

Complete set

R=2 Z=1

19/7/57

	$(S_{ij} + u_{ij})$	$RK_{ij}(1-2\alpha_i + \alpha_j)$	$RJ_{ij} + (1-2\alpha_i)KL_{ij}$	A_{ij}	B_{ij}	
+2.0000						
00	+1.586453	+0.812012	+0.945053	-2.10754300	+1.00000000	15
01	-1.063897	-0.360894	-0.380948	+1.08972455	-0.64203875	2
02	+0.586453	+0.541341	+0.307686	-1.29505819	+0.52908486	3
03	+0.144358	+0.000000	-0.097683	-0.02811113	+0.08694422	4
04	-0.265202	-0.073667	+0.023934	+0.33789199	-0.28453386	5
05	+0.331748	+0.255191	+0.127766	-0.49354949	+0.22909315	6
06	+0.048119	+0.036089	+0.000000	-0.05084048	+0.02905170	7
07	-0.064559	-0.072629	-0.049146	+0.21471133	-0.07439082	8
08	+0.012030	+0.072179	+0.076932	-0.10473431	+0.00781884	9
09	+0.139877	+0.096838	+0.049118	-0.27015445	+0.13220470	10
11	+1.730811	+0.000000	-0.293050	-0.83068615	+1.00000000	21
12	-0.216536	+0.000000	-0.278372	+0.42747051	-0.18703033	
13	-1.015778	+0.096238	-0.185582	+0.63723492	-0.58571787	
14	+0.419903	-0.103134	+0.113628	-0.44209442	+0.43131557	
15	+0.008506	-0.034025	-0.146734	+0.11388347	+0.00562388	
16	+0.151232	-0.024060	-0.097683	-0.01704504	+0.08741484	
17	-0.239789	+0.080698	+0.081919	+0.08513555	-0.26453524	
18	+0.202788	-0.132328	-0.046438	-0.01494828	+0.12618719	
19	+0.043039	-0.053799	-0.062698	+0.06647039	+0.03894505	2p
22	+0.774441	+0.000000	-0.014678	-0.98104708	+1.00000000	
23	-0.243604	+0.096238	-0.009785	+0.13546768	-0.20999252	
24	+0.081639	-0.147334	-0.173429	+0.36719901	+0.12536380	
25	-0.433824	+0.119089	+0.334924	-0.01995446	-0.42878252	
26	+0.109987	+0.000000	+0.051288	-0.13936031	+0.09504146	
27	-0.202899	+0.032279	-0.140902	+0.51377429	-0.33462885	
28	+0.274967	-0.108268	+0.135601	-0.28121698	+0.25579012	
29	-0.275143	+0.145257	+0.127603	+0.00308764	-0.37220132	
33	+1.737685	-0.302750	-0.835996	-0.34467630	+0.99999999	3s
34	-0.130496	+0.073667	-0.135547	+0.19721371	-0.13377755	
35	-0.188355	+0.130431	+0.011452	+0.03066366	-0.12428230	
36	-1.022652	+0.232003	-0.120460	+0.52559510	-0.58994189	
37	+0.406374	-0.251702	+0.049108	-0.22436460	+0.44742318	
38	-0.021482	+0.017185	-0.050781	+0.03420496	-0.01334079	
39	-0.073013	+0.053799	+0.008902	+0.00931241	-0.06593671	
44	+0.547593	+0.078194	-0.744892	+0.21750686	+1.00000000	3p
45	+0.238128	-0.125017	-0.116886	+0.00443666	+0.27989785	
46	-0.247838	+0.224510	-0.015979	+0.04039339	-0.25468585	
47	+0.017854	-0.282385	-0.093546	+0.70230464	+0.03501832	
48	-0.325188	+0.119271	+0.091500	+0.12657816	-0.35975183	
49	+0.015531	+0.031376	-0.055257	+0.01343256	+0.02498563	
55	+1.321797	-0.142353	-0.558637	-0.46966954	+1.00000000	5s
56	-0.023696	+0.097215	+0.037459	-0.07340454	-0.01567345	
57	+0.136134	-0.173904	-0.078907	+0.14729217	+0.17185568	
58	-0.758365	+0.255191	+0.009307	+0.35166201	-0.53999936	
59	+0.499839	-0.388568	+0.220643	-0.34368226	+0.51756091	
66	+1.729284	-53.567842	-1.107469	+30.61731189	+1.00000000	6s
67	-0.081467	+0.047266	-0.098235	+0.14616738	-0.08991388	
68	-0.199160	+0.262937	+0.024294	-0.05482692	-0.12398443	
69	-0.043381	+0.090690	+0.017996	-0.05911839	-0.03927152	
77	+0.474727	+0.238963	-1.044102	+0.69600428	+0.99999999	4p
78	+0.184453	-0.205204	-0.100385	+0.14392902	+0.21916055	
79	+0.127516	-0.143326	-0.033711	+0.08556380	+0.22032122	
88	+1.492124	-0.278834	-0.987519	-0.15130849	+0.99999999	4s
89	-0.195555	+0.094917	-0.003556	+0.10154435	-0.19058097	
99	+0.705623	+0.191532	-0.934618	+0.05309267	+1.00000000	4p
99	+0.499839	-0.388568	+0.220643	-0.34368226	+0.51756091	
99						

69	-0.043381	+0.090690	+0.017998	-0.05911859	-0.05927152
77	+0.474727	+0.238963	-1.044102	+0.69600428	+0.99999999
78	+0.184453	-0.205204	-0.100385	+0.14392902	+0.21916055
79	+0.127516	-0.143326	-0.033711	+0.08556380	+0.22032122
88	+1.492124	-0.278834	-0.987519	-0.15130849	+0.99999999
89	-0.195555	+0.094917	-0.003556	+0.10154435	-0.19058097
99	+0.705623	+0.191532	-0.934618	+0.05309267	+1.00000000
59	+0.499839	-0.388568	+0.220643	-0.34368226	+0.51756091
66	+1.729284	-0.440377	-1.107469	-0.10492093	+1.00000000

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