833	-1.04976
H	4.04130	-2.48466	-0.48235
H	3.74509	-1.97183	-1.90881

6 – Cu

Cu	2.12038	1.37020	1.47836
Cu	0.84833	1.52735	-0.80471
Cu	0.56051	-1.83421	-1.34007
Cu	-1.67373	-1.41703	-0.17412
Cu	2.28125	-0.52595	-0.20607
Cu	-0.77597	0.09092	-2.20733
Pt	0.00000	0.00000	1.22095
Pt	1.69290	-0.00001	-2.60416
Pt	-1.75669	1.29490	-0.11674
Pt	0.32010	-2.54757	1.03900
Pt	2.09386	-1.10939	2.22753
Pt	-3.19707	-0.05438	-1.62123
Pt	-0.14169	2.61456	1.30040
O	-1.24511	0.03895	-4.31641
H	-2.18620	-0.16298	-4.21738
H	-0.83314	-0.73330	-4.71808

2 – Cu

Cu	2.04759	1.48870	1.37071
Cu	0.71779	1.52207	-0.88445
Cu	0.60215	-1.86200	-1.33641
Cu	-1.62476	-1.53853	-0.12744
Cu	2.27389	-0.43576	-0.27361
Cu	-0.85673	-0.03335	-2.21513
Pt	0.00000	0.00000	1.19493
Pt	1.60387	0.00000	-2.66834
Pt	-1.85449	1.16554	-0.12966
Pt	0.45468	-2.53014	1.06328

Pt	2.17348	-0.97004	2.17636
Pt	-3.25247	-0.29534	-1.56847
Pt	-0.28254	2.60421	1.21839
O	0.40110	3.51184	-2.00984
H	-0.05215	3.20001	-2.80055
H	-0.30218	3.70072	-1.37096

9 – Pt [7-9]

Cu	2.05305	1.46829	1.45048
Cu	0.81314	1.52338	-0.85490
Cu	0.68343	-1.85760	-1.32578
Cu	-1.58605	-1.51760	-0.20363
Cu	2.32555	-0.45169	-0.19207
Cu	-0.72255	-0.01156	-2.25303
Pt	0.00000	0.00000	1.18810
Pt	1.75415	-0.00000	-2.60930
Pt	-1.79002	1.18853	-0.20307
Pt	0.43563	-2.53384	1.06336
Pt	2.12406	-0.99473	2.24974
Pt	-3.14417	-0.25315	-1.70192
Pt	-0.25869	2.60669	1.21180
O	-2.98811	3.22317	-1.21426
H	-3.57606	3.46820	-0.49297
H	-2.19225	3.74964	-1.08190

S5.3.6. Pd_{13}

13(10) [9-13]

Pd	-0.00000	0.00000	2.85186
Pd	1.45833	-0.00001	0.51887
Pd	-0.14162	-1.01492	-1.68833
Pd	-1.90493	1.07448	-1.96502
Pd	1.73615	-2.49544	-0.33430
Pd	0.69073	1.62405	-1.35205
Pd	-1.27033	0.47664	0.53944
Pd	2.36894	-0.34226	-1.95077
Pd	0.53580	2.32673	1.47995
Pd	1.62562	-2.00399	2.22143
Pd	-2.59080	-1.36099	-0.84804
Pd	-0.66797	-2.02624	0.85532
Pd	-1.34379	2.97988	-0.27978
O	-2.76688	4.26061	-1.60083
H	-2.27468	4.83489	-2.19482
H	-3.39146	4.82088	-1.13042

13(10) [4-13]

Pd	0.00000	0.00000	2.84422
Pd	1.44320	0.00000	0.50184
Pd	-0.16647	-1.02806	-1.69218
Pd	-1.94077	1.05276	-1.96314
Pd	1.72656	-2.49653	-0.34629
Pd	0.65633	1.61547	-1.36850
Pd	-1.28737	0.46465	0.53876
Pd	2.33934	-0.34505	-1.97271
Pd	0.51660	2.32527	1.46251
Pd	1.63038	-1.99853	2.20874
Pd	-2.60860	-1.38262	-0.83509
Pd	-0.67188	-2.03467	0.85759
Pd	-1.37720	2.96527	-0.28678
O	-1.43298	5.17176	0.40305
H	-0.57496	5.57351	0.23498
H	-1.56392	5.20986	1.35590

5(4)

Pd	-0.00000	-0.00000	2.85954
Pd	1.40325	-0.00000	0.49302
Pd	-0.31044	-0.81126	-1.71309
Pd	-1.93271	1.40180	-1.86117
Pd	1.49126	-2.47038	-0.46708
Pd	0.70725	1.74924	-1.29105
Pd	-1.28544	0.65785	0.60051
Pd	2.23379	-0.29859	-2.01030
Pd	0.66300	2.34104	1.57002
Pd	1.47081	-2.08053	2.10840
Pd	-2.75843	-1.02682	-0.82698
Pd	-0.84847	-1.89096	0.79985
Pd	-1.20590	3.19258	-0.11466
O	1.63389	-4.77140	-0.31079
H	0.79351	-5.03754	0.07544
H	1.68831	-5.20805	-1.16598

9(1)

Pd	0.00000	0.00000	2.81543
Pd	1.42302	-0.00001	0.46076
Pd	-0.21215	-1.00863	-1.72342
Pd	-1.97496	1.08487	-1.97082
Pd	1.68264	-2.49489	-0.39974
Pd	0.63080	1.62813	-1.39631
Pd	-1.30402	0.48238	0.52302
Pd	2.29561	-0.34092	-2.02278
Pd	0.52004	2.32740	1.43859
Pd	1.61167	-2.00659	2.15800
Pd	-2.64912	-1.35063	-0.84677
Pd	-0.70228	-2.02218	0.82658
Pd	-1.38444	2.98685	-0.29177
O	1.14085	4.59091	1.67273
H	0.38579	5.12399	1.93915
H	1.34097	4.85060	0.76723

8(11)

Pd	0.00000	0.00000	2.89211
Pd	1.38563	0.00000	0.51523

Pd	-0.31398	-0.91639	-1.66038
Pd	-2.01407	1.23497	-1.84117
Pd	1.55371	-2.48518	-0.39466
Pd	0.61600	1.68639	-1.29885
Pd	-1.32369	0.56540	0.63013
Pd	2.20850	-0.32123	-1.98782
Pd	0.57116	2.33554	1.54976
Pd	1.53773	-2.04290	2.17236
Pd	-2.74656	-1.19908	-0.75102
Pd	-0.79596	-1.96185	0.87827
Pd	-1.33837	3.08597	-0.13744
O	2.76557	0.29915	-4.10463
H	2.26714	1.12209	-4.17172
H	2.28579	-0.33137	-4.65239

6(12)

Pd	0.00000	0.00000	2.88699
Pd	1.41572	0.00000	0.52791
Pd	-0.23461	-0.98367	-1.65623
Pd	-1.98043	1.12584	-1.88752
Pd	1.65163	-2.49257	-0.34600
Pd	0.63157	1.64419	-1.31839
Pd	-1.30693	0.50503	0.60111
Pd	2.27777	-0.33561	-1.96002
Pd	0.53544	2.32991	1.52036
Pd	1.59264	-2.01673	2.21438
Pd	-2.67168	-1.30958	-0.77373
Pd	-0.72545	-2.00603	0.89012
Pd	-1.36871	3.01420	-0.20070
O	1.31663	3.22505	-3.02020
H	1.29924	2.63035	-3.77684
H	2.24746	3.40125	-2.85255

3

Pd	-0.00000	-0.00000	2.89668
Pd	1.43269	-0.00000	0.54788
Pd	-0.23672	-0.87096	-1.66938
Pd	-1.90022	1.30763	-1.86408
Pd	1.58143	-2.47926	-0.38133
Pd	0.72500	1.71401	-1.26554
Pd	-1.26955	0.60565	0.61417
Pd	2.30048	-0.31147	-1.94121
Pd	0.63303	2.33840	1.58747
Pd	1.52082	-2.05965	2.18882
Pd	-2.69097	-1.12457	-0.81111
Pd	-0.78505	-1.93148	0.84949
Pd	-1.23087	3.13287	-0.13031
O	-0.18483	-2.12846	-3.66850
H	0.75356	-1.94228	-3.79926
H	-0.65292	-1.57382	-4.30021

S5.3.7. Co_{13}

8(12,13)

Co	0.00000	0.00000	2.70014
Co	0.90606	0.00000	0.27808
Co	-0.39009	0.81206	-1.62421
Co	1.33097	-2.24047	-0.94141
Co	1.54857	2.23144	-0.85996
Co	0.58189	2.18479	1.56420
Co	-0.98191	-1.36569	-0.44898
Co	-1.92935	-1.32285	1.88379
Co	1.91520	0.03964	-2.06987
Co	-1.33257	0.85690	0.73876
Co	0.39639	-2.23421	1.40990
Co	-0.05678	-1.38568	-2.80744
Co	-0.76212	3.01434	-0.42822
O	-3.95966	-1.96936	1.98356
H	-4.49172	-1.64580	2.71834
H	-4.35043	-1.60472	1.18039

1(4,5,6,9,11)

Co	0.00000	0.00000	2.68088
Co	0.80102	0.00000	0.22208
Co	-0.67137	0.52075	-1.65383
Co	1.49297	-2.21951	-0.91035
Co	1.07349	2.23665	-1.04696
Co	0.21926	2.18211	1.41891
Co	-0.89991	-1.65373	-0.35253
Co	-1.75147	-1.62189	2.01709
Co	1.70124	0.05757	-2.16938
Co	-1.51712	0.55686	0.74561
Co	0.66008	-2.22104	1.47889
Co	-0.07468	-1.66748	-2.74782
Co	-1.30650	2.70870	-0.54553
O	0.93094	3.63623	2.78119
H	0.52269	4.49994	2.65400
H	0.66077	3.32194	3.65227

3(7,10)

Co	0.00000	0.00000	2.77159
Co	0.88244	0.00000	0.34083
Co	-0.42554	0.82820	-1.54635
Co	1.27735	-2.24013	-0.88932
Co	1.53187	2.22961	-0.79687
Co	0.58846	2.18344	1.63645
Co	-1.02349	-1.34824	-0.37180
Co	-1.94783	-1.30480	1.97020
Co	1.86900	0.03859	-2.01672
Co	-1.34460	0.87351	0.82582
Co	0.36576	-2.23343	1.47100
Co	-0.12152	-1.36858	-2.73921

Co	-0.76811	3.02979	-0.34033
O	-3.05409	-1.98623	-0.96053
H	-3.18034	-1.35596	-1.68176
H	-3.58885	-1.64984	-0.22964

S5.3.8. Rh_{13} – 2S+1=2

1(7) [1-7]

Rh	0.00000	0.00000	3.10855
Rh	1.40266	0.00000	1.11748
Rh	2.86410	-0.01184	-0.80356
Rh	-1.49021	-1.53208	2.04962
Rh	-0.09353	-1.52902	0.08467
Rh	1.36092	-1.56156	-1.89673
Rh	-1.23810	1.83159	2.20219
Rh	0.19401	1.78789	0.23266
Rh	1.61643	1.83383	-1.71688
Rh	-2.72884	0.30028	1.14284
Rh	-1.30734	0.26659	-0.80391
Rh	0.11914	0.27542	-2.80576
Rh	-1.20890	-1.92252	-2.27448
O	2.82532	1.47745	2.41631
H	3.71224	1.12918	2.27483
H	2.74895	2.23909	1.82875

3(9) [3-9]

Rh	0.00000	0.00000	3.13269
Rh	1.43004	0.00000	1.13172
Rh	2.86755	0.04291	-0.86489
Rh	-1.55153	-1.50859	2.07847
Rh	-0.14772	-1.47245	0.10580
Rh	1.24749	-1.49182	-1.91500
Rh	-1.18376	1.81266	2.30775
Rh	0.22767	1.84114	0.29382
Rh	1.67541	1.86841	-1.69566
Rh	-2.74776	0.32316	1.24485
Rh	-1.33026	0.33833	-0.71828
Rh	0.05627	0.33226	-2.74513
Rh	-1.32470	-1.84021	-2.26330
O	4.68503	-1.29884	-0.58968
H	4.40907	-2.19165	-0.82324
H	4.89427	-1.32135	0.35003

6(12) [6-12]

Rh	0.00000	0.00000	3.17907
Rh	1.47481	0.00000	1.21087
Rh	2.95621	0.04310	-0.75339
Rh	-1.49966	-1.55062	2.11088
Rh	-0.05237	-1.51461	0.16988
Rh	1.38843	-1.53487	-1.81866
Rh	-1.19738	1.77956	2.30328
Rh	0.25862	1.80752	0.32132
Rh	1.75036	1.83526	-1.63538
Rh	-2.70965	0.24768	1.22587
Rh	-1.24850	0.26311	-0.70500
Rh	0.18351	0.25590	-2.69997
Rh	-1.16847	-1.93509	-2.21982
O	-1.07298	1.41149	-4.19209
H	-1.31147	2.25826	-3.80093
H	-1.87110	0.87151	-4.16154

4(10) [4-10]

Rh	0.00000	0.00000	3.08667
Rh	1.47904	0.00000	1.12164
Rh	2.96596	0.04278	-0.83845
Rh	-1.54318	-1.47987	1.98077
Rh	-0.09062	-1.44367	0.04370
Rh	1.35386	-1.46243	-1.94218
Rh	-1.14085	1.83441	2.24943
Rh	0.32026	1.86323	0.27125
Rh	1.81704	1.89017	-1.68161
Rh	-2.69604	0.37386	1.13471
Rh	-1.23029	0.38884	-0.79266
Rh	0.20582	0.38355	-2.78469
Rh	-1.21297	-1.77584	-2.35696
O	-1.10348	-3.64360	2.58548
H	-0.70653	-4.01400	1.78880
H	-0.39970	-3.61847	3.24161

13 [11-13]

Rh	0.00000	0.00000	3.17167
Rh	1.47876	0.00000	1.20643
Rh	2.96545	0.04276	-0.75383
Rh	-1.54489	-1.47738	2.06482
Rh	-0.09256	-1.44117	0.12758
Rh	1.35162	-1.45988	-1.85852
Rh	-1.13904	1.83627	2.33604
Rh	0.32182	1.86512	0.35767
Rh	1.81835	1.89203	-1.59537
Rh	-2.69592	0.37822	1.22039
Rh	-1.23043	0.39319	-0.70718
Rh	0.20540	0.38796	-2.69942
Rh	-1.21559	-1.77027	-2.27318
O	-1.20885	-3.93318	-2.86217
H	-0.95288	-4.30879	-2.01035
H	-0.40392	-3.95048	-3.39461

2(8) [2-8]

Rh	0.00000	0.00000	3.13257
Rh	1.47437	0.00000	1.16404
Rh	2.95487	0.04320	-0.80090
Rh	-1.48247	-1.57610	2.07776

Rh	-0.03601	-1.54017	0.13614
Rh	1.40458	-1.56098	-1.85254
Rh	-1.21729	1.75874	2.24228
Rh	0.23796	1.78637	0.25976
Rh	1.72896	1.81438	-1.69749
Rh	-2.71258	0.20116	1.17809
Rh	-1.25203	0.21674	-0.75323
Rh	0.17963	0.20884	-2.74845
Rh	-1.14777	-1.99300	-2.24966
O	-0.95141	3.58333	-0.66871
H	-1.83974	3.35570	-0.36658
H	-0.92411	3.30199	-1.59253

5(11) [5-11]

Rh	0.00000	0.00000	3.11512
Rh	1.46149	0.00000	1.13701
Rh	2.93087	0.04278	-0.83627
Rh	-1.55181	-1.48172	2.02386
Rh	-0.11658	-1.44552	0.07392
Rh	1.31018	-1.46432	-1.92473
Rh	-1.14969	1.83303	2.28701
Rh	0.29373	1.86183	0.29589
Rh	1.77304	1.88879	-1.67023
Rh	-2.71360	0.37062	1.18703
Rh	-1.26508	0.38562	-0.75333
Rh	0.15325	0.38027	-2.75806
Rh	-1.25999	-1.77997	-2.31646
O	0.75486	-3.48778	0.86237
H	0.66819	-3.98225	0.03937
H	1.69797	-3.33590	0.98513

S5.3.9. Rh_{13} – 2S+1=10

1(7) [1-7]

Rh	0.00000	0.00000	3.07942
Rh	1.41657	0.00000	1.09823
Rh	2.89121	-0.01365	-0.81269
Rh	-1.50805	-1.49421	1.99201
Rh	-0.09759	-1.49136	0.03692
Rh	1.37015	-1.52488	-1.93464
Rh	-1.20086	1.86271	2.18648
Rh	0.24427	1.81827	0.22650
Rh	1.68106	1.86338	-1.71248
Rh	-2.70942	0.36928	1.09865
Rh	-1.27489	0.33476	-0.83850
Rh	0.16571	0.34332	-2.83022
Rh	-1.20259	-1.83814	-2.33441
O	1.17776	-1.32657	4.43239
H	2.06190	-1.33548	4.04805
H	0.80697	-2.20038	4.25999

3(9) [3-9]

Rh	0.00000	0.00000	3.14356
Rh	1.38763	0.00000	1.14200
Rh	2.83436	-0.01364	-0.79014
Rh	-1.52351	-1.49447	2.07829
Rh	-0.14161	-1.49162	0.10292
Rh	1.29734	-1.52513	-1.88976
Rh	-1.21392	1.86250	2.26802
Rh	0.20259	1.81807	0.28724
Rh	1.61106	1.86318	-1.67241
Rh	-2.73795	0.36882	1.20233
Rh	-1.33171	0.33430	-0.75545
Rh	0.07981	0.34286	-2.76789
Rh	-1.28090	-1.83872	-2.25208
O	4.55987	-1.34223	-0.34818
H	4.22653	-2.23083	-0.51869
H	4.70658	-1.29221	0.60288

6(12) [6-12]

Rh	0.00000	0.00000	3.18983
Rh	1.43607	0.00000	1.22273
Rh	2.92974	-0.01170	-0.67336
Rh	-1.47019	-1.53493	2.10732
Rh	-0.04055	-1.53186	0.16622
Rh	1.44718	-1.56432	-1.79032
Rh	-1.22494	1.82919	2.26102
Rh	0.24027	1.78555	0.31598
Rh	1.69534	1.83155	-1.60931
Rh	-2.69565	0.29503	1.17807
Rh	-1.24144	0.26140	-0.74438
Rh	0.21860	0.27026	-2.72188
Rh	-1.11544	-1.92890	-2.21107
O	-0.97154	1.68443	-3.98042
H	-0.99867	2.46316	-3.41104
H	-1.85533	1.29916	-3.94279

4(10) [4-10]

Rh	0.00000	0.00000	3.10182
Rh	1.43590	0.00000	1.13460
Rh	2.92899	-0.01513	-0.76193
Rh	-1.51744	-1.46267	1.98501
Rh	-0.08788	-1.46000	0.04386
Rh	1.39864	-1.49431	-1.91358
Rh	-1.16654	1.88765	2.21580
Rh	0.29711	1.84262	0.26961
Rh	1.75343	1.88703	-1.65476
Rh	-2.68448	0.42577	1.09857
Rh	-1.23152	0.39058	-0.82479
Rh	0.22862	0.39891	-2.80222
Rh	-1.17406	-1.76835	-2.34143
O	-0.92458	-3.57416	2.64901

H	-0.40924	-3.83051	1.87217
H	-0.27468	-3.44111	3.34794

13 [11-13]

Rh	0.00000	0.00000	3.17384
Rh	1.43606	0.00000	1.20673
Rh	2.92927	-0.01535	-0.68970
Rh	-1.52029	-1.45797	2.05475
Rh	-0.09056	-1.45532	0.11372
Rh	1.39604	-1.48975	-1.84365
Rh	-1.16266	1.89130	2.29049
Rh	0.30105	1.84618	0.34436
Rh	1.75762	1.89048	-1.57983
Rh	-2.68345	0.43412	1.17099
Rh	-1.23041	0.39883	-0.75230
Rh	0.22992	0.40713	-2.72960
Rh	-1.17717	-1.75798	-2.27211
O	-1.71967	-3.87892	-2.14289
H	-1.48471	-3.97386	-1.20801
H	-1.05821	-4.38298	-2.62977

2(8) [2-8]

Rh	0.00000	0.00000	3.14789
Rh	1.43645	0.00000	1.18107
Rh	2.93060	-0.01060	-0.71465
Rh	-1.45441	-1.55758	2.07646
Rh	-0.02442	-1.55438	0.13562
Rh	1.46401	-1.58624	-1.82040
Rh	-1.24308	1.80988	2.20546
Rh	0.22294	1.76670	0.26102
Rh	1.67792	1.81319	-1.66432
Rh	-2.69802	0.25306	1.13359
Rh	-1.24310	0.21995	-0.78833
Rh	0.21724	0.22897	-2.76561
Rh	-1.09471	-1.97969	-2.23885
O	-0.93574	3.56486	-0.67612
H	-1.82130	3.35785	-0.34926
H	-0.93119	3.24648	-1.58961

5(11) [5-11]

Rh	0.00000	0.00000	3.12486
Rh	1.42019	0.00000	1.14626
Rh	2.89814	-0.01504	-0.76209
Rh	-1.52507	-1.46460	2.02104
Rh	-0.11100	-1.46192	0.06856
Rh	1.35990	-1.49618	-1.90063
Rh	-1.17513	1.88615	2.24702
Rh	0.27301	1.84116	0.28927
Rh	1.71393	1.88561	-1.64667
Rh	-2.70070	0.42234	1.14279
Rh	-1.26307	0.38719	-0.79206
Rh	0.18128	0.39553	-2.78106
Rh	-1.21589	-1.77261	-2.30782
O	0.82756	-3.42638	0.83167
H	0.77318	-3.95584	0.02729
H	1.75704	-3.18530	0.93088

1(7) [4-1]

Rh	0.00000	0.00000	3.07544
Rh	1.41360	0.00000	1.09214
Rh	2.88555	-0.01236	-0.82087
Rh	-1.49178	-1.52114	2.00304
Rh	-0.08428	-1.51815	0.04582
Rh	1.38091	-1.55097	-1.92765
Rh	-1.22417	1.84071	2.16864
Rh	0.21856	1.79680	0.20687
Rh	1.65192	1.84249	-1.73464
Rh	-2.71646	0.32034	1.09581
Rh	-1.28442	0.28640	-0.84320
Rh	0.15310	0.29516	-2.83714
Rh	-1.18851	-1.89809	-2.32078
O	1.59659	0.62924	4.56939
H	2.36417	0.58941	3.98427
H	1.49192	1.55564	4.81026

2(8) [5-2]

Rh	0.00000	0.00000	3.10855
Rh	1.40266	0.00000	1.11748
Rh	2.86410	-0.01184	-0.80356
Rh	-1.49021	-1.53208	2.04962
Rh	-0.09353	-1.52902	0.08467
Rh	1.36092	-1.56156	-1.89673
Rh	-1.23810	1.83159	2.20219
Rh	0.19401	1.78789	0.23266
Rh	1.61643	1.83383	-1.71688
Rh	-2.72884	0.30028	1.14284
Rh	-1.30734	0.26659	-0.80391
Rh	0.11914	0.27542	-2.80576
Rh	-1.20890	-1.92252	-2.27448
O	2.82532	1.47745	2.41631
H	3.71224	1.12918	2.27483
H	2.74895	2.23909	1.82875

S5.3.10. Ir_{13}

6

Ir	0.00000	0.00000	3.07586
Ir	1.45345	-0.00001	-0.00245
Ir	-0.64661	0.15951	-2.82106
Ir	-2.32811	-1.10896	-1.65675
Ir	1.65205	1.31321	1.96232
Ir	3.19273	-0.92312	-1.38614

Ir	1.01475	-1.40110	-2.09846
Ir	-0.00258	2.84233	1.17639
Ir	-0.28758	1.47486	-0.80182
Ir	-0.28507	-1.30495	1.05587
Ir	-0.64404	-2.66785	-0.93159
Ir	-1.66216	1.52817	2.28850
Ir	-1.96308	0.20287	0.30575
O	5.21212	-1.38690	-2.03197
H	5.39539	-2.33225	-1.98679
H	5.37918	-1.08705	-2.93267

5 [2-5]

Ir	0.00001	-0.00001	3.03617
Ir	1.47937	0.00065	-0.02941
Ir	-0.59680	0.09507	-2.86740
Ir	-2.26463	-1.19439	-1.70645
Ir	1.63770	1.33371	1.92544
Ir	3.24915	-0.90254	-1.38919
Ir	1.08759	-1.42796	-2.11610
Ir	-0.03875	2.82484	1.11114
Ir	-0.28048	1.43475	-0.85704
Ir	-0.24258	-1.32790	1.02561
Ir	-0.55825	-2.71489	-0.95253
Ir	-1.68336	1.48968	2.22052
Ir	-1.94168	0.14141	0.24723
O	2.19436	2.59345	3.97853
H	2.57168	3.45175	3.76382
H	2.89925	2.08600	4.39195

4 [13-4]

Ir	0.00000	0.00000	3.08887
Ir	1.51225	0.00000	0.03901
Ir	-0.53239	0.17879	-2.81891
Ir	-2.24297	-1.08329	-1.69057
Ir	1.68041	1.30685	2.01086
Ir	3.27260	-0.92920	-1.31361
Ir	1.10607	-1.39306	-2.06888
Ir	0.04972	2.84733	1.19755
Ir	-0.20488	1.48673	-0.78952
Ir	-0.25350	-1.29796	1.06019
Ir	-0.58185	-2.65355	-0.93755
Ir	-1.63821	1.53958	2.27400
Ir	-1.90838	0.22125	0.28219
O	-3.20603	-2.07083	-3.69629
H	-2.75550	-2.88819	-3.93304
H	-3.02412	-1.45115	-4.41090

12 [13-12]

Ir	0.00000	0.00000	3.03357
Ir	1.50117	0.00000	-0.02176
Ir	-0.55719	0.09362	-2.87388
Ir	-2.23222	-1.19629	-1.72391
Ir	1.64396	1.33452	1.93348
Ir	3.27916	-0.90206	-1.36967
Ir	1.12209	-1.42821	-2.11109
Ir	-0.02701	2.82443	1.10776
Ir	-0.25492	1.43386	-0.86173
Ir	-0.22851	-1.32844	1.02171
Ir	-0.53032	-2.71593	-0.95822
Ir	-1.67845	1.48879	2.20632
Ir	-1.92300	0.14004	0.23164
O	-1.59650	2.81629	4.36490
H	-2.01606	3.67258	4.23691
H	-2.15032	2.34328	4.99324

1(8) [10-1]

Ir	-0.00001	0.00001	3.02882
Ir	1.49037	0.00000	-0.03178
Ir	-0.57739	0.11489	-2.87631
Ir	-2.25628	-1.16816	-1.72429
Ir	1.64827	1.32771	1.92694
Ir	3.25802	-0.90890	-1.38868
Ir	1.09517	-1.41953	-2.12403
Ir	-0.01638	2.83035	1.11161
Ir	-0.25979	1.44716	-0.86123
Ir	-0.24374	-1.32093	1.01382
Ir	-0.56110	-2.70054	-0.96919
Ir	-1.67215	1.50157	2.21199
Ir	-1.93196	0.16034	0.23415
O	0.09917	1.25010	5.24846
H	0.89748	0.97621	5.72743
H	-0.64633	0.94218	5.79292

11(2) [10-11]

Ir	-0.00000	0.00000	3.08371
Ir	1.49865	0.00000	0.02715
Ir	-0.55729	0.20426	-2.82094
Ir	-2.27210	-1.04931	-1.68955
Ir	1.68520	1.29837	2.00294
Ir	3.24608	-0.93719	-1.33667
Ir	1.07285	-1.38233	-2.08393
Ir	0.06232	2.85377	1.20250
Ir	-0.21112	1.50235	-0.78832
Ir	-0.27207	-1.28865	1.05150
Ir	-0.61928	-2.63448	-0.94964
Ir	-1.63041	1.55455	2.28174
Ir	-1.91914	0.24553	0.28640
O	-0.70794	-4.26992	-2.83541
H	-1.36702	-4.00262	-3.48307
H	0.14707	-4.16104	-3.26700

11(3) [7-11]

Ir	0.00000	0.00000	3.06238
Ir	1.50718	0.00000	0.01002
Ir	-0.54067	0.20645	-2.84373
Ir	-2.25943	-1.04638	-1.71753
Ir	1.68903	1.29764	1.98673
Ir	3.25782	-0.93787	-1.34921
Ir	1.08640	-1.38140	-2.10267
Ir	0.06938	2.85431	1.18225
Ir	-0.19936	1.50368	-0.80975
Ir	-0.26721	-1.28784	1.02902
Ir	-0.60968	-2.63284	-0.97350
Ir	-1.62718	1.55584	2.25635
Ir	-1.91117	0.24762	0.25981
O	-1.66821	-4.45863	0.03562
H	-1.51484	-4.35322	0.98216
H	-2.62116	-4.39524	-0.09368

7 [2-7]

Ir	-0.00000	-0.00000	3.09091
Ir	1.49073	0.00012	0.03041
Ir	-0.57378	0.18239	-2.81287
Ir	-2.27768	-1.07852	-1.67317
Ir	1.67415	1.30560	2.00180
Ir	3.24056	-0.93033	-1.33496
Ir	1.06831	-1.39162	-2.07517
Ir	0.03936	2.84825	1.20074
Ir	-0.23063	1.48893	-0.78519
Ir	-0.26912	-1.29666	1.06341
Ir	-0.61294	-2.65087	-0.93266
Ir	-1.64230	1.54169	2.28837
Ir	-1.92785	0.22467	0.29785
O	0.82642	-2.71759	-4.19934
H	1.39230	-2.17342	-4.75612
H	1.35885	-3.48506	-3.96751

12 [8-12]

Ir	0.00000	0.00000	3.03974
Ir	1.51856	0.00000	-0.00698
Ir	-0.52247	0.12645	-2.87027
Ir	-2.21619	-1.15286	-1.73592
Ir	1.66278	1.32398	1.95531
Ir	3.29562	-0.91260	-1.34902
Ir	1.13794	-1.41479	-2.10514
Ir	0.01074	2.83350	1.12716
Ir	-0.21905	1.45436	-0.85013
Ir	-0.22956	-1.31681	1.02038
Ir	-0.53315	-2.69214	-0.96776
Ir	-1.65953	1.50849	2.21001
Ir	-1.90553	0.17134	0.22764
O	-3.68744	0.78085	3.05519
H	-4.08902	0.32232	2.30422
H	-4.27347	1.50970	3.28607

11(3) [4-11]

Ir	0.00000	0.00000	3.06683
Ir	1.49029	-0.00000	0.00618
Ir	-0.57257	0.21837	-2.83585
Ir	-2.28940	-1.03045	-1.70227
Ir	1.68754	1.29364	1.98404
Ir	3.23014	-0.94159	-1.36428
Ir	1.05307	-1.37634	-2.10647
Ir	0.06885	2.85725	1.19115
Ir	-0.21555	1.51095	-0.80161
Ir	-0.28289	-1.28345	1.03281
Ir	-0.64106	-2.62384	-0.97005
Ir	-1.62622	1.56281	2.27242
Ir	-1.92575	0.25898	0.27528
O	0.54458	-4.45433	-0.68466
H	1.45300	-4.11681	-0.63278
H	0.50313	-5.00089	-1.47822

1(8) [12-1]

Ir	-0.00001	-0.00001	3.03368
Ir	1.48195	-0.00001	-0.03101
Ir	-0.59168	0.16339	-2.86889
Ir	-2.28534	-1.10380	-1.72093
Ir	1.66379	1.31194	1.93624
Ir	3.23296	-0.92434	-1.39900
Ir	1.06114	-1.39949	-2.13175
Ir	0.01825	2.84334	1.13582
Ir	-0.24993	1.47725	-0.84569
Ir	-0.26777	-1.30355	1.01043
Ir	-0.60983	-2.66498	-0.98102
Ir	-1.65306	1.53048	2.23177
Ir	-1.93706	0.20657	0.24559
O	0.95248	-1.75701	4.09740
H	0.93260	-2.42779	3.39720
H	0.39146	-2.08473	4.80941

1(8) [5-1]

Ir	0.00000	-0.00000	3.03343
Ir	1.50350	0.00002	-0.02077
Ir	-0.55015	0.16251	-2.87319
Ir	-2.25152	-1.10498	-1.73702
Ir	1.67114	1.31221	1.94756
Ir	3.26432	-0.92406	-1.37628
Ir	1.09784	-1.39987	-2.12423
Ir	0.03089	2.84311	1.13538
Ir	-0.22299	1.47670	-0.84780
Ir	-0.25320	-1.30387	1.00849
Ir	-0.58087	-2.66564	-0.98514
Ir	-1.64777	1.52995	2.21970

Ir	-1.91743	0.20573	0.23174
O	-1.33825	-1.25755	4.37366
H	-1.25023	-2.16670	4.05934
H	-2.23608	-0.97104	4.15098

10(9) [5-10]

Ir	0.00000	-0.00000	3.04930
Ir	1.50574	-0.00009	-0.00372
Ir	-0.54466	0.18510	-2.85716
Ir	-2.25512	-1.07489	-1.72632
Ir	1.68049	1.30481	1.96885
Ir	3.26152	-0.93118	-1.36098
Ir	1.09254	-1.39036	-2.11207
Ir	0.05087	2.84894	1.16044
Ir	-0.21043	1.49061	-0.82731
Ir	-0.26019	-1.29566	1.02000
Ir	-0.59526	-2.64885	-0.97826
Ir	-1.63713	1.54329	2.23931
Ir	-1.91395	0.22726	0.24689
O	-2.07817	-2.88053	1.83637
H	-2.83016	-2.45526	1.40500
H	-2.19822	-2.72792	2.78032

5 [8-5]

Ir	-0.00000	-0.00000	3.04368
Ir	1.46774	0.00012	-0.02793
Ir	-0.62004	0.14018	-2.85658
Ir	-2.29978	-1.13465	-1.69669
Ir	1.64981	1.31946	1.93435
Ir	3.21861	-0.91698	-1.40097
Ir	1.04669	-1.40919	-2.12205
Ir	-0.00972	2.83720	1.13658
Ir	-0.27781	1.46289	-0.83924
Ir	-0.26832	-1.31190	1.02590
Ir	-0.61037	-2.68209	-0.95954
Ir	-1.66705	1.51669	2.24451
Ir	-1.95127	0.18443	0.26396
O	3.38840	0.03369	2.67973
H	3.27994	-0.74345	2.10720
H	4.20401	0.45659	2.38653

13 [9-13]

Ir	0.00000	0.00000	3.05437
Ir	1.51963	0.00000	0.00819
Ir	-0.51926	0.15425	-2.85526
Ir	-2.22360	-1.11596	-1.72660
Ir	1.67374	1.31493	1.97581
Ir	3.28981	-0.92145	-1.33689
Ir	1.12846	-1.40330	-2.09574
Ir	0.03416	2.84095	1.15314
Ir	-0.20595	1.47161	-0.82973
Ir	-0.23936	-1.30685	1.02968
Ir	-0.55324	-2.67174	-0.96404
Ir	-1.64708	1.52505	2.23013
Ir	-1.90306	0.19786	0.24234
O	-3.89936	-0.83547	1.22348
H	-4.45789	-1.13421	0.49687
H	-4.38269	-0.13295	1.67257

10(9) [2-10]

Ir	0.00000	0.00000	3.05192
Ir	1.48105	0.00000	-0.01315
Ir	-0.59230	0.18718	-2.84988
Ir	-2.29427	-1.07212	-1.70556
Ir	1.67248	1.30415	1.95833
Ir	3.22519	-0.93173	-1.38487
Ir	1.04996	-1.38948	-2.11850
Ir	0.03725	2.84949	1.16355
Ir	-0.24089	1.49194	-0.82238
Ir	-0.27729	-1.29476	1.02450
Ir	-0.62937	-2.64730	-0.97146
Ir	-1.64269	1.54455	2.25569
Ir	-1.93647	0.22909	0.26506
O	1.47564	-2.85595	1.65767
H	2.15936	-2.56180	1.03129
H	1.20641	-3.72924	1.35046

4 [3-4]

Ir	0.000000	0.000000	3.067723
Ir	1.522212	0.000000	0.020869
Ir	-0.515710	0.176828	-2.841391
Ir	-2.229288	-1.084994	-1.717819
Ir	1.683165	1.306236	1.994288
Ir	3.285156	-0.929684	-1.324428
Ir	1.119563	-1.395688	-2.087173
Ir	0.054715	2.846690	1.175525
Ir	-0.194169	1.485688	-0.811756
Ir	-0.247974	-1.298544	1.038626
Ir	-0.569928	-2.654959	-0.959547
Ir	-1.636099	1.539133	2.247670
Ir	-1.900542	0.220128	0.255518
O	-4.155442	-2.211110	-1.189960
H	-4.199482	-2.294057	-0.232526
H	-4.962737	-1.763811	-1.459451

S5.3.11. Ru_{13}

9(10)

Ru	0.00000	0.00000	2.91217
Ru	1.14915	0.00000	0.90252
Ru	-1.56500	1.41319	1.95914
Ru	-0.34754	1.35150	-0.00892

Ru	-1.19690	-1.82619	2.16219
Ru	-0.01901	-1.89370	0.15674
Ru	-2.75771	-0.41679	1.21170
Ru	-1.59591	-0.46976	-0.80354
Ru	2.93101	1.03835	-0.42118
Ru	1.39943	2.42136	-1.35388
Ru	0.28463	0.52396	-2.42781
Ru	1.86694	-0.90486	-1.46423
Ru	-0.26400	-1.97179	-2.38734
O	0.81994	4.53207	-1.25881
H	0.34846	4.84233	-2.04066
H	0.15651	4.44836	-0.55678

1(3)

Ru	0.00000	0.00000	2.85186
Ru	1.18238	0.00000	0.86157
Ru	-1.53742	1.43039	1.87979
Ru	-0.28793	1.36796	-0.06806
Ru	-1.19902	-1.81280	2.07332
Ru	0.01148	-1.88056	0.08740
Ru	-2.73233	-0.38624	1.10387
Ru	-1.53764	-0.43929	-0.89206
Ru	2.99438	1.02991	-0.42736
Ru	1.48978	2.42977	-1.37867
Ru	0.37766	0.54660	-2.48009
Ru	1.93209	-0.89962	-1.49727
Ru	-0.19178	-1.94474	-2.46075
O	-2.07043	3.51567	2.41982
H	-2.82368	3.77669	1.87771
H	-1.32376	4.04021	2.10759

13

Ru	0.00000	0.00000	2.93471
Ru	1.16417	0.00000	0.93372
Ru	-1.46790	1.53862	2.02229
Ru	-0.23966	1.47146	0.06112
Ru	-1.29933	-1.72231	2.11289
Ru	-0.11062	-1.79156	0.11391
Ru	-2.76330	-0.18782	1.20291
Ru	-1.58969	-0.24124	-0.80546
Ru	3.01718	0.97314	-0.34095
Ru	1.58061	2.47891	-1.23389
Ru	0.36166	0.69186	-2.38144
Ru	1.84581	-0.86378	-1.45893
Ru	-0.33813	-1.76559	-2.43287
O	-1.24429	-3.75419	-3.34579
H	-0.81522	-4.46685	-2.85976
H	-2.18095	-3.81397	-3.12832

11(12) [12-11]

Ru	0.00000	0.00000	2.89501
Ru	1.12287	0.00000	0.87055
Ru	-1.49823	1.52318	2.00630
Ru	-0.30998	1.45670	0.02063
Ru	-1.30247	-1.73592	2.10750
Ru	-0.15449	-1.80496	0.08484
Ru	-2.79669	-0.21682	1.22116
Ru	-1.66412	-0.27020	-0.81064
Ru	2.94171	0.98165	-0.44609
Ru	1.47546	2.47231	-1.31584
Ru	0.24718	0.67082	-2.43038
Ru	1.76199	-0.86921	-1.53184
Ru	-0.43437	-1.79214	-2.45681
O	3.21728	-2.53771	-1.15514
H	3.25935	-2.55220	-0.19072
H	2.69513	-3.31030	-1.40436

6(8) [8-6]

Ru	0.00000	0.00000	2.87044
Ru	1.14499	0.00000	0.85841
Ru	-1.47237	1.54401	1.97447
Ru	-0.26312	1.47661	0.00155
Ru	-1.31180	-1.71750	2.05842
Ru	-0.14244	-1.78682	0.04805
Ru	-2.78023	-0.17763	1.16485
Ru	-1.62602	-0.23107	-0.85473
Ru	2.98836	0.97013	-0.43242
Ru	1.54742	2.48117	-1.30926
Ru	0.31271	0.69923	-2.44786
Ru	1.80137	-0.86186	-1.54198
Ru	-0.39421	-1.75623	-2.49639
O	0.84631	-3.86957	0.18864
H	1.30915	-3.82843	-0.65875
H	1.53045	-3.77435	0.86109

7(5)

Ru	0.00000	0.00000	2.84315
Ru	1.19897	0.00000	0.86282
Ru	-1.48953	1.48751	1.88232
Ru	-0.22555	1.42259	-0.05608
Ru	-1.24119	-1.76644	2.02514
Ru	-0.01600	-1.83501	0.04827
Ru	-2.72673	-0.28291	1.06688
Ru	-1.51686	-0.33618	-0.91987
Ru	3.04931	1.00077	-0.39420
Ru	1.59158	2.45653	-1.33452
Ru	0.43811	0.62263	-2.47581
Ru	1.94412	-0.88134	-1.50435
Ru	-0.19906	-1.85219	-2.50215
O	-4.89514	-0.35637	1.13019
H	-5.23553	0.47871	1.46898
H	-5.20342	-1.05085	1.72209