

Anna Kaleta
Piotr Chojnacki
IV rok informatyki chemicznej





Wrocław, 2 czerwca 2006 roku


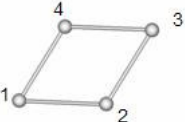
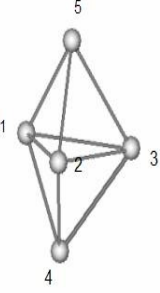
Przedmiot specjalizacyjny II

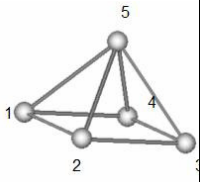

**Przewidywanie najbardziej stabilnych struktur i stanu spinowego
klasterów metali przejściowych w fazie gazowej przy użyciu metody
ZINDO/1**

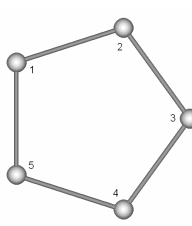
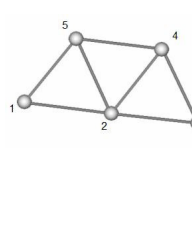
TABELA I

Ni

n	Rysunek klasteru	Multipletowość	Energia względna	Długość wiązania	Kąty walencyjne	Kąty torsyjne	Liczba ujemnych częstości
1		Singlet	-16.0224	-	-	-	-
		Tryplet	0	-	-	-	-
		Kwintet	-6.06141	-	-	-	-
2		Singlet	0	3.91399	-	-	0
		Tryplet	-1.8766	2.87877	-	-	0
		Kwintet	-3.7723	2.90223	-	-	0
3		Singlet	-154.269	r ₁₋₂ 3.85163 r ₂₋₃ 3.87898 r ₁₋₃ 3.87808	< ₁₋₂₋₃ 60.2176 < ₂₋₁₋₃ 60.2407 < ₁₋₃₋₂ 59.5417	-	0
		Tryplet	-59.7279	r ₁₋₂ 4.67526 r ₂₋₃ 4.67994 r ₁₋₃ 4.67995	< ₁₋₂₋₃ 60.0333 < ₂₋₁₋₃ 60.0329 < ₁₋₃₋₂ 59.9338	-	2
		Kwintet	0	r ₁₋₂ 4.47055 r ₂₋₃ 3.94506 r ₁₋₃ 4.35683	< ₁₋₂₋₃ 61.9861 < ₂₋₁₋₃ 53.0724 < ₁₋₃₋₂ 64.9415	-	2
4		Singlet	-165.864	r ₁₋₂ 3.9333 r ₂₋₃ 3.8908 r ₁₋₃ 3.8459 r ₁₋₄ 3.9147 r ₂₋₄ 3.9140 r ₃₋₄ 3.9014	< ₁₋₂₋₃ 58.8808 < ₂₋₁₋₃ 60.0080 < ₁₋₃₋₂ 61.1112 < ₁₋₄₋₂ 60.3218 < ₁₋₄₋₃ 58.9502 < ₂₋₄₋₃ 59.7144	< ₁₋₂₋₃₋₄ -70.8026 < ₂₋₃₋₁₋₄ -70.1735 < ₃₋₁₋₂₋₄ -71.0280 < ₄₋₁₋₂₋₃ 71.028 < ₄₋₂₋₃₋₁ 70.8026 < ₄₋₃₋₁₋₂ 70.1735	0
		Tryplet	-32.6027	r ₁₋₂ 4.55469 r ₂₋₃ 4.49576 r ₁₋₃ 4.62337 r ₁₋₄ 4.39988 r ₂₋₄ 3.93367 r ₃₋₄ 4.2809	< ₁₋₂₋₃ 61.4362 < ₂₋₁₋₃ 58.6541 < ₁₋₃₋₂ 59.9098 < ₁₋₄₋₂ 65.9851 < ₁₋₄₋₃ 64.3453 < ₂₋₄₋₃ 66.2058	< ₁₋₂₋₃₋₄ -72.0494 < ₂₋₃₋₁₋₄ -62.6031 < ₃₋₁₋₂₋₄ -69.9394 < ₄₋₁₋₂₋₃ 69.9394 < ₄₋₂₋₃₋₁ 72.0494 < ₄₋₃₋₁₋₂ 62.6031	2
		Kwintet	0	r ₁₋₂ 4.5445 r ₂₋₃ 4.2618 r ₁₋₃ 4.46372 r ₁₋₄ 4.46692 r ₂₋₄ 4.39144 r ₃₋₄ 3.95296	< ₁₋₂₋₃ 60.812 < ₂₋₁₋₃ 56.4633 < ₁₋₃₋₂ 62.7247 < ₁₋₄₋₂ 61.7225 < ₁₋₄₋₃ 63.6866 < ₂₋₄₋₃ 61.1585	< ₁₋₂₋₃₋₄ -72.2403 < ₂₋₃₋₁₋₄ -73.3886 < ₃₋₁₋₂₋₄ -63.3625 < ₄₋₁₋₂₋₃ 63.3625 < ₄₋₂₋₃₋₁ 72.2403 < ₄₋₃₋₁₋₂ 73.3886	3

		Singlet	-237.978	r_{1-2} 3.8422 r_{2-3} 3.8410 r_{3-4} 3.84010 r_{1-4} 3.8416	\langle_{1-2-3} 89.9880 \langle_{2-3-4} 90.0211 \langle_{3-4-1} 90.0931 \langle_{4-1-2} 89.9816	$\langle_{1-2-3-4}$ -3.62225e-6	2
		Tryplet	-131.645	r_{1-2} 4.85294 r_{2-3} 4.82930 r_{3-4} 4.83340 r_{1-4} 4.83250	\langle_{1-2-3} 89.8993 \langle_{2-3-4} 90.1386 \langle_{3-4-1} 90.0093 \langle_{4-1-2} 89.8690	$\langle_{1-2-3-4}$ -2.39666e-5	4
		Kwintet	0	r_{1-2} 3.8422 r_{2-3} 3.8410 r_{3-4} 3.84010 r_{1-4} 3.8416	\langle_{1-2-3} 89.9880 \langle_{2-3-4} 90.0211 \langle_{3-4-1} 90.0093 \langle_{4-1-2} 89.9816	$\langle_{1-2-3-4}$ -7.45819e-5	3
		Singlet	-98.1426	r_{1-2} 3.91515 r_{2-3} 3.93842 r_{1-3} 3.87677 r_{1-4} 3.81718	\langle_{1-2-3} 60.5742 \langle_{2-3-4} 118.531 \langle_{3-4-1} 61.2611	$\langle_{1-2-3-4}$ -8.20015e-5	1
		Tryplet	0	r_{1-2} 4.86062 r_{2-3} 4.85489 r_{1-3} 4.84295 r_{1-4} 4.85611	\langle_{1-2-3} 89.8962 \langle_{2-3-4} 90.1194 \langle_{3-4-1} 90.0892	$\langle_{1-2-3-4}$ 4.50239e-5	4
		Kwintet	-2.6673	r_{1-2} 4.58926 r_{2-3} 4.63020 r_{1-3} 4.59041 r_{1-4} 4.59930	\langle_{1-2-3} 90.9786 \langle_{2-3-4} 88.6359 \langle_{3-4-1} 91.3577	$\langle_{1-2-3-4}$ -0.000772516	4
5		Singlet	-163.881	r_{1-2} 3.85466 r_{1-3} 3.94560 r_{1-4} 3.90303 r_{2-3} 3.89991 r_{2-4} 3.93221 r_{2-5} 3.89380 r_{3-5} 3.91295 r_{5-4} 3.92473	\langle_{1-2-3} 61.1658 \langle_{2-3-4} 60.2757 \langle_{3-4-2} 59.4615 \langle_{1-4-2} 58.9382 \langle_{1-4-5} 108.799 \langle_{1-2-4} 60.1632 \langle_{2-3-5} 59.7859 \langle_{1-4-2} 59.4168 \langle_{3-4-5} 59.7429	$\langle_{1-2-3-4}$ -69.0026 $\langle_{2-3-1-4}$ 71.7735 $\langle_{3-1-2-4}$ -71.3528 $\langle_{4-1-2-3}$ 71.3528 $\langle_{4-2-3-1}$ 70.8026 $\langle_{4-3-1-2}$ 70.1735 $\langle_{5-2-1-3}$ -36.3273 $\langle_{5-4-3-2}$ -70.1258 $\langle_{2-4-5-3}$ 70.5571	5
		Tryplet	-46.3434	r_{1-2} 4.37952 r_{1-3} 4.34219 r_{1-4} 4.93303 r_{2-3} 4.87991 r_{2-4} 4.81251 r_{2-5} 4.83370 r_{3-5} 4.87245 r_{5-4} 4.95413	\langle_{1-2-3} 52.5982 \langle_{2-3-4} 51.2757 \langle_{3-4-2} 50.4615 \langle_{1-4-2} 49.9382 \langle_{1-4-5} 96.3153 \langle_{1-2-4} 61.1632 \langle_{2-3-5} 52.7859 \langle_{1-4-2} 53.4168 \langle_{3-4-5} 56.7429	$\langle_{1-2-3-4}$ -69.0056 $\langle_{2-3-1-4}$ 71.7778 $\langle_{3-1-2-4}$ -71.3603 $\langle_{4-1-2-3}$ 71.3502 $\langle_{4-2-3-1}$ 70.8026 $\langle_{4-3-1-2}$ 70.1335 $\langle_{5-2-1-3}$ -36.3243 $\langle_{5-4-3-2}$ -70.1270 $\langle_{2-4-5-3}$ 70.5569	4

		Kwintet	0	r_{1-2} 3.76751 r_{1-3} 4.83465 r_{1-4} 4.40869 r_{2-3} 4.82991 r_{2-4} 4.85251 r_{2-5} 4.87370 r_{3-5} 4.81245 r_{5-4} 4.87413	\langle_{1-2-3} 71.8751 \langle_{2-3-4} 58.6630 \langle_{3-4-2} 57.5410 \langle_{1-4-2} 55.4121 \langle_{1-4-5} 84.7536 \langle_{1-2-4} 54.2345 \langle_{2-3-5} 51.2314 \langle_{1-4-2} 52.2144 \langle_{3-4-5} 57.2147	$\langle_{1-2-3-4}$ -69.0061 $\langle_{2-3-1-4}$ 71.7801 $\langle_{3-1-2-4}$ -71.3609 $\langle_{4-1-2-3}$ 71.3511 $\langle_{4-2-3-1}$ 70.8030 $\langle_{4-3-1-2}$ 70.1339 $\langle_{5-2-1-3}$ -36.3132 $\langle_{5-4-3-2}$ -70.1245 $\langle_{2-4-5-3}$ 70.5596	4
		Singlet	-177.299	r_{1-2} 3.92989 r_{1-3} 3.92478 r_{1-4} 3.91474 r_{1-5} 3.89261 r_{3-2} 3.83387 r_{3-4} 3.83603 r_{4-5} 3.83980 r_{5-2} 3.83884	\langle_{1-2-3} 60.7176 \langle_{1-2-4} 60.1381 \langle_{1-5-4} 60.8278 \langle_{1-4-3} 60.8351 \langle_{3-2-5} 89.9540 \langle_{2-5-4} 90.0225 \langle_{5-1-2} 58.7536	$\langle_{1-2-3-4}$ -55.0065 $\langle_{4-2-1-3}$ 54.98602 $\langle_{1-3-2-5}$ -55.0032 $\langle_{3-1-2-5}$ -56.4664 $\langle_{5-3-2-1}$ 54.4734 $\langle_{4-3-5-2}$ 00.00452	7
		Tryplet	75.6616	r_{1-2} 3.99971 r_{1-3} 3.93578 r_{1-4} 3.94574 r_{1-5} 3.88561 r_{3-2} 3.84287 r_{3-4} 3.85203 r_{4-5} 3.84280 r_{5-2} 3.84184	\langle_{1-2-3} 84.6938 \langle_{1-2-4} 60.0161 \langle_{1-5-4} 60.8178 \langle_{1-4-3} 60.8451 \langle_{3-2-5} 88.9640 \langle_{2-5-4} 92.0325 \langle_{5-1-2} 59.7636	$\langle_{1-2-3-4}$ -55.0084 $\langle_{4-2-1-3}$ 54.98632 $\langle_{1-3-2-5}$ -55.0030 $\langle_{3-1-2-5}$ -56.4701 $\langle_{5-3-2-1}$ 54.4734 $\langle_{4-3-5-2}$ 00.00463	1
		Kwintet	0	r_{1-2} 5.23456 r_{1-3} 5.08638 r_{1-4} 5.94374 r_{1-5} 5.84561 r_{3-2} 5.87212 r_{3-4} 5.75203 r_{4-5} 4.63159 r_{5-2} 5.84184	\langle_{1-2-3} 61.72.95 \langle_{1-2-4} 61.01520 \langle_{1-5-4} 60.8578 \langle_{1-4-3} 60.8251 \langle_{3-2-5} 88.4540 \langle_{2-5-4} 92.0525 \langle_{5-1-2} 59.7236	$\langle_{1-2-3-4}$ -55.0088 $\langle_{4-2-1-3}$ 54.98703 $\langle_{1-3-2-5}$ -55.0032 $\langle_{3-1-2-5}$ -56.4679 $\langle_{5-3-2-1}$ 54.4734 $\langle_{4-3-5-2}$ 00.00469	5
		Singlet	-333.102	r_{1-2} 3.97921 r_{1-3} 3.99712 r_{1-4} 3.94777 r_{1-5} 3.95721 r_{3-2} 3.92145 r_{3-4} 3.91425 r_{4-5} 3.92457 r_{5-2} 3.95214	\langle_{1-2-3} 59.71571 \langle_{1-2-4} 61.7766 \langle_{1-5-4} 59.3256 \langle_{1-4-3} 59.5418 \langle_{3-2-5} 57.1245 \langle_{2-5-4} 58.24789 \langle_{5-1-2} 59.87412	$\langle_{1-2-3-4}$ 70.1176 $\langle_{2-3-4-1}$ -70.1176 $\langle_{3-4-2-1}$ -70.3602 $\langle_{4-2-1-3}$ 70.3602 $\langle_{1-3-2-5}$ 36.4664 $\langle_{3-1-2-5}$ -36.4664 $\langle_{5-3-2-1}$ -36.4734 $\langle_{1-3-5-2}$ 36.4734	1

		Tryplet	-80.0068	r_{1-2} 5.56039 r_{1-3} 4.49349 r_{1-4} 4.41210 r_{1-5} 4.48731 r_{3-2} 4.47174 r_{3-4} 4.42429 r_{4-5} 4.43487 r_{5-2} 4.58275	$<_{1-2-3}$ 53.1796 $<_{1-2-4}$ 52.7766 $<_{1-5-4}$ 54.3256 $<_{1-4-3}$ 55.5418 $<_{3-2-5}$ 55.1245 $<_{2-5-4}$ 54.2472 $<_{5-1-2}$ 54.8741	$<_{1-2-3-4}$ 70.2103 $<_{2-3-4-1}$ -70.2103 $<_{3-4-2-1}$ -70.1623 $<_{4-2-1-3}$ 70.1623 $<_{1-3-2-5}$ 36.5002 $<_{3-1-2-5}$ -36.5001 $<_{5-3-2-1}$ -36.3531 $<_{1-3-5-2}$ 36.3531	3
		Kwintet	0	r_{1-2} 3.95894 r_{1-3} 3.51859 r_{1-4} 3.81210 r_{1-5} 3.48722 r_{3-2} 3.67155 r_{3-4} 3.22452 r_{4-5} 3.43477 r_{5-2} 3.88254	$<_{1-2-3}$ 59.8183 $<_{1-2-4}$ 59.7766 $<_{1-5-4}$ 58.3417 $<_{1-4-3}$ 54.5418 $<_{3-2-5}$ 59.1345 $<_{2-5-4}$ 55.2378 $<_{5-1-2}$ 55.8741	$<_{1-2-3-4}$ 70.1176 $<_{2-3-4-1}$ -70.1176 $<_{3-4-2-1}$ -70.3602 $<_{4-2-1-3}$ 70.3602 $<_{1-3-2-5}$ 36.4664 $<_{3-1-2-5}$ -36.4664 $<_{5-3-2-1}$ -36.4734 $<_{1-3-5-2}$ 36.4734	1
		Singlet	0	r_{1-2} 3.845 r_{2-3} 3.845 r_{3-4} 3.845 r_{4-5} 3.845 r_{1-5} 3.8461	$<_{1-2-3}$ 108.14 $<_{3-4-5}$ 108.10 $<_{1-5-2}$ 108.02 $<_{4-5-1}$ 108.04 $<_{2-4-3}$ 107.79	$<_{1-2-3-4}$ -3.54225e-3	
		Tryplet	-102.494	r_{1-2} 3.849 r_{2-3} 3.849 r_{3-4} 3.849 r_{4-5} 3.849 r_{1-5} 3.8460	$<_{1-2-3}$ 108.04 $<_{3-4-5}$ 108.05 $<_{1-5-2}$ 108.02 $<_{4-5-1}$ 108.00 $<_{2-4-3}$ 107.80	$<_{1-2-3-4}$ -2.40663e-4	3
		Kwintet	-66.5165	r_{1-2} 3.849 r_{2-3} 3.849 r_{3-4} 3.849 r_{4-5} 3.849 r_{1-5} 3.860	$<_{1-2-3}$ 108.04 $<_{3-4-5}$ 108.05 $<_{1-5-2}$ 108.02 $<_{4-5-1}$ 108.00 $<_{2-4-3}$ 107.80	$<_{1-2-3-4}$ -3.45820e-4	3
		Singlet	-66.5165	r_{1-2} 3.66946 r_{1-3} 2.67184 r_{2-4} 2.64551 r_{1-5} 3.48722 r_{3-2} 2.68325 r_{3-4} 2.68325 r_{4-5} 3.66946 r_{5-2} 3.88254	$<_{1-2-3}$ 59.8857 $<_{3-4-5}$ 59.8886 $<_{1-5-2}$ 59.4475 $<_{4-5-1}$ 59.5214 $<_{2-4-3}$ 59.6324	$<_{1-2-3-4}$ 75.7328 $<_{2-3-1-4}$ -75.7328 $<_{3-1-2-4}$ -71.3603 $<_{4-1-2-3}$ 71.3502 $<_{4-2-3-1}$ 70.8026 $<_{4-3-1-2}$ 70.1335 $<_{5-2-1-3}$ 0.00001 $<_{5-4-3-2}$ -70.1270 $<_{2-4-5-3}$ 70.5569	1

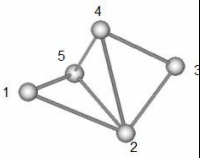


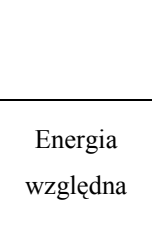
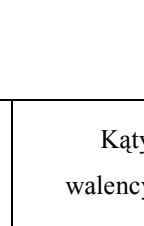
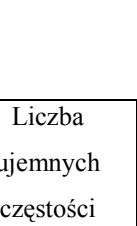
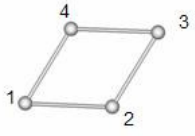
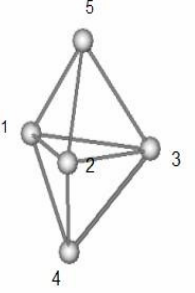
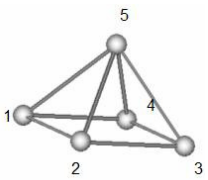
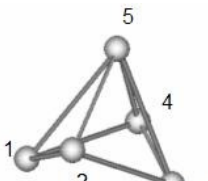
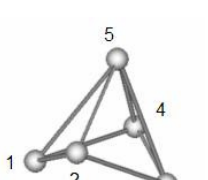
	Tryplet	0	r_{1-2} 2.49985 r_{1-3} 2.28526 r_{2-4} 2.2574 r_{1-5} 2.24787 r_{3-2} 2.58324 r_{3-4} 2.38323 r_{4-5} 2.76944 r_{5-2} 2.98251	\angle_{1-2-3} 61.9952 \angle_{3-4-5} 62.8425 \angle_{1-5-2} 59.6321 \angle_{4-5-1} 59.7452 \angle_{2-4-3} 60.3245	$1-2-3-4$ 75.7328 $\angle_{2-3-1-4}$ -75.7328 $\angle_{3-1-2-4}$ -71.3603 $\angle_{4-1-2-3}$ 71.3502 $\angle_{4-2-3-1}$ 70.8026 $\angle_{4-3-1-2}$ 70.1335 $\angle_{5-2-1-3}$ -150.034 $\angle_{5-4-3-2}$ -70.1270 $\angle_{2-4-5-3}$ 70.5569	2
	Kwintet	-29.08	r_{1-2} 2.5794 r_{1-3} 2.2925 r_{2-4} 2.26551 r_{1-5} 2.25722 r_{3-2} 2.29325 r_{3-4} 2.654325 r_{4-5} 2.641946 r_{5-2} 2.41254	\angle_{1-2-3} 63.512 \angle_{3-4-5} 63.2142 \angle_{1-5-2} 62.4157 \angle_{4-5-1} 62.5478 \angle_{2-4-3} 61.2453	$1-2-3-4$ 75.7321 $\angle_{2-3-1-4}$ -75.7321 $\angle_{3-1-2-4}$ -71.3634 $\angle_{4-1-2-3}$ 71.3521 $\angle_{4-2-3-1}$ 70.8026 $\angle_{4-3-1-2}$ 70.1335 $\angle_{5-2-1-3}$ -168.034 $\angle_{5-4-3-2}$ -70.1270 $\angle_{2-4-5-3}$ 70.5569	1

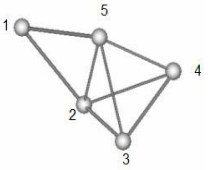
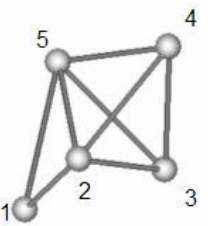
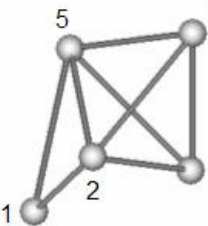
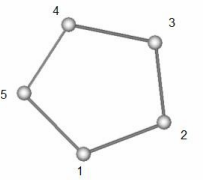
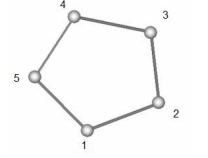
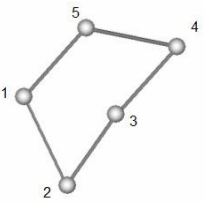
TABELA II

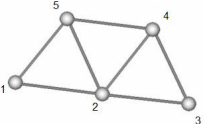
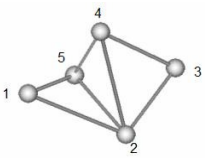
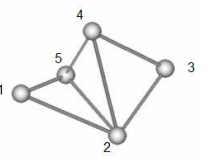
Pd

n	Rysunek klasteru	Multipletowość	Energia względna	Długość wiązania	Kąty walencyjne	Kąty torsyjne	Liczba ujemnych częstości
1		Singlet	0	—	—	—	—
		Tryplet	-546,051	—	—	—	—
		Kwintet	-9504,28	—	—	—	—
2		Singlet	-15,9279	2.11399	—	—	0
		Tryplet	-1,6766	2.23046	—	—	0
		Kwintet	0	2.06391	—	—	0
3		Singlet	-1,2719	2.68239	60.0001	—	0
		Tryplet	0	r1-2 2.59872 r2-3 2.27145 r3-1 2.59820	64.0706	—	0
		Kwintet	-20,7461	r1-2 2.46645 r2-3 2.64589 r3-1 2.46634	57.5599	—	1
4		Singlet	-10,3255	r1-2 2.69775 r2-3 2.69765 r3-1 2.69769 r1-4 2.69778 r2-4 2.69774 r3-4 2.69769	< ₁₄₂ 59.9998 < ₂₄₃ 59.9984 < ₃₄₁ 59.9990	-70.5292	0
		Tryplet	0	r1-2 2.47195 r2-3 2.36497 r3-1 2.36470 r1-4 2.47290 r2-4 2.47184 r3-4 2.36471	< ₁₄₂ 59.9887 < ₂₄₃ 58.4968 < ₃₄₁ 58.4745	-71.7997	2
		Kwintet	-28,9974	r1-2 2.64792 r2-3 2.65424 r3-1 2.32861 r1-4 2.69399 r2-4 2.32861 r3-4 2.64792	< ₁₄₂ 63.1407 < ₂₄₃ 64.0882 < ₃₄₁ 51.6781	-58.2166	0
		Singlet	-1,9111	r1-2 2.59446 r2-3 2.59445 r3-4 2.59445 r4-1 2.59445	90	0	2

		Tryplet	0	r1-2 2.40148 r2-3 2.40149 r3-4 2.40135 r4-1 2.40132	< ₁₂₃ 89.9952 < ₂₃₄ 90.0007 < ₃₄₁ 90.0025 < ₄₁₂ 90.0017	5.56e-006	1
		Kwintet	-49,7443	r1-2 2.27457 r2-3 2.27458 r3-4 2.27467 r4-1 2.27469	< ₁₂₃ 89.2292 < ₂₃₄ 90.7736 < ₃₄₁ 90.7736 < ₄₁₂ 90.7734	0	1
4		Singlet	0	r1-2 2.66464 r2-3 2.66467 r3-4 2.66464 r4-1 2.66467	< ₁₂₃ 119.065 < ₂₃₄ 60.9346 < ₃₄₁ 119.065 < ₄₁₂ 60.9345	-2.41e-006	1
		Tryplet	-0,9883	r1-2 2.57635 r2-3 2.57634 r3-4 2.57651 r4-1 2.57650	< ₁₂₃ 127.327 < ₂₃₄ 52.6797 < ₃₄₁ 127.313 < ₄₁₂ 52.6797	3.41e-006	0
		Kwintet	-14,4434	r1-2 2.54080 r2-3 2.54041 r3-4 2.54030 r4-1 2.54121	< ₁₂₃ 125.393 < ₂₃₄ 54.6208 < ₃₄₁ 125.380 < ₄₁₂ 54.6058	0.169818	2
5		Singlet	-19,5558	r1-2 2.70360 r2-3 2.70363 r3-1 2.70361 r1-4 2.67856 r2-4 2.67859 r3-4 2.67859 r1-5 2.67856 r2-5 2.67859 r3-5 2.67859	< ₁₅₂ 60.6203 < ₂₅₃ 60.6199 < ₃₅₁ 60.6205 < ₁₄₂ 60.6203 < ₂₄₃ 60.6199 < ₃₄₁ 60.6205 < ₁₂₃ 59.9993	—	0
		Tryplet	0	r1-2 2.58761 r2-3 2.60494 r3-1 2.58764 r1-4 2.32733 r2-4 2.52111 r3-4 2.52090 r1-5 2.32733 r2-5 2.52110 r3-5 2.52091	< ₁₅₂ 64.3661 < ₂₅₃ 62.2150 < ₃₅₁ 64.3703 < ₁₄₂ 64.3660 < ₂₄₃ 62.2150 < ₃₄₁ 64.3704 < ₁₂₃ 59.7791	—	1

		Kwintet	-22,949	r1-2 2.54430 r2-3 2.54393 r3-1 2.54430 r1-4 2.62543 r2-4 2.62526 r3-4 2.62527 r1-5 2.35370 r2-5 2.35388 r3-5 2.62527	< 152 65.4312 < 253 65.4174 < 351 65.4311 < 142 57.9679 < 243 57.9605 < 341 57.9679 < 123 60.0049	—	2
5		Singlet	-34,8517	r1-2 2.62831 r2-3 2.62831 r3-4 2.62831 r4-1 2.62831 r1-5 2.68353 r2-5 2.68363 r3-5 2.68353 r4-5 2.68353	< 152 58.6419 < 253 58.4620 < 354 58.6419 < 451 58.642	—	1
		Tryplet	0	r1-2 2.28532 r2-3 2.56799 r3-4 2.28526 r4-1 2.56800 r1-5 2.59420 r2-5 2.49945 r3-5 2.59416 r4-5 2.49964	< 152 61.2382 < 253 61.5670 < 354 61.2446 < 451 61.5654	—	3
		Kwintet	-36,3373	r1-2 2.32250 r2-3 2.62598 r3-4 2.32248 r4-1 2.62597 r1-5 2.70382 r2-5 2.57111 r3-5 2.70382 r4-5 2.57110	< 152 60.9729 < 253 62.6884 < 354 60.9729 < 451 62.6886	—	0

		Singlet	-43,3728	r1-2 2.62432 r2-3 2.65617 r3-4 2.17371 r4-5 2.65617 r5-2 2.75813 r2-4 2.65617 r3-5 2.65617	< 215 63.4033 < 253 58.7218 < 354 61.4385 < 452 58.7217 < 234 59.2807	—	1
		Tryplet	0	r1-2 2.28518 r2-3 2.59424 r3-4 2.50002 r4-5 2.28523 r5-2 2.61855 r2-4 2.56771 r3-5 2.59397	< 215 62.7251 < 253 59.6825 < 354 53.2708 < 452 65.0058 < 234 60.5019	—	3
		Kwintet	-36,3373	r1-2 2.32250 r2-3 2.70383 r3-4 2.57071 r4-5 2.32253 r5-2 2.70552 r2-4 2.62610 r3-5 2.70383	< 215 51.6217 < 253 59.9792 < 354 52.1752 < 452 65.9528 < 234 62.6922	—	0
5		Singlet	1,1348	r1-2 2.58171 r2-3 2.58184 r3-4 2.58180 r4-5 2.58172 r5-1 2.58172	< 123 108.000 < 234 107.998 < 345 108.000 < 451 108.001 < 512 108.001	—	4
		Tryplet	-34,7846	r1-2 2.38145 r2-3 2.38179 r3-4 2.38396 r4-5 2.38491 r5-1 2.38349	< 123 108.056 < 234 108.017 < 345 107.937 < 451 107.981 < 512 108.009	—	4
		Kwintet	0	r1-2 2.69783 r2-3 2.42166 r3-4 2.52820 r4-5 2.27729 r5-1 2.58095	< 123 52.9625 < 234 173.443 < 345 64.3826 < 451 115.507 < 512 120.591	—	4

	Singlet	-66,5164	r1-2 2.67186 r2-3 2.67193 r3-4 2.66961 r4-5 2.64555 r5-2 2.68325 r2-4 2.68317	< 152 59.8864 < 524 59.0737 < 234 59.8892	—	2
	Tryplet	0	r1-2 2.56797 r2-3 2.28515 r3-4 2.56772 r4-5 2.59413 r5-2 2.59406 r2-4 2.61858	< 152 60.5112 < 524 59.6886 < 234 52.2747	—	3
	Kwintet	-36,3373	r1-2 2.62612 r2-3 2.32249 r3-4 2.62610 r4-5 2.70383 r5-2 2.70383 r2-4 2.70538	< 152 62.6896 < 524 60.0380 < 234 51.6231	—	0

Na podstawie wykonanych przez nas obliczeń możemy stwierdzić, że:

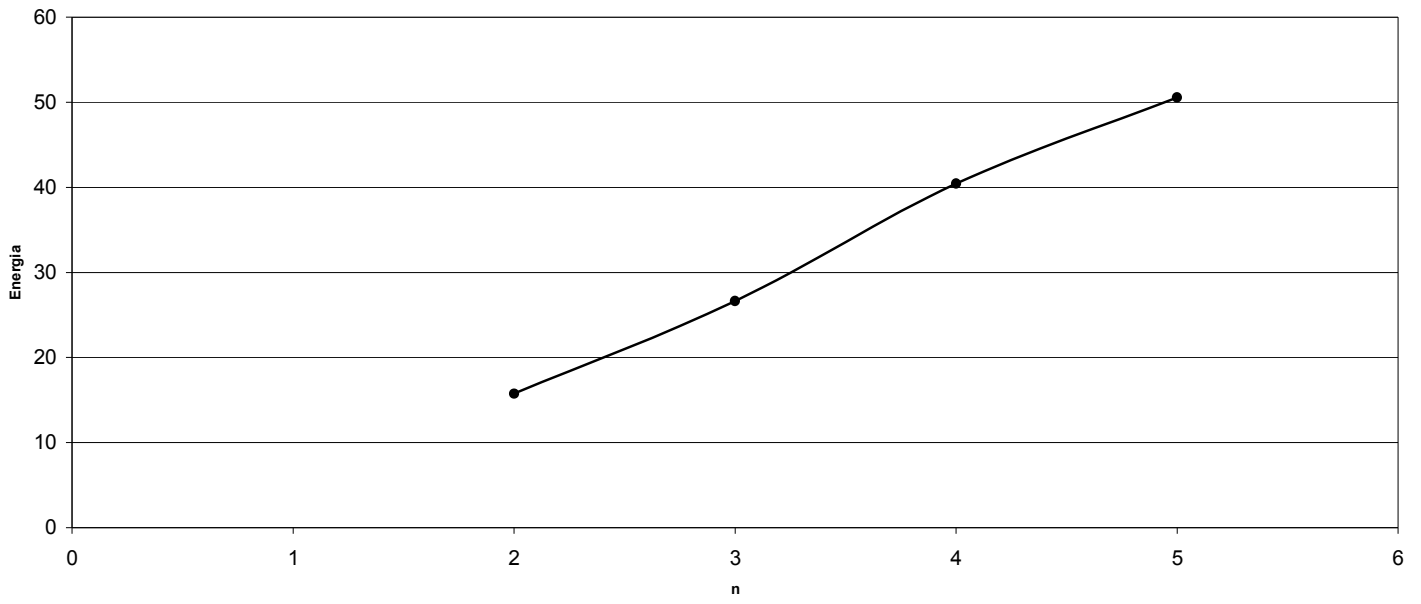
- pod względem uzyskanych wyników dotyczących energii widać, że stabilność struktury zależy od liczby atomów budujących klaster najlepsze wyniki uzyskujemy dla liczby atomów $n=5$, a pod względem natury atomu struktury Ni_n uzyskały korzystniejszą wartość energii, czyli są bardziej stabilne od struktur Pd_n
- pod względem preferowanych stanów spinowych, widać że nie są one identyczne dla oby metalu. W przypadku atomów palladu bardziej preferowane są stany trypletowi, natomiast kwintet jest stanem spinowym preferowanym przez atomy Ni
- dla atomu niklu najkorzystniejsza struktura to piramida tetragonalna o multipletowości kwintetu – odpowiada jej najniższa energia 531.617
- dla atomu palladu najkorzystniejsza struktura to trapezoid o multipletowości trypletu – odpowiada jej najniższa energia -282.441

Choć niekoniecznie musi być to prawdą. W przypadku atomu niklu mamy dość kłopotliwą sytuację jeśli chodzi o izolowany atom. Polega on na tym, że atom niklu ma położony nisko stan wzbudzony

i być może traktowany jest on jako stan podstawowy co oczywiście uniemożliwi nam uzyskanie poprawnych wyników.

Drugi, bardziej namacalny fakt to długości wiązań, które przekraczają wartości oczekiwane.

Wykres zależności $(\Delta E_n/n)=f(n)$ dla Pd



Wykres zależności $(\Delta E_n/n)=f(n)$ dla Ni

