Table

Global minima of LJ_N for N less than 110. The references in which each minimum was first reported, to the best of our knowledge, is given. The unit of energy is the pair well depth.

Click on a label to access the points file for the structure in Cartesian coordinates.
Or click here for a tar file of all the points.
The unit of length is sigma.

N	PG	Energy	Ref.	N	PG	Energy	Ref.
2	$D_{infty\ h}$	-1.000000		57	C_s	-288.342625	Northby
3	D_{3h}	-3.000000		58	C_{3v}	-294.378148	Northby
4	T_d	-6.000000		59	C_{2v}	-299.738070	Northby
5	D_{3h}	-9.103852	Hoare	60	C_s	-305.875476	Northby
6	O_h	-12.712062	Hoare	61	C_{2v}	-312.008896	Northby
7	D_{5h}	-16.505384	Hoare	62	C_s	-317.353901	Northby
8	C_s	-19.821489	Hoare	63	C_1	-323.489734	Northby
9	C_{2v}	-24.113360	Hoare	64	C_s	-329.620147	Northby
10	C_{3v}	-28.422532	Hoare	65	C_2	-334.971532	Xue
11	C_{2v}	-32.765970	Hoare	66	C_1	-341.110599	Coleman/Xue
12	C_{5v}	-37.967600	Hoare	67	C_s	-347.252007	Northby
13	I_h	-44.326801	Hoare	68	C_1	-353.394542	Northby
14	C_{3v}	-47.845157	Hoare	69	C_{5v}	-359.882566	Wales
15	C_{2v}	-52.322627	Hoare	70	C_{5v}	-366.892251	Northby
16	C_s	-56.815742	Hoare	71	C_{5v}	-373.349661	Northby
17	C_2	-61.317995	Freeman	72	C_s	-378.637253	Coleman
18	C_{5v}	-66.530949	Hoare	73	C_s	-384.789377	Northby
19	D_{5h}	-72.659782	Hoare	74	C_s	-390.908500	Northby
20	C_{2v}	-77.177043	Hoare	75	D_{5h}	-397.492331	Doye1
21	C_{2v}	-81.684571	Hoare	76	C_s	-402.894866	Doye1
22	C_s	-86.809782	Northby	77	C_{2v}	-409.083517	Doye1
23	D_{3h}	-92.844472	Farges	78	C_s	-414.794401	Wales
24	C_s	-97.348815	Wille	79	C_{2v}	-421.810897	Northby
25	C_s	-102.372663	Hoare	80	C_s	-428.083564	Northby
26	T_d	-108.315616	Hoare	81	C_{2v}	-434.343643	Northby
27	C_{2v}	-112.873584	Northby	82	C_1	-440.550425	Northby
28	C_s	-117.822402	Northby	83	C_{2v}	-446.924094	Northby
29	D_{3h}	-123.587371	Hoare	84	C_1	-452.657214	Northby
30	C_{2v}	-128.286571	Northby	85	C_{3v}	-459.055799	Northby

31	C_s	-133.586422	Northby	86	C_1	-465.384493	Northby
32	C_{2v}	-139.635524	Northby	87	C_s	-472.098165	Northby
33	C_s	-144.842719	Northby	88	C_s	-479.032630	Deaven
34	C_{2v}	-150.044528	Northby	89	C_{3v}	-486.053911	Northby
35	C_1	-155.756643	Northby	90	C_s	-492.433908	Northby
36	C_s	-161.825363	Northby	91	C_s	-498.811060	Northby
37	C_1	-167.033672	Northby	92	C_{3v}	-505.185309	Northby
38	O_h	-173.928427	Pillardy/Doye1	93	C_1	-510.877688	Northby
39	C_{5v}	-180.033185	Northby	94	C_1	-517.264131	Northby
40	C_s	-185.249839	Northby	95	C_1	-523.640211	Northby
41	C_s	-190.536277	Northby	96	C_1	-529.879146	Northby
42	C_s	-196.277534	Northby	97	C_1	-536.681383	Northby
43	C_s	-202.364664	Northby	98	C_s	-543.642957	Deaven
44	C_1	-207.688728	Northby	99	C_{2v}	-550.666526	Northby
45	C_1	-213.784862	Northby	100	C_s	-557.039820	Northby
46	C_{2v}	-220.680330	Northby	101	C_{2v}	-563.411308	Northby
47	C_1	-226.012256	Northby	102	C_{2v}	-569.363652	Doye2
48	C_s	-232.199529	Northby	103	C_s	-575.766131	Doye2
49	C_{3v}	-239.091864	Northby	104	C_{2v}	-582.086642	Doye2
50	C_s	-244.549926	Northby	105	C_1	-588.266501	Northby
51	C_{2v}	-251.253964	Northby	106	C_1	-595.061072	Northby
52	C_{3v}	-258.229991	Northby	107	C_s	-602.007110	Wales
53	C_{2v}	-265.203016	Northby	108	C_s	-609.033011	Northby
54	C_{5v}	-272.208631	Northby	109	C_1	-615.411166	Northby
55	I_h	-279.248470	Hoarec	110	C_s	-621.788224	Northby
56	C_{3v}	-283.643105	Northby				

Lowest energy icosahedral minima at sizes with non-icosahedral global minima.

N	PG	Energy	Ref.
38	C_{5v}	-173.252378	Deaven
75	C_1	-396.282249	Doye1
76	C_1	-402.384580	Xue
77	C_1	-408.518265	Xue
102	C_s	-569.277721	Northby
103	C_1	-575.658879	Northby
104	C_s	-582.038429	Northby

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