

Supporting Information: A Theoretical Indicator for Transition-Metal Nanoclusters Applied in the Carbon Nanotube Nucleation Process: A DFT Study

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A CNT Fragments Tests

Below are provided different unit cell sizes for the armchair and zigzag carbon nanotube fragments.

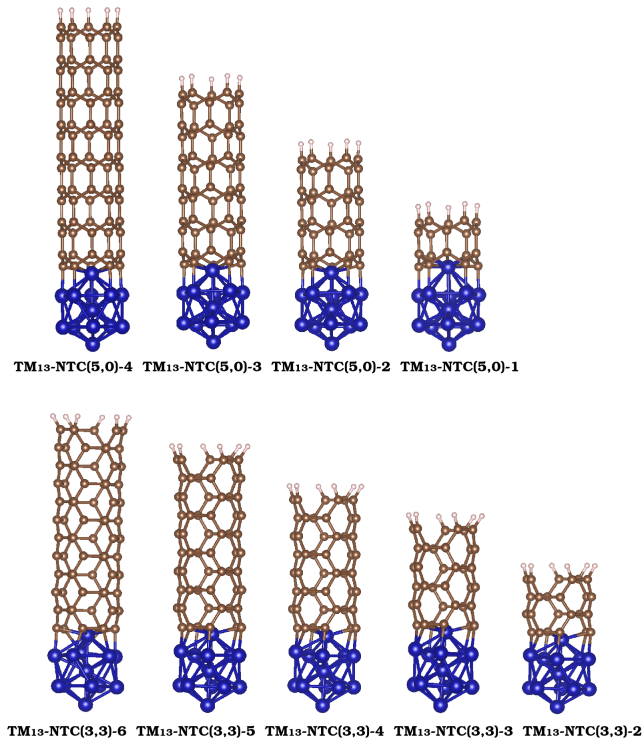


Figure 1: Armchair and zigzag carbon nanotube fragments containing different unit cell sizes and connected to transition-metal nanoclusters. $TM_{13}\text{-CNT}(x,y)\text{-}z$ indicates the transition-metal species, in nanocluster configuration associated with the carbon nanotube CNT (x,y) , where (x,y) indicates the chirality. The unit cell number z ranges from 1 to 4 for zigzag and from 2 to 6 for armchair.

We have calculated the adhesion energy for all $TM_{13}\text{-CNT}(x,y)\text{-}z$ as provide below.

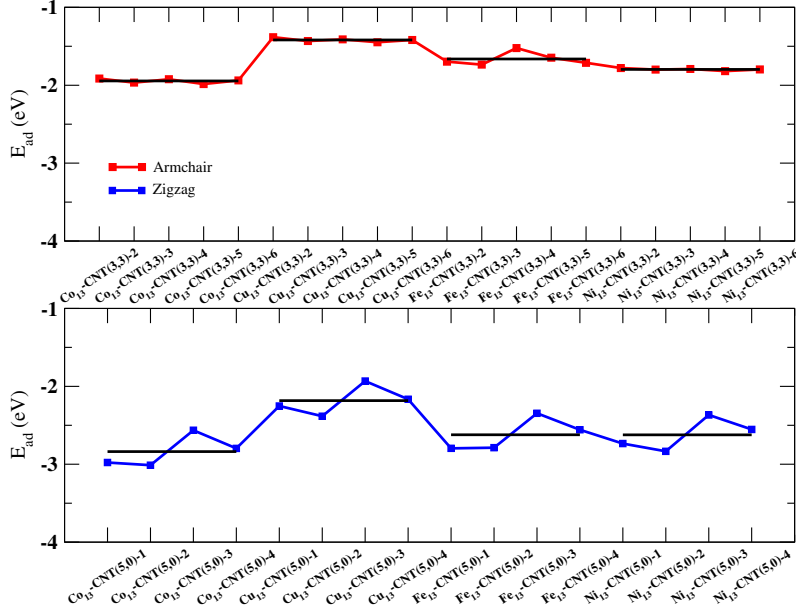


Figure 2: Adhesion energy for TM_{13} -CNT (x,y) - z systems. TM_{13} -CNT (x,y) - z indicates the transition-metal species, in nanocluster configuration associated with the carbon nanotube CNT (x,y) , where (x,y) indicates the chirality. The unit cell number z ranges from 1 to 4 for zigzag and from 2 to 6 for armchair.

Here, we provided the total magnetic moment for the previous systems with their respective magnetic isomers, calculated by DFT-PBE.

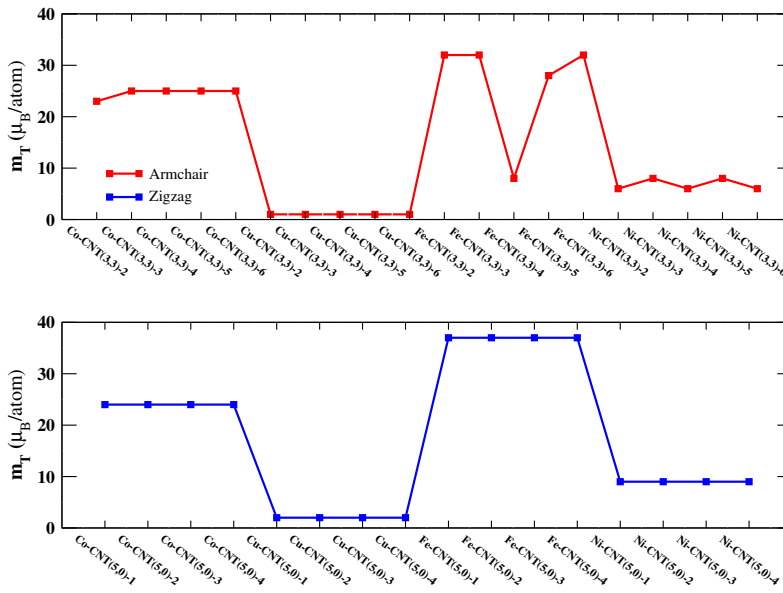


Figure 3: Total magnetic moments for TM_{13} -CNT (x,y) - z systems, calculated by DFT-PBE.

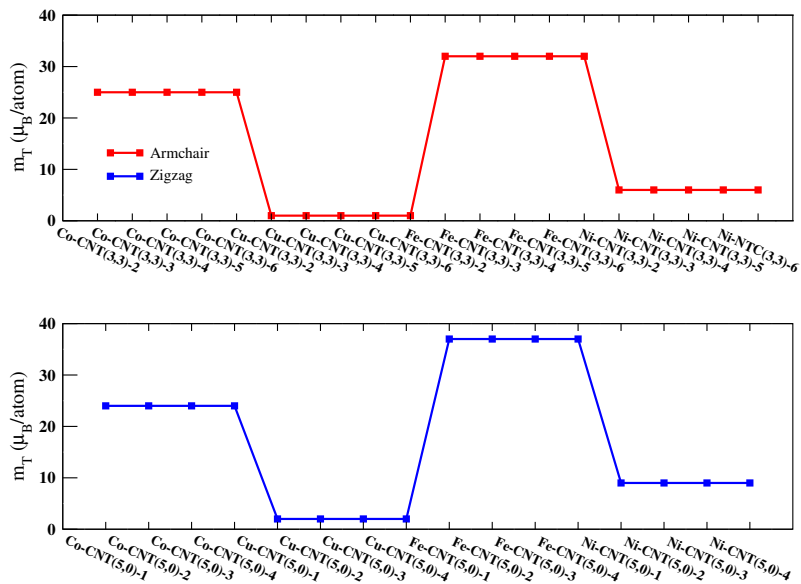


Figure 4: Corrected total magnetic moments for the systems TM₁₃-CNT(x,y)-z, calculated by DFT-PBE.

B The Lowest Energy Configurations – Tests

Below are shown some examples for the calculations of the lowest energy configurations, for the cases where the icosahedral (ICO) is not the most stable configuration. We showed an armchair CNT fragment (3,3) adhered to the lowest configurations for TM_{13} , where $\text{TM} = \text{Co}, \text{Ir}, \text{and Rh}$.

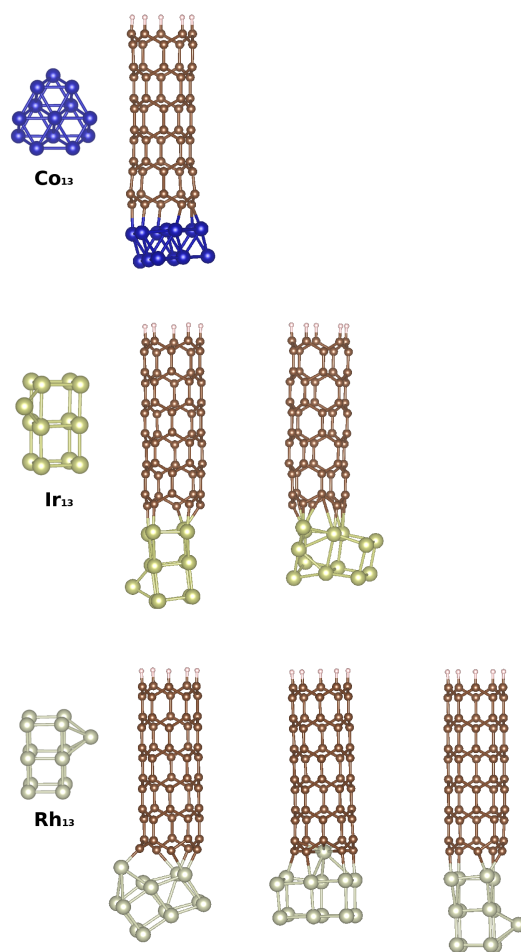


Figure 5: Armchair CNT fragment (3,3) adhered to the lowest energy configurations for TM_{13} , where $\text{TM} = \text{Co}, \text{Ir}, \text{and Rh}$.

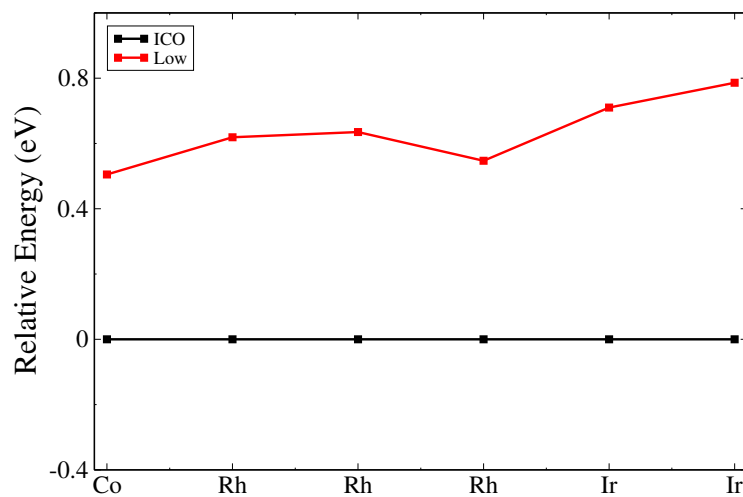


Figure 6: Relative energy between armchair CNT fragment (3,3) adhered to TM₁₃ with ICO configuration and armchair CNT fragment (3,3) adhered to the lowest configurations for TM₁₃, where TM = Co, Ir, and Rh.

C Nucleation Tests

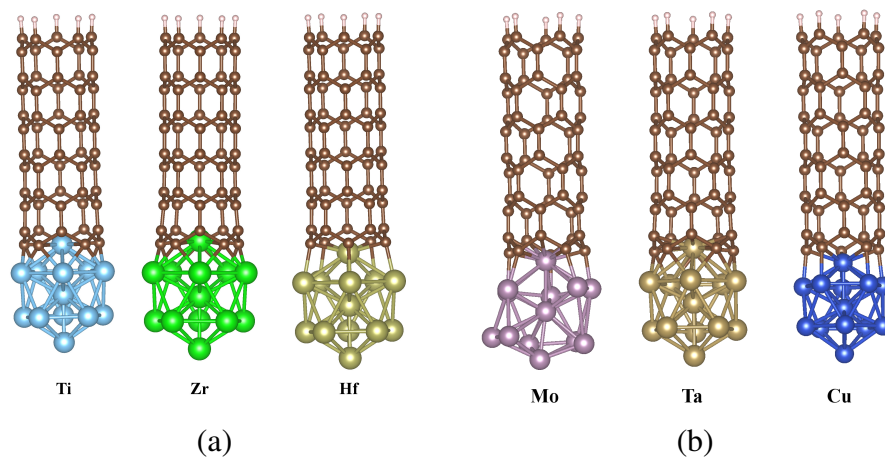


Figure 7: (a) CNT fragments adhered to nanoclusters by bridge site interactions between C and TM atoms, where TM = Ti, Zr, and Hf. (b) CNT fragments adhered to nanoclusters by top site interactions between C and Cu or Mo atoms and between C and Ta atoms adhered by bridge interaction sites.

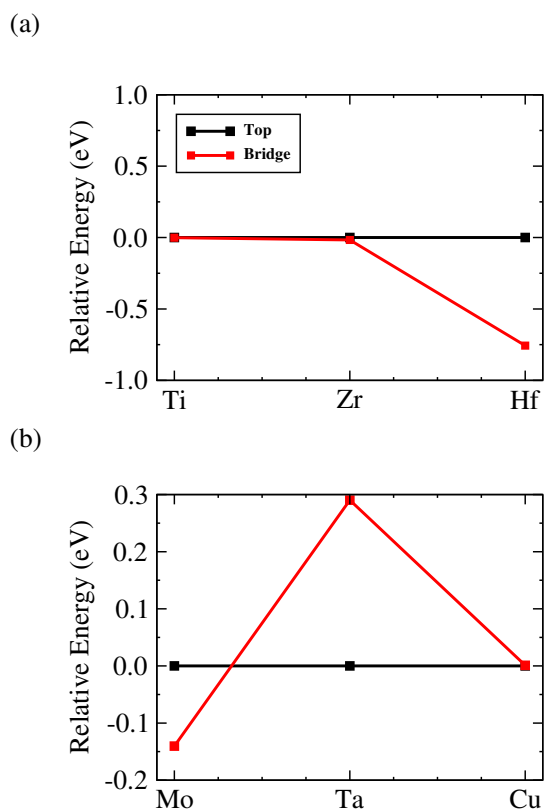


Figure 8: (a) Relative Energy between CNT fragments adhered on Ti_{13} , Zr_{13} , and Hf_{13} nanoclusters by top and bridge site interactions. (b) Relative Energy between CNT fragments adhered on Mo_{13} , Ta_{13} , and Cu_{13} nanoclusters by top and bridge site interactions.

D Results by DFT-PBE-vdW and DFT-PBE-vdW-SOC

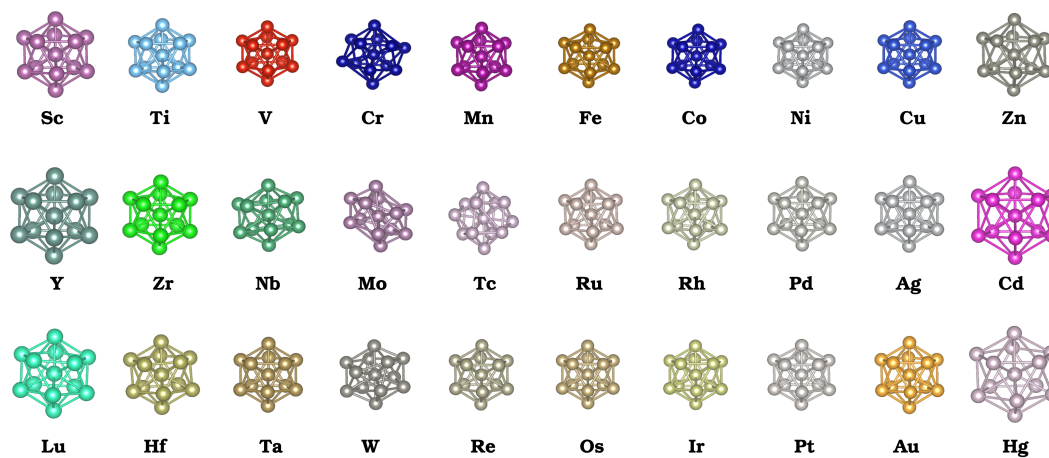


Figure 9: The ICO TM_{13} configurations obtained for all $3d$, $4d$, and $5d$ elements in gas-phase, by DFT-PBE-vdW-SOC.

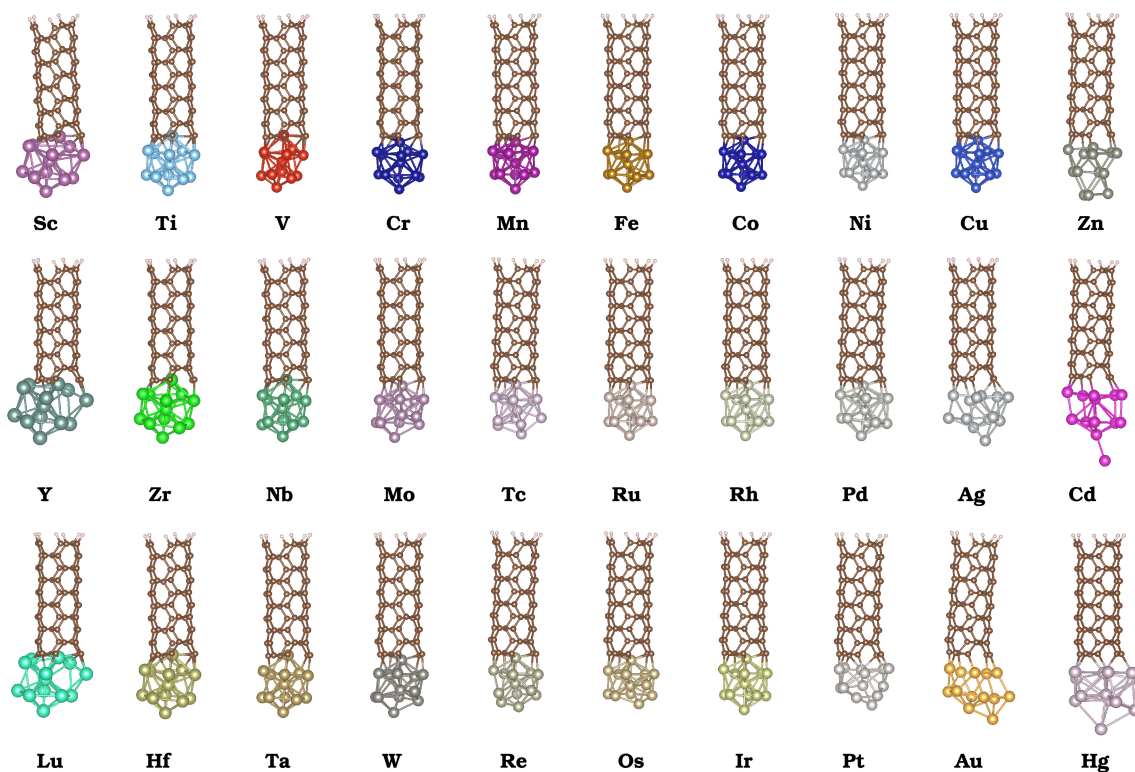


Figure 10: Configurations for (3,3) armchair CNT fragments adhered to $3d$, $4d$, and $5d$ TM_{13} nanoclusters obtained by DFT-PBE-vdW-SOC.

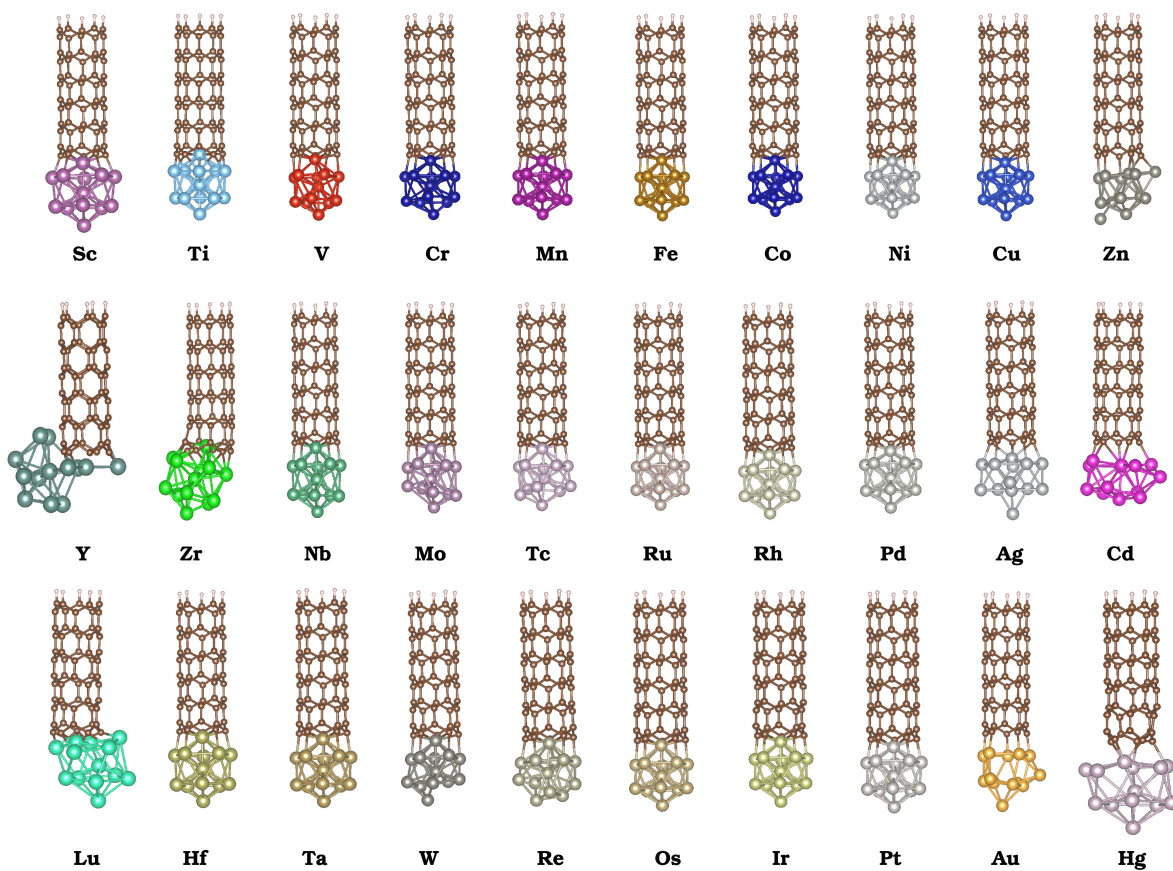


Figure 11: Configurations for (5,0) zigzag CNT fragments adhered to $3d$, $4d$, and $5d$ TM_{13} nanoclusters obtained by DFT-PBE-vdW-SOC.

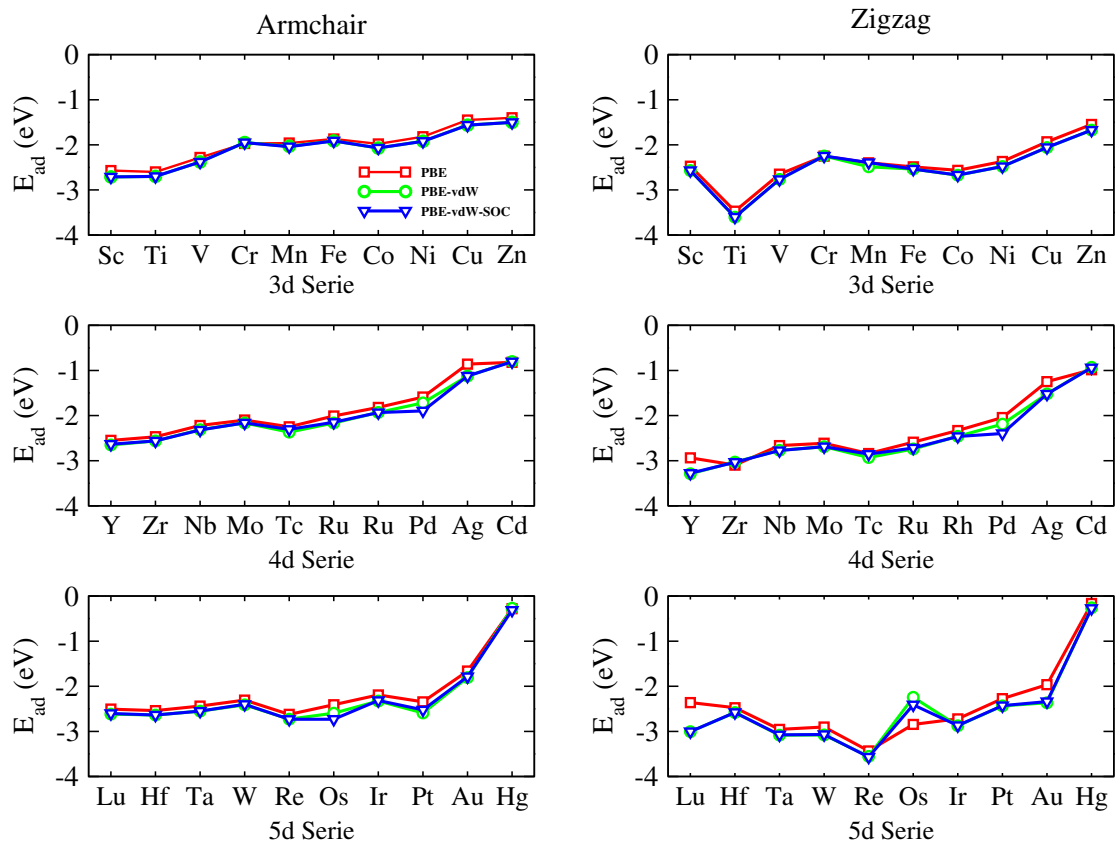


Figure 12: Adhesion energy values for CNT fragments adhered to TM_{13} nanoclusters using three approaches, PBE, PBE-vdW, and PBE-vdW-SOC.

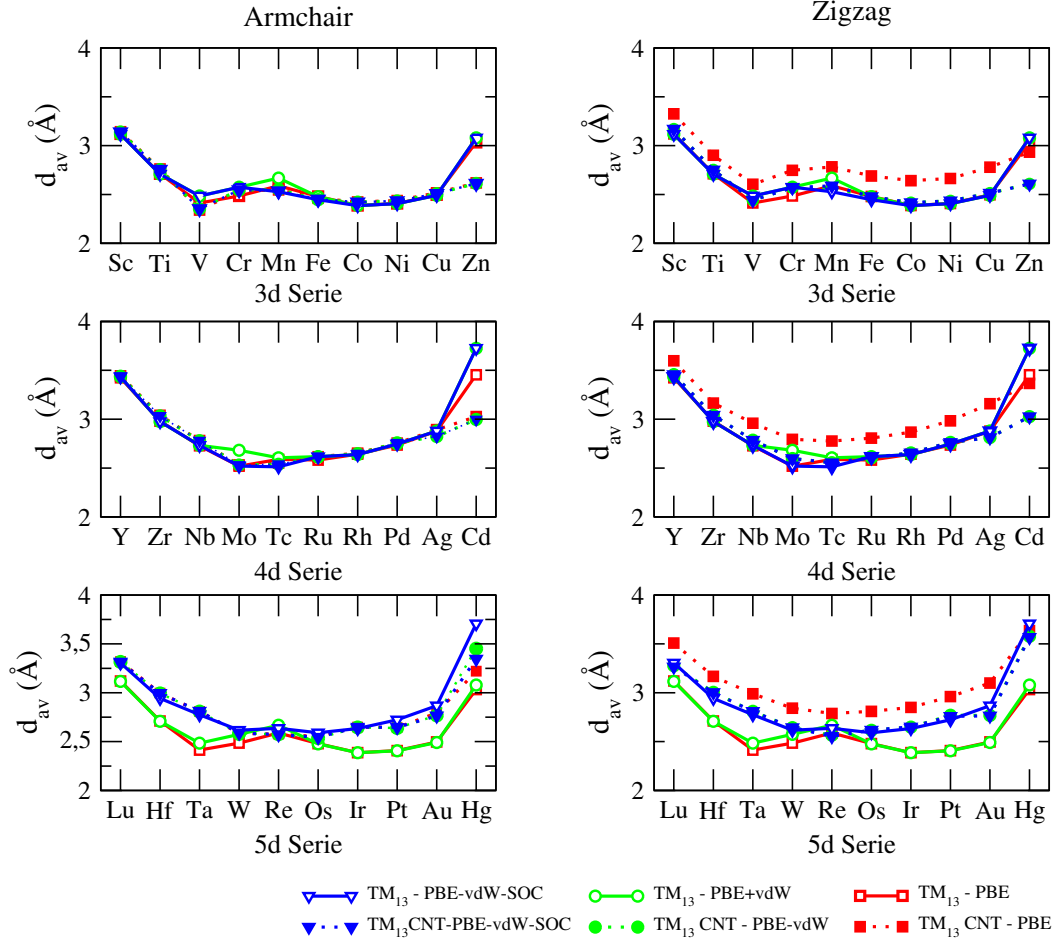


Figure 13: Average bond length, d_{av} , values for CNT fragments adhered to TM_{13} nanoclusters using three approaches, PBE, PBE-vdW, and PBE-vdW-SOC.

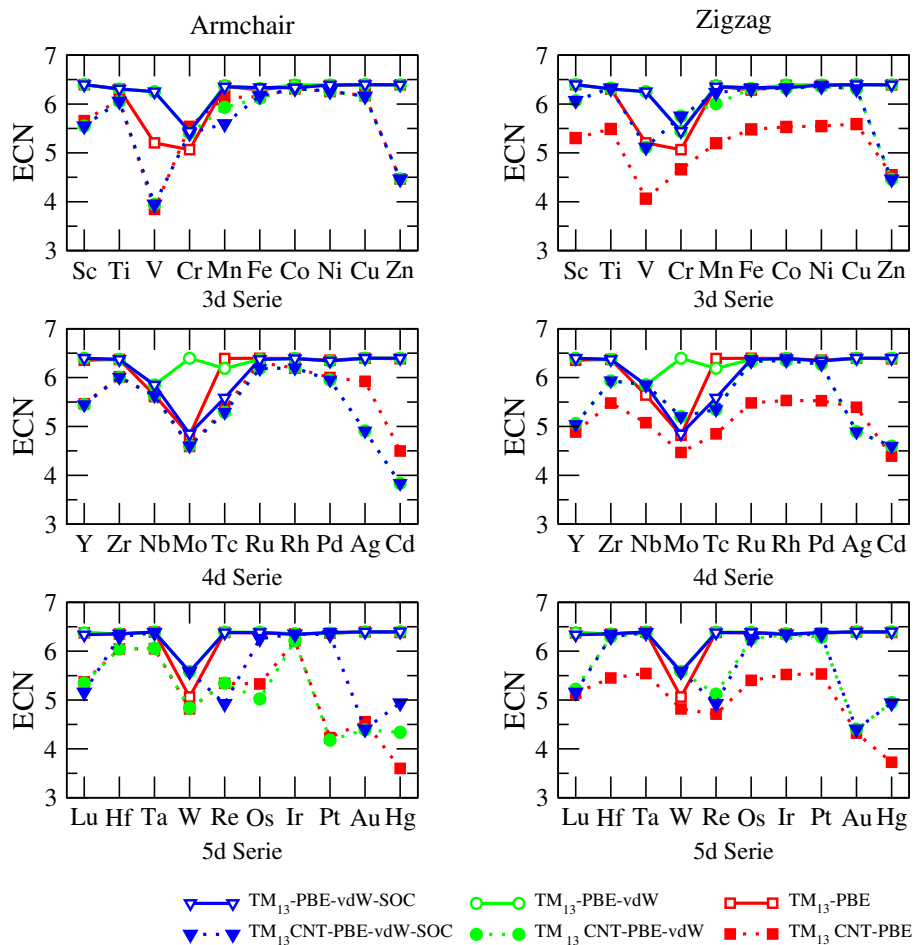


Figure 14: Effective Coordination Number, ECN, values for CNT fragments adhered to TM_{13} nanoclusters using three approaches, PBE, PBE-vdW, and PBE-vdW-SOC.

E Vibrational Frequencies

Table S1: 3d Series – 3N-6 vibrational frequencies for the 13-atom nanoclusters (cm^{-1}), obtained by VASP.

$\nu(\text{Sc}_{13})$	$\nu(\text{Ti}_{13})$	$\nu(\text{V}_{13})$	$\nu(\text{Cr}_{13})$	$\nu(\text{Mn}_{13})$	$\nu(\text{Fe}_{13})$	$\nu(\text{Co}_{13})$	$\nu(\text{Ni}_{13})$	$\nu(\text{Cu}_{13})$	$\nu(\text{Zn}_{13})$
257.54	316.67	476.15	314.43	316.10	345.67	339.88	371.09	280.62	86.98
256.90	315.66	464.68	313.18	253.02	298.64	321.84	364.41	280.47	85.21
256.36	286.36	358.98	246.79	243.08	291.26	316.61	363.34	279.92	82.74
202.96	261.93	342.97	198.46	232.11	258.13	286.51	265.09	214.59	82.33
202.49	260.49	314.31	198.13	225.52	258.13	240.48	232.20	188.30	63.01
202.16	257.52	308.48	196.17	221.23	232.48	228.91	230.62	188.18	61.98
201.85	256.20	293.39	187.60	197.07	232.48	214.16	223.25	187.73	60.44
201.68	217.13	280.50	185.31	193.72	224.29	208.47	219.16	187.58	47.92
201.48	216.71	278.71	171.67	186.06	208.92	205.67	218.70	187.36	47.34
183.94	212.31	276.18	171.32	181.31	200.17	183.83	184.57	157.35	47.02
182.96	211.99	271.97	169.69	175.03	184.59	174.77	180.45	157.13	46.61
182.83	196.20	271.48	163.74	172.06	181.09	169.44	176.56	156.66	46.24
181.90	186.59	260.02	163.43	168.06	166.65	168.82	175.52	152.71	31.77
181.31	184.48	259.79	160.45	154.67	163.16	158.52	169.31	152.55	31.52
180.81	173.20	213.76	159.42	150.03	156.11	156.25	168.20	152.36	30.78
180.61	171.55	193.87	157.00	148.93	153.37	155.16	165.03	152.08	29.83
150.56	167.09	191.45	143.72	144.31	148.51	141.99	162.21	129.01	28.70
150.32	165.98	178.30	143.30	136.96	144.15	120.63	158.09	128.82	26.89
150.07	164.90	175.30	133.25	130.75	134.51	113.39	156.51	128.15	26.06
149.56	164.37	168.79	124.96	126.33	132.74	97.77	145.42	120.89	25.19
149.19	160.57	163.64	124.29	118.35	126.75	95.63	141.42	120.78	23.72
148.85	158.89	162.78	120.34	113.97	120.80	86.12	132.58	120.23	22.56
148.38	139.96	138.94	119.60	108.10	106.75	82.71	129.64	119.87	21.37
145.34	138.63	127.41	109.22	105.59	103.67	75.36	118.42	119.68	20.70
144.61	138.25	93.20	105.68	96.44	50.72	67.32	116.37	118.74	18.73
144.29	135.93	91.08	104.89	93.32	41.15	60.11	111.12	118.51	12.27
143.96	117.50	89.02	102.44	74.53	35.74	27.77	98.73	118.23	10.62
143.51	116.08	80.00	101.39	53.62	30.57	19.20	97.140	117.42	8.78
117.53	115.66	78.73	89.31	47.70	26.14	16.59	92.00	87.48	6.41
117.05	113.23	58.26	88.70	37.14	11.23	13.77	82.07	87.46	1.87
116.58	81.12	54.80	81.55	30.08	9.44	4.29	80.72	86.69	4.32
115.88	79.82	10.14	77.82	14.77	12.39	14.07	73.18	86.35	5.11
115.28	21.84	7.57	77.05	48.57	38.17	22.28	21.15	85.66	8.69

Table S2: 4d Series – 3N-6 vibrational frequencies for the 13-atom nanoclusters (cm^{-1}), obtained by VASP.

$\nu(\text{Y}_{13})$	$\nu(\text{Zr}_{13})$	$\nu(\text{Nb}_{13})$	$\nu(\text{Mo}_{13})$	$\nu(\text{Tc}_{13})$	$\nu(\text{Ru}_{13})$	$\nu(\text{Rh}_{13})$	$\nu(\text{Pd}_{13})$	$\nu(\text{Ag}_{13})$	$\nu(\text{Cd}_{13})$
172.40	256.40	371.15	344.25	279.23	373.59	281.85	247.73	182.75	62.20
171.86	255.97	358.81	343.93	248.08	340.78	268.48	246.76	181.94	60.94
156.79	255.37	290.74	329.95	233.47	337.05	266.75	226.83	179.63	60.20
133.66	192.24	261.97	305.80	231.62	326.87	226.57	183.89	137.50	55.74
130.31	189.74	244.23	292.54	219.26	299.45	177.19	151.01	118.77	41.06
129.16	189.68	239.43	292.51	217.56	270.44	170.38	145.67	118.02	40.60
120.34	178.73	225.42	240.86	215.09	239.62	169.90	144.82	117.54	38.81
119.25	178.69	221.63	237.76	211.55	230.34	162.52	133.98	117.28	31.75
118.07	178.60	216.94	237.59	208.67	223.98	153.82	132.38	116.88	31.21
117.41	170.56	215.32	236.17	176.32	214.71	153.52	117.37	99.42	30.32
111.56	170.12	212.33	201.96	169.04	209.37	134.46	116.58	98.59	29.81
109.08	169.83	209.77	201.80	166.20	202.35	132.82	115.79	97.70	28.99
106.12	159.82	204.64	195.82	165.64	187.82	132.44	102.69	91.61	28.84
103.60	158.09	200.25	195.41	160.34	179.10	130.79	101.32	91.00	28.69
98.17	142.05	171.05	182.80	159.53	157.99	130.20	100.73	89.90	27.51
97.16	141.70	154.21	182.71	135.84	147.77	122.50	99.90	89.44	27.19
96.03	141.52	144.28	174.94	134.84	143.62	119.29	96.97	78.82	25.67
95.21	138.27	135.90	155.73	133.37	119.61	116.71	95.31	78.54	25.06
93.93	138.17	125.01	154.88	126.75	104.03	111.02	93.65	75.67	23.85
91.76	132.77	124.71	133.05	120.32	60.33	110.50	92.82	73.83	23.21
91.33	132.67	117.86	124.97	118.05	53.24	108.30	91.22	73.37	22.62
90.93	132.60	111.10	124.86	107.23	18.69	107.77	90.87	73.00	21.32
79.03	95.94	110.05	120.42	87.77	82.79	102.26	84.03	72.37	20.50
78.53	95.64	93.97	119.23	73.84	116.45	101.86	80.52	71.29	20.14
73.34	89.00	84.03	114.97	72.32	129.41	95.19	74.04	68.62	19.64
72.26	88.85	74.14	114.84	62.51	143.30	94.77	73.34	68.58	18.70
69.64	88.23	73.06	83.44	60.56	194.55	87.68	71.32	67.71	18.16
67.14	80.99	60.05	82.58	55.68	204.22	86.94	65.41	67.05	16.65
66.77	80.51	52.10	55.01	53.96	223.61	68.96	62.61	49.13	14.42
65.26	80.20	51.49	54.42	49.69	287.60	68.59	60.97	48.68	14.32
60.63	76.53	42.20	39.05	46.22	296.48	62.68	60.41	46.86	11.73
55.87	73.30	19.05	37.76	42.79	346.77	38.00	52.52	46.61	9.84
36.44	71.34	12.88	11.13	13.68	370.15	36.55	48.04	45.27	8.23

Table S3: 5d Series – 3N-6 vibrational frequencies for the 13-atom nanoclusters (cm^{-1}), obtained by VASP.

$\nu(\text{Lu}_{13})$	$\nu(\text{Hf}_{13})$	$\nu(\text{Ta}_{13})$	$\nu(\text{W}_{13})$	$\nu(\text{Re}_{13})$	$\nu(\text{Os}_{13})$	$\nu(\text{Ir}_{13})$	$\nu(\text{Pt}_{13})$	$\nu(\text{Au}_{13})$	$\nu(\text{Hg}_{13})$
147.60	205.54	264.30	259.07	226.65	273.45	253.54	228.60	163.65	39.18
130.54	183.59	263.06	249.58	212.15	272.79	243.61	225.16	163.36	34.49
123.67	150.52	258.42	234.91	203.87	255.75	229.83	224.90	162.95	33.80
101.55	145.52	189.35	229.21	203.56	227.99	200.97	168.31	127.31	32.11
96.62	135.15	168.97	220.55	178.05	167.86	153.29	129.59	104.38	30.94
95.16	131.95	167.68	213.22	168.76	167.76	144.50	123.74	103.47	30.41
93.63	124.75	164.13	189.04	168.01	167.43	143.09	123.37	103.42	30.09
90.62	121.16	153.72	180.72	162.24	166.75	137.42	113.17	102.19	29.64
89.88	114.75	152.79	178.57	161.40	163.06	134.60	112.82	101.71	28.77
83.48	111.90	149.82	170.32	138.64	152.31	132.87	103.88	82.68	26.46
82.00	107.07	135.53	165.63	130.40	149.16	131.80	103.50	82.26	26.00
80.39	106.31	130.87	165.51	129.43	148.51	122.25	100.99	81.35	25.11
75.93	103.98	128.77	143.66	118.48	140.32	121.20	88.74	78.10	23.30
72.44	100.44	118.25	138.82	115.38	139.60	120.84	88.36	75.74	21.59
70.76	96.74	116.26	132.42	114.94	135.58	120.12	85.17	75.21	20.53
67.49	94.25	114.83	125.74	114.80	135.10	119.69	82.81	74.49	18.04
65.79	93.55	108.55	123.93	113.68	128.04	115.61	82.53	65.10	16.80
61.34	87.24	108.07	121.18	113.28	111.46	112.87	81.94	64.55	15.25
57.89	85.59	107.23	119.92	101.81	108.23	97.76	81.18	63.27	14.83
56.43	81.20	102.09	115.62	63.53	107.61	96.43	80.47	61.98	14.30
54.45	80.21	99.67	109.16	62.18	79.59	93.74	76.61	61.69	12.63
50.02	78.11	94.07	105.78	62.00	78.77	92.98	76.44	60.92	10.87
36.57	75.92	92.64	99.62	56.07	57.85	90.78	73.56	59.89	7.86
25.81	69.29	89.18	94.77	53.86	56.91	79.53	73.30	58.57	4.72
22.96	68.68	87.55	91.34	47.99	52.19	75.15	72.40	55.65	3.25
20.10	61.41	79.13	89.76	6.26	50.00	73.74	71.76	54.52	3.54
12.10	56.92	72.41	81.85	4.21	49.53	72.92	67.53	49.71	8.37
5.74	47.40	72.07	80.21	2.03	48.58	71.52	65.09	48.50	9.76
4.46	40.56	71.31	41.54	1.77	44.75	61.00	64.68	43.61	11.96
14.14	3.36	70.64	34.91	3.11	30.84	59.76	59.18	40.68	16.02
20.25	1.05	69.59	20.75	5.11	28.52	56.43	57.20	36.90	17.17
37.63	0.76	58.57	7.28	35.49	21.20	50.72	54.62	34.14	18.09
52.07	5.16	44.22	6.26	40.38	16.22	50.28	53.77	32.86	19.68

F Coefficients of Linear Regression

Below, are provided the equations and coefficients for the linear regressions employed in Figure 5(b) for the data of the adhesion energy in relation to the center of gravity of the occupied d -states for the cases armchair and zigzag, respectively.

For $3d$ systems:

$$y = -2.3231 - (0.18311)x, \quad (1)$$

where the regression constant is given by -2.3231 , the regression coefficient is given by -0.18311 , and the correlation coefficient is -0.71889 .

$$y = -2.8253 - (0.22654)x, \quad (2)$$

where the regression constant is given by -2.8253 , the regression coefficient is given by -0.22654 , and the correlation coefficient is -0.72854 .

For $4d$ systems:

$$y = -2.5104 - (0.25748)x, \quad (3)$$

where the regression constant is given by -2.5104 , the regression coefficient is given by -0.25748 , and the correlation coefficient is -0.83333 .

$$y = -3.0913 - (0.30573)x, \quad (4)$$

where the regression constant is given by -3.0913 , the regression coefficient is given by -0.30573 , and the correlation coefficient is -0.85111 .

For $5d$ systems:

$$y = -3.4059 - (0.56161)x, \quad (5)$$

where the regression constant is given by -3.4059 , the regression coefficient is given by -0.56161 ,

and the correlation coefficient is -0.75884 .

$$y = -3.4651 - (0.46446)x, \quad (6)$$

where the regression constant is given by -3.4651 , the regression coefficient is given by -0.46446 , and the correlation coefficient is -0.795399 . And, where y represents the adhesion energy values, while x represents the values for the center of gravity of the occupied d -states.

G Atomic Positions

Below we provided the atomic positions (xyz coordinates) for the TM_{13} nanoclusters composed by all $3d$, $4d$, and $5d$ elements obtained by DFT-PBE as implemented in VASP.

13Sc	Ti 4.325710 2.815981 14.117537
Sc 15.573111 14.509049 45.215668	Ti 1.794512 4.006123 14.034704
Sc 15.032967 17.267918 46.663231	Ti 1.319422 5.202412 16.518650
Sc 17.893135 15.928914 46.829731	Ti 3.556709 4.752739 18.137171
Sc 13.879761 16.750488 43.763798	Ti 5.415524 3.277666 16.653826
Sc 18.508657 14.584298 44.033699	Ti 3.894035 5.280594 15.397282
Sc 16.026739 15.093502 42.138474	
Sc 16.829241 17.070650 44.258900	13V
Sc 18.625513 16.873375 41.854572	V 1.797556 1.222236 17.176781
Sc 15.765346 18.212387 41.688080	V 1.352398 3.118034 18.319431
Sc 15.149823 19.556992 44.484100	V 3.754176 2.290921 18.445799
Sc 17.631742 19.047789 46.379333	V 0.348659 2.976711 15.985495
Sc 19.778719 17.390800 44.754013	V 4.349717 1.295218 16.081388
Sc 18.085369 19.632250 43.302143	V 2.112471 1.745346 14.464012
	V 2.829241 3.070650 16.258900
	V 4.306083 3.023266 14.198380
13Ti	V 1.904304 3.850370 14.072011
Ti 1.764445 0.860696 17.120520	V 1.308764 4.846072 16.436420
Ti 1.332771 3.325319 18.400263	V 3.546009 4.395953 18.053799
Ti 3.863968 2.135168 18.483107	V 5.309819 3.164578 16.532316
Ti 0.242956 2.863634 15.863985	V 3.860926 4.919064 15.341030
Ti 4.339058 0.938878 15.999160	
Ti 2.101772 1.388562 14.380638	13Cr
Ti 2.829241 3.070650 16.258900	

Cr 1.741287 0.820800 17.136179
Cr 1.772523 3.019865 18.404276
Cr 3.870344 2.059238 18.474333
Cr 0.583408 2.519146 15.644621
Cr 3.854527 0.908670 16.210163
Cr 2.116882 1.320255 14.403274
Cr 2.829241 3.070650 16.258900
Cr 3.885958 3.121435 14.113536
Cr 1.788136 4.082050 14.043477
Cr 1.803953 5.232620 16.307648
Cr 3.541599 4.821035 18.114527
Cr 5.075071 3.622154 16.873192
Cr 3.917192 5.320499 15.381630

13Mn

Mn 1.826965 0.927728 17.062946
Mn 1.395539 3.250250 18.293571
Mn 3.808932 2.123114 18.351696
Mn 0.374510 2.800215 15.879389
Mn 4.198662 0.990378 16.081244
Mn 2.076768 1.407084 14.552559
Mn 2.829241 3.070650 16.258900
Mn 4.262941 2.891041 14.224237
Mn 1.849546 4.018174 14.166112
Mn 1.459818 5.150921 16.436565
Mn 3.581713 4.734205 17.965240
Mn 5.283969 3.341076 16.638420

Mn 3.831515 5.213573 15.454862

13Fe

Fe 1.876347 1.064895 17.036047
Fe 1.571284 3.199188 18.220362
Fe 3.737084 2.112564 18.275211
Fe 0.548517 2.911286 15.902571
Fe 4.152136 1.066619 16.083153
Fe 2.249460 1.494137 14.639601
Fe 2.829241 3.070650 16.258900
Fe 4.087196 2.942112 14.297450
Fe 1.921395 4.028726 14.242599
Fe 1.506344 5.074670 16.434656
Fe 3.409019 4.647153 17.878208
Fe 5.109963 3.230016 16.615229
Fe 3.782134 5.076404 15.481752

13Co

Co 1.918964 1.099601 17.020098
Co 1.503334 3.217010 18.136469
Co 3.688953 2.170536 18.192514
Co 0.559999 2.830956 15.938990
Co 4.084167 1.152292 16.071388
Co 2.173500 1.550488 14.660158
Co 2.829241 3.070650 16.258900
Co 4.155146 2.924281 14.381340
Co 1.969528 3.970753 14.325294

Co 1.574313 4.988999 16.446423
Co 3.484980 4.590800 17.857651
Co 5.098482 3.310334 16.578821
Co 3.739516 5.041699 15.497713

13Ni

Ni 1.870635 1.075781 17.003710
Ni 1.474660 3.218130 18.123793
Ni 3.702328 2.171648 18.199493
Ni 0.531368 2.825674 15.952351
Ni 4.127718 1.140551 16.077236
Ni 2.167068 1.532602 14.668083
Ni 2.829241 3.070650 16.258900
Ni 4.183821 2.923161 14.394016
Ni 1.956151 3.969643 14.318316
Ni 1.530762 5.000750 16.440565
Ni 3.491411 4.608688 17.849728
Ni 5.127111 3.315617 16.565460
Ni 3.787846 5.065508 15.514100

13Cu

Cu 1.843101 1.024241 17.052980
Cu 1.445873 3.233137 18.221291
Cu 3.735140 2.156727 18.291784
Cu 0.459051 2.819298 15.929066
Cu 4.161604 1.078519 16.044737
Cu 2.136553 1.488360 14.583416

Cu 2.829241 3.070650 16.258900
Cu 4.212606 2.908163 14.296520
Cu 1.923341 3.984564 14.226027
Cu 1.496877 5.062780 16.473064
Cu 3.521927 4.652929 17.934395
Cu 5.199429 3.322002 16.588734
Cu 3.815380 5.117058 15.464828

13Zn

Zn 15.613031 14.582300 45.220119
Zn 15.155750 17.277468 46.656151
Zn 17.930935 15.953722 46.717453
Zn 13.956667 16.755901 43.865921
Zn 18.457611 14.646111 44.012657
Zn 16.002718 15.153851 42.222565
Zn 16.829241 17.070650 44.258900
Zn 18.502729 16.863831 41.861649
Zn 15.727545 18.187569 41.800354
Zn 15.200870 19.495180 44.505154
Zn 17.655762 18.987440 46.295246
Zn 19.701813 17.385399 44.651894
Zn 18.045448 19.559000 43.297684

13Y

Y 15.401808 14.260170 45.357994
Y 14.870461 17.238934 46.901436
Y 18.024090 15.791150 47.102673

Y 13.553255 16.732788 43.702877
Y 18.615765 14.367111 44.092018
Y 15.847326 14.938393 41.977997
Y 16.829241 17.070650 44.258900
Y 18.788019 16.902357 41.616375
Y 15.634388 18.350140 41.415127
Y 15.042715 19.774189 44.425789
Y 17.811153 19.202898 46.539814
Y 20.105225 17.408510 44.814934
Y 18.256672 19.881119 43.159817

13Zr

Zr 15.726022 14.601047 45.235023
Zr 15.281343 17.238482 46.673374
Zr 17.982533 16.049944 46.685009
Zr 13.979683 16.765099 43.979790
Zr 18.478878 14.737920 43.982826
Zr 15.956647 15.118980 42.340508
Zr 16.829241 17.070650 44.258900
Zr 18.377136 16.902809 41.844425
Zr 15.675945 18.091356 41.832802
Zr 15.179603 19.403370 44.534985
Zr 17.701832 19.022308 46.177299
Zr 19.678799 17.376190 44.538025
Zr 17.932457 19.540243 43.282776

13Nb

Nb 1.955189 0.765452 17.177849
Nb 1.506698 3.414155 18.462234
Nb 3.947956 2.125410 18.661104
Nb 0.318036 2.794139 15.585135
Nb 4.204030 0.731161 16.113928
Nb 2.055499 1.217696 14.292299
Nb 2.829241 3.070650 16.258900
Nb 4.151781 2.727145 14.055577
Nb 1.710523 4.015890 13.856705
Nb 1.454451 5.410129 16.403881
Nb 3.602983 4.923594 18.225510
Nb 5.340445 3.347150 16.932674
Nb 3.703292 5.375838 15.339962

13Mo

Mo 1.583369 1.213589 17.496473
Mo 1.293741 3.268596 18.464220
Mo 3.828495 2.003983 18.519220
Mo 0.180972 2.739843 15.891587
Mo 4.696484 1.318437 16.120552
Mo 1.987694 1.864629 14.163525
Mo 2.829241 3.070650 16.258909
Mo 4.364739 2.872695 14.053591
Mo 1.829985 4.137316 13.998590
Mo 0.961997 4.822864 16.397259
Mo 3.670787 4.276670 18.354284
Mo 5.477508 3.401447 16.626223

Mo 4.075111 4.927702 15.021337

13Tc

Tc 1.785566 0.913878 16.964779

Tc 1.384734 3.144228 18.292597

Tc 3.785583 2.061313 18.330450

Tc 0.375665 2.762840 15.893310

Tc 4.211382 1.014741 15.952818

Tc 2.076378 1.484744 14.480581

Tc 2.829241 3.070650 16.258900

Tc 4.273746 2.997064 14.225204

Tc 1.872896 4.079988 14.187359

Tc 1.447098 5.126560 16.564993

Tc 3.582101 4.656558 18.037220

Tc 5.282815 3.378458 16.624502

Tc 3.872914 5.227413 15.553031

13Ru

Ru 1.810577 0.953741 17.078320

Ru 1.398935 3.236650 18.287939

Ru 3.766413 2.125834 18.361305

Ru 0.378717 2.809620 15.916809

Ru 4.209160 1.012414 16.035847

Ru 2.115694 1.435125 14.525001

Ru 2.829241 3.070650 16.258900

Ru 4.259544 2.904650 14.229872

Ru 1.892067 4.015467 14.156506

Ru 1.449320 5.128887 16.481964

Ru 3.542788 4.706165 17.992800

Ru 5.279762 3.331669 16.601002

Ru 3.847902 5.187550 15.439489

13Rh

Rh 1.770290 0.906867 17.096741

Rh 1.352438 3.241144 18.331333

Rh 3.803007 2.107885 18.410538

Rh 0.341344 2.807693 15.913357

Rh 4.254072 0.967326 16.034092

Rh 2.081480 1.396321 14.486344

Rh 2.829241 3.070650 16.258900

Rh 4.306042 2.900146 14.186476

Rh 1.855472 4.033403 14.107270

Rh 1.404407 5.173964 16.483707

Rh 3.577000 4.744968 18.031466

Rh 5.317137 3.333607 16.604454

Rh 3.888189 5.234434 15.421070

13Pd

Pd 1.802619 0.857786 17.100548

Pd 1.369305 3.271552 18.377987

Pd 3.851259 2.051017 18.535173

Pd 0.289368 2.819088 15.871176

Pd 4.316933 0.835297 16.023804

Pd 2.060909 1.299197 14.377547

Pd 2.829241 3.070650 16.258900
Pd 4.289175 2.869748 14.139823
Pd 1.807222 4.090283 13.982635
Pd 1.341547 5.305994 16.494005
Pd 3.597571 4.842103 18.140253
Pd 5.369113 3.322203 16.646624
Pd 3.855860 5.283502 15.417262

13Ag

Ag 1.693363 0.713115 17.177256
Ag 1.235139 3.258416 18.519484
Ag 3.874346 2.018173 18.603975
Ag 0.097535 2.780386 15.877230
Ag 4.365759 0.775149 16.011986
Ag 2.031623 1.246666 14.327800
Ag 2.829241 3.070650 16.258900
Ag 4.423341 2.882884 13.998325
Ag 1.784135 4.123127 13.913833
Ag 1.292720 5.366142 16.505823
Ag 3.626857 4.894634 18.190002
Ag 5.560946 3.360905 16.640572
Ag 3.965116 5.428173 15.340555

13Cd

Cd 15.491232 14.217154 45.362099
Cd 14.901931 17.310989 46.957932
Cd 18.067699 15.816149 47.098209

Cd 13.562712 16.723227 43.807278
Cd 18.671921 14.312493 43.965836
Cd 15.843655 14.896830 41.922211
Cd 16.829241 17.070650 44.258900
Cd 18.756550 16.830303 41.559875
Cd 15.590779 18.325142 41.419601
Cd 14.986558 19.828796 44.551964
Cd 17.814825 19.244469 46.595596
Cd 20.095766 17.418064 44.710533
Cd 18.167248 19.924137 43.155701

13Lu

Lu 15.509009 14.334886 45.325592
Lu 15.028469 17.307636 46.903816
Lu 18.017714 15.888572 46.996841
Lu 13.664433 16.725458 43.809113
Lu 18.612816 14.408911 43.953571
Lu 15.935969 14.991356 41.982361
Lu 16.829241 17.070650 44.258900
Lu 18.630011 16.833654 41.613983
Lu 15.640767 18.252720 41.520966
Lu 15.045666 19.732380 44.564240
Lu 17.722507 19.149944 46.535446
Lu 19.994038 17.415831 44.708694
Lu 18.149471 19.806406 43.192219

13Hf

Hf 1.751569 0.616608 17.193586
Hf 1.185114 3.250811 18.620527
Hf 3.910840 1.997761 18.638565
Hf 0.039526 2.795283 15.833562
Hf 4.426395 0.747033 16.028690
Hf 1.961253 1.190651 14.309428
Hf 2.829241 3.070650 16.258900
Hf 4.473366 2.890479 13.897281
Hf 1.747640 4.143528 13.879242
Hf 1.232084 5.394256 16.489107
Hf 3.697227 4.950638 18.208382
Hf 5.618955 3.346006 16.684248
Hf 3.906913 5.524692 15.324223

13Ta

Ta 1.749016 0.792551 17.153765
Ta 1.306735 3.218107 18.443558
Ta 3.852903 2.056203 18.509163
Ta 0.196890 2.784676 15.888012
Ta 4.341715 0.874627 16.022974
Ta 2.055807 1.334013 14.377567
Ta 2.829241 3.070650 16.258900
Ta 4.351747 2.923183 14.074252
Ta 1.805576 4.085098 14.008636
Ta 1.316763 5.266664 16.494839
Ta 3.602672 4.807287 18.140244
Ta 5.461590 3.356624 16.629797

Ta 3.909464 5.348740 15.364045

13W

W 1.763111 0.844016 16.596569
W 1.183544 3.678853 18.184534
W 4.239252 2.256481 18.299009
W 0.140382 2.790166 15.915057
W 4.350499 0.827278 16.071877
W 2.137804 1.442969 14.252605
W 2.829241 3.070650 16.258900
W 4.474936 2.462438 14.333277
W 1.419228 3.884820 14.218801
W 1.307981 5.314011 16.445934
W 3.520675 4.698332 18.265194
W 5.518097 3.351125 16.602753
W 3.895370 5.297272 15.921241

13Re

Re 1.772691 0.932615 17.085619
Re 1.355021 3.197802 18.303844
Re 3.770651 2.098066 18.389643
Re 0.341689 2.786467 15.937973
Re 4.242039 0.993005 16.016602
Re 2.103903 1.418452 14.493593
Re 2.829241 3.070650 16.258900
Re 4.303459 2.943489 14.213965
Re 1.887829 4.043234 14.128167

Re 1.416441 5.148285 16.501209
Re 3.554577 4.722847 18.024218
Re 5.316792 3.354834 16.579836
Re 3.885790 5.208685 15.432191

13Os

Os 1.799990 0.919783 16.980900
Os 1.373044 3.175949 18.277294
Os 3.781340 2.047562 18.353119
Os 0.375686 2.791582 15.932438
Os 4.217699 1.027874 15.934926
Os 2.132528 1.466787 14.485730
Os 2.829241 3.070650 16.258900
Os 4.285435 2.965351 14.240506
Os 1.877141 4.093729 14.164690
Os 1.440782 5.113426 16.582884
Os 3.525953 4.674513 18.032080
Os 5.282795 3.349709 16.585373
Os 3.858490 5.221506 15.536909

13Ir

Ir 1.743530 0.910083 17.081564
Ir 1.398579 3.253578 18.323902
Ir 3.781206 2.120880 18.447672
Ir 0.315235 2.763302 15.927875
Ir 4.248970 0.947266 15.988401
Ir 2.129288 1.423766 14.485948

Ir 2.829241 3.070650 16.258909
Ir 4.259901 2.887722 14.193896
Ir 1.877274 4.020420 14.070139
Ir 1.409510 5.194035 16.529409
Ir 3.529194 4.717533 18.031864
Ir 5.343245 3.377989 16.589926
Ir 3.914949 5.231218 15.436245

13Pt

Pt 1.741196 0.797160 17.151423
Pt 1.282700 3.250320 18.433996
Pt 3.779924 2.073374 18.434095
Pt 0.288773 2.805815 15.936985
Pt 4.303999 0.853759 16.012568
Pt 2.111660 1.359308 14.474168
Pt 2.829241 3.070650 16.258900
Pt 4.375780 2.890980 14.083816
Pt 1.878556 4.067915 14.083715
Pt 1.354481 5.287542 16.505243
Pt 3.546822 4.781992 18.043633
Pt 5.369707 3.335485 16.580824
Pt 3.917284 5.344130 15.366386

13Au

Au 1.695486 0.718107 17.174358
Au 1.238760 3.258039 18.514912
Au 3.871570 2.020387 18.598520

Au 0.103180 2.781791 15.878147	Hg 14.785282 17.278782 47.135361
Au 4.362361 0.780302 16.012331	Hg 18.066395 15.692934 47.243172
Au 2.032915 1.250703 14.332340	Hg 13.360032 16.667980 43.717964
Au 2.829241 3.070650 16.258900	Hg 18.839947 14.204887 43.964565
Au 4.419720 2.883252 14.002897	Hg 15.880189 14.746624 41.795990
Au 1.786909 4.120901 13.919290	Hg 16.829241 17.070650 44.258900
Au 1.296120 5.360989 16.505482	Hg 18.873198 16.862509 41.382446
Au 3.625564 4.890585 18.185457	Hg 15.592085 18.448357 41.274643
Au 5.555298 3.359500 16.639662	Hg 14.818533 19.936413 44.553246
Au 3.962994 5.423183 15.343442	Hg 17.778292 19.394667 46.721825
	Hg 20.298447 17.473320 44.799835
13Hg	Hg 18.285179 20.078024 43.147881
Hg 15.373301 14.063266 45.369926	

Here, we provided the atomic positions (xyz coordinates) of the five-layered hydrogen-terminated fragment for the (3,3) armchair CNT and tree-layered hydrogen terminated fragment for the (5,0) zigzag CNT.

6H60C	C 11.965842 14.823107 23.031551
H 12.990671 16.482792 22.150349	C 12.964539 12.049039 23.035122
H 11.377527 14.559064 22.151907	C 14.296043 11.816928 23.032227
H 15.811480 16.000870 22.155907	C 15.019041 15.785959 24.245264
H 16.664545 13.638066 22.149296	C 13.654816 16.025560 24.244669
H 14.816623 11.433596 22.153572	C 11.946513 13.987636 24.245405
H 12.342887 11.864201 22.158146	C 12.414574 12.683718 24.246574
C 16.197315 14.083983 23.028267	C 15.033370 12.228002 24.241488
C 15.739350 15.355471 23.032410	C 15.925013 13.288244 24.239681
C 12.834482 15.858871 23.031147	C 12.958774 15.802435 25.509983

C 12.039211 14.713631 25.510063
C 12.958396 12.195615 25.511845
C 14.361697 11.945552 25.509199
C 16.081467 13.999550 25.507187
C 15.598701 15.340347 25.509975
C 11.875502 14.003374 26.740860
C 12.375134 12.634405 26.741991
C 15.059645 12.158177 26.738895
C 15.996448 13.273837 26.737391
C 15.064188 15.836010 26.740408
C 13.629377 16.089867 26.739864
C 12.951131 12.179621 27.965929
C 14.363729 11.928532 27.964392
C 16.104124 13.999462 27.962151
C 15.612400 15.347111 27.964077
C 12.947440 15.821337 27.964439
C 12.024780 14.722836 27.965065
C 15.042103 12.206024 29.213902
C 15.951624 13.282764 29.212879
C 15.031639 15.796198 29.213131
C 13.644950 16.044909 29.214485
C 11.929921 13.997780 29.215483
C 12.409157 12.673388 29.215763
C 16.087456 14.000046 30.466311
C 15.604367 15.342879 30.466034
C 12.955603 15.809819 30.467752
C 12.031910 14.721813 30.468777

C 12.958300 12.194541 30.468481
C 14.362204 11.939629 30.467365
C 15.068205 15.839485 31.697477
C 13.631250 16.091640 31.699409
C 11.870314 14.009599 31.700096
C 12.373087 12.639159 31.699368
C 15.058787 12.155328 31.698448
C 15.995335 13.273579 31.698280
C 12.892574 15.868074 32.940254
C 11.967019 14.778214 32.941734
C 12.936307 12.111248 32.939430
C 14.344888 11.853176 32.939610
C 16.169798 14.025865 32.938042
C 15.687441 15.373191 32.938465
C 11.874907 13.887639 34.035690
C 12.279797 12.711883 34.041176
C 15.160780 12.223937 34.031120
C 15.986185 13.154640 34.040798
C 14.957137 15.889886 34.031219
C 13.740182 16.146866 34.042328

60C5H

H 12.308657 15.218826 34.236565
H 14.619741 15.920985 34.252598
H 16.046104 13.970243 34.252026
H 12.317490 12.802344 34.232544
H 14.622478 12.020251 34.241112

C 15.476085 13.557748 21.892653
C 15.173874 14.846399 22.392008
C 14.045584 15.546910 21.896261
C 13.199739 16.306187 22.685364
C 12.606986 15.340456 21.792526
C 12.134322 14.105618 22.426807
C 12.521301 12.933456 21.796650
C 13.498232 12.177697 22.421911
C 14.822956 12.250509 21.802063
C 15.922740 12.516397 22.686781
C 15.491716 15.075755 23.835951
C 14.631948 15.970232 24.630581
C 13.293814 16.203629 24.053934
C 12.301275 15.323949 24.676132
C 12.065317 14.111676 23.876152
C 12.485022 12.902663 24.578049
C 13.483635 12.105588 23.871828
C 14.712472 11.970904 24.675518
C 15.852235 12.638285 24.057665
C 16.063469 13.974756 24.634140
C 14.661940 15.953660 26.041895
C 13.387817 16.002209 26.779751
C 12.341755 15.255700 26.067022
C 11.995646 14.026507 26.756886
C 12.426699 12.863412 26.004618
C 13.386462 12.081889 26.762136
C 14.659212 12.034136 26.069868

C 15.695055 12.786779 26.782581
C 16.055717 14.009071 26.044453
C 15.648654 15.189219 26.771780
C 13.385205 15.983572 28.175634
C 12.362549 15.216206 28.889875
C 11.968488 14.015409 28.162954
C 12.354555 12.815924 28.888700
C 13.368667 12.063747 28.167238
C 14.632181 12.059037 28.895681
C 15.680663 12.787852 28.179167
C 16.048822 13.997813 28.907326
C 15.661220 15.196602 28.181757
C 14.648076 15.941541 28.905760
C 12.343300 15.220798 30.294695
C 11.980351 14.011977 31.015491
C 12.331176 12.800467 30.292553
C 13.370361 12.090502 31.020828
C 14.630703 12.043246 30.299532
C 15.636142 12.800004 31.030943
C 16.063412 13.991625 30.311844
C 15.630648 15.168930 31.037195
C 14.648252 15.950805 30.312002
C 13.384755 15.921289 31.028625
C 11.943686 14.009513 32.438950
C 12.377751 12.841606 33.143414
C 13.356668 12.063611 32.445671
C 14.603286 12.093225 33.152634

C 15.650836 12.778042 32.452202
C 15.985817 13.974762 33.162334
C 15.647322 15.179199 32.464565
C 14.607810 15.869560 33.162445

C 13.368615 15.940743 32.453167
C 12.372539 15.178343 33.147999

Below, we provided the atomic positions of the lowest energy configurations for the armchair CNT fragment (3,3) and the zigzag (5,0) CNT fragment, respectively, adhered to *3d*, *4d*, and *5d* TM₁₃ nanoclusters.

06H60C13Sc
H 13.191867 16.320583 20.528164
H 11.611984 14.396585 20.516582
H 15.886662 15.910986 20.647249
H 16.762318 13.579559 20.725973
H 15.027840 11.469974 20.706676
H 12.568402 11.854147 20.610130
C 16.315514 14.047696 21.604389
C 15.838265 15.316477 21.560890
C 12.969087 15.764930 21.440407
C 12.108794 14.715702 21.433968
C 13.130835 12.004334 21.532890
C 14.470174 11.795811 21.586111
C 15.108416 15.796164 22.738890
C 13.713587 16.015289 22.679585
C 12.004207 13.927759 22.666039
C 12.503823 12.605762 22.714140
C 15.162198 12.185810 22.818485

C 16.057259 13.278776 22.826742
C 12.973395 15.815771 23.896372
C 12.048988 14.684027 23.888084
C 13.007337 12.151071 23.980837
C 14.447766 11.920500 24.038292
C 16.164364 14.020422 24.054588
C 15.647511 15.386300 24.006725
C 11.895030 13.994111 25.122101
C 12.403108 12.641319 25.172018
C 15.076506 12.212186 25.279301
C 15.992777 13.333076 25.287449
C 15.035877 15.865809 25.197721
C 13.608342 16.093794 25.138575
C 12.930799 12.218128 26.443920
C 14.338780 11.998966 26.497726
C 16.040854 14.083449 26.514538
C 15.544326 15.418652 26.469496
C 12.892772 15.839427 26.362736

C 11.990579 14.733832 26.354053
C 14.975712 12.272237 27.760176
C 15.890752 13.389688 27.768419
C 14.953136 15.929310 27.680511
C 13.527118 16.144039 27.619434
C 11.806997 14.038992 27.601519
C 12.301592 12.683985 27.653992
C 15.987068 14.135424 28.979998
C 15.490296 15.514331 28.938889
C 12.800022 15.913227 28.824686
C 11.875674 14.784466 28.815187
C 12.802653 12.226464 28.912607
C 14.253439 12.015323 28.962948
C 14.862117 15.983011 30.134876
C 13.446260 16.171377 30.072618
C 11.741599 14.087297 30.055403
C 12.208122 12.736955 30.109285
C 14.881122 12.336389 30.203072
C 15.788780 13.444157 30.211969
C 12.712790 15.956312 31.321617
C 11.799061 14.835176 31.313982
C 12.722798 12.313711 31.425026
C 14.157814 12.094848 31.456463
C 15.873744 14.190651 31.472584
C 15.370975 15.552114 31.449482
C 11.418829 14.100119 32.506817
C 11.967016 12.734324 32.621292

C 14.936761 12.212025 32.685551
C 15.902188 13.395258 32.695286
C 14.793082 16.198650 32.645641
C 13.349458 16.466120 32.522911
Sc 13.742668 14.171497 32.670815
Sc 14.199947 13.786643 35.911133
Sc 16.301378 12.075888 34.319683
Sc 11.354540 13.684862 34.524124
Sc 16.423267 15.214125 33.836372
Sc 13.722794 16.586641 34.546478
Sc 13.251122 11.323933 33.805828
Sc 14.414525 13.560678 38.826843
Sc 15.256590 16.151663 37.379520
Sc 12.243767 15.319023 37.480606
Sc 12.074134 12.220718 37.313721
Sc 14.986902 11.108320 36.950340
Sc 16.961044 13.542846 36.970440

06H60C13Ti

H 13.095462 16.382835 20.597153
H 11.538610 14.432076 20.581211
H 15.806587 15.965158 20.672091
H 16.699896 13.636494 20.727089
H 14.985029 11.481683 20.721828
H 12.519478 11.860603 20.651199
C 16.254332 14.096242 21.610268
C 15.768967 15.362111 21.580431

C 12.896040 15.804340 21.500359
C 12.051079 14.744952 21.492105
C 13.095350 12.025046 21.563017
C 14.434723 11.818760 21.601503
C 15.048158 15.826973 22.772449
C 13.655929 16.038710 22.735355
C 11.976019 13.941445 22.719395
C 12.481280 12.627973 22.752689
C 15.134417 12.219816 22.827089
C 16.014212 13.319778 22.831833
C 12.930631 15.823352 23.961950
C 12.016322 14.686702 23.953184
C 12.994460 12.163626 24.016838
C 14.432816 11.944812 24.055229
C 16.129368 14.055902 24.065910
C 15.605596 15.413307 24.035122
C 11.870629 13.987588 25.181969
C 12.390720 12.634885 25.216581
C 15.073543 12.228316 25.290258
C 15.984279 13.356922 25.295832
C 15.008983 15.886764 25.237654
C 13.575967 16.101599 25.197876
C 12.938233 12.212099 26.476501
C 14.346904 12.003756 26.509602
C 16.037510 14.098604 26.523396
C 15.532917 15.430554 26.496727
C 12.878340 15.826859 26.426638

C 11.981771 14.717944 26.418446
C 14.992670 12.279822 27.767771
C 15.894241 13.393575 27.774031
C 14.947098 15.920132 27.724167
C 13.524424 16.123779 27.681747
C 11.819819 14.015590 27.667675
C 12.323090 12.669108 27.703964
C 16.014492 14.127592 28.996746
C 15.503177 15.504211 28.975317
C 12.807042 15.892912 28.896393
C 11.887225 14.757446 28.888584
C 12.836849 12.201373 28.954817
C 14.289824 11.995399 28.982944
C 14.884820 15.960540 30.178675
C 13.466932 16.157728 30.132338
C 11.762450 14.047022 30.119064
C 12.253128 12.701727 30.158726
C 14.940790 12.304793 30.204454
C 15.839804 13.415878 30.210766
C 12.762609 15.899289 31.384916
C 11.860397 14.781770 31.378292
C 12.809769 12.299534 31.459974
C 14.233560 12.074471 31.471090
C 15.905836 14.145950 31.483263
C 15.387730 15.491327 31.479982
C 11.562357 14.073605 32.598610
C 12.125557 12.724745 32.697205

C 14.974388 12.176579 32.715881
C 15.955291 13.391826 32.722828
C 14.820268 16.062649 32.717281
C 13.385090 16.332687 32.612118
Ti 13.865318 14.077327 32.648533
Ti 14.188697 13.799895 35.549034
Ti 16.150644 12.220382 34.397301
Ti 11.658882 13.763341 34.560524
Ti 16.158651 15.075050 34.153645
Ti 13.698924 16.287315 34.576103
Ti 13.362850 11.615369 34.135193
Ti 14.392360 13.619558 38.144264
Ti 15.180861 15.847330 36.807266
Ti 12.540229 15.125280 37.038971
Ti 12.387641 12.392143 36.785435
Ti 14.845847 11.454531 36.576637
Ti 16.613823 13.640831 36.590691

06H60C13V

H 13.164381 16.395079 20.610010
H 11.580785 14.464306 20.573292
H 15.880121 15.946904 20.711866
H 16.753483 13.606876 20.768673
H 15.002123 11.472014 20.736668
H 12.538587 11.877611 20.647509
C 16.297663 14.069015 21.645483
C 15.824042 15.337563 21.614948

C 12.954438 15.811623 21.507498
C 12.095418 14.763758 21.487415
C 13.111012 12.033753 21.562908
C 14.447035 11.813699 21.611544
C 15.092829 15.804448 22.802120
C 13.706493 16.031248 22.749945
C 12.004025 13.956758 22.711926
C 12.496420 12.640933 22.749992
C 15.139807 12.203856 22.846937
C 16.030157 13.292361 22.863523
C 12.963186 15.824445 23.970169
C 12.041187 14.698524 23.948711
C 12.993118 12.165485 24.019529
C 14.427644 11.930029 24.071482
C 16.142704 14.022583 24.103466
C 15.632668 15.384930 24.072050
C 11.874160 13.997159 25.174068
C 12.385147 12.638868 25.214029
C 15.063877 12.200768 25.313601
C 15.983311 13.323329 25.330288
C 15.027495 15.864003 25.267567
C 13.595729 16.098434 25.213268
C 12.921784 12.212608 26.477966
C 14.326681 11.985080 26.528631
C 16.030876 14.065961 26.559336
C 15.530380 15.398488 26.530268
C 12.880571 15.826482 26.430935

C 11.979581 14.725537 26.408607
C 14.967853 12.253256 27.795797
C 15.874997 13.360779 27.810074
C 14.931138 15.886207 27.754265
C 13.514174 16.111057 27.700787
C 11.801979 14.022203 27.659004
C 12.307507 12.680955 27.699476
C 15.989264 14.091366 29.037399
C 15.471495 15.468017 29.011719
C 12.772719 15.898546 28.905470
C 11.837962 14.766866 28.878777
C 12.805842 12.208101 28.956293
C 14.255473 11.975717 29.008942
C 14.836469 15.931067 30.201286
C 13.420661 16.153904 30.148603
C 11.697053 14.050819 30.097462
C 12.206209 12.713585 30.142897
C 14.902036 12.264626 30.239895
C 15.814951 13.372745 30.245796
C 12.702787 15.880610 31.395054
C 11.802285 14.766827 31.364407
C 12.751340 12.321413 31.445324
C 14.159689 12.062576 31.494221
C 15.828050 14.101031 31.514833
C 15.301160 15.440186 31.503372
C 11.521220 14.072337 32.594955
C 12.083357 12.726444 32.703407

C 14.799680 12.224547 32.806042
C 15.788168 13.370944 32.784023
C 14.729496 16.012186 32.750290
C 13.289440 16.276724 32.657639
V 13.767209 14.066308 32.587643
V 14.326096 13.862437 35.271702
V 16.047405 12.187685 34.513535
V 11.889297 14.352722 34.522064
V 15.916355 14.946221 34.018955
V 13.402624 16.021832 34.606293
V 13.264162 12.080000 34.295719
V 14.726648 13.352960 37.851768
V 15.578528 15.401829 36.718582
V 12.780065 14.810887 36.942627
V 12.472607 12.877062 36.552208
V 15.043249 11.824986 36.679729
V 16.702385 13.864908 36.295433

06H60C13Cr

H 13.018420 16.405535 20.618141
H 11.404248 14.492175 20.647053
H 15.770434 15.896827 20.620560
H 16.623802 13.544848 20.656574
H 14.809675 11.408411 20.690893
H 12.349171 11.860942 20.684568
C 16.186226 14.010459 21.540915
C 15.723852 15.282953 21.521290

C 12.844851 15.813309 21.517820
C 11.971625 14.778711 21.533890
C 12.960519 12.023899 21.573320
C 14.291895 11.779578 21.576721
C 15.028820 15.753049 22.729416
C 13.654688 16.008564 22.729382
C 11.930946 13.968822 22.760870
C 12.403454 12.654967 22.778833
C 15.033170 12.173594 22.784866
C 15.937758 13.238113 22.768307
C 12.955513 15.815375 23.985157
C 12.023520 14.713782 24.003111
C 12.938086 12.174922 24.038977
C 14.357796 11.914071 24.042774
C 16.102303 13.970312 24.011152
C 15.608765 15.327506 23.988752
C 11.876499 14.019545 25.237825
C 12.371001 12.651073 25.254753
C 15.050424 12.160322 25.262262
C 15.989688 13.271640 25.246422
C 15.065294 15.833655 25.204521
C 13.634922 16.094959 25.204845
C 12.948854 12.217162 26.491230
C 14.352507 11.961556 26.497326
C 16.087822 14.017633 26.467619
C 15.604996 15.360594 26.444910
C 12.958218 15.839496 26.443420

C 12.035847 14.750354 26.460592
C 15.037869 12.231300 27.744385
C 15.953070 13.322613 27.728743
C 15.047933 15.850078 27.686401
C 13.648160 16.100323 27.689373
C 11.916421 14.047981 27.721163
C 12.395264 12.707312 27.733353
C 16.105488 14.057387 28.953979
C 15.625581 15.418015 28.930220
C 12.955988 15.891011 28.934938
C 12.023938 14.784893 28.950977
C 12.933895 12.226063 28.973494
C 14.361621 11.976305 28.984432
C 15.082801 15.931454 30.149729
C 13.639221 16.175552 30.156612
C 11.874327 14.079306 30.185318
C 12.350126 12.696063 30.188282
C 15.063434 12.224986 30.209774
C 16.001162 13.346230 30.195066
C 12.965841 15.901156 31.400021
C 12.043066 14.805984 31.416460
C 12.938798 12.260036 31.418259
C 14.350662 12.028056 31.438835
C 16.104612 14.101411 31.407358
C 15.630571 15.446628 31.379166
C 11.897662 14.081509 32.686199
C 12.406347 12.749740 32.688007

C 14.991005 12.343554 32.720783
C 15.939578 13.420835 32.694675
C 15.069515 15.909220 32.655960
C 13.674082 16.179554 32.656536
Cr 13.943037 14.163489 33.322758
Cr 13.976585 13.849195 35.474449
Cr 15.916773 12.789088 34.620911
Cr 11.749464 14.415063 34.672821
Cr 15.969891 15.267657 34.374565
Cr 13.116735 16.207075 34.602184
Cr 13.386453 11.844988 34.234535
Cr 13.863064 13.247403 37.806618
Cr 14.768005 15.864383 36.511963
Cr 12.400272 15.213457 37.118423
Cr 12.001287 12.389649 36.303192
Cr 14.722652 11.424097 36.436035
Cr 16.252134 13.841182 36.823978

06H60C13Mn

H 13.024093 16.462603 20.628256
H 11.428503 14.526900 20.611370
H 15.815951 15.981634 20.668030
H 16.698322 13.638010 20.692308
H 14.895454 11.449054 20.674088
H 12.426763 11.878248 20.632828
C 16.227295 14.085511 21.568914
C 15.750693 15.351555 21.556379

C 12.852648 15.846855 21.512463
C 11.992895 14.803037 21.503395
C 13.026845 12.050809 21.527514
C 14.359464 11.818866 21.549486
C 15.021634 15.794305 22.756657
C 13.650372 16.026995 22.737562
C 11.956099 13.973781 22.719923
C 12.446468 12.671823 22.730392
C 15.075191 12.219228 22.773010
C 15.958984 13.295006 22.781195
C 12.936009 15.811472 23.988878
C 12.022138 14.703574 23.979095
C 12.965275 12.182247 23.999527
C 14.382539 11.940575 24.021608
C 16.093061 14.016155 24.036831
C 15.588532 15.360312 24.025257
C 11.854165 13.994788 25.205542
C 12.369064 12.630956 25.214273
C 15.056759 12.174438 25.254772
C 15.984953 13.297016 25.262642
C 15.028775 15.849668 25.241505
C 13.591783 16.093981 25.223843
C 12.933145 12.192487 26.454231
C 14.342823 11.952071 26.475426
C 16.063019 14.028360 26.488544
C 15.560412 15.366214 26.477173
C 12.899691 15.815261 26.445866

C 11.987354 14.715181 26.436274
C 15.006243 12.223356 27.731735
C 15.910996 13.313918 27.738678
C 14.971844 15.822508 27.719501
C 13.575671 16.057066 27.707235
C 11.863480 13.999315 27.692207
C 12.363249 12.672893 27.696165
C 16.043236 14.034794 28.979073
C 15.542875 15.385462 28.967499
C 12.871330 15.835920 28.947845
C 11.949558 14.724895 28.938168
C 12.893800 12.188527 28.944864
C 14.312271 11.954893 28.967918
C 14.986264 15.889740 30.184547
C 13.541070 16.122971 30.176294
C 11.792857 14.010854 30.165226
C 12.285652 12.631393 30.164349
C 15.001786 12.182002 30.205460
C 15.939296 13.307482 30.208633
C 12.852367 15.847309 31.408813
C 11.943108 14.737951 31.398861
C 12.862773 12.171864 31.384529
C 14.275188 11.953513 31.416683
C 16.024998 14.053919 31.426258
C 15.525646 15.396802 31.413319
C 11.843534 13.992867 32.650818
C 12.345597 12.678230 32.661037

C 14.877749 12.293300 32.717083
C 15.828296 13.370042 32.706966
C 14.938873 15.841187 32.688232
C 13.543262 16.139154 32.665222
Mn 13.896408 14.075190 33.219982
Mn 14.130120 13.985353 35.658009
Mn 15.983633 12.431787 34.494038
Mn 11.817383 14.251982 34.611416
Mn 16.020185 15.037606 34.249222
Mn 13.468062 16.107973 34.618790
Mn 13.358850 11.924219 34.271385
Mn 14.260508 13.778491 37.838158
Mn 15.154952 15.851145 36.576050
Mn 12.608778 15.396774 36.913467
Mn 12.149373 12.820354 36.764374
Mn 14.680279 11.766401 36.602776
Mn 16.491426 13.739625 36.654053

06H60C13Fe

H 13.107695 16.492954 20.661455
H 11.424817 14.639355 20.656488
H 15.846415 15.898506 20.659376
H 16.608953 13.513314 20.656500
H 14.729755 11.431664 20.655367
H 12.281305 11.958986 20.653908
C 16.188841 13.982007 21.547709
C 15.776261 15.271142 21.549158

C 12.914293 15.890392 21.550102
C 12.004344 14.888133 21.546703
C 12.899044 12.095951 21.542713
C 14.222175 11.810678 21.543644
C 15.094939 15.742065 22.764853
C 13.730701 16.035458 22.765182
C 11.935863 14.057784 22.759418
C 12.360426 12.728917 22.757761
C 14.970762 12.166700 22.760359
C 15.908469 13.199765 22.761734
C 13.024831 15.841556 24.019535
C 12.055534 14.776730 24.016632
C 12.875261 12.210514 24.013088
C 14.285427 11.907269 24.014399
C 16.096710 13.904762 24.018528
C 15.658674 15.277011 24.019831
C 11.875339 14.068569 25.239559
C 12.319868 12.682380 25.235992
C 14.982903 12.110923 25.238422
C 15.963614 13.186906 25.241896
C 15.133269 15.780115 25.245033
C 13.709725 16.084068 25.244892
C 12.879677 12.211870 26.467607
C 14.275945 11.914318 26.469051
C 16.090302 13.905766 26.474113
C 15.655526 15.265290 26.474226
C 13.020909 15.829185 26.473629

C 12.059132 14.774834 26.472286
C 14.966823 12.141045 27.719011
C 15.925406 13.193552 27.724827
C 15.105314 15.745214 27.724556
C 13.717912 16.039352 27.724726
C 11.907218 14.058852 27.722887
C 12.339204 12.701320 27.716661
C 16.097269 13.899050 28.964331
C 15.661090 15.275135 28.965015
C 13.014777 15.839844 28.963926
C 12.042260 14.773203 28.961872
C 12.864985 12.190362 28.951456
C 14.275963 11.890081 28.952814
C 15.134685 15.791197 30.188156
C 13.703166 16.094517 30.188921
C 11.873063 14.060397 30.192301
C 12.303689 12.663934 30.182667
C 14.980242 12.087448 30.186214
C 15.949563 13.180306 30.194046
C 13.006590 15.848401 31.423737
C 12.058487 14.774868 31.422394
C 12.859783 12.150661 31.394102
C 14.259768 11.848325 31.397652
C 16.076954 13.908830 31.422695
C 15.666983 15.281311 31.422489
C 11.936985 14.009938 32.664165
C 12.394669 12.684472 32.675301

C 14.894986 12.151434 32.682533
C 15.864396 13.166452 32.662994
C 15.120672 15.827237 32.669250
C 13.729124 16.126595 32.670856
Fe 14.018130 14.117682 33.237293
Fe 14.023780 14.045693 35.593113
Fe 15.914757 13.116953 34.581947
Fe 11.892445 14.043356 34.589172
Fe 15.621685 15.576547 34.543457
Fe 13.234685 16.109116 34.566689
Fe 13.530212 11.964750 34.205299
Fe 14.046173 14.019738 37.837494
Fe 14.522590 16.190317 36.666893
Fe 12.217926 15.126948 36.721512
Fe 12.420607 12.495675 36.423641
Fe 14.709994 11.974954 36.450665
Fe 16.147287 14.279103 36.679115

06H60C13Co

H 13.095500 16.514534 20.673727
H 11.416277 14.660881 20.668819
H 15.828965 15.937650 20.663628
H 16.596132 13.555423 20.652697
H 14.727795 11.486254 20.645878
H 12.278687 12.001219 20.651756
C 16.179092 14.020622 21.547230
C 15.763798 15.309344 21.553148

C 12.900734 15.914690 21.563835
C 11.991886 14.911449 21.561153
C 12.894633 12.128690 21.543251
C 14.219178 11.849434 21.540163
C 15.086340 15.776917 22.772427
C 13.718006 16.061493 22.777164
C 11.924456 14.078416 22.771156
C 12.354506 12.749560 22.762852
C 14.969008 12.197490 22.756840
C 15.906116 13.234001 22.760227
C 13.016315 15.860237 24.030840
C 12.046745 14.792013 24.028687
C 12.874107 12.228431 24.013725
C 14.286941 11.933944 24.010529
C 16.095612 13.935590 24.016466
C 15.654453 15.309480 24.022774
C 11.875861 14.078709 25.248905
C 12.321083 12.693730 25.240238
C 14.985873 12.138136 25.234600
C 15.962175 13.215795 25.238405
C 15.128167 15.806752 25.249462
C 13.704102 16.100145 25.253592
C 12.884549 12.220893 26.469751
C 14.282767 11.933922 26.466446
C 16.089088 13.932450 26.472996
C 15.654812 15.292397 26.477364
C 13.019742 15.839531 26.483990

C 12.061904 14.781564 26.482922
C 14.973450 12.159494 27.716772
C 15.927358 13.218731 27.721373
C 15.109466 15.773630 27.727615
C 13.716292 16.058231 27.730967
C 11.912856 14.062907 27.729752
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C 16.095840 13.923946 28.960625
C 15.664445 15.301293 28.964483
C 13.017392 15.847795 28.968252
C 12.052570 14.775116 28.967937
C 12.871480 12.191681 28.954647
C 14.285648 11.900565 28.950830
C 15.139641 15.819008 30.190804
C 13.705089 16.111692 30.193922
C 11.883141 14.059354 30.198347
C 12.312271 12.661724 30.189705
C 14.990443 12.098345 30.183296
C 15.954112 13.199810 30.188927
C 13.008458 15.860674 31.424631
C 12.068622 14.776419 31.423452
C 12.872299 12.143378 31.397745
C 14.271873 11.848162 31.393339
C 16.083420 13.929697 31.413012
C 15.675780 15.305245 31.418859
C 11.980374 14.011377 32.666058
C 12.443632 12.683811 32.691238

C 14.890003 12.168421 32.682476
C 15.854822 13.192443 32.652905
C 15.114082 15.809144 32.678787
C 13.729305 16.100315 32.681900
Co 14.035736 14.139190 33.117390
Co 14.017687 13.975025 35.561810
Co 15.896384 12.984735 34.530300
Co 11.887532 13.854808 34.548515
Co 15.579659 15.404846 34.533722
Co 13.174688 15.927628 34.548397
Co 13.601144 12.089070 34.264065
Co 14.005331 13.856678 37.850838
Co 14.461193 15.982707 36.635658
Co 12.216918 14.943336 36.646023
Co 12.476155 12.534125 36.528950
Co 14.833340 12.022716 36.517082
Co 16.071285 14.107338 36.625130

06H60C13Ni

H 13.092707 16.525410 20.691650
H 11.415051 14.670615 20.676344
H 15.829251 15.948594 20.684448
H 16.604311 13.569099 20.661316
H 14.733793 11.497041 20.639002
H 12.285190 12.011947 20.642935
C 16.184284 14.027822 21.557486
C 15.765217 15.315040 21.570169

C 12.898873 15.920787 21.578697
C 11.990108 14.917236 21.570139
C 12.898795 12.133616 21.536627
C 14.223840 11.854886 21.534618
C 15.083837 15.773137 22.789652
C 13.716410 16.059677 22.792988
C 11.923965 14.076634 22.774693
C 12.356386 12.748128 22.758560
C 14.972272 12.196959 22.753542
C 15.909536 13.233367 22.764694
C 13.014194 15.851291 24.044964
C 12.045616 14.784425 24.036419
C 12.877514 12.223136 24.006893
C 14.288048 11.927433 24.004169
C 16.095707 13.927234 24.025972
C 15.652066 15.298937 24.038345
C 11.872679 14.065146 25.254524
C 12.322074 12.682493 25.236809
C 14.986486 12.122877 25.230856
C 15.963064 13.199541 25.244442
C 15.124849 15.790074 25.267189
C 13.701582 16.085249 25.270535
C 12.883142 12.200528 26.462194
C 14.282738 11.908873 26.458565
C 16.089645 13.908853 26.483234
C 15.652514 15.269960 26.492155
C 13.014317 15.822115 26.497858

C 12.053735 14.762549 26.492954
C 14.972408 12.131091 27.709499
C 15.925305 13.187660 27.726723
C 15.104075 15.740666 27.742207
C 13.712879 16.027613 27.744127
C 11.909355 14.035203 27.734827
C 12.344752 12.680292 27.715195
C 16.091944 13.885751 28.975161
C 15.661158 15.262191 28.978354
C 13.012696 15.812841 28.981920
C 12.050606 14.738467 28.983204
C 12.870584 12.155179 28.944904
C 14.283808 11.859072 28.940617
C 15.137203 15.779179 30.202618
C 13.703759 16.074980 30.204388
C 11.893495 14.011204 30.209408
C 12.309534 12.610559 30.180874
C 14.989088 12.047720 30.172560
C 15.938743 13.157550 30.200718
C 13.007163 15.827635 31.436758
C 12.092098 14.714581 31.444572
C 12.868589 12.064828 31.378187
C 14.266539 11.770254 31.373598
C 16.052326 13.878279 31.438782
C 15.674641 15.270735 31.434879
C 12.052921 13.929953 32.680054
C 12.470484 12.586170 32.678993

C 14.855427 12.079507 32.668736
C 15.780216 13.139816 32.671593
C 15.116220 15.817631 32.670780
C 13.738962 16.105082 32.672928
Ni 14.049852 14.165796 33.200603
Ni 14.039335 14.061199 35.527786
Ni 15.985568 13.100012 34.519489
Ni 11.860796 13.969247 34.530693
Ni 15.618254 15.542945 34.492451
Ni 13.165989 16.050434 34.492527
Ni 13.616410 12.061700 34.150005
Ni 13.985688 14.010527 37.836838
Ni 14.405899 16.059614 36.638836
Ni 12.184052 15.132298 36.587654
Ni 12.477278 12.677589 36.500565
Ni 14.845488 12.170260 36.499249
Ni 16.074615 14.305984 36.600498

06H60C13Cu

H 13.134131 16.442596 20.641983
H 11.460913 14.590349 20.646654
H 15.826760 15.892794 20.651024
H 16.590012 13.514298 20.654697
H 14.748071 11.463206 20.660795
H 12.302916 11.971919 20.655794
C 16.187225 13.986336 21.551950
C 15.773461 15.276706 21.549711

C 12.923059 15.867803 21.544956
C 12.014030 14.862040 21.546745
C 12.909558 12.093628 21.554464
C 14.236423 11.816978 21.556992
C 15.099618 15.756063 22.764273
C 13.725546 16.042639 22.762007
C 11.930555 14.047496 22.765779
C 12.357636 12.709613 22.768917
C 14.983115 12.167498 22.772488
C 15.924868 13.208179 22.769487
C 13.021089 15.843827 24.009995
C 12.047638 14.773086 24.011290
C 12.882265 12.205480 24.017450
C 14.299847 11.907099 24.020287
C 16.104187 13.918887 24.016613
C 15.664904 15.298303 24.014357
C 11.885337 14.067146 25.238050
C 12.331697 12.686360 25.240383
C 14.991428 12.130293 25.243896
C 15.965464 13.205934 25.242804
C 15.126643 15.790411 25.237118
C 13.705643 16.086323 25.236814
C 12.888288 12.217308 26.474874
C 14.288036 11.929544 26.479023
C 16.095079 13.925872 26.475677
C 15.653433 15.283998 26.471809
C 13.019180 15.837093 26.471628

C 12.062285 14.777553 26.472445
C 14.981341 12.155964 27.723602
C 15.948373 13.211912 27.725058
C 15.109292 15.769567 27.717705
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C 11.905457 14.064042 27.720501
C 12.340395 12.702514 27.718868
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C 15.672811 15.302979 28.951107
C 13.014888 15.843735 28.955593
C 12.033071 14.783257 28.956060
C 12.879318 12.207096 28.949734
C 14.290732 11.905457 28.954937
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C 13.710339 16.079470 30.186104
C 11.875053 14.072254 30.187010
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C 14.984961 12.117924 30.189959
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C 12.868009 12.170953 31.401855
C 14.265356 11.880822 31.409910
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C 15.672558 15.303392 31.411657
C 11.883389 13.984782 32.647057
C 12.302861 12.645632 32.660469

C 14.951803 12.178570 32.659882
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Cu 13.925803 14.156045 33.214611
Cu 13.978168 14.057074 35.633926
Cu 15.773142 12.625157 34.524689
Cu 11.725727 14.250834 34.570843
Cu 15.873060 15.151488 34.351475
Cu 13.251171 16.245041 34.549931
Cu 13.331530 12.009513 34.254482
Cu 14.051515 13.951255 38.038055
Cu 14.756281 16.034452 36.608742
Cu 12.359199 15.334747 36.760281
Cu 12.212248 12.832901 36.595840
Cu 14.546819 11.947726 36.540218
Cu 16.147467 13.952065 36.575214

06H60C13Zn

H 12.902134 16.609045 20.661993
H 11.256139 14.717786 20.650494
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H 16.508217 13.683788 20.522387
H 14.663040 11.558135 20.510040
H 12.207355 12.045389 20.559528
C 16.085836 14.121720 21.427799
C 15.636124 15.398026 21.461016

C 12.748960 15.972012 21.534485
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C 12.837952 12.174932 21.440340
C 14.164701 11.911748 21.413754
C 14.962883 15.827537 22.697313
C 13.595166 16.098351 22.732609
C 11.845221 14.087400 22.720358
C 12.308279 12.773143 22.677385
C 14.928718 12.257421 22.623129
C 15.844510 13.308448 22.630459
C 12.918782 15.867454 23.997581
C 11.971545 14.781388 23.992542
C 12.855851 12.237906 23.912384
C 14.270300 11.964108 23.883471
C 16.041819 13.991680 23.896978
C 15.564227 15.350843 23.931938
C 11.833114 14.044103 25.202662
C 12.313141 12.668217 25.155643
C 14.988184 12.152161 25.097790
C 15.950609 13.245720 25.107321
C 15.054942 15.817846 25.176483
C 13.624160 16.094376 25.212355
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C 12.969250 15.798347 26.450033

C 12.029522 14.726350 26.448423
C 15.024833 12.133316 27.578861
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C 15.149085 15.718360 30.111626
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Zn 16.083805 16.025284 34.373920
Zn 13.131554 16.553961 34.478859
Zn 13.706085 11.676477 34.106979
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06H60C13Y

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H 12.724497 11.735898 20.686226
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C 16.183735 14.001019 24.177744
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C 12.407223 12.629960 25.223282
C 15.075309 12.226004 25.424988
C 15.977992 13.352136 25.427668
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C 12.818237 15.858978 26.339170

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06H60C13Zr

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C 12.067565 14.689802 23.885660
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C 11.899307 14.003429 25.119852
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C 13.620782 16.096336 25.144041
C 12.922461 12.229873 26.456619
C 14.328179 11.999141 26.524422
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C 14.957147 12.275146 27.792660
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C 12.448619 15.115107 25.390644
C 12.066414 13.902083 26.106400
C 12.566925 12.721032 25.423752
C 13.550965 11.995658 26.210266
C 14.859899 12.037163 25.562954
C 15.812695 12.832725 26.335419
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Ti 11.355471 15.100500 36.541283
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C 13.839457 11.969543 21.979351
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C 12.441607 15.096895 25.418554
C 12.061953 13.886858 26.135244
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C 13.577452 12.006497 26.251102
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V 11.543523 13.871431 36.940231
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C 13.572753 15.846341 23.362768
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05H60C13Co

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C 16.278341 14.034112 24.280115
C 14.710875 15.937689 25.576885
C 13.407278 15.907510 26.226480
C 12.462091 15.110580 25.456598
C 12.049317 13.905231 26.167646
C 12.538174 12.712152 25.484390
C 13.535974 11.998738 26.275751
C 14.840624 12.061798 25.627916
C 15.800370 12.840808 26.398540
C 16.181395 14.050896 25.681734
C 15.731489 15.257565 26.368576
C 13.332139 15.907668 27.627802
C 12.288201 15.142118 28.295553
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C 12.358190 12.729682 28.325691
C 13.455859 12.023945 27.674019
C 14.676506 12.081503 28.470560

C 15.705804 12.864070 27.799904
C 16.029285 14.083158 28.529112
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C 14.550983 15.981874 28.422258
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C 15.541016 12.893394 30.639206
C 15.945644 14.099624 29.930964
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C 12.139202 12.805143 32.615520
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C 15.452545 12.911164 32.051907
C 15.733339 14.131133 32.819622
C 15.407349 15.324813 32.018742
C 14.285763 15.983755 32.713131
C 13.078812 15.947419 31.877033
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Co 13.693448 14.053323 33.175858

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Co 15.694287 14.157953 34.770947
Co 15.106285 15.377385 36.808563
Co 13.540930 14.088129 35.666111
Co 11.953301 12.782125 34.560135
Co 11.406835 13.994026 36.594574
Co 14.311570 12.115418 34.698696
Co 13.396679 14.114754 37.962593
Co 15.207004 12.960168 36.821537
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05H60C13Ni

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C 13.049064 15.967547 31.878319
C 12.049177 15.156051 32.584801
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Ni 11.834623 15.241382 34.488926
Ni 13.683257 14.044377 33.238266
Ni 12.770313 16.020725 36.612114

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Ni 15.109790 15.392863 36.742966
Ni 13.541948 14.049607 35.598438
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Ni 11.375251 14.005606 36.527870
Ni 14.328484 12.050509 34.666519
Ni 13.394452 14.120762 37.958679
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05H60C13Cu

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H 12.751169 15.096490 20.111311
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C 15.900238 15.180293 22.070885
C 14.900908 15.870539 21.315784
C 13.616257 15.918195 21.955929
C 12.734540 15.069734 21.202421
C 12.371986 13.864995 21.883215
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C 12.450892 15.112214 25.440296
C 12.072523 13.896281 26.152271
C 12.575003 12.713459 25.471346
C 13.561558 11.994114 26.261686
C 14.871692 12.037151 25.612926
C 15.817396 12.845318 26.381866
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C 15.701714 15.261217 26.350597
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Cu 13.677003 14.059712 33.407757
Cu 12.760543 16.090080 36.731083
Cu 15.814578 14.111520 34.756397

Cu 15.115204 15.432783 36.876804
Cu 13.513053 14.060420 35.820187
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C 13.823325 12.010498 21.945679
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C 16.122389 12.688916 22.135012
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C 15.816447 14.155169 32.813457
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Re 13.875107 16.428341 34.661282
Re 11.729153 15.419791 34.631157
Re 13.649986 14.064790 33.159874
Re 12.650655 15.648278 37.546803
Re 15.992428 14.296100 34.917488
Re 15.128435 15.912329 36.683506
Re 13.631336 14.105102 35.771526
Re 11.809006 12.561764 34.601547
Re 11.127036 13.814606 36.625710
Re 14.205335 11.864793 34.846977
Re 14.302489 13.866295 38.189598
Re 15.756746 12.622576 36.589146
Re 12.825270 12.161772 37.259136

05H60C13Os

H 12.844193 12.655183 20.121307
H 15.165698 11.976892 20.263565
H 16.505186 13.983213 20.319469
H 15.019777 15.891465 20.212124
H 12.745545 15.072588 20.093098
C 16.379147 13.993814 21.403469

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C 14.940697 15.840124 21.299278
C 13.654517 15.855337 21.931286
C 12.740340 15.044363 21.184069
C 12.317483 13.863334 21.874475
C 12.832087 12.703813 21.211494
C 13.794262 11.971542 21.977207
C 15.079118 12.050447 21.348955
C 16.046959 12.789668 22.102608
C 15.856040 15.188475 23.490538
C 14.796711 15.933764 24.146366
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C 13.460272 12.023734 27.649147
C 14.679998 12.077096 28.442835
C 15.712868 12.853824 27.770296
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C 14.548712 15.979191 28.391581
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C 12.287084 12.755371 29.702206
C 13.288826 12.048501 30.491753
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C 15.558642 12.876271 30.614958
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C 13.199254 12.044976 31.898796
C 14.446992 12.067821 32.742851
C 15.494806 12.879477 32.022625

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H 15.015518 15.906986 20.214249
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C 14.938390 15.860866 21.301949
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C 12.735508 15.032764 21.186962
C 12.284120 13.863570 21.874548
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C 13.779791 11.995878 21.968254
C 15.057491 12.116528 21.339022
C 16.027113 12.846999 22.090298
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C 14.788859 15.948250 24.150982
C 13.579669 15.825803 23.361141
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C 13.705738 12.029960 23.391165
C 14.921906 12.069192 24.185043
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C 14.711056 15.943301 25.551609
C 13.414168 15.866491 26.203018
C 12.456952 15.092206 25.434065
C 12.018172 13.889059 26.141991
C 12.514162 12.696182 25.449638
C 13.531887 12.001926 26.236883
C 14.835257 12.092378 25.586849
C 15.793794 12.869505 26.355696
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C 15.758707 15.288242 26.341599
C 13.342768 15.860502 27.609644
C 12.290604 15.108418 28.271330
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C 12.094003 12.731627 32.572586
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C 15.484990 12.892800 31.996790
C 15.826343 14.121060 32.782616

C 15.506129 15.358727 31.973307
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C 13.108624 15.869493 31.850695
C 12.008248 15.144777 32.554001
Ir 14.250313 16.308266 34.723259
Ir 11.682871 15.356823 34.577896
Ir 13.715980 14.008543 33.204514
Ir 12.684583 16.234127 36.861458
Ir 15.951918 14.161268 34.847073
Ir 15.208548 15.476246 37.056351
Ir 13.539880 14.094382 35.804779
Ir 11.765677 12.618317 34.612011
Ir 11.238109 14.016453 36.816418
Ir 14.404530 11.900295 34.768299
Ir 13.355878 14.138602 38.483170
Ir 15.290067 12.882448 37.091736
Ir 12.859076 11.982583 36.947052

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H 12.861342 12.659916 20.120096
H 15.171780 12.004650 20.263023
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H 15.015387 15.885940 20.213272
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C 12.839346 12.701874 21.210340
C 13.804318 11.976072 21.976868
C 15.087305 12.066442 21.349287
C 16.048893 12.807895 22.104925
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C 14.787138 15.943260 24.151295
C 13.576164 15.843687 23.355808
C 12.523625 15.103889 24.028696
C 12.264871 13.874859 23.298420
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C 14.701943 15.948302 25.550270
C 13.393675 15.917073 26.198908
C 12.453237 15.110188 25.428242
C 12.052670 13.900122 26.140152
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C 13.545526 11.997560 26.244967
C 14.852549 12.058719 25.597202
C 15.811177 12.843578 26.369759
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C 15.719801 15.263794 26.342632

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C 15.517189 12.866654 31.998116
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C 15.423273 15.342719 31.966581

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Pt 11.566947 15.431479 34.499004
Pt 13.682005 14.051949 33.331520
Pt 12.657031 16.305950 36.920406
Pt 16.052071 14.161978 34.781372
Pt 15.309849 15.552303 37.087093
Pt 13.532555 14.084407 35.835064
Pt 11.679408 12.551125 34.540676
Pt 11.118595 14.008728 36.856770
Pt 14.453439 11.768400 34.714497
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Pt 15.412221 12.790134 37.127335
Pt 12.822264 11.837058 36.984024

05H60C13Au

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H 14.969903 15.833915 20.157917
H 12.708387 15.006894 20.082497
C 16.339897 13.951678 21.359695
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C 13.629592 15.829986 21.895868

C 12.712029 15.002940 21.173754
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C 13.763982 11.941755 22.005239
C 15.037825 12.010085 21.356112
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C 14.801291 15.941990 24.094696
C 13.576508 15.841885 23.320618
C 12.532659 15.115146 24.021021
C 12.260027 13.875873 23.316402
C 12.617291 12.698554 24.085751
C 13.710235 12.004702 23.428812
C 14.935049 12.025074 24.209099
C 15.931337 12.813921 23.506031
C 16.279999 14.033246 24.212883
C 14.736852 15.966682 25.496990
C 13.440197 15.958527 26.166998
C 12.487057 15.142954 25.424131
C 12.088177 13.949089 26.158405
C 12.564831 12.744605 25.487638
C 13.569548 12.040943 26.276432
C 14.865968 12.080516 25.609903
C 15.840074 12.868888 26.354940
C 16.202877 14.071530 25.614971
C 15.756497 15.285138 26.286486
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C 12.419659 12.809466 28.327740
C 13.507462 12.087590 27.674715
C 14.737034 12.154239 28.452381
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C 14.668979 12.189655 29.852951
C 15.614291 13.002353 30.603395
C 16.024199 14.185997 29.863897
C 15.553627 15.384287 30.538626
C 14.555962 16.085281 29.748669
C 13.267701 16.026453 30.419167
C 11.821152 14.094775 31.800123
C 12.185755 12.891044 32.582397
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C 14.517610 12.274343 32.707619
C 15.550810 13.039546 32.013176
C 15.914354 14.258522 32.716255
C 15.496369 15.428665 31.954618
C 14.424488 16.169212 32.609882

C 13.197346 16.063217 31.833384
C 12.146375 15.315959 32.506393
Au 14.472026 16.526903 34.625248
Au 11.600368 15.773533 34.460930
Au 13.522197 13.859724 34.090977
Au 12.718565 16.329641 36.868996
Au 16.225927 14.320765 34.741226
Au 15.501717 15.655861 37.081970
Au 11.227126 14.079189 36.679539
Au 11.241864 12.245089 34.313164
Au 10.282946 11.518897 36.665291
Au 14.898004 11.548623 34.663761
Au 13.512503 14.097921 38.295929
Au 15.543098 12.755947 37.011139
Au 12.996254 11.847614 36.732338

05H60C13Hg

H 12.814360 12.730942 20.034687
H 15.092173 12.070458 20.116474
H 16.368711 14.097604 20.167519
H 14.913113 16.069138 20.138777
H 12.700695 15.130678 20.050003
C 16.308006 14.093507 21.257246
C 15.868192 15.262507 21.943768
C 14.864264 15.999872 21.226616
C 13.579399 15.931852 21.883825
C 12.690017 15.102328 21.141319

C 12.302977 13.897177 21.814178
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C 13.766938 11.991605 21.863228
C 15.037901 12.111614 21.205959
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C 15.801615 15.234814 23.373423
C 14.768541 15.979681 24.073505
C 13.531648 15.890286 23.304024
C 12.523191 15.093492 23.985802
C 12.259703 13.878880 23.242746
C 12.628696 12.680487 23.971308
C 13.717782 12.001390 23.284094
C 14.953798 12.036174 24.049484
C 15.933241 12.863811 23.364065
C 16.256123 14.069902 24.104496
C 14.716021 15.948394 25.471825
C 13.424696 15.885953 26.154331
C 12.477388 15.079484 25.391884
C 12.108295 13.853698 26.093273
C 12.592230 12.682535 25.375959
C 13.611778 11.971713 26.134668
C 14.901530 12.041790 25.450195
C 15.879110 12.820594 26.206821
C 16.208326 14.061288 25.506674
C 15.740969 15.236419 26.224453
C 13.376288 15.863191 27.553612
C 12.342900 15.076254 28.218790

C 12.059208 13.844320 27.494684
 C 12.521976 12.683377 28.246765
 C 13.573655 11.979985 27.536959
 C 14.821034 11.989766 28.284304
 C 15.846884 12.796182 27.599108
 C 16.137661 14.026871 28.341465
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 C 14.606663 15.871419 28.337442
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 C 11.919863 13.865707 30.324484
 C 12.498945 12.708175 29.665930
 C 13.561006 12.084362 30.447262
 C 14.816178 11.956629 29.678705
 C 15.891376 12.680833 30.346951
 C 16.124908 13.985251 29.742403
 C 15.499485 15.063872 30.529116
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 C 13.220165 15.859912 30.376070
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 C 12.476784 12.904548 32.534653
 C 13.554483 12.256971 31.883247

C 14.855261 12.313452 32.571037
 C 15.965682 12.590364 31.723640
 C 15.706582 13.679476 32.569801
 C 15.289092 14.932982 31.957367
 C 14.253010 15.644747 32.615070
 C 13.123127 15.867859 31.787046
 C 12.061444 15.135406 32.452679
 Hg 14.662602 17.902798 34.911087
 Hg 9.622059 16.540676 34.795322
 Hg 12.994292 14.426729 34.348198
 Hg 12.093851 17.137194 37.129429
 Hg 16.620569 14.082296 34.804043
 Hg 16.192650 16.070101 37.277252
 Hg 13.588819 14.013046 37.014290
 Hg 10.360888 11.569401 34.854713
 Hg 10.164897 14.108864 37.198917
 Hg 14.827160 11.267812 34.719147
 Hg 12.595507 14.716385 39.817581
 Hg 15.961082 12.211298 37.813431
 Hg 12.770646 10.841663 37.098343

We also provided the atomic positions (xyz coordinates) of the TM_{13} nanoclusters composed by all *3d*, *4d*, and *5d* elements obtained by DFT-PBE-D3 as implemented in VASP.

13Sc
 Sc 15.575130 14.512575 45.214104
 Sc 15.035377 17.267689 46.659462

Sc 17.891581 15.929853 46.825279
 Sc 13.883965 16.750658 43.764328
 Sc 18.506348 14.587898 44.034073

Sc 16.028294 15.096132 42.142029
Sc 16.829241 17.070650 44.258900
Sc 18.623104 16.873602 41.858337
Sc 15.766900 18.211447 41.692535
Sc 15.152133 19.553391 44.483727
Sc 17.630188 19.045158 46.375782
Sc 19.774517 17.390633 44.753479
Sc 18.083351 19.628723 43.303707

13Ti

Ti 1.765024 0.862929 17.119574
Ti 1.334839 3.324299 18.396711
Ti 3.862261 2.136650 18.479761
Ti 0.246180 2.863374 15.864527
Ti 4.336623 0.941865 15.999340
Ti 2.102481 1.390585 14.383582
Ti 2.829241 3.070650 16.258900
Ti 4.323642 2.817001 14.121089
Ti 1.796219 4.004642 14.038050
Ti 1.321857 5.199425 16.518469
Ti 3.556000 4.750716 18.134228
Ti 5.412300 3.277925 16.653284
Ti 3.893456 5.278360 15.398226

13V

V 1.797465 1.219423 17.176270
V 1.353187 3.118291 18.318169

V 3.754744 2.291046 18.445034
V 0.349222 2.976837 15.984899
V 4.350247 1.292660 16.081087
V 2.112281 1.742626 14.463104
V 2.829241 3.070650 16.258900
V 4.305294 3.023009 14.199640
V 1.903735 3.850245 14.072777
V 1.308233 4.848630 16.436722
V 3.546199 4.398674 18.054707
V 5.309256 3.164452 16.532911
V 3.861016 4.921877 15.341541

13Cr

Cr 1.741287 0.820800 17.136179
Cr 1.772523 3.019865 18.404276
Cr 3.870344 2.059238 18.474333
Cr 0.583408 2.519146 15.644621
Cr 3.854527 0.908670 16.210163
Cr 2.116882 1.320255 14.403274
Cr 2.829241 3.070650 16.258900
Cr 3.885958 3.121435 14.113536
Cr 1.788136 4.082050 14.043477
Cr 1.803953 5.232620 16.307648
Cr 3.541599 4.821035 18.114527
Cr 5.075071 3.622154 16.873192
Cr 3.917192 5.320499 15.381630

13Mn

Mn 1.800024 0.909570 17.131046
Mn 1.423071 3.136215 18.360668
Mn 3.774656 2.100548 18.415047
Mn 0.509062 2.909231 16.029028
Mn 4.181060 0.933553 16.161348
Mn 2.275583 1.499033 14.619730
Mn 2.829241 3.070650 16.258900
Mn 4.235409 3.005076 14.157143
Mn 1.883823 4.040740 14.102762
Mn 1.477419 5.207747 16.356464
Mn 3.382898 4.642255 17.898069
Mn 5.149417 3.232060 16.488781
Mn 3.858456 5.231731 15.386763

13Fe

Fe 1.876347 1.064895 17.036047
Fe 1.571284 3.199188 18.220362
Fe 3.737084 2.112564 18.275211
Fe 0.548517 2.911286 15.902571
Fe 4.152136 1.066619 16.083153
Fe 2.249460 1.494137 14.639601
Fe 2.829241 3.070650 16.258900
Fe 4.087196 2.942112 14.297450
Fe 1.921395 4.028726 14.242599
Fe 1.506344 5.074670 16.434656
Fe 3.409019 4.647153 17.878208

Fe 5.109963 3.230016 16.615229

Fe 3.782134 5.076404 15.481752

13Co

Co 1.918995 1.100056 17.019714
Co 1.503674 3.216987 18.136415
Co 3.688792 2.170841 18.192108
Co 0.560357 2.831024 15.939013
Co 4.084268 1.152979 16.071606
Co 2.173408 1.550959 14.660371
Co 2.829241 3.070650 16.258900
Co 4.154806 2.924304 14.381393
Co 1.969690 3.970449 14.325700
Co 1.574212 4.988312 16.446205
Co 3.485072 4.590330 17.857441
Co 5.098124 3.310266 16.578796
Co 3.739486 5.041245 15.498095

13Ni

Ni 1.871728 1.078020 17.002729
Ni 1.475565 3.218178 18.122265
Ni 3.701644 2.172476 18.197889
Ni 0.533703 2.825935 15.952356
Ni 4.126512 1.142426 16.077034
Ni 2.167469 1.534289 14.669310
Ni 2.829241 3.070650 16.258900
Ni 4.182916 2.923113 14.395545

Ni 1.956835 3.968815 14.319919
Ni 1.531968 4.998876 16.440767
Ni 3.491010 4.607001 17.848501
Ni 5.124776 3.315356 16.565454
Ni 3.786753 5.063269 15.515081

13Cu

Cu 1.845062 1.028949 17.051310
Cu 1.449359 3.232922 18.216459
Cu 3.733073 2.159025 18.287525
Cu 0.464358 2.820082 15.929809
Cu 4.158824 1.083180 16.044945
Cu 2.138457 1.492079 14.587105
Cu 2.829241 3.070650 16.258900
Cu 4.209120 2.908378 14.301352
Cu 1.925408 3.982266 14.230286
Cu 1.499657 5.058119 16.472857
Cu 3.520023 4.649210 17.930706
Cu 5.194122 3.321218 16.587992
Cu 3.813419 5.112350 15.466497

13Zn

Zn 15.593801 14.543217 17.235647
Zn 15.129402 17.280365 18.694336
Zn 17.947754 15.936098 18.756392
Zn 13.915940 16.751108 15.859512
Zn 18.484030 14.607304 16.008289

Zn 15.989948 15.122842 14.190655
Zn 16.829241 17.070650 16.258900
Zn 18.529078 16.860935 13.823463
Zn 15.710727 18.205193 13.761418
Zn 15.174452 19.533987 16.509521
Zn 17.668531 19.018448 18.327156
Zn 19.742540 17.390192 16.658298
Zn 18.064678 19.598083 15.282152

13Y

Y 15.403497 14.263514 45.356041
Y 14.871913 17.237598 46.898026
Y 18.022963 15.793410 47.100189
Y 13.556325 16.733269 43.703468
Y 18.613562 14.370529 44.093498
Y 15.849266 14.941632 41.982243
Y 16.829241 17.070650 44.258900
Y 18.786568 16.903690 41.619789
Y 15.635517 18.347879 41.417610
Y 15.044919 19.770771 44.424316
Y 17.809214 19.199657 46.535568
Y 20.102154 17.408031 44.814342
Y 18.254984 19.877775 43.161766

13Zr

Zr 15.728557 14.604703 17.233170
Zr 15.284309 17.238579 18.669487

Zr 17.980452 16.051994 18.681494
Zr 13.984066 16.765934 15.980330
Zr 18.476669 14.741290 15.983276
Zr 15.958402 15.122153 14.343241
Zr 16.829241 17.070650 16.258900
Zr 18.374170 16.902710 13.848315
Zr 15.678026 18.089306 13.836315
Zr 15.181812 19.400000 16.534533
Zr 17.700077 19.019136 18.174570
Zr 19.674414 17.375355 16.537481
Zr 17.929922 19.536587 15.284631

13Nb

Nb 1.951703 0.765818 17.174316
Nb 1.501656 3.412740 18.456398
Nb 3.947765 2.128620 18.654123
Nb 0.315719 2.793139 15.593289
Nb 4.200588 0.732613 16.112698
Nb 2.055660 1.221163 14.294991
Nb 2.829241 3.070650 16.258900
Nb 4.156823 2.728560 14.061413
Nb 1.710714 4.012680 13.863686
Nb 1.457893 5.408677 16.405111
Nb 3.602821 4.920127 18.222820
Nb 5.342762 3.348150 16.924519
Nb 3.706778 5.375472 15.343493

13Mo

Mo 1.583516 1.210849 17.494034
Mo 1.296821 3.270378 18.459106
Mo 3.826020 2.004573 18.513563
Mo 0.187053 2.738226 15.892720
Mo 4.694552 1.315612 16.118773
Mo 1.988435 1.860961 14.164494
Mo 2.829241 3.070650 16.258909
Mo 4.361660 2.870913 14.058704
Mo 1.832460 4.136727 14.004246
Mo 0.963928 4.825689 16.399036
Mo 3.670046 4.280338 18.353315
Mo 5.471427 3.403065 16.625090
Mo 4.074965 4.930442 15.023777

13Tc

Tc 1.791614 0.852669 16.933201
Tc 1.298900 3.177340 18.205233
Tc 3.838752 2.000810 18.245119
Tc 0.361833 2.653238 15.875657
Tc 4.112115 0.916603 15.919746
Tc 2.054518 1.357009 14.515673
Tc 2.829241 3.070650 16.258900
Tc 4.359580 2.963951 14.312567
Tc 1.819728 4.140491 14.272692
Tc 1.546365 5.224698 16.598064
Tc 3.603963 4.784293 18.002129

Tc 5.296647 3.488060 16.642153

Tc 3.866866 5.288621 15.584609

13Ru

Ru 1.811886 0.956312 17.077316

Ru 1.400539 3.236410 18.285515

Ru 3.765271 2.126942 18.358717

Ru 0.381571 2.809964 15.917232

Ru 4.207606 1.014882 16.036034

Ru 2.116455 1.437094 14.527168

Ru 2.829241 3.070650 16.258900

Ru 4.257939 2.904890 14.232295

Ru 1.893209 4.014359 14.159094

Ru 1.450874 5.126419 16.481777

Ru 3.542027 4.704196 17.990631

Ru 5.276908 3.331325 16.600578

Ru 3.846593 5.184979 15.440492

13Rh

Rh 1.771610 0.909769 17.095564

Rh 1.354326 3.241042 18.328289

Rh 3.801915 2.109228 18.407522

Rh 0.345107 2.808021 15.913864

Rh 4.252262 0.970198 16.034460

Rh 2.082402 1.398604 14.488663

Rh 2.829241 3.070650 16.258900

Rh 4.304154 2.900248 14.189520

Rh 1.856564 4.032060 14.110287

Rh 1.406217 5.171092 16.483337

Rh 3.576079 4.742685 18.029146

Rh 5.313374 3.333280 16.603947

Rh 3.886868 5.231532 15.422245

13Pd

Pd 1.803586 0.861492 17.099508

Pd 1.371177 3.271197 18.373894

Pd 3.851315 2.050908 18.535374

Pd 0.293648 2.819248 15.872496

Pd 4.317310 0.835433 16.023428

Pd 2.060899 1.299001 14.377348

Pd 2.829241 3.070650 16.258900

Pd 4.287302 2.870103 14.143917

Pd 1.807166 4.090392 13.982433

Pd 1.341170 5.305858 16.494381

Pd 3.597580 4.842299 18.140451

Pd 5.364833 3.322043 16.645304

Pd 3.854893 5.279796 15.418302

13Pd

Pd 1.803586 0.861492 17.099508

Pd 1.371177 3.271197 18.373894

Pd 3.851315 2.050908 18.535374

Pd 0.293648 2.819248 15.872496

Pd 4.317310 0.835433 16.023428

Pd 2.060899 1.299001 14.377348
Pd 2.829241 3.070650 16.258900
Pd 4.287302 2.870103 14.143917
Pd 1.807166 4.090392 13.982433
Pd 1.341170 5.305858 16.494381
Pd 3.597580 4.842299 18.140451
Pd 5.364833 3.322043 16.645304
Pd 3.854893 5.279796 15.418302

13Lu

Lu 15.510445 14.337078 45.324982
Lu 15.030842 17.306873 46.901695
Lu 18.016035 15.890838 46.994453
Lu 13.667156 16.724936 43.808018
Lu 18.611336 14.411219 43.954460
Lu 15.936624 14.994143 41.983967
Lu 16.829241 17.070650 44.258900
Lu 18.627638 16.834417 41.616100
Lu 15.642446 18.250452 41.523357
Lu 15.047146 19.730072 44.563351
Lu 17.721855 19.147156 46.533844
Lu 19.991314 17.416355 44.709793
Lu 18.148037 19.804214 43.192825

13Hf

Hf 1.751820 0.617136 17.192984
Hf 1.185262 3.250770 18.619883

Hf 3.910858 1.998369 18.638086
Hf 0.039815 2.795331 15.833909
Hf 4.426107 0.747565 16.029009
Hf 1.961375 1.191103 14.309643
Hf 2.829241 3.070650 16.258900
Hf 4.473218 2.890521 13.897927
Hf 1.747621 4.142921 13.879721
Hf 1.232373 5.393724 16.488791
Hf 3.697105 4.950186 18.208168
Hf 5.618666 3.345958 16.683899
Hf 3.906662 5.524164 15.324827

13Ta

Ta 1.748854 0.791862 17.153992
Ta 1.306332 3.218093 18.444241
Ta 3.853144 2.055936 18.509651
Ta 0.196253 2.784715 15.887862
Ta 4.341886 0.874016 16.023157
Ta 2.055490 1.333501 14.377001
Ta 2.829241 3.070650 16.258900
Ta 4.352149 2.923197 14.073568
Ta 1.805335 4.085364 14.008149
Ta 1.316593 5.267274 16.494654
Ta 3.602988 4.807798 18.140808
Ta 5.462227 3.356585 16.629948
Ta 3.909626 5.349430 15.363821

13W

W 1.762288 0.841786 16.598831
W 1.183877 3.676906 18.186169
W 4.237682 2.255341 18.300665
W 0.143515 2.789663 15.915588
W 4.347805 0.829133 16.072472
W 2.138380 1.444422 14.254507
W 2.829241 3.070650 16.258900
W 4.474602 2.464385 14.331641
W 1.420798 3.885959 14.217146
W 1.310675 5.312156 16.445337
W 3.520099 4.696879 18.263294
W 5.514964 3.351628 16.602222
W 3.896192 5.299502 15.918980

13Re

Re 1.756664 0.915488 17.095860
Re 1.336358 3.193921 18.321396
Re 3.773787 2.093090 18.398769
Re 0.317607 2.780054 15.940689
Re 4.248688 0.984446 16.015120
Re 2.100279 1.410791 14.487065
Re 2.829241 3.070650 16.258900
Re 4.322123 2.947370 14.196413
Re 1.884693 4.048210 14.119041
Re 1.409792 5.156844 16.502693
Re 3.558201 4.730508 18.030745

Re 5.340874 3.361248 16.577120

Re 3.901817 5.225812 15.421948

13Os

Os 1.800199 0.920096 16.980904
Os 1.373419 3.175813 18.276991
Os 3.781193 2.047631 18.352873
Os 0.376240 2.791760 15.932446
Os 4.217427 1.027999 15.934946
Os 2.132747 1.466865 14.485901
Os 2.829241 3.070650 16.258900
Os 4.285060 2.965487 14.240810
Os 1.877287 4.093660 14.164935
Os 1.441054 5.113301 16.582863
Os 3.525734 4.674435 18.031910
Os 5.282241 3.349530 16.585365
Os 3.858281 5.221193 15.536904

13Ir

Ir 1.744937 0.913348 17.080730
Ir 1.400554 3.253254 18.320910
Ir 3.779905 2.121840 18.444227
Ir 0.319047 2.763246 15.928205
Ir 4.247059 0.950156 15.988931
Ir 2.130096 1.426235 14.488509
Ir 2.829241 3.070650 16.258909
Ir 4.257926 2.888046 14.196890

Ir 1.878575 4.019460 14.073582
Ir 1.411421 5.191145 16.528879
Ir 3.528386 4.715064 18.029301
Ir 5.339433 3.378045 16.589596
Ir 3.913543 5.227952 15.437078

13Pt

Pt 1.742479 0.799540 17.150558
Pt 1.284456 3.250105 18.431524
Pt 3.778439 2.074798 18.430620
Pt 0.292603 2.806185 15.937366
Pt 4.302339 0.856200 16.012783
Pt 2.112817 1.361771 14.476892
Pt 2.829241 3.070650 16.258900
Pt 4.374023 2.891195 14.086286
Pt 1.880042 4.066491 14.087190
Pt 1.356142 5.285101 16.505028
Pt 3.545665 4.779529 18.040909
Pt 5.365877 3.335114 16.580444
Pt 3.916001 5.341750 15.367252

13Au

Au 1.693597 0.714340 17.175465
Au 1.236251 3.258530 18.518452
Au 3.873209 2.019047 18.601860
Au 0.098996 2.781455 15.877550

Au 4.364552 0.776790 16.011904
Au 2.031769 1.248072 14.329682
Au 2.829241 3.070650 16.258900
Au 4.422229 2.882761 13.999358
Au 1.785269 4.122241 13.915949
Au 1.293929 5.364500 16.505907
Au 3.626710 4.893217 18.188116
Au 5.559482 3.359836 16.640261
Au 3.964883 5.426950 15.342336

13Hg

Hg 15.365132 13.997663 45.391815
Hg 14.725081 17.266541 47.137497
Hg 18.140669 15.706888 47.287777
Hg 13.322480 16.658237 43.717514
Hg 18.851700 14.136105 43.947258
Hg 15.867680 14.722689 41.741047
Hg 16.829241 17.070650 44.258900
Hg 18.933397 16.874748 41.380310
Hg 15.517812 18.434402 41.230034
Hg 14.806781 20.005196 44.570549
Hg 17.790800 19.418602 46.776764
Hg 20.335999 17.483063 44.800285
Hg 18.293346 20.143627 43.125992

Here, we provided the atomic positions (xyz coordinates) of the five-layered hydrogen-

terminated fragment for the (3,3) armchair CNT and tree-layered hydrogen terminated fragment for the (5,0) zigzag CNT, obtained by DFT-PBE-D3.

6H60C	C 15.599827 15.340401 25.510559
H 13.005339 16.468914 22.144638	C 11.875553 14.003577 26.740343
H 11.389912 14.545991 22.147240	C 12.376068 12.634940 26.741928
H 15.792711 15.991688 22.150881	C 15.060675 12.159607 26.740080
H 16.652323 13.630962 22.146757	C 15.998642 13.274532 26.738808
H 14.823399 11.453792 22.150383	C 15.064177 15.835799 26.740396
H 12.349002 11.882095 22.153847	C 13.629359 16.089897 26.739447
C 16.193329 14.080676 23.027973	C 12.951795 12.180631 27.966057
C 15.731491 15.350370 23.030842	C 14.364069 11.930295 27.965181
C 12.839761 15.852162 23.028719	C 16.104254 14.000517 27.963556
C 11.969955 14.817511 23.029978	C 15.611677 15.347245 27.965010
C 12.968205 12.056302 23.034451	C 12.947358 15.821362 27.964371
C 14.299779 11.824984 23.032225	C 12.025287 14.723168 27.964737
C 15.018500 15.783732 24.246199	C 15.041893 12.206817 29.215240
C 13.654435 16.024345 24.245087	C 15.951303 13.283712 29.214649
C 11.946064 13.986931 24.246315	C 15.031120 15.796709 29.214043
C 12.415905 12.683487 24.247908	C 13.644578 16.045212 29.214937
C 15.035376 12.228824 24.244171	C 11.929665 13.998074 29.215166
C 15.928272 13.287804 24.242260	C 12.408370 12.673538 29.215616
C 12.957834 15.803468 25.509703	C 16.087337 14.000588 30.467669
C 12.038196 14.713866 25.509796	C 15.603815 15.343401 30.467100
C 12.959207 12.195413 25.512350	C 12.954837 15.810571 30.467896
C 14.363142 11.946157 25.510588	C 12.031543 14.722116 30.468355
C 16.085907 13.999823 25.508753	C 12.956669 12.194352 30.468189

C 14.361127 11.940164 30.467693
C 15.067332 15.839093 31.698166
C 13.630624 16.091452 31.699623
C 11.869676 14.010068 31.699455
C 12.371658 12.639624 31.698547
C 15.057214 12.156637 31.698589
C 15.994059 13.273767 31.699036
C 12.892202 15.867536 32.940723
C 11.966765 14.778514 32.941593
C 12.934795 12.111907 32.938885
C 14.342317 11.854381 32.939575
C 16.168402 14.025556 32.939404
C 15.686209 15.372191 32.939556
C 11.875175 13.888199 34.035908
C 12.279177 12.712198 34.041695
C 15.156781 12.223863 34.033085
C 15.982123 13.154372 34.041920
C 14.956687 15.889014 34.032753
C 13.739760 16.145103 34.043400

60C5H

H 12.310753 15.216245 34.235756
H 14.617910 15.921550 34.251255
H 16.042645 13.973272 34.250999
H 12.319292 12.803721 34.231586
H 14.623028 12.023699 34.240917
C 15.478099 13.558344 21.893448

C 15.175496 14.847034 22.392265
C 14.046200 15.545435 21.896118
C 13.199313 16.303982 22.685192
C 12.608005 15.336711 21.793839
C 12.134204 14.102478 22.428019
C 12.521804 12.930779 21.797764
C 13.499383 12.176304 22.423195
C 14.824375 12.250908 21.803181
C 15.923927 12.516928 22.688269
C 15.491633 15.076426 23.836731
C 14.630762 15.969997 24.631014
C 13.292558 16.202772 24.054131
C 12.300065 15.321989 24.676243
C 12.064726 14.108786 23.877319
C 12.485250 12.900082 24.579567
C 13.484674 12.103690 23.873343
C 14.713662 11.970195 24.677038
C 15.853385 12.638488 24.059145
C 16.063871 13.975745 24.634863
C 14.660942 15.953850 26.042051
C 13.386240 16.002579 26.779249
C 12.340458 15.254821 26.067265
C 11.995140 14.025207 26.756983
C 12.426389 12.861516 26.005743
C 13.386741 12.080120 26.763065
C 14.660229 12.033463 26.071146
C 15.695978 12.787191 26.782944

C 16.056091 14.009954 26.044907	C 15.636569 12.801427 31.030224
C 15.648325 15.190102 26.771723	C 16.062782 13.993776 30.311352
C 13.383908 15.984332 28.174984	C 15.629988 15.171711 31.035923
C 12.361591 15.215853 28.889214	C 14.646942 15.953147 30.310951
C 11.968170 14.014302 28.163143	C 13.383201 15.922933 31.027561
C 12.354455 12.814482 28.888941	C 11.944144 14.009057 32.437901
C 13.368954 12.062208 28.167791	C 12.379038 12.841723 33.142563
C 14.633123 12.058653 28.895592	C 13.357722 12.063305 32.445175
C 15.681181 12.788455 28.179443	C 14.604209 12.094775 33.152267
C 16.048519 13.999038 28.907261	C 15.650963 12.780825 32.451439
C 15.660821 15.197703 28.181553	C 15.984765 13.977924 33.161182
C 14.647176 15.943282 28.904840	C 15.647043 15.182057 32.463184
C 12.342568 15.220369 30.293888	C 14.607184 15.871402 33.161205
C 11.980034 14.011271 31.014507	C 13.367624 15.941788 32.452259
C 12.331177 12.799366 30.292475	C 12.372366 15.178153 33.147057
C 13.370694 12.089222 31.020576	
C 14.631533 12.043091 30.299273	

The lowest energy configurations obtained from DFT-PBE-D3 for the (3,3) armchair fragment and (5,0) zigzag fragment adhered to *3d*, *4d*, and *5d* TM₁₃ nanoclusters are provided below.

06H60C13Sc	H 12.718701 11.827477 20.688486
H 13.404922 16.224083 20.537163	C 16.432673 13.930167 21.774981
H 11.800575 14.320746 20.513882	C 15.968545 15.201973 21.681534
H 16.031441 15.760777 20.746988	C 13.132393 15.702011 21.455204
H 16.882584 13.427933 20.917578	C 12.257874 14.664231 21.442688
H 15.161794 11.395823 20.883469	C 13.243321 11.964307 21.634888

C 14.576341 11.728578 21.741467
C 15.220240 15.727325 22.826725
C 13.829075 15.975468 22.715240
C 12.093048 13.911301 22.688816
C 12.578671 12.582585 22.784143
C 15.230083 12.115325 22.994278
C 16.143475 13.198626 23.010616
C 13.044164 15.813803 23.905655
C 12.103104 14.691582 23.892099
C 13.032941 12.148014 24.072840
C 14.468199 11.890997 24.188932
C 16.211229 13.966855 24.219372
C 15.708859 15.337764 24.118050
C 11.906198 14.028364 25.135929
C 12.399284 12.674959 25.232174
C 15.056722 12.204232 25.446785
C 15.984572 13.311474 25.462231
C 15.060421 15.849030 25.276031
C 13.642813 16.101849 25.163389
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C 15.975811 13.312197 25.334507
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V 13.238041 12.055419 34.279793
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V 12.784520 14.792009 36.931095
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V 15.024333 11.785792 36.659790
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C 14.976187 15.893831 25.225924
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Fe 13.560017 11.948898 34.213284
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C 13.717403 16.060364 27.729828
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C 16.096048 13.925106 28.965164
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C 14.284349 11.905456 28.956284
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C 11.879548 14.066332 30.197443
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C 14.988495 12.102506 30.189411
C 15.954246 13.202072 30.194302
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C 12.868201 12.151207 31.400873
C 14.267986 11.853356 31.398617
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C 11.975728 14.022609 32.662605
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C 14.886316 12.173795 32.688110
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Co 15.884684 12.980222 34.528301
Co 11.880803 13.855548 34.540203
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Co 13.169846 15.928568 34.544209
Co 13.591067 12.089984 34.265079
Co 13.992686 13.854926 37.841263
Co 14.452040 15.981619 36.627956
Co 12.207597 14.945198 36.632488
Co 12.463015 12.535571 36.514801
Co 14.818529 12.020898 36.507225
Co 16.060349 14.104572 36.616699

06H60C13Ni

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H 15.821710 15.898369 20.667904
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Ni 14.417303 16.084805 36.620926
Ni 12.191423 15.173265 36.572651
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Ni 14.827398 12.193371 36.489571
Ni 16.071009 14.320264 36.585793

06H60C13Cu

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H 14.751482 11.489798 20.658163
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C 12.926394 15.862389 21.548443
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C 12.910666 12.103517 21.557051

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C 15.925529 13.208684 22.773956
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C 12.045226 14.773422 24.015978
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C 14.991235 12.131021 25.246870
C 15.964220 13.206715 25.245707
C 15.124968 15.790613 25.240911
C 13.704836 16.086336 25.240730
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C 14.288760 11.930099 26.482651
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C 13.018749 15.837471 26.475819
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Cu 13.265954 16.243525 34.549095
Cu 13.312418 12.014517 34.258957
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06H60C13Zn

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C 12.327185 14.821970 24.096180
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05H60C13V

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V 11.114457 13.698515 36.645164
V 14.381721 12.162221 34.801785
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H 12.748600 15.053842 20.103470
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C 13.646136 15.851423 21.940758
C 12.736955 15.032231 21.194525
C 12.317335 13.851166 21.888990
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Cr 13.707737 14.048728 33.255913

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Cr 15.294030 15.542614 37.029144
Cr 13.671006 14.008108 35.524055
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Cr 11.302266 13.824318 36.465118
Cr 14.485147 11.754977 34.707024
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C 12.844313 12.690762 21.230198
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Fe 11.379505 14.036037 36.722370
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05H60C13Co

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Co 11.863336 15.231587 34.502476
Co 13.690628 14.052588 33.201603
Co 12.808599 16.076254 36.579945
Co 15.712050 14.171979 34.762089
Co 15.132112 15.398110 36.766357

Co 13.542248 14.085593 35.604759
Co 11.936234 12.763448 34.547760
Co 11.384244 13.961287 36.546379
Co 14.309691 12.101709 34.688835
Co 13.399247 14.107347 37.821671
Co 15.229761 12.967966 36.763836
Co 12.843707 12.094419 36.658871

05H60C13Ni

H 12.867932 12.650930 20.159201
H 15.175162 11.999988 20.300377
H 16.494938 14.005086 20.354908
H 15.014842 15.884389 20.248075
H 12.769525 15.050739 20.125889
C 16.383165 14.014690 21.440483
C 15.955572 15.206066 22.107536
C 14.936817 15.848900 21.336018
C 13.651469 15.855047 21.964569
C 12.748725 15.033985 21.216848
C 12.327549 13.855270 21.908846
C 12.845927 12.695374 21.249397
C 13.811695 11.971290 22.016413
C 15.093549 12.062125 21.386808
C 16.054440 12.810055 22.138308
C 15.852491 15.205569 23.531096
C 14.787431 15.943930 24.187208
C 13.576435 15.847107 23.388737

C 12.524302 15.104632 24.061098
C 12.268827 13.873113 23.333647
C 12.626282 12.686380 24.089907
C 13.735472 12.011640 23.439146
C 14.949731 12.032429 24.236736
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C 16.283922 14.048599 24.294428
C 14.701182 15.945175 25.588470
C 13.392785 15.918447 26.235558
C 12.455043 15.110353 25.462095
C 12.057220 13.899233 26.173059
C 12.553759 12.709150 25.489937
C 13.554585 11.999878 26.283123
C 14.861772 12.062733 25.636600
C 15.819700 12.845177 26.411081
C 16.186127 14.063035 25.695078
C 15.718025 15.262348 26.381876
C 13.312404 15.922193 27.631439
C 12.275382 15.140491 28.299915
C 11.983776 13.911552 27.570297
C 12.372365 12.726452 28.329563
C 13.472582 12.020676 27.679039
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C 15.727072 12.862954 27.807512
C 16.025146 14.089960 28.540588
C 15.626525 15.270660 27.779034
C 14.532634 15.985255 28.431782

C 12.186725 15.155119 29.698229
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C 12.285784 12.738127 29.727024
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C 15.558393 12.883171 30.649200
C 15.940820 14.102254 29.939337
C 15.455144 15.299821 30.618681
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C 12.146179 12.794631 32.611794
C 13.207982 12.046667 31.923887
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C 15.476048 12.892365 32.056458
C 15.714490 14.126130 32.818432
C 15.370781 15.313695 32.025833
C 14.255260 15.980094 32.709312
C 13.044613 15.977642 31.876495
C 12.044491 15.160084 32.580208
Ni 14.162254 16.110638 34.614994
Ni 11.780713 15.261527 34.467621
Ni 13.678058 14.047630 33.245720
Ni 12.749635 16.061741 36.579082
Ni 15.709583 14.153079 34.737377
Ni 15.068857 15.375998 36.751251
Ni 13.512236 14.061147 35.592224

Ni 11.923487 12.730168 34.510410
Ni 11.430227 14.033484 36.558090
Ni 14.322624 12.018598 34.654236
Ni 13.392490 14.125535 37.948483
Ni 15.208317 12.931627 36.765835
Ni 12.945382 12.130653 36.688568

05H60C13Cu

H 12.948115 12.696109 20.136452
H 15.229502 11.868526 20.292679
H 16.419640 13.971233 20.332041
H 14.985182 15.906844 20.233459
H 12.760091 15.104928 20.113966
C 16.344099 13.983875 21.421024
C 15.910974 15.176644 22.079042
C 14.913691 15.867791 21.322121
C 13.628722 15.918691 21.960043
C 12.741850 15.076557 21.205183
C 12.375281 13.871578 21.883121
C 12.890681 12.711318 21.226551
C 13.827174 11.961596 21.988518
C 15.136339 11.947835 21.376801
C 16.057228 12.779747 22.119125
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C 14.781711 15.953206 24.165276
C 13.555508 15.907475 23.373669
C 12.522115 15.118157 24.040848

C 12.301105 13.887879 23.312494
C 12.656515 12.704439 24.063560
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C 15.951440 12.818458 23.540316
C 16.247646 14.038573 24.266272
C 14.698094 15.949205 25.567503
C 13.390129 15.924664 26.215279
C 12.453739 15.113855 25.442047
C 12.070151 13.897688 26.151039
C 12.569831 12.713593 25.468830
C 13.553745 11.990704 26.258732
C 14.866231 12.031100 25.613409
C 15.812099 12.835901 26.385536
C 16.164612 14.052988 25.671715
C 15.707363 15.252588 26.357088
C 13.311600 15.923227 27.611586
C 12.277045 15.137451 28.278702
C 11.984222 13.908377 27.549707
C 12.373280 12.723114 28.305689
C 13.468184 12.009106 27.656540
C 14.689138 12.067236 28.454662
C 15.720428 12.853995 27.783802
C 16.017405 14.081675 28.513004
C 15.626493 15.266176 27.755810
C 14.534044 15.981666 28.409201
C 12.187342 15.151443 29.675200

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C 13.294138 12.044824 30.499428
C 14.602996 12.078665 29.853270
C 15.543231 12.883969 30.624390
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C 13.207559 12.053576 31.908043
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C 15.463408 12.893685 32.032475
C 15.730764 14.118491 32.788357
C 15.374615 15.304332 32.002533
C 14.268409 15.994949 32.681519
C 13.054187 15.956314 31.854753
C 12.040826 15.156982 32.550941
Cu 14.181968 16.204088 34.635246
Cu 11.788295 15.349397 34.494225
Cu 13.671831 14.055587 33.415264
Cu 12.697433 16.115673 36.734829
Cu 15.804933 14.222801 34.753838
Cu 15.171827 15.395899 36.894821
Cu 13.525411 14.121781 35.808506
Cu 11.831887 12.746838 34.530174

Cu 11.334709 13.983998 36.665321
Cu 14.385881 12.009651 34.695290
Cu 13.376505 14.150905 38.224659
Cu 15.210468 12.896616 36.907799
Cu 12.903066 12.082053 36.766953

05H60C13Zn

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H 15.204726 11.964979 20.265028
H 16.515265 13.906622 20.344238
H 14.982402 15.751019 20.218132
H 12.609108 15.185909 20.088314
C 16.397070 13.919995 21.429615
C 15.921846 15.100332 22.076498
C 14.914083 15.767473 21.307615
C 13.641558 15.840072 21.925083
C 12.604116 15.144403 21.178856
C 12.311386 13.885907 21.843822
C 12.857341 12.756771 21.184574
C 13.808909 12.008504 21.949989
C 15.106487 12.015922 21.351070
C 16.104370 12.700494 22.130165
C 15.835003 15.106367 23.504807
C 14.780107 15.852973 24.150387
C 13.571670 15.824816 23.350664
C 12.485363 15.112939 24.013750
C 12.248178 13.880562 23.270529

C 12.621388 12.699427 24.023008
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C 12.415292 15.103537 25.409966
C 12.019585 13.884480 26.114073
C 12.515870 12.701172 25.427292
C 13.491660 11.967794 26.217896
C 14.806436 11.986814 25.584448
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H 12.156853 14.394484 20.477205
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C 13.413779 15.867493 26.202824
C 12.457121 15.092083 25.434237
C 12.018720 13.888720 26.142611
C 12.515079 12.695077 25.451939
C 13.532537 12.000653 26.239489
C 14.836902 12.089572 25.590227
C 15.795262 12.867912 26.358625
C 16.203087 14.075123 25.648746
C 15.757979 15.287215 26.343863
C 13.340660 15.862909 27.608904

C 12.288319 15.110436 28.270409
C 11.942898 13.895102 27.532612
C 12.335856 12.701486 28.290644
C 13.451131 12.019224 27.633255
C 14.672688 12.105186 28.427286
C 15.704112 12.885942 27.758801
C 16.054743 14.095775 28.492460
C 15.679804 15.295930 27.732109
C 14.558749 15.967204 28.395016
C 12.205102 15.113633 29.667543
C 11.744715 13.904491 30.372303
C 12.247478 12.703834 29.684019
C 13.279513 12.017061 30.468904
C 14.591900 12.111097 29.824593
C 15.542376 12.904420 30.586967
C 15.983318 14.105191 29.888845
C 15.551349 15.330907 30.585161
C 14.484118 15.972512 29.793383
C 13.191868 15.846044 30.428453
C 11.628647 13.914568 31.757597
C 12.093682 12.732897 32.570702
C 13.192052 11.991655 31.863987
C 14.439834 12.082314 32.709290
C 15.485137 12.894342 31.996506
C 15.821667 14.125179 32.780113
C 15.501884 15.362821 31.971363
C 14.334634 16.011776 32.681641

C 13.104197 15.871932 31.848568
C 12.005562 15.146000 32.551220
Ir 14.244839 16.312147 34.719162
Ir 11.679896 15.359946 34.574211
Ir 13.712737 14.009928 33.204681
Ir 12.683084 16.236866 36.851810
Ir 15.945867 14.168247 34.843643
Ir 15.205842 15.482514 37.042793
Ir 13.536728 14.101231 35.795059
Ir 11.764603 12.624023 34.609859
Ir 11.241641 14.022038 36.808353
Ir 14.401165 11.907314 34.766453
Ir 13.358706 14.143568 38.471073
Ir 15.287427 12.891361 37.078537
Ir 12.860370 11.992911 36.937366

05H60C13Pt

H 12.850998 12.661228 20.131813
H 15.159719 11.990693 20.273300
H 16.493612 13.986061 20.329323
H 15.016357 15.880722 20.222412
H 12.757493 15.064146 20.103094
C 16.376101 13.997317 21.414179
C 15.955647 15.191491 22.080423
C 14.939092 15.839866 21.310188
C 13.654171 15.854807 21.941525
C 12.743411 15.042413 21.194115

C 12.317749 13.864241 21.884922
C 12.831912 12.705008 21.222113
C 13.792858 11.972873 21.988186
C 15.076193 12.055266 21.359497
C 16.042238 12.794558 22.113182
C 15.854342 15.192550 23.503569
C 14.793750 15.936483 24.159451
C 13.580091 15.845243 23.365494
C 12.525556 15.107679 24.038542
C 12.261564 13.878736 23.310030
C 12.614073 12.690065 24.065950
C 13.717948 12.010231 23.411524
C 14.932809 12.023953 24.209614
C 15.938118 12.825064 23.534790
C 16.279650 14.032532 24.265766
C 14.710268 15.938358 25.560873
C 13.403584 15.915068 26.208961
C 12.460019 15.112056 25.440336
C 12.054753 13.904837 26.151926
C 12.541935 12.711827 25.467758
C 13.539348 11.998039 26.258787
C 14.844820 12.054766 25.610037
C 15.807300 12.833699 26.381067
C 16.182608 14.048233 25.665749
C 15.725214 15.251094 26.351959
C 13.326929 15.916576 27.606846
C 12.289256 15.143296 28.277565

C 11.986166 13.918221 27.551079
C 12.367858 12.733840 28.309793
C 13.460737 12.022741 27.657261
C 14.681231 12.077351 28.452702
C 15.713786 12.855301 27.779005
C 16.022886 14.077459 28.510126
C 15.634197 15.258963 27.750172
C 14.546053 15.977552 28.403957
C 12.198404 15.161568 29.677343
C 11.788693 13.947439 30.381489
C 12.281002 12.746050 29.709898
C 13.286029 12.029238 30.494959
C 14.600262 12.087147 29.854422
C 15.570860 12.868574 30.620295
C 15.945193 14.092280 29.912029
C 15.484447 15.304518 30.587620
C 14.462166 15.996954 29.804195
C 13.145748 15.973467 30.440397
C 11.647561 13.961948 31.781965
C 12.053509 12.737751 32.586086
C 13.187231 11.992356 31.899626
C 14.452390 12.053700 32.737759
C 15.532406 12.853254 32.028023
C 15.844180 14.125693 32.797081
C 15.444016 15.353170 31.994551
C 14.308212 16.092886 32.681816
C 13.042089 16.040529 31.842304

C 11.965663 15.235198 32.549675
Pt 14.283824 16.451591 34.648949
Pt 11.556400 15.455496 34.494541
Pt 13.711422 14.051856 32.887718
Pt 12.669469 16.289825 36.866119
Pt 16.069435 14.159419 34.784996
Pt 15.291944 15.535688 37.034721
Pt 13.540881 14.087605 35.640266
Pt 11.655971 12.553399 34.537045
Pt 11.141369 14.021671 36.801937
Pt 14.452318 11.754321 34.715931
Pt 13.375153 14.121701 38.372997
Pt 15.385963 12.803139 37.075912
Pt 12.821389 11.868061 36.928368

05H60C13Au

H 12.813511 12.733389 20.031422
H 15.122799 12.098443 20.144955
H 16.442719 14.108082 20.217731
H 14.947860 15.987359 20.155977
H 12.706395 15.138418 20.036728
C 16.336136 14.099767 21.303658
C 15.909359 15.278490 21.993990
C 14.879091 15.927979 21.243464
C 13.598827 15.915007 21.883057
C 12.695713 15.102949 21.127249
C 12.286053 13.910903 21.804726

C 12.801090 12.763866 21.122156
C 13.776209 12.034241 21.873180
C 15.050518 12.145107 21.232857
C 16.016659 12.882876 21.985735
C 15.819070 15.255689 23.418049
C 14.755336 15.976263 24.094320
C 13.538015 15.881863 23.308537
C 12.496798 15.123572 23.977770
C 12.238928 13.904576 23.231613
C 12.606439 12.709440 23.971924
C 13.713466 12.053576 23.298725
C 14.934546 12.071133 24.084372
C 15.925330 12.891052 23.411077
C 16.260969 14.088372 24.160801
C 14.680661 15.954558 25.496424
C 13.380160 15.909257 26.155914
C 12.438780 15.109398 25.380911
C 12.051730 13.889755 26.081244
C 12.548023 12.712399 25.375341
C 13.560679 11.998078 26.147640
C 14.859007 12.079457 25.487307
C 15.820370 12.853522 26.264786
C 16.175888 14.081413 25.563332
C 15.710071 15.269407 26.270687
C 13.313371 15.896631 27.555817
C 12.290708 15.102662 28.225807
C 11.990388 13.884143 27.480841

C 12.393946 12.689933 28.217134
C 13.493008 12.000849 27.546694
C 14.719731 12.058796 28.332359
C 15.743143 12.853207 27.664190
C 16.047009 14.070719 28.409630
C 15.633286 15.259196 27.670378
C 14.540689 15.955862 28.341948
C 12.224534 15.090428 29.628822
C 11.869173 13.869452 30.323635
C 12.323911 12.685989 29.616678
C 13.352654 12.022549 30.397305
C 14.642482 12.062943 29.735958
C 15.566319 12.863166 30.515574
C 15.974216 14.065282 29.810032
C 15.473934 15.231742 30.514221
C 14.469005 15.940688 29.745302
C 13.185759 15.840489 30.416182
C 11.785233 13.858864 31.734810
C 12.155427 12.662315 32.467701
C 13.281108 12.017089 31.812967
C 14.485082 12.071043 32.613167
C 15.491574 12.855860 31.931675
C 15.851902 14.057446 32.663975
C 15.412890 15.228645 31.927229
C 14.340970 15.915811 32.615288
C 13.116405 15.823931 31.836735
C 12.068103 15.058327 32.491707

Au 14.323097 16.205761 34.615700
Au 11.692711 15.215515 34.471718
Au 14.364463 15.546702 37.318714
Au 12.370909 17.136854 36.363739
Au 16.228798 14.155955 34.633324
Au 16.972408 15.021380 37.068672
Au 11.823128 14.596202 37.180687
Au 11.616523 12.417712 34.385063
Au 10.248716 12.492844 36.700291
Au 14.445389 11.880636 34.634830
Au 13.528769 13.640678 39.115074
Au 15.353357 12.839341 37.032921
Au 12.898568 11.916703 36.897858

05H60C13Hg

H 12.906652 12.678206 20.002163
H 15.193443 11.932259 20.134754
H 16.436825 14.041457 20.172165
H 15.011737 15.965709 20.087887
H 12.809790 15.080078 19.973700
C 16.362686 14.047259 21.260960
C 15.946344 15.241618 21.932264
C 14.941025 15.921234 21.176031
C 13.652279 15.920857 21.812189
C 12.780808 15.067922 21.064953
C 12.376641 13.883206 21.752577
C 12.876897 12.712597 21.092878

C 13.817236 11.959414 21.855354
C 15.114450 12.012388 21.219952
C 16.032629 12.845846 21.950081
C 15.852749 15.245503 23.355310
C 14.800431 15.993532 24.021393
C 13.579259 15.911675 23.231831
C 12.547720 15.135528 23.904928
C 12.310112 13.903460 23.180639
C 12.660384 12.718127 23.930719
C 13.743015 12.001005 23.271290
C 14.970983 12.030800 24.062731
C 15.939328 12.871099 23.377512
C 16.267958 14.077091 24.107695
C 14.727049 15.988157 25.421247
C 13.424534 15.943511 26.082203
C 12.490205 15.136271 25.308899
C 12.105749 13.926777 26.020691
C 12.588717 12.733203 25.334736
C 13.586629 12.008878 26.117767
C 14.891156 12.064743 25.459061
C 15.829601 12.875339 26.226084
C 16.196123 14.086962 25.510553
C 15.753683 15.295773 26.199196
C 13.366496 15.933561 27.483427
C 12.374831 15.134290 28.177530
C 12.032419 13.934270 27.421280
C 12.404599 12.731258 28.154482

C 13.511442 12.028983 27.514246
C 14.724266 12.136402 28.322111
C 15.744975 12.899746 27.628466
C 16.075630 14.117451 28.345276
C 15.696434 15.317784 27.591633
C 14.596145 16.037148 28.256525
C 12.327496 15.109958 29.596968
C 11.840609 13.905085 30.245869
C 12.279125 12.701048 29.544266
C 13.301482 12.020411 30.333578
C 14.620673 12.173890 29.735313
C 15.492359 13.035255 30.527721
C 16.033573 14.162919 29.746523
C 15.688309 15.450299 30.335403
C 14.564298 16.076818 29.649704
C 13.309874 15.833185 30.397446
C 11.731314 13.874802 31.653454
C 12.039880 12.651693 32.379108
C 13.173107 12.005112 31.741123
C 14.254167 12.350105 32.592659

C 15.232906 13.154557 31.951494
C 15.515882 14.446785 32.546173
C 15.728943 15.549818 31.711761
C 14.580927 15.708813 32.540924
C 13.286338 15.660869 31.834942
C 12.258719 14.918300 32.460384
Hg 14.409088 16.902094 34.663589
Hg 10.631161 16.415079 34.741817
Hg 12.878334 13.448750 34.290642
Hg 12.382738 17.273071 37.727905
Hg 16.562725 14.073692 34.785290
Hg 15.999101 16.100172 37.947731
Hg 13.569016 14.290638 36.788971
Hg 10.000162 11.222556 35.035568
Hg 10.219495 14.060037 37.505791
Hg 15.081247 10.305652 34.969414
Hg 13.212845 14.135659 39.838234
Hg 16.159731 12.388756 37.903671
Hg 12.582316 11.065742 37.769196

We provide the atomic positions (xyz coordinates) of the TM_{13} nanoclusters composed by all *3d*, *4d*, and *5d* elements obtained by DFT-PBE-D3-SOC as implemented in VASP.

13Sc
Sc 15.575329 14.513142 17.214172
Sc 15.035522 17.267540 18.658884

Sc 17.891430 15.930015 18.824642
Sc 13.884626 16.750471 15.764420
Sc 18.505980 14.588339 16.034237

Sc 16.028242 15.096640 14.142237
Sc 16.829241 17.070650 16.258900
Sc 18.622957 16.873753 13.858918
Sc 15.767050 18.211287 13.693169
Sc 15.152501 19.552950 16.483562
Sc 17.630239 19.044651 18.375574
Sc 19.773853 17.390818 16.753391
Sc 18.083151 19.628157 15.303637

13Ti

Ti 1.765145 0.863309 17.119303
Ti 1.335012 3.324016 18.396446
Ti 3.861928 2.136607 18.479509
Ti 0.246538 2.863062 15.864744
Ti 4.336219 0.942003 15.999476
Ti 2.102419 1.390565 14.384016
Ti 2.829241 3.070650 16.258900
Ti 4.323469 2.817284 14.121355
Ti 1.796552 4.004684 14.038299
Ti 1.322261 5.199286 16.518332
Ti 3.556062 4.750736 18.133793
Ti 5.411942 3.278238 16.653067
Ti 3.893335 5.277981 15.398500

13V

V 1.797465 1.219423 17.176270
V 1.353187 3.118291 18.318169

V 3.754744 2.291046 18.445034
V 0.349222 2.976837 15.984899
V 4.350247 1.292660 16.081087
V 2.112281 1.742626 14.463104
V 2.829241 3.070650 16.258900
V 4.305294 3.023009 14.199640
V 1.903735 3.850245 14.072777
V 1.308233 4.848630 16.436722
V 3.546199 4.398674 18.054707
V 5.309256 3.164452 16.532911
V 3.861016 4.921877 15.341541

13Cr

Cr 1.742573 0.838220 17.132729
Cr 1.761868 3.024344 18.402693
Cr 3.869158 2.062695 18.459505
Cr 0.577638 2.527297 15.651253
Cr 3.864957 0.910996 16.207184
Cr 2.127355 1.330778 14.412259
Cr 2.829241 3.070650 16.258900
Cr 3.896613 3.116956 14.115120
Cr 1.789322 4.078593 14.058306
Cr 1.793523 5.230294 16.310629
Cr 3.531126 4.810512 18.105541
Cr 5.080841 3.614003 16.866560
Cr 3.915906 5.303079 15.385080

13Mn

Mn 1.870080 1.021647 17.109804
Mn 1.363415 3.190125 18.402071
Mn 3.707074 2.127691 18.306387
Mn 0.590215 2.848076 15.970486
Mn 4.235255 0.904182 16.108217
Mn 2.199149 1.561776 14.679757
Mn 2.829241 3.070650 16.258900
Mn 4.295065 2.951165 14.115739
Mn 1.951405 4.013597 14.211422
Mn 1.423224 5.237118 16.409595
Mn 3.459332 4.579513 17.838043
Mn 5.068264 3.293215 16.547323
Mn 3.788401 5.119654 15.408005

13Fe

Fe 1.874903 1.063120 17.036116
Fe 1.570861 3.199713 18.219971
Fe 3.738516 2.113474 18.275112
Fe 0.547432 2.912959 15.901602
Fe 4.152771 1.069155 16.082674
Fe 2.249198 1.494194 14.639462
Fe 2.829241 3.070650 16.258900
Fe 4.087619 2.941587 14.297839
Fe 1.919963 4.027816 14.242699
Fe 1.505709 5.072134 16.435135
Fe 3.409281 4.647096 17.878347

Fe 5.111049 3.228343 16.616196

Fe 3.783578 5.078179 15.481683

13Co

Co 1.918845 1.085664 16.996561
Co 1.493787 3.232471 18.127760
Co 3.641980 2.211061 18.227346
Co 0.564540 2.767724 15.955435
Co 4.060336 1.136809 16.010778
Co 2.123632 1.557446 14.669459
Co 2.829241 3.070650 16.258900
Co 4.164693 2.908820 14.390051
Co 2.016500 3.930229 14.290464
Co 1.598144 5.004482 16.507032
Co 3.534848 4.583842 17.848352
Co 5.093941 3.373566 16.562374
Co 3.739635 5.055637 15.521248

13Ni

Ni 1.871728 1.078020 17.002729
Ni 1.475565 3.218178 18.122265
Ni 3.701644 2.172476 18.197889
Ni 0.533703 2.825935 15.952356
Ni 4.126512 1.142426 16.077034
Ni 2.167469 1.534289 14.669310
Ni 2.829241 3.070650 16.258900
Ni 4.182916 2.923113 14.395545

Ni 1.956835 3.968815 14.319919
Ni 1.531968 4.998876 16.440767
Ni 3.491010 4.607001 17.848501
Ni 5.124776 3.315356 16.565454
Ni 3.786753 5.063269 15.515081

13Cu

Cu 1.845062 1.028949 17.051310
Cu 1.449359 3.232922 18.216459
Cu 3.733073 2.159025 18.287525
Cu 0.464358 2.820082 15.929809
Cu 4.158824 1.083180 16.044945
Cu 2.138457 1.492079 14.587105
Cu 2.829241 3.070650 16.258900
Cu 4.209120 2.908378 14.301352
Cu 1.925408 3.982266 14.230286
Cu 1.499657 5.058119 16.472857
Cu 3.520023 4.649210 17.930706
Cu 5.194122 3.321218 16.587992
Cu 3.813419 5.112350 15.466497

13Zn

Zn 15.593801 14.543217 17.235647
Zn 15.129402 17.280365 18.694336
Zn 17.947754 15.936098 18.756392
Zn 13.915940 16.751108 15.859512
Zn 18.484030 14.607304 16.008289

Zn 15.989948 15.122842 14.190655
Zn 16.829241 17.070650 16.258900
Zn 18.529078 16.860935 13.823463
Zn 15.710727 18.205193 13.761418
Zn 15.174452 19.533987 16.509521
Zn 17.668531 19.018448 18.327156
Zn 19.742540 17.390192 16.658298
Zn 18.064678 19.598083 15.282152

13Y

Y 15.422443 14.269724 17.331465
Y 14.868258 17.320286 18.912851
Y 18.001465 15.811725 19.085728
Y 13.576104 16.750181 15.731050
Y 18.649944 14.313865 16.014336
Y 15.911713 14.892768 13.941000
Y 16.829241 17.070650 16.258900
Y 18.790222 16.821005 13.604960
Y 15.657014 18.329565 13.432074
Y 15.008536 19.827436 16.503475
Y 17.746767 19.248524 18.576811
Y 20.082375 17.391117 16.786758
Y 18.236038 19.871565 15.186344

13Zr

Zr 15.728557 14.604703 17.233170
Zr 15.284309 17.238579 18.669487

Zr 17.980452 16.051994 18.681494
Zr 13.984066 16.765934 15.980330
Zr 18.476669 14.741290 15.983276
Zr 15.958402 15.122153 14.343241
Zr 16.829241 17.070650 16.258900
Zr 18.374170 16.902710 13.848315
Zr 15.678026 18.089306 13.836315
Zr 15.181812 19.400000 16.534533
Zr 17.700077 19.019136 18.174570
Zr 19.674414 17.375355 16.537481
Zr 17.929922 19.536587 15.284631

13Nb

Nb 1.951703 0.765818 17.174316
Nb 1.501656 3.412740 18.456398
Nb 3.947765 2.128620 18.654123
Nb 0.315719 2.793139 15.593289
Nb 4.200588 0.732613 16.112698
Nb 2.055660 1.221163 14.294991
Nb 2.829241 3.070650 16.258900
Nb 4.156823 2.728560 14.061413
Nb 1.710714 4.012680 13.863686
Nb 1.457893 5.408677 16.405111
Nb 3.602821 4.920127 18.222820
Nb 5.342762 3.348150 16.924519
Nb 3.706778 5.375472 15.343493

13Mo

Mo 1.592409 1.202857 17.500767
Mo 1.303701 3.256125 18.461777
Mo 3.840052 1.994844 18.507179
Mo 0.191500 2.741940 15.866820
Mo 4.688284 1.309913 16.152014
Mo 1.970178 1.864706 14.174608
Mo 2.829241 3.070650 16.258909
Mo 4.354780 2.885166 14.056032
Mo 1.818428 4.146456 14.010632
Mo 0.970196 4.831388 16.365797
Mo 3.688303 4.276593 18.343201
Mo 5.466980 3.399351 16.650990
Mo 4.066072 4.938434 15.017044

13Tc

Tc 1.705072 0.855787 16.927633
Tc 1.194505 3.204674 18.191975
Tc 3.795354 2.104098 18.307556
Tc 0.332242 2.641453 15.945065
Tc 4.165473 0.976869 15.735432
Tc 2.040991 1.355829 14.543651
Tc 2.829241 3.070650 16.258900
Tc 4.463974 2.936617 14.325825
Tc 1.863126 4.037201 14.210254
Tc 1.493008 5.164433 16.782379
Tc 3.617489 4.785472 17.974150

Tc 5.326238 3.499845 16.572746

Tc 3.953408 5.285503 15.590175

13Ru

Ru 1.809120 0.950695 17.083529

Ru 1.395001 3.232400 18.288977

Ru 3.765560 2.124919 18.364584

Ru 0.374191 2.809353 15.916661

Ru 4.208317 1.012943 16.033913

Ru 2.114462 1.436796 14.528068

Ru 2.829241 3.070650 16.258900

Ru 4.263478 2.908900 14.228834

Ru 1.892920 4.016382 14.153228

Ru 1.450163 5.128358 16.483898

Ru 3.544020 4.704494 17.989733

Ru 5.284288 3.331936 16.601149

Ru 3.849359 5.190596 15.434280

13Rh

Rh 1.795373 0.909646 17.092699

Rh 1.353323 3.248523 18.326929

Rh 3.793901 2.086728 18.407991

Rh 0.322133 2.812622 15.920892

Rh 4.227054 0.979161 16.036707

Rh 2.101751 1.377926 14.493818

Rh 2.829241 3.070650 16.258900

Rh 4.305157 2.892766 14.190881

Rh 1.864578 4.054560 14.109818

Rh 1.431425 5.162129 16.481091

Rh 3.556729 4.763363 18.023991

Rh 5.336349 3.328678 16.596920

Rh 3.863106 5.231656 15.425110

13Pd

Pd 1.803033 0.857103 17.100496

Pd 1.369527 3.272504 18.377964

Pd 3.852073 2.050502 18.536148

Pd 0.289501 2.818862 15.870559

Pd 4.316242 0.835359 16.023661

Pd 2.061337 1.298834 14.377062

Pd 2.829241 3.070650 16.258900

Pd 4.288953 2.868796 14.139847

Pd 1.806408 4.090798 13.981659

Pd 1.342238 5.305932 16.494148

Pd 3.597143 4.842466 18.140739

Pd 5.368980 3.322429 16.647242

Pd 3.855446 5.284185 15.417313

13Ag

Ag 1.693363 0.713115 17.177256

Ag 1.235139 3.258416 18.519484

Ag 3.874346 2.018173 18.603975

Ag 0.097535 2.780386 15.877230

Ag 4.365759 0.775149 16.011986

Ag 2.031623 1.246666 14.327800
Ag 2.829241 3.070650 16.258900
Ag 4.423341 2.882884 13.998325
Ag 1.784135 4.123127 13.913833
Ag 1.292720 5.366142 16.505823
Ag 3.626857 4.894634 18.190002
Ag 5.560946 3.360905 16.640572
Ag 3.965116 5.428173 15.340555

13Cd

Cd 15.368800 14.005666 45.443642
Cd 14.762527 17.318851 47.182304
Cd 18.168444 15.710871 47.303398
Cd 13.304740 16.692883 43.759315
Cd 18.813566 14.090014 43.940533
Cd 15.797910 14.704220 41.753380
Cd 16.829241 17.070650 44.258900
Cd 18.895954 16.822441 41.335495
Cd 15.490036 18.430420 41.214409
Cd 14.844913 20.051277 44.577271
Cd 17.860569 19.437080 46.764435
Cd 20.353739 17.448410 44.758492
Cd 18.289680 20.135624 43.074158

13Lu

Lu 15.500263 14.383204 45.403549
Lu 15.012271 17.255962 46.907619

Lu 17.990593 15.869074 47.012432
Lu 13.715356 16.665026 43.815441
Lu 18.575558 14.437923 43.969944
Lu 15.918982 15.032913 41.958721
Lu 16.829241 17.070650 44.258900
Lu 18.646210 16.885330 41.610180
Lu 15.667889 18.272217 41.505379
Lu 15.082924 19.703365 44.547867
Lu 17.739496 19.108387 46.559090
Lu 19.943115 17.476263 44.702366
Lu 18.158218 19.758087 43.114262

13Hf

Hf 1.750181 0.616257 17.203480
Hf 1.195024 3.238860 18.618221
Hf 3.900447 2.016013 18.642544
Hf 0.046963 2.796075 15.847599
Hf 4.433764 0.749773 16.043665
Hf 1.963135 1.207233 14.289242
Hf 2.829241 3.070650 16.258900
Hf 4.463456 2.902430 13.899588
Hf 1.758033 4.125277 13.875265
Hf 1.224717 5.391516 16.474134
Hf 3.695345 4.934056 18.228569
Hf 5.611518 3.345214 16.670212
Hf 3.908301 5.525043 15.314329

13Ta

Ta 1.749465 0.792247 17.146498
Ta 1.295142 3.215847 18.450474
Ta 3.859195 2.059254 18.510057
Ta 0.194092 2.781753 15.885148
Ta 4.332823 0.873039 16.023239
Ta 2.051620 1.331288 14.384646
Ta 2.829241 3.070650 16.258900
Ta 4.363339 2.925443 14.067335
Ta 1.799284 4.082046 14.007740
Ta 1.325655 5.268251 16.494572
Ta 3.606859 4.810012 18.133163
Ta 5.464388 3.359547 16.632660
Ta 3.909016 5.349044 15.371313

13W

W 1.731130 0.852561 16.604784
W 1.170847 3.655649 18.172518
W 4.243584 2.254832 18.297689
W 0.131065 2.776568 15.918686
W 4.344951 0.838511 16.076302
W 2.128721 1.447047 14.262154
W 2.829241 3.070650 16.258900
W 4.487632 2.485642 14.345293
W 1.414897 3.886468 14.220120
W 1.313529 5.302777 16.441509
W 3.529757 4.694253 18.255646

W 5.527414 3.364723 16.599125

W 3.927350 5.288727 15.913026

13Re

Re 1.772424 0.916118 17.088404
Re 1.321412 3.220719 18.312294
Re 3.785293 2.096060 18.393833
Re 0.308989 2.811323 15.947748
Re 4.267295 0.989530 16.008316
Re 2.110886 1.411356 14.483706
Re 2.829241 3.070650 16.258900
Re 4.337069 2.920572 14.205515
Re 1.873188 4.045240 14.123978
Re 1.391185 5.151760 16.509495
Re 3.547594 4.729943 18.034103
Re 5.349493 3.329978 16.570061
Re 3.886057 5.225182 15.429407

13Os

Os 1.760243 0.935359 17.021002
Os 1.428400 3.169351 18.366404
Os 3.770598 2.022132 18.355104
Os 0.345118 2.811540 15.834675
Os 4.297159 1.057651 15.932109
Os 2.114465 1.443568 14.465431
Os 2.829241 3.070650 16.258900
Os 4.230079 2.971949 14.151397

Os 1.887883 4.119159 14.162704
Os 1.361322 5.083649 16.585701
Os 3.544016 4.697732 18.052380
Os 5.313363 3.329751 16.683136
Os 3.898237 5.205930 15.496807

13Ir

Ir 1.802227 0.937072 17.142015
Ir 1.328082 3.255771 18.284130
Ir 3.808117 2.088579 18.429146
Ir 0.317645 2.739259 15.932857
Ir 4.203738 0.947643 15.985648
Ir 2.128270 1.406629 14.465543
Ir 2.829241 3.070650 16.258909
Ir 4.330398 2.885529 14.233668
Ir 1.850363 4.052721 14.088663
Ir 1.454742 5.193658 16.532162
Ir 3.530212 4.734670 18.052267
Ir 5.340836 3.402032 16.584944
Ir 3.856252 5.204229 15.375793

13Pt

Pt 1.768033 0.859998 17.125336
Pt 1.306171 3.247876 18.452831
Pt 3.816576 2.071118 18.512997
Pt 0.272969 2.809296 15.904360
Pt 4.261611 0.920923 16.023054

Pt 2.088405 1.339690 14.421114
Pt 2.829241 3.070650 16.258900
Pt 4.352309 2.893424 14.064981
Pt 1.841904 4.070171 14.004813
Pt 1.396869 5.220378 16.494757
Pt 3.570077 4.801610 18.096685
Pt 5.385511 3.332004 16.613451
Pt 3.890447 5.281292 15.392475

13Au

Au 1.701612 0.699265 17.168961
Au 1.247215 3.260470 18.501547
Au 3.864785 2.010634 18.582834
Au 0.118478 2.778644 15.880508
Au 4.354420 0.762877 16.012897
Au 2.038720 1.236208 14.344837
Au 2.829241 3.070650 16.258900
Au 4.411265 2.880821 14.016262
Au 1.793694 4.130653 13.934976
Au 1.304061 5.378413 16.504913
Au 3.619759 4.905081 18.172962
Au 5.540000 3.362647 16.637302
Au 3.956868 5.442025 15.348839

13Hg

Hg 15.377580 14.000903 45.387299
Hg 14.733319 17.263012 47.133911

Hg 18.135378 15.709266 47.279404
Hg 13.326102 16.656122 43.719337
Hg 18.847237 14.138782 43.949127
Hg 15.868284 14.725914 41.745945
Hg 16.829241 17.070650 44.258900
Hg 18.925159 16.878277 41.383896

Hg 15.523104 18.432026 41.238411
Hg 14.811243 20.002520 44.568680
Hg 17.790195 19.415377 46.771866
Hg 20.332376 17.485178 44.798462
Hg 18.280901 20.140387 43.130512

Here, we provided the atomic positions (xyz coordinates) of the five-layered hydrogen-terminated fragment for the (3,3) armchair CNT and tree-layered hydrogen terminated fragment for the (5,0) zigzag CNT obtained by DFT-PBE-vdW-SOC.

6H60C	
H 13.005339 16.468914 22.144638	C 12.415905 12.683487 24.247908
H 11.389912 14.545991 22.147240	C 15.035376 12.228824 24.244171
H 15.792711 15.991688 22.150881	C 15.928272 13.287804 24.242260
H 16.652323 13.630962 22.146757	C 12.957834 15.803468 25.509703
H 14.823399 11.453792 22.150383	C 12.038196 14.713866 25.509796
H 12.349002 11.882095 22.153847	C 12.959207 12.195413 25.512350
C 16.193329 14.080676 23.027973	C 14.363142 11.946157 25.510588
C 15.731491 15.350370 23.030842	C 16.085907 13.999823 25.508753
C 12.839761 15.852162 23.028719	C 15.599827 15.340401 25.510559
C 11.969955 14.817511 23.029978	C 11.875553 14.003577 26.740343
C 12.968205 12.056302 23.034451	C 12.376068 12.634940 26.741928
C 14.299779 11.824984 23.032225	C 15.060675 12.159607 26.740080
C 15.018500 15.783732 24.246199	C 15.998642 13.274532 26.738808
C 13.654435 16.024345 24.245087	C 15.064177 15.835799 26.740396
C 11.946064 13.986931 24.246315	C 13.629359 16.089897 26.739447
	C 12.951795 12.180631 27.966057

C 14.364069 11.930295 27.965181
C 16.104254 14.000517 27.963556
C 15.611677 15.347245 27.965010
C 12.947358 15.821362 27.964371
C 12.025287 14.723168 27.964737
C 15.041893 12.206817 29.215240
C 15.951303 13.283712 29.214649
C 15.031120 15.796709 29.214043
C 13.644578 16.045212 29.214937
C 11.929665 13.998074 29.215166
C 12.408370 12.673538 29.215616
C 16.087337 14.000588 30.467669
C 15.603815 15.343401 30.467100
C 12.954837 15.810571 30.467896
C 12.031543 14.722116 30.468355
C 12.956669 12.194352 30.468189
C 14.361127 11.940164 30.467693
C 15.067332 15.839093 31.698166
C 13.630624 16.091452 31.699623
C 11.869676 14.010068 31.699455
C 12.371658 12.639624 31.698547
C 15.057214 12.156637 31.698589
C 15.994059 13.273767 31.699036
C 12.892202 15.867536 32.940723
C 11.966765 14.778514 32.941593
C 12.934795 12.111907 32.938885
C 14.342317 11.854381 32.939575

C 16.168402 14.025556 32.939404
C 15.686209 15.372191 32.939556
C 11.875175 13.888199 34.035908
C 12.279177 12.712198 34.041695
C 15.156781 12.223863 34.033085
C 15.982123 13.154372 34.041920

60C5H

H 12.310753 15.216245 34.235756
H 14.617910 15.921550 34.251255
H 16.042645 13.973272 34.250999
H 12.319292 12.803721 34.231586
H 14.623028 12.023699 34.240917
C 15.478099 13.558344 21.893448
C 15.175496 14.847034 22.392265
C 14.046200 15.545435 21.896118
C 13.199313 16.303982 22.685192
C 12.608005 15.336711 21.793839
C 12.134204 14.102478 22.428019
C 12.521804 12.930779 21.797764
C 13.499383 12.176304 22.423195
C 14.824375 12.250908 21.803181
C 15.923927 12.516928 22.688269
C 15.491633 15.076426 23.836731
C 14.630762 15.969997 24.631014
C 13.292558 16.202772 24.054131
C 12.300065 15.321989 24.676243

C 12.064726 14.108786 23.877319	C 16.048519 13.999038 28.907261
C 12.485250 12.900082 24.579567	C 15.660821 15.197703 28.181553
C 13.484674 12.103690 23.873343	C 14.647176 15.943282 28.904840
C 14.713662 11.970195 24.677038	C 12.342568 15.220369 30.293888
C 15.853385 12.638488 24.059145	C 11.980034 14.011271 31.014507
C 16.063871 13.975745 24.634863	C 12.331177 12.799366 30.292475
C 14.660942 15.953850 26.042051	C 13.370694 12.089222 31.020576
C 13.386240 16.002579 26.779249	C 14.631533 12.043091 30.299273
C 12.340458 15.254821 26.067265	C 15.636569 12.801427 31.030224
C 11.995140 14.025207 26.756983	C 16.062782 13.993776 30.311352
C 12.426389 12.861516 26.005743	C 15.629988 15.171711 31.035923
C 13.386741 12.080120 26.763065	C 14.646942 15.953147 30.310951
C 14.660229 12.033463 26.071146	C 13.383201 15.922933 31.027561
C 15.695978 12.787191 26.782944	C 11.944144 14.009057 32.437901
C 16.056091 14.009954 26.044907	C 12.379038 12.841723 33.142563
C 15.648325 15.190102 26.771723	C 13.357722 12.063305 32.445175
C 13.383908 15.984332 28.174984	C 14.604209 12.094775 33.152267
C 12.361591 15.215853 28.889214	C 15.650963 12.780825 32.451439
C 11.968170 14.014302 28.163143	C 15.984765 13.977924 33.161182
C 12.354455 12.814482 28.888941	C 15.647043 15.182057 32.463184
C 13.368954 12.062208 28.167791	C 14.607184 15.871402 33.161205
C 14.633123 12.058653 28.895592	
C 15.681181 12.788455 28.179443	

Here, we provided the atomic positions of the lowest energy configurations for the armchair CNT fragment (3,3) and the zigzag (5,0) CNT fragment, respectively, adhered to *3d*, *4d*, and *5d* TM₁₃ nanoclusters, obtained by DFT-PBE-D3-SOC.

06H60C13Sc

H 13.404928 16.224073 20.537170	C 15.056719 12.204233 25.446785
H 11.800587 14.320743 20.513891	C 15.984571 13.311474 25.462231
H 16.031441 15.760767 20.746998	C 15.060424 15.849020 25.276031
H 16.882582 13.427931 20.917587	C 13.642818 16.101837 25.163391
H 15.161795 11.395823 20.883476	C 12.876571 12.274337 26.531969
H 12.718710 11.827477 20.688496	C 14.277399 12.027104 26.647003
C 16.432671 13.930163 21.774986	C 16.003725 14.089101 26.675976
C 15.968547 15.201967 21.681538	C 15.516604 15.426560 26.576166
C 13.132401 15.702006 21.455212	C 12.878576 15.888343 26.368830
C 12.257881 14.664222 21.442696	C 11.965373 14.794615 26.355217
C 13.243329 11.964305 21.634890	C 14.880818 12.312137 27.922541
C 14.576344 11.728580 21.741474	C 15.810950 13.423235 27.936493
C 15.220253 15.727317 22.826733	C 14.889074 15.973624 27.747452
C 13.829069 15.975465 22.715242	C 13.466795 16.218748 27.640625
C 12.093050 13.911304 22.688818	C 11.725044 14.134004 27.612511
C 12.578681 12.582575 22.784151	C 12.214142 12.775084 27.705162
C 15.230076 12.115311 22.994287	C 15.864034 14.198533 29.132710
C 16.143488 13.198633 23.010628	C 15.371402 15.575141 29.027517
C 13.044177 15.813801 23.905655	C 12.692858 16.030630 28.823624
C 12.103108 14.691567 23.892097	C 11.757667 14.909709 28.809008
C 13.032932 12.148017 24.072838	C 12.672626 12.347144 28.985390
C 14.468217 11.890995 24.188929	C 14.112864 12.103276 29.106644
C 16.211235 13.966839 24.219368	C 14.705402 16.080723 30.184624
C 15.708858 15.337770 24.118048	C 13.299657 16.301670 30.093948
C 11.906209 14.028361 25.135927	C 11.584614 14.245087 30.066917
C 12.399297 12.674958 25.232174	C 12.043230 12.897409 30.143713
	C 14.707387 12.432272 30.366739

C 15.630556 13.535379 30.379761	06H60C13Ti
C 12.523818 16.139410 31.338457	H 13.103241 16.369825 20.597702
C 11.590138 15.018874 31.323851	H 11.540508 14.422770 20.584312
C 12.495982 12.475418 31.474974	H 15.777282 15.950106 20.666733
C 13.930654 12.249456 31.595428	H 16.674902 13.623172 20.720215
C 15.659856 14.312432 31.619280	H 14.984761 11.500422 20.717209
C 15.185385 15.686629 31.513821	H 12.521093 11.888314 20.649004
C 11.161894 14.287807 32.512711	C 16.243593 14.087844 21.607916
C 11.684336 12.903153 32.608719	C 15.755806 15.352298 21.578817
C 14.628644 12.434524 32.892799	C 12.896721 15.797069 21.502764
C 15.582245 13.574454 32.905842	C 12.048983 14.740402 21.495613
C 14.609167 16.391417 32.650455	C 13.095591 12.035102 21.564436
C 13.155772 16.668196 32.544052	C 14.434357 11.823324 21.601877
Sc 13.442104 14.400280 32.677238	C 15.045103 15.820418 22.774366
Sc 14.638109 13.375335 35.141525	C 13.653412 16.034370 22.738585
Sc 16.665077 11.700827 33.539005	C 11.972207 13.940843 22.725023
Sc 11.079681 13.683686 34.514133	C 12.481538 12.628816 22.757467
Sc 16.346962 15.445592 33.691818	C 15.134884 12.214502 22.829836
Sc 13.717546 16.829954 34.551491	C 16.014973 13.314924 22.833281
Sc 12.909978 11.347187 33.645573	C 12.929432 15.822325 23.965368
Sc 14.985458 13.054768 38.196014	C 12.014207 14.685755 23.957916
Sc 15.697312 15.732564 36.843864	C 12.995977 12.163065 24.020041
Sc 12.758079 14.929576 37.013969	C 14.433999 11.940860 24.057835
Sc 12.488434 11.899403 36.801521	C 16.131378 14.051498 24.066629
Sc 15.398320 10.703122 36.191303	C 15.605299 15.408236 24.035692
Sc 17.393286 13.084535 36.219864	C 11.872150 13.985764 25.186405
	C 12.394566 12.634391 25.220793

C 15.076759 12.224472 25.292679
C 15.987113 13.352983 25.297262
C 15.010083 15.882454 25.238605
C 13.577608 16.099112 25.199934
C 12.943088 12.211315 26.480436
C 14.351567 12.000745 26.513189
C 16.040764 14.095115 26.525118
C 15.534571 15.426262 26.497807
C 12.879963 15.826368 26.428934
C 11.983983 14.717078 26.421631
C 14.998295 12.276677 27.771276
C 15.899634 13.390951 27.776657
C 14.949655 15.916858 27.725096
C 13.527388 16.123047 27.683088
C 11.824163 14.014647 27.670532
C 12.328574 12.668353 27.707573
C 16.018820 14.125825 28.999128
C 15.506382 15.501994 28.976435
C 12.810057 15.893265 28.897518
C 11.890854 14.757080 28.890324
C 12.842575 12.201069 28.958174
C 14.294991 11.993055 28.986315
C 14.887591 15.959955 30.179176
C 13.470186 16.158207 30.132679
C 11.766749 14.046483 30.119938
C 12.257740 12.701678 30.160950
C 14.944787 12.303533 30.207756

C 15.843536 13.414672 30.213737
C 12.765150 15.899557 31.384340
C 11.863934 14.782350 31.377678
C 12.813320 12.300693 31.462473
C 14.236305 12.075768 31.474344
C 15.906902 14.145815 31.485594
C 15.388975 15.490770 31.480947
C 11.564816 14.075637 32.596779
C 12.127589 12.726992 32.697701
C 14.975975 12.178288 32.718613
C 15.955979 13.392784 32.724995
C 14.820892 16.062988 32.717037
C 13.385805 16.333538 32.610802
Ti 13.866018 14.079212 32.650364
Ti 14.184542 13.807112 35.537903
Ti 16.148628 12.225938 34.401237
Ti 11.659496 13.766696 34.556263
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Ti 13.699071 16.290676 34.571728
Ti 13.364323 11.620685 34.133377
Ti 14.381707 13.634181 38.129005
Ti 15.171724 15.855301 36.790810
Ti 12.534007 15.134926 37.016247
Ti 12.383326 12.403849 36.770748
Ti 14.838391 11.468000 36.570343
Ti 16.603127 13.652292 36.583408

06H60C13V

H 13.219901 16.418728 20.614498	C 15.045445 12.199545 25.313345
H 11.617649 14.502551 20.567825	C 15.975811 13.312197 25.334507
H 15.884166 15.935595 20.714399	C 15.051364 15.864694 25.276445
H 16.730030 13.587102 20.767893	C 13.623070 16.118149 25.222706
H 14.984741 11.478777 20.736393	C 12.900204 12.235935 26.472301
H 12.528774 11.923811 20.642839	C 14.301529 11.990437 26.525135
C 16.293940 14.057635 21.649885	C 16.030575 14.051331 26.565880
C 15.834593 15.331690 21.621239	C 15.546922 15.389959 26.539228
C 12.990153 15.843550 21.512266	C 12.903393 15.850489 26.439051
C 12.121593 14.804184 21.486759	C 11.989337 14.761250 26.411499
C 13.100151 12.065365 21.561113	C 14.944145 12.247396 27.793276
C 14.432813 11.824036 21.611471	C 15.864091 13.344425 27.813797
C 15.118324 15.810344 22.811531	C 14.951818 15.881253 27.764116
C 13.734997 16.057232 22.758986	C 13.538249 16.123085 27.711306
C 12.012786 14.001080 22.711796	C 11.801800 14.054814 27.658842
C 12.489984 12.678702 22.747187	C 12.288747 12.706325 27.694221
C 15.128429 12.202209 22.848213	C 15.984691 14.068924 29.043571
C 16.026873 13.284112 22.868187	C 15.486442 15.453115 29.021887
C 12.988938 15.855734 23.977066	C 12.794046 15.913116 28.915003
C 12.054391 14.740693 23.950205	C 11.846046 14.792290 28.882708
C 12.977490 12.194615 24.015121	C 12.778646 12.220713 28.949883
C 14.409586 11.936512 24.069708	C 14.226526 11.970529 29.003168
C 16.144604 14.011979 24.108757	C 14.856440 15.917837 30.212950
C 15.650805 15.379889 24.079830	C 13.443122 16.156631 30.159954
C 11.878479 14.038470 25.173977	C 11.695060 14.072399 30.098406
C 12.372963 12.674366 25.208790	C 12.183914 12.727772 30.138142
	C 14.873586 12.247247 30.235447

C 15.798149 13.345251 30.246721	06H60C13Cr
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C 11.808792 14.781473 31.368700	H 11.404840 14.421516 20.626900
C 12.721596 12.323493 31.440142	H 15.678699 16.055622 20.636766
C 14.126830 12.048135 31.487152	H 16.642735 13.743649 20.642406
C 15.819876 14.066650 31.517460	H 14.964075 11.510342 20.647871
C 15.311729 15.412739 31.512833	H 12.477663 11.832592 20.637533
C 11.515253 14.086004 32.595383	C 16.186771 14.179397 21.532280
C 12.058208 12.731937 32.699688	C 15.666126 15.428606 21.529373
C 14.771504 12.193505 32.797367	C 12.769735 15.806837 21.520905
C 15.772107 13.327150 32.778221	C 11.954741 14.726755 21.518269
C 14.746490 15.986925 32.760712	C 13.080431 12.020659 21.527153
C 13.309696 16.268299 32.669071	C 14.422505 11.847077 21.532970
V 13.761806 14.050556 32.588371	C 14.946544 15.846595 22.743338
V 14.322518 13.823901 35.258755	C 13.565141 16.025423 22.739292
V 16.027023 12.133152 34.499416	C 11.955434 13.899169 22.734850
V 11.891970 14.334023 34.522572	C 12.490427 12.612915 22.738764
V 15.925694 14.898941 34.007877	C 15.133977 12.269346 22.750265
V 13.425484 15.997578 34.614269	C 15.973829 13.381473 22.750467
V 13.238041 12.055419 34.279793	C 12.872929 15.777151 23.994133
V 14.721799 13.324459 37.835060	C 12.004910 14.629272 23.991360
V 15.582952 15.367313 36.692966	C 13.041484 12.142421 23.998890
V 12.784520 14.792009 36.931095	C 14.469064 11.959121 24.005377
V 12.464946 12.851426 36.542900	C 16.099428 14.104155 24.005861
V 15.024333 11.785792 36.659790	C 15.543531 15.432038 24.002880
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	C 12.443898 12.567729 25.219187

C 15.146694 12.221807 25.230558
C 16.028730 13.380194 25.231428
C 14.976179 15.893804 25.225933
C 13.531530 16.079359 25.221647
C 13.038695 12.151816 26.452579
C 14.455147 11.971889 26.460060
C 16.091236 14.110606 26.461527
C 15.537600 15.427034 26.458166
C 12.865121 15.767366 26.450211
C 11.997037 14.633791 26.447609
C 15.118512 12.265430 27.712910
C 15.984258 13.390079 27.714907
C 14.948251 15.859413 27.709200
C 13.540662 16.033701 27.705793
C 11.906258 13.909158 27.700115
C 12.457405 12.602516 27.698477
C 16.099173 14.110429 28.955954
C 15.544204 15.444312 28.953428
C 12.854794 15.778228 28.945713
C 11.976136 14.632134 28.945030
C 13.014836 12.135106 28.939806
C 14.445292 11.962034 28.949383
C 14.974717 15.920840 30.177212
C 13.517966 16.084993 30.172630
C 11.845972 13.907376 30.169479
C 12.401013 12.549723 30.162115
C 15.128836 12.215193 30.181067

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C 12.844639 15.763721 31.398550
C 11.975267 14.630606 31.406128
C 13.006302 12.128972 31.385912
C 14.421843 11.959850 31.398670
C 16.071108 14.121199 31.401741
C 15.541690 15.442948 31.403736
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C 12.429143 12.587092 32.664173
C 15.063993 12.275917 32.679264
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C 14.949951 15.816370 32.700893
C 13.541693 16.040485 32.649086
Cr 13.882262 14.043946 33.345642
Cr 14.028053 14.099155 35.423752
Cr 15.748846 12.324478 34.596695
Cr 11.632832 14.165973 34.693295
Cr 16.050480 14.816827 34.295292
Cr 13.573852 16.376457 34.564529
Cr 13.226444 11.715891 34.332550
Cr 13.702940 13.974611 38.087975
Cr 15.016241 16.022879 36.850433
Cr 12.432460 15.616940 36.674919
Cr 12.311253 12.582922 36.614658
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Cr 16.019423 13.884031 36.981949

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H 15.875685 15.840169 20.637260
H 16.633869 13.451900 20.684702
H 14.755874 11.402200 20.710806
H 12.304675 11.915504 20.693584
C 16.209385 13.939410 21.563404
C 15.801277 15.229240 21.537861
C 12.940500 15.838117 21.519833
C 12.027420 14.839258 21.536085
C 12.916289 12.059655 21.585062
C 14.241009 11.782356 21.594147
C 15.115131 15.723479 22.743000
C 13.751274 16.010166 22.734667
C 11.950357 14.036966 22.766371
C 12.370938 12.707752 22.789288
C 14.983109 12.153983 22.807175
C 15.923448 13.183458 22.792297
C 13.041499 15.843788 23.992611
C 12.071859 14.779696 24.009472
C 12.883986 12.212379 24.054497
C 14.293123 11.918151 24.062527
C 16.114058 13.910715 24.034616
C 15.676933 15.283556 24.009151
C 11.890402 14.095533 25.246321
C 12.328953 12.707633 25.270002

C 14.991597 12.141927 25.283117
C 15.976099 13.214298 25.268835
C 15.148720 15.809751 25.222292
C 13.724257 16.112514 25.213823
C 12.888920 12.261007 26.508423
C 14.285621 11.964972 26.514675
C 16.102440 13.955883 26.486378
C 15.667807 15.316068 26.462708
C 13.035741 15.882330 26.448048
C 12.073404 14.827049 26.464390
C 14.977956 12.217046 27.759388
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C 15.121175 15.821165 27.704042
C 13.731437 16.119295 27.697353
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C 12.062222 14.920964 31.407518	H 11.422981 14.641965 20.645304
C 12.879004 12.322302 31.440357	H 15.852228 15.916602 20.648363
C 14.284183 12.025288 31.446093	H 16.619101 13.529065 20.645548
C 16.119425 14.046396 31.423033	H 14.738169 11.445033 20.643057
C 15.675285 15.400488 31.394112	H 12.285697 11.967244 20.641821
C 11.973571 14.253027 32.705154	C 16.192152 13.997620 21.533346
C 12.398632 12.863452 32.719971	C 15.778765 15.285550 21.535089
C 14.934577 12.328173 32.730343	C 12.912074 15.895138 21.536556
C 15.901767 13.402889 32.724201	C 12.004921 14.891546 21.533604
C 15.110187 15.826164 32.689995	C 12.904537 12.103516 21.529778
C 13.729731 16.096556 32.683456	C 14.228039 11.822345 21.530399
Mn 13.967268 14.039359 33.324638	C 15.092451 15.752347 22.751154
Mn 13.993628 14.004480 35.482388	C 13.731007 16.039116 22.751307
Mn 15.969017 12.455359 34.523739	C 11.942057 14.061556 22.747026
Mn 11.444115 13.373749 34.481632	C 12.368419 12.737535 22.745440
Mn 16.093666 15.075302 34.250984	C 14.975655 12.183722 22.746599
Mn 12.520498 15.827023 34.246750	C 15.908954 13.215594 22.748646
Mn 13.493470 11.738089 34.221981	C 13.025297 15.845263 24.009684
Mn 13.997645 14.024858 38.053326	C 12.061373 14.781496 24.006973
Mn 14.398023 15.940273 36.387646	C 12.885599 12.220536 24.004057
Mn 12.015398 14.883217 36.610786	C 14.291121 11.925038 24.005095
Mn 12.449923 12.472143 36.558197	C 16.098036 13.921450 24.009022
Mn 14.652521 11.975624 36.584362	C 15.657609 15.288346 24.010092
Mn 16.151630 14.013508 36.611908	C 11.878389 14.073492 25.231045
	C 12.324256 12.686615 25.228703

C 14.991284 12.124998 25.230957
C 15.970210 13.203591 25.234951
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C 13.708469 16.095770 25.235611
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C 14.284770 11.923361 26.458454
C 16.095407 13.924359 26.465481
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C 13.020419 15.839812 26.463348
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C 14.971689 12.162541 27.710417
C 15.918959 13.215556 27.716846
C 15.103416 15.762304 27.715687
C 13.718534 16.047752 27.714062
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C 12.350463 12.711616 27.707626
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C 13.697390 16.117924 30.183449
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C 14.994852 12.094371 30.180624

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C 14.267595 11.860161 31.384150
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C 15.673123 15.302679 31.412107
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C 12.465413 12.715668 32.677395
C 14.868289 12.204346 32.676552
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Fe 14.013144 14.110475 33.266396
Fe 13.975306 13.999531 35.572872
Fe 15.845177 13.060961 34.606201
Fe 11.892697 13.887225 34.608265
Fe 15.488240 15.565506 34.606030
Fe 13.117857 15.998380 34.539272
Fe 13.559832 11.948492 34.212708
Fe 14.166319 13.932563 37.946526
Fe 14.311445 16.163733 36.643623
Fe 12.246639 14.906893 36.863388
Fe 12.537682 12.405815 36.542068
Fe 14.813596 12.014476 36.584518
Fe 16.118357 14.303648 36.661026

06H60C13Co

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H 11.438389 14.641621 20.659939	C 15.964869 13.213278 25.243877
H 15.822788 15.926318 20.662548	C 15.131112 15.804949 25.250343
H 16.588903 13.542701 20.654217	C 13.707033 16.100128 25.251799
H 14.737381 11.494266 20.648010	C 12.885663 12.222326 26.473091
H 12.287798 12.010994 20.650810	C 14.283355 11.933752 26.471998
C 16.180635 14.011933 21.550220	C 16.090405 13.931272 26.477390
C 15.766084 15.300636 21.554188	C 15.656236 15.291193 26.479513
C 12.914085 15.902988 21.559065	C 13.021585 15.841165 26.482183
C 12.004658 14.900422 21.555538	C 12.063842 14.783547 26.480915
C 12.901240 12.128558 21.545000	C 14.972901 12.161476 27.722355
C 14.225782 11.849366 21.543573	C 15.928150 13.218893 27.726200
C 15.092250 15.770872 22.773697	C 15.110238 15.773603 27.728664
C 13.724246 16.055546 22.775864	C 13.717493 16.060347 27.729918
C 11.929252 14.074844 22.770035	C 11.913583 14.066905 27.728354
C 12.359317 12.745729 22.765238	C 12.343958 12.707808 27.723415
C 14.973292 12.193239 22.762693	C 16.096226 13.925033 28.965055
C 15.910919 13.229226 22.765680	C 15.664321 15.301922 28.966475
C 13.019949 15.858727 24.028521	C 13.017411 15.851441 28.966801
C 12.050128 14.790560 24.026304	C 12.051517 14.780466 28.966116
C 12.877842 12.226091 24.016697	C 12.871180 12.198421 28.957830
C 14.290758 11.930879 24.015629	C 14.284330 11.905473 28.956278
C 16.099957 13.931618 24.021311	C 15.139452 15.821548 30.192059
C 15.659105 15.305820 24.025139	C 13.705200 16.116199 30.193153
C 11.879080 14.078755 25.247574	C 11.879609 14.066374 30.197374
C 12.323820 12.693741 25.242136	C 12.310161 12.668385 30.191755
	C 14.988493 12.102456 30.189413

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C 12.868382 12.151360 31.400930	H 15.822020 15.897697 20.668312
C 14.267956 11.853588 31.398582	H 16.583706 13.512508 20.660572
C 16.083591 13.933708 31.416689	H 14.727442 11.469243 20.654419
C 15.675422 15.308836 31.420576	H 12.279114 11.988550 20.657282
C 11.975680 14.022635 32.662621	C 16.177624 13.983733 21.556505
C 12.437657 12.694372 32.692478	C 15.765892 15.273295 21.560652
C 14.886205 12.173858 32.688141	C 12.915092 15.880947 21.566238
C 15.850456 13.199092 32.656151	C 12.002971 14.880337 21.564489
C 15.110823 15.810254 32.679729	C 12.892600 12.106198 21.551426
C 13.727370 16.102753 32.680668	C 14.217019 11.825235 21.550220
Co 14.029703 14.139972 33.120331	C 15.093724 15.744981 22.780367
Co 14.008396 13.975777 35.555283	C 13.726619 16.032961 22.782675
Co 15.884912 12.980175 34.528214	C 11.926905 14.055642 22.778561
Co 11.880359 13.855600 34.539818	C 12.351759 12.724300 22.771675
Co 15.573265 15.402947 34.532646	C 14.965226 12.168265 22.768587
Co 13.169697 15.929008 34.543888	C 15.905085 13.201904 22.771872
Co 13.590864 12.089733 34.264885	C 13.022454 15.837801 24.035831
Co 13.992454 13.854953 37.841656	C 12.050188 14.773739 24.033875
Co 14.452134 15.982058 36.628231	C 12.871464 12.206732 24.022688
Co 12.207162 14.945545 36.632477	C 14.281508 11.907369 24.020639
Co 12.462421 12.535489 36.515030	C 16.095751 13.904608 24.027710
Co 14.818636 12.020632 36.507484	C 15.658972 15.278461 24.032185
Co 16.060587 14.104635 36.616909	C 11.873586 14.063104 25.256401
	C 12.318755 12.678964 25.248526

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C 15.961277 13.184797 25.250597
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C 13.709951 16.075912 25.260504
C 12.878958 12.202773 26.475986
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C 16.090593 13.899514 26.485685
C 15.656968 15.261034 26.487101
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C 15.924429 13.184594 27.732578
C 15.109365 15.739749 27.734800
C 13.719453 16.032858 27.735899
C 11.910183 14.047346 27.736567
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C 15.664175 15.265888 28.973866
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C 12.053511 14.756419 28.980797
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C 14.278296 11.868599 28.954159
C 15.141623 15.790211 30.195866
C 13.709227 16.092104 30.197048
C 11.894171 14.034917 30.210556
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C 13.011130 15.852616 31.429930
C 12.090456 14.743627 31.442310
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C 12.047327 13.964799 32.679520
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C 13.745841 16.128796 32.664169
Ni 14.046757 14.188892 33.197651
Ni 14.035673 14.090182 35.518295
Ni 15.975383 13.109736 34.517673
Ni 11.856987 14.006658 34.526897
Ni 15.622934 15.554705 34.481747
Ni 13.174018 16.078798 34.481491
Ni 13.603085 12.093658 34.159935
Ni 13.983169 14.042114 37.822189
Ni 14.418028 16.085564 36.620941
Ni 12.191664 15.174307 36.573349
Ni 12.465742 12.716653 36.490578
Ni 14.827307 12.194046 36.489975
Ni 16.071650 14.320883 36.586487

06H60C13Cu

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H 16.573629 13.512236 20.654892
H 14.751492 11.489779 20.658171
H 12.307071 11.998047 20.654617
C 16.180525 13.986461 21.555101
C 15.766137 15.276628 21.553795
C 12.926398 15.862393 21.548414
C 12.016949 14.857055 21.550716
C 12.910655 12.103498 21.557055
C 14.237378 11.826652 21.559240
C 15.098087 15.758085 22.769831
C 13.722925 16.043743 22.767164
C 11.927321 14.047779 22.771755
C 12.356527 12.709253 22.774475
C 14.983007 12.167023 22.776865
C 15.925510 13.208672 22.773970
C 13.018961 15.845342 24.014175
C 12.045235 14.773424 24.015976
C 12.881291 12.204857 24.021301
C 14.299889 11.906517 24.023323
C 16.104301 13.919563 24.019627
C 15.663867 15.299810 24.017918
C 11.885689 14.067163 25.242731
C 12.331934 12.687055 25.244600

C 14.991246 12.131029 25.246792
C 15.964216 13.206714 25.245722
C 15.124971 15.790621 25.240927
C 13.704809 16.086336 25.240738
C 12.889199 12.218318 26.479086
C 14.288744 11.930102 26.482687
C 16.094439 13.926128 26.478979
C 15.652455 15.284412 26.475477
C 13.018822 15.837495 26.475777
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C 14.981953 12.156007 27.726782
C 15.950017 13.212384 27.728077
C 15.109509 15.770985 27.720428
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C 12.033269 14.784019 28.958521
C 12.880202 12.208842 28.952934
C 14.291600 11.907549 28.958458
C 15.138256 15.807238 30.176754
C 13.710131 16.080292 30.188425
C 11.874294 14.073572 30.189201
C 12.323853 12.688316 30.182541
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C 12.061811 14.778060 31.432747	H 11.301010 14.690685 20.633091
C 12.867328 12.173991 31.404779	H 15.669805 16.058029 20.588980
C 14.266428 11.885338 31.413603	H 16.504711 13.696756 20.526203
C 16.106636 13.938313 31.420219	H 14.693062 11.572285 20.513521
C 15.673526 15.305499 31.411806	H 12.232523 12.043162 20.557119
C 11.874795 13.987868 32.647404	C 16.089334 14.136961 21.433527
C 12.297607 12.647549 32.660851	C 15.637849 15.412235 21.467293
C 14.950977 12.187158 32.662312	C 12.766654 15.967756 21.529366
C 15.902665 13.196838 32.654533	C 11.886948 14.939842 21.518690
C 15.129598 15.839014 32.641911	C 12.859847 12.172293 21.440117
C 13.757200 16.202129 32.661400	C 14.188755 11.918280 21.416569
Cu 13.914386 14.151978 33.211761	C 14.966517 15.840622 22.704889
Cu 13.980494 14.051702 35.613773	C 13.597538 16.106316 22.735706
Cu 15.755572 12.589710 34.518826	C 11.861813 14.082274 22.715054
Cu 11.728324 14.273101 34.567574	C 12.325186 12.767578 22.675909
Cu 15.885674 15.099896 34.325848	C 14.947159 12.266603 22.628508
Cu 13.265971 16.243540 34.549099	C 15.855404 13.324207 22.637285
Cu 13.312397 12.014516 34.258980	C 12.917310 15.870440 23.997004
Cu 14.063538 13.950994 38.012642	C 11.976348 14.777726 23.987087
Cu 14.790090 16.016569 36.571522	C 12.871330 12.235995 23.911491
Cu 12.387191 15.344028 36.748680	C 14.287699 11.968250 23.885967
Cu 12.209010 12.849689 36.576595	C 16.049377 14.007726 23.903585
Cu 14.523741 11.943057 36.526760	C 15.565512 15.365241 23.939648
Cu 16.146629 13.920784 36.547951	C 11.837911 14.039384 25.196850
	C 12.324909 12.667006 25.151958

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C 12.922889 12.187177 26.361607
C 14.323936 11.925471 26.335896
C 16.084652 13.958297 26.360308
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C 12.960546 15.797230 26.450779
C 12.026461 14.720677 26.444817
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C 15.963978 13.215927 27.603317
C 15.069475 15.743797 27.666033
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C 11.919621 13.970833 27.685169
C 12.393474 12.632584 27.634005
C 16.143829 13.900661 28.859940
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C 12.990411 15.766836 28.937847
C 12.049391 14.661338 28.940662
C 12.947241 12.092579 28.842575
C 14.376872 11.828097 28.816118
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Zn 13.061427 16.565025 34.454876
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H 12.762678 11.755000 20.684551	C 14.330952 12.047001 26.640120
C 16.394129 13.968194 21.743860	C 15.994170 14.156716 26.646921
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C 13.040012 15.651566 21.432533	C 12.805798 15.854418 26.342606
C 12.199432 14.584709 21.426926	C 11.920977 14.736651 26.337654
C 13.281830 11.910650 21.631266	C 14.939425 12.348639 27.908836
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C 12.066137 13.829210 22.675035	C 11.702371 14.080857 27.599072
C 12.598461 12.516295 22.775597	C 12.247841 12.737704 27.695889
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Y 15.860346 16.020443 37.041241	C 13.018385 12.145391 24.004658
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C 12.286050 12.704903 27.667164	Zr 16.458857 11.942776 34.280312
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C 12.775442 12.256512 28.933006	Zr 14.587298 13.432863 38.458187
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C 12.998104 15.836842 23.921902	C 12.824319 15.954246 28.865238
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Nb 14.169653 13.719101 35.483871	C 13.652422 16.026352 22.696281
Nb 16.245750 12.209283 34.607105	C 11.977018 13.942984 22.676294
Nb 11.440222 13.851960 34.580948	C 12.489711 12.640922 22.688744
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Nb 12.979287 16.066109 34.753712	C 16.011152 13.316849 22.747482
Nb 13.219977 11.713769 34.195873	C 12.939992 15.799029 23.936026
Nb 14.451816 13.766972 38.314110	C 12.031328 14.673429 23.925535
Nb 15.093090 15.815077 36.822342	C 13.014156 12.158318 23.950338
Nb 12.182650 14.772679 37.159882	C 14.445791 11.932693 23.977058
Nb 12.427586 12.278340 36.856632	C 16.138201 14.038465 23.995857
Nb 15.221515 11.703038 37.131035	C 15.611444 15.388787 23.981396
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06H60C13Tc

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C 14.703808 15.957033 25.565409	C 15.460464 15.275853 30.590294
C 13.397619 15.924352 26.213634	C 14.454594 15.986025 29.815613
C 12.466967 15.110126 25.442316	C 13.145159 15.951967 30.468359

C 11.744244 13.922534 31.783352
C 12.126190 12.728012 32.560997
C 13.247791 12.021788 31.902317
C 14.469264 12.060469 32.746872
C 15.499571 12.861034 32.033936
C 15.813416 14.101638 32.776951
C 15.378011 15.281545 31.999773
C 14.298420 16.017670 32.698128
C 13.061284 15.961250 31.880970
C 12.030579 15.150412 32.553185
V 14.537476 16.158535 34.719578
V 11.455677 14.837320 34.489059
V 13.717331 14.019228 33.157799
V 12.479383 15.943627 36.859947
V 15.839080 14.231028 34.778366
V 15.202826 15.271883 37.091759
V 13.418006 14.301274 35.625809
V 11.916498 12.510434 34.543304
V 11.114457 13.698515 36.645164
V 14.381721 12.162221 34.801785
V 13.007937 14.342843 38.143990
V 15.212478 13.256880 37.098141
V 12.891837 12.240337 36.977184

05H60C13Cr

H 12.856101 12.640569 20.142548
H 15.169676 11.972655 20.286863

H 16.498440 13.983994 20.339287
H 15.015938 15.883292 20.225945
H 12.748267 15.052381 20.103409
C 16.377432 13.995780 21.423855
C 15.951308 15.190844 22.086145
C 14.934291 15.837653 21.313311
C 13.645857 15.850739 21.940620
C 12.737047 15.030886 21.194492
C 12.317562 13.850016 21.889145
C 12.838105 12.689535 21.232796
C 13.800036 11.960384 22.000784
C 15.084387 12.043376 21.372604
C 16.048159 12.790777 22.123432
C 15.844385 15.193610 23.509054
C 14.784636 15.942941 24.159481
C 13.570843 15.845799 23.362825
C 12.520338 15.102220 24.036850
C 12.260076 13.870339 23.312693
C 12.614958 12.682780 24.072147
C 13.723848 12.004867 23.423534
C 14.937881 12.021878 24.219847
C 15.942295 12.824698 23.543901
C 16.271210 14.037504 24.272068
C 14.694201 15.944605 25.561033
C 13.385469 15.924513 26.208015
C 12.451499 15.110256 25.440468
C 12.046103 13.905009 26.153021

C 12.543244 12.711802 25.473951
C 13.546879 12.016273 26.267599
C 14.848511 12.060180 25.621733
C 15.819934 12.832329 26.392311
C 16.169867 14.055133 25.674252
C 15.695513 15.247352 26.354771
C 13.305986 15.930194 27.607437
C 12.279365 15.145823 28.274563
C 11.974036 13.922020 27.552734
C 12.359892 12.738178 28.319105
C 13.467637 12.048060 27.673426
C 14.685760 12.084414 28.461441
C 15.733539 12.850748 27.787025
C 16.016272 14.085668 28.515831
C 15.601005 15.253227 27.760742
C 14.527931 15.991778 28.412067
C 12.190216 15.164426 29.684118
C 11.777769 13.964257 30.391123
C 12.280204 12.765924 29.717213
C 13.309976 12.119567 30.510021
C 14.604904 12.107183 29.864849
C 15.609857 12.852122 30.631168
C 15.929888 14.095414 29.920425
C 15.409711 15.261614 30.598438
C 14.437062 15.999071 29.810837
C 13.120683 15.978147 30.450178
C 11.693714 13.989862 31.797167

C 12.107753 12.832926 32.612492
C 13.229043 12.149614 31.937468
C 14.458574 12.148030 32.742455
C 15.540791 12.857414 32.022781
C 15.766814 14.097884 32.797863
C 15.317819 15.266171 32.026203
C 14.238974 16.014189 32.702866
C 13.031024 15.986714 31.856270
C 12.025774 15.192164 32.562794
Cr 14.367422 16.251240 34.682701
Cr 11.664679 15.375945 34.587708
Cr 13.707692 14.048805 33.255741
Cr 12.907222 16.226994 36.539146
Cr 16.083771 14.149333 34.776279
Cr 15.293369 15.542537 37.029163
Cr 13.670064 14.008618 35.524216
Cr 11.888478 12.541367 34.577286
Cr 11.301949 13.824848 36.465851
Cr 14.483476 11.756165 34.707066
Cr 13.087682 14.322464 38.115128
Cr 14.983192 13.088982 37.081665
Cr 12.834736 11.862925 36.922169

05H60C13Mn

H 12.866961 12.640942 20.139511
H 15.185762 11.989454 20.284739
H 16.509768 13.999232 20.339897

H 15.012701 15.879745 20.226210	C 13.553563 11.998331 26.263258
H 12.757499 15.043498 20.104431	C 14.860499 12.063374 25.617329
C 16.388205 14.010444 21.424377	C 15.815069 12.850718 26.388783
C 15.955105 15.202891 22.087433	C 16.182562 14.067641 25.673136
C 14.933926 15.841084 21.314001	C 15.712770 15.267388 26.357447
C 13.646473 15.846829 21.941826	C 13.309090 15.920236 27.608458
C 12.741939 15.024955 21.195526	C 12.275647 15.139307 28.279261
C 12.322428 13.845225 21.888706	C 11.983438 13.909599 27.553104
C 12.847517 12.687868 21.229721	C 12.372143 12.725329 28.311846
C 13.816051 11.966931 21.997522	C 13.471715 12.019951 27.660078
C 15.099817 12.057794 21.370554	C 14.691948 12.084445 28.455917
C 16.061682 12.804993 22.123373	C 15.722300 12.870143 27.785984
C 15.849449 15.205931 23.509216	C 16.024240 14.096901 28.516781
C 14.781896 15.942951 24.161787	C 15.623448 15.276887 27.755709
C 13.570483 15.840876 23.365768	C 14.528296 15.986903 28.407978
C 12.518862 15.098196 24.039062	C 12.186962 15.156560 29.677994
C 12.264705 13.864882 23.312824	C 11.799145 13.938928 30.386206
C 12.626048 12.680295 24.070423	C 12.285151 12.737911 29.710344
C 13.737387 12.007072 23.419626	C 13.297703 12.038889 30.499300
C 14.951519 12.029788 24.217812	C 14.608509 12.094398 29.856514
C 15.954199 12.837500 23.543922	C 15.563424 12.887572 30.624628
C 16.283157 14.050219 24.273682	C 15.943976 14.108887 29.916294
C 14.694562 15.946735 25.563885	C 15.461758 15.310138 30.595251
C 13.387970 15.915949 26.210407	C 14.444921 16.004843 29.807827
C 12.451166 15.104962 25.440931	C 13.132822 15.961953 30.446815
C 12.056007 13.895254 26.154123	C 11.713866 13.955913 31.794044
C 12.552137 12.704700 25.471497	C 12.164852 12.813643 32.591251

C 13.212214 12.054779 31.907803
C 14.407745 12.193241 32.734367
C 15.476718 12.900936 32.033001
C 15.695855 14.132113 32.790726
C 15.373896 15.323608 32.003021
C 14.251038 15.975085 32.684772
C 13.046516 15.977164 31.855576
C 12.062710 15.155925 32.559719
Mn 14.260775 16.279253 34.630260
Mn 11.658113 15.319230 34.481537
Mn 13.674362 14.061212 33.361973
Mn 12.648684 16.272457 36.864746
Mn 15.947273 14.192780 34.755104
Mn 15.093933 15.399808 36.852436
Mn 13.531662 14.091417 35.692436
Mn 11.741946 12.636342 34.515057
Mn 11.408615 14.016934 36.625004
Mn 14.399551 11.918588 34.698391
Mn 13.372910 14.113584 38.176033
Mn 15.322991 12.833534 36.968391
Mn 12.857295 11.898031 36.845322

05H60C13Fe

H 12.866741 12.648074 20.137232
H 15.184005 11.993667 20.280249
H 16.510353 14.000409 20.338057
H 15.012943 15.881150 20.226213

H 12.754265 15.049235 20.103827
C 16.388605 14.010056 21.422602
C 15.954659 15.201450 22.086290
C 14.933888 15.841824 21.314072
C 13.646670 15.848272 21.941601
C 12.739306 15.029535 21.194927
C 12.320851 13.848535 21.887623
C 12.845834 12.691993 21.227602
C 13.814539 11.970308 21.993429
C 15.098713 12.058538 21.366383
C 16.061047 12.804198 22.119915
C 15.848653 15.202483 23.509050
C 14.782741 15.939737 24.161402
C 13.570997 15.841145 23.365633
C 12.519247 15.099422 24.039003
C 12.264544 13.866725 23.312338
C 12.626724 12.682096 24.068449
C 13.736554 12.009169 23.417038
C 14.950067 12.028833 24.214970
C 15.953776 12.835275 23.541050
C 16.282679 14.046751 24.271534
C 14.696186 15.941436 25.564751
C 13.390599 15.914608 26.211721
C 12.453561 15.104563 25.441717
C 12.056814 13.895641 26.153673
C 12.554870 12.707157 25.471382
C 13.553914 11.999232 26.261990

C 14.859517 12.062016 25.615788
C 15.816592 12.845407 26.387531
C 16.181038 14.062885 25.672276
C 15.713438 15.261986 26.356674
C 13.313007 15.916333 27.611332
C 12.276800 15.139213 28.280762
C 11.987244 13.909525 27.554296
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C 13.473014 12.023213 27.661427
C 14.692540 12.078865 28.456802
C 15.721355 12.866347 27.786196
C 16.024303 14.091867 28.516262
C 15.621447 15.268866 27.757113
C 14.532185 15.984708 28.409657
C 12.192289 15.153359 29.681547
C 11.804143 13.937291 30.388498
C 12.291052 12.740608 29.713217
C 13.299250 12.041630 30.504034
C 14.607778 12.093117 29.858616
C 15.565611 12.882687 30.625170
C 15.938621 14.104161 29.917955
C 15.459437 15.301634 30.599766
C 14.447572 15.997379 29.811697
C 13.135942 15.961590 30.450182
C 11.721670 13.952291 31.795980
C 12.134581 12.790209 32.603947
C 13.215497 12.060897 31.913944

C 14.432773 12.143167 32.738419
C 15.480058 12.897573 32.030075
C 15.746895 14.125298 32.797405
C 15.370099 15.311756 32.010250
C 14.262854 16.001188 32.697247
C 13.051804 15.971811 31.855791
C 12.031766 15.173757 32.554249
Fe 14.149255 16.110502 34.672035
Fe 11.849767 15.243858 34.491310
Fe 13.691505 14.052497 33.162525
Fe 12.726456 16.047276 36.783134
Fe 15.711094 14.119100 34.757816
Fe 15.105494 15.389289 36.906845
Fe 13.527471 14.087948 35.702354
Fe 11.927367 12.779613 34.576187
Fe 11.378756 14.035699 36.722755
Fe 14.365203 12.102744 34.696907
Fe 13.356844 14.124414 38.176647
Fe 15.165308 12.954813 36.973980
Fe 12.895311 12.082726 36.805870

05H60C13Co

H 12.841282 12.643541 20.158041
H 15.154999 11.997596 20.300953
H 16.497444 13.998158 20.353355
H 15.020215 15.887094 20.245853
H 12.767466 15.047894 20.127630

C 16.381216 14.009809 21.438425
C 15.963575 15.205652 22.105957
C 14.942761 15.847803 21.333683
C 13.656938 15.847805 21.963409
C 12.750074 15.030585 21.218832
C 12.316207 13.856151 21.909508
C 12.824781 12.691033 21.248173
C 13.792315 11.966576 22.016338
C 15.073812 12.061919 21.387554
C 16.037292 12.807907 22.135689
C 15.861856 15.206634 23.526863
C 14.792909 15.942035 24.183952
C 13.582623 15.838617 23.388847
C 12.528133 15.101740 24.060888
C 12.258531 13.872892 23.333565
C 12.607701 12.682817 24.090200
C 13.717648 12.007654 23.438368
C 14.933576 12.035598 24.234652
C 15.934144 12.839556 23.559692
C 16.282284 14.043284 24.290743
C 14.709613 15.943019 25.586170
C 13.405980 15.902816 26.234694
C 12.462627 15.104943 25.464329
C 12.048772 13.899099 26.173920
C 12.536798 12.705667 25.489988
C 13.537714 11.994827 26.282906
C 14.843543 12.068596 25.636459

C 15.797843 12.851740 26.407804
C 16.184593 14.060188 25.692057
C 15.735315 15.268856 26.378826
C 13.330179 15.901720 27.636362
C 12.288262 15.133276 28.302271
C 11.978106 13.910450 27.571848
C 12.353290 12.719416 28.331133
C 13.455611 12.016917 27.679186
C 14.676035 12.086962 28.476793
C 15.702341 12.874144 27.809521
C 16.029469 14.092095 28.538559
C 15.647834 15.279702 27.774519
C 14.548316 15.986213 28.430645
C 12.204241 15.143115 29.702473
C 11.790302 13.932819 30.408726
C 12.269177 12.730655 29.730019
C 13.277149 12.022593 30.520451
C 14.589262 12.101245 29.877035
C 15.525251 12.907484 30.643744
C 15.944123 14.108658 29.939262
C 15.499284 15.326612 30.622929
C 14.464864 15.999695 29.831367
C 13.160881 15.924937 30.471704
C 11.705969 13.947908 31.813944
C 12.138251 12.794245 32.614918
C 13.193640 12.037723 31.923813
C 14.401400 12.156399 32.762787

C 15.435480 12.924337 32.059242
C 15.730612 14.141764 32.823029
C 15.415138 15.340631 32.023109
C 14.283687 15.985636 32.716583
C 13.075737 15.935092 31.885151
C 12.048691 15.154729 32.587822
Co 14.203317 16.103737 34.649368
Co 11.863039 15.231322 34.502098
Co 13.690448 14.052408 33.201496
Co 12.807944 16.075968 36.580490
Co 15.712294 14.172149 34.761532
Co 15.132163 15.398150 36.766380
Co 13.542316 14.085320 35.604816
Co 11.936269 12.762888 34.547134
Co 11.383971 13.961152 36.546425
Co 14.310070 12.101242 34.688068
Co 13.399175 14.107052 37.821987
Co 15.229787 12.967499 36.764156
Co 12.844047 12.093838 36.658775

05H60C13Ni

H 12.867932 12.650930 20.159201
H 15.175162 11.999988 20.300377
H 16.494938 14.005086 20.354908
H 15.014842 15.884389 20.248075
H 12.769525 15.050739 20.125889
C 16.383165 14.014690 21.440483

C 15.955572 15.206066 22.107536
C 14.936817 15.848900 21.336018
C 13.651469 15.855047 21.964569
C 12.748725 15.033985 21.216848
C 12.327549 13.855270 21.908846
C 12.845927 12.695374 21.249397
C 13.811695 11.971290 22.016413
C 15.093549 12.062125 21.386808
C 16.054440 12.810055 22.138308
C 15.852491 15.205569 23.531096
C 14.787431 15.943930 24.187208
C 13.576435 15.847107 23.388737
C 12.524302 15.104632 24.061098
C 12.268827 13.873113 23.333647
C 12.626282 12.686380 24.089907
C 13.735472 12.011640 23.439146
C 14.949731 12.032429 24.236736
C 15.951288 12.839442 23.561161
C 16.283922 14.048599 24.294428
C 14.701182 15.945175 25.588470
C 13.392785 15.918447 26.235558
C 12.455043 15.110353 25.462095
C 12.057220 13.899233 26.173059
C 12.553759 12.709150 25.489937
C 13.554585 11.999878 26.283123
C 14.861772 12.062733 25.636600
C 15.819700 12.845177 26.411081

C 16.186127 14.063035 25.695078
C 15.718025 15.262348 26.381876
C 13.312404 15.922193 27.631439
C 12.275382 15.140491 28.299915
C 11.983776 13.911552 27.570297
C 12.372365 12.726452 28.329563
C 13.472582 12.020676 27.679039
C 14.693984 12.077386 28.476694
C 15.727072 12.862954 27.807512
C 16.025146 14.089960 28.540588
C 15.626525 15.270660 27.779034
C 14.532634 15.985255 28.431782
C 12.186725 15.155119 29.698229
C 11.805533 13.937067 30.406851
C 12.285784 12.738127 29.727024
C 13.297016 12.039034 30.517151
C 14.608562 12.086701 29.875565
C 15.558393 12.883171 30.649200
C 15.940820 14.102254 29.939337
C 15.455144 15.299821 30.618681
C 14.446050 16.001879 29.830368
C 13.133587 15.958339 30.471611
C 11.714346 13.950398 31.815018
C 12.146179 12.794631 32.611794
C 13.207982 12.046667 31.923887
C 14.414780 12.155071 32.755077
C 15.476048 12.892365 32.056458

C 15.714490 14.126130 32.818432
C 15.370781 15.313695 32.025833
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C 13.044613 15.977642 31.876495
C 12.044491 15.160084 32.580208
Ni 14.162254 16.110638 34.614994
Ni 11.780713 15.261527 34.467621
Ni 13.678058 14.047630 33.245720
Ni 12.749635 16.061741 36.579082
Ni 15.709583 14.153079 34.737377
Ni 15.068857 15.375998 36.751251
Ni 13.512236 14.061147 35.592224
Ni 11.923487 12.730168 34.510410
Ni 11.430227 14.033484 36.558090
Ni 14.322624 12.018598 34.654236
Ni 13.392490 14.125535 37.948483
Ni 15.208317 12.931627 36.765835
Ni 12.945382 12.130653 36.688568

05H60C13Cu

H 12.948115 12.696109 20.136452
H 15.229502 11.868526 20.292679
H 16.419640 13.971233 20.332041
H 14.985182 15.906844 20.233459
H 12.760091 15.104928 20.113966
C 16.344099 13.983875 21.421024
C 15.910974 15.176644 22.079042

C 14.913691 15.867791 21.322121
C 13.628722 15.918691 21.960043
C 12.741850 15.076557 21.205183
C 12.375281 13.871578 21.883121
C 12.890681 12.711318 21.226551
C 13.827174 11.961596 21.988518
C 15.136339 11.947835 21.376801
C 16.057228 12.779747 22.119125
C 15.820609 15.191969 23.507996
C 14.781711 15.953206 24.165276
C 13.555508 15.907475 23.373669
C 12.522115 15.118157 24.040848
C 12.301105 13.887879 23.312494
C 12.656515 12.704439 24.063560
C 13.744111 12.002618 23.412704
C 14.959420 11.992993 24.218180
C 15.951440 12.818458 23.540316
C 16.247646 14.038573 24.266272
C 14.698094 15.949205 25.567503
C 13.390129 15.924664 26.215279
C 12.453739 15.113855 25.442047
C 12.070151 13.897688 26.151039
C 12.569831 12.713593 25.468830
C 13.553745 11.990704 26.258732
C 14.866231 12.031100 25.613409
C 15.812099 12.835901 26.385536
C 16.164612 14.052988 25.671715

C 15.707363 15.252588 26.357088
C 13.311600 15.923227 27.611586
C 12.277045 15.137451 28.278702
C 11.984222 13.908377 27.549707
C 12.373280 12.723114 28.305689
C 13.468184 12.009106 27.656540
C 14.689138 12.067236 28.454662
C 15.720428 12.853995 27.783802
C 16.017405 14.081675 28.513004
C 15.626493 15.266176 27.755810
C 14.534044 15.981666 28.409201
C 12.187342 15.151443 29.675200
C 11.812480 13.932929 30.384872
C 12.280647 12.730856 29.703939
C 13.294138 12.044824 30.499428
C 14.602996 12.078665 29.853270
C 15.543231 12.883969 30.624390
C 15.941370 14.093636 29.912743
C 15.454195 15.287584 30.595669
C 14.452164 15.998457 29.806639
C 13.143414 15.938187 30.449413
C 11.719418 13.945926 31.791340
C 12.131407 12.783177 32.585106
C 13.207559 12.053576 31.908043
C 14.416638 12.143379 32.731125
C 15.463408 12.893685 32.032475
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Cu 12.697433 16.115673 36.734829
Cu 15.804933 14.222801 34.753838
Cu 15.171827 15.395899 36.894821
Cu 13.525411 14.121781 35.808506
Cu 11.831887 12.746838 34.530174
Cu 11.334709 13.983998 36.665321
Cu 14.385881 12.009651 34.695290
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Cu 12.903066 12.082053 36.766953

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