

Supporting Information

Structure and Thermodynamics of Li^+Ar_n Clusters beyond the Second Solvation Shell

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Li⁺-Ar and Ar-Ar pair potentials

The Li⁺-Ar two-body terms were represented by the expression:

$$\begin{aligned} V_{\text{Li}^+ - \text{Ar}}(R) &= aR^c \exp(-bR) - \chi_{pol}(d_{pol}, R) \frac{C_4}{R^4} \\ &\quad - \chi_{disp}(d_{disp}, R) \frac{C_6}{R^6} \end{aligned} \quad (\text{S1})$$

where a , b , c , C_4 , and C_6 are fitting parameters. In addition, χ_{pol} and χ_{disp} are, respectively, the damping functions for polarization and dispersion terms. Both χ_{pol} and χ_{disp} can be described by the following general function:

$$\chi(d, R) = \begin{cases} 1 & R > d; \\ \exp[-(d/R - 1)^2] & R \leq d. \end{cases} \quad (\text{S2})$$

In this equation, d represents either d_{pol} or d_{disp} fitting parameters that are employed in the corresponding χ_{pol} and χ_{disp} functions. As detailed in our previous work,¹ the parameters a , b , c , C_4 , C_6 , d_{pol} , and d_{disp} were fitted to *ab initio* data and the corresponding numerical values, so obtained, are (in units of a_0 for distance and E_h for the potential energy): 18.6423546335389, 2.47462560510424, 2.41048244693289, 5.00251140429571, 85.4275134083190, 4.01847424072307, and 6.39278969540634. Note that all the figures in the values of the parameters are given just to allow the reproduction of the interaction potential employed in this work and, of course, do not reflect the accuracy of the fitting data.

The two-body terms employed for Ar - Ar are the Rydberg-London functions of Cahill and Parsegian:²

$$V_{\text{Ar} - \text{Ar}}(R) = A(1 - CR) \exp(-BR) - \frac{D}{R^6 + ER^{-6}}. \quad (\text{S3})$$

where the parameters A , B , C , D , and E take the values 1720 eV, 2.6920 Å⁻¹, 0.2631 Å⁻¹, 37.943 eV Å⁶, and 177588 Å¹², respectively.

Fraction of binding energy corresponding to 3-body interactions

In order to estimate the fraction of binding energy corresponding to three-body interactions, we have followed the procedure for each cluster size:

1. Obtain the energy of the putative global minimum structure as modeled with the 2-body potential energy surface ($E_{min,2}$).
2. Obtain the energy of the minimum structure as modeled with the potential that includes both 2-body and 3-body terms ($E_{min,3}$) by local optimization departing from the structures from step 1. As described in previous work,^{1,3} the 3-body potential function includes all Li^+Ar_2 and Ar_3 contributions, with the former accounting for the interaction between the dipoles on argon atoms induced by the lithium ion, whereas the latter is represented by the Axilrod–Teller–Muto term.^{4–6}
3. Calculate the fraction of the energy (in %) corresponding to three-body interactions by using the expression:

$$100 \times \frac{(E_{min,2} - E_{min,3})}{E_{min,3}}$$

The calculated contribution of three-body interactions to the binding energy is represented in Figure S1. Because $E_{min,3}$ results from a local optimization of geometry, we have no guarantee of reaching the global minimum for the potential energy surface that includes three-body terms, and hence the estimated result displayed in Figure S1 may constitute an upper bound to the true value.

We observe in Figure S1 that, after an increase up to $n = 14$, the estimated contribution of three-body interactions to the total binding energy tends to decrease with the cluster size. However, such decrease of the three-body contribution becomes slower for larger cluster sizes, thus appearing to approach a plateau. For $n \geq 85$, three-body interactions contribute with less than 20% to the total binding energy of the cluster.

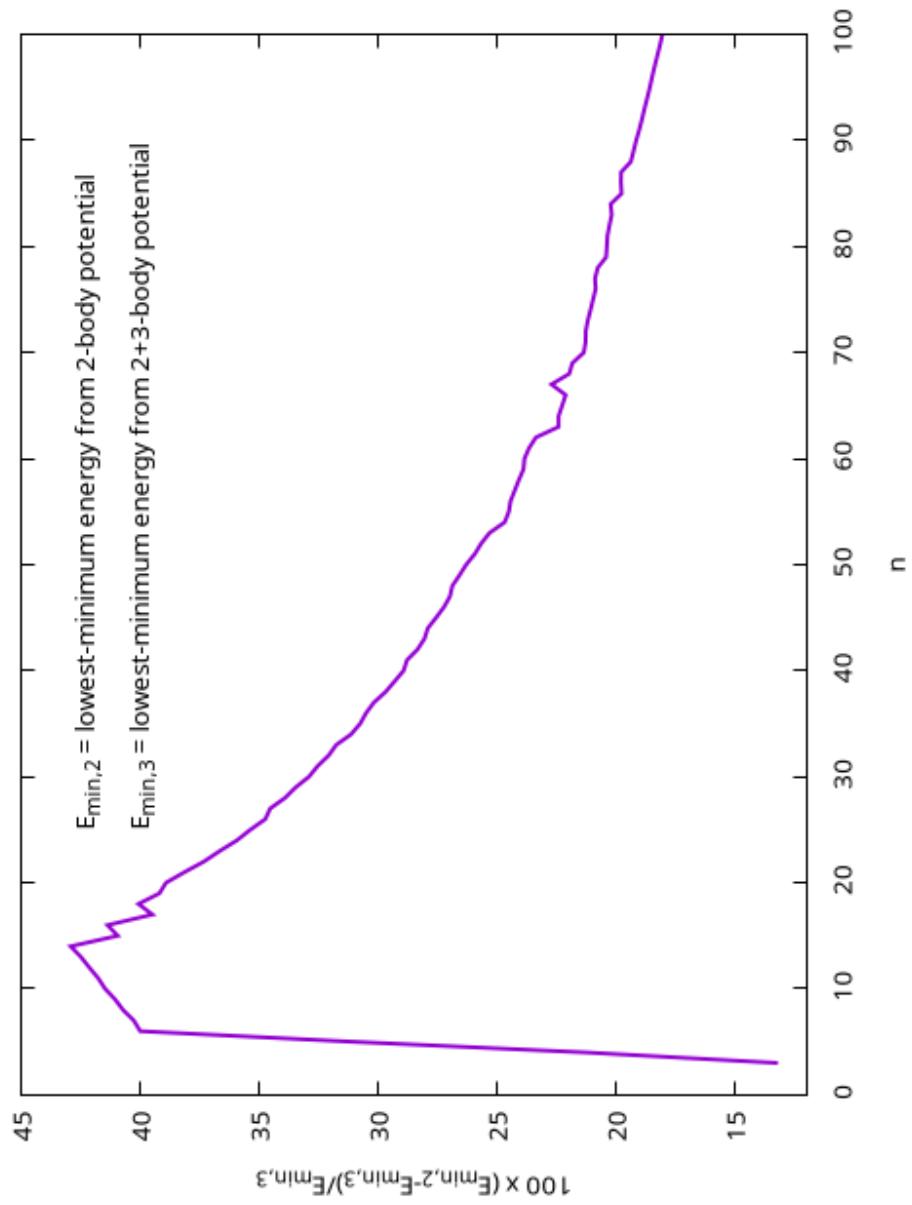


Figure S1: Fraction of the total binding energy corresponding to three-body interactions in Li^+Ar_n as function of the cluster size (n). The represented values are linked by straight lines to guide the eye.

Table S1: Values of the parameters employed in the parallel-tempering Monte Carlo calculations.

Parameter	Meaning	Value
N_{MC}	Total number of Monte-Carlo moves	4×10^7
$N_{MC,each}$	Number of sampling steps between two temperature exchanges	50
T_{min}/K	Minimum value of temperature sampled	0.5
T_{max}/K	Maximum value of temperature sampled	500
$\Delta T_1/\text{K}$	Temperature spacing over the lower-temperature interval	0.5
$\Delta T_2/\text{K}$	Temperature spacing over the higher-temperature interval	10
# runs	Number of Monte Carlo Simulations	2
$R_{cut}/\text{\AA}$	Distance at which the rigid-wall potential begins to act for the cluster:	
$\text{Li}^+\text{Ar}_{41}$		19.735
$\text{Li}^+\text{Ar}_{42}$		19.879
$\text{Li}^+\text{Ar}_{44}$		20.742
$\text{Li}^+\text{Ar}_{50}$		19.977
$\text{Li}^+\text{Ar}_{52}$		20.876
$\text{Li}^+\text{Ar}_{53}$		20.624
$\text{Li}^+\text{Ar}_{63}$		22.751
$\text{Li}^+\text{Ar}_{85}$		24.556

Building up the solvation shells in small clusters

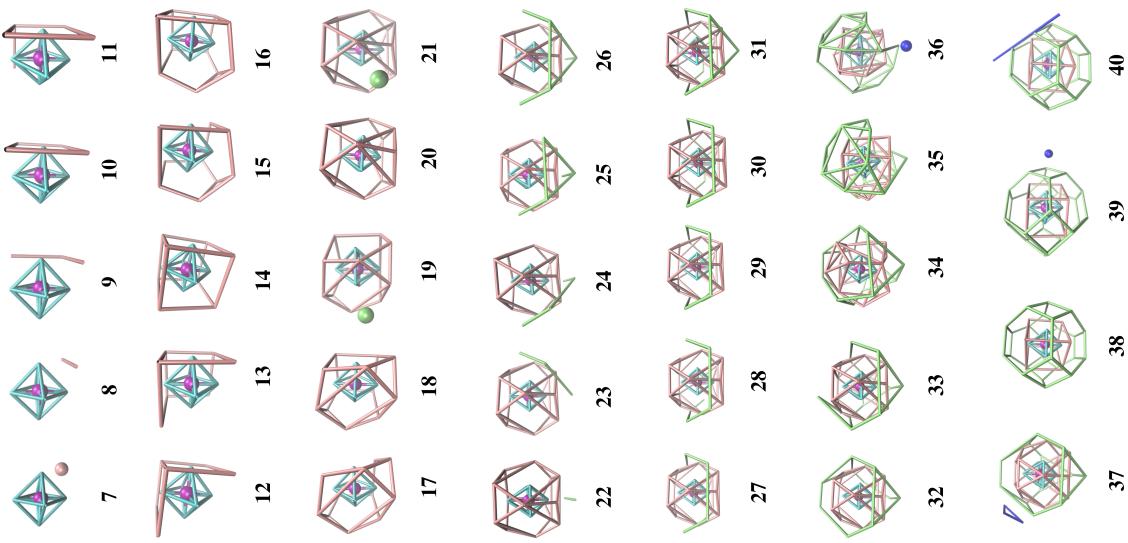


Figure S2: Global minimum structures of Li^+Ar_n ($7 \leq n \leq 40$) clusters, where the organization of the argon atoms around the lithium ion (in magenta) are indicated by different colors according to the Li^+ -Ar distance ($d_{\text{Li}^+-\text{Ar}}$): $d_{\text{Li}^+-\text{Ar}} \leq 4.8 a_0$ (cyan tubes); $4.8 a_0 < d_{\text{Li}^+-\text{Ar}} \leq 10.0 a_0$ (pink tubes); $10.0 a_0 < d_{\text{Li}^+-\text{Ar}} \leq 12.0 a_0$ (blue tubes); $12.0 a_0 < d_{\text{Li}^+-\text{Ar}} \leq 15.0 a_0$ (green tubes).

Table S2: Distribution of argon atoms by different “solvation shells”, according to the distance from Li^+ (d), for the Li^+Ar_n clusters (with $6 \leq n \leq 40$).

Cluster size (n)	1st shell ($d \leq 4.8 a_0$)	2nd shell ($4.8 < d/a_0 \leq 10.0$)	3rd shell ($10.0 < d/a_0 \leq 12.0$)	4th shell ($12.0 < d/a_0 \leq 15.0$)	external atoms ($d > 15.0 a_0$)
6	6	—	—	—	—
7	6	1	—	—	—
8	6	2	—	—	—
9	6	3	—	—	—
10	6	4	—	—	—
11	6	5	—	—	—
12	6	6	—	—	—
13	6	7	—	—	—
14	6	8	—	—	—
15	6	9	—	—	—
16	6	10	—	—	—
17	6	11	—	—	—
18	6	12	—	—	—
19	6	12	1	—	—
20	6	14	—	—	—
21	6	14	1	—	—
22	6	14	2	—	—
23	6	14	3	—	—
24	6	14	4	—	—
25	6	14	5	—	—
26	6	14	6	—	—
27	6	16	5	—	—
28	6	16	6	—	—
29	6	16	7	—	—
30	6	16	8	—	—
31	6	16	9	—	—
32	6	16	10	—	—
33	6	16	11	—	—
34	6	16	12	—	—
35	6	11	18	—	—
36	6	11	18	1	—
37	6	16	12	3	—
38	6	8	24	—	—
39	6	8	24	1	—
40	6	8	24	2	—

Table S3: Distribution of argon atoms by different “solvation shells”, according to the distance from Li^+ (d), for the Li^+Ar_n clusters (with $41 \leq n \leq 100$).

Cluster size (n)	1st shell ($d \leq 4.8 a_0$)	2nd shell ($4.8 < d/a_0 \leq 10.0$)	3rd shell ($10.0 < d/a_0 \leq 12.0$)	4th shell ($12.0 < d/a_0 \leq 15.0$)	external atoms ($d > 15.0 a_0$)
41	6	8	24	3	—
42	6	16	12	7	1
43	6	16	12	8	1
44	6	16	12	10	—
45	6	16	12	10	1
46	6	16	12	10	2
47	6	16	12	11	2
48	6	16	12	13	1
49	6	16	12	13	2
50	6	16	12	13	3
51	6	16	12	14	3
52	6	16	12	14	4
53	6	16	12	14	5
54	6	16	10	13	9
55	6	16	10	14	9
56	6	16	11	14	9
57	6	16	12	14	9
58	6	16	12	15	9
59	6	16	12	15	10
60	6	16	12	17	9
61	6	16	12	17	10
62	6	16	12	18	10
63	6	16	10	13	18
64	6	16	12	12	18
65	6	16	12	13	18
66	6	16	12	14	18
67	6	16	12	21	12
68	6	16	12	16	18
69	6	16	12	17	18
70	6	16	10	16	22
71	6	16	10	17	22
72	6	16	11	17	22
73	6	16	12	17	22
74	6	16	12	18	22
75	6	16	12	19	22
76	6	16	12	19	23
77	6	16	12	21	22
78	6	16	12	21	23
79	6	16	12	19	26
80	6	16	12	20	26
81	6	16	12	21	26
82	6	16	12	22	26
83	6	16	12	22	27
84	6	16	12	24	26
85	6	14	15	24	26

Cluster size (n)	1st shell ($d \leq 4.8 a_0$)	2nd shell ($4.8 < d/a_0 \leq 10.0$)	3rd shell ($10.0 < d/a_0 \leq 12.0$)	4th shell ($12.0 < d/a_0 \leq 15.0$)	external atoms ($d > 15.0 a_0$)
86	6	16	12	22	30
87	6	16	12	23	30
88	6	14	15	23	30
89	6	14	15	24	30
90	6	14	15	24	31
91	6	14	15	24	32
92	6	14	15	24	33
93	6	14	15	24	34
94	6	14	15	24	35
95	6	14	15	24	36
96	6	14	15	24	37
97	6	14	15	24	38
98	6	14	15	24	39
99	6	14	15	24	40
100	6	14	15	24	41

Cartesian coordinates, energy and symmetry of the putative global-minimum structures of the Li^+Ar_n clusters (with $41 \leq n \leq 100$)

All coordinates are in a_0 , while the energies are in E_h . The symmetry point group of each structure is also indicated.

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	Energy= -0.16102097470099999	Symmetry:	C3
Ar	12.970664566697	10.345494022967	11.185761435001
Ar	22.993988081493	18.287090913099	17.426945337963
Ar	2.760480893426	15.8929985272209	12.309002571578
Ar	13.218909670920	16.800602179160	17.810070677114
Ar	12.562329118173	16.886668846661	11.257912961891
Ar	24.950562626193	5.095678553880	14.723202719370
Ar	8.502434862221	13.221852854487	14.926108770746
Ar	22.547351413316	9.8469989419630	9.369710744428
Ar	7.767675410671	13.276340136501	8.140863734310
Ar	13.695657304026	10.321082370190	17.678208897701
Ar	12.100830069554	10.707687843763	3.543511916749
Ar	14.719623998544	9.127785919441	24.211399727539
Ar	3.621983095721	16.503418185468	19.193975647953
Ar	9.020802121042	6.367268095264	14.940524116998
Ar	17.704047325939	20.724088054732	21.263700308000
Ar	7.899703381269	19.955308640029	15.074895808652
Ar	20.280768448814	6.959306471046	20.279848357556
Ar	3.688913862053	8.974895527223	11.488659610484
Ar	6.747022875187	20.090265687501	8.304851549743
Ar	17.677507671076	13.926792803004	13.960371353805

Ar	17.176916291285	13.761926647593	7.233813980915
Ar	14.064812402939	16.166430970389	25.014294773438
Ar	8.969795697857	20.035249345537	22.104018970870
Ar	13.932894956503	2.586070900305	11.731037676620
Ar	3.769326391190	9.614156365601	18.392910361311
Ar	18.272025931966	7.257897736107	13.868956461473
Ar	9.043090510316	6.046328967088	7.832119305897
Ar	21.150167590767	2.485871961426	9.515423946077
Ar	16.629682805572	6.767440239882	6.810106010940
Ar	8.742102771187	6.219568484675	21.912943588358
Ar	18.723689274456	13.757326548771	20.582922384726
Ar	9.036616260343	13.028545721435	21.665221173903
Ar	14.270446913858	3.703411179841	18.780382323186
Ar	17.464320336475	20.622657899236	14.189623225316
Ar	19.732616989400	0.703986983957	16.087438517880
Ar	11.950994865810	17.623010600307	4.437311471767
Ar	12.696332815541	24.047996790044	17.799505658989
Ar	23.651665108183	11.626029773359	16.047129103944
Ar	17.467070295851	20.620535494795	7.381889928020
Ar	12.153884191459	23.710811069172	10.790085245230
Ar	22.641351597788	16.897325729665	10.541053383939
Li	13.096120452429	13.594139193902	14.470728935594

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Energy= -0.16352808737499999 Symmetry: Cs

Ar	3.020963522564	14.032132395272	13.792555067067
Ar	8.269531165252	10.060102242513	11.875873987050
Ar	8.736434909893	13.783425187497	17.650094578548

Ar	3.644337887632	20.918503423239	13.659169550033
Ar	9.324968026871	20.285258084024	17.523776808092
Ar	3.354073238383	17.589680159178	19.726131098412
Ar	5.144162972922	13.724815598547	7.012232627164
Ar	4.664695102834	8.057009509928	17.327249103833
Ar	9.019911740598	16.925071156604	11.911843207248
Ar	5.764322261226	20.577479681760	6.8793989985804
Ar	5.015260928745	11.589442704561	23.203155029863
Ar	14.0028866690810	13.178371110302	13.872896530592
Ar	25.388665600300	19.195308297066	17.631824553783
Ar	12.238617231440	13.040700525297	7.221218557724
Ar	11.782343392445	7.561014539852	17.192077013625
Ar	9.513925667718	23.806721529346	11.608737057938
Ar	8.956208430583	17.159169850879	23.661498670475
Ar	14.601283443376	19.789151451313	13.744401928657
Ar	12.867325620423	19.984933798179	7.086217042945
Ar	14.324150951657	16.592253988583	19.494424917634
Ar	9.244459594162	16.713783238885	2.085024413868
Ar	6.346820685559	26.633220338604	16.966655831282
Ar	12.129378915945	11.125901969564	23.089301236745
Ar	6.077336408652	23.323889655873	22.975206539536
Ar	14.359747627324	7.105319908835	10.54877888435
Ar	18.072164455055	16.053292049856	9.226154765624
Ar	13.436947244167	25.837454802810	16.836693975267
Ar	17.759063472471	10.518617238628	19.102543234567
Ar	13.158738493264	22.498298533323	22.868157022770
Ar	19.698906005287	16.032216189996	15.710061740036

Ar	16.338065063975	16.077446687941	2.385489016198
Ar	18.480677650883	10.143006076551	5.642013242744
Ar	16.031121916931	25.566586238347	10.189760082956
Ar	20.291048805557	10.119527064389	12.444182652872
Ar	15.283292869497	16.638903844281	26.360162345357
Ar	18.792176431993	21.931001598393	18.880751176217
Ar	19.523341912724	21.651260675807	5.418471765267
Ar	21.331569330086	21.612097084265	12.220974015993
Ar	20.894508734762	16.053228875910	22.356787449730
Ar	23.088626117134	15.506906461792	4.517802281658
Ar	24.896433058561	15.476872702263	11.352345709725
Ar	24.734934997290	11.975439283243	17.772262550227
Li	11.708862471501	16.754849693083	15.679536993285
	44		
	Energy= -0.16586594911700001	Symmetry: C1	
Ar	9.523393474676	25.938082364814	6.847282730222
Ar	8.465504926692	19.066272437315	5.914127079381
Ar	13.542603987092	18.729793524775	0.884044399742
Ar	9.147880918504	13.012424303450	2.213133265833
Ar	2.5042661172137	16.757968976506	8.834718369348
Ar	12.667822081050	24.758223493673	13.052118855523
Ar	14.218929626687	11.870024883931	12.380040441046
Ar	18.166743436346	17.021033034112	11.268630752366
Ar	14.487453353135	8.324771627997	18.207093936254
Ar	11.707879415926	18.019108064478	12.136097981211
Ar	5.822498074021	15.87448939671	15.012694936933
Ar	16.280067061968	11.976435200502	1.071219680213

Ar	12.008627841263	14.762946129470	17.802516263890
Ar	19.827056038796	17.386180514481	4.266674264810
Ar	24.273224096616	19.486063700356	9.136472320418
Ar	13.910189893619	15.099177590234	6.605485806468
Ar	15.046286220181	21.713585203889	7.260665126205
Ar	3.181052295109	10.644914014198	5.173851883224
Ar	12.826673691801	8.416834206201	6.274622949131
Ar	6.127045338098	22.123246605297	11.686788785176
Ar	19.436874651153	23.775822048537	12.165711434764
Ar	13.209342913968	5.016609940357	12.288636063452
Ar	9.264332562986	21.091723485393	17.720504513240
Ar	2.221691584805	10.524428046805	12.212660118906
Ar	19.277018363959	11.132604144619	7.647898923626
Ar	18.428184118753	13.827832443136	16.938193601344
Ar	15.962740327590	19.866542396924	16.707122482992
Ar	2.992156269555	11.120027852499	19.274876499936
Ar	8.219794999995	12.874036741220	9.328494036908
Ar	24.976308797755	13.748593163185	19.516859973123
Ar	8.459641201867	9.427794911789	15.258806897079
Ar	20.517389947617	24.644804849151	19.153539384706
Ar	22.765679359314	19.084842241483	15.859746661475
Ar	6.892263395218	6.076256105727	9.247167600859
Ar	19.626703451720	7.801084842653	13.718811713888
Ar	13.785730951566	25.666471276067	20.032907814424
Ar	19.996359055865	18.172713486861	22.069885380654
Ar	6.699345474684	16.465376632137	22.063778774187
Ar	23.756553432978	13.197449268074	12.515970724788

Ar	9.297923082139	10.098621372146	22.302644119312
Ar	15.806252516787	12.788471527192	23.240099688038
Ar	20.839746115507	8.407928292216	20.726243090256
Ar	13.206861035114	19.191893203056	22.991825665650
Li	15.053600251121	15.887401830668	14.497950156505
	45		

Energy= -0.1685470642939999		Symmetry: Cs	
Ar	19.472810050331	19.865926924570	15.756606669809
Ar	24.388594507076	15.182612755320	17.994701707800
Ar	18.723065216022	13.130278176423	14.569613279007
Ar	18.165543579872	15.630827833295	20.930862517102
Ar	13.422067778652	16.605812669970	16.074968920823
Ar	20.792238654318	9.363624312790	19.962253319315
Ar	20.851168908880	24.271338806171	10.439472182580
Ar	14.642684018822	21.034274031323	10.931473954413
Ar	4.203582406789	18.697403036683	6.558958047733
Ar	14.656127068134	21.563931742846	20.758535879035
Ar	14.151630105438	10.580190647012	18.457418780719
Ar	16.978242854849	14.791392526180	3.547110251556
Ar	14.142795425489	14.249933873374	9.953979821622
Ar	19.503575463850	10.749091529518	8.421981849483
Ar	14.887936363720	8.218634944066	12.433554624771
Ar	16.135450246716	10.685534035214	25.199174883719
Ar	25.820535594823	19.677905950272	12.734397778485
Ar	16.115866762591	26.040540122262	15.490102568025
Ar	6.661966167693	16.695593689880	17.794712645058
Ar	9.857604933922	22.777846163808	15.908927320429

Ar	25.173673281293	12.736157643174	11.559225493907
Ar	16.773845014719	4.211194098732	17.712310507470
Ar	8.819695801043	6.211541337412	9.768774417916
Ar	17.543941393075	21.741457517697	4.632640966326
Ar	9.597879639805	11.687082215442	13.935792598030
Ar	7.492787764822	10.296613323012	20.347890106319
Ar	8.790439704965	17.773114241944	11.464297557292
Ar	11.509687495442	15.449936106050	22.598414377497
Ar	21.638195912451	6.876596465149	13.541823955993
Ar	25.049705936147	7.083168563328	7.114827383358
Ar	24.093364524786	13.880608236483	4.508969593879
Ar	10.125132086107	5.321499881172	16.420080475043
Ar	13.641333009232	8.8806196058341	5.593967825272
Ar	13.647113422216	1.423591486663	11.933051239135
Ar	19.948206304239	8.374479349286	2.087915826284
Ar	12.141906574576	5.567156720673	22.955783574334
Ar	20.237830296773	17.365801537116	9.342531517568
Ar	8.550033641797	24.071415618905	8.923346134055
Ar	11.285290110360	18.524600883729	5.164103288583
Ar	3.319185018298	21.330354783882	13.285855761199
Ar	7.987518914189	12.567589967312	7.199307120249
Ar	18.486633627970	4.101284353113	7.766945937650
Ar	3.912840483245	7.805822617249	14.697646561802
Ar	3.102854547082	14.187492177633	12.135157717114
Li	14.163584675673	12.443282745548	14.198207918219

Energy= -0.17121919700800001 Symmetry: C1

Ar	26.837673426815	13.245887267691	15.070005644407
Ar	4.027108850230	14.809613872817	19.486574423738
Ar	17.044521082588	18.118636109842	29.231508871926
Ar	21.078395783702	18.355137734160	23.471920607924
Ar	19.022612292805	27.634565259887	13.816025114921
Ar	8.670239678959	20.302789454492	18.694278262145
Ar	18.719466276890	29.222566800598	20.703635382600
Ar	7.665504853441	17.399229832637	25.256104572141
Ar	24.348423383474	23.026788117742	15.187456658131
Ar	17.975369786214	24.251473934922	25.706928408485
Ar	18.276404446748	22.602162381548	18.837108555385
Ar	12.539576405900	25.627811138221	21.341949665929
Ar	12.831705962608	24.045459733361	14.498466211678
Ar	24.056940415320	24.606504192867	22.049063971182
Ar	20.061516252167	12.172149566156	26.904127046891
Ar	14.622632916110	17.475224617617	16.270525090312
Ar	23.457660739412	10.813409295300	9.549601398098
Ar	14.184056976007	19.026098536799	22.984506164350
Ar	13.183300438710	12.891046630020	26.452503315766
Ar	17.306900817723	13.335081269479	20.648601453932
Ar	10.710195653965	13.974217458477	20.235178713186
Ar	6.876234947697	10.165406954809	24.321440605420
Ar	21.188039622825	16.805843775296	16.736261590356
Ar	27.142892731421	18.636114556767	19.753134565459
Ar	15.530563674547	25.166581410123	7.897125106837
Ar	8.584771040056	15.037056957285	13.887431863566
Ar	20.567900057802	10.388864716298	15.8277275370223

Ar	7.502396380335	8.839070539806	17.236873117382
Ar	18.540560431142	21.020272347100	12.333597356388
Ar	17.966770852644	14.487777977143	11.483311791241
Ar	20.041774001651	7.125883077937	21.895283369537
Ar	24.102995333874	17.664878018580	10.467647796682
Ar	12.113108533471	11.935881652981	8.820783241963
Ar	14.100907710514	11.002806613019	15.384490520411
Ar	11.014087275779	5.717917922568	12.147595242660
Ar	24.098669524730	12.638179859829	21.331153962371
Ar	22.807995817170	4.479927678468	12.753986019971
Ar	13.148762317005	7.788986478315	21.487493231868
Ar	26.163090787342	6.893397208343	18.241541511500
Ar	18.128708513641	12.129317171508	4.977269985576
Ar	22.759402464200	24.494226423043	8.331585227556
Ar	17.341461213224	7.773725721820	10.280647057168
Ar	16.672514792101	4.686746018469	16.375170680947
Ar	18.751692618896	18.964343197569	5.907816648302
Ar	12.718178747136	18.759555089745	9.718219061559
Li	17.602522506378	13.961661951811	16.074644295494

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Energy= -0.17390761362599999 Symmetry: Cs

Ar	17.081029844143	6.781659803904	11.604579485925
Ar	14.377152404293	8.866235265400	17.511573970773
Ar	16.580860367439	11.160176346593	6.174017559836
Ar	13.871296830071	12.987775463280	12.400549664797
Ar	22.820750053330	10.230751030890	9.353419255673
Ar	19.906466483693	12.019291796448	15.437784779250

Ar	9.555832559945	19.167001625685	17.780131637488
Ar	20.173915424111	5.339499433855	17.938827466604
Ar	13.800717073542	2.247437364734	16.188668381041
Ar	19.420729094142	16.271857244037	10.163445241900
Ar	25.949971812172	8.725787930270	15.638579148838
Ar	9.514005052842	11.592168793087	7.199190923001
Ar	9.675661450838	24.637071069830	22.179472348962
Ar	14.843642039270	15.427754980967	18.470842628903
Ar	9.057386186719	12.741290226459	16.835293164562
Ar	18.718079994927	10.821062136232	22.332139228930
Ar	8.559266831478	6.073082264999	19.486318082132
Ar	14.810532080727	4.816054411262	22.923013403166
Ar	13.435336103705	17.111674631336	7.284986974454
Ar	25.719078837203	15.377627909603	13.236317295728
Ar	14.378036559260	19.503986484844	13.415190971038
Ar	8.592054330558	16.815189819397	11.782554277846
Ar	10.011277499122	7.238977318329	12.598279288322
Ar	20.543556755838	18.807627567041	16.478466728777
Ar	24.496028516083	14.185727395667	20.115686530667
Ar	25.085236211970	16.296531334895	6.248828903251
Ar	11.650245546395	11.375593940033	23.164411318466
Ar	18.809589420807	17.283969240937	3.124382180507
Ar	12.419026572205	14.343600454392	1.186161611400
Ar	3.639491982986	21.831671474914	20.473438686518
Ar	19.209679289129	17.648197471885	23.365008984399
Ar	2.965361602711	10.099682816242	18.781181467733
Ar	17.371593744931	22.609599345395	7.711110686519

Ar	23.637852936229	21.699078357018	10.797101216208
Ar	7.207561806920	17.907198320256	4.808892479775
Ar	15.520784849615	22.149592285590	19.635573935997
Ar	4.448008735777	11.281693935011	11.892848262352
Ar	10.333275629679	22.905803278025	8.863847411748
Ar	12.132340119348	18.232347303081	24.140568736551
Ar	6.052428982138	15.414957367611	22.423989362855
Ar	12.900707876711	21.536598726189	2.185011635233
Ar	18.354726688977	25.133141531830	14.0816299915544
Ar	2.109700602868	17.590710430748	9.490175811725
Ar	11.315945635306	25.379718018448	15.275892528313
Ar	5.236577355740	22.557531958478	13.565206146215
Ar	3.362703900729	16.494028271757	16.195342884150
Li	11.758650754214	16.080030451495	15.088313002779
	48		
	Energy= -0.17633248422400000	Symmetry: Cs	
Ar	13.012231573357	22.840704011063	3.985400583508
Ar	7.468987091956	16.322397206310	19.198362662609
Ar	27.037554712479	16.783277951042	10.305948327811
Ar	15.122319288137	16.105325598816	3.434642936821
Ar	18.228730122932	16.519765462151	14.349966438179
Ar	7.433427054764	20.741634630456	8.035446995719
Ar	16.016619862938	12.858566312415	9.344010817158
Ar	11.752374804027	25.915056530396	10.238350823726
Ar	15.849711116447	24.617624558933	21.821355790892
Ar	11.416103769195	27.474104962405	17.146633308213
Ar	18.889600399278	3.646244218839	15.680534372587

Ar	16.749743210841	10.214218732242	15.366613711690
Ar	13.936786164258	19.212081999461	9.762251285015
Ar	9.602118823348	14.055596807812	7.525440118654
Ar	22.329557404705	11.741506297106	11.492612310271
Ar	12.257527108460	5.494198186305	17.586192271343
Ar	16.041294587754	11.891316840743	26.244815461520
Ar	24.374884950696	17.046965132104	23.749247083802
Ar	10.959372185145	16.441178459913	25.107719972686
Ar	11.613629166084	6.551645511701	24.605345248073
Ar	13.611212786123	8.999292935460	4.331607674008
Ar	18.413730710978	24.410291308234	8.438323366709
Ar	21.452018829219	26.807469014838	17.919722658447
Ar	9.260192937796	22.498701901027	21.734134379973
Ar	22.860866762839	10.360902013933	24.768582776867
Ar	22.866350001277	21.649851489257	13.151621344883
Ar	7.173710751571	10.041026994652	16.446079463241
Ar	17.656895386314	7.227188037268	21.465593482863
Ar	20.542352598463	17.720015794187	7.833466070513
Ar	23.130448150561	8.994382022426	17.768071341425
Ar	17.025765514949	29.624302094268	13.166154802275
Ar	24.642233055526	15.651469101850	16.784268341348
Ar	14.066603860540	18.193671544933	19.220040176819
Ar	20.544579554400	11.319083754591	4.546769285566
Ar	11.908739805605	14.545690230564	20.304745603469
Ar	18.907931613065	13.862760860240	14.282739142404
Ar	5.293796162633	15.792337987920	12.658108933979
Ar	12.703690978854	11.900681216179	20.177454416980

Ar	11.447840798654	8.268232816805	11.270125349454
Ar	6.560260856344	11.065776210954	23.480035943743
Ar	16.188500659494	23.018433389954	14.913824750214
Ar	26.902109200249	22.067856773022	19.094135075562
Ar	9.582652046163	21.048568241650	14.782439688777
Ar	22.464125376108	23.966432163447	24.589822903799
Ar	20.383681474043	20.241376875756	19.336310351421
Ar	18.096442781326	6.433678947150	9.384982306507
Ar	17.557676333402	18.595898064993	25.249042557141
Li	15.449694507856	14.248559892701	17.242586843862
	49		
	Energy= -0.17885767556200000	Symmetry: Cs	
Ar	19.845017879885	8.644508763393	5.992695669923
Ar	15.816562350172	10.706329394101	0.757135437663
Ar	20.621732699046	15.07222483476	3.713040453013
Ar	22.967434051296	7.593433051237	12.019303105875
Ar	13.274060067205	6.645662810665	6.044339913940
Ar	18.281290215949	2.858612481455	9.448209619484
Ar	25.969622890733	11.699269513968	7.014991081207
Ar	16.214717498445	9.011259189907	11.823026906920
Ar	20.387064524824	13.815540446652	10.503696994648
Ar	15.610514155322	18.242278735142	11.340976242641
Ar	16.984577706784	13.921366341072	16.102217502208
Ar	11.389488434229	13.375105800115	12.652796420324
Ar	14.877314148906	13.277459803354	7.106994321024
Ar	15.557506362581	19.718364557945	4.543500728552
Ar	19.343874941447	7.648542280205	17.920576023529

Ar	8.184569991663	11.269051474839	6.879742112622
Ar	23.810287800552	12.794843600331	16.514427626768
Ar	9.620221650034	6.699882086532	11.926625068007
Ar	21.458117946450	20.293720794161	8.180849306781
Ar	10.733026823061	15.345419260514	1.610527785895
Ar	14.634352181123	2.935244894536	15.346795960485
Ar	26.794189525209	16.912619778440	11.512789491967
Ar	12.734376142438	9.054240681319	17.461146598851
Ar	21.205043569657	18.813370370663	14.793493351763
Ar	10.009426483916	17.720358627562	7.891409235211
Ar	7.427156067380	16.413084090647	24.904919030276
Ar	11.071336622296	15.326784035857	19.165564395419
Ar	15.443867581147	20.438768064956	17.873294106620
Ar	9.578951681171	19.866025420980	14.257690823016
Ar	4.754668647163	15.414917943209	11.581753817654
Ar	16.069152337458	11.769581836921	22.741535435088
Ar	6.202672448295	10.806429103325	16.659314084137
Ar	18.217052229335	24.606650268863	12.810777605310
Ar	20.562449377492	16.959057367100	21.327747334935
Ar	12.266965180958	24.025831513027	9.143060123762
Ar	14.418365324810	4.740908350889	22.391057074252
Ar	8.225858003951	4.136876213092	18.573983722138
Ar	26.882101019802	19.063823632960	18.460525168383
Ar	25.405041968824	23.849808103900	13.128985620503
Ar	4.226995684032	16.851995689154	4.493422774750
Ar	9.143115187745	9.765437106605	23.174155308853
Ar	21.454622491405	23.894544189799	19.287261584063

Ar	5.198253684442	22.307011225679	9.266153585506
Ar	4.495749821612	17.405291665493	18.402167216883
Ar	14.344816783806	18.366988971775	24.474259546789
Ar	8.933380658596	22.242369297167	2.975142579104
Ar	12.049912851849	26.184081601526	15.859008440910
Ar	9.331395132903	21.962842813110	20.937021420698
Li	15.884434335129	13.638754895680	11.625768743811
	50		
	Energy= -0.18153540830100001	Symmetry: Cs	
Ar	5.167189703329	8.365862431164	20.864025782806
Ar	1.931559018100	7.811833911498	9.644179451375
Ar	9.916084892518	4.294075436371	17.452161850245
Ar	10.639515844348	23.328388528001	22.971200673025
Ar	5.747508421979	14.730830188051	18.066591296134
Ar	0.212785753995	10.529852461282	16.186183771665
Ar	6.580934710599	9.331625177900	14.309838705584
Ar	8.086407681701	3.935926454415	10.474693411119
Ar	10.222654439863	14.738146562910	13.285924038092
Ar	17.779309492404	25.598808860267	11.448669345898
Ar	16.819351524421	14.085121062918	11.612116367870
Ar	14.832807876050	6.147775769845	22.088908966371
Ar	15.807814537747	12.829403007188	23.075375876623
Ar	9.362424997904	20.035294646236	17.038546031130
Ar	13.038053663341	8.536372677467	12.687543877228
Ar	13.431233244859	15.555195023216	28.778351964522
Ar	12.241888555444	16.389002081639	6.751341769522
Ar	8.345416114143	10.672994738294	7.859516848519

Ar	7.426241706590	20.331708790236	10.311148956458
Ar	17.900949601889	10.266995241866	17.21445478119
Ar	10.286241523362	16.458253102134	22.384679462723
Ar	20.315443550513	19.554784121032	14.494958276329
Ar	14.835467918561	16.471799444048	17.666524254536
Ar	14.919469753919	3.229773935650	8.740278037789
Ar	10.036024724370	10.206452282215	25.484326088976
Ar	21.430331211244	9.024144622260	23.214710281950
Ar	16.690622002387	3.506525352955	15.749050494887
Ar	20.545148195812	14.932413330743	27.418600811747
Ar	16.470748769067	8.954869870264	28.577754612395
Ar	21.657571227227	13.118432816565	6.822885290681
Ar	18.716045883577	19.533153351458	7.452512579558
Ar	15.196678410334	9.977435175695	6.216094530211
Ar	10.730791360139	25.964982486588	13.193855849679
Ar	15.408079293006	23.394917509854	17.951183115497
Ar	21.325693133401	15.674332726269	20.242163509018
Ar	2.927959459475	3.805296331294	15.672106701795
Ar	11.180156420661	11.107967261632	18.706146266404
Ar	-0.687635920271	16.166322871118	20.129839643512
Ar	2.677578381066	20.282795879688	15.358627992550
Ar	3.556026314537	14.653528172197	11.412783908637
Ar	13.919071792793	20.099757367022	12.222844861665
Ar	19.867991236515	7.726029579780	11.020985776419
Ar	7.664496445786	19.349920235396	28.090866660349
Ar	16.409847553796	19.558396177749	23.671091000744
Ar	23.315955926447	13.228946398136	13.864129202712

Ar	12.704140233468	23.618468551196	6.580367609821
Ar	5.968458169405	25.931987693428	18.238809863062
Ar	4.289023745078	14.010782933464	24.776259104747
Ar	4.570426458435	20.272608412977	21.967195520499
Li	10.311078262672	15.558250738193	17.8228285369534

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	Energy= -0.18421701676499999	Symmetry: C3v	
Ar	19.809683808125	13.320086729578	29.487293767832
Ar	18.699360819749	7.420263013937	12.500796772679
Ar	17.517631417373	19.104016600721	25.759179398003
Ar	7.775456785292	6.529046729304	18.018417317430
Ar	8.276211066257	13.567744012127	18.001117288290
Ar	2.162210196849	10.637197057509	19.073703072400
Ar	16.737395027032	24.930530955475	10.786721065717
Ar	12.224900709960	22.843413023909	23.214309623933
Ar	7.846083729636	17.232191213078	24.018728959265
Ar	24.074492093071	9.464704644907	24.961938850423
Ar	18.841827673655	13.156355863836	22.800005024051
Ar	15.074807323956	13.591520763977	3.208851070338
Ar	20.636412639686	9.661481047443	5.883369887677
Ar	17.130210427689	7.444659715775	26.052543785576
Ar	5.384049036515	10.278387818931	12.572391240470
Ar	9.258473736662	4.221494106419	11.539395563311
Ar	20.015383081336	18.632075461572	19.241199564373
Ar	20.837529231597	16.939026861743	6.152247619998
Ar	16.500797876587	13.290716538053	9.808834564423
Ar	15.073121392708	22.124062498628	16.864816154164

Ar	9.8007299624110	26.916809227030	17.864820482061
Ar	2.601079533229	17.710211047760	19.066236805217
Ar	16.346839009179	28.910356467364	16.705474688756
Ar	5.786251152340	17.350840250459	12.586292997432
Ar	8.806397796800	20.246919852931	17.974593832975
Ar	14.235940653681	4.023468669013	16.827627795831
Ar	18.862446402150	18.698252947510	12.843302039333
Ar	13.170447213706	13.470493125948	26.578771019780
Ar	13.850634086103	16.733212725689	20.378615426040
Ar	10.190742093625	22.960581794246	11.924565746211
Ar	25.447653586424	22.480616720485	21.081106081795
Ar	17.692848114678	13.259541522974	16.300931886165
Ar	3.775007828013	23.807010718709	15.200728603230
Ar	19.941519910788	7.348850896045	19.392995063866
Ar	13.455395686420	9.908227582907	20.491390808716
Ar	24.194544696110	16.746929076826	24.785956490030
Ar	23.324810482930	22.602191240343	9.300579170651
Ar	13.740906208422	7.639243574677	7.244317022135
Ar	11.419067359390	4.096429801210	23.523466688364
Ar	9.868267933166	13.659877500027	8.254380107668
Ar	18.764157483808	24.814190306566	22.034560503192
Ar	24.204553519142	13.058663113612	18.663171675505
Ar	14.248825452670	19.291587537669	7.617625483661
Ar	25.425824864389	18.791273971982	14.964764360852
Ar	12.246865355087	9.977819768764	13.786609722095
Ar	21.477248939036	24.366182577994	15.733916933186
Ar	5.072295074532	23.732397509900	22.401021481270

Ar	22.969784204570	13.129378396944	11.811395118804
Ar	7.449837977026	10.159017322789	24.031153241520
Ar	12.681642360262	16.800422899257	13.891239315742
Li	16.325463911773	17.659452068647	16.592905207792

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Energy= -0.18679859894199999 Symmetry: C1			
Ar	14.909116136445	16.546292626230	17.094937226446
Ar	18.288583255496	25.159459471865	23.606580007100
Ar	22.539033564365	7.826605115221	23.037734411895
Ar	21.009031688347	18.011799352066	15.077354595274
Ar	19.993336232110	12.738032023771	18.882611612139
Ar	16.772494941158	23.048943578060	16.932149487696
Ar	10.516885161825	11.701009542090	18.959512369055
Ar	12.117215353007	20.766420655356	12.438448069889
Ar	16.634770703615	15.773831511359	10.803156900507
Ar	12.832039328488	20.681110967556	22.385735896974
Ar	19.326894680592	18.817674467468	21.439653242594
Ar	5.502257587013	18.528588440048	11.077620186017
Ar	13.262334195934	10.304235477620	8.057014111384
Ar	15.076301151192	14.0566660605189	23.429574820433
Ar	25.604002964581	16.705552183321	20.158179775998
Ar	18.533764772945	22.372963000906	10.319392606357
Ar	15.747581651090	7.668778213516	20.933904371965
Ar	6.109306884310	11.804943853686	8.253513920545
Ar	10.961053168912	16.896729092028	6.570948374427
Ar	27.344146012236	15.865223198604	13.484522491092
Ar	19.698874006458	11.895549405415	5.998621322950

Ar	17.384274803127	18.442876409063	4.458455161879
Ar	18.637107334765	6.354200200492	9.992845032056
Ar	23.558025056564	23.474593249633	18.984509743912
Ar	21.638542880032	12.020016188365	12.629110024043
Ar	25.356454463456	22.639849326045	12.345338183787
Ar	10.589655861167	9.012819958591	25.488829399452
Ar	14.059292034655	27.484919297250	12.156453170354
Ar	10.492216304728	14.261750405118	12.775536471234
Ar	8.144290650550	18.269547426031	17.789293575472
Ar	9.288518447665	4.968307710956	19.810252818021
Ar	12.975223213810	23.673590949980	6.210403752484
Ar	4.420638453733	12.643900216186	15.344138994173
Ar	21.815934469286	14.186523608094	25.680865502162
Ar	26.627293469496	11.782371236966	7.682958129728
Ar	10.160094898915	25.066198096597	17.600835449358
Ar	22.880807074445	17.445707532177	8.511837170690
Ar	15.636339067886	10.485672247510	14.606418028058
Ar	20.874654002705	27.848396471336	14.142302457410
Ar	20.762151752937	6.351280070924	16.519884094001
Ar	12.663598197588	14.185120788277	29.8666276685860
Ar	26.279305300824	10.327186382235	17.486696970160
Ar	15.630555274288	29.585745581962	18.753753023544
Ar	25.571736742854	6.280422879335	11.655969517625
Ar	14.523936727685	3.679412032751	15.181255825240
Ar	17.330705883622	9.127576460789	27.691346327439
Ar	4.549776509493	9.987166098959	21.916076286041
Ar	23.976498622148	21.082727130029	25.788202362196

Ar	17.200839275641	19.254707541101	27.871729723620
Ar	9.175071834685	7.649330999824	13.288863643330
Ar	8.328845622612	15.607310131946	24.316069656957
Li	18.256877442545	14.293108965964	14.882110860165
	53		
	Energy= -0.189485299645900000	Symmetry: C2v	
Ar	18.873552958216	16.183611539373	12.284972897603
Ar	16.876599585020	10.134458374110	10.258117099776
Ar	12.288259240983	14.693650423672	11.546424537392
Ar	15.606839260625	11.924570331195	16.517594726614
Ar	14.136064223885	20.894378007331	13.611623569116
Ar	17.716762978246	18.109101013181	18.801769520572
Ar	24.627627062712	18.880636000826	9.664585596266
Ar	24.280637229747	16.674386867567	16.534181565293
Ar	18.199228534804	21.638901767392	7.991478626410
Ar	20.937237321182	22.572776190828	14.451597932553
Ar	22.258002265302	10.285921490588	14.336255997008
Ar	16.233053268430	15.237388212238	5.761826046955
Ar	22.612970445333	12.446284551048	7.468226075659
Ar	6.148528632711	5.382526976360	22.683088394230
Ar	11.079092191817	16.426905704669	17.785586267975
Ar	20.963000461552	12.135067495639	20.885316303886
Ar	11.372407994214	20.071008154162	7.122990255406
Ar	11.167629232572	8.405960147147	13.159530198270
Ar	11.307036508500	10.186450261287	6.561327417844
Ar	17.157523981334	5.299622801558	14.953530304295
Ar	15.935641570188	24.972469872538	18.871253595828

Ar	7.702245343706	19.257232448733	12.8272899903159
Ar	21.532611703731	5.380923833317	9.084144256011
Ar	17.651600147985	8.513664239536	3.715469897046
Ar	14.596902067130	13.779070097019	23.037406191672
Ar	9.9869999922355	10.195102677968	19.302317983246
Ar	6.639795035847	12.908299756172	14.427562551675
Ar	6.569637330163	14.897304880471	7.887931128048
Ar	15.829765069153	7.196438022423	21.504510879899
Ar	12.639681578583	20.412109375992	23.216392651963
Ar	9.127961308293	23.342014903267	18.013367065368
Ar	14.453738226143	4.100066934958	8.433517097558
Ar	10.267559898444	15.352360129407	1.991628487359
Ar	9.357050852504	25.627899225997	11.180915925333
Ar	7.888865012499	15.093196134089	23.728208802318
Ar	11.165580704328	3.499383628617	17.975712130354
Ar	5.333765072439	8.294576386936	9.434903161577
Ar	4.331966076648	18.052707195319	18.544987742963
Ar	11.689764362538	8.626392934093	-0.122092284114
Ar	4.395562400333	21.695277546029	7.427550838200
Ar	5.256972589936	6.376212075419	15.972369186320
Ar	8.500348396896	2.257495588694	11.458390300533
Ar	1.323817182793	17.156127113272	12.110088610465
Ar	5.402477355535	10.260002513879	2.700461211442
Ar	10.779661634715	9.053854605932	26.186680034323
Ar	8.524593797298	4.186104373938	4.615731178551
Ar	2.962229223447	23.846466260125	14.284405470964
Ar	3.224322898116	11.396028871988	20.199853226038

Ar	16.208006391130	27.252711447413	12.022430097373
Ar	3.270484215357	16.998350287914	2.235454812847
Ar	0.179383917616	12.484275248151	6.952364211687
Ar	0.176961730828	10.534030186519	13.789180595118
Li	11.144621919998	12.458064585343	15.400764371518

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Energy= -0.19202907977000000		Symmetry: Cs	
Ar	26.763465561134	18.134704651583	23.213725387667
Ar	25.869014169390	16.893320558826	16.249422298228
Ar	20.378915721412	17.116815905320	26.247060809252
Ar	24.991568850486	24.743625995708	22.121547995007
Ar	28.972712642395	11.903770217091	20.267028513935
Ar	29.267673046261	20.514914801108	11.321120948296
Ar	20.693965403644	19.821453628577	19.820652656340
Ar	22.406240240377	13.506729629904	20.913197616313
Ar	22.518142788493	18.680813956751	10.540546246637
Ar	25.514200211156	6.955676385686	9.134669868092
Ar	27.446166656276	13.734136286838	10.184843262809
Ar	20.713852498749	12.043127402560	9.504562264299
Ar	13.707052860757	19.011514781803	26.428506895310
Ar	19.182664132848	26.436084996726	18.811352381821
Ar	18.581674432688	10.252917509799	25.438749921466
Ar	19.359585803912	27.759690528613	12.024031372607
Ar	23.779661747136	6.901334624460	21.679291991446
Ar	24.571245900387	24.792936621689	8.151882883364
Ar	18.598723013670	23.723115949047	25.098720992856
Ar	16.030465108867	15.328888391283	21.088793949810

Ar	17.580936198249	21.499792279489	14.356663489040
Ar	19.278071841890	5.865177089375	12.405839460546
Ar	19.825529214563	16.771434950499	4.174411084128
Ar	14.415603293001	21.554492526906	20.039251437800
Ar	17.883546538610	9.200451831986	18.420849191890
Ar	12.928007437431	17.016991466237	15.621764789366
Ar	14.609118835275	11.061479162426	12.691092440185
Ar	16.093775328834	16.930479087080	9.827891697359
Ar	17.820091193736	22.938366539444	7.306324386765
Ar	19.526239881174	6.713163018163	5.315884292443
Ar	24.704935659781	11.701632907432	3.908097212302
Ar	13.631793100965	28.098790746961	22.459475363138
Ar	13.635045521287	5.926483411212	22.794296844026
Ar	9.388927885703	17.000979216344	21.474287766771
Ar	11.922818427007	12.153777813107	25.675307789310
Ar	14.713938435928	11.847857224244	5.564501229488
Ar	13.175812383466	26.646305712834	15.496639985331
Ar	19.267700158153	15.204417236755	15.385623566306
Ar	11.196317713762	11.051856235289	18.650929097477
Ar	8.280195442930	21.929061072045	16.826515559021
Ar	11.601489724730	21.850672112011	10.733558532577
Ar	13.062772647625	4.903598685883	15.727502964900
Ar	8.080349529371	8.906100792788	12.635248426949
Ar	9.628256632388	15.048371873453	9.534252552875
Ar	13.232901416942	5.675885193248	8.643697939271
Ar	8.773030395929	23.419333698912	23.778368922956
Ar	12.800768700333	18.765064048387	4.215186395023

Ar	30.203401442459	21.888389884795	18.288596084573
Ar	25.497310463506	11.936244389505	26.716155484513
Ar	24.133338014647	10.118005479414	15.259587021248
Ar	26.6000299915075	18.554061985973	5.008803626354
Ar	24.142703760285	23.524337659140	15.130501594792
Ar	6.271379612290	15.150104017236	15.583432997743
Li	16.848442433123	18.364547353385	17.684429718295
	55		
	Energy= -0.19482310354099999	Symmetry: Cs	
Ar	12.683938837782	4.501572764548	16.165034794362
Ar	10.461757652663	15.436743435913	20.360326684842
Ar	24.093606417790	23.775759913095	13.304782644352
Ar	13.228288133995	11.853979190315	25.837803030370
Ar	23.569353940963	16.332425353328	23.112578330289
Ar	17.455213721230	25.508807683789	15.091309601768
Ar	22.683675387509	25.878148945202	19.924206457086
Ar	8.200382575239	9.639579934771	17.399500201025
Ar	13.925160565196	21.407743692002	19.520967221495
Ar	17.729940870993	4.429509619028	20.812708376805
Ar	19.916173748600	10.227568601403	23.880660461110
Ar	12.148462163842	21.478501814484	12.896082194235
Ar	7.633917851458	19.300368789079	7.858844657233
Ar	8.291758276735	11.967761018118	7.665867905812
Ar	8.698403280242	15.503345772984	13.777010481613
Ar	24.558042277083	13.287397902151	6.942954833948
Ar	14.740151339928	4.487603860238	9.626693117122
Ar	20.438684193136	19.757976369911	17.730934973215

Ar	18.666354077065	7.450816746209	14.574023129348
Ar	24.185675450162	20.456322792911	7.069438406943
Ar	13.187695784605	10.440267497772	12.680603387875
Ar	3.295402987601	11.408018408128	12.575363220725
Ar	24.528323460843	16.711728759748	13.095991156356
Ar	15.222408353079	15.981040547721	15.525068065600
Ar	14.867700553276	10.378955885509	18.979021186722
Ar	7.962132102776	6.099184277352	11.317300017018
Ar	19.091062648911	21.839744993101	24.447891182344
Ar	9.413584780770	24.743160468935	23.482038462561
Ar	6.426991311210	11.308511230714	24.096123837209
Ar	13.482338493489	16.044387713174	9.027067673002
Ar	10.775354312712	27.096056520147	16.917973787611
Ar	14.204949127084	22.146960775360	6.127314882756
Ar	6.268929955085	24.913507605339	11.895959920320
Ar	20.740741435989	12.922763771248	17.431050396351
Ar	15.95398556743	27.575676567498	21.758740210025
Ar	16.941813806045	15.912754961140	21.936607445897
Ar	5.837094936340	18.581542681389	24.364038014645
Ar	2.675982095052	18.715525580772	12.800298645200
Ar	3.676931513321	14.932807839686	18.685730732074
Ar	18.788315121750	16.514578749171	4.899227378957
Ar	23.917759676920	7.110040280612	19.181974301546
Ar	27.234352147550	20.320646999203	18.612318118410
Ar	12.836897600947	27.758792321433	10.165329009564
Ar	19.050219175386	12.979462866487	11.135419710391
Ar	20.954018286795	7.178670824990	7.989049930881

Ar	19.610441921963	26.050451785236	8.337265860475
Ar	24.901503105824	9.793373348560	12.944811613972
Ar	15.156247192004	10.315823204206	5.963630687487
Ar	7.155229065238	21.047624397725	17.805695841380
Ar	11.044610567053	6.033846705586	22.758615799670
Ar	18.725126760869	15.764291867049	28.459357733961
Ar	18.674318768145	19.824203120706	11.147784341254
Ar	27.579397192721	13.195696787278	18.400376764062
Ar	12.640222059199	19.046151813511	26.147786522045
Li	16.933639242164	11.754473281518	15.072189538355
	56		
	Energy= -0.19781781491900000	Symmetry: C2v	
Ar	22.582774208837	17.220697533904	26.915583395924
Ar	19.633328639690	23.588189496776	25.559804528162
Ar	12.989677175124	21.175198809157	19.032398418079
Ar	9.209976740391	22.582398842237	13.428787875369
Ar	18.417512863348	16.014988278040	10.438468196428
Ar	21.880230352552	10.147160384550	26.204174243152
Ar	7.976035343277	14.232978423244	5.500686879594
Ar	6.107634188546	12.486086653086	21.999670436569
Ar	5.322159898883	7.210650589870	17.343841463876
Ar	11.875264888572	9.168974945480	24.860123906131
Ar	25.107302890325	15.221975914716	10.725719279547
Ar	20.689128269484	11.700550561230	15.028752191054
Ar	11.452108267713	10.258735424029	17.807475163811
Ar	4.807213578399	17.679796612173	10.831718887185
Ar	10.942222287850	7.802904153078	6.698098940518

Ar	18.233540534214	18.158804999871	21.632905200459
Ar	13.567201607121	27.325931708247	15.992934749782
Ar	3.290219841911	20.840764617476	16.984601359086
Ar	13.367693546798	20.687612677234	26.040418153744
Ar	20.746006438086	10.103382740768	8.054154084583
Ar	27.463654573721	10.735157353165	15.628065046787
Ar	23.025213566047	5.576386249079	12.963770857096
Ar	21.270159059841	18.478675634359	15.880590856878
Ar	8.597726086323	16.494977809875	16.621462995184
Ar	19.518967167827	27.338482134169	12.563097968700
Ar	7.815038418076	25.715039660190	19.592329337780
Ar	13.354843726591	26.298892771800	9.098153817789
Ar	25.047220298594	24.158778073646	15.304734227926
Ar	17.414233233884	4.985090388274	23.593148815482
Ar	18.894947781069	23.893610777371	18.614432383953
Ar	14.648583763884	10.595418144892	11.752372810879
Ar	8.873506282642	21.428911494369	6.408736065429
Ar	9.136640694352	15.112035223720	28.106218556681
Ar	24.478028990364	21.049829609625	21.403573224686
Ar	10.690828616817	4.990481112088	13.231921240486
Ar	12.251571120599	15.365440080695	22.118626319041
Ar	14.105334510964	26.768324570694	22.818274140734
Ar	7.682675885037	11.305878092407	11.995143326981
Ar	14.978759879638	13.421535127312	5.194170419181
Ar	23.037463424229	7.193281021649	19.872467466147
Ar	16.305587925441	14.295586136616	27.399462154101
Ar	2.365163022433	13.641977985990	16.130314191641

Ar	28.122234593606	17.804142353488	16.421000544420
Ar	23.799466200118	14.190283762796	20.663830300850
Ar	16.02631522399	21.495083877441	13.280114926621
Ar	16.784605958471	4.441728960199	9.595576357645
Ar	21.600543675435	16.425138006231	4.495543542732
Ar	22.035319795442	21.600469240000	9.622737589917
Ar	11.164632235338	3.850054440232	20.241810745004
Ar	7.060758199332	19.612377084309	22.814678757013
Ar	15.863178025902	20.540372941443	6.141716683861
Ar	17.514032542430	11.366130625505	21.043317595079
Ar	15.331975913154	15.684301616097	16.276862090548
Ar	16.883605043621	6.013170646865	16.558106929267
Ar	11.77743227517	16.829461719640	10.606895305134
Li	17.096413168068	19.749717386484	17.434507488169
	57		
	Energy= -0.2004114556499999	Symmetry: Cs	
Ar	15.265954924006	26.479337632407	27.939807526549
Ar	17.526877404958	17.343757884671	18.761299472620
Ar	15.737753963263	23.093782430114	21.992889418509
Ar	13.910543023518	12.222409313332	20.764348341510
Ar	18.821959438654	14.159528399765	13.150482003910
Ar	9.994083475546	6.809344362999	19.160266833522
Ar	11.244120781760	18.276211207037	20.600041878104
Ar	15.231497856508	9.159046166146	15.186441425474
Ar	20.089031103518	11.283992648652	18.945508752383
Ar	23.797902616141	16.369511166802	16.904294491901
Ar	19.566500277217	8.159464760872	9.866830045944

Ar	16.474435079789	5.849924427372	21.116059331387
Ar	12.639593693108	15.098515070273	14.970514068274
Ar	24.773445018050	10.496819340431	13.796171847040
Ar	23.253215041824	6.355086063568	22.600383089616
Ar	20.898441014581	5.1532575117181	15.950370531877
Ar	13.819767728939	11.800749356972	9.028003730472
Ar	15.8144388823709	16.978440188333	25.319348834504
Ar	20.119499212291	20.865682653173	13.566875083718
Ar	8.657833876263	9.816527598991	13.0781500031912
Ar	7.205130553205	13.165086523391	18.968406981325
Ar	22.250526842982	22.104607399723	20.075533162516
Ar	13.654875068786	21.847534099763	15.469893243650
Ar	9.196859674477	14.430483199175	25.743845620352
Ar	24.881520467983	16.747875526514	10.262238204679
Ar	8.383085863967	16.107770683514	9.639636406261
Ar	18.536116785398	10.645964897661	25.645079418769
Ar	14.997691376409	18.606539556075	9.518062776213
Ar	11.961908116697	8.070061514436	25.924148143771
Ar	14.254016749347	2.464835517773	15.319652380398
Ar	27.116704105846	11.708460439595	20.467962016934
Ar	19.684885909216	14.391055560927	6.312537005017
Ar	6.954322277942	19.470460143667	15.539814897407
Ar	22.280217966716	15.996378875512	23.415823151482
Ar	20.924841831445	21.421438626848	6.769312701103
Ar	20.640444799114	15.609715769438	30.231975904519
Ar	14.060619058807	13.012435966016	30.646257275630
Ar	27.084609773769	21.924926082809	14.810826923032

Ar	25.427917575825	11.286215231247	27.299608329855
Ar	9.017176441538	24.668947634353	20.129750431943
Ar	30.178289886236	15.296223309902	14.976442207397
Ar	4.808931079731	19.149257634474	22.445260640966
Ar	16.221418929459	25.555729531153	10.090411286251
Ar	26.758637245950	18.440308466720	28.017210628709
Ar	28.482160964816	18.778810081391	21.181411253372
Ar	9.554448547936	23.148319192919	10.116501223501
Ar	11.683540346353	28.3888388386554	14.754622028031
Ar	20.602727607668	21.856605411314	26.880808859340
Ar	10.415197553882	21.523211071223	26.500300273702
Ar	25.294397995483	27.929765580310	18.112719989767
Ar	18.373017300000	26.879594292149	16.716489055621
Ar	20.514296419467	28.042767020595	23.389087765109
Ar	15.331887746138	20.175836037794	31.381102876916
Ar	23.111755530906	26.652694546136	11.390053325863
Ar	26.711170188052	24.740918075081	24.570092137133
Ar	13.848657589016	29.668117780973	21.482569817769
Li	16.389943319752	13.278795299304	16.996219072262
	58		
	Energy= -0.20330820519900000	Symmetry: C2v	
Ar	14.595622227628	8.210683980386	16.608763314598
Ar	15.503864761316	4.076866096671	10.993934189497
Ar	13.729781150480	12.183473456564	21.930057829820
Ar	8.457206095209	13.955664824427	11.677149140652
Ar	19.264992316795	13.578844638012	25.476707633781
Ar	14.629730805863	11.028551929017	10.403900344887

Ar	8.422997315419	11.121125173238	17.918867979271
Ar	10.868667229058	6.039163116227	22.314224517807
Ar	18.964341743059	2.932706238191	17.083105168827
Ar	19.377918597357	12.744341024834	18.526701679005
Ar	22.040970385034	18.619538901369	17.634226330943
Ar	13.759886407810	14.916974492812	15.907448514435
Ar	18.013429260523	7.048335111243	22.734700984064
Ar	11.746388220295	1.955828732091	16.624593590441
Ar	20.493117021054	8.606484287278	13.078454408371
Ar	13.795817132883	17.653126205142	9.886030995991
Ar	9.646539122735	17.355145563142	20.734594401614
Ar	5.378600467008	4.971389748591	17.968761060695
Ar	9.680568396023	20.172961906088	14.529720105143
Ar	25.299394522051	13.026771288911	15.112112023344
Ar	19.024587975749	7.894436810719	6.157461791555
Ar	5.438755851167	9.958768325680	6.986224004821
Ar	23.941596900413	7.606634344164	19.202994613713
Ar	19.410366500295	15.436307730197	12.599078617055
Ar	25.187388732006	14.156048071511	21.893519777088
Ar	11.806688460612	6.936352545132	5.657769548949
Ar	2.942702499495	10.080296244287	13.651590611968
Ar	16.462064660489	18.132180253707	20.957598376275
Ar	24.001013295361	12.546211831419	8.326882676961
Ar	2.138609722201	10.957584181509	20.669994159863
Ar	13.798574338513	9.437838261023	28.097761921113
Ar	7.764926126026	19.821830827685	7.647501426832
Ar	7.669844302800	11.949773060443	24.981279711647

Ar	8.702179938073	26.966739636870	14.762338405099
Ar	9.197239026189	7.016044162811	12.294218020297
Ar	4.089137587393	16.453680263773	16.552335633099
Ar	10.963478717403	13.911043885615	4.980727374020
Ar	16.494456408126	20.824149906732	15.029951754152
Ar	12.884923826611	16.524493852928	27.010202956266
Ar	3.453592305373	22.369320586145	12.621013891846
Ar	22.117354113105	19.828928978479	24.453155471860
Ar	12.369632862212	23.616235475182	19.850707529846
Ar	2.198845136341	15.945441882353	9.686742689771
Ar	29.035215307327	18.252352572469	17.505829586919
Ar	3.393483702004	17.389139225675	23.587770944735
Ar	13.931884632963	20.490226235188	3.760958678186
Ar	15.803289808619	27.693360861033	15.161531130312
Ar	25.244406219369	18.876666102554	11.499449607963
Ar	19.357270696711	21.218862838884	8.653139127525
Ar	18.107311102935	14.862057974895	5.528564717236
Ar	12.979448800070	24.338431748269	9.804405688832
Ar	8.642299614729	22.005096983475	25.688110060040
Ar	19.155546808856	24.378939879635	20.234127897212
Ar	15.743839569314	22.754220026473	26.037212936467
Ar	22.174067607979	24.549382640792	14.058748685700
Ar	25.989851721374	23.879341682541	20.044387222430
Ar	5.376738548766	22.788480460794	19.436222402692
Li	17.871924448265	16.755520678715	16.764919163414

Energy= -0.20564748026800000 Symmetry: C1

Ar	16.286696330080	21.230435263191	17.745910425307
Ar	18.529099951631	16.752788267108	7.924262818085
Ar	7.088928199607	18.864959124423	10.794642670836
Ar	9.232720527350	25.170311993734	12.475907462178
Ar	9.856766953683	19.975857702476	16.950502051670
Ar	11.676717616555	26.393065732494	18.829455072269
Ar	8.045950652291	20.564750894263	28.277978473327
Ar	15.088373543815	21.910829372470	29.129639202978
Ar	3.480918976586	22.245815771068	15.652812065726
Ar	11.312926377261	14.440876838037	13.864720545850
Ar	1.023174142548	18.502853048181	21.232044926792
Ar	13.739045510335	15.549379654960	19.863093072039
Ar	12.265562973134	21.174486078193	23.000354042395
Ar	4.822247926946	15.284129923432	16.163091979540
Ar	10.818397577581	27.021738580759	26.042145947238
Ar	5.994225495127	23.439086398336	21.996932628392
Ar	11.766745185919	15.441987247076	7.094268329717
Ar	12.895811695637	15.561326739123	26.663854226819
Ar	8.678170306909	14.559743614852	31.982854641979
Ar	9.015149270843	10.713636851418	19.151553251864
Ar	21.512068357127	19.075191293797	29.842679317456
Ar	15.993902016646	26.464563833670	13.352615815189
Ar	2.527761876945	11.590534985469	21.720886618866
Ar	16.996770225258	30.886392690953	18.757448371455
Ar	3.107994171501	15.561191825406	27.578495332852
Ar	6.121212548839	12.058914000635	9.976902460436
Ar	18.411322837288	18.600539033211	23.726819780730

Ar	19.921846114752	12.795363340778	20.496874594784
Ar	15.817155016016	15.930863099927	32.859839987476
Ar	21.601479849631	25.651662522488	17.864509278660
Ar	13.857967060856	20.069196034927	11.812452611611
Ar	14.414385167420	9.723363752563	23.409718179894
Ar	15.204412077534	9.914663614998	16.722146441378
Ar	13.572346821776	9.643259289796	30.383130658120
Ar	3.695685895235	8.290164175828	15.546455863676
Ar	17.335737706481	25.583976290377	23.344821793072
Ar	17.733693270751	15.675900373046	14.657775965905
Ar	20.629304725719	21.464649129121	12.463379822521
Ar	7.999362936721	10.582666247175	26.092803088537
Ar	10.589323986534	22.386430529981	6.062113412789
Ar	10.209779127120	7.362386147693	12.995130528755
Ar	5.777347661238	5.288730828908	21.862205244345
Ar	15.874301848773	10.708606218500	10.083485424949
Ar	24.846917489783	15.862725284164	24.466805192987
Ar	17.291395858051	23.707382812542	6.912384126626
Ar	18.490028579869	5.648848233885	27.135487874215
Ar	23.794376695633	22.862131145214	24.046571501690
Ar	22.725907121564	18.704728996743	18.368528250267
Ar	19.257075461431	12.737074944149	27.478399337366
Ar	12.255901535065	4.337630393049	19.231817507189
Ar	7.500949961887	16.514139283771	22.386997751184
Ar	26.443590428545	12.648055976940	18.344308115696
Ar	24.182880795686	8.810390380511	24.129660831069
Ar	24.183054883387	15.525372895645	12.195007831234

Ar	11.352921511021	4.282294616326	26.257835708449
Ar	21.509352148242	9.528305580265	14.386799994064
Ar	16.702752535169	4.220060987718	13.417605069006
Ar	19.303367977327	5.684930217201	20.099587032519
Li	13.799905523521	17.801755058925	15.869238353212
	60		
	Energy= -0.2082262659599999	Symmetry: Cs	
Ar	8.482706689978	7.761109101511	19.313905397837
Ar	3.302310714670	11.219157505242	22.154407223581
Ar	14.152275058463	5.533916870391	16.222899605596
Ar	14.252670847261	11.391138581352	19.932343107262
Ar	11.157018940361	11.453841165001	14.208575919249
Ar	7.933375058906	5.519674081142	12.785192998502
Ar	9.782863290834	11.195329064868	25.137482779788
Ar	13.624722575884	5.403705687895	23.307846769238
Ar	4.352392465719	11.305773740697	15.098006868052
Ar	8.682696201591	14.693356789857	19.281614499346
Ar	16.806619183786	14.735580406775	14.888185687930
Ar	19.994470629304	9.099788851423	16.975854638957
Ar	16.753165398595	9.165474371454	10.982616304371
Ar	14.272812995237	17.969866925983	20.010072736090
Ar	3.314391922965	18.094881764260	22.221327645972
Ar	11.163278036056	18.032776584346	14.260592359076
Ar	19.542311458462	3.004671101831	20.108831751146
Ar	15.766149964298	14.628196751530	25.962814752913
Ar	9.825498722423	18.142165124896	25.223152002360
Ar	6.968830570134	14.805702601879	9.696808590199

Ar	4.368225605829	18.253196148801	15.131486362472
Ar	19.585958156527	8.845347043109	24.074494905619
Ar	10.587190908635	9.027576157788	7.435363344216
Ar	19.955698753213	14.666412726848	20.707147413244
Ar	13.660490460922	14.793878751110	9.067491306194
Ar	8.514234668978	21.542418088395	19.447612132616
Ar	20.011581812588	3.274840167014	13.029276741922
Ar	15.566802561338	30.531605892067	15.731554424036
Ar	20.099527165014	20.269078409368	17.055503238628
Ar	16.846334559046	20.334961719376	11.040416688379
Ar	14.286485907627	23.723693424269	16.349573818326
Ar	20.402748631531	14.734283102586	9.045189859795
Ar	23.664712208534	14.668141807134	15.076414155058
Ar	23.766636082488	8.930639375274	11.060372296742
Ar	19.543938513296	20.501387627190	24.095013698194
Ar	10.653313143098	20.681250768571	7.657322118393
Ar	25.667838297735	5.223894540108	16.848790655905
Ar	13.605500301703	24.066315063820	23.318460961271
Ar	25.680566457413	11.022129764772	20.882270788682
Ar	8.085542343420	24.178432153618	13.111767917820
Ar	16.614609384882	11.206030889717	4.119116033262
Ar	23.036185521945	14.660304838013	26.704242544446
Ar	10.328386071934	14.917843781088	3.207927834089
Ar	19.929584642163	5.340219917422	6.238894821641
Ar	25.714369052765	18.246647733893	20.948338812645
Ar	16.643653695821	18.430765643774	4.177487980908
Ar	9.719162600477	28.311398527767	18.869908859234

Ar	23.865918034544	20.455240046764	11.132959640572
Ar	19.531175466960	26.420800417951	20.155869017482
Ar	13.997336670860	26.532825523056	9.923376478439
Ar	13.827900898859	3.120446273033	9.543387885586
Ar	29.446907118225	10.981441162789	14.876573535110
Ar	23.701580414265	11.097783930848	4.253606559480
Ar	27.432414665264	14.686743354921	9.140730175141
Ar	20.247324934837	26.085583261191	13.151714282878
Ar	29.483399148316	18.297541768599	14.946660940531
Ar	23.729672073433	18.414243306623	4.308604645831
Ar	25.792092182914	24.099829800818	17.017420003584
Ar	20.029576494003	24.216724532387	6.362672256059
Li	12.771847903323	14.723507006170	17.0703772709373
	61		
	Energy= -0.2109086236449999	Symmetry: Cs	
Ar	10.804032970610	4.675162666295	13.630809569347
Ar	12.129172236609	9.914251136723	18.349560351662
Ar	14.269735964944	10.268066736900	12.015454170356
Ar	17.530624513790	5.928271025720	15.995150994191
Ar	16.462733727409	4.692949066826	8.927760984534
Ar	8.503496209690	4.420834078424	20.304987480253
Ar	10.142936067839	7.923498308848	7.178339042011
Ar	7.682740088930	11.093938723075	13.134779113877
Ar	15.307703421507	5.641132312697	22.684043302987
Ar	3.908083784126	5.655388916774	14.930806916192
Ar	17.321628959536	15.980140051647	10.865769965002
Ar	20.947835812808	10.025969524700	11.180230185823

Ar	23.333732728374	27.664568267166	8.639713235737
Ar	12.259947807222	15.828248500434	15.016073683454
Ar	5.301601143431	10.769024258686	19.714813465211
Ar	16.482011331497	11.206396258773	5.691685331455
Ar	21.449866567168	8.853386461745	20.907545280017
Ar	11.029903265102	14.890366003573	8.390219082612
Ar	9.871432471893	9.575264552872	24.993161759644
Ar	3.231333392928	8.921328533665	8.396620350548
Ar	15.997073040937	12.687157824011	23.341558912529
Ar	17.981665114607	13.099359833545	16.727496438098
Ar	10.057197051139	15.630017825825	21.435908912411
Ar	0.833786338772	12.051328502336	14.340558526306
Ar	5.598458802415	16.844074225906	16.239595460639
Ar	24.829780207311	12.987896944228	16.094626721769
Ar	6.692240640404	12.848525219200	3.477889494263
Ar	4.180536413110	15.917217830743	9.427469976042
Ar	16.005497995975	18.550913368559	19.671257235592
Ar	21.931404885097	15.730135232103	21.689894402138
Ar	21.013572595833	18.721055507661	15.535039537884
Ar	24.164416430299	16.069038709371	9.900370504417
Ar	8.956417531211	20.610600932811	11.478961356142
Ar	13.091321918742	16.093345240302	1.926159480147
Ar	4.840283274456	14.526954894393	25.761714090679
Ar	15.322527404870	21.495246527935	13.843826817217
Ar	10.240376130651	21.384298959506	18.017832995810
Ar	19.703598536180	17.296956857673	4.408330678136
Ar	11.664374284289	15.692520465572	28.111532022290

Ar	14.165618786359	20.833823963799	7.025484657714
Ar	0.243940479571	15.763527766748	20.388708304116
Ar	7.650832230101	19.775441027939	4.611694204123
Ar	17.819923794282	18.866976445595	26.315049650463
Ar	20.351782681922	21.681958224726	9.607600067715
Ar	5.009445230564	20.660883323303	22.262201011855
Ar	-0.441281453238	19.053174485502	13.867130481125
Ar	11.783056347437	21.785143791176	24.557325418588
Ar	27.119852217008	19.228049368152	18.696756967102
Ar	21.357584165260	22.565320759596	21.266958176489
Ar	4.350471266720	23.903813592570	15.806836954761
Ar	3.028144624359	22.956599724149	8.935671411289
Ar	15.331958131273	25.518653884418	19.545746848196
Ar	26.423027465868	22.317582715659	12.504977738713
Ar	10.782327455858	26.93035556373	14.182111229090
Ar	20.681808694841	25.677842103077	15.089600836886
Ar	9.471851249983	26.078724326481	7.317903475488
Ar	25.564145699656	21.510282557396	5.315626617289
Ar	16.159050496147	27.075852697369	9.689239495626
Ar	19.128812907435	24.505917510498	3.558284486707
Ar	8.338328733588	27.105638710748	21.030059277491
Li	16.609855407075	17.279024838066	15.249354976515

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Energy= -0.21359625026800000 Symmetry: Cs

Ar	19.870365924164	10.875325136459	8.109454642058
Ar	15.686533227246	16.535741135011	9.184436614749
Ar	21.459631014437	15.737194481539	12.482484426854

Ar	22.026850278420	17.438052214744	5.949637712138
Ar	22.827686865873	9.460734562865	14.506265388016
Ar	26.729063887524	12.914234687855	9.377627678099
Ar	13.744866653506	11.707698432633	4.706373864707
Ar	19.933886886318	24.017333160250	4.344302148612
Ar	14.489078234737	6.914485087921	9.964032880811
Ar	16.301271997144	18.400674309485	15.689240103871
Ar	16.283179120535	11.986161270627	14.272753631262
Ar	15.895092274595	18.356096335311	2.565925801812
Ar	19.606174483541	22.013657685325	10.893215823291
Ar	24.477511936861	26.629757584915	9.485082079390
Ar	13.584004412960	23.004136875456	7.457211215061
Ar	26.507597159017	20.022398200867	11.026880422083
Ar	22.618392336004	20.585986977074	16.965406601255
Ar	26.982477210636	15.057407124889	16.348794795438
Ar	15.282276262100	10.613894043637	20.548276646905
Ar	10.294996292701	12.569532836983	10.863283851043
Ar	10.989202515642	7.915120959432	15.871666112737
Ar	17.424636602422	5.543735971592	16.382421508803
Ar	20.377555884278	14.341956302633	18.813571507409
Ar	21.549195322036	19.160276801957	23.527117995424
Ar	11.223074785052	14.604148467514	17.407018257744
Ar	21.740272695859	8.020501816335	21.238887118952
Ar	17.294155635854	23.340481245078	20.263267117758
Ar	10.382523893470	19.279898716978	12.469731009963
Ar	14.269533953081	24.774645651300	14.198874766397
Ar	23.656413982377	16.029775945673	29.543084086303

Ar	11.137466889057	21.077493980855	18.8760708885636
Ar	17.607472917757	28.556527902081	9.315399715658
Ar	20.736419509175	27.174174261653	15.521483636575
Ar	15.241209083946	16.999322579781	21.995085775305
Ar	9.6195723666710	17.390624006960	5.745883751438
Ar	28.082752696023	20.114431300742	21.198169059033
Ar	27.612380132936	25.125695482767	15.785733084752
Ar	4.407739899549	16.538457037680	10.489699812390
Ar	19.398966574629	13.013653629552	25.189792466288
Ar	25.878596284682	13.611233940226	23.110925771270
Ar	12.661410437501	4.326259171724	21.568452745014
Ar	16.968539397972	6.841039799274	26.422300549700
Ar	5.191537459133	11.725170762664	15.723225802032
Ar	23.773124287487	25.655971532787	21.692050116252
Ar	6.51432024471	23.2098351549524	8.376696670329
Ar	8.527784667433	10.146445531180	21.893295709035
Ar	12.445558588816	22.577360911372	25.353070390972
Ar	15.076672866313	31.493042909378	15.308147761431
Ar	7.183047381313	25.118460034835	15.144237544998
Ar	23.782281430001	8.828461470470	28.160018271202
Ar	18.079334021094	11.778966896930	31.692417784813
Ar	11.665281151593	27.701304018510	20.221334383081
Ar	16.846280793195	18.284571238191	28.706186894697
Ar	18.199619739481	29.995764333468	21.616254832469
Ar	19.019702943026	24.803141641513	26.811282247326
Ar	10.543210522312	28.876166696334	10.161082833404
Ar	5.926875961900	23.676842793169	22.262427200531

Ar	8.433461366139	16.907272639554	23.421315419951
Ar	25.853226663944	22.526091729679	27.665837712150
Ar	5.145711252734	18.493820809983	17.229475374212
Ar	12.811825451901	12.640173377234	26.769274180072
Li	15.808751269539	14.537111783647	18.121213575183
	63		

Energy= -0.21607467270899999 Symmetry: Cs

Ar	20.174842453977	17.188094894371	9.862984998260
Ar	15.423003375155	31.310948913565	16.244729598011
Ar	21.192053205129	8.740226919320	20.001802667251
Ar	25.280011845674	24.552888797537	23.137627790326
Ar	12.187115200132	21.944734697359	22.341554763566
Ar	11.370347374435	8.179880107452	13.928722967555
Ar	15.333808357951	24.603565569935	17.007741771467
Ar	14.831512582639	5.171814366770	8.584140625234
Ar	24.106405877385	22.897604586501	9.572503602366
Ar	24.275119291729	10.642032744235	3.834335765719
Ar	10.982496462277	11.044244202037	7.630077607899
Ar	26.316168169308	16.863285275571	6.522796523166
Ar	8.9349911251539	19.060089754383	27.866907486857
Ar	3.633865164493	12.152237618687	19.113201445129
Ar	26.749859520690	11.944090204453	17.379623106144
Ar	9.582190398677	8.774939980996	20.891507372095
Ar	19.722452114413	25.063214303180	27.835367184537
Ar	18.610527941441	26.678652937246	11.518244171769
Ar	26.787935693887	23.828152368668	16.183008817723
Ar	9.569356070639	14.520001148972	16.603103443969

Ar	15.800517183556	28.095408204566	22.811695543274
Ar	25.220331192208	12.597050933684	24.315233744409
Ar	18.897639209335	1.674549253486	13.360406644081
Ar	5.416521834018	11.466744831446	12.069913308038
Ar	20.553820030298	14.552043402059	15.814943613108
Ar	6.301202872997	12.789435039480	25.733989913511
Ar	21.931707037134	5.419682594294	8.107248775185
Ar	12.149531570666	15.130080793664	23.031212707660
Ar	14.911682194600	14.230051815678	12.326188530893
Ar	15.402177309076	4.725061402250	18.731429908577
Ar	9.658908130585	27.745036580940	19.013628124149
Ar	9.611894074093	21.296660434803	15.918000558835
Ar	5.456848087879	23.422088478575	10.879663077634
Ar	20.569720397681	21.008609424955	15.129872088749
Ar	18.220189029357	22.562386561497	5.933584779111
Ar	18.497846669770	8.535269038968	13.373578541465
Ar	23.071455584263	18.891863624978	26.814103984261
Ar	14.984226972464	20.689857695770	11.676135570884
Ar	21.287171496470	27.537076259314	18.141218591036
Ar	15.721078367851	9.125221837328	24.687545073257
Ar	18.114988392523	11.243687044167	7.064622093286
Ar	14.369702920597	16.872161223632	6.035546403147
Ar	15.252604312395	11.467447491496	18.351196965961
Ar	24.675514819402	5.733665552795	14.670529380811
Ar	24.678542500347	18.214074579335	19.982639067044
Ar	12.523380350426	13.144448374162	29.581348588348
Ar	3.685812809959	24.148033805493	17.918682883094

Ar	11.441546794127	26.975138091763	12.052233261760
Ar	16.017822500338	18.987389683332	27.413880148107
Ar	26.191087779742	17.546695158428	13.345161212228
Ar	12.570949460986	25.160146734386	28.391521239551
Ar	3.620824667229	17.781946615579	14.786427991117
Ar	9.061196439448	17.322787931237	10.325685890441
Ar	6.204903476748	18.427394573341	21.345993569780
Ar	11.054434461907	22.930063565141	6.4544424436784
Ar	24.075402096234	11.583721198908	10.749974635920
Ar	15.303248060913	18.025468738283	17.664110269895
Ar	20.459701867980	16.530183647443	2.901653099356
Ar	19.667806858312	13.067003281550	29.027737138435
Ar	6.352047034665	24.805270318523	24.545744244947
Ar	19.081236799294	15.062821439479	22.484833963313
Ar	19.115675659822	21.838981729361	21.794935461154
Li	17.724475976613	17.599120478394	13.787868184371
	64		
	Energy= -0.2186035576700000	Symmetry: C1	
Ar	7.350047081441	11.275193319736	12.723105047051
Ar	14.183688753967	17.292148189277	19.924788768432
Ar	5.240166995521	17.443386605503	9.734979356454
Ar	11.893401650209	15.111217414612	8.811375738481
Ar	16.311311097695	15.138640125548	14.181932713264
Ar	10.716013239628	22.068486319086	9.923816892727
Ar	9.616013880194	5.231115035674	15.770262886443
Ar	3.327194230451	21.070065932047	21.442078987377
Ar	5.403718642405	9.729844248472	19.452108424331

Ar	17.410605457233	19.634386360869	9.142294965669
Ar	14.150776550070	9.023522554124	11.863927342167
Ar	20.351031102302	18.561322556170	18.323336737180
Ar	18.430386948033	12.369977370410	19.906786154240
Ar	16.572860364258	23.172342749614	21.906996094508
Ar	12.083559381841	19.478039740744	25.842910561224
Ar	13.307293262844	12.671329818600	24.618454886966
Ar	18.401386280728	12.932275011170	8.137014152689
Ar	16.301885295553	26.526815860900	10.235408548073
Ar	18.632870263024	17.176100139144	24.832881439711
Ar	21.666206179686	23.201482850694	13.511391871756
Ar	22.474451771986	16.372455688134	12.601359330363
Ar	20.603824044611	10.293742384845	14.166084102360
Ar	5.509979039831	27.688075968935	19.693877177660
Ar	12.273699157089	28.590349069075	21.848613469928
Ar	16.377710535575	6.163169073751	17.850012603391
Ar	5.545205789383	18.072686760926	27.632750524208
Ar	7.634643785775	24.783753979008	25.895418948033
Ar	6.817105327297	11.057769192754	26.386806059402
Ar	10.859767946283	27.216468737859	14.914653001478
Ar	23.092378591365	24.635184802362	20.302904907025
Ar	7.888916020254	15.858229508111	21.504342452319
Ar	14.479650551050	25.598542245466	28.040749837540
Ar	17.734594757228	7.417188257043	24.721832939598
Ar	11.114288307065	14.771025622027	30.837324115928
Ar	22.037637584782	24.194689977045	6.617398636071
Ar	23.152001967871	17.247821019879	5.695407136274

Ar	19.760429945166	6.218305410972	8.530408597786
Ar	26.844170848342	19.915585967957	16.776087540409
Ar	24.543327526805	13.632255827790	18.179137296927
Ar	16.619644764387	19.414106098641	31.074676103390
Ar	23.139050765913	12.048311981160	24.919758521604
Ar	21.213772027838	23.202539345186	27.046446690276
Ar	22.909411030273	7.250659980974	20.031587059264
Ar	12.415111213064	7.855694939950	29.489340650734
Ar	17.873054566209	12.440332710810	29.817764355219
Ar	9.903297931393	21.741940227321	31.979655662666
Ar	24.937865037672	11.103027987467	8.811711450130
Ar	17.673979372615	28.002519817009	17.066926701119
Ar	21.887945622759	3.386185825580	14.430855044873
Ar	27.268854549862	20.766732363047	9.959038656341
Ar	29.114207296176	14.632779694214	13.024534195209
Ar	27.123822214611	8.187941386616	14.685185978717
Ar	23.283333466226	17.055768610935	29.972205754908
Ar	19.072998314379	29.276637769560	23.958493310766
Ar	1.360059457427	14.374849660961	23.145018093025
Ar	9.790990645610	17.371708719166	14.935790840936
Ar	3.196173636676	15.899989332322	16.404700280385
Ar	11.947023824095	11.390878493647	17.887975865282
Ar	5.291117115563	22.614320427044	14.664314819613
Ar	25.145997775740	18.499395399982	23.263075177168
Ar	9.925174131397	22.397753206355	19.811943926404
Ar	15.188919642559	21.826270636065	15.196749323844
Ar	10.970775004616	6.464038002944	22.637091224398

Li	20.355384870888	14.440305046855	16.264675813398
	65		
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Ar	19.199724629255	5.698314535613	17.541847259302
Ar	13.329027622554	9.365852450744	17.774323609286
Ar	21.997344903302	10.730428403062	13.184430698089
Ar	12.897651805505	2.717612628870	15.938109206446
Ar	14.253913362376	4.601381406801	22.702127189200
Ar	15.748387603133	7.607544460709	11.600906508352
Ar	20.568875974078	7.693495181682	24.308281939951
Ar	25.395908246638	8.827912121382	19.128209694587
Ar	19.452211341859	12.374808747861	19.319759605418
Ar	7.745020045739	5.824343074296	19.802523369302
Ar	14.669883904124	11.315363691783	24.371010954947
Ar	8.733498215911	7.665181016375	12.879494644580
Ar	16.083038782806	14.239160254701	13.647275791659
Ar	15.613609958174	6.703595983886	29.407264093042
Ar	18.467293630487	12.514159208174	7.565935834509
Ar	13.755192495232	15.763639272526	19.516993760082
Ar	24.272105771915	13.846744191814	24.053384497393
Ar	25.046950616091	15.629300868485	17.099987216736
Ar	9.109751660911	7.845108808412	26.605641060028
Ar	11.674761753890	12.670450588512	8.586641963080
Ar	8.327002400758	12.507107251786	21.545621100591
Ar	9.326622262676	14.277718408577	14.809603390749
Ar	21.273894614502	17.473189991073	11.520849321208
Ar	19.358222415518	12.801033228354	29.254591984286

Ar	25.250553369525	13.376774387311	7.432426349683
Ar	19.011752712563	18.943661392658	17.407072324679
Ar	18.279129294053	17.317681231446	24.128999154200
Ar	17.624173335848	24.323204134860	5.794038635129
Ar	3.605097235492	10.881175440760	16.751896421915
Ar	15.379597486000	18.581266148358	8.895548087550
Ar	12.048916573390	24.599376460786	9.790378485687
Ar	12.271618296591	12.924567971170	30.664641300458
Ar	11.407937236588	17.456695157495	25.500983890758
Ar	2.699486414161	9.129900059110	23.654676535645
Ar	4.692732275441	12.718877181924	9.906451979654
Ar	28.254282851212	18.200431926861	11.289400066610
Ar	23.884906811641	20.678324552164	22.046562326502
Ar	8.088363597708	19.232515790885	19.590022207864
Ar	20.835040610259	18.276164269875	4.680602235792
Ar	14.244920860276	22.178942246342	21.1240111613501
Ar	8.446147451200	18.749529113864	9.705600203417
Ar	5.762230715017	14.147410473645	27.765236561710
Ar	24.530429061888	22.253051199610	15.349620470464
Ar	22.999346806999	18.945902511983	28.906661465877
Ar	18.242887891610	23.180470525807	12.571384224024
Ar	16.010790414978	19.103512746710	30.414209294405
Ar	3.363279117686	17.775779873422	14.740090757554
Ar	2.341110993674	15.998326354061	21.674735267476
Ar	23.869250070621	23.148552828175	8.575447138990
Ar	19.738481717412	25.62404467054	18.939094133451
Ar	18.889489376631	23.980904858634	25.918205362073

Ar	14.612630087892	15.376071925727	2.694747321468
Ar	11.433259014607	21.362918594278	3.796928445862
Ar	7.134034500661	23.826040373747	14.585554680738
Ar	5.502576808737	21.077417123431	25.733923320470
Ar	8.972325793606	19.207556950327	31.707816120863
Ar	12.982588540914	20.076830626966	14.721674934967
Ar	13.459870136709	26.803988108751	16.142877534516
Ar	11.844666231063	24.118693674695	27.330576479479
Ar	8.446931790238	25.942783606353	21.267125560665
Ar	2.202394220202	22.853361616890	19.643605918888
Ar	22.784307219350	28.501177173329	13.185030160406
Ar	14.748828857928	28.874074128174	22.817176561025
Ar	16.600936011385	29.663639918901	10.431863506972
Li	17.117085554046	18.709457322263	13.212117301378
	66		
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Ar	25.845879920850	24.953089187787	21.486859665580
Ar	8.528545728573	20.219446533956	8.868002830848
Ar	5.050265862802	19.356318898348	19.354092737954
Ar	15.714203687703	17.033013481992	17.259174643879
Ar	10.558443433560	16.478595649441	21.175851414256
Ar	14.887491961210	11.221153553582	20.347538167585
Ar	10.207758453009	19.990661188672	15.497324131910
Ar	5.263893977601	16.267793195567	13.578398682132
Ar	17.335447261838	11.592084428904	13.802065492846
Ar	9.117899364468	13.212086447635	8.651997108879

Ar	5.716065923068	9.350681812235	13.166244795080
Ar	5.598319017801	12.839211028850	19.153061818511
Ar	9.690860079847	7.233238249913	18.354009774511
Ar	13.945521752054	22.425197670078	20.693551669579
Ar	14.286791996839	17.112830370598	10.786741544526
Ar	5.293659330075	15.906618283927	25.367823266678
Ar	2.605163875078	6.515393486711	18.551444772404
Ar	12.220412550486	7.551301533503	11.666864937463
Ar	16.999568458437	16.939827246106	23.774612639187
Ar	4.553715152305	23.175400689128	13.592576101805
Ar	21.274669098481	13.906262136085	19.117470699134
Ar	1.041464673063	25.117867599468	19.125075109392
Ar	5.548440379918	16.595659345755	3.719433498025
Ar	-0.683455931671	19.186730659259	15.520290594274
Ar	14.602494386211	28.588556415644	17.630353083725
Ar	16.195140850353	10.933447299980	27.128793679661
Ar	16.547624804848	5.453251501139	16.916083019355
Ar	14.040625021458	5.154450212211	23.573941139077
Ar	8.522063372755	21.947577002598	24.839598448759
Ar	15.903262697808	11.541529032558	7.021353636663
Ar	2.406152465643	9.758072641023	24.599509385431
Ar	20.684634330174	20.923735943108	19.334323198584
Ar	15.221770894939	22.510826539930	27.486363938891
Ar	20.889412284180	17.595884642550	13.124047548116
Ar	8.146326744779	25.604641785175	18.920817321510
Ar	1.416273678087	21.522214719590	24.961572839615
Ar	10.658956469132	26.123254121594	12.239945098331

Ar	11.656180323645	16.359076827792	28.036365323014
Ar	-0.321057789389	15.555650244456	21.424706297443
Ar	22.696118155887	12.004233675717	9.452463631266
Ar	14.931992644448	23.095624807727	7.378106019925
Ar	-0.103144523122	12.284707486818	15.306744715646
Ar	12.715209285928	17.188974387794	4.033954336710
Ar	19.002752399369	5.930275904644	10.208087326893
Ar	20.586282403387	7.827649776807	22.358941638697
Ar	26.554373816449	17.819679942217	21.297267851925
Ar	2.012444673614	12.700306007008	8.491102963977
Ar	1.436462221557	19.546608151853	8.702549644262
Ar	19.539263313702	17.692272780319	6.322038995906
Ar	23.097500304731	8.217795698770	15.604287955767
Ar	9.482038290960	10.532542660865	24.48730575474
Ar	21.514935924582	27.041036946951	16.185571070272
Ar	22.750467617726	13.730138672275	25.886981377486
Ar	16.387312937615	22.869648681926	14.150368428651
Ar	21.719169297260	23.624807131628	9.8111352559215
Ar	18.314264853788	16.840863267337	30.556996466681
Ar	19.008666724913	26.592137964526	22.938632460945
Ar	26.764180706293	14.405570270919	14.924921227772
Ar	22.145305181082	20.928305767728	26.109377644193
Ar	17.068169582420	28.939689481471	10.918492332394
Ar	12.115100981023	28.056237519826	24.281062879690
Ar	26.158740899291	21.605050334852	15.147265560466
Ar	27.046811676459	10.670048527409	21.045642110866
Ar	26.255009873206	18.179113493386	8.840304535885

Li 8.008413881253 16.382691727227 17.334591935839

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Energy= -0.22686085551400001 Symmetry: Cs			
Ar 9.570548870345	25.899327457990	13.651932060979	
Ar 9.418888482061	19.244841413406	12.058465463318	
Ar 6.908204533706	27.222517674087	19.826644344862	
Ar 3.760866829388	15.512503096633	13.652980295240	
Ar 13.266669226199	23.814311079693	8.189853572630	
Ar 15.059136602486	22.074950587175	14.697165788100	
Ar 10.061555299055	21.183857407131	18.717571829561	
Ar 3.982354408188	22.387342117875	15.436017507311	
Ar 13.747925524933	26.592015660507	19.147976892388	
Ar 10.635751055750	32.148420453710	16.213160755475	
Ar 31.321379847538	10.758716467309	17.605172966032	
Ar 4.239831462557	17.652610574139	20.408618135743	
Ar 15.799288680155	28.605802774541	12.803108536594	
Ar 9.683187355464	14.405599649802	17.149666564740	
Ar 13.262634263270	16.891504984385	6.4666714535611	
Ar 14.996693979467	15.432335080547	13.000466230488	
Ar 7.152626733041	22.444847472769	24.846617708257	
Ar 9.354529391341	12.372515139984	10.3777808331893	
Ar 15.307268679108	17.471338204736	19.551785753114	
Ar 18.823388492120	19.940738212960	9.267637182629	
Ar 13.973518511536	22.083052888717	23.892707666607	
Ar 10.088542023788	16.346734604959	23.700772060911	
Ar 11.055889100951	28.170777853337	25.302488356275	
Ar 19.059012440058	22.975272091527	19.989748096985	

Ar	21.3173233364308	24.705193044135	13.737847645060
Ar	19.808025736536	26.494090420963	7.230331098920
Ar	20.344292827523	18.403900814292	15.555929889939
Ar	17.234978131057	21.542704614001	2.736109624518
Ar	14.751893034480	33.074282238539	21.636312544039
Ar	20.006205426562	29.549851545647	18.354641165708
Ar	17.057707880226	35.0191666312897	15.206204179943
Ar	13.691555672840	8.903521937306	14.863309706703
Ar	17.873322876988	27.767409928784	24.609736302836
Ar	15.996503322487	10.503139524794	8.252227736206
Ar	13.972524855636	10.986063710653	21.693821592742
Ar	22.268616866539	31.318398348732	11.884920131048
Ar	19.246424110198	12.134233641106	17.461182667777
Ar	21.502101703694	13.699602286250	11.007184100777
Ar	19.969839727244	15.154704621589	4.409285015167
Ar	11.292916629211	19.281817559900	29.750981982449
Ar	16.487257897422	15.967275488547	26.170665887699
Ar	21.731993924682	16.955144601081	21.879978808804
Ar	25.465609104471	19.514546857938	11.469185802934
Ar	15.150479729147	24.940323407462	30.201500245448
Ar	24.039002688342	21.124633459817	4.883547833526
Ar	20.399880448985	21.707019979470	26.627492364778
Ar	25.6103611170619	21.470437602825	18.203141429206
Ar	26.603763797247	26.064620330492	9.489418914557
Ar	24.420204454644	26.313248315944	22.912688723216
Ar	26.750160606901	28.061561696355	16.386622733108
Ar	25.730769086191	14.652093080080	16.566061203034

Ar	20.403816422875	7.111421977870	12.850690664127
Ar	20.677970261185	10.472271680193	24.033149357586
Ar	18.094172355506	5.619165840911	19.451470299312
Ar	26.815417689494	14.698190784961	6.681226049865
Ar	22.706844219349	8.820618004303	6.294764745078
Ar	27.193886022482	20.030913683893	24.792846006041
Ar	23.191972839569	15.435822869972	28.473402315661
Ar	31.031301967530	22.702513108442	14.089683944727
Ar	24.746869140627	8.085797377034	18.551094705550
Ar	27.087161237575	9.709847526536	11.909126029687
Ar	30.778132855398	20.661934006722	7.235447208021
Ar	27.321645431550	13.047452710597	23.11080809588
Ar	31.077396334717	24.666624186975	20.965190986287
Ar	31.153377006382	15.675511482023	12.382823586107
Ar	31.308164176095	17.711073825821	19.315591841271
Li	14.605028923933	22.019628263246	19.280544482725
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	Energy= -0.22919643474300000	Symmetry: C1	
Ar	20.785706373547	10.239573000887	11.472292082266
Ar	15.785757411899	14.704072050390	12.118067271222
Ar	25.293482373309	10.071669985557	16.739393869470
Ar	27.203716989048	12.996864087115	10.508563035035
Ar	20.549182876044	4.830454688147	15.995445100288
Ar	21.876531413652	17.272718018910	11.152340628083
Ar	15.558274997595	9.553495482423	16.299324886811
Ar	20.099640007051	14.574006294173	17.191318592153
Ar	18.244755037469	14.018185635550	5.862074079358

Ar	14.085181956873	8.831085390000	9.268570729754
Ar	26.476569922800	17.065403302568	16.294265691025
Ar	24.629997503560	16.890781054092	4.880044890139
Ar	20.058047272710	9.231902169045	21.533833505557
Ar	17.415221577669	20.267549939511	15.314304133275
Ar	13.711843403137	15.793361619719	18.272304707877
Ar	9.534946133953	18.092242278697	30.714227441169
Ar	16.209786062617	20.363928217146	8.555855115489
Ar	9.580615257507	12.412461858947	13.622225977136
Ar	11.234014983639	15.317554092737	7.156488724901
Ar	24.695891201827	14.210788665263	22.285029023760
Ar	28.252020190730	20.020776813375	10.131236325555
Ar	15.298665080293	4.124753285828	20.752418873536
Ar	13.777132581615	3.402971934804	13.855048393835
Ar	23.547816083597	23.026638903799	14.403073697668
Ar	22.512071131849	23.202512060310	7.460340489917
Ar	21.683645598146	20.055348377524	20.291664643152
Ar	18.785054200415	20.084880642472	2.215507907142
Ar	11.040760299119	19.329767277066	13.053875184134
Ar	18.008548662991	15.601421175500	23.261710490640
Ar	13.366507107978	10.642773552378	22.656669896253
Ar	9.353280287896	7.053110233276	18.228753916698
Ar	17.889046651057	26.145790501363	11.830781630454
Ar	30.165626271063	23.143199370034	16.216987902667
Ar	28.233287379754	20.174264966399	22.432143417839
Ar	11.677382690136	21.396662785682	3.527220590414
Ar	15.363765825088	21.307379615549	21.444946676783

Ar	21.429919156963	11.927849142193	27.973403420512
Ar	7.345343993805	13.552684902528	20.149595496727
Ar	16.679744464183	6.693856740081	27.226199754376
Ar	19.037941337051	25.868301801047	18.464017057949
Ar	16.658970452296	26.334370954344	4.914909611179
Ar	27.594305655645	27.080610652370	10.620091134556
Ar	12.724849622519	25.090799373937	16.328817111808
Ar	11.557815684027	16.843663576775	24.417653464702
Ar	11.318609434852	25.321881368979	9.465442991300
Ar	8.864243719398	20.426844019333	19.421769653877
Ar	22.808913614922	18.871785414720	26.974869375299
Ar	6.320567650754	20.304024601072	8.199398236461
Ar	4.632016857053	17.355481465987	14.777257008323
Ar	25.448027890518	26.215296815328	20.477926756201
Ar	9.885984211279	5.298953393395	25.191219297981
Ar	14.690721689700	13.188207015602	29.153693191538
Ar	21.745426399023	30.286311512639	7.960529615773
Ar	22.930201236673	30.155066284580	14.949708261087
Ar	20.053576203000	24.938483433178	25.061439258607
Ar	16.083383752627	20.142795687736	28.222488654939
Ar	6.111255260153	24.214404506004	14.087793391318
Ar	7.883939662620	11.845255254720	27.114000180897
Ar	14.643425420674	31.617257246021	9.2777370831938
Ar	15.912105291039	31.458169439988	16.245923903179
Ar	14.133418599462	28.190002708076	22.526491521186
Ar	10.141039587679	23.376852502493	25.697385975459
Ar	4.966931223260	18.323132903202	24.987873322333

Ar	9.289352544979	30.527289314288	13.965091259496
Ar	20.618457629392	31.479175811700	21.832525753999
Ar	7.464217180650	27.218267666393	20.310992625431
Ar	2.256391737550	22.190877711518	19.653215456042
Li	17.676195681626	17.935716942977	19.268193140573
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Energy= -0.23190769820900001

Symmetry: C1

Ar	6.359822574729	19.617066008375	17.016233596214
Ar	16.980029027005	14.989545298949	16.658229203656
Ar	3.731260915291	13.398750938296	19.183314180084
Ar	16.771864641585	30.676985902399	22.260014864603
Ar	8.773109282157	20.285936850391	10.312903788570
Ar	6.141001570431	14.042019400374	12.516883079134
Ar	4.415566362233	26.000258645017	19.465325295792
Ar	23.440207442884	15.944752444883	15.462506680092
Ar	7.883971356018	17.318926934164	23.405928563915
Ar	15.527397562200	26.002276183939	17.361393360443
Ar	11.841165662371	27.713732231874	26.110844608564
Ar	10.492638117798	14.221112689403	17.897802237272
Ar	14.3883866646209	19.033789581356	6.046989943759
Ar	8.718462917045	14.695675207201	5.886929553729
Ar	16.899163925201	23.863056211367	23.383077710582
Ar	12.921966094207	14.849917388899	11.365218958065
Ar	21.776270116993	27.819561634463	26.499037499163
Ar	19.393787601583	12.114191369786	11.183041497120
Ar	14.590607227506	17.993891106780	21.921457089919
Ar	18.488715808241	18.506040613172	27.561941276888

Ar	12.701285500497	4.867351532547	20.340525908448
Ar	10.162652003753	8.756459028016	9.622397461127
Ar	13.171984676870	20.119011077171	15.780427528485
Ar	18.280128529972	29.932809481585	8.745887711335
Ar	14.387648123090	9.083783571611	15.107238572629
Ar	15.296174782177	11.867571049543	5.598856413585
Ar	15.386167998617	11.077027422175	21.771002648197
Ar	26.126215363984	13.001736544969	9.813165509609
Ar	10.337922493300	30.009302825852	19.710068872680
Ar	9.359310305275	25.336895175087	14.914024423683
Ar	14.512958012324	24.454045713402	10.633739825204
Ar	5.563273439737	30.881235304898	14.234112064932
Ar	5.906344459942	23.714370089171	25.837873646723
Ar	12.689201106092	30.909796007145	13.011578554884
Ar	18.507580230467	19.047482072336	11.626977282655
Ar	20.919286015595	15.363952857927	21.973761660326
Ar	21.007315586071	25.216590128324	13.157496330626
Ar	12.044160811226	20.974054214396	27.453934721846
Ar	25.040032446601	15.721356583092	27.510929050108
Ar	20.055218032204	23.355575971855	6.403932456456
Ar	25.175607818371	20.153303235662	10.223417633084
Ar	10.846013950954	23.187498473126	21.037284424920
Ar	19.346709923697	20.855457471314	18.199193101312
Ar	21.025764942597	16.238317682548	5.842962498136
Ar	7.640078754751	8.112489507016	16.339591040392
Ar	19.086080787081	31.658617423563	15.573044853534
Ar	26.089545343562	22.074129082828	17.046377992603

Ar	19.435536501335	11.329052602784	27.381845478641
Ar	23.457268872646	21.499340212632	23.675700809091
Ar	8.661624413902	10.149544054526	23.168744734833
Ar	18.397254447542	3.527838163733	16.096835172368
Ar	11.725599806145	2.936357731948	13.508840343672
Ar	16.880507217611	24.874874884646	30.318954611005
Ar	12.858659471336	14.090264498980	27.395706713022
Ar	21.913491932804	9.115454337096	5.520749783753
Ar	30.159410798137	16.936639054825	14.229129128516
Ar	8.361260390579	27.269139084071	8.481267623476
Ar	13.740226031278	7.006981900171	27.098207866934
Ar	19.405429422418	5.580464947896	22.967336468697
Ar	23.535140369344	6.640225551626	12.069629224132
Ar	3.125446303332	24.172798429896	12.525730139623
Ar	16.822909117375	5.928769884395	9.446849787179
Ar	25.117101297138	9.985563781583	23.177793850028
Ar	27.705763572801	10.598713872780	16.462410502055
Ar	27.684265135903	16.308784251988	20.920793022854
Ar	25.035436555223	4.346118011367	18.712673835141
Ar	20.933512346168	9.773008435117	17.668498514893
Ar	21.943708451653	26.938036334814	19.716484383199
Li	15.070189665642	21.932080161165	19.556868358578

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Energy= -0.23470877620500000 Symmetry: Cs

Ar	20.752115694347	18.906031075694	15.820345771211
Ar	6.002872108727	23.122901625299	28.701039662982
Ar	20.310333117831	21.430021987037	9.876353191434

Ar	19.304285122845	15.047435366766	10.838991517950
Ar	16.047820882468	20.298411489961	20.105154981689
Ar	14.615167722981	16.407338047449	15.169852362080
Ar	15.672505730194	22.900462879381	14.145528997953
Ar	25.752941235272	17.409797249094	11.4862993877864
Ar	20.334304237569	25.134957650148	18.639042447246
Ar	23.503281890306	12.611544955153	15.818360582925
Ar	25.322567015526	23.760953972419	14.140020779962
Ar	18.559771632893	14.148941574962	20.272178797308
Ar	27.238062432645	18.195683797161	18.208667064355
Ar	22.164477098269	19.650784139704	22.594569385818
Ar	14.289549363296	18.990951450943	9.185479477465
Ar	17.043024835888	9.992774121122	15.102555861682
Ar	20.012636306140	27.936465690069	12.389437029046
Ar	26.739074436597	24.653610803341	21.186273079773
Ar	24.905677900935	13.278147975458	22.840233862698
Ar	22.861438399769	16.958942820363	5.267705952791
Ar	9.987181911742	20.890048903226	17.445811587215
Ar	26.682120946409	22.681429061788	7.229365561317
Ar	24.649756124072	11.094635342483	8.931151043003
Ar	13.540676403918	26.431827330332	19.751494190734
Ar	11.748276970033	15.342380279076	21.325906933853
Ar	17.596393561529	24.360915030365	25.097171149483
Ar	16.472458140383	17.454973033635	26.085416368071
Ar	13.191539229723	12.491634188095	10.148071813930
Ar	15.174697674870	25.728287825516	7.998548695904
Ar	24.802403922980	30.191087963444	17.145021258737

Ar	21.172124661971	7.715392727494	20.354006919414
Ar	28.527300380251	18.988463266051	25.184505839996
Ar	8.415864487575	16.777187852576	12.258028374780
Ar	17.595413213627	21.099805832202	3.531507585785
Ar	16.473336798754	14.303826402824	4.519122158280
Ar	21.454144034259	26.792587355344	5.505825291099
Ar	9.506521676801	23.617972863030	11.203455697953
Ar	18.272591226843	8.459372250555	8.253635084722
Ar	13.088493070333	29.321836502266	13.543695874463
Ar	22.496969684941	6.086600170623	13.455720151929
Ar	11.108207302221	21.673039438965	24.317027389780
Ar	10.112107597919	11.081751040160	16.124790969817
Ar	17.910788860529	31.595484614540	18.275805934419
Ar	14.232255024273	8.880180284366	21.536898478103
Ar	22.061106978172	29.475898633048	23.753568577953
Ar	19.078328775556	11.027413218094	26.409125105373
Ar	22.791922747257	16.733474525398	28.829906386858
Ar	23.943527841046	23.812181449992	27.818711517278
Ar	10.573694084121	22.164429964294	4.290035493445
Ar	9.441113377697	15.405658598834	5.340995079329
Ar	5.390304423902	15.833398689451	18.621902637364
Ar	7.210647022042	27.192368249681	17.006137253693
Ar	12.363645946296	5.921124586937	11.607663851360
Ar	12.066525768344	12.306578866602	27.529513342709
Ar	15.054007277678	30.802211243705	24.888189424846
Ar	18.074928505164	21.570678131794	31.4137008277871
Ar	3.684341553964	21.466978012599	14.588224314702

Ar	10.942623901319	32.815323921217	19.387019085725
Ar	7.296136689539	10.219822781670	22.611454368431
Ar	4.719714944994	22.318421974955	21.675357404871
Ar	6.565156241154	16.632629738876	25.715918733874
Ar	8.404373804386	28.046774689543	24.086749612648
Ar	6.781146455534	10.311847358617	9.766663037582
Ar	19.199615066401	28.578194405510	30.292309612635
Ar	16.926141095193	14.533652100870	32.302021906603
Ar	12.568323380849	25.900479999855	29.598552879424
Ar	11.422071466412	18.822129431883	30.616028367988
Ar	4.625748649705	20.139898630891	7.562880297058
Ar	11.903630030216	8.605253704295	4.784603104695
Li	17.455740507937	18.936664291232	12.587252610337
	71		
	Energy= -0.23745703089299999	Symmetry: Cs	
Ar	23.921333824665	29.285470729804	18.715573770425
Ar	20.605472426690	23.438492600577	20.334680432094
Ar	19.751572076591	26.381938156002	14.006954135177
Ar	24.706402890886	26.210162589159	25.139799669290
Ar	22.964305863998	32.205470231801	12.237959063462
Ar	10.253724064741	21.105666098945	16.911034458544
Ar	17.565538446236	32.236289405379	16.979438591464
Ar	18.447261476688	29.221218652379	23.456336767758
Ar	27.438607436990	22.997715702063	19.343504103405
Ar	14.445482777637	26.278956816199	18.642892914252
Ar	23.192053183660	20.255353071173	14.616331262466
Ar	16.655469517869	20.778774779851	15.713456090868

Ar	18.579402686679	22.937572464539	26.880991442174
Ar	16.284749047054	30.854153074241	10.010715761595
Ar	21.837330101344	26.990556752233	7.431024410445
Ar	24.131635701621	19.122357511482	24.466778623060
Ar	29.959931810005	19.722496477395	13.482477802004
Ar	12.157984104587	32.051022934440	21.689220219644
Ar	19.975341167239	16.550771469607	19.597920816657
Ar	18.586064315122	21.201488643617	9.365325189125
Ar	14.612566304419	20.210421248593	21.880096750615
Ar	13.199140713982	24.959553202646	11.891475048776
Ar	25.360241151696	20.684263926465	8.060896623784
Ar	26.565269098777	26.019185054719	12.820872142156
Ar	10.858983059960	30.779576729218	14.805891128297
Ar	12.304728879462	25.807957493836	25.119709714634
Ar	18.756821033343	15.143294810424	12.854677593814
Ar	8.237027476183	20.446004681112	23.038236640594
Ar	25.503817035923	14.402465391708	11.661689575433
Ar	15.084565741464	25.535231766275	5.259604339687
Ar	7.744438007427	26.744565141356	19.921168030801
Ar	17.892938097548	15.917636014128	26.094262652992
Ar	13.579667543332	15.371597652056	17.437307025042
Ar	12.616427117943	18.062164340044	11.208633393124
Ar	20.584665712564	21.648515601706	2.794262036321
Ar	23.363975422394	12.095016670025	23.667144834639
Ar	12.535896526398	19.729696325067	28.352346356812
Ar	9.605291563209	29.311289246401	7.924619399303
Ar	20.773476306872	15.374122532462	6.268908676703

Ar	26.769901744828	15.841934428650	18.605160747249
Ar	22.174949530054	10.585293685564	16.823521480582
Ar	6.441943701498	25.430160414451	13.044423430259
Ar	9.731884451043	5.403923755527	14.043714882589
Ar	16.732661442753	10.905839039435	21.398101335822
Ar	11.484479754250	14.797131649310	23.578244605803
Ar	14.450616391407	18.372158730828	4.560843940264
Ar	8.933884164322	22.243500377160	7.140849305841
Ar	7.194226601590	15.678349017353	18.687433028559
Ar	5.876622962821	18.385765787427	12.395673237418
Ar	15.508176747094	9.459771025504	14.680415768207
Ar	3.564810471444	21.572382428186	18.125739141918
Ar	14.591975725768	12.142499249089	8.179092389041
Ar	20.834704430334	9.217784831085	9.964376165754
Ar	9.400117731391	12.411751116252	13.039092440081
Ar	18.456169658533	9.046711688717	27.779864351960
Ar	12.905668152813	13.001170070001	30.106088729006
Ar	10.396600848802	9.772802440331	19.220713098040
Ar	8.367503529297	15.174874695473	6.571133184525
Ar	21.131401011318	5.633977847404	21.822362999415
Ar	6.694347703618	16.123946483198	28.292537789622
Ar	2.138219624409	17.059088994577	23.098460238032
Ar	11.872206819935	7.908335011439	25.529631777833
Ar	19.856711845119	4.150009996557	14.864348522069
Ar	5.565164789125	11.088702740820	23.696896738687
Ar	14.574017105465	4.409409202190	19.562389999724
Ar	0.730576872079	15.502642103408	16.226830851506

Ar	15.031866444880	5.140639174229	9.365411948304
Ar	3.112036226976	12.198519285385	10.288047701438
Ar	4.141934523832	9.497008870608	16.718579394302
Ar	8.703779353599	8.186234379771	7.655769706689
Li	10.9666986947972	17.938232283129	20.191663866799
	72		
	Energy= -0.24040308401300001	Symmetry: Cs	
Ar	23.767371991368	12.247217226818	7.719438501841
Ar	20.018873045531	15.091309804830	12.813529890428
Ar	23.440261316476	9.091163775237	13.818167664155
Ar	27.219654412397	6.080068114810	8.902141691190
Ar	20.330717938161	18.287995903986	6.791243615621
Ar	20.085366323924	6.153807133374	8.493992849445
Ar	25.825029429039	18.241302876349	10.966300463602
Ar	16.678844879343	12.409313253335	7.450163427055
Ar	29.432925403407	12.081292221933	12.096759693596
Ar	16.496146933430	9.214219189244	13.518124196621
Ar	25.490893672796	14.988331682062	16.977631750859
Ar	14.694343728194	18.179847338913	10.810218257610
Ar	19.901687078356	21.577327663891	12.809229008751
Ar	19.819762410297	11.987685915915	18.558010784359
Ar	23.391814960948	2.179536774497	13.546531425835
Ar	29.217086294788	5.845215279364	15.785101264788
Ar	13.951231626917	17.893485820485	3.964854811920
Ar	12.962385583403	6.411616781426	8.253638721091
Ar	31.446746138321	18.089487717535	15.347900697685
Ar	14.529103460870	15.023593827507	16.532073439654

Ar	19.797467979413	18.519811132316	18.529661172303
Ar	19.637447026086	5.347869064150	18.418549105544
Ar	25.316263734599	8.935101809451	20.602088184570
Ar	25.593262781061	21.830644627131	16.950517680845
Ar	10.953181084343	12.429333917349	11.398703578463
Ar	16.171101877984	2.333291219899	13.206580099101
Ar	31.353241282164	11.931101247730	19.038411481023
Ar	16.250720539579	23.809678103166	7.278211619907
Ar	3.270581522979	11.707099981960	22.374907949257
Ar	14.476134413343	21.559555024832	16.444974803178
Ar	13.982726212085	9.121033838766	20.051334539863
Ar	23.063696070370	14.922864248971	23.540459152324
Ar	10.349914544888	6.256867153761	14.857751779431
Ar	29.047136501185	18.054010218806	22.053475433026
Ar	25.311147734937	2.011085899235	20.532290431970
Ar	8.150728689799	17.847905795283	7.797982402469
Ar	9.134272137985	18.127778646519	14.461223543527
Ar	16.121846002192	15.007980267863	23.177776026762
Ar	10.580272969495	18.202055445627	21.023476067061
Ar	19.403293690153	8.974425750960	24.464788028659
Ar	19.472248689090	-1.526772021022	18.278418028067
Ar	31.035257809585	5.764438204362	22.725560444092
Ar	19.875076603048	25.344595629334	18.556081183779
Ar	10.470161346083	23.787383997715	11.118636250031
Ar	8.405461615300	12.349778725913	17.898645839724
Ar	23.150708513499	21.796470059264	23.639121117397
Ar	13.594065876847	2.249017272908	19.934088096727

Ar	28.829125049664	11.857079752146	25.806698233240
Ar	16.067852686918	21.867950158389	23.219613827559
Ar	5.495098078697	17.730606243598	25.594725787206
Ar	19.227811858978	2.060574809080	24.489834601602
Ar	25.070921629101	5.732787551597	26.736583381439
Ar	4.086687845218	14.040329473434	12.476732519548
Ar	9.964529614169	12.223410714483	24.805568417285
Ar	19.312809416226	18.115520023737	28.436081871024
Ar	7.841130860055	6.279244093778	21.517722212562
Ar	26.452211650023	17.965497514399	28.715140159120
Ar	22.764014673868	11.902890336774	29.756382657815
Ar	13.353638235861	5.971614435172	26.140312938586
Ar	13.335052270480	27.431550688268	19.867133698146
Ar	7.763923256956	23.833761364601	17.778919206776
Ar	3.514745422338	7.927056638745	16.071805317115
Ar	3.642631608668	21.369208236495	12.304404439488
Ar	10.169817581206	11.850924388328	4.619729960270
Ar	6.123284624856	8.005139936371	9.379612454908
Ar	15.544815786114	12.027884730910	29.369462259321
Ar	3.845177261675	17.776655114039	18.706970718380
Ar	16.020202862338	27.379494801106	13.229807774604
Ar	12.200638489656	18.205572280881	27.916751052398
Ar	18.995627213738	5.851666778252	30.579580321526
Ar	9.393087733405	23.876531616750	24.669716763549
Li	17.224251741615	18.244550891372	14.704536074018

Energy= -0.24302021282100000 Symmetry: C1

Ar	9.831096395362	18.883831322299	30.604841181963
Ar	14.446301223003	22.579242689729	27.100600082770
Ar	11.503277434912	16.993240247562	24.143353818259
Ar	6.910234519934	13.311734291933	27.577398033720
Ar	13.607010514260	13.007316486495	29.325997781731
Ar	16.768134344778	18.705993250202	32.376892829781
Ar	5.203594106625	19.534359500987	25.215112734494
Ar	12.946796211190	24.639862233225	33.506374269673
Ar	8.228293392772	25.409424049909	28.183538736228
Ar	18.158935915973	16.823858874014	25.895690812852
Ar	11.473883847684	10.604135648660	23.141871745814
Ar	9.792066536828	7.085947477498	28.817181726518
Ar	9.881093709158	23.240022157195	21.832239381303
Ar	21.941423975147	9.922779266898	9.236001502738
Ar	6.695870862523	14.322347654390	20.730511039010
Ar	20.494788049678	12.775852749658	31.016721699760
Ar	15.885164847132	20.612408038124	20.933664157510
Ar	0.824563057694	13.946704627006	24.0666151451287
Ar	18.123001996260	10.149048156047	24.882633827114
Ar	19.605990748438	25.185669398622	30.896873047513
Ar	21.797810236621	11.006928968082	19.007113114241
Ar	16.714439845140	6.753891556075	30.662052194505
Ar	5.088585570270	8.129363387407	23.496485241886
Ar	14.300112655904	29.381073208121	28.306836024098
Ar	10.965371537930	17.976632883427	17.555228488101
Ar	23.438030759631	19.177599293865	29.652615900134
Ar	20.957660325337	23.060780267339	24.451940922420

Ar	3.637536127118	26.044972173059	22.780482587440
Ar	4.629472787118	20.556133014143	18.352608040753
Ar	15.774715809939	27.145871028749	21.918811798052
Ar	9.585225870058	30.081725254090	22.878236207582
Ar	10.946649667999	11.567613229582	16.654660002649
Ar	14.382578175603	4.143897292131	24.510848606417
Ar	24.293209701709	13.661797986277	25.080215367606
Ar	21.833866849734	17.733659883691	20.005529570882
Ar	15.855757888215	7.766719158881	19.023009402367
Ar	4.542629518838	9.115947964587	16.673070697912
Ar	13.509312483767	24.249086154443	15.924036203238
Ar	9.668296124480	5.145903965191	19.166778521674
Ar	23.499394518723	7.143162556723	27.883832224401
Ar	15.893465421070	14.255229949690	19.985946742205
Ar	17.231859139224	18.479712819222	14.783868591952
Ar	7.266124618582	27.114911556619	16.743914168699
Ar	20.989380782111	29.883718853939	25.560021372458
Ar	5.752303825883	15.327875276100	14.011481709619
Ar	26.663376514142	9.118346369070	14.587101198873
Ar	20.374348710739	24.098109107395	17.498323593537
Ar	26.198476250408	25.618924232572	28.095034070635
Ar	27.205390264989	20.119935352053	23.584615038792
Ar	17.201676119231	11.799114369596	13.813663903903
Ar	8.290350644597	21.614646958072	12.303266479972
Ar	21.114493729181	4.466056053819	21.774039150048
Ar	15.661447688350	33.942197649981	22.942988743277
Ar	12.083600497814	15.711584202226	11.178389719562

Ar	13.331172775917	31.101357161539	16.784312241318
Ar	25.706301164552	26.736651199750	21.023456019993
Ar	20.389918143514	30.947744366182	18.427404745975
Ar	27.272020541271	8.039645075663	21.837937790469
Ar	13.413670424277	5.850334772086	13.043251227981
Ar	15.733198567594	1.110951762375	18.043478863480
Ar	27.919906095760	14.583731042808	19.026543882238
Ar	23.338031807279	15.367407658178	13.638976310505
Ar	8.263586007412	9.804313999656	10.564823205399
Ar	26.606615006269	21.184930913910	16.446243772092
Ar	14.842598220055	22.125923396949	9.448175146689
Ar	20.511515853254	5.532997406650	14.611798041783
Ar	18.041211803998	27.967510037900	12.257138575538
Ar	11.031697109257	28.038437516860	10.727390965471
Ar	21.879740659921	21.951086447348	11.062861901701
Ar	18.599585276601	16.146429015926	8.401816893633
Ar	14.786196371065	10.183448407505	7.614146937955
Ar	25.011455188030	27.729884343564	13.9505388823945
Li	11.335404735896	14.331462935998	20.371573028182

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Energy= -0.24594684121200000 Symmetry: Cs

Ar	11.814931426014	7.871839250714	6.286753330553
Ar	14.178249404299	14.119155488321	7.123897734661
Ar	5.965746334957	10.049201816436	14.344133543421
Ar	16.022199012066	2.646200955154	8.564917350126
Ar	18.163547548659	9.120187175505	9.195173487228
Ar	12.561667329860	10.984331595473	12.761131758058

Ar	7.620969421984	13.350392259796	8.426655231834
Ar	10.448784862372	13.233556401478	1.593470466815
Ar	17.258005124062	10.509199636997	2.260338157529
Ar	10.114191472940	4.574320865753	12.141141350407
Ar	21.531067313386	5.350147248484	4.564803047925
Ar	16.081152471979	11.776657386503	18.130145366650
Ar	24.566227083897	15.844136125820	12.149720221641
Ar	11.706529769880	17.489393027781	12.296092887431
Ar	28.264066441168	17.553857040618	29.268342569455
Ar	20.871959368947	14.955682886707	6.515023649240
Ar	10.304009811191	19.368119952087	5.464642902349
Ar	16.315574961340	17.682316602831	1.747496791734
Ar	10.864921955200	7.447100679345	18.409304170659
Ar	22.410676401719	3.915053935820	11.471723065536
Ar	16.524760194687	5.664291624407	14.976194063047
Ar	21.837068522004	9.979844357725	14.798544662950
Ar	10.142540331791	14.352190903912	17.805112350120
Ar	16.705242083469	20.213668663259	8.402285069000
Ar	5.064062181136	16.908824264308	13.853184860861
Ar	24.313655895778	11.363600265044	1.817730287745
Ar	25.220945090445	9.821983012412	8.731240424139
Ar	20.372481300114	21.120075513993	14.002485615067
Ar	32.685929684349	17.298415307335	17.560355769418
Ar	7.704965868320	22.902546204377	10.830633855820
Ar	23.360484343567	18.619547210484	1.299687067467
Ar	16.591679430363	6.101593091136	22.092164267557
Ar	5.581234872129	10.535671531912	21.480596296719

Ar	22.571855977177	4.282732103521	18.607466700363
Ar	21.206563794770	15.814589345694	17.915270231208
Ar	15.212001520614	18.387682307463	17.657590368109
Ar	9.053420525151	21.225038341909	17.424182475594
Ar	14.126745551887	23.905435905409	13.672328961498
Ar	12.245562463916	11.523771548930	23.820653694320
Ar	12.983051278028	25.765520680806	6.912405452400
Ar	27.899996407520	15.848534542473	6.080291145830
Ar	19.074356496063	24.037050181888	3.229183157386
Ar	21.893944492462	10.446582715059	21.742395741062
Ar	28.033073895269	6.956163725606	14.732440499338
Ar	17.730836240153	14.975714195578	12.572510653525
Ar	4.685708523553	17.342134160865	20.992662094776
Ar	17.645397316155	15.745011946733	23.491021609438
Ar	11.336040242467	18.438035539788	23.326292638487
Ar	27.246282709888	13.049670237616	17.9777817051930
Ar	30.835389206956	13.002562040016	12.016504862288
Ar	19.428106024909	26.601349743372	9.850367588548
Ar	26.329819306140	20.020246313629	17.479786772379
Ar	20.419634210470	21.659404416322	20.941174628325
Ar	29.895174735800	20.154777655174	11.505511878847
Ar	14.172561284472	24.499087847927	20.777565695114
Ar	23.712995315234	21.292799795778	7.9111710757521
Ar	18.280772539312	10.256843103714	27.6395114448716
Ar	22.612134945185	4.873784771171	25.739078652561
Ar	28.127055256864	7.456815166303	21.955235573656
Ar	25.582428617191	25.595558392360	13.400469007090

Ar	19.546784304211	27.289230836633	16.963478030768
Ar	24.665800985359	16.667004029690	23.479647340086
Ar	13.980442849244	15.680837065254	29.338852445159
Ar	16.771220425460	21.735875381862	26.819483537264
Ar	33.501120374252	10.192446502642	18.069890648154
Ar	25.486312512288	11.161011627587	27.599701391393
Ar	21.119431221782	16.625061089967	29.418429778758
Ar	30.992190359509	13.861351538147	23.730532327107
Ar	25.668920535821	26.150927710981	20.619303849621
Ar	31.636380836664	24.374089623312	17.056553923588
Ar	19.606436110634	27.731400082835	24.105866984629
Ar	30.051626746693	21.012448952409	23.219786066921
Ar	23.966417247343	22.718764512130	26.773782052597
Li	13.987714806084	14.671614812390	15.201658201325
	75		
	Energy= -0.24868034404500000	Symmetry: Cs	
Ar	11.743102507833	26.691002339596	29.686796917679
Ar	19.132125691642	22.111446115689	24.873192893246
Ar	14.151842475094	26.813183449858	23.208122189907
Ar	12.340576203069	20.696660407740	26.273070822984
Ar	16.850422109700	21.869220919971	31.394485240950
Ar	9.922058403720	20.410099534851	32.697160213141
Ar	18.713664773963	28.140726277668	28.231276308360
Ar	8.501469207002	23.252650878636	20.969105079370
Ar	5.918291814444	23.038776915035	27.371637786986
Ar	12.845020472628	26.171416026572	16.376057317664
Ar	7.780363816691	29.308718878453	24.230082806864

Ar	14.172030285529	15.246998396660	30.130876700007
Ar	13.608842225165	32.849907805319	26.454465897507
Ar	7.441815903389	15.968862453256	27.575375815952
Ar	21.133814352292	16.702305955011	28.694576749515
Ar	16.514971208048	15.687816170352	23.648064804126
Ar	23.738050206361	23.287034651625	29.840955281291
Ar	19.006098697565	31.615538642167	21.867213411512
Ar	11.719800788721	10.851693683233	24.897744042395
Ar	9.999768271306	16.409518429682	21.169310698542
Ar	6.481310929303	28.701484753268	17.155850713492
Ar	21.243322751128	21.357835248736	1.508393054480
Ar	14.666162771698	20.971862661310	20.093910134804
Ar	12.279475489446	32.330849396144	19.419742309352
Ar	19.383147538937	25.491140225997	18.746492871753
Ar	2.092510380004	25.618519998987	21.902644326151
Ar	3.518564253097	18.593818527239	22.155921874483
Ar	24.113997482294	26.793123593509	23.574828756374
Ar	10.463427648164	19.818468821457	15.236734443443
Ar	25.595144993683	19.760165329338	23.871556381222
Ar	18.423932110131	10.201094923798	27.362441178970
Ar	15.194413317364	15.352590691839	16.818280864269
Ar	3.947147845289	22.130863071546	15.958345474648
Ar	16.833453521688	21.123990122890	14.040682878976
Ar	20.806062249863	18.656254391663	19.037563386204
Ar	5.124973809825	11.625975785953	22.242806693835
Ar	17.123771463854	9.692259112518	20.363306196820
Ar	17.641573357081	30.936705839774	14.784342205840

Ar	24.281948166598	30.126436642693	17.181594122409
Ar	10.527855010150	10.482881373477	17.802647774843
Ar	10.991939467362	31.548998909904	12.399110995938
Ar	22.921473349734	13.181798531438	22.651885739089
Ar	5.537771277125	15.193436253576	16.134448285800
Ar	21.660756077383	25.637087853757	12.344458503410
Ar	11.025315817403	14.240238543113	11.976665688337
Ar	15.125824382291	26.296883259579	10.017773121590
Ar	8.424701467684	25.063161500810	11.261402195239
Ar	25.836278911819	23.200640325725	17.523873986598
Ar	23.050025774992	18.816509159379	12.666827532734
Ar	12.663733918034	19.905413661593	9.159258930345
Ar	5.979508220525	18.740024496523	10.249032580289
Ar	17.308244526057	15.521125215937	10.711838624059
Ar	27.200160462308	16.248495575171	17.817423826661
Ar	15.836756929155	9.435402876461	13.544212094533
Ar	4.184956375607	8.372246136912	15.867822724555
Ar	21.462481513060	12.755738483228	15.619808232189
Ar	19.041894692573	21.277099588100	7.866306294700
Ar	16.432059020877	32.709720102455	7.974611442926
Ar	23.153706808380	32.017355301087	10.375655931333
Ar	28.334709454173	27.126633610506	12.108301261733
Ar	10.515333085013	29.014612194211	5.744966368400
Ar	8.018290679920	22.369905061223	4.707754311648
Ar	4.779044142823	12.011641899078	9.791211353581
Ar	27.031746136030	13.423459375020	11.266075632682
Ar	29.778720498144	20.110268965470	12.436084226297

Ar	9.645700550292	7.417528294753	11.418591038770
Ar	20.546786139708	27.482611521000	5.541064761709
Ar	14.234034171840	10.675326450691	6.979000475522
Ar	9.337798767759	15.297635531386	5.342071182052
Ar	14.673892521233	23.779442209628	3.399737810975
Ar	25.669683429230	22.647241846633	7.253872842170
Ar	21.110806033493	10.011322367104	9.084078346529
Ar	16.032312882380	16.701829881171	3.950124887619
Ar	22.885912215124	16.028299922827	6.144711442762
Li	13.938970493906	17.706643770577	13.048955772263

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Energy= -0.25102344834300000 Symmetry: C1

Ar	26.326827999920	23.338018892676	12.100077334541
Ar	23.767667937259	18.532039178719	16.343820399837
Ar	27.475971508242	24.118306867518	18.911004288727
Ar	22.735387825972	18.011773105868	9.568186798661
Ar	19.361404322909	22.880184200040	13.039502554259
Ar	22.880103188676	28.448119968570	15.717765025509
Ar	32.679542268520	21.927226494275	14.726007121534
Ar	20.498155810980	23.518270296048	19.837332142724
Ar	30.040896244036	17.262620052465	19.161163610019
Ar	18.114306915148	16.217998700622	14.203321977943
Ar	4.439224933015	11.190126142558	27.966457324862
Ar	23.426297876602	12.515606559706	13.805591373810
Ar	24.834316585867	19.354552709733	22.854934433995
Ar	28.866441052391	16.510600170225	12.285887116472
Ar	15.9963099937249	18.941530383283	8.164797378293

Ar	25.858987811878	12.366824158205	7.267618430786
Ar	15.840195286524	27.827085426839	16.656583316524
Ar	30.762037673668	21.781400720105	24.904536921251
Ar	19.138142310281	16.945846479154	20.686764364360
Ar	14.610162801642	21.064625331247	17.616825472242
Ar	18.838736139247	12.427509321213	8.582859010637
Ar	24.510801663781	13.257056697725	20.209672003970
Ar	9.252501307857	25.373541066395	18.103769362634
Ar	29.674685136460	10.935163260606	16.322678039419
Ar	19.792188400168	29.923877840229	22.180238216823
Ar	24.491862950000	25.668631419734	25.338772122146
Ar	25.336725662893	19.879666255126	29.607006910635
Ar	18.889390461071	10.858118557500	18.129157727049
Ar	11.336059125249	17.159096234662	12.875973587413
Ar	26.642274615060	6.838820877084	11.301884182067
Ar	19.168329083388	20.982302023475	26.189185223644
Ar	14.447068984070	25.288556712755	23.127633556300
Ar	13.544823545227	14.576617062031	18.568956146775
Ar	28.857473912812	14.823479320021	25.801600540658
Ar	14.107539827923	10.734059577788	13.215516021995
Ar	24.357859620867	6.839662880849	17.762495456040
Ar	19.657986049425	6.772344961486	12.727989923227
Ar	21.809615378277	14.538405424207	26.429373104670
Ar	11.812204575885	13.229024013044	7.194666299878
Ar	9.017052523745	19.829543479561	6.956693603850
Ar	21.803016977067	6.641642692050	6.105851601726
Ar	12.369285573516	23.941041404813	11.765526504764

Ar	13.251496243970	18.487006169027	23.964398211423
Ar	19.276261621570	21.426889005527	33.016026643976
Ar	28.572035643441	8.476849529996	23.026192374370
Ar	18.426251565080	27.297699684540	28.708443325455
Ar	15.932404235958	12.041340279621	24.229585486185
Ar	8.254962378229	18.560970875480	19.056694252559
Ar	21.526458818166	8.104150501434	23.874393864615
Ar	5.807497801699	21.304229787359	13.196421246477
Ar	14.746516233400	6.722845964136	7.620404772768
Ar	12.656388092831	8.077384682697	19.536114534280
Ar	7.878954985015	12.067459911510	16.272442398980
Ar	18.166130830907	4.010623657545	19.116769537472
Ar	13.121152123227	22.569534451678	29.555269488267
Ar	15.802366320671	16.000182602926	29.938509317494
Ar	5.421573869170	14.649466790355	10.337706786003
Ar	7.850236318178	22.703135261740	24.633107384804
Ar	25.613626347882	9.702255698291	29.449980229736
Ar	9.079274707266	12.917517122637	23.194950073846
Ar	13.163024692348	3.934413063622	14.011544204746
Ar	8.286873778547	8.015361290921	10.664009967041
Ar	22.007248392842	14.803348561905	33.271525565531
Ar	18.520617275358	9.456969522233	30.129190923899
Ar	2.764438759824	22.670670147263	19.548642196633
Ar	15.086051245947	5.306541789997	25.430327752926
Ar	8.693976640958	16.914907172819	28.878279692141
Ar	2.248503392981	16.075136965556	16.705067904274
Ar	11.455698561860	10.280553499573	29.168755185774

Ar	3.499176495890	16.953925288371	23.810486359745
Ar	6.782527029896	5.294377378513	17.196935010646
Ar	11.710177014907	1.319421761708	20.530161682043
Ar	1.989128521170	9.458255062538	13.883462491568
Ar	8.011876349566	6.170688197910	24.293325631604
Ar	3.093248976407	10.287015079091	20.949424169047
Li	21.243815200069	14.739440475360	17.260346758529
	77		
	Energy= -0.25367182962300000	Symmetry: C1	
Ar	23.571658370781	26.009973627161	7.880539672426
Ar	22.013960220242	17.760510893100	13.060733097936
Ar	21.761504076907	24.527241673250	14.431672958523
Ar	19.908307222058	23.176336379853	2.504220285518
Ar	27.450965328849	21.732751024398	11.976671930189
Ar	23.847491133527	19.004014848883	6.665655802064
Ar	27.006591128588	23.215517006961	2.275209083369
Ar	21.542318574083	12.844827399833	8.782959104231
Ar	30.708316585379	26.012178175021	7.750099852898
Ar	16.771816411140	28.103964895782	6.696186859756
Ar	20.438700369906	30.908755592704	12.220271904134
Ar	18.186425650088	21.790304287839	9.079768635780
Ar	17.776549360573	9.551851304282	12.979246960181
Ar	15.153057445607	26.508036862599	13.262221661041
Ar	30.969297355169	19.024221741272	6.381092742293
Ar	15.141431088524	18.771779637733	21.649763524101
Ar	13.103665342895	22.318563468560	4.452112151552
Ar	27.2258988858583	23.977881331250	18.702733268796

Ar	9.944292762130	14.276834858260	22.665207749727
Ar	33.018580182442	24.730723312972	14.591993085468
Ar	18.262321722706	14.386178729881	17.304187056282
Ar	23.640259493673	11.705423107423	14.902523785968
Ar	27.514960973273	15.077227710063	10.696357715207
Ar	13.615892999665	32.843532375927	11.083352966136
Ar	11.598390787781	20.845192050063	11.068756146865
Ar	16.118282964892	15.519339454364	11.068000054398
Ar	27.147230661356	13.207751395467	4.243366918932
Ar	11.644579071704	16.127167587812	16.209013504607
Ar	17.673517292687	16.748586393704	4.469974821797
Ar	9.911291954655	27.149438716652	8.789874137094
Ar	27.191004619062	28.688801624803	13.383412282574
Ar	30.602549017040	13.268605121715	21.847132041972
Ar	17.357711929854	25.242552887605	19.846736648142
Ar	33.258960829047	17.763092025578	13.144173700527
Ar	15.849857882030	31.673571788961	17.802604137430
Ar	20.600835286815	6.145202914728	7.658609406977
Ar	22.700829121533	29.614495121570	18.971148803166
Ar	20.942123326204	10.876136472923	2.212374767406
Ar	21.737167516105	19.823816084332	19.592828696613
Ar	11.007642523813	22.951219014225	17.760381458381
Ar	33.103926743376	12.230754252333	8.263880951346
Ar	15.476433328759	10.545587716039	6.477581089680
Ar	32.964725579868	19.906635414112	19.894145454656
Ar	9.319369305597	29.330705920489	15.673277606894
Ar	22.681189300655	24.763355057239	24.293365066128

Ar	11.034682118405	10.993527798079	11.700308180730
Ar	14.931127844747	5.447425842840	23.275913963609
Ar	6.361744544239	21.322911062726	6.603414514723
Ar	26.884066926746	8.443387236795	9.679307066667
Ar	13.869986772957	4.754783325438	9.881537062293
Ar	13.583365952682	17.127254346357	28.154287906407
Ar	30.848431483184	11.201537009687	15.071929151584
Ar	20.390711436616	18.162701430625	26.148530360283
Ar	18.099024273745	30.272708563608	24.469816011739
Ar	23.512237596538	13.539872658315	21.679612711197
Ar	5.661170840893	23.504277576061	13.396531782546
Ar	11.577850003533	28.024968077124	22.427472699983
Ar	13.345607162610	9.897828544905	18.182625853188
Ar	15.998773724544	3.607978352553	16.353578200893
Ar	6.297713316945	16.463291841612	11.840642398824
Ar	27.135466079345	19.161057753262	23.905473493840
Ar	15.823564782789	23.735513838049	26.419479819277
Ar	26.847769328266	7.649175235353	19.460676859101
Ar	22.776541065238	4.925660597623	14.118112887645
Ar	16.736772444479	12.425069082085	23.829220875925
Ar	6.465009556252	11.636360497346	17.013297891405
Ar	10.922721153122	15.808661005745	6.454205666807
Ar	27.383117130141	17.046365162928	17.127549650714
Ar	5.699125978468	18.583192150363	18.705977956890
Ar	5.173347121069	25.604074585674	20.233567609087
Ar	9.312259825001	21.365182960725	24.283199355525
Ar	9.193559074834	5.231195781689	15.318846150825

Ar	23.204688447623	17.341777194677	0.055386243580
Ar	8.276046094978	7.328081328674	22.191277486220
Ar	19.967572694199	8.196117913542	19.420104404241
Ar	16.620214741393	20.393212841427	15.382935167893
Li	19.879284535117	13.698468955200	13.038757660055
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	Energy= -0.25643835054100000	Symmetry: C1	
Ar	10.5689233367781	9.588642033869	19.793055273157
Ar	15.946289062452	26.288355548569	21.904355807280
Ar	15.169545712684	14.204107307223	17.556314785093
Ar	24.863045948336	11.565976883585	12.314554969699
Ar	28.109687527422	8.521063800050	25.247505970591
Ar	15.590782654979	4.598962597176	19.473473003169
Ar	26.951500932455	7.952490111325	18.149025832072
Ar	31.818110428139	10.507684006908	13.573289386117
Ar	18.352119493755	17.073608483208	22.403711663953
Ar	29.573914755197	16.816833974502	11.090177743829
Ar	28.111495281678	14.743701547447	17.551803454126
Ar	22.610845223664	17.913136509432	10.090629668679
Ar	27.853118254318	13.071330644145	30.881235599496
Ar	33.058693811190	11.024483221727	20.617236648100
Ar	14.561031242372	10.306389014309	6.729391325811
Ar	21.394924715258	15.938638499326	16.592314347466
Ar	24.577107154995	18.836170704432	21.433631149337
Ar	16.569955019484	14.847687762299	28.732527761420
Ar	30.810538661757	20.722103498474	20.192027626424
Ar	15.175545706308	25.411242228648	15.28229799388

Ar	8.528282349306	16.109634265345	17.665784858108
Ar	21.787363498150	9.976021452070	28.370080169630
Ar	21.55900994125	12.298466051151	5.884020462382
Ar	18.174699811104	13.052245889746	11.698767482401
Ar	20.994602634125	24.325207469799	12.080089349910
Ar	13.745045753235	8.369062182732	13.725431600661
Ar	21.981229565737	5.594205470442	22.711714575464
Ar	34.650993020880	16.556286672018	16.221984430119
Ar	34.118617492456	11.686438904640	27.684776302857
Ar	25.901902012533	20.932948407996	15.255253450486
Ar	20.044577235641	9.243356593731	16.978965197983
Ar	19.915736838224	22.088334040098	18.392528751967
Ar	29.252787924204	15.322165067498	24.486690576204
Ar	14.774821752169	23.995943605226	8.679400704763
Ar	11.903925885725	15.216233434130	23.586833455383
Ar	11.638233882978	14.878446693369	11.574752089012
Ar	27.651987897022	21.972468746490	26.384462197113
Ar	16.385720579308	17.419404220676	6.776228860056
Ar	32.312029549107	22.950455754016	13.773900878846
Ar	20.827259369047	22.889300702237	25.121765523996
Ar	16.841153043348	10.438639377561	23.135556094519
Ar	27.167410474508	23.126178263753	8.783862891114
Ar	32.586463764412	18.440105044925	29.690785413483
Ar	23.060141557392	16.740506048323	27.530136018206
Ar	21.518825186467	14.561528345324	33.880033687483
Ar	37.278769396589	22.670439067477	18.940658916945
Ar	10.398810258059	27.035248773103	25.844507578197

Ar	25.570109175820	25.375051508027	20.618350729177
Ar	9.533491682770	26.201993828057	18.859535303042
Ar	31.976287673231	27.525970839872	19.323186315246
Ar	20.906964944772	22.843478727765	5.371205384471
Ar	16.636207076407	19.201343973106	13.550781672268
Ar	19.176135783861	20.905206665390	31.508676536102
Ar	20.646057757614	28.794478106813	17.405543480825
Ar	14.294404039304	21.109222200003	26.218936359055
Ar	23.853425455983	26.266235631528	30.309136795847
Ar	23.327631291655	12.357704086857	22.083149052780
Ar	26.213206834554	19.881423172336	32.818722843651
Ar	26.874273110048	27.715097367592	14.184458576690
Ar	13.695755786581	20.311210693129	19.304931427422
Ar	34.168911428323	23.989681601620	25.272193272267
Ar	35.826099570631	17.165644084560	23.344782798936
Ar	10.042734524869	21.431868949947	13.458625763810
Ar	30.859539699849	25.199948561838	31.525247485302
Ar	19.922199920288	6.666299446982	10.315394166671
Ar	7.951148910202	20.898089428961	23.042810878355
Ar	28.738598115290	28.807391161335	25.668174764121
Ar	16.856325653563	27.144893452495	28.885909718820
Ar	14.129120751785	31.699246206638	17.603051640005
Ar	26.454795614217	32.174400071784	19.695923433345
Ar	15.088464492576	32.531723099285	24.582955031264
Ar	21.662323106182	29.743260476861	24.357466995406
Ar	17.374582864621	30.380205762448	11.225870554285
Ar	10.271987248072	28.665835479739	12.045045873266

Ar	23.571918785641	29.192486484800	8.008874380751
Ar	23.202710851630	33.795110941161	13.511226253425
Ar	19.932241128118	35.099629098643	19.958016034305
Li	17.591522305170	18.148887779624	17.968859189813

79

Energy=	-0.25913695461800001	Symmetry:	C1
Ar	25.894265352859	16.281061783841	9.373061360511
Ar	21.550794556198	18.509165774919	13.851948483341
Ar	30.429476491309	13.997286915127	4.719917636527
Ar	27.445859709976	20.494061387793	4.121334772245
Ar	32.201157730720	19.091844104605	9.439642447645
Ar	21.225728635792	12.121289253023	12.468466057109
Ar	31.087942679830	12.278120822064	11.649371301914
Ar	23.469222741880	14.533991762855	3.104861062681
Ar	25.698651008278	9.604482726193	7.791395466884
Ar	19.103994506420	16.833208318107	7.914006760225
Ar	26.431963072249	14.658773758716	16.138902227275
Ar	27.539707238414	21.278983377742	14.062028797485
Ar	22.897471135771	22.645982132685	8.868308211557
Ar	29.125346735767	25.644911486552	8.933649227122
Ar	3.927866836140	9.629479505190	13.712669374251
Ar	26.190478614962	7.951310205113	14.707122385449
Ar	32.757634678493	17.371230907628	16.464847919475
Ar	18.751045402614	10.165266527401	6.353745548658
Ar	20.372630109759	21.032788427433	2.601355760389
Ar	20.017926602605	14.392446991445	18.606287157183
Ar	15.776027817629	15.636480112042	13.761127689423

Ar	23.864772501845	19.942090110422	19.930117562974
Ar	31.466978978833	10.588483936368	18.590877561787
Ar	21.012543202059	5.496409906722	10.885821337455
Ar	21.651711054475	24.943643407093	15.433874775220
Ar	16.457342169329	22.163327408221	11.602134047694
Ar	33.764211620111	24.165037761504	14.257116630124
Ar	16.462549887351	15.048895475505	1.760853979365
Ar	24.319678865747	26.944486544393	3.710176104247
Ar	18.477725950345	10.216309033111	23.398309922365
Ar	19.671405768700	7.998020516989	17.200393215095
Ar	15.431108162082	9.251487025771	12.422546858827
Ar	28.962285216875	15.981188913235	22.467386214384
Ar	13.044325925139	13.827698976319	7.851322040621
Ar	30.106616556817	22.860482806638	20.296827211988
Ar	17.097594818006	20.566452939801	18.357093634256
Ar	27.845245779148	28.001754374841	15.662052950608
Ar	13.739233142340	20.481514975196	5.429191944098
Ar	23.063771576501	29.396445105913	10.341250815584
Ar	17.662197355546	26.513015520876	6.412438784493
Ar	28.274248101970	4.476002263594	20.512341422903
Ar	22.881239172894	1.941097452090	16.539777220407
Ar	14.222873864826	11.419188822910	18.496907677427
Ar	22.354821029516	15.622366676712	25.131737893003
Ar	14.968307779346	4.304453222895	7.674699141000
Ar	10.370983152892	19.124403392711	11.519055333393
Ar	24.076640519055	26.625928660058	21.690716493863
Ar	12.638546070859	9.128065337815	2.892161657152

Ar	16.386173188979	28.868839802248	13.139206745366
Ar	24.806098420860	10.358409206653	21.095664398966
Ar	9.887490915090	12.723192225718	13.686761781398
Ar	15.967413502839	2.773787882919	14.669684173416
Ar	30.004772826081	9.528632039240	25.464691877040
Ar	26.292259329260	21.472982615808	26.197187226056
Ar	11.064253881648	17.525018513717	18.259469860232
Ar	15.474332961817	16.279259476435	23.432078018353
Ar	19.328946884089	22.109493073666	24.714744493392
Ar	21.779997755353	31.619099169507	17.045044991697
Ar	17.033035204145	27.213431487571	20.119345657192
Ar	11.672642630936	24.300472696029	16.198600173904
Ar	11.068423443195	25.829981636992	9.289383547375
Ar	21.624080575279	4.256008000394	22.958404701689
Ar	9.399987961546	15.698300598501	2.366951777082
Ar	9.213100636484	7.959241331375	8.984379258446
Ar	14.717297843230	5.050879152757	21.123614923107
Ar	23.345567486205	9.106914567535	27.983620851319
Ar	10.157166479210	6.375856936633	15.969712105876
Ar	5.948888919025	14.442248217761	8.439365896509
Ar	6.663404413674	21.151263293849	6.142112133939
Ar	12.395574793958	22.599798003812	23.048907891062
Ar	11.872355505146	10.409394601397	25.035439633065
Ar	17.197758867255	12.930203059519	29.457858915403
Ar	7.290146566746	11.724890110450	19.854732444665
Ar	4.684902120656	16.793830779097	15.211593957513
Ar	5.355412781002	23.532484245956	12.970064212184

Ar	16.693679581136	5.760337270931	28.107424327569
Ar	8.558591553651	16.787166951628	24.614102166142
Ar	6.061013697985	21.895457093053	19.928718386175
Li	17.740013421169	11.865327547766	15.500554499125
	80		
	Energy= -0.26184673029400002	Symmetry: Cs	
Ar	24.2669183325641	34.515379612723	24.563272557133
Ar	27.488853992430	17.115667548767	20.005860106882
Ar	27.917918851401	22.419397148217	12.416972975675
Ar	23.573315812413	27.789429767287	26.782924371310
Ar	29.164900106795	26.119314082522	22.673904669714
Ar	29.937373366224	32.864225998788	20.658847635122
Ar	37.602182934412	21.504580833246	21.053085622356
Ar	23.748757315069	29.512823197239	19.892592723641
Ar	30.212703145570	16.529606974431	14.158354936099
Ar	24.991519439468	21.273820634506	24.884930840600
Ar	23.831678868843	17.805703413852	14.512880266099
Ar	30.193741714203	12.977103546003	24.888731105050
Ar	19.489516588613	32.850141930435	11.611297379138
Ar	18.034163168067	31.156935794426	23.841444157656
Ar	17.078437225595	13.548002633613	22.350319184015
Ar	21.095189066671	18.424236203385	20.355062960307
Ar	22.807260515231	12.306329475576	18.494233817386
Ar	22.422597799985	22.205041708127	31.220377081885
Ar	27.198330613800	23.221067234347	5.432092112052
Ar	23.010841390472	27.229659711317	13.361222639793
Ar	35.239998738583	11.806687462556	14.142856622310

Ar	26.624785192928	17.174856377173	8.456392913810
Ar	31.701824972040	19.938598883448	24.627144894463
Ar	36.682386988797	18.896345756709	14.364342805972
Ar	20.246705189726	35.231085649539	18.417811153221
Ar	23.500009193790	14.463202506529	25.091047250751
Ar	18.809160492311	22.397162821694	15.561935402375
Ar	23.731998311017	5.758833806569	9.463390193751
Ar	17.219091969190	28.942247221238	17.142065633230
Ar	31.417807046156	12.436912416285	8.404732240643
Ar	27.570663799892	17.327913159426	29.921676453199
Ar	28.551222161184	28.773139259504	9.388990733057
Ar	18.456154876473	19.205157690394	26.381334969677
Ar	17.336645551864	15.603477598997	15.653258097619
Ar	25.302038142970	8.013500822641	23.283997508184
Ar	20.203164968996	14.957799371014	9.520237245064
Ar	22.044110990101	28.051580094378	6.520924998286
Ar	20.844908963605	15.132516182961	31.437487611122
Ar	25.984180858399	10.341924806555	30.025359851767
Ar	14.613456423944	19.892741614138	20.509629504478
Ar	32.923336885399	19.606782054195	8.555504322548
Ar	29.481640315866	10.823491817953	18.131430281875
Ar	16.497527257797	26.544681840726	10.532333512073
Ar	24.712152072342	11.411779454695	5.370700436792
Ar	10.298470686608	14.909520383655	22.573036378649
Ar	18.740640484049	7.085584546213	20.446231244801
Ar	17.062547030639	22.891267594887	4.515476728149
Ar	16.806609650059	25.667431362489	28.335544275948

Ar	22.113728814413	18.084242140471	3.441528876576
Ar	31.484022424015	21.748795026792	17.8777865703354
Ar	10.588121418919	17.010940178931	15.639372841163
Ar	19.050912712202	9.221502620887	13.550982607187
Ar	12.119657697150	24.048782970524	15.530271189198
Ar	14.232609857337	14.205261459607	28.620782599640
Ar	24.621747868774	5.942003816405	16.488240774528
Ar	14.954482022282	19.646294730073	10.518515405419
Ar	19.432243025706	9.331909353544	27.304419949981
Ar	18.094866975758	9.166806067883	6.498965412653
Ar	12.867812977468	26.369321060839	22.308020728287
Ar	15.722187510175	20.007214715739	32.632671614745
Ar	30.404313025993	6.731087125838	12.4261956838911
Ar	13.535584740856	12.688197894568	10.681008411200
Ar	11.716580618886	20.733213615380	26.723270351226
Ar	13.112590502046	10.497861533143	17.526412999724
Ar	34.113859604017	15.640884284365	19.810598977287
Ar	15.514553301132	15.808300090369	4.577534290966
Ar	12.917868311780	8.490593403080	24.426314365459
Ar	7.909637229757	21.407510519667	20.675254742636
Ar	35.090445751020	25.969842803835	26.137190830942
Ar	34.274428652802	25.151931894228	12.507845800250
Ar	25.110993157540	23.057640781189	18.255579621763
Ar	25.648416302741	11.681646944283	12.385064386972
Ar	29.881812954532	31.007614628367	27.457284220838
Ar	35.144605750828	27.737250395126	19.308837146703
Ar	29.0911291171761	24.291660892011	29.565045103074

Ar	29.230604491636	27.871752241413	16.079359139148
Ar	25.890333834315	33.583741942056	14.486297730982
Ar	19.539797327163	24.647942395303	22.098269834520
Ar	21.677788814148	21.757697853797	9.461917544078
Li	27.611744880940	19.777824810518	16.228216107059
	81		
	Energy= -0.26474641421599998	Symmetry: C1	
Ar	13.139385953170	26.877298069888	16.751258246947
Ar	16.757635514461	21.306776145555	16.768664819105
Ar	15.815110055423	32.495066583081	19.858572847335
Ar	9.387732803802	32.631939455181	16.715033004891
Ar	6.298259829197	26.184040296892	17.379878751374
Ar	9.413041849423	28.169320903083	11.083904270532
Ar	15.329891040346	32.055727393300	12.678787057059
Ar	10.326412937109	28.865269389926	22.789572250582
Ar	14.103831705461	23.111772766143	22.606710013260
Ar	19.395759050027	26.618010902842	19.763093268809
Ar	15.439662474129	27.484243624575	7.063196124996
Ar	13.247208490881	22.414428120805	11.278877968683
Ar	10.219077978325	20.485842265737	17.399029551411
Ar	16.852312509306	28.606365579656	25.897395422401
Ar	21.347871258708	31.235852299162	8.785365130763
Ar	22.018115612589	24.402543714899	6.886637158501
Ar	6.394261535369	21.608271464180	11.748738396953
Ar	7.326082538375	22.313787913949	23.456800826096
Ar	20.357563986874	20.203139855956	22.004297234428
Ar	23.201875922833	21.981080683755	16.370115916408

Ar	27.883241718949	17.979796460975	32.706352527908
Ar	19.615716939915	19.448896459445	11.097832795814
Ar	14.804335929413	16.396655322938	20.777463404114
Ar	14.250664195433	15.922695374126	13.844135484801
Ar	28.451249753010	29.964620463049	25.363717313792
Ar	9.596599953037	23.556447155979	5.581083349669
Ar	3.436691964698	19.632881580784	18.028847873340
Ar	11.490639517126	24.932519239490	28.747661358970
Ar	24.135721695323	14.866580042495	22.194797976166
Ar	23.19102024113	25.454217631784	25.243772225659
Ar	21.819408072882	31.778847418128	15.855610757859
Ar	17.908457536201	21.951234277192	28.1209299929245
Ar	20.507785535196	15.943475863884	16.945055695375
Ar	31.685913660201	29.255720651248	15.461612499949
Ar	27.385306344793	33.535779643956	11.824828423125
Ar	16.126953036281	20.543016591474	5.250420002077
Ar	7.433137732986	14.927216784091	14.37177476481
Ar	12.086016364941	18.076744612525	26.948213015299
Ar	10.535795867239	16.901888721235	8.101480543766
Ar	8.035201537474	15.395221478094	21.588974797305
Ar	26.124245523511	27.314486033247	19.351110945607
Ar	18.951366996037	26.194501371208	12.841152152715
Ar	18.590136223149	15.264816435733	26.264122310147
Ar	12.131455916785	10.721572446487	17.927915153900
Ar	17.119983485045	13.892254600113	7.866061854136
Ar	22.552155660101	30.490419174921	29.819771762162
Ar	22.219905818988	32.099575832626	22.920832217711

Ar	17.083276250291	26.872359039486	32.798843851485
Ar	24.011711160511	19.106597606756	27.341854335879
Ar	29.859845731855	22.723441245223	15.967204769188
Ar	25.705793493151	26.907940875123	12.421751607706
Ar	26.938078315328	16.645271588182	16.575937672722
Ar	26.336027131239	20.181356841490	10.697786683320
Ar	22.656392285029	17.529858317532	5.197371036784
Ar	23.529886495427	13.822610997129	11.170829812686
Ar	12.844146058954	11.288715801801	25.028424725710
Ar	11.619726031772	10.340980912395	10.786850950015
Ar	18.644261896363	10.720726128612	21.008289146033
Ar	18.0412041179545	10.201159703612	13.925558322585
Ar	14.038031730439	20.214219373831	33.482828307277
Ar	27.502123593553	28.870934392698	6.096636840656
Ar	27.832351523413	33.947103560431	19.057773644015
Ar	23.499722248860	23.858378859623	32.162976645393
Ar	32.334429872330	25.198546748441	21.797506793583
Ar	29.352960733409	23.247174157792	27.810277629395
Ar	24.25939468777	10.272017549301	17.044318620963
Ar	31.808681611356	24.563676948429	9.706440892254
Ar	20.498358131166	17.271645203348	32.848909994490
Ar	28.156302706911	21.902873703872	4.296235664292
Ar	14.735212262564	13.330885682495	31.582278805362
Ar	32.919169811655	18.085049194016	19.822509542808
Ar	29.926492335025	16.235970651183	25.850297162115
Ar	32.704628044981	17.714281459453	12.477749593423
Ar	29.102022176511	15.106342662553	6.999821758379

Ar	24.563772614570	12.609755301755	29.025567275943
Ar	18.852762474553	8.596781186797	27.783983362246
Ar	29.888654572314	11.428862138049	13.171758271035
Ar	24.709727638998	8.181121988656	23.666751038662
Ar	30.026540655310	11.819337823077	20.422557472866
Ar	26.853480374555	20.815023783794	21.623237371929
Li	23.615374703969	18.447757284468	19.2839066953909
	82		
	Energy= -0.2676363407569999	Symmetry: Cs	
Ar	35.205139459894	14.724733368512	20.515888741762
Ar	29.441680038376	16.701320591890	17.421141663583
Ar	35.503637855976	20.156701312726	15.904440249505
Ar	30.087226384067	17.880359984789	24.385623647600
Ar	29.117269080315	11.255417102229	21.968776056190
Ar	36.087793697047	21.448931838566	22.861740621758
Ar	31.874520158291	10.653074998066	15.364640641879
Ar	30.289130811638	23.238545752464	19.699221590410
Ar	32.194924728662	16.126858350743	10.822105289341
Ar	24.061547693374	15.949596222445	21.517238288613
Ar	24.856618735706	11.394681490542	16.290815878041
Ar	29.582445061680	21.946058573460	13.128292908787
Ar	25.414447969417	13.459177630428	27.780066035417
Ar	30.912832418590	24.561832412881	26.640414903450
Ar	24.388160109515	21.256136852512	17.089228854125
Ar	24.945552382074	22.515463062481	23.787031959999
Ar	25.228552791127	16.957220916988	11.893389147925
Ar	33.611511367616	27.089564990084	14.734794374540

Ar	34.248380243558	28.458371781671	21.664782547610
Ar	27.509800042647	10.928303128970	9.634131272466
Ar	34.778185341774	22.753010813625	8.964160685053
Ar	26.341158286667	20.210730691370	30.125568608281
Ar	22.145302010283	9.447807987028	22.711540060851
Ar	19.876104701011	16.196687418003	15.971193767496
Ar	26.472150078914	27.285652901305	15.642978997586
Ar	27.196906838058	28.850787165464	22.401807056788
Ar	20.425546731677	18.252906442357	27.058705398036
Ar	28.144357984054	20.609823503140	6.629375927926
Ar	19.275365178691	20.545371075294	20.972206198669
Ar	7.160988305955	29.076632856981	12.755275826218
Ar	23.549282242516	23.619830072931	11.059730815368
Ar	20.549106523613	11.748239870292	10.687702587970
Ar	17.237753324392	14.332997674811	22.115947639759
Ar	29.041174449046	27.367443741670	9.138428774755
Ar	21.365097538154	26.598466269101	19.559140237661
Ar	24.610515720728	27.112085309800	28.904127285819
Ar	17.825230734073	9.708052865746	16.945020264763
Ar	21.595068636555	15.881481503650	33.385587912175
Ar	30.377349923706	32.672067067507	17.328464108777
Ar	18.350712591276	11.802036875777	28.440263412375
Ar	23.371690810588	15.422387113890	5.382355089367
Ar	18.398251857212	22.835536815557	14.996440471361
Ar	18.972725533095	18.606705932250	9.707665569599
Ar	18.752707222315	25.002334432932	25.831965427679
Ar	19.887443080711	22.766795436145	32.268229569912

Ar	15.122454770564	7.916245200511	23.327525478138
Ar	20.500986953076	28.860096262654	13.556636591324
Ar	23.490339040625	32.939126838598	18.261162520224
Ar	13.674907349721	18.688391697227	17.888198339079
Ar	25.752945322835	32.916937983248	11.768345393729
Ar	20.891054940315	31.399160488793	24.538918999614
Ar	21.697197630483	22.309072344581	4.376666544948
Ar	14.184392378718	14.208568719829	12.562551275842
Ar	13.911387831366	19.970580270796	24.782865779734
Ar	14.649839190848	25.230199645224	20.189623065657
Ar	14.923557702255	17.581611823846	31.191173016392
Ar	22.608883813984	29.063112045068	6.890805585223
Ar	17.502474620575	25.131110378622	8.907624886720
Ar	11.397355007289	12.281835926580	18.956175998874
Ar	16.081272328134	13.941736983855	5.641717100303
Ar	11.654067094926	13.568025994787	26.100470228745
Ar	18.190617850415	29.606398989051	30.914515121970
Ar	16.738251726977	31.608268596162	18.747682056669
Ar	12.759434627095	21.099851265839	11.592543528968
Ar	13.219393621914	24.524964613725	29.938651603952
Ar	13.741687187726	27.601740990068	13.917413392813
Ar	13.910723636032	29.933362226282	25.165534298897
Ar	14.506094479950	20.790587769519	4.642790827422
Ar	19.246746691708	35.607036014735	13.439998133722
Ar	7.982306160538	18.055924654235	21.689422029696
Ar	8.759289043971	23.504259930659	16.933581104368
Ar	7.902645664835	16.849414880800	14.557026589424

Ar	16.103915207785	31.706254011198	8.617572192665
Ar	8.966476976075	24.792287944520	24.055077127979
Ar	8.358071500395	19.371858565804	28.760834379293
Ar	9.637679132285	16.515277514277	7.596406158606
Ar	16.775809260779	27.499282769714	2.674627616003
Ar	9.833721503838	30.119909295314	19.275589690292
Ar	11.065603918371	26.601119616802	7.366165478567
Ar	12.213004525231	34.268544948615	13.965531522148
Ar	6.159993265636	22.383580276108	10.367543099898
Li	22.425021996858	25.023784655429	15.337048176634
	83		
	Energy= -0.2700693558899997	Symmetry: Cs	
Ar	27.417039741920	11.785988348210	22.982904132006
Ar	23.223850141053	17.109397248159	21.549161020035
Ar	25.236437909608	12.848911710712	16.440595627424
Ar	25.289534500343	16.176064425669	28.107864576662
Ar	29.377330750994	7.4589982712028	17.707494810159
Ar	20.596736333448	11.877583362062	24.943483065346
Ar	22.609104045694	7.586717808998	19.858000743887
Ar	27.243505908166	4.744745779216	24.003571027135
Ar	25.136005169107	9.183480626294	29.275821507958
Ar	31.828574954775	14.273783303247	17.818232232141
Ar	29.728002948659	18.670286403766	23.131358046720
Ar	12.470784817413	20.205288499819	24.757392658834
Ar	27.448313110781	19.531541384880	16.608390807250
Ar	20.450990703019	4.873440331723	26.134156139731
Ar	18.699487395958	18.257360837542	26.448900777764

Ar	24.105061895392	6.946176180040	12.955161736602
Ar	20.495415184770	27.436257562316	29.358005087108
Ar	29.804124262700	11.246289857939	11.559015343020
Ar	25.184006345043	1.657147405758	17.647190602525
Ar	21.133457323172	17.964072326321	15.292666952748
Ar	19.706215900091	13.693353710140	31.592782930204
Ar	16.136085944399	7.880130882694	21.849071587647
Ar	33.982035152815	21.159755581354	17.942516912164
Ar	16.822739404339	19.069649159981	19.9777874396034
Ar	8.425677742440	10.697961002953	30.070282649510
Ar	19.969884215017	12.420517777753	11.847869241838
Ar	17.373920726633	7.192455124118	15.2677858144974
Ar	22.083840106498	23.450005281633	18.942098137250
Ar	25.465493685989	16.579783475087	10.502171525864
Ar	15.085187394582	9.296391349047	28.395857844969
Ar	28.566576924853	25.242756214543	20.406543130507
Ar	32.092440725493	18.162802032957	11.689786478635
Ar	18.404238118654	1.809366225330	19.867503648843
Ar	14.227380977907	14.033733758418	23.245412834447
Ar	21.667923789403	20.845449672927	32.027654827016
Ar	14.861484443189	16.336468845822	14.285838582685
Ar	12.377585953528	11.339938067519	17.553707264734
Ar	17.546337256687	24.611066409092	23.875172855362
Ar	23.488529824527	23.227638611832	12.070839998437
Ar	13.121663995665	15.899052073387	29.953860646222
Ar	19.800409988069	1.240920841006	12.924704587479
Ar	24.391242645277	10.787665432792	6.824874527398

Ar	30.059597803166	24.998561097179	13.302795028953
Ar	13.393185060819	2.870510480569	25.361242560179
Ar	10.565011479250	17.435026362401	18.991949686691
Ar	16.845395954744	22.927106432845	14.327069205237
Ar	18.892269418818	18.754170307594	9.119798960764
Ar	18.732280806602	6.585049001241	8.331672818278
Ar	22.938036219575	29.112123557613	22.816910027654
Ar	9.652627996086	8.855221270426	23.435759104329
Ar	11.714380894872	4.204048490530	18.347874992954
Ar	15.081237921720	22.930067605847	30.394910789426
Ar	18.638613424807	12.963512123466	18.537032651680
Ar	7.978502212321	21.078230552765	29.657652528079
Ar	13.438009534110	10.653825834162	10.695881506198
Ar	24.513461344490	29.036976358483	15.757022190864
Ar	28.040952040309	21.969934400890	7.021639460005
Ar	12.352476382164	24.077873722800	19.252248231260
Ar	7.691166659621	15.450943194713	24.992122663539
Ar	17.631295622746	28.715230119297	18.091930363225
Ar	17.685521192883	13.030595322859	5.378825453393
Ar	13.016569611288	3.600706015070	11.404736065239
Ar	23.304921139934	17.385515860348	3.984270632619
Ar	24.177302914115	22.680124528518	25.553554983169
Ar	29.959596689785	15.166771100546	5.518809946406
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Ar	8.364822320343	14.697856496503	13.042475018811
Ar	19.118242228083	28.518954078020	11.008865717239
Ar	10.263592233128	21.328307870996	13.214699343725

Ar	21.281298334184	24.190265347843	5.589961264930
Ar	12.348362091341	17.104231393010	7.864895060543
Ar	16.369503468492	31.297294978911	24.641270935259
Ar	10.989341941727	26.743123898731	25.751033228123
Ar	4.387367433169	19.184386190391	16.580900756071
Ar	7.768626340681	7.814381449756	13.897961371690
Ar	6.392160145436	22.100841925152	22.570913724339
Ar	14.437789070367	23.951590368319	7.955813118842
Ar	6.327700342627	26.093079368577	16.712182698890
Ar	5.750679535247	12.513886890817	19.003349240325
Ar	12.334240312374	28.099469892020	13.408357723035
Ar	16.603116186729	19.591962697090	2.684344910374
Ar	11.022513106604	30.757970337457	19.889736313644
Li	14.636418673229	15.210237618870	18.775072631489
	84		
	Energy= -0.27258508361500000	Symmetry: C1	
Ar	16.564879723773	12.955689979158	19.181377320317
Ar	11.508113937503	24.446581664686	22.462883696543
Ar	21.662981075772	17.125780218429	19.532703851327
Ar	21.054992015287	12.194726581902	23.788083597481
Ar	13.716385275256	7.008249201145	16.920357553771
Ar	15.898903168773	7.734640367506	23.454140689590
Ar	9.457690877145	17.860908261141	23.390921290924
Ar	14.503204788176	12.338330701168	12.596783481670
Ar	17.163683580111	17.928065964364	14.960606897529
Ar	20.706526804422	7.514391560860	18.596519292465
Ar	11.007308055672	16.499895927282	16.927483827609

Ar	18.863942973243	16.427291423651	8.7666620853143
Ar	8.034665778996	10.690843994730	14.628206929337
Ar	23.794944883520	27.554963641025	27.181114601030
Ar	24.512431469857	22.594384682971	22.381912451101
Ar	20.180051810931	18.377796143071	25.765612959489
Ar	26.252112188715	16.342252803444	24.169098428163
Ar	23.419742835922	19.387070064869	13.232104823426
Ar	14.165226596836	20.573809014801	27.360435825404
Ar	5.068506324799	26.648533336494	23.072437641062
Ar	10.362992875880	11.388268498112	21.312743897653
Ar	2.952284260159	19.842952551784	24.037363933700
Ar	21.300985390342	12.792926187956	14.238504619048
Ar	15.079647875215	14.283003811947	25.363273538517
Ar	18.727875197391	6.910234646734	11.740370091312
Ar	12.386715367268	18.763209615053	10.472239021281
Ar	4.269529419572	8.252953600829	20.311406651007
Ar	26.013595299958	11.987709907742	19.029648498226
Ar	23.204559807451	11.079061458817	7.8556071532180
Ar	19.807969869827	23.440481144567	17.584707644740
Ar	17.931295086182	23.117474034712	10.899962040247
Ar	11.749308896380	6.572430711127	10.067668015907
Ar	9.813135773314	4.598166672153	22.566387979849
Ar	9.522310072210	13.030811744550	7.872825912128
Ar	25.666435066262	7.460286942701	13.567995065150
Ar	13.067099934634	23.086379916381	15.979769385960
Ar	4.600607819183	15.082390608715	19.068134227609
Ar	15.671866514496	19.217001727376	21.113007374141

Ar	5.876816905201	17.289040294129	12.417444618165
Ar	22.220574723556	5.595837774003	25.294694771096
Ar	28.154374705189	18.547868358520	18.045695973632
Ar	27.277315252603	5.369306065726	20.212376880254
Ar	10.976123834374	9.356204408828	27.992984038990
Ar	15.700780036443	28.882243183970	18.821820585878
Ar	16.161422569497	10.653330727371	6.102791597832
Ar	5.229880021404	12.973082529725	25.790684839757
Ar	13.984341434196	17.232236667799	3.931931411179
Ar	6.598052632708	21.739687635958	18.133924808698
Ar	27.890394108548	14.118058331123	12.500188726764
Ar	24.420217126986	24.728761951829	9.011464380231
Ar	27.637391460146	9.925761112770	25.639119381444
Ar	18.134233627022	9.809377753394	29.572946651875
Ar	18.258052876525	24.784350911947	24.038030290972
Ar	19.371571941501	23.237289678261	30.814962754745
Ar	8.021252867751	24.095681074715	11.420166077029
Ar	25.382324370903	17.881442223948	6.819797817126
Ar	7.809054203016	22.704250952419	28.346516410464
Ar	25.821328425727	20.974940039550	29.110034044613
Ar	20.610481697855	14.874649320779	2.324168488098
Ar	13.030453731909	24.105957821228	6.137051936823
Ar	13.532862293847	27.179108500265	28.771041785168
Ar	17.194940233334	16.370549186977	31.685802039600
Ar	10.088696850972	15.959716206846	30.149959411072
Ar	7.436942311069	19.606559954525	5.801887652438
Ar	32.227011695263	14.106499306057	21.866974630399

Ar	29.965536875350	20.864393261751	11.579797527963
Ar	8.814474578887	28.406527911988	17.203797602975
Ar	31.857145284962	9.616016085036	16.373680921765
Ar	22.575004679642	29.135515115375	20.423151724821
Ar	20.696680137259	28.932274746389	13.545533126767
Ar	34.048773832711	16.370097570778	15.356541930860
Ar	26.340332730076	25.095105811755	15.988502380696
Ar	31.207645188581	20.968710045376	24.075681185211
Ar	19.695692245090	21.708435557180	4.379125710767
Ar	13.705224153502	28.555193670553	11.857074346865
Ar	33.036753657314	23.309827883615	17.601025391381
Ar	29.259217352005	27.497473167738	22.097292143368
Ar	18.719232433799	28.463174850855	6.670867711271
Ar	10.852348029262	31.169199453245	23.510426743057
Ar	23.624118586937	14.103040413946	29.981987231328
Ar	30.794329349060	15.564309379017	29.041225538497
Ar	17.851616252844	31.508903239558	25.152245895254
Ar	12.754806595476	21.814101684779	33.789924804953
Li	18.365314762167	15.726383217316	22.416037140809
	85		
	Energy= -0.27530099411699999	Symmetry: Cs	
Ar	29.312979736361	20.915613141574	13.632065194786
Ar	15.908489210947	27.631405763582	18.633453368632
Ar	25.265278054442	15.589270228844	15.499847770157
Ar	26.517463028337	27.155081065692	14.439406655282
Ar	28.249130585797	23.748361652667	20.060476722689
Ar	21.121880324047	26.154849239809	3.780640197324

Ar	31.535188123470	14.126425718799	13.078513561785
Ar	26.399372013944	16.546153095385	8.728382748455
Ar	30.698399857714	17.072187642829	19.542105865262
Ar	33.117041694939	26.735783484751	15.807573571912
Ar	30.396921511010	26.401399176958	8.963700330866
Ar	20.160398488589	17.916185652696	11.353788479698
Ar	24.314165788493	18.424983355738	21.801991744384
Ar	24.140659238468	31.247296387881	25.346506865906
Ar	19.959048554879	27.246264279202	13.510600237138
Ar	6.920983077030	20.314988897019	22.562086939942
Ar	22.851233763495	22.021222450999	16.146506251053
Ar	25.892551049279	9.912633845659	11.614642246002
Ar	28.573023817292	10.240294278394	18.356527531810
Ar	28.539109806107	30.822602355859	19.829073091237
Ar	24.174114579430	30.287387895804	8.846357460689
Ar	29.956680083915	32.685196650464	12.802397515886
Ar	21.133005411700	19.050508253810	4.583865617047
Ar	29.622523220843	20.090302445831	25.938976657293
Ar	18.748664215415	22.384352549508	21.279376954938
Ar	16.337071711935	22.089226894986	15.213044955760
Ar	17.156927846444	23.328113694465	8.616484924497
Ar	23.823547308098	24.144317119067	25.386957971359
Ar	19.643153887142	11.500005564653	14.106715521274
Ar	22.265529846358	11.821066889046	20.702695250801
Ar	23.226920580618	33.020826953131	15.461716649142
Ar	20.633306999265	12.396075284263	7.283063689740
Ar	27.631910608315	13.252733986787	24.885720557873

Ar	29.927073288853	27.233613551927	25.932280493078
Ar	24.039790839706	23.232741120663	9.471694243486
Ar	22.378521698196	27.542493544234	19.597096082361
Ar	14.015885997699	15.714746187850	13.851380860354
Ar	18.205556012837	16.227371467972	24.389540493084
Ar	14.859843008291	16.783962644630	7.025197793839
Ar	23.461445900085	17.836436673669	28.660451229678
Ar	21.045940112002	27.613049001298	30.955994903157
Ar	17.179583956461	30.394925321345	7.832697059473
Ar	22.803349942108	6.047559391747	16.942649212887
Ar	18.272767882312	27.927591289026	24.792194326341
Ar	13.399331164624	27.331375074736	12.532466276697
Ar	13.175680111507	18.528596430126	20.162707999632
Ar	15.257657073031	11.912888769976	19.657172125596
Ar	18.898427261026	33.441754871647	20.926437708604
Ar	16.319422607406	33.126281161074	14.438669717401
Ar	20.104804063935	5.857334318698	10.247353127654
Ar	25.434348599523	6.509566613678	23.651784254354
Ar	26.804283341119	23.497881122804	31.505652872762
Ar	15.155088948950	22.071498269829	2.201244608375
Ar	11.009006033156	21.158751990503	11.082048716490
Ar	17.733546546561	21.981432018499	27.997056006376
Ar	21.321292781504	10.976438909713	27.541019510012
Ar	14.298214802683	10.116984488350	9.876958531708
Ar	12.712155536272	24.259387384084	23.751828679997
Ar	10.188254994869	23.950836922856	17.402829159462
Ar	15.612268936507	6.163600011533	15.857819812951

Ar	11.205458437568	26.409228164872	6.198549908305
Ar	18.310930121759	6.493800665221	22.644947765324
Ar	20.517965874366	21.269334023101	34.189510074654
Ar	8.621957945597	14.620231756723	9.675846575197
Ar	17.178339777924	15.666735976250	31.198019209134
Ar	7.653203412137	17.439345237663	16.128623508825
Ar	11.958055851787	17.965734750008	26.956717879573
Ar	12.501787774460	31.297479838949	23.605985271396
Ar	9.900528639585	30.979324045662	17.062122034099
Ar	14.148200831491	11.076211487004	26.465627570061
Ar	9.812823216494	10.545878685989	15.561583897328
Ar	8.815542471339	19.838657565530	4.753585318459
Ar	17.787267475794	33.683243576079	28.181824989710
Ar	10.533202131434	32.796152470420	9.929328853454
Ar	8.930562641961	13.484770738828	22.095944075399
Ar	6.674375669157	26.811879702443	11.921406662345
Ar	13.814669782232	27.684845979265	29.885049379941
Ar	19.195864079374	16.912875903465	17.848143770796
Ar	11.204387235541	6.709511335255	21.522000248888
Ar	6.665022045987	27.351849424552	22.321995072140
Ar	3.417981183442	23.162776724050	17.0833310309604
Ar	8.031130715903	23.725637067646	28.687928715459
Ar	4.256826435059	20.255433963805	10.539146574180
Ar	13.223093125967	21.352217243521	33.092156188336
Li	19.364028874803	24.782307153375	17.398380975373

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Energy= -0.27816385715500003 Symmetry: Cs

S116

Ar	25.983278921692	14.680748637896	26.695310042041
Ar	21.326909534184	18.962697269084	23.919822104328
Ar	21.427210582774	20.509045431915	17.207572880721
Ar	30.906518737677	12.050746251064	22.500608088528
Ar	34.415099140150	25.192704339353	18.397322044932
Ar	32.741002105724	18.613911103683	20.500973110253
Ar	29.483468107590	27.792262765279	22.616614947859
Ar	31.120189071651	13.741036317224	15.675907630306
Ar	25.900737060234	9.699445185594	18.084476757862
Ar	23.374315693899	20.164320708171	30.363252141269
Ar	27.830396898446	21.209437892494	24.749322375374
Ar	26.127845756190	16.390789883179	19.819937648396
Ar	25.66715554349	7.931686111327	24.933926829721
Ar	14.976869561547	15.107267835716	13.3393688875069
Ar	21.021337647486	12.375508090142	22.191437365782
Ar	10.052237420107	7.113752007021	16.7450038834048
Ar	32.811010159163	20.280363135492	13.630675720863
Ar	26.236158744378	18.013390121931	13.138785176589
Ar	20.742783838450	5.581244141009	20.495445370502
Ar	19.232058726735	14.447743620842	28.742431945113
Ar	23.923070772653	24.428603486838	12.277170447799
Ar	27.843523126896	22.855228880660	17.830907529160
Ar	16.866423879917	23.067130373077	21.265729323141
Ar	21.011023350806	7.382390576523	13.694855422784
Ar	25.271427253363	26.821027421867	28.290623274340
Ar	18.661185094401	24.536077325899	27.617207324364
Ar	30.468230444130	26.889789790677	12.736215926930

Ar	17.248875438982	29.638616181592	22.818018275979
Ar	21.147959183401	14.219473182715	15.502886147376
Ar	14.662214417225	18.822243286957	25.833280165057
Ar	26.107588080160	11.390326999561	11.328110915228
Ar	18.860097367973	7.699553252459	26.946686072745
Ar	23.018824641700	25.394384375862	21.952664301123
Ar	14.315202171730	12.216851478799	24.112718296232
Ar	23.819731678701	32.073233299039	23.361826109912
Ar	19.139490707166	26.955246659278	16.422928828210
Ar	16.237007183220	10.150272419878	17.782287468310
Ar	31.317685574469	15.371279461582	8.833986425816
Ar	15.862711314701	3.218088769980	16.010925802406
Ar	15.303521474401	21.389609127535	15.058842282436
Ar	25.550877735534	29.527138434255	16.951430965167
Ar	10.874142362266	20.455628536449	20.261028230395
Ar	14.468619879104	8.324256664039	11.400971438321
Ar	16.592417972689	16.707103668103	19.452607991871
Ar	28.875259780412	21.915282195355	8.004679973086
Ar	24.730855162402	16.393945900790	6.635475706784
Ar	16.444361585001	19.879836893754	32.389274569473
Ar	11.982384258935	25.495765853297	25.264428401417
Ar	26.410517538166	28.439198843814	7.116500577995
Ar	12.427106956346	26.910582897728	18.214668440513
Ar	17.455139985556	25.361005499411	10.013698009992
Ar	12.357952440223	14.323266686987	30.569744913456
Ar	13.946054092741	5.445743159728	22.390442875494
Ar	9.148196310544	18.828924279350	13.871110187806

Ar	19.849782317369	18.939026127270	11.076612470538
Ar	13.567896343396	19.839971950310	8.697226949871
Ar	12.613100348392	33.677646290900	19.393268030422
Ar	9.574977351625	20.869800175681	29.976871483223
Ar	19.586599895473	12.461851895417	9.164151663054
Ar	10.508556945794	13.879971733643	18.506054849918
Ar	19.663318990240	33.693294507098	17.674752325369
Ar	12.001298310467	7.568198676541	28.803950787215
Ar	10.695924035242	25.322260714938	11.796662903391
Ar	8.356374238166	16.005195098637	24.935852123987
Ar	8.037516105877	9.251426933308	23.150958920616
Ar	14.686772138108	31.095292941400	13.130663815928
Ar	22.284529657790	22.855015706347	5.743953048771
Ar	18.272169709409	17.327490367959	4.371166505827
Ar	21.511657328812	31.022609946181	11.364821159539
Ar	5.682305168310	22.698524166224	24.167245736711
Ar	15.722762011721	23.819572969946	3.403768881644
Ar	6.059578820035	24.311188557757	17.137140760324
Ar	4.610122196028	17.731435072755	19.212948201077
Ar	13.106190997522	13.265180713929	6.769975834448
Ar	8.697929881977	12.171425724862	12.052631609734
Ar	7.204880993337	29.423873309294	21.905934716538
Ar	7.279406816793	17.180521397425	7.324163227740
Ar	19.772950009931	29.4009666825758	4.800546605323
Ar	2.833729528964	16.081253175977	12.665742021837
Ar	12.895579796680	29.438928127252	6.578861481366
Ar	7.771195182652	30.864912486994	14.885658785852

Ar	11.727909079197	18.213353251359	1.980068428321
Ar	4.324660207152	22.699371655182	10.559165078124
Ar	4.230613419664	10.997814237348	17.414563447700
Ar	8.891109291889	23.759344307740	5.262800404830
Li	18.216939518737	17.810712041085	15.272323211795

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Energy= -0.2807668312059999 Symmetry: Cs

Ar	16.800120520661	11.240336803814	34.617062687145
Ar	16.718284452838	17.451636125164	31.595390673174
Ar	14.238442506941	14.590342681569	25.668150456059
Ar	24.073253640938	11.257562116068	34.187599016598
Ar	19.930361609861	18.031737511848	25.831809217037
Ar	14.210836941327	8.312045116326	28.478668605999
Ar	20.139040890059	23.343569973251	29.799321388779
Ar	10.751881904895	13.886799837040	31.555860531166
Ar	20.271548759966	5.786482612410	31.4645696937508
Ar	27.772331976562	16.886869631101	36.723075163351
Ar	8.293705474042	11.078782457903	25.347094947875
Ar	25.379228318707	31.025355486673	16.619337954312
Ar	9.675542190564	25.501144685480	14.713214777934
Ar	19.732080326796	23.824611525545	22.861151422052
Ar	10.447229280248	15.327389477130	20.071472130452
Ar	25.553365643008	14.616964642782	24.982887434014
Ar	14.340303268030	27.122961780422	30.487504175846
Ar	22.652321930744	24.50037889314	17.082237119429
Ar	19.518353118347	29.828669402858	19.843526970189
Ar	22.872538617171	18.762915629743	20.067318454055

Ar	22.757758585345	13.618261011071	15.688321642126
Ar	25.536096094665	21.539909032022	25.777457069221
Ar	14.320327774500	21.508752244821	26.458201951861
Ar	25.945568463234	27.154082208181	29.796054631185
Ar	7.297616479430	9.488074106143	18.425501142223
Ar	25.923004038848	8.337336370266	27.784201469669
Ar	13.814634213309	9.193814529988	21.291330979566
Ar	29.704325562158	13.929584801190	30.433099840450
Ar	3.777135376395	15.162009887146	21.558566054852
Ar	10.824097190918	21.054316078548	32.365641913180
Ar	25.451463278562	9.214458749694	20.603069657939
Ar	12.637855114693	19.416299491914	15.126529669201
Ar	20.356758733187	28.931558790061	33.828215469580
Ar	19.842212561040	6.519466542159	24.342899525979
Ar	31.511084002243	18.183609632031	24.845416965767
Ar	22.329139421141	16.352615426150	9.262488277794
Ar	16.328532901350	18.735634264463	20.507991283940
Ar	10.546790239750	22.247063681741	20.884049949246
Ar	16.433351501554	33.901886056492	30.533848224580
Ar	28.609811800581	22.290491224620	19.779445355880
Ar	14.116115636801	27.546388851118	23.376132805568
Ar	16.125067949540	24.536450992003	17.490588946781
Ar	13.406206087859	16.851229951025	37.572013019109
Ar	20.597069537992	16.859885000032	37.279852680353
Ar	20.092396667535	12.013388911973	28.593670042546
Ar	16.863614409610	22.938238976614	35.842774662318
Ar	24.102418991122	22.958025154691	35.415988790298

Ar	23.780763868413	17.469970487919	31.178427436378
Ar	19.683798851570	12.863714574109	21.686324858312
Ar	29.696454215428	21.103508116750	31.245772627733
Ar	25.329078763119	27.578387883826	22.697824359257
Ar	8.467560922737	25.150283378787	27.032695671205
Ar	31.408851065337	11.118075130376	23.996641298642
Ar	12.954539402453	7.709303858293	14.329188903756
Ar	7.661724842856	28.543401521967	20.935025404264
Ar	31.374732172374	25.215149128879	25.682105719887
Ar	8.270560946313	18.130033586315	26.224143515322
Ar	19.935084836253	29.406988990643	26.711343486432
Ar	35.456846426015	15.186255486934	19.761714920873
Ar	10.366182159463	31.958351223994	27.037279815432
Ar	29.445601597567	32.015755139822	25.912517436057
Ar	25.942574583394	19.474399806183	14.128694546389
Ar	35.412577119376	22.398100710711	20.604465408972
Ar	28.704647498631	25.665371964841	13.661250618113
Ar	9.435278601292	13.774564418750	13.157998190940
Ar	15.912683094854	13.5989987392043	16.110024527873
Ar	8.993877435718	20.225487636031	9.566175700321
Ar	28.819104388168	13.665534933950	12.072100508510
Ar	19.254780282722	19.492236179037	14.706162706706
Ar	15.404655925936	23.614156790344	10.631934636082
Ar	28.643660104568	15.370842922716	18.964400382983
Ar	31.588232167126	9.475707796274	17.052631193385
Ar	19.405533435392	7.521136822366	17.301586997244
Ar	23.831238260494	33.923986285277	30.103028874167

Ar	19.077535132548	29.006569868131	13.146296522319
Ar	13.285790260321	30.927882181168	17.307619182240
Ar	5.953246697888	19.386240069173	16.256447724436
Ar	32.714429509295	19.414236318889	14.798821491859
Ar	15.326540918178	16.393570839722	9.685168561774
Ar	31.444693599903	28.636114673545	19.562393646312
Ar	3.889161061225	22.319745135471	22.394763842378
Ar	22.383724236752	23.677388436944	10.204899895031
Ar	18.987267183828	10.290213021827	10.859148797663
Ar	15.984225705739	34.352260008628	23.489671559599
Ar	25.441059885338	7.661488201078	13.626944772728
Ar	23.432179881639	34.375346256371	23.055959118426
Li	19.485956061646	21.625354288739	18.821864654007
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	Energy= -0.28361666348300002	Symmetry: Cs	
Ar	27.221885542216	26.342617581300	17.175212721096
Ar	21.986140085643	23.510351466244	13.669307870946
Ar	20.670926944673	27.891917944086	18.921573410737
Ar	28.433753800102	21.858584057026	11.804128481926
Ar	30.767789405888	25.740769669951	23.292622744769
Ar	25.761836258532	30.775770413779	22.554223118310
Ar	24.182062314192	23.830505548333	23.114788816095
Ar	25.479361041678	19.461031510159	17.850305184286
Ar	32.111862517710	21.168039699517	17.802635323653
Ar	24.289978922731	32.830963728406	15.777563643551
Ar	25.666962667558	28.270681673232	10.342310729089
Ar	19.143261548049	21.123168556147	19.478128487437

Ar	19.156033773919	29.739139438957	12.280914029569
Ar	29.204723405761	18.861044312351	23.814290296026
Ar	23.159773238866	17.089476175014	11.843018162574
Ar	19.738265808163	28.737715065073	25.760947526904
Ar	15.791876256965	25.028821608375	15.467746084186
Ar	23.284113025907	22.280700621010	6.971767951245
Ar	25.996281269074	27.268278147117	28.766793867247
Ar	19.621791193475	34.324927463846	21.133547892500
Ar	29.481454194891	15.259336343681	13.989960873760
Ar	22.630843257668	17.128636292865	23.632193632590
Ar	22.635746188115	34.636504092328	8.987236222131
Ar	16.914334364390	18.892053744205	13.725871881553
Ar	14.756351335599	25.824267164110	21.964205221501
Ar	20.253031015594	14.950683869701	17.740765578036
Ar	16.837515809426	23.958347622251	8.989621258339
Ar	18.256148385685	21.772816753007	26.137777925007
Ar	14.597666825313	31.198014808671	17.510915364568
Ar	26.535061670832	12.882455090201	20.006644296022
Ar	20.329409362787	28.746515068836	5.503686358726
Ar	24.400265221356	20.399031146131	29.3265966674785
Ar	18.033307470407	36.250272854102	14.291014531367
Ar	-0.332384644024	21.139457585069	18.972082248224
Ar	27.847398192033	16.747748955059	6.896185665425
Ar	12.709881726271	20.237668546014	18.550024756416
Ar	16.053802586010	16.294653497142	22.558718419430
Ar	18.019343611871	17.513234574353	7.154448159961
Ar	12.212536591666	28.735921298314	11.313977262227

Ar	13.497050609401	32.165694414199	24.304944270555
Ar	19.810948522898	25.105456080823	31.915672508673
Ar	24.118051746217	10.425873583116	13.898504357397
Ar	15.576567689529	33.714300746205	7.911816757980
Ar	18.046461209444	12.681289047695	11.912674975053
Ar	10.961763036442	21.932840813115	12.121392647992
Ar	9.543999577931	26.292589485496	17.357745390388
Ar	13.666181222474	26.584880099825	28.747380294089
Ar	17.947074345242	22.692893169965	2.290562524753
Ar	13.371586171964	37.601573330880	19.616262469921
Ar	20.199473481125	10.816424107193	23.273624380027
Ar	18.743991125506	15.375606185202	28.945782419790
Ar	13.833007686314	14.032541258396	16.827699310420
Ar	22.560312454502	11.985241484212	6.908354943171
Ar	22.538703734220	17.186893493108	2.040431508668
Ar	11.527978456866	20.812191733046	25.188702132843
Ar	13.216324483465	27.718973385038	4.514249963359
Ar	10.885354252854	35.216094793721	13.294372972533
Ar	12.137727300086	15.513349300271	10.296984077534
Ar	11.883153079236	20.639493709498	5.379762545826
Ar	8.301848411631	27.075692431323	24.161481002302
Ar	17.889237494408	8.424873052791	17.157150551522
Ar	8.108782820707	32.657909941830	19.524755371941
Ar	14.175790840307	20.158087821015	31.551714379088
Ar	9.542176176218	15.402999452289	21.669975338937
Ar	7.735938623751	16.922129963927	15.347444255553
Ar	6.302085305146	21.263284499513	20.598174532402

Ar	8.520372201450	32.595349061583	7.019138029084
Ar	7.124085310977	25.595402210145	7.755024715633
Ar	15.295874713308	16.137627571845	1.041721286556
Ar	5.666684815842	30.135608290511	13.176535039777
Ar	15.394868240187	10.951642600928	5.924218015977
Ar	13.363910159879	9.873284689520	22.349191092936
Ar	11.880512638896	14.342897977165	27.939287312847
Ar	19.167124118396	6.294110745463	10.256462469132
Ar	4.383639369429	23.039720185685	13.984515980295
Ar	12.494979731887	8.782639393772	12.332010208049
Ar	7.556540868520	23.241053962051	30.177563082162
Ar	5.947821279559	18.613110068572	8.677225462514
Ar	3.046168463769	27.461962735075	19.387191677598
Ar	9.207776645836	14.062138859299	4.308773378252
Ar	7.946764305593	10.238393512449	17.550208220143
Ar	5.392031971803	17.479788441911	26.606167763992
Ar	6.233051715083	11.901115771327	10.798104574485
Ar	2.146879899524	23.713194585371	25.437271930818
Ar	2.944261483090	14.9366388763074	20.209498060035
Ar	6.474941741311	10.356522748643	24.819619170412
Ar	1.163923897155	16.636160705038	13.538273841969
Li	16.471568195355	17.618934564298	18.127056027676

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Energy= -0.28652096411599998 Symmetry: Cs

Ar	23.434623768275	25.442210227086	31.783095476473
Ar	22.731300414342	21.716346001503	25.837012367703
Ar	17.898270737093	21.543281296494	30.604874516722

Ar	18.358441905930	25.289299305385	36.652489994394
Ar	28.484229823110	25.665078025396	27.028094389822
Ar	26.401144371588	13.952082587763	34.521955256993
Ar	17.217575574565	28.375152963665	30.439913867771
Ar	22.349410821892	19.602503540982	35.596493894286
Ar	22.249149653171	28.456336341377	25.624764739302
Ar	21.816196391502	15.966111748971	29.650204857378
Ar	16.414706981085	20.981030352284	19.101429603994
Ar	12.192311004985	24.396574423511	33.395097354075
Ar	15.361501641912	18.900222214640	36.553470053789
Ar	21.675189094322	24.690721352401	20.039345705946
Ar	27.765788628045	21.965146193448	21.289332030423
Ar	27.443438305884	19.844712446977	30.733963203525
Ar	24.500274626202	28.133699102889	14.576097145691
Ar	32.599724219384	20.076731885148	25.920988015801
Ar	27.368534810327	28.808096002092	20.901828383089
Ar	16.110246472219	31.493733719342	24.360564380390
Ar	9.096534547986	18.040313666071	33.346895174379
Ar	11.824692500546	20.683023072646	27.482438138553
Ar	19.419432644794	13.167965636547	35.586342093910
Ar	16.243641542263	7.563347392775	7.831277736497
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Ar	17.468911538194	18.012250967379	24.888313709162
Ar	31.553415113824	14.187290447307	29.662337954507
Ar	21.208961195175	31.710908747411	19.563620226152
Ar	25.876929445657	10.224228665460	28.632700514295
Ar	21.335404452526	12.376012596688	23.920814712789

Ar	16.875229148640	24.483813641619	24.565430921754
Ar	15.724754138644	27.664619690751	18.672503574815
Ar	14.915234998872	15.245037759423	30.651246426026
Ar	11.902700039004	8.849206799528	30.617814151198
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Ar	28.287132046385	15.824296252083	18.044029060440
Ar	22.258626348042	18.220027378187	20.371265601792
Ar	14.482572256852	11.671416147102	24.868688656501
Ar	6.027567403058	23.566244871838	30.103266985088
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Ar	26.858358863110	16.183600892943	24.897437617842
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Ar	10.715353628249	23.806998459262	21.393213066504
Ar	15.002556514859	34.742512354352	18.225845531689
Ar	27.349265424727	9.770586220325	21.741533230381
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Ar	18.906102487501	24.161144761902	13.675475023531
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Ar	19.542230632633	17.424848175248	14.078922903745
Ar	5.570709903331	19.807265830984	24.225341815355
Ar	4.894072703416	26.758086992992	23.881139605285
Ar	18.265990323438	31.104235593281	13.176640123356
Ar	22.278764923469	5.555812464359	24.605861220931

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Ar	17.752171154579	7.912216425864	19.914182427007
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Ar	12.672281806412	16.768353657464	14.932851666047
Ar	11.390420664403	17.071117459218	21.761690445655
Ar	11.265716867116	30.437193288213	14.064841866423
Ar	15.164941837196	4.835474255266	25.570279436821
Ar	33.046428744087	13.765055515260	22.735632773863
Ar	11.502323761622	10.862520388943	18.556744208925
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Ar	25.484984439440	15.019854700407	11.509101511965
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Ar	14.561174806102	26.851669677300	8.912649750925
Ar	22.530366536529	8.452673298187	11.207936761602
Ar	19.261313668613	14.051494898862	8.044229254470
Ar	18.540034299437	1.098075832400	20.435556866972
Ar	12.120387154802	3.989941377231	19.047366694606
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Ar	6.894221730672	13.132995063770	13.891635354237

Ar	17.394727107389	4.219286396710	14.075640451199
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Ar	5.806196338538	7.109519244727	17.669370567200
Ar	10.9600051170803	7.257260408335	12.677732203705
Li	19.562409849287	21.332923205113	22.459532242034
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Ar	19.422895362695	20.670632733248	18.320085434331
Ar	16.180786519655	19.010533133675	9.480253503428
Ar	12.042745363003	12.709549640735	20.217227982102
Ar	23.830767142580	24.054139892144	5.744356364909
Ar	24.759016655618	16.182422405377	19.067222362023
Ar	14.220307228901	17.528652939863	15.781522779718
Ar	28.246447580688	24.478012326975	11.292790622406
Ar	22.877717165069	29.029863209038	10.627401392502
Ar	17.297002339477	25.663576710938	7.952042067284
Ar	25.958276888405	22.739136469234	17.670732156830
Ar	15.250927306394	23.810006090331	14.439481913900
Ar	20.613530602069	27.150748711055	16.939502607672
Ar	1.101498348628	15.805302808405	23.566787645672
Ar	20.521443497565	15.786612289676	13.568377308055
Ar	31.330120836309	18.204826071777	18.425925328855
Ar	9.882500504645	20.669608915687	11.703095273022
Ar	27.179492898111	29.437441019857	16.243979293067
Ar	16.344056124244	30.583464266698	12.796673623474
Ar	18.404181956493	14.373526130382	19.657043281668

Ar	14.439127189168	18.862022586839	22.228113687508
Ar	20.893763340998	18.054837471024	24.535711767538
Ar	21.865129470807	34.016339881286	15.476539382909
Ar	15.470052498595	25.146566954699	20.901088726498
Ar	18.235247391680	20.675114554185	3.013622938176
Ar	11.437313759427	13.969582588508	10.585098209661
Ar	22.698493852072	17.314220313059	7.215842173141
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Ar	29.137645739822	11.700100761376	16.163589934946
Ar	28.632175012019	26.832179664471	22.674774975728
Ar	10.875621542926	27.280894612662	10.128417112837
Ar	16.576286831286	32.001496756977	19.650215493094
Ar	17.134883499087	7.992837578415	21.019693528353
Ar	15.824853680699	10.787237838658	14.708190855597
Ar	29.377505645788	13.158764968043	23.217140919112
Ar	7.662252618447	15.918826425238	16.160244560650
Ar	16.785038735191	22.693059742910	27.284273967918
Ar	10.255391606888	21.997029121868	18.356621005176
Ar	27.490232948906	20.054616801548	24.125908303663
Ar	22.030248262457	24.596688098908	23.170960096028
Ar	23.257171347623	31.347075996519	21.828297923402
Ar	11.150559032246	28.554962438720	16.969762444901
Ar	27.103099117868	17.696182178500	12.722419702220
Ar	13.443730081518	15.538004487544	4.068932775848
Ar	24.758072648412	11.293870892263	10.445433053148
Ar	17.966257797818	12.178242288019	8.264216878861
Ar	6.955881541936	17.223088233928	6.375481157081

Ar	22.697587719328	11.351878174317	23.733514042115
Ar	16.200961608365	13.076673839288	25.778246124283
Ar	10.333752241820	23.420003038491	25.000313978457
Ar	23.458605882842	21.945295004147	29.606823424966
Ar	19.884652224264	6.112550406904	11.648863627697
Ar	17.907946608919	29.391600449881	25.974880267495
Ar	3.088710232751	19.165216522644	11.987139701872
Ar	22.463183798476	9.926441264759	16.841171359148
Ar	13.831624879881	11.854371081211	32.147949623628
Ar	7.892486480653	17.322508584992	22.945433146276
Ar	12.048227125033	17.6910666378883	28.578363291175
Ar	25.384865390303	15.110410949511	28.899916722290
Ar	18.738110711717	16.878352528252	30.989335373072
Ar	24.592234688067	28.701417099302	28.210316245798
Ar	11.337781336644	30.100115343380	23.758044358104
Ar	19.232766039756	26.756000241682	32.413354659779
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Ar	4.644006369230	12.343875861923	10.969021481291
Ar	5.576962603910	25.357755532850	14.283282482798
Ar	26.996185574226	6.699700477576	20.951792707321
Ar	9.149997531103	8.978740575386	15.177841320804
Ar	5.806943411479	26.759279839104	21.059226933228
Ar	21.268067819877	3.240924783917	18.157176953890
Ar	14.431580485308	4.133554472435	15.925340306867
Ar	0.866479160099	14.370847438681	16.633415310839
Ar	3.363102288984	20.606695592981	18.877838859249

Ar	14.452599597095	21.686081351255	33.793907438461
Ar	21.509468997183	4.708613758786	25.254379938837
Ar	27.142692995090	8.235791995249	27.959655560230
Ar	10.490902536264	6.116035218292	21.633620130124
Ar	5.388121947512	11.031715459788	20.790320651956
Ar	20.514076178049	9.942100226929	30.167600373739
Ar	5.288791072644	24.004729218134	7.388776734843
Ar	26.665201399475	5.331427034525	13.915440577212
Ar	9.534737133481	11.320477256974	26.499062917834
Ar	3.556481866217	22.018108738511	25.777733027607
Ar	7.806413696004	22.406261046149	31.435401436638
Ar	5.985922117026	28.253155604089	27.928547824434
Ar	14.821178010387	6.504623681023	27.390330384049
Ar	5.266340781583	16.138249415686	29.311997676935
Ar	15.808065485322	1.391292879319	22.429861411874
Li	14.851791446224	21.318918880690	18.341040820748
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Ar	13.998841347504	11.146924441474	10.644127340076
Ar	16.408387324217	14.288781994854	16.134311064468
Ar	15.110723502828	7.576382789032	16.543315009294
Ar	14.876403100187	20.179717555414	13.650383358176
Ar	11.563916320142	8.002635579474	4.903964273057
Ar	27.430133158223	11.862010553627	19.254866086763
Ar	22.993711172404	11.830876665526	6.691207346019
Ar	9.931882492191	15.383135834069	14.038004507236
Ar	22.739472013803	15.728982424771	15.682238865035

Ar	21.379529396015	18.028388877653	4.079795350716
Ar	18.819792717241	16.160773246189	10.386892813499
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Ar	18.781967142051	19.751032109283	18.926267606009
Ar	6.102941143796	20.556065364840	28.852682758375
Ar	20.683119816853	10.404449362871	19.666057974228
Ar	11.028016683632	11.845584639804	19.914918603137
Ar	25.394739880074	17.605395934544	9.753557574435
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Ar	13.953798315542	24.695500562153	18.784655540258
Ar	12.431921033548	18.314258806732	19.408619450334
Ar	27.151808509446	11.373115671993	12.307992862451
Ar	24.919923115810	5.990069905972	16.283173390308
Ar	16.577685111530	14.639707524268	23.011038154470
Ar	17.269632165861	22.187544081241	7.679230385678
Ar	19.282563058901	3.159649526486	13.092438079963
Ar	21.735039594705	22.797199793689	24.344942842316
Ar	29.643157276771	17.120689439100	15.250147554385
Ar	20.435604822588	10.028780451050	12.802936393247
Ar	12.381805984579	17.354343050672	8.028673194635
Ar	18.124206955905	6.742538790887	7.111651551531
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Ar	8.411197798987	8.636383258895	14.354930142702
Ar	21.200123994191	21.645414484861	13.188631752542
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Ar	14.837234055162	19.358301048532	1.795956111227
Ar	29.989209620632	17.689076817521	22.274036975128

Ar	15.299684881363	7.867700417822	23.658198233922
Ar	23.174510239389	16.161464861708	22.611612894589
Ar	10.837128425671	23.975037725225	9.632289391920
Ar	9.632999336837	5.112117840105	20.394335255148
Ar	8.382536506683	21.964152074473	15.652222018948
Ar	23.904729611953	23.845515554979	7.051880285103
Ar	25.326213251196	21.303737445978	18.572852825190
Ar	3.243251585085	13.644748001586	14.081586845866
Ar	16.436400193806	26.707722050341	12.799309333716
Ar	5.990745106438	16.720678373560	19.660346326392
Ar	8.282510695242	21.100785602131	3.780038385302
Ar	10.035937694476	29.342164480321	22.062301416646
Ar	25.190311275619	6.488491312529	23.292383926208
Ar	27.318299742792	27.946527838096	17.951102004832
Ar	4.380660735593	9.990775051299	20.186129354087
Ar	20.932844188245	10.824344754612	26.742031055083
Ar	19.812804573376	24.310832103346	1.355215779670
Ar	28.010240303030	23.394878919287	12.605838774883
Ar	10.178473616988	16.261523300174	25.307194619566
Ar	15.115504918625	21.228465819611	24.714040658094
Ar	13.318856615312	26.061220641751	3.441322988485
Ar	13.862161677725	0.733835944446	16.907124512662
Ar	8.669301667332	9.518765863885	25.974961766508
Ar	23.131835396012	28.365483019941	12.301628839751
Ar	18.053768862773	24.270779432303	30.178463992504
Ar	18.964262673448	28.863886292034	6.645767644458
Ar	9.906088205718	14.356744030689	2.230754285947

Ar	8.479745921237	22.626303738129	22.695298537452
Ar	19.544609521793	3.525250806552	20.152288228342
Ar	14.432264089723	12.396310609280	29.190194017068
Ar	19.481647150866	17.484403661284	28.590591780594
Ar	1.637552153996	20.455025809639	15.758572543970
Ar	27.734820919402	12.378185699731	26.308510742636
Ar	9.871737966570	28.693436555355	14.877414429109
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Ar	12.462531475671	30.727471173006	8.687857635651
Ar	5.698058218495	19.036755843903	9.965623272334
Ar	32.255211088319	22.947045093963	18.193050036258
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Ar	20.545199637738	26.253113555982	18.361643202162
Ar	3.484426908343	14.550593912135	25.735225599689
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Ar	26.301090995978	19.094053334535	28.135089073719
Ar	16.765155853130	27.942701559075	24.194261856036
Ar	15.594323950812	31.345707410567	18.099600442926
Ar	4.224303905910	26.473238360229	18.792596333271
Ar	28.491899253920	24.403258769282	23.978224822317
Ar	12.916278173432	19.224764936976	30.952826168735
Ar	1.752447136258	21.031050858502	22.986920431819
Ar	18.178176946844	33.418286803423	11.946608770422
Ar	11.260998252459	25.704859364556	28.258538981672
Ar	7.861217125415	14.114373177678	31.425365106332
Ar	23.590554477372	29.517804834847	23.741509779755
Ar	22.380609478727	32.953733530652	17.638786092572

Li 18.792869312741

17.959505335376

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Ar	24.973340871500	6.995316936129
Ar	31.196603209683	10.232516412275
Ar	21.111969009117	5.676712616113
Ar	25.300859928620	13.725684395653
Ar	23.482641100782	7.539917020030
Ar	19.177534974706	10.640524042450
Ar	31.603061556116	16.939542207810
Ar	23.917134630304	14.284501202030
Ar	26.704464755850	11.968950239110
Ar	16.608487692848	8.371330791638
Ar	2.838744198068	27.600801058567
Ar	25.693610935378	20.239746195997
Ar	19.572642622391	17.131962926189
Ar	21.932804024344	18.953963106749
Ar	18.755104094479	3.765067778294
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Ar	20.809831346215	15.521575446142
Ar	32.973571538150	15.222151777211
Ar	31.195663945574	21.914586027312
Ar	20.531090856232	8.771465994260
Ar	27.286028744529	20.599047206825

Ar	14.799588584577	13.282738471044	22.733207693019
Ar	17.047484803675	15.102763560247	29.291983727047
Ar	14.299019458134	6.543171831444	20.941221599348
Ar	30.790612837727	23.709510832764	17.428440217290
Ar	14.649991246565	15.256795241961	16.056691383101
Ar	16.303911764872	19.900161953946	11.663155994013
Ar	20.003058726878	23.376764615283	21.690004478025
Ar	25.164433375455	25.143518646225	25.489613617279
Ar	13.996595652904	8.490804467298	14.164202114573
Ar	20.553472411422	20.311578686687	32.867489217578
Ar	15.243585299526	19.801918972807	24.542848783582
Ar	28.508638922854	16.907993452093	7.475807145527
Ar	22.267670176167	13.641627168598	7.053440290282
Ar	9.796778595885	9.331502345386	25.575587238660
Ar	32.135057040448	22.016348868420	10.745671866012
Ar	24.764514692184	26.889406416612	18.697910932882
Ar	15.083081378659	21.494643629502	17.851567162010
Ar	22.584977741527	20.193448318341	9.091280853751
Ar	15.802799336965	13.467654554931	9.638868240129
Ar	18.598504586086	24.863796791298	28.016116880220
Ar	9.524886016958	11.234628171638	18.756106730432
Ar	30.516405001090	26.959841845929	29.414349733389
Ar	10.276321684707	16.045911234425	27.466223472191
Ar	26.137623232491	25.300487570960	12.221838447916
Ar	21.223176112712	21.760175006747	15.494004733914
Ar	30.218074730703	28.814982461322	22.474743405417
Ar	10.071534378778	17.876910594873	20.603166454151

Ar	23.865182450162	26.713521569678	32.101748401257
Ar	13.616096332829	21.175471698844	31.119014577747
Ar	18.037442654142	27.679673763755	17.088612325417
Ar	20.362252359688	29.810196362295	23.3263032227855
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Ar	14.224831960347	26.444318275323	22.763417538561
Ar	29.701352353985	30.4688920861976	15.459797917198
Ar	19.352323756377	26.073036311282	10.634270401267
Ar	27.540135466073	23.677467690261	5.606915472049
Ar	9.914608498052	19.641729290868	13.951343382604
Ar	17.488563223349	18.285706940050	4.900185299887
Ar	25.682689477133	31.807721860283	27.270874135535
Ar	24.021401547691	18.527885493423	2.310636006878
Ar	17.130433107794	26.388452367114	34.564495289386
Ar	9.120907155816	22.805056423254	25.721199661992
Ar	4.959034013710	14.032428478541	23.396367133183
Ar	22.832243525093	31.443489743067	13.843314668996
Ar	12.884222408975	25.791790187995	13.109757632307
Ar	25.297027826692	33.597327162986	20.257948195873
Ar	9.031424680201	24.548244480676	18.805782856445
Ar	11.030006138914	18.004350876977	7.376059233175
Ar	4.689248154189	15.881427190429	16.611517764624
Ar	18.920436320120	31.519185011702	29.874390241121
Ar	12.576637461151	28.063192629172	29.273958783996
Ar	20.695538454317	24.500707093456	3.955911654987
Ar	24.196231536912	29.731721476470	7.169255268063
Ar	14.134381265565	24.184391437643	6.501462839382

Ar	3.806271167756	20.811572693935	21.598261759755
Ar	18.319207799321	34.427873665668	18.578876193237
Ar	12.018617764782	30.969569611888	17.997083601841
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Ar	15.979079453397	32.122506949239	12.251974382689
Ar	4.44454344063	17.671658375507	9.813929085564
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Ar	8.180116764134	29.577081374949	23.804058109362
Ar	7.550514267637	23.926296537091	8.994232368434
Ar	3.668639625610	22.627464476950	14.759932798803
Ar	17.304171327705	30.449722938118	5.593768215615
Ar	6.703095285771	28.958723389887	13.8885240516827
Ar	10.689484987542	30.160663450110	8.124561277242
Li	17.944860944740	18.521273719206	15.784679144198
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Ar	27.514952294439	20.546851939916	22.681802407704
Ar	31.199798555831	27.837442806713	17.179627334981
Ar	30.868392616470	22.918711543154	28.325001002457
Ar	36.830211490917	23.930858488001	15.619378294524
Ar	28.2512771127581	27.377498073890	23.481060047776
Ar	33.108238067965	17.050646697347	24.994423659826
Ar	35.996821425827	17.583931371817	18.55614194422
Ar	29.643094602864	14.787690857406	19.343082191553
Ar	24.864006234118	24.808500153183	17.856115271012

Ar	31.733676384610	24.847274235905	10.867790200066
Ar	34.732320450462	18.508069317992	11.660678609422
Ar	24.221638462576	18.368470409425	17.188603689462
Ar	22.013595632534	24.477131955490	24.199892347460
Ar	25.705956469518	31.762941876559	18.695278217210
Ar	24.554809313223	20.023242841372	29.120027940028
Ar	25.237876705597	26.939871713267	29.878489338056
Ar	26.774837332528	14.156754156845	25.842063847900
Ar	25.366933582363	21.989626416895	11.906034611475
Ar	28.372103857254	15.740395119868	12.537604204581
Ar	18.998982158971	22.100385327110	18.6299819215363
Ar	26.144722007177	28.683174236527	12.464743496160
Ar	33.991071608578	12.103073677325	14.553341189840
Ar	5.962019790023	10.402964926513	19.421506209263
Ar	21.378068041102	17.768249498403	23.450621854260
Ar	22.677983125856	31.383449301826	25.058251823863
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Ar	19.568365676939	28.765959076880	19.402138569786
Ar	23.477490601186	12.032781451126	20.126466831538
Ar	28.865008685502	8.349952612631	22.325360045161
Ar	29.655128650205	19.514916999655	6.885825600251
Ar	20.124708474239	25.735345209336	13.352303917860
Ar	27.658206010941	9.200190554996	15.3777870348639
Ar	26.766951349112	25.818217720159	6.148089907428
Ar	19.499875200845	19.291998120745	12.701854507265
Ar	32.615351359999	13.123169087821	7.653680316836
Ar	17.552925836684	20.747326633378	28.387944972426

Ar	18.210826417212	27.694527631407	29.104668531892
Ar	18.352142596349	15.646710567005	17.982268834453
Ar	20.446647963979	14.204471361459	29.300278523047
Ar	22.230349805789	12.984856415063	13.352477958516
Ar	20.678328502150	32.745959882799	13.917303486785
Ar	20.178402551411	35.828622057276	20.213474353639
Ar	11.195412614072	28.382119749009	28.132361303097
Ar	23.399106749053	16.713519633267	7.811429274739
Ar	22.608731803365	8.257710935120	25.847236359096
Ar	20.602342344569	22.970677357462	7.169801262151
Ar	14.509367699580	18.441649378817	22.602671103384
Ar	17.319739955867	12.072773778887	23.493085046582
Ar	21.205669937507	29.791802018146	7.681748583282
Ar	35.216764183668	11.218167040903	21.506566737474
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Ar	27.527793631536	14.120172505615	2.8164224465425
Ar	24.624147979292	20.485366085574	2.054188206041
Ar	13.933476384997	26.057984784214	16.521109012956
Ar	15.699930517177	32.086293167152	24.155156929382
Ar	23.157367785988	5.175978942450	19.340874627857
Ar	13.334268369726	19.342123581711	15.808255131686
Ar	17.854591303467	9.068752194534	17.150969203831
Ar	14.460999593589	23.099176114515	10.277300740150
Ar	14.464421949997	32.990380983341	17.251714531944
Ar	21.879585131159	6.159235776174	12.315640342256
Ar	15.032722253693	29.962064423448	10.918382017056
Ar	15.368167687554	13.619558342365	12.422363041505

Ar	16.505573796575	17.356849419841	6.858602929489
Ar	21.776651930157	26.874391301547	1.313530135901
Ar	19.319118887277	10.831257057330	7.455668442133
Ar	13.326764902774	14.891161581027	28.410701423017
Ar	12.267829800740	13.061401984490	18.693876328013
Ar	20.525317312173	14.736715214482	1.754723959032
Ar	10.555533110577	21.434525544701	27.381222718356
Ar	16.263869102136	8.386901288153	29.207885713914
Ar	15.537262108051	26.976404253909	4.560009904567
Ar	16.788555396331	5.210597542949	22.793669219954
Ar	9.217294539857	22.377575018081	20.468968776696
Ar	9.894164693915	29.321155667338	21.199989134370
Ar	17.648991505041	21.171430698140	1.118429629718
Ar	14.763844300427	6.818278208978	11.367304461530
Ar	10.101005313350	17.419652679755	9.999847558876
Ar	8.141777291803	23.234547754356	13.526275378830
Ar	17.354252958341	2.261312412064	16.275325080731
Ar	8.773066034282	30.161521238809	14.229524245244
Ar	8.143813995106	15.905014034230	23.487245524855
Ar	11.034002814111	9.323025918960	24.383039245835
Ar	11.324604271524	21.308937211278	4.291378079217
Ar	9.312449214435	27.131427233169	7.840668904602
Ar	11.584885823700	6.228963007359	17.850231968118
Ar	6.917367596533	16.851884031837	16.446901289698
Ar	12.308644613009	11.589590614141	6.596381397104
Ar	9.032412156075	10.914787438936	12.950030219532
Ar	13.503178813320	15.463063024357	0.868119296267

Li 22.171765403159

22.036404492393

94

Energy= -0.30002673687699999 Symmetry: C1

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Ar	19.750142936992	32.197647192537	15.362535776944
Ar	22.772346731886	31.725818856645	21.628744298372
Ar	22.775769057857	27.570849728265	11.129100569371
Ar	29.651970429950	26.522072765080	11.471554418129
Ar	33.496674549240	29.995558425016	16.220031522718
Ar	29.708308198612	30.604142708620	22.115140179953
Ar	22.075125858252	25.943281037034	17.655310017449
Ar	24.987268627066	21.660880362907	13.559418068909
Ar	25.129332845665	25.632257026134	23.903799212095
Ar	11.025984754392	6.203216438663	25.108877657840
Ar	34.754794070973	25.671565677175	21.634504334649
Ar	34.758442186091	23.181822838466	15.014569104641
Ar	24.324905120915	20.257246332513	19.878856886322
Ar	15.416415617651	27.205253357184	17.219483200093
Ar	18.487740187973	22.741281344922	13.129889474151
Ar	18.305931348341	26.771588358624	23.450768631794
Ar	15.944113951254	28.799975193852	10.561428925192
Ar	25.893083554420	23.167012405056	6.726960900288
Ar	15.841674990802	32.910939939990	21.192853257668
Ar	25.871617481399	31.247759452420	27.981067975503
Ar	30.900687299232	19.781587989469	10.203092583033
Ar	30.092501819541	18.334352527102	16.915818641812

Ar	17.847491760698	21.334826740918	19.449074796368
Ar	30.139924460514	20.762598766810	23.476489674224
Ar	18.997038101396	24.312598276363	6.270040036568
Ar	31.013958065079	26.354365851659	27.604789602591
Ar	12.847843961742	33.426182663053	14.849457068702
Ar	18.891926450257	32.418283763459	27.514760389747
Ar	20.748061261249	17.067937986041	15.367724612125
Ar	21.404864836951	18.401129647469	8.799583981197
Ar	20.684512469975	20.844255713985	25.719402559959
Ar	21.311125021375	26.297081853321	29.867218729587
Ar	26.331504389497	14.974001588049	12.164338695518
Ar	36.121563772465	18.842044509340	20.413660436008
Ar	26.422165259848	21.421301093478	29.541318196382
Ar	12.192055099880	21.305320854085	15.737430286098
Ar	12.767226895570	22.790979492600	9.006900841592
Ar	12.106997619183	23.762497792108	22.278960148549
Ar	9.625040058183	27.355023880375	13.352703978151
Ar	35.996835650387	16.367726437154	13.758500673770
Ar	20.092084063838	15.644582258146	21.695641310345
Ar	27.106838536954	16.352778930464	5.357555898419
Ar	25.621575822503	13.571882537099	18.754403154353
Ar	9.583872238747	29.853386399133	19.967050524926
Ar	25.643554354064	15.997829446435	25.293344268299
Ar	12.542985750576	29.425937475976	26.380746512288
Ar	36.062860364220	21.386305950019	27.080233845999
Ar	22.101209030635	19.823855542532	1.842859279094
Ar	15.248570877069	16.811190512750	11.439351186092

Ar	31.500856805597	13.888007905118	22.304498163721
Ar	14.990562881299	23.306888202641	28.782876961150
Ar	14.603992713032	15.402245125224	18.040557940331
Ar	14.528308190348	17.832171914004	24.554994359465
Ar	15.838957247612	18.220714454677	4.616840553901
Ar	32.148305878237	12.936094419260	8.885324073116
Ar	31.407077424641	11.460198259443	15.676471357789
Ar	20.184425777808	11.889386700670	10.928284561319
Ar	31.431256785465	16.452955120686	28.985436754913
Ar	20.063399386242	19.805069528940	32.525644595472
Ar	19.513274156568	10.503320741691	17.550702221401
Ar	6.248274162346	23.799930293926	18.442403183576
Ar	20.864308306476	13.271618081975	4.113319094512
Ar	19.460299856463	14.421888100923	28.201125259692
Ar	8.689011680681	17.669546912454	20.825320911871
Ar	37.452858188795	14.548620007785	25.876721917759
Ar	6.432220324615	21.278687825027	11.797708480591
Ar	25.937657088865	9.737929386567	7.554477134583
Ar	25.245646752672	8.236083069050	14.371185344388
Ar	6.274852865300	26.312183418848	25.100383092160
Ar	22.582425182416	9.862887242741	23.837961117523
Ar	25.199789533073	14.766724990253	32.076100929918
Ar	8.902571234044	15.194438875334	14.199230136910
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Ar	8.748323087888	20.185310420001	27.466111766292
Ar	15.644356634233	11.001561801792	23.380412190454
Ar	28.392511508283	7.579982896270	20.827530816574

Ar	13.816642860206	10.134296222391	13.621698742895
Ar	14.528384787646	11.629236802785	6.804462595614
Ar	28.428394016585	10.101914185687	27.584607394253
Ar	13.688357660262	16.668883970178	31.314103987286
Ar	9.836327774982	10.651373021821	19.613055489377
Ar	9.772244019140	13.161622926825	26.367889014407
Ar	19.626094816122	6.686024170408	6.337350348136
Ar	18.929801121138	5.225245338016	13.166404782852
Ar	22.043924972634	4.407783357732	19.589821934808
Ar	22.016518644017	8.450283649808	30.582746043575
Ar	18.812043108305	13.174952437981	34.937957536829
Ar	14.933014481894	5.577529441127	19.119670556978
Ar	14.867134819184	9.619425334394	30.115198722728
Ar	18.074664442860	4.925573150642	25.620922674115
Ar	25.168276445995	3.880794432419	26.040780284420
Li	21.410077072129	21.488574044353	16.517986646889
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Ar	9.774616004401	12.630337996432	20.276809988963
Ar	5.140773190718	4.162734775722	13.391270988907
Ar	2.312261694279	17.385432443997	12.379016263089
Ar	2.405264010128	10.349538619691	11.228703670418
Ar	10.704585385311	7.540138386045	15.845256232427
Ar	8.541157379289	6.195902533279	22.510235028501
Ar	4.107782118842	16.414988238969	19.144955026403
Ar	4.531516363154	11.800973045684	24.689238181340

Ar	31.430845844769	15.348261817550	20.789327076978
Ar	8.898605090266	8.447168530195	9.145486305662
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Ar	9.581958472162	0.967913845463	17.952097231139
Ar	13.537762594304	16.857284541132	16.146999291907
Ar	16.224883703892	10.852552004934	18.195503361306
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Ar	14.174412045299	9.604228225948	24.671116402132
Ar	9.863305929612	19.534311773051	21.440382757089
Ar	11.635819227824	2.312584989738	11.315111080309
Ar	6.199539756573	14.645817630994	7.066249885331
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Ar	15.143317912291	4.512350433325	20.301829665085
Ar	10.301002647829	15.015261342463	26.831548563372
Ar	4.650875800028	18.911721722278	25.939214667704
Ar	9.098400587406	8.640375451659	29.268296195917
Ar	15.223671942881	15.721258643263	22.415673172025
Ar	17.127133016529	5.800049496804	13.835271336522
Ar	11.772689994011	18.004185787245	9.606150414169
Ar	13.122170602588	3.211273607308	26.989171789364
Ar	5.209728436322	14.268013993257	31.396985737443
Ar	12.746290370325	12.785914545230	5.046847236133
Ar	15.398672039038	6.603137972134	7.130725224963
Ar	16.095676315631	-0.787191868376	15.845152229087
Ar	14.154154968700	-2.039664358605	22.490792114186
Ar	20.085299775761	16.187748950634	18.095707430171
Ar	21.468389997664	7.067284608198	18.905787501209

Ar	21.069363689116	11.330535323508	13.879157557532
Ar	18.534291837373	17.400178116570	11.614372637522
Ar	20.479137387850	11.936779100724	23.104564473210
Ar	16.361510163515	21.819895232485	20.063980285587
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Ar	17.063962493226	14.517912914290	28.664756825154
Ar	14.401113516576	20.725510052073	26.706450782934
Ar	19.621866803300	5.658586865192	25.470163096348
Ar	10.912508523731	25.927237102854	18.974167668256
Ar	16.018927872739	8.132415133997	31.155999429196
Ar	8.868295801692	24.790787930437	25.818893458148
Ar	12.097808391664	13.746816930322	33.405534573421
Ar	9.323922388207	20.137701471032	31.368278017024
Ar	18.096462349679	0.450559904553	9.217587249064
Ar	19.535872173184	12.300199742450	7.052129641057
Ar	20.654979877193	0.409995999725	21.082495491983
Ar	20.725490222185	18.710626457865	24.482471550228
Ar	22.146078314807	6.192391080203	9.167739528188
Ar	16.911211005042	18.517861832846	4.913798588775
Ar	22.573435646069	1.669871287312	14.500492569067
Ar	18.738159906109	-0.875646578937	27.773997115539
Ar	25.333823167420	12.418229946646	18.801213803659
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Ar	15.566062671560	27.153502997018	24.370457247347
Ar	25.081269886833	16.805272024418	13.622324333450
Ar	16.304639277134	19.598687749404	33.279435365543

Ar	26.538110017233	7.393475613393	14.440564894760
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Ar	19.865924191674	23.666010392863	8.829694643616
Ar	17.617503884253	28.112655521040	17.561870474104
Ar	21.689940816095	4.063298542830	31.948276158141
Ar	19.096634763966	13.185905528830	35.122756550685
Ar	13.572060959333	25.906474137038	31.150547479803
Ar	26.197558352199	11.799865460537	9.057947986437
Ar	8.005665706366	13.664728718783	13.752235609928
Ar	23.650384981880	18.016422891239	6.903934173918
Ar	26.201637215243	14.797401748724	25.288397767538
Ar	27.043522031830	2.814963182871	19.664171059950
Ar	22.124282856146	25.066169417186	22.123841100484
Ar	25.196732984416	1.538656461566	26.353765803116
Ar	22.833126892174	17.593407215692	30.960710595997
Ar	20.111049992180	23.948431589337	28.953149150837
Ar	30.726369823516	12.955235847684	14.278949375096
Ar	26.599229248290	23.042016049492	10.910875970437
Ar	26.499583576042	21.786099092604	26.610595620460
Ar	31.142599349561	8.492001652037	19.553098756157
Ar	22.842358460260	28.678869183263	12.909077209145
Ar	28.148881638192	6.549833578176	30.410338906721
Ar	25.790881476513	19.269276486379	20.009870973912
Ar	27.348629309781	25.589464021780	17.469194285900
Ar	28.490819205458	13.504060217128	31.763271451514
Ar	31.041635856006	19.912771400568	15.438340554575
Ar	30.375169080147	17.449818244241	8.884869623122

Ar	31.641954242297	3.921534368914	24.871584901302
Ar	31.888794714060	10.828056043341	26.172436414574
Ar	31.738344467175	22.325712868473	22.009651557265
Ar	32.158938745161	17.755332817710	27.408539960863
Li	20.761545615802	11.641331380973	18.504519111736
	96		

Energy= -0.30551586123500002 Symmetry: C1

Ar	22.904606822245	36.399761322215	15.447328444812
Ar	19.388622760950	16.670921112939	15.3533144486979
Ar	16.813808279562	17.450516979202	24.216694690001
Ar	15.597553447593	20.816862862029	18.790320721095
Ar	14.397666156948	14.421104019490	18.870353132434
Ar	27.188818919743	15.604494804106	20.788091535410
Ar	21.795065915079	19.690541720852	20.683571544434
Ar	20.588234648387	23.080020060574	15.255479680659
Ar	15.529602867839	10.818057197819	24.479453479621
Ar	18.195291880588	10.043569864113	15.326863339287
Ar	23.159510225786	16.279208725079	26.324562765981
Ar	10.370291842654	18.594179923608	22.407089430858
Ar	15.280428242314	21.021320901028	11.937311507831
Ar	14.035748993544	14.340893920522	11.925879704540
Ar	10.042421585717	18.703192001069	15.542116386903
Ar	24.655917038456	12.427183733474	15.171917565700
Ar	25.857755677569	19.100621257111	15.141102488446
Ar	14.168465826881	23.885428751753	24.641423670072
Ar	20.696150164331	22.702065332545	26.639356522178
Ar	20.618652391307	13.293400826990	20.776452074242

Ar	19.388578843069	26.163890106128	20.959519250761
Ar	8.929510066977	11.881957740943	22.530740910326
Ar	19.515961702959	6.329239016236	20.950264867318
Ar	11.490049060449	15.096877497731	28.206537344057
Ar	22.045920368274	9.507233392137	26.555633040305
Ar	18.008955879849	13.918890481575	30.204203845873
Ar	12.917385458861	7.525187551386	18.924326342532
Ar	20.543110708218	13.165244856594	9.578966061761
Ar	21.784363140890	19.862987509121	9.597154716512
Ar	27.221288168457	21.591953253241	24.395379077920
Ar	15.234825150445	26.991521719890	15.447931327216
Ar	25.877422334857	25.066392818499	18.709894533740
Ar	9.978341838522	24.710239017419	19.108344884443
Ar	15.423805896059	20.389579412091	30.473991309019
Ar	26.040691909987	8.785432693431	20.887097935307
Ar	8.681458652995	11.922249966243	15.560083675452
Ar	23.498964198678	5.533361475961	15.178750735181
Ar	8.782061422428	21.612169228772	28.477327507694
Ar	22.051270116658	19.212058083169	32.543576832008
Ar	4.591706544636	16.346737188536	19.212864193235
Ar	28.648368763752	11.996600842412	26.591982601782
Ar	12.713068565671	7.482312807900	11.868106266889
Ar	16.339166707475	17.597166224861	6.134100841530
Ar	19.151652714836	26.353847588332	9.648082661245
Ar	21.728492518697	29.624897271074	15.337182104265
Ar	25.793214173903	25.192870074843	11.693213954675
Ar	9.576889010449	24.933600771345	12.002590948350

Ar	13.829242561171	30.267075039959	21.386946511395
Ar	27.242835513162	15.617681681563	9.311448833529
Ar	31.476225841295	20.975590056454	18.710692092219
Ar	24.774685579727	28.289756026427	24.744405870799
Ar	9.763823999663	18.840706358748	8.470059748239
Ar	31.317485593592	14.919469788270	15.049975781673
Ar	18.125444994880	29.326654132520	26.932648654136
Ar	4.839155552139	16.231912798500	26.241159467735
Ar	24.596256821584	12.658501274075	32.300741829258
Ar	16.927669321895	3.024611550488	15.311825308476
Ar	19.293044449228	6.299105432926	9.543936685836
Ar	28.638516575271	18.051133762819	30.249413516248
Ar	4.555334381801	22.405745447648	22.862026323877
Ar	15.030214592041	10.703531185954	6.041096109093
Ar	26.117297838415	24.655735825491	30.595005965926
Ar	32.797748360772	17.349708508695	24.568821412156
Ar	8.438338458301	27.852125046583	25.174755696614
Ar	4.198564410237	22.519913705859	15.796455577929
Ar	25.939548063926	8.726209415636	9.3674482996250
Ar	12.764074857580	26.954121369631	30.746902253569
Ar	4.374423775514	16.403301505660	12.171087556082
Ar	30.077344809087	8.038583149739	15.110481436539
Ar	19.443717438482	25.744995140403	32.792342089745
Ar	8.474462519803	11.963022716282	8.467742046749
Ar	32.669982970298	11.281019567141	20.862636800874
Ar	13.605929981161	24.248497893620	6.059618699436
Ar	31.382457418882	21.099587657718	11.499544466790

Ar	20.509368069475	32.974800171448	21.281805375352
Ar	22.940966116721	16.455066978747	3.731255533905
Ar	9.628350845817	30.982593898663	15.703939870830
Ar	31.353425597465	27.059971474146	22.373145964471
Ar	20.309954792659	23.061352929844	3.653879567346
Ar	13.573748420030	30.468226544277	9.711055795648
Ar	16.212664375167	33.822847515717	15.549532514452
Ar	27.225491462324	31.836534203417	18.936398598049
Ar	27.133015254564	21.895975442397	5.734834623803
Ar	31.394957497227	27.288997275239	15.192839785077
Ar	21.654317324832	9.555142502103	3.736871627228
Ar	4.220024966006	28.601246547245	19.490829116588
Ar	10.799728800199	15.204349188097	2.596177325453
Ar	32.722044669553	23.448529321392	28.234533871465
Ar	24.453881699575	28.605927559012	5.824104767941
Ar	17.372766281116	14.011670154293	0.236399499555
Ar	20.275902563412	33.175469608360	9.575424705652
Ar	27.112235640573	31.978253756366	11.684165788390
Ar	14.705851591445	20.623313995669	0.106279587600
Ar	17.637674577848	29.693567316872	3.827132121571
Ar	31.185964601984	27.359684957283	8.010568152303
Li	18.106633767858	17.069415521248	19.769191468378

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Energy= -0.30777432578600000 Symmetry: C1

Ar	12.393715061985	21.587670435440	23.130842688783
Ar	21.174281045938	17.987790907204	14.360337275545
Ar	27.729768803481	10.915098772879	12.235142830261

Ar	15.065575309589	11.126578737865	6.912389254776
Ar	20.164373718325	19.601705088278	7.745550193755
Ar	22.291319175216	6.225034183652	11.922394337932
Ar	16.289469876495	21.945744439877	28.882706597837
Ar	10.460141836748	13.080817414207	15.404737265844
Ar	26.613148518688	17.702984421206	10.094040148908
Ar	21.257926011243	12.887638556916	9.696422878539
Ar	16.347152422530	14.860820052250	18.141850552996
Ar	16.118014834905	4.437071805163	9.098566289706
Ar	27.466327248451	16.133215874589	16.789678926421
Ar	14.007936142984	17.875586006666	4.928461976795
Ar	16.704149801936	22.911679084672	13.008559082844
Ar	23.676441563632	23.968357666709	12.032081052898
Ar	22.107532323835	16.473312705843	20.717655251583
Ar	25.988907375951	30.204037413255	9.913095105563
Ar	26.640533226759	6.259869412799	17.643292445358
Ar	15.224994622544	16.283662329441	11.617880484296
Ar	4.216955716022	11.201341795026	12.511207141161
Ar	9.125004572532	14.508163352076	8.714888500293
Ar	32.997745867383	15.786546476848	12.716574539711
Ar	13.348018658987	26.075456660154	18.119547982966
Ar	19.483274003251	10.779174601060	22.755085071201
Ar	24.613848439504	22.231195649200	18.640893919173
Ar	26.409110828563	11.595099865450	22.065347630311
Ar	15.542885979271	24.656289985938	6.356773667023
Ar	12.004498743512	19.534093728813	16.867508865212
Ar	13.520354913304	9.021828899009	20.050896703858

Ar	10.628051829815	21.240854959011	10.161361202356
Ar	19.492302134509	5.406522466595	18.396253601669
Ar	30.16574526678	22.132565503238	14.534446789738
Ar	32.032208585717	11.101790929405	18.066555750874
Ar	16.732977036617	16.902338783997	24.382363636966
Ar	27.865356376801	18.345940364471	23.469813891931
Ar	10.991591284832	15.272848945523	21.807504098495
Ar	20.161558367103	27.210564497002	17.298192237385
Ar	19.044856987644	29.082169071737	10.671211407134
Ar	16.691530609157	4.864219304076	24.872211982234
Ar	33.525454906566	18.065653436497	19.506778879003
Ar	5.8013288853261	17.904659781400	13.929259095382
Ar	10.173466979425	7.838006856257	10.824025712340
Ar	15.789041301227	27.229521457353	33.424117412484
Ar	4.727267049421	13.382307758834	19.17104922356
Ar	21.8183977272566	21.464597760275	25.012394578990
Ar	22.911077828330	14.960106397035	27.124192494934
Ar	17.359324981928	26.421161929791	23.695507757191
Ar	12.125852251588	27.984906842364	11.535093908750
Ar	23.766452778600	5.557126239507	24.212667859352
Ar	27.145638273881	28.271380386354	16.562278486465
Ar	30.841431639361	6.528429124098	23.465751535212
Ar	17.748584009951	21.158313759191	19.457975518350
Ar	13.927219945580	11.175608127640	26.623285936009
Ar	30.565618762504	24.390583133791	21.404935594710
Ar	32.448652819346	13.385166419892	24.936405397787
Ar	7.272877422105	24.526041705885	15.314003358679

Ar	16.283671286621	9.685317376991	13.665579863184
Ar	13.306080313798	3.646096285707	15.589268055983
Ar	22.249416634711	11.444015141536	16.409545546354
Ar	24.264139433300	27.501502524097	22.987733718219
Ar	7.816328811530	9.351298493270	23.94943238074
Ar	6.346474296058	20.018508883791	20.541371883935
Ar	20.174807571450	9.025008681949	29.415676412551
Ar	27.330159688025	9.908249790192	28.728608263510
Ar	15.592726701649	32.306769386725	15.934102108755
Ar	16.852612454192	20.578231762108	35.707914799481
Ar	11.257314201450	17.303510498791	28.280649995247
Ar	17.358615684857	15.382043196580	31.025284209308
Ar	22.521535033523	33.397957234439	15.181753523505
Ar	27.681923740900	23.612764931804	27.975645712583
Ar	28.828672152313	16.834931450727	30.163685491444
Ar	5.133342264372	15.535907351245	25.733530009137
Ar	33.801212152954	20.336061756492	26.3222821442395
Ar	7.687770821890	26.705533369104	21.956799023141
Ar	10.940103044732	5.271202058290	28.831923356974
Ar	7.387614272560	7.120531831993	17.284078853147
Ar	8.670930379883	31.272455746043	16.706254676828
Ar	19.716478724970	32.672725311568	21.654940609297
Ar	22.620019729226	20.123352231802	31.748566541230
Ar	12.799266064944	31.552098806065	22.395276532714
Ar	21.505798211265	26.693406228494	29.460436538669
Ar	23.646376040895	13.410288665125	33.792927100475
Ar	8.214796986523	11.503521420138	30.642833397760

Ar	6.623114983702	22.238389466853	27.135116070736
Ar	26.676863270358	33.7263337577590	20.920647859990
Ar	14.408536378245	9.487115140755	33.388276625314
Ar	11.713800040952	26.979229148833	27.640628443260
Ar	30.127565889979	29.879069021890	25.831527243736
Ar	10.524324351428	3.066016702082	22.107184358344
Ar	16.904251641948	31.789703492591	28.114331997295
Ar	23.870271824051	32.930049480372	27.376360271129
Ar	11.677145063908	15.796347034146	35.0704524485161
Ar	10.629498801524	22.458602108328	32.936826221913
Ar	17.896674567026	13.856053038272	37.794037694810
Ar	5.451358067612	17.729847639511	32.401708890115
Li	14.389033318897	18.218895531840	20.631269327008
	98		
	Energy= -0.3107605697329998	Symmetry: C1	
Ar	19.575668512439	22.352324538660	32.477740476078
Ar	17.850816450464	20.193838313990	26.168804178582
Ar	19.041843220466	26.945465491066	27.091081357571
Ar	15.000907561266	16.993517884396	31.591902485701
Ar	17.357620550469	24.536003328860	20.810091821925
Ar	23.806204895954	18.219437015790	36.276082331242
Ar	21.918040515730	16.148106731051	29.919716377443
Ar	26.223293701341	24.322316067950	33.476849280735
Ar	19.242115007694	12.777892378349	35.384890217423
Ar	13.124065946511	23.734841454045	29.724134539427
Ar	24.307398744750	22.133612843530	27.156328779756
Ar	13.382901424323	14.900109769109	25.161971579452

Ar	20.157868440282	14.134790931873	23.644778646473
Ar	11.587504030007	21.467036453693	23.335324370097
Ar	17.377868936986	10.750031536840	28.938674390670
Ar	22.488379289129	19.933957577791	20.921436129359
Ar	16.268268976027	18.064285852207	20.085432423724
Ar	8.503879348426	18.295298503949	28.676411935790
Ar	26.603463141659	16.030117060451	24.639397568775
Ar	28.552974083999	18.092520954547	31.015702830104
Ar	12.604415824255	28.277014030638	24.152943971162
Ar	10.515178233148	11.558064805091	30.464939158767
Ar	23.779904220915	26.517430270003	21.741140726226
Ar	24.205297828783	10.051696263506	27.324114588334
Ar	25.703358964618	28.924536585974	28.032729815068
Ar	16.758105321156	16.968069966629	2.359971960046
Ar	26.094508877921	11.999992922812	33.720972884579
Ar	6.756899303576	25.018477161624	26.703412927337
Ar	15.342872250718	11.556541905574	19.325025370259
Ar	28.867733681059	21.888176285280	21.908105790669
Ar	9.942666096523	16.068880884143	19.062311870802
Ar	30.906815591195	24.139372430289	28.188785895743
Ar	21.034217634498	14.896560521592	16.923933727598
Ar	18.518587370761	31.279706211760	21.527920315266
Ar	12.417620206863	8.045659349274	24.516671159028
Ar	6.903513585800	12.738350211748	24.339180219949
Ar	19.387944981569	7.394140801712	22.980987922376
Ar	12.563348188143	22.093232282022	16.389853187153
Ar	24.131546404210	17.868147491744	12.045073959077

Ar	21.540386181709	6.570181334492	32.692238366582
Ar	25.069933399150	10.722719055415	20.429736496554
Ar	5.021130264579	19.573104822283	22.410109236142
Ar	30.816676792476	11.903771301252	28.419441700864
Ar	27.218185502801	16.753484715320	17.771882928083
Ar	7.638256777935	25.747737073990	19.576130021463
Ar	25.588900164099	22.912480697907	16.047916502958
Ar	20.535636097177	27.685314561038	15.724344445480
Ar	13.596962537263	28.919849797523	17.042670579061
Ar	33.214580244526	17.945248688464	25.707984314530
Ar	14.866859077818	15.962761351100	14.005483575598
Ar	16.657558643101	3.803451609623	28.275162789968
Ar	30.373214095144	28.626859871227	22.732401954233
Ar	25.141280026715	33.318437777072	22.453723232887
Ar	31.64289784937	12.587310172664	21.414683389878
Ar	8.946367848546	9.245512379553	18.273967003202
Ar	23.545292782597	3.163118502165	26.715397948916
Ar	20.259783000360	8.142253814321	16.062280754296
Ar	29.254480754690	6.495033252972	24.128562083590
Ar	27.071256482039	29.781272514114	16.612226081096
Ar	6.034870304334	20.276534473588	15.169973957800
Ar	19.412275627389	21.036789436834	15.214589775703
Ar	14.498891316206	4.768355678595	18.549210818551
Ar	15.708494182206	25.263495697879	11.246581432689
Ar	35.615166914236	23.948648589609	22.946268642462
Ar	33.965531443334	18.580757298925	18.718787439707
Ar	25.264005431422	4.622416718460	12.710942969839

Ar	32.244730755563	25.120852318427	16.886173651779
Ar	24.426494878511	3.814270144182	19.693258118562
Ar	21.828756226282	34.522661851208	16.294796156651
Ar	13.902287556878	9.170819494171	12.993480188330
Ar	8.431454962304	13.859542451574	12.677218867826
Ar	19.753361276086	12.601991500852	10.701771680990
Ar	22.501345878733	24.179316043147	10.131842970869
Ar	8.825509472118	26.340166691483	12.440434543612
Ar	18.045266744110	19.076473154345	8.892691433585
Ar	11.016081260020	20.013898670107	9.958604266163
Ar	18.698753881781	0.519071382512	22.248828206545
Ar	30.585115880453	19.768593112640	12.745131291612
Ar	16.908614281754	32.138249698575	11.747503842948
Ar	30.103418771175	7.180694514268	17.169916794196
Ar	32.436161855021	13.293287308718	14.524965482521
Ar	28.995525737586	26.289386893679	10.885416686332
Ar	23.774003559378	31.016411415065	10.503752717553
Ar	13.459978531707	13.786801812790	7.635819147084
Ar	19.562630772199	1.273124150566	15.201788778929
Ar	25.865517437081	11.504059804958	13.671302574318
Ar	18.996331685158	5.720093581224	9.629680607728
Ar	29.167028180164	14.475033541918	8.441267650090
Ar	27.448770870989	20.935594385939	6.637651023751
Ar	22.998557372011	15.694940349632	5.438110445530
Ar	18.910466054992	28.505848201059	5.991722948021
Ar	14.342113203853	23.242713542793	4.683544918714
Ar	24.727709540040	9.103767929202	7.246592740658

Ar	21.245677593927	22.261852335955	3.556789831757
Ar	30.980508293916	7.920241166135	10.232677174006
Ar	25.781657300913	27.502529239203	4.750337173864
Ar	18.498144009014	10.342762741967	4.227253691513
Li	23.297718561827	18.894721013702	16.499968129312
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Ar	22.295579356573	27.058034652441	4.685564816134
Ar	11.645827681267	21.312322949462	6.122443522148
Ar	19.309372461795	25.389413387559	10.770350991266
Ar	8.297348799839	27.493208158835	6.051241057054
Ar	15.296449410871	27.306343611033	5.381277099892
Ar	18.582246331165	21.071220202376	5.414543874982
Ar	12.463831472506	25.518831527852	11.489404087603
Ar	19.294057851673	32.071557296242	8.742412457692
Ar	12.259237855782	32.191739352935	9.500071686798
Ar	16.337979020124	30.245514740166	14.830249796854
Ar	15.651865847183	19.524674696336	11.638672113425
Ar	6.372793502897	22.475954104831	10.585584622610
Ar	6.682141558321	29.213075995753	12.676599453088
Ar	16.392002006561	23.644384986488	16.619093729641
Ar	22.569422651337	19.272313987345	10.769394495176
Ar	14.888858253991	15.198373032375	6.113629282453
Ar	26.3801366675667	25.239007211683	10.058503791979
Ar	25.636667888195	20.799235183223	4.703133905706
Ar	16.216380823487	36.935341413418	12.928184219487
Ar	23.431789424108	30.243865762426	14.106933107237

Ar	10.684035358289	20.621119140303	15.845342752328
Ar	10.835799548906	27.263218145054	17.948111165569
Ar	9.743707334217	16.379811861567	10.662157584487
Ar	10.573024509356	34.004181961227	16.128928759192
Ar	20.754106623591	11.204139921289	34.011344379623
Ar	23.268433914242	23.585894991932	15.959740148621
Ar	21.912897295538	14.863150629629	5.380427169040
Ar	19.484840242312	17.839532651195	16.607262348351
Ar	18.834264308654	13.528307871390	11.471679293278
Ar	20.319436429438	28.403323762164	20.021373062787
Ar	20.328436679811	35.063187245505	18.304333885607
Ar	4.716247919491	24.136613473406	17.151505014356
Ar	13.782763262314	14.791894481697	15.846675325283
Ar	14.692367966946	32.168045534426	21.507277858872
Ar	4.407002474400	17.510229983205	14.995649948050
Ar	14.517336524506	18.934429924008	20.813116397606
Ar	5.030260699166	30.883837263744	19.308991583251
Ar	28.878734465039	19.975093334081	14.074000325438
Ar	28.100383697496	15.478945719288	8.743577486422
Ar	20.237065470970	21.981657516854	21.595155307008
Ar	29.371659594147	26.802757745631	16.345681604320
Ar	14.834575337597	25.444620215620	23.105669176052
Ar	12.909554187645	10.177062039895	10.589938106343
Ar	18.135455516992	8.965208196763	6.040781131552
Ar	24.919311722330	14.073506199804	14.800516734630
Ar	26.317631459568	31.786660647916	20.565338497282
Ar	8.871195193864	22.298378334777	22.366526025590

Ar	25.606806648540	18.451828653131	19.973819265211
Ar	26.099807107887	25.058120021017	22.199209030515
Ar	24.244623570184	9.593296331416	9.497917275189
Ar	8.605502841459	15.784958109433	20.143513276354
Ar	9.171362202912	29.030433411415	24.632730458242
Ar	7.703530617875	11.324323071423	15.006897281297
Ar	19.344001203004	11.189582605063	17.892423764386
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Ar	18.653429644753	6.644765973066	12.657456128785
Ar	31.792627520186	21.451925224229	20.529692672463
Ar	2.687448849888	19.109129463168	21.658113390895
Ar	3.015869249163	25.804159654559	23.821505508719
Ar	14.120928621591	12.345571045003	22.337319925322
Ar	17.091155997375	20.301412627046	27.188333521217
Ar	13.352697563102	7.846132064277	17.151347062398
Ar	15.198716772055	29.921488750873	28.359310142292
Ar	31.116804729286	14.695582052312	18.264614022701
Ar	30.379476345892	10.179503263030	12.953003842977
Ar	32.162200866371	28.242407871293	22.802468942601
Ar	24.084446412663	19.983916604088	26.635874941294
Ar	11.106788240834	17.105115173761	26.506873182107
Ar	25.452177624846	11.752683806478	21.390766774548
Ar	11.402745712159	23.839446374067	28.896846620965
Ar	24.782800625215	7.185318165508	16.127349876448
Ar	26.842680750751	29.495364460717	27.444092282617

Ar	2.357042094460	12.447461715515	19.433697829046
Ar	8.060145012234	8.988139039269	21.666376399119
Ar	5.238470199304	20.566323608004	28.081559065373
Ar	29.714088881079	16.216410661006	25.065481494755
Ar	30.216780085936	23.055637769280	27.403869799852
Ar	19.830772522517	8.930075090795	24.473172910034
Ar	5.018204079878	13.843770608768	25.820396792962
Ar	19.120761164871	4.341253452417	19.286318835908
Ar	16.847513377293	13.615574513415	28.763712571957
Ar	21.372561981631	30.593394844500	31.949943600938
Ar	17.553890262058	24.544909961705	32.597890269566
Ar	23.962941939445	13.280391494981	28.172640850267
Ar	24.772623026302	24.247230399006	32.0218122262044
Ar	30.902745390887	7.806258388006	19.648312945445
Ar	13.800253077181	5.520742854069	23.825808225113
Ar	10.740179184697	10.281288684283	28.094384350403
Ar	20.915177959496	18.150888188667	32.530450937355
Ar	13.745233676886	18.405873344229	32.933924622503
Ar	25.262100842385	4.904652495195	22.823622471037
Ar	28.022287073149	17.781706164329	31.839036651295
Ar	29.474381590824	9.281304277051	26.494630708358
Ar	16.592321922870	6.809086126289	30.254725829642
Ar	19.589183649053	2.045764945826	25.956205348682
Ar	23.741317497855	6.445490986438	29.639992256994
Li	15.100203915358	19.227931195202	16.244077301893
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Energy= -0.31648195694600001 Symmetry: C1

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Ar	23.835774196557	20.262720397784	28.543089875010
Ar	26.149616309361	10.947432884437	21.574784688684
Ar	29.962047691044	9.120373312383	16.004088466275
Ar	21.185558388501	13.621935238321	17.776476194332
Ar	34.550653534344	14.267734861568	17.573880275085
Ar	29.252739000999	20.537632502482	12.133583426039
Ar	31.493178850059	14.019987347498	11.198592139662
Ar	30.704216255211	15.952160639862	23.201707942318
Ar	24.824385079685	11.779038987794	11.977784459937
Ar	16.280869284135	16.073911141496	13.756828241628
Ar	32.298057792938	20.834678228112	18.432689328210
Ar	7.416566530175	20.624459682320	29.631386801239
Ar	19.251794751747	19.795449778872	18.525817525481
Ar	26.344842959635	16.694282521881	7.118865625380
Ar	36.059417318842	19.249795931063	12.750115453348
Ar	28.591143159107	22.383437815407	23.984449523525
Ar	23.287080475391	6.963037217813	16.776138410291
Ar	32.895106035925	9.378267471376	22.418321190361
Ar	23.993393270617	25.152191963429	11.848916010849
Ar	29.950570451632	26.745376345199	15.330231171611
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Ar	25.895841786642	13.838951940163	27.812650667150
Ar	17.420656940232	22.857554880479	12.677062282294
Ar	19.729381663474	14.436462215214	7.896475775368

Ar	33.002207990391	18.958895754978	6.371228519630
Ar	18.262462975404	9.573874789650	12.795745677973
Ar	39.070977206894	19.505283445442	19.162028921544
Ar	37.462390644320	14.529388186943	24.030688226975
Ar	35.304775074620	21.140415225870	24.862744585081
Ar	28.372265208957	4.219395976034	20.782982581663
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Ar	15.284241143078	15.002311985834	20.391408467432
Ar	20.991721842095	21.312618960421	6.829752610123
Ar	24.042604607858	17.309804301389	22.320466802740
Ar	27.669608402148	23.606218875715	6.097898680095
Ar	26.281759628825	28.234332587934	20.936307841958
Ar	36.824853069535	25.525200296652	15.968645075561
Ar	18.161608443160	18.691845739259	24.915895906825
Ar	22.700782200564	18.283717880950	12.878968709499
Ar	15.454820650829	10.178552647776	32.722312000458
Ar	17.112340405614	8.539913155374	19.588140792432
Ar	33.101354238271	27.138109910676	21.749503684403
Ar	22.111546468029	5.777786272953	23.581892989761
Ar	28.057513135534	7.224539474163	27.127952785641
Ar	32.655073279707	12.317678353078	28.843059118074
Ar	30.551771091972	18.956915040087	29.666154468172
Ar	28.380694380198	29.909714866343	9.267137660985
Ar	15.682235861185	24.505768210635	22.093499868628
Ar	24.656387095379	31.538591580041	15.038016470372
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Ar	14.356901222240	19.011066209135	7.730609554904
Ar	19.694954136871	15.293863930044	30.555801401447
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Ar	21.744083726336	8.716578934987	29.889031365148
Ar	31.896314945617	26.0111713447908	28.821730923037
Ar	11.994303111713	11.032585585734	15.567033930238
Ar	13.139960655684	12.133919559753	8.715169734857
Ar	18.637517833389	29.806054700120	11.639018840079
Ar	22.295737844527	28.220515362744	5.857341057506
Ar	34.372322064739	31.469317567137	12.841756756366
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Ar	18.510007852007	24.751957949439	28.461516771812
Ar	14.012158085672	13.808185103929	26.956563557737
Ar	15.926169337983	7.239975691584	26.327337506004
Ar	27.680099102764	10.202192255451	33.486786248386
Ar	25.591199984677	16.831198155635	34.241174066449
Ar	18.189386431682	33.152596914158	17.919333688722
Ar	11.511263246672	19.544063087061	24.075898478953
Ar	15.587460924595	25.895797686840	6.694784967536
Ar	29.513145474430	32.046978615153	25.698728681053
Ar	9.503779253476	16.862787120474	12.430967708261
Ar	26.956636008518	23.802546690823	33.592961868447
Ar	10.837869499571	9.881023620771	22.296653312425
Ar	10.612973366260	23.767446771172	11.379475595298
Ar	20.400675514171	26.652406514370	17.494726391811
Ar	8.357244874169	15.669510936569	19.285202308265

Ar	24.301026500037	34.797034615659	21.508868120464
Ar	14.312643479215	19.795006543411	30.509247104162
Ar	20.195749527909	21.393465458341	34.289838354330
Ar	15.876229531746	16.240261747097	36.328665998288
Ar	21.334860182477	11.681661308368	36.299995207525
Ar	8.950653342750	25.465247640701	21.073341827784
Ar	13.216510896315	30.917305845241	22.743838607216
Ar	11.710933395215	25.792078659525	27.587792384729
Ar	23.049553461570	33.632850548652	28.653058892080
Ar	28.220704406943	30.794338966356	32.6900643877843
Ar	21.440600707861	28.452022060530	33.510605471964
Ar	5.843465796341	21.542858025338	16.191453008048
Ar	7.133213997015	14.496731975350	26.130978807453
Ar	16.173650166692	31.160171102446	29.405562019168
Ar	9.619840349206	8.629719159107	29.109813697363
Ar	10.022465700170	14.740217594954	32.610244154802
Ar	14.676852087987	25.880456137292	34.084642123159
Ar	4.645355997966	20.340574613323	23.085676108358
Li	19.677760166465	16.173983119297	21.352096157406
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Ar	27.567524589422	11.869665310847	15.271495482386
Ar	30.453871124724	16.802311527145	11.470792613763
Ar	29.101721348926	10.496059608698	8.727170908157
Ar	17.058701904613	6.875700078164	17.634671935635
Ar	30.212057385262	5.626304664900	13.733672509974

Ar	22.421161025221	11.223619607100	10.885029772030
Ar	23.701560964067	17.163705974971	13.464119651958
Ar	25.756119310018	16.436719058419	20.046875904017
Ar	30.339166956431	13.734850405049	24.562067619367
Ar	25.539394936415	9.606043550137	21.532431839601
Ar	11.230800401329	9.353142190777	29.443476283561
Ar	25.193595294180	15.995498123507	6.974609633385
Ar	28.557013520569	21.491299443963	16.270312893205
Ar	23.537723123612	6.301842667272	15.705919592942
Ar	21.119336246881	12.444314560392	17.131660827194
Ar	26.648354383327	22.278261772948	9.609927487774
Ar	23.947575978377	9.744174719580	4.166682314114
Ar	18.791548304590	16.446282056501	9.110467559041
Ar	23.774808039621	21.086111228022	24.856509973993
Ar	18.384315041190	5.552752999442	11.127323871366
Ar	32.219883056535	9.025164923137	19.620587158949
Ar	24.962142142278	4.898441654029	9.086172818444
Ar	28.115367847845	3.280852380457	20.064984468904
Ar	26.011655233392	-0.009655448419	14.102768109892
Ar	30.088256342872	6.787533903189	25.975583373789
Ar	30.478175202437	20.643422505314	23.031034410119
Ar	1.944612321871	14.240863178895	22.698569146710
Ar	21.412145460237	3.799874481680	22.068514310194
Ar	20.745462789120	-0.782832650233	9.405058231009
Ar	19.731044008186	4.092978022639	4.428460574956
Ar	23.607568906866	14.257327062968	26.413283047055
Ar	17.459433896427	10.399057482269	6.322265792191

Ar	20.093873078850	15.288885355338	2.282685090859
Ar	19.338779204431	0.574318942326	16.116898216135
Ar	12.191380683911	14.463568298494	8.099521985503
Ar	14.585474757523	1.594776331696	21.340711271174
Ar	21.439788155784	21.520575871786	4.981101338386
Ar	17.492363942379	17.663356388990	15.358348772002
Ar	21.937490970826	21.931734710287	18.179657178562
Ar	19.017342632064	10.144279930658	23.418252957152
Ar	19.246968885372	16.938445443320	21.911288788462
Ar	23.378219142439	7.312797794978	27.925447724170
Ar	24.701152773799	27.085090484180	14.396836308446
Ar	28.130222430789	11.535382776212	30.927817647705
Ar	28.469485050483	25.378755093159	27.887812581542
Ar	26.582400719676	26.249750053997	21.125899466115
Ar	28.302878436833	18.473323877333	29.441494884405
Ar	18.779482546452	8.985276533710	-0.538275301418
Ar	14.897944340630	12.942954985199	19.047742492462
Ar	22.852483452513	27.867283083687	7.6558175840597
Ar	14.141676608208	1.218526591109	7.662460918775
Ar	11.908208642266	7.609815075015	9.467582094863
Ar	16.224022157628	11.740213537537	12.796071657826
Ar	12.751254161174	2.533774117881	14.414178487118
Ar	14.828046055569	19.480085035159	4.131549673008
Ar	13.529315564581	20.703322806374	10.812602079490
Ar	16.625984974508	5.015897276738	27.359120900664
Ar	15.473074678741	24.091058049633	16.610524415071
Ar	5.786242858805	8.529272588755	24.694348380359

Ar	13.193312501241	6.217658306157	2.742100627245
Ar	15.399509194858	29.854082277215	24.703058041937
Ar	13.433904420356	13.153258498132	1.349834963883
Ar	20.067760385801	28.515501831023	19.539574055703
Ar	18.105555368039	11.543012483146	30.127795823430
Ar	16.406730048494	25.129690656532	29.986470247163
Ar	18.321098595552	18.543906030206	28.528565125278
Ar	10.614013959123	8.932179949911	16.005936155973
Ar	10.894569108211	15.745341800259	14.620949586006
Ar	12.396850333925	8.016505973426	22.743400906112
Ar	16.165540432864	25.838198696379	6.866105688055
Ar	12.802968688771	19.086321461169	20.379780153468
Ar	13.806362563043	14.360686809843	25.452678184332
Ar	18.176838457049	29.232993358357	12.754172456086
Ar	21.939858519340	27.629407232369	26.330184118316
Ar	22.972655305012	22.797502898194	31.532097260176
Ar	8.532534531018	13.577069605175	20.854044835223
Ar	7.767389391875	10.389659230435	4.546179446172
Ar	6.366257246582	11.721417068318	11.292312996732
Ar	7.908947606576	3.732686984743	19.662224594973
Ar	11.426121566904	27.296423071603	11.905131068743
Ar	8.632752926799	22.188859278043	15.820087199935
Ar	7.580001575622	3.419688769887	5.990159573938
Ar	32.448669882889	15.936463676769	18.185399768877
Ar	8.124958710352	17.376036813364	3.235288301688
Ar	6.217899850514	4.769290104512	12.745624655007
Ar	11.675622908154	20.794466215853	26.984143255488

Ar	17.310796416154	23.318019788440	23.334526284459
Ar	20.093846143901	22.623808058906	11.617365609155
Ar	6.765690576973	18.665702094794	9.969947707578
Ar	9.822356848903	2.905398325256	26.550323268972
Ar	10.734753078103	25.506019196532	21.743440800799
Ar	13.509872494579	30.643955624167	17.869398984459
Ar	12.788090625760	15.906346360957	32.084864546199
Ar	3.942165690076	9.440955189973	17.722591305449
Ar	22.859658314665	15.845150648025	33.141599782047
Ar	4.2228912411278	16.497277225789	16.277194712244
Ar	6.232900157993	19.970721130866	22.277558964522
Ar	7.253740527845	15.075473916254	27.499086594298
Ar	9.493422947214	23.758630886964	6.027331728784
Li	19.948568930254	14.446679476605	13.143602049066

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