Supplementary Information of

Revisiting the Potential Energy Surface of $C_nBe_{3n+2}H_{2n+2}^{2+}$ (n=2-4) Clusters: Are Planar Pentacoordinate Carbon Structures the Global Minima?

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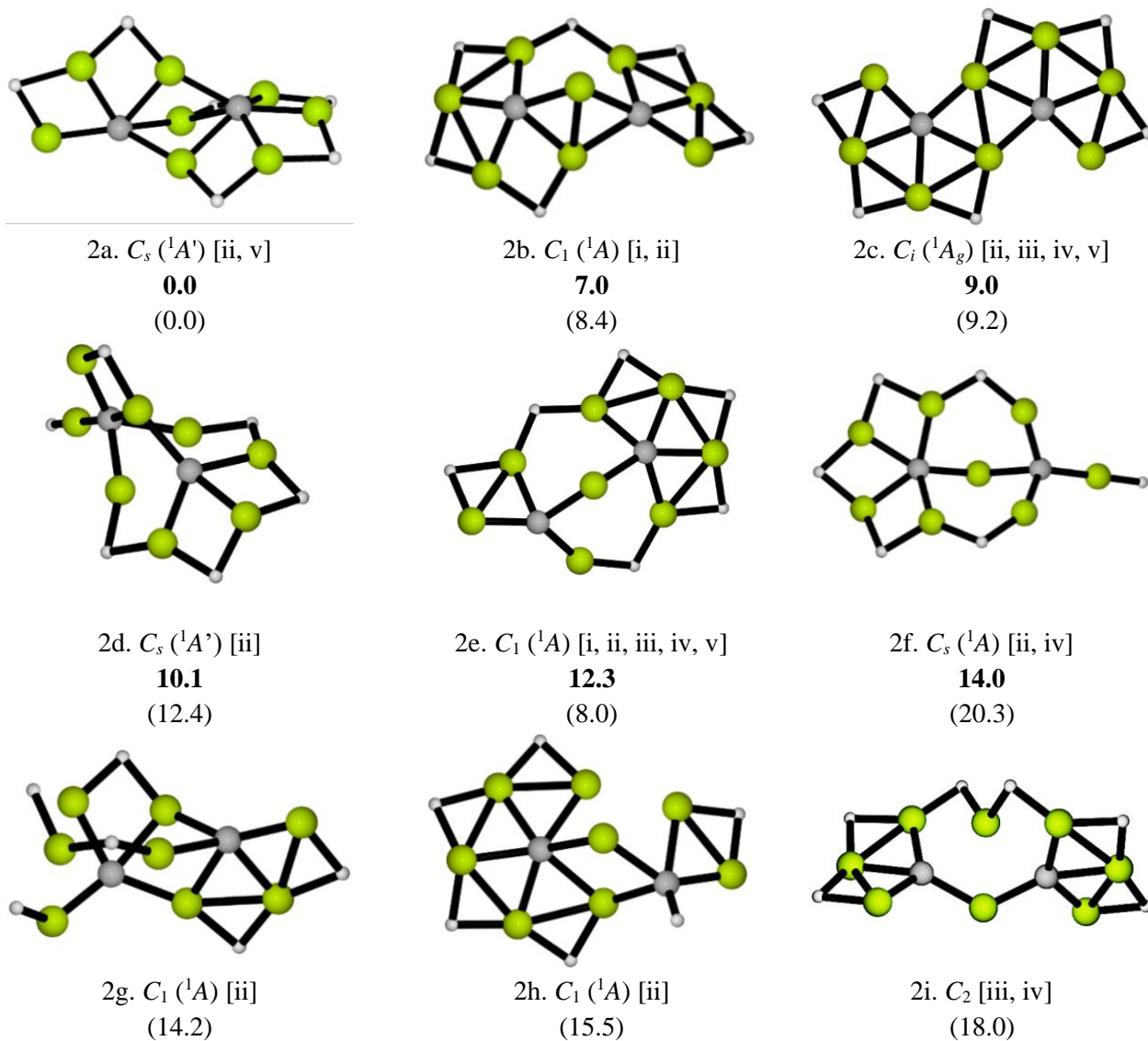* Correspondence: wtiznado@unab.cl (W.T.)

Figure S1. The employed methodology involved permutation; we have used as molecular templates the acenes $C_{4n+2}H_{2n+4}$ (n=2-4). Carbon atoms were introduced to the center of each ring, whereas the perimeter of carbon was replaced by beryllium. Additionally, Be-H fragments were eliminated from each ring until the targeted stoichiometry was achieved.
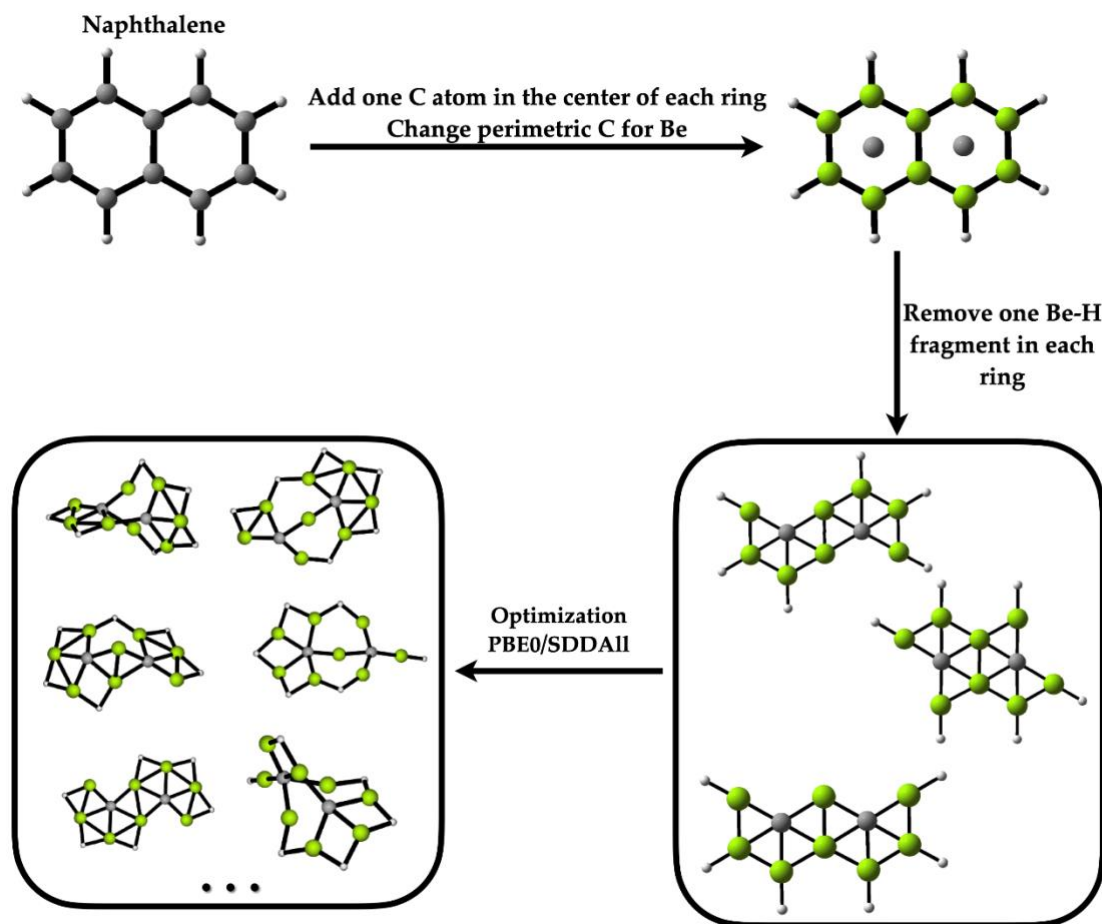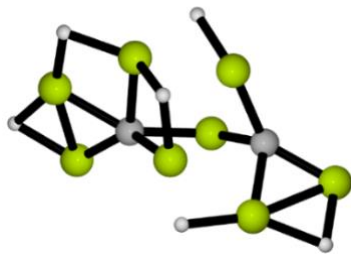
Figures S2. Minimum energy isomers of $CBe_5H_4^+$ and their respective point group symmetries and spectroscopic states. Relative energies are shown in kcal·mol^{-1} at PBE0-D3/def2-TZVP levels, including zero-point energy (ZPE) corrections. Within the brackets the methodology by which it was identified; (i) standard AUTOMATON; (ii) guided AUTOMATON, (iii) Fragment Kick, (iv) Permutation, and (v) exposed in BOMD; a special tag (ref) identifies the isomer discussed in the main text. To facilitate the connection of the structures with their Cartesian coordinates (at end of the ESI), a number-letter label was assigned to each structure.

1a. C_{2v} ($^2A_1$) [i, ii]
0.0

1b. C_s ($^2A'$) [i]
27.6

1c. C_1 (^2A) [i]
27.6

1d. C_1 (^2A) [ref]
54.2
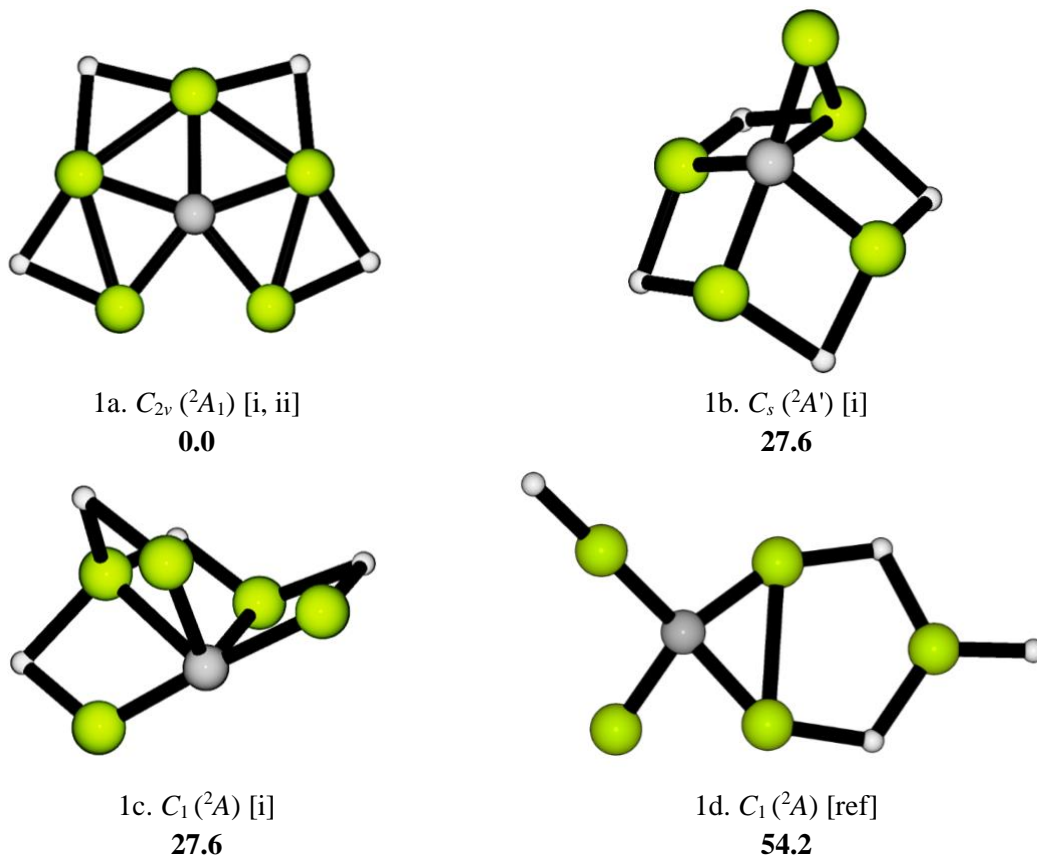
Figures S3. Minimum energy isomers of $C_2Be_8H_6^{2+}$ and their respective point group symmetries and spectroscopic states. Relative energies are shown in kcal·mol⁻¹ at led as DLPNO-CCSD(T)/CBS (in **black**) and PBE0-D3/def2-TZVP (in parentheses) levels including zero-point energy (ZPE) corrections. Within the brackets the methodology by which it was identified; (i) standard AUTOMATON; (ii) guided AUTOMATON, (iii) Fragment Kick, (iv) Permutation, and (v) exposed in BOMD. To facilitate the connection of the structures with their Cartesian coordinates (at end of the ESI), a number-letter label was assigned to each structure.
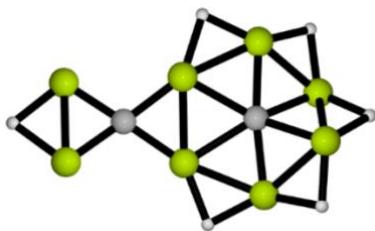

2a. C_s ($^1A'$) [ii, v]
0.0
(0.0)

2b. C_1 (^1A) [i, ii]
7.0
(8.4)

2c. C_i (^1A_g) [ii, iii, iv, v]
9.0
(9.2)

2d. C_s ($^1A'$) [ii]
10.1
(12.4)

2e. C_1 (^1A) [i, ii, iii, iv, v]
12.3
(8.0)

2f. C_s (^1A) [ii, iv]
14.0
(20.3)

2g. C_1 (^1A) [ii]
(14.2)

2h. C_1 (^1A) [ii]
(15.5)

2i. C_2 [iii, iv]
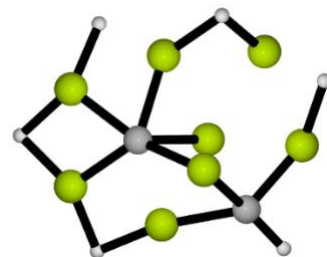(18.0)

2j. C_1 (^1A) [i]
(18.9)

2k. C_1 (^1A) [iv]
(19.5)

2l. C_1 (^1A) [ii]
(20.1)

2m. C_1 (^1A) [i, ii]
(20.2)

2n. C_1 (^1A) [ii]
(20.4)
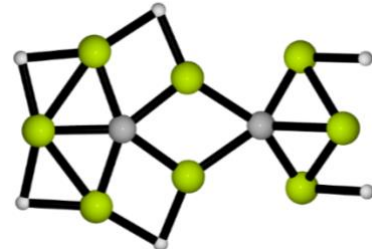
2o. C_s ($^1A'$) [ii, iv]
(21.1)
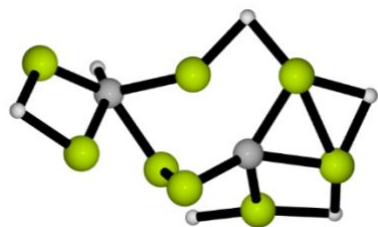
2p. C_1 (^1A) [ii]
(21.5)
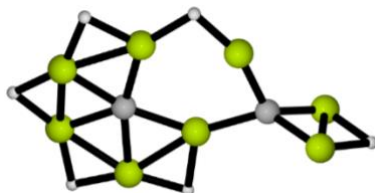
2q. C_1 (^1A) [ii]
(21.8)
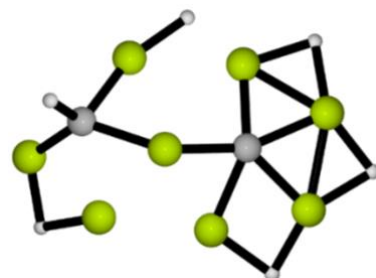
2r. C_1 (^1A) [ii, iii]
(22.3)
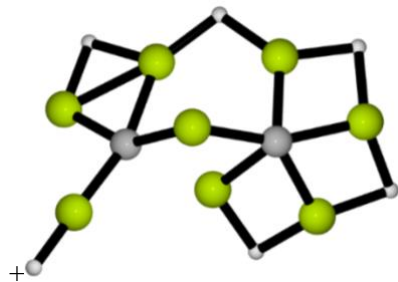
2s. C_1 (^1A) [iv]
(22.5)
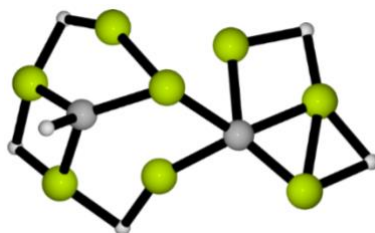
2t. C_1 (^1A) [iii]
(23.0)
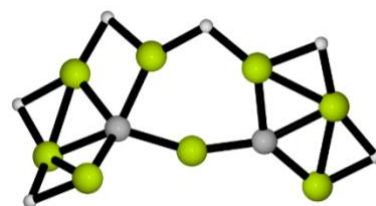
2u. C_1 (^1A) [ii, iii, iv]
(23.1)

2v. C_1 (^1A) [ii, iii]
(23.4)
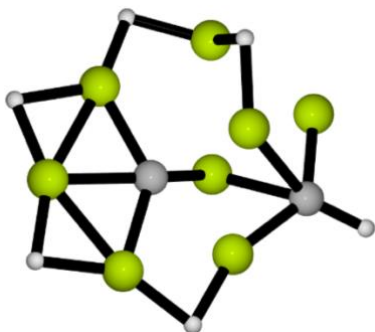
2w. C_1 (^1A) [ii]
(24.9)
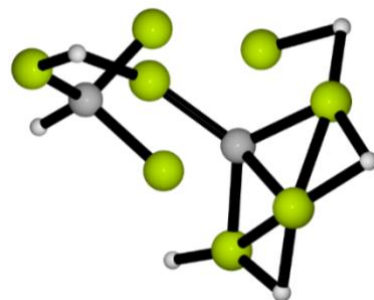
2x. C_1 (^1A) [ii]
(25.9)
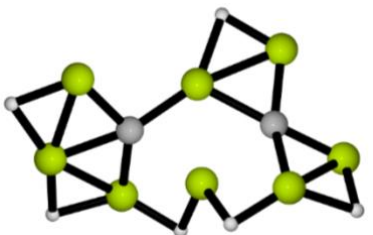
2y. C_1 (^1A) [iv]
(26.4)
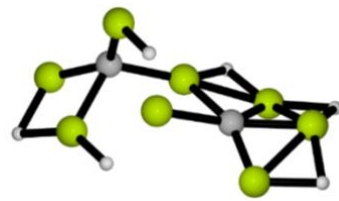
2z. C_1 (^1A) [ii]
(27.2)
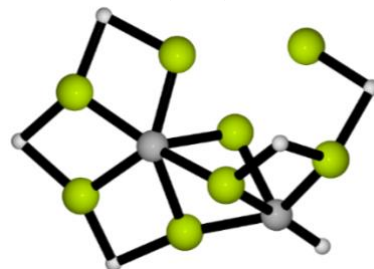
2ab. C_1 (^1A) [i]
(27.4)
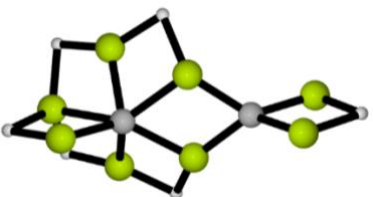
2ac. C_1 (^1A) [ii]
(28.0)
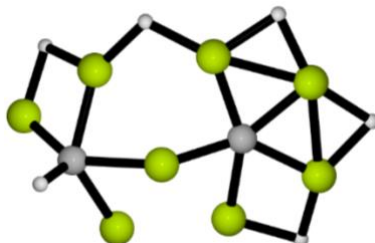
2ad. C_1 (^1A) [ii]
(28.8)
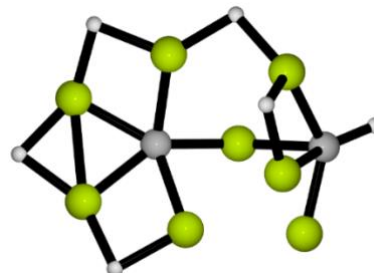
2ae. C_1 (^1A) [ii]
(29.2)
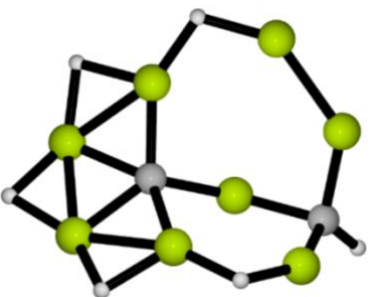
2af. C_1 (^1A) [ii]
(30.6)
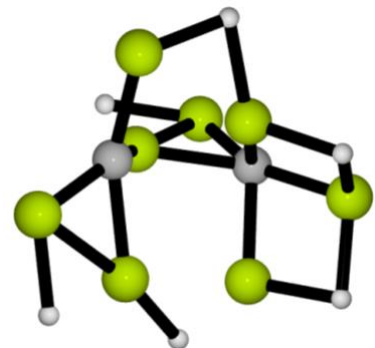
2ag. C_1 (^1A) [ii]
(30.8)

Figures S4. Minimum energy isomers of $C_3Be_{11}H_8^{2+}$ and their respective point group symmetries and spectroscopic states. Relative energies are shown in kcal·mol^{-1} at PBE0-D3/def2-TZVP levels including zero-point energy (ZPE) corrections. Within the brackets the methodology by which it was identified; (i) standard AUTOMATON; (ii) guided AUTOMATON, (iii) Fragment Kick, (iv) Permutation, and (v) exposed in BOMD. To facilitate the connection of the structures with their Cartesian coordinates (at end of the ESI), a number-letter label was assigned to each structure.
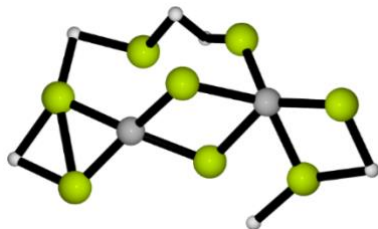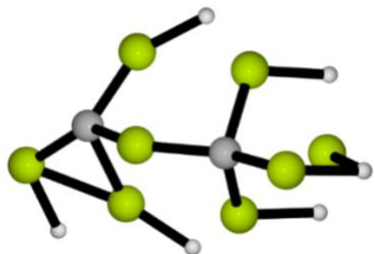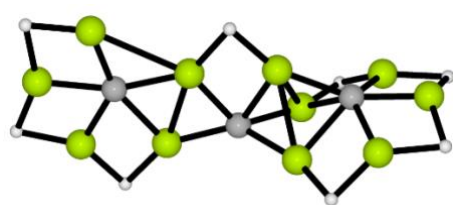
3a. C_s ($^1A'$) [iv]
0.0
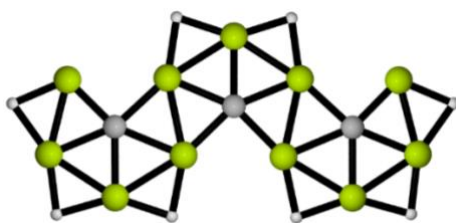
3b. C_{2v} ($^1A_1$) [iv, v]
11.8
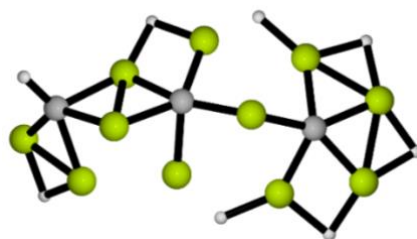
3c. C_1 (^1A) [iv]
13.8
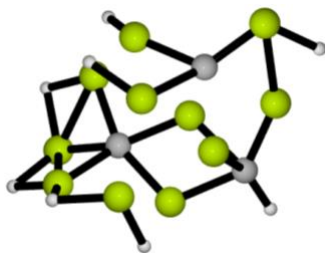
3d. C_1 (^1A) [ii]
20.1
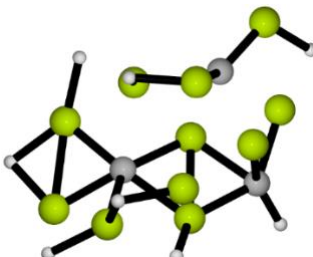
3e. C_1 (^1A) [ii]
20.1
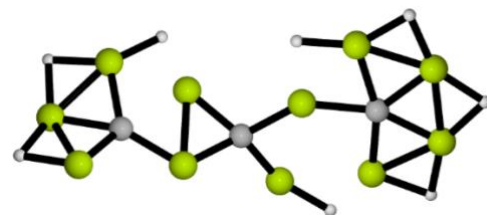
3f. C_1 (^1A) [iv]
21.1
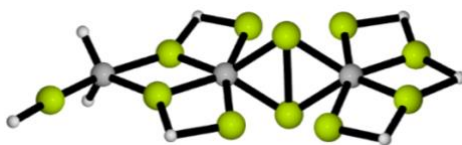
3g. C_1 (^1A) [iv]
22.2
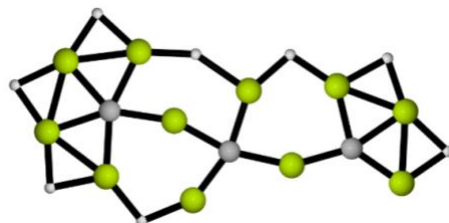
3h. C_s (^1A) [iv]
22.5
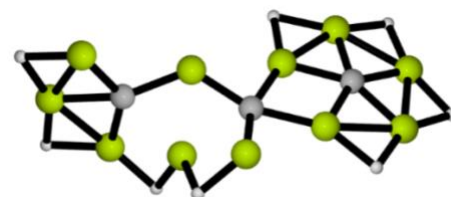
3i. C_1 (^1A) [iv]
22.9
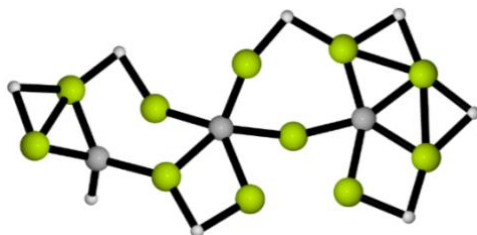
3j. C_1 (^1A) [iv]
23.4
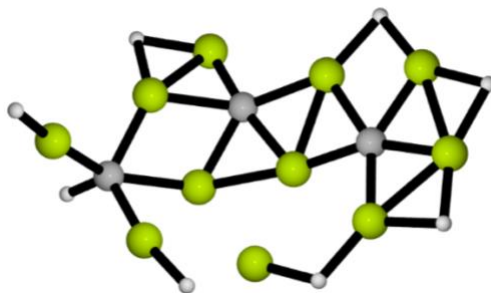
3k. C_1 (^1A) [iv]
26.6
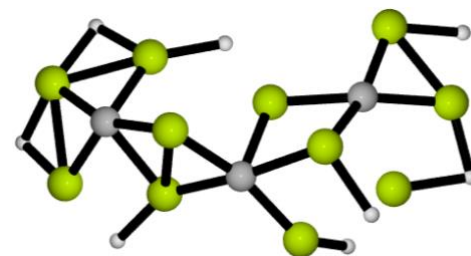
3l. C_1 (^1A) [ii]
26.9
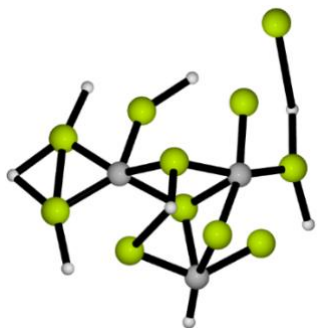
3m. C_1 (^1A) [i]
27.6
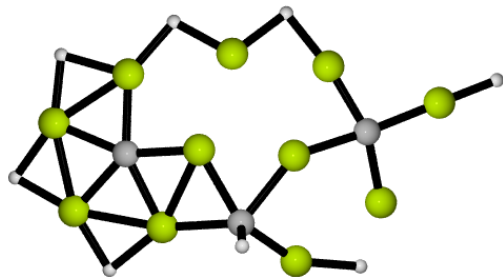
3n. C_1 (^1A) [ii]
28.6

Figures S5. Minimum energy isomers of $C_4Be_{14}H_{10}^{2+}$ and their respective point group symmetries and spectroscopic states. Relative energies are shown in kcal·mol^{-1} at led as DLPNO-CCSD(T)/CBS (in **black**) and PBE0-D3/def2-TZVP (in parentheses) levels including zero-point energy (ZPE) corrections. Within the brackets the methodology by which it was identified; (i) standard AUTOMATON; (ii) guided AUTOMATON, (iii) Fragment Kick, (iv) Permutation, and (v) exposed in BOMD. To facilitate the connection of the structures with their Cartesian coordinates (at end of the ESI), a number-letter label was assigned to each structure.

4a. C_{2h} (^1A_g) [iv, v]
0.0
(0.0)

4b. C_s (^1A) [iv]
0.2
(0.1)

4c. C_1 (^1A) [v]
(15.6)

4d. C_s (^1A) [v]
(19.7)

4e. C_1 (^1A) [v]
(23.1)
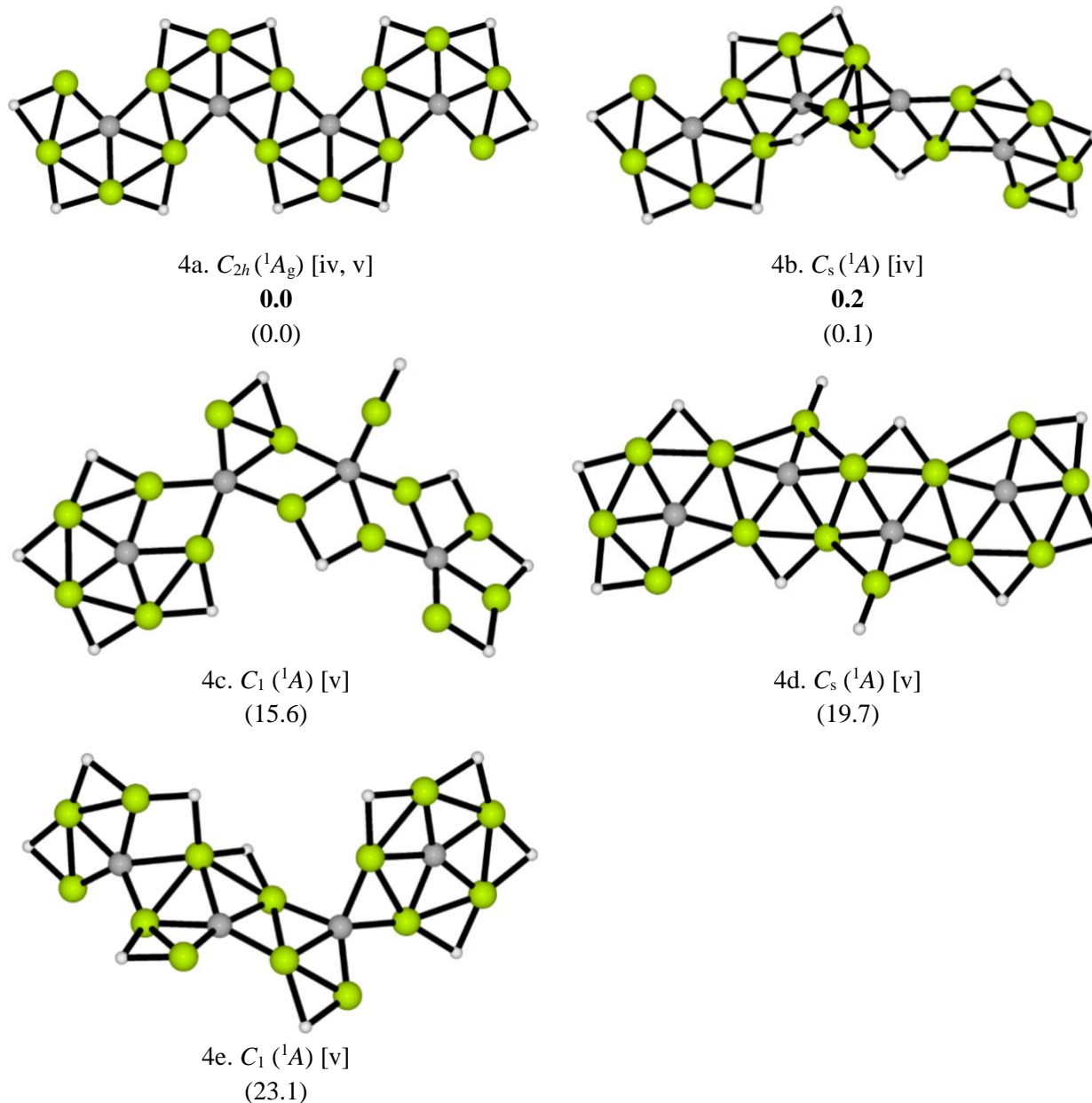
Table S1. HOMO-LUMO energy gaps and smallest vibrational frequencies for the $CBe_5H_4^+$ clusters.

System	$\Delta E_{H\text{-}L}$ (eV)	ν_{min} (cm^{-1})
1a	4.28	118.0
1b	3.24	189.9
1c	3.07	221.9
1d	3.08	23.7

Table S2. HOMO-LUMO energy gaps and smallest vibrational frequencies for the $C_2Be_8H_6^{2+}$ clusters.

System	$\Delta E_{H\text{-}L}$ (eV)	ν_{min} (cm^{-1})
2a	5.58	79.0
2b	5.07	75.6
2c	4.85	30.6
2d	5.08	64.2
2e	5.19	98.9
2f	4.60	108.5
2g	5.14	93.3
2h	4.32	68.3
2i	5.08	62.8
2j	5.42	92.9
2k	4.91	28.1
2l	4.25	145.5
2m	5.40	72.8
2n	5.19	115.5
2o	4.20	65.4
2p	4.25	102.1
2q	4.77	40.5
2r	3.92	88.0

System	$\Delta E_{H\text{-}L}$ (eV)	ν_{min} (cm^{-1})
2s	4.97	45.0
2t	3.90	65.7
2u	3.93	47.4
2v	4.98	75.3
2w	4.35	94.1
2x	3.77	72.7
2y	4.58	27.4
2z	5.14	53.7
2ab	4.29	136.1
2ac	5.07	35.9
2ad	3.57	81.4
2ae	3.85	75.0
2af	4.42	70.2
2ag	4.92	98.7

Table S3. HOMO-LUMO energy gaps and smallest vibrational frequencies for the $C_3Be_{11}H_8^{2+}$ clusters.

System	$\Delta E_{H\text{-}L}$ (eV)	ν_{min} (cm^{-1})
3a	4.84	27.2
3b	3.96	39.3
3c	3.93	72.3
3d	4.65	107.0
3e	4.67	123.7
3f	4.15	20.0
3g	3.57	47.6
3h	4.13	29.8
3i	3.91	40.1
3j	3.37	47.8

System	ΔE_{H-L} (eV)	ν_{min} (cm^{-1})
3k	3.88	48.3
3l	4.48	59.8
3m	4.47	73.0
3n	4.01	42.2

Table S4. HOMO-LUMO energy gaps and smallest vibrational frequencies for the $C_4Be_{14}H_{10}{}^{2+}$ clusters.

System	ΔE_{H-L} (eV)	ν_{min} (cm^{-1})
4a	3.51	20.4
4b	4.33	30.5
4c	4.01	26.2
4d	4.30	34.2
4e	3.83	21.5

Table S5. Cartesian coordinates of the C-Be-H systems with their label for easier identification.

1a				1b			
4	0.000000000	1.584622020	0.487687327	4	1.791115739	0.639797350	0.000000000
1	0.000000000	-2.405445048	-0.746925189	1	-1.888753235	0.032898858	1.257848873
6	0.000000000	0.000000000	-0.073811162	1	0.069087520	-1.649197573	1.300620762
4	0.000000000	-1.584622020	0.487687327	1	-1.888753235	0.032898858	-1.257848873
1	0.000000000	2.405445048	-0.746925189	1	0.069087520	-1.649197573	-1.300620762
4	0.000000000	-1.042691023	-1.380600180	4	-1.468160280	0.709531154	0.000000000
4	0.000000000	0.000000000	1.609784888	4	0.694912580	-1.194511338	0.000000000
4	0.000000000	1.042691023	-1.380600180	4	-0.441349775	-0.270691383	1.346236490
1	0.000000000	-1.444599522	1.973450370	4	-0.441349775	-0.270691383	-1.346236490
1	0.000000000	1.444599522	1.973450370	6	0.204137203	0.561807606	0.000000000

1c				1d			
4	1.728628000	0.411544000	0.237887000	4	-1.391565000	1.528201000	0.379371000
1	-2.276753000	-0.402166000	0.111160000	4	-2.051659000	-0.869559000	-0.276684000
4	0.101148000	1.266255000	-0.750797000	4	0.509076000	1.076508000	-0.304817000
4	0.680799000	-1.214301000	-0.009329000	4	0.385147000	-0.999528000	0.422245000
6	0.128388000	0.273310000	0.623305000	1	-3.108027000	-1.622318000	-0.535000000
1	-0.846865000	0.728950000	-1.737324000	1	1.910314000	1.070656000	-0.394725000
1	2.122745000	-0.954499000	-0.226432000	4	2.570829000	-0.230602000	-0.085017000
4	-1.005375000	-0.414596000	-0.763461000	1	3.873877000	-0.419735000	-0.208021000
4	-1.382718000	0.129301000	1.086154000	1	1.719905000	-1.386832000	0.412273000
1	-0.280161000	-1.721245000	-0.998863000	6	-0.753662000	0.076531000	0.107556000

2a				2b			
1	3.239027000	1.165533000	0.396601000	1	2.318969000	1.854761000	-0.868619000
1	-1.523789000	-0.808461000	2.019735000	1	-2.681134000	1.736436000	-0.372279000
1	0.766861000	2.392432000	-0.005325000	4	2.768730000	0.526779000	-0.519730000
4	-2.448986000	-0.390091000	0.961638000	4	-2.906990000	0.311045000	-0.042708000
4	1.786215000	1.424942000	0.405524000	1	3.827254000	-0.561610000	-0.417017000
1	-3.854017000	-0.193290000	0.406484000	1	-3.329635000	-0.782831000	-0.943393000
4	2.803803000	-0.240682000	0.316800000	4	1.022203000	1.364410000	-0.276901000
4	-3.071690000	0.314018000	-0.716753000	4	-2.056328000	-1.367585000	-0.499977000
4	-0.069657000	1.184584000	-0.241474000	1	-0.130758000	2.241988000	-0.248561000
6	-1.488099000	0.193500000	-0.365522000	1	-0.878096000	-1.950573000	-1.213042000
1	3.136391000	-1.380048000	-0.556408000	4	2.718958000	-1.206780000	0.264679000
4	-0.507985000	-0.366536000	1.023678000	6	-1.385647000	-0.196548000	0.540818000
6	1.073831000	-0.152391000	0.268940000	6	1.404495000	-0.247164000	0.240518000
4	1.667929000	-1.477567000	-0.678942000	4	-0.123882000	-0.952393000	-0.435430000
4	-0.147221000	-0.742638000	-0.959609000	4	-1.305051000	1.426203000	0.066188000
1	0.597960000	-1.857132000	-1.604951000	4	0.072437000	-0.070653000	1.287602000

2c				2d			
1	-3.748396364	-1.205183691	0.039912248	1	-1.275900000	1.252506000	2.185535000
1	3.748396364	1.205183691	-0.039912248	1	0.494065000	-2.424993000	0.321822000
4	-3.145801395	0.155229565	0.281368630	4	-2.263383000	0.773944000	1.239592000
4	3.145801395	-0.155229565	-0.281368630	1	0.545405000	1.652710000	-1.712475000
1	-3.329982942	1.592111496	0.111299619	1	3.133071000	0.978650000	-0.935506000
1	3.329982942	-1.592111496	-0.111299619	4	-2.852778000	-0.557448000	-0.937738000
4	-2.355117902	-1.462804532	-0.231839633	4	-0.353014000	0.573153000	1.177433000
4	2.355117902	1.462804532	0.231839633	4	1.648218000	-1.538984000	0.483946000
6	-1.457718425	-0.130214933	-0.030893814	4	2.807527000	-0.019769000	0.093288000
4	1.896106161	-1.530209822	0.167581348	4	-0.250977000	-1.162779000	0.097162000
4	-1.896106161	1.530209822	-0.167581348	6	-1.563133000	-0.013766000	0.003821000
6	1.457718425	0.130214933	0.030893814	4	-0.220906000	0.702346000	-0.872532000
4	0.050136594	-0.957640601	0.099964867	4	1.683615000	1.244035000	-0.883690000
1	0.667187507	-2.310023659	0.195261039	1	3.099516000	-1.454281000	0.251844000
1	-0.667187507	2.310023659	-0.195261039	6	1.074398000	0.090397000	0.268627000
4	-0.050136594	0.957640601	-0.099964867	1	-3.854047000	-0.982647000	-1.681509000

2e				2f			
1	-3.677662000	-0.478597000	0.024265000	4	1.509550000	1.392702000	-0.680712000
1	3.282372000	-1.526941000	-0.295690000	4	3.482662000	0.038441000	0.609624000
1	-2.501108000	1.972438000	-0.368230000	4	1.493258000	-1.450508000	-0.736342000
4	3.352377000	-0.212043000	0.309064000	4	0.439177000	-0.033040000	0.642269000
4	-2.749348000	0.644981000	0.203706000	1	0.354830000	2.192079000	-0.926852000
4	1.798960000	-1.104236000	-0.439562000	4	-0.935436000	1.563670000	-0.498727000
4	-2.430538000	-1.248599000	0.136384000	1	0.307767000	-2.227289000	-0.907528000
6	1.891105000	0.450632000	0.266240000	4	-0.987072000	-1.592045000	-0.506512000
4	-1.095269000	1.507705000	-0.376422000	4	-2.554963000	1.009691000	0.599015000
1	0.741158000	-2.058862000	-0.743297000	4	-2.596502000	-0.989020000	0.567468000
1	-1.754974000	-2.415430000	-0.420967000	1	-2.212950000	2.294956000	-0.082751000
4	1.231595000	1.730048000	-0.443926000	1	-2.300118000	-2.277267000	-0.123113000
1	0.012132000	2.394357000	-0.808462000	1	-3.700491000	0.029246000	0.720111000
4	0.369646000	0.159808000	0.823661000	6	-1.166316000	-0.015922000	0.170430000
6	-1.183786000	-0.068123000	0.285883000	6	1.927293000	-0.041278000	-0.046210000
4	-0.563882000	-1.523168000	-0.387991000	1	4.645167000	0.136916000	1.232544000
2g				2h			
1	1.081714000	-0.717890000	1.978753000	4	1.915770000	1.166389000	0.067345000
1	-1.738899000	2.059562000	-0.560779000	1	-2.879858000	-1.790490000	-0.068011000
1	3.018732000	0.882973000	1.123837000	1	3.209307000	1.237838000	-0.752433000
4	-0.607574000	1.089979000	-0.414332000	4	-2.730329000	-0.397158000	0.360006000
4	2.124434000	-0.353364000	0.984494000	4	0.443632000	0.204563000	1.011117000
4	-2.516899000	0.899623000	-0.118325000	1	-3.473338000	0.838945000	0.126975000
1	2.689388000	-1.425545000	0.131912000	4	3.189721000	-0.160382000	-0.466924000
1	-3.835639000	0.249658000	0.277763000	4	-1.458002000	-1.634280000	-0.386003000
4	0.077279000	-0.288960000	1.014370000	1	2.217274000	-1.477712000	0.956299000
1	0.786298000	-1.847940000	-1.471117000	1	-0.267334000	-2.286361000	-0.865500000
6	-1.412581000	-0.416598000	0.137125000	6	1.855069000	-0.602609000	0.391749000
4	2.248424000	1.407946000	0.050485000	6	-1.043307000	0.009991000	0.050379000
4	-2.929558000	-0.878442000	0.493674000	4	-0.202958000	1.586677000	-0.277515000
4	1.830430000	-0.965313000	-0.942280000	4	0.395664000	-1.001242000	-0.521228000
6	1.015511000	0.475209000	-0.434498000	1	-1.337266000	2.525440000	-0.461471000
4	-0.131331000	-0.799589000	-0.992117000	4	-2.138338000	1.362444000	-0.183955000
2i				2j			
4	-2.457004000	-0.914672000	1.233354000	1	3.553505000	-1.044312000	0.572916000
4	-3.118954000	-0.130987000	-0.348792000	1	-3.683879000	-1.014209000	0.008080000
4	0.005938000	-1.016431000	0.048518000	4	3.114824000	-0.309193000	-0.610133000
4	-1.715074000	0.969679000	-1.054160000	1	-2.602867000	1.595695000	0.542832000
4	0.010521000	0.957747000	-0.058173000	4	2.109108000	-0.738622000	0.968843000
1	-0.558478000	1.780017000	-1.196819000	4	-2.779593000	0.183290000	0.258069000
4	1.681404000	1.003718000	1.032311000	1	1.028843000	-0.884908000	1.921628000
4	2.458175000	-1.079631000	-1.116470000	4	-1.189121000	1.337345000	0.131707000
4	3.133986000	-0.016319000	0.287336000	1	-0.020836000	1.330743000	1.221245000
1	0.531814000	1.831948000	1.070327000	4	-2.386730000	-1.563123000	-0.354055000
1	3.841288000	-0.897660000	-0.713799000	4	0.179799000	-0.165112000	0.906640000
1	3.149675000	1.096213000	1.220238000	1	-0.344518000	2.227569000	-0.728649000
6	1.468605000	-0.254751000	-0.139189000	6	1.578283000	0.125114000	-0.438906000
6	-1.460797000	-0.250033000	0.147776000	6	-1.237794000	-0.448930000	-0.183253000
1	-3.173248000	0.958142000	-1.311023000	4	0.816648000	1.599991000	-0.147604000
1	-3.833866000	-0.832364000	0.783855000	4	0.141772000	-0.411497000	-1.104743000
2k				2l			
4	3.193175000	-0.934167000	-0.100377000	1	-2.803744000	1.286824000	-0.308940000
4	3.237549000	0.901018000	0.018860000	1	3.288944000	0.051734000	0.469771000
4	0.544797000	-0.903522000	0.310556000	4	-1.593473000	1.850403000	0.342024000
4	0.547732000	0.952339000	-0.281863000	4	2.267663000	1.012054000	-0.002852000
1	0.038473000	-2.291086000	0.432462000	1	-0.729286000	2.542555000	-0.584695000
4	-1.232375000	-1.689479000	0.175440000	1	1.688390000	-2.246724000	0.561958000
1	0.066628000	2.348169000	-0.412309000	4	-2.389596000	-0.019411000	0.184768000
4	-1.208710000	1.775524000	-0.115727000	1	1.743497000	2.336714000	0.235740000
4	-2.624140000	-0.624924000	-0.566065000	1	-2.069448000	-2.097447000	0.134645000
4	-2.553651000	0.756656000	0.767886000	4	2.239416000	-0.943717000	0.176430000

1	-2.498993000	-2.070011000	-0.408136000	6	-1.302736000	-1.322380000	-0.004492000
1	-2.410758000	2.194973000	0.569288000	4	0.392594000	-1.674002000	0.136663000
1	-3.676240000	0.081078000	0.140921000	4	0.421105000	1.721703000	-0.120037000
6	-1.100358000	0.043273000	0.044962000	4	-0.492504000	0.055730000	0.866361000
6	1.897452000	0.012669000	-0.011791000	4	-0.446379000	-0.532979000	-1.230222000
1	4.387854000	-0.041653000	-0.066305000	6	0.896713000	0.022979000	-0.365790000
2m				**2n**			
4	-0.000573000	0.433420000	1.039781000	1	-3.598308000	-0.435787000	-0.120101000
1	-2.720619000	1.585857000	-0.347283000	4	1.177931000	1.655381000	0.462420000
4	0.306495000	-0.917880000	-0.383861000	4	-2.653037000	-0.246014000	-1.168983000
1	-0.252419000	1.765497000	-1.458422000	1	3.164561000	-1.593718000	0.398739000
4	3.140614000	0.208047000	0.465685000	4	-2.366567000	-0.264164000	0.789374000
4	-1.265311000	1.283454000	-0.438507000	4	3.328232000	-0.289731000	-0.209318000
1	1.176534000	-2.059037000	-0.887095000	1	0.573672000	-1.966871000	0.765821000
4	0.767081000	1.602216000	-0.445546000	4	0.443236000	0.196416000	-1.046180000
4	-2.323111000	-1.619493000	0.121994000	6	-1.137655000	-0.017493000	-0.652750000
4	-2.828690000	0.199171000	0.080935000	6	1.897135000	0.431901000	-0.283453000
6	-1.234117000	-0.436263000	0.175115000	1	-2.158845000	1.044694000	1.468106000
6	1.553207000	0.246874000	0.199597000	4	1.688693000	-1.108399000	0.433076000
4	2.247337000	-1.183315000	-0.477077000	4	-1.127207000	1.291692000	0.463044000
1	-3.663567000	-1.071716000	0.009554000	1	-1.734492000	-1.441706000	1.422276000
1	3.712100000	-0.995315000	-0.120960000	1	-0.053924000	2.218483000	0.914639000
1	-0.341934000	1.888559000	0.702318000	4	-0.677082000	-1.304732000	0.409373000
2o				**2p**			
4	2.250267000	-1.336537000	-0.438693000	1	0.481232000	2.335167000	-0.375680000
4	3.004222000	0.002405000	0.690827000	1	3.069464000	-1.132661000	-0.742083000
4	-0.086746000	-1.004880000	0.003562000	4	-3.101506000	0.582718000	-0.066798000
4	2.247569000	1.334538000	-0.444934000	4	2.797985000	0.061014000	0.076601000
4	-0.085352000	1.003065000	0.004008000	1	-3.321546000	-0.020489000	1.201748000
4	-1.959403000	-1.576611000	0.016073000	4	1.624131000	-1.371507000	-0.566376000
4	-1.957378000	1.577141000	0.019249000	4	-0.248852000	1.025615000	-0.256194000
4	-3.103533000	0.001123000	0.044314000	4	0.038752000	-0.602466000	1.549894000
1	-0.654821000	-2.373130000	-0.111687000	1	-1.965900000	0.213420000	-1.813299000
1	-0.650945000	2.372124000	-0.109361000	6	1.100524000	-0.022245000	0.408536000
1	-3.434970000	-1.461280000	-0.052606000	6	-1.677742000	0.119682000	-0.750925000
1	-3.432815000	1.464502000	-0.051095000	1	0.496614000	-2.028381000	-1.167576000
6	-1.421268000	-0.000051000	0.127795000	1	3.068630000	1.496439000	-0.106631000
6	1.406066000	-0.001136000	-0.089776000	4	-0.363832000	-1.014446000	-0.466024000
1	3.511597000	1.348837000	0.256486000	4	1.621632000	1.610296000	0.149539000
1	3.514574000	-1.344904000	0.262527000	4	-1.959606000	-0.653252000	0.843823000
2q				**2r**			
1	-0.207924000	2.429475000	0.093072000	4	-1.684077000	-1.435101000	0.029626000
1	2.560882000	-2.322315000	0.142648000	4	2.784998000	0.647613000	-0.041290000
4	-1.241742000	1.478715000	0.074897000	6	-2.014819000	0.433616000	0.356255000
4	1.220420000	-1.778344000	-0.098338000	1	1.724524000	-2.509528000	-0.256210000
4	0.988296000	1.568116000	0.024846000	1	-2.895365000	-1.636505000	-0.910003000
1	-0.155112000	-2.116005000	-0.126381000	4	-1.130290000	1.701995000	-0.250889000
4	2.758901000	0.942408000	-0.198833000	1	2.519397000	2.056886000	-0.351257000
4	2.868378000	-0.899388000	0.248896000	1	-2.567797000	0.814804000	1.236795000
6	-1.943310000	0.039962000	0.003806000	4	-3.128755000	-0.254144000	-0.644341000
4	-3.210702000	-0.358851000	0.935965000	4	1.120380000	1.588396000	-0.193065000
6	1.365290000	-0.067674000	-0.010515000	1	3.688190000	-0.488591000	-0.252735000
4	-3.225513000	-0.275026000	-0.940640000	1	-0.011792000	2.513627000	-0.535085000
4	-0.314662000	-0.586622000	-0.040499000	6	1.225461000	-0.050198000	0.170792000
1	2.261947000	2.306234000	-0.143502000	4	0.526532000	-1.662005000	-0.062870000
1	3.923035000	0.095846000	0.053070000	4	2.437638000	-1.249722000	-0.070164000
1	-4.351497000	-0.604595000	-0.006229000	4	-0.356680000	-0.099832000	0.709547000
2s				**2t**			
4	-1.367386000	1.396175000	-0.287226000	1	-2.255098000	1.795444000	-0.865200000
4	-2.860359000	0.144755000	-0.100419000	6	-1.506444000	-0.153521000	0.662343000
4	-1.910854000	-1.392487000	0.617768000	4	-2.722054000	0.482879000	-0.445104000
4	0.230212000	-0.156632000	-1.195963000	4	-1.155201000	1.580827000	0.111120000

4	0.906935000	1.566158000	0.202607000	4	-2.010770000	-1.355236000	-0.554049000
4	-0.029595000	-0.785298000	0.655322000	4	0.106677000	0.414193000	1.101219000
4	2.654280000	0.877091000	0.641384000	1	-3.052146000	-0.660998000	-1.327627000
4	2.448631000	-1.404920000	-0.370145000	1	-0.822075000	-2.067661000	-0.996960000
1	-0.285091000	2.349809000	-0.009937000	1	3.832595000	-0.545739000	-0.418149000
1	-0.752334000	-1.757702000	1.487072000	6	1.390973000	-0.281521000	0.186771000
1	2.166447000	2.206689000	0.828971000	4	2.765715000	0.530479000	-0.505075000
1	3.181168000	-2.476041000	-0.598274000	1	-1.989449000	-0.541634000	1.580216000
6	1.495612000	-0.060590000	-0.039247000	4	2.706889000	-1.238817000	0.181429000
6	-1.252984000	-0.279824000	-0.506934000	4	1.038940000	1.441146000	-0.287651000
1	-3.263471000	-0.879396000	0.884163000	4	-0.073420000	-1.127837000	-0.092252000
1	-2.789943000	1.619752000	0.031780000	1	2.360921000	1.880633000	-0.818929000
2u				2v			
4	0.747970000	1.400176000	-0.285792000	1	-0.592743000	1.985380000	1.067581000
4	2.442360000	1.039559000	0.633245000	1	3.425384000	-1.335261000	0.868906000
4	2.986052000	-0.803573000	0.480136000	1	-3.060402000	0.767014000	1.445530000
4	2.050368000	-1.334669000	-1.095641000	4	3.066724000	0.058445000	0.704742000
4	-0.178307000	-0.632141000	0.135424000	4	-1.692273000	1.082183000	0.979661000
4	-1.564912000	1.183166000	-0.404133000	4	2.072791000	-1.468933000	0.187742000
1	3.304719000	-1.840676000	-0.575141000	4	-0.017942000	1.123766000	-0.052498000
4	-2.948974000	-1.322543000	0.661850000	6	1.643984000	0.184623000	-0.052021000
4	-3.265084000	0.402669000	-0.006857000	4	-2.868712000	-0.374652000	0.557371000
1	-0.439825000	2.052142000	-0.708209000	1	0.873091000	-2.253733000	0.116583000
1	-2.948061000	1.740445000	-0.485253000	6	-1.308072000	-0.144526000	-0.167395000
1	-4.227512000	-0.654476000	0.514586000	4	1.590290000	1.350896000	-1.172316000
6	-1.759989000	-0.381925000	0.150413000	1	-3.585376000	-1.182814000	-0.504935000
6	1.453153000	-0.189959000	-0.106246000	4	0.222692000	-0.903390000	-0.127894000
1	3.687447000	0.355625000	1.025765000	4	-2.292093000	-0.983700000	-1.130935000
1	1.748644000	2.277785000	0.425144000	1	0.418512000	2.088301000	-1.288433000
2w				2x			
1	-3.161238000	-1.044816000	0.011538000	1	-3.365789000	0.511871000	-0.601727000
4	2.435768000	0.493971000	-0.273862000	1	2.862380000	-0.993281000	0.673034000
4	-2.514894000	0.265057000	-0.057070000	4	-2.489047000	-0.655936000	-0.575416000
1	2.544324000	-1.697961000	0.102072000	4	2.451578000	-0.263772000	-1.317794000
4	-1.773955000	-1.528050000	0.050084000	1	-2.625232000	-1.956647000	0.086366000
4	0.687413000	0.122312000	1.049588000	6	2.100534000	-0.293687000	0.293821000
1	-2.653365000	1.703578000	-0.082232000	4	-2.148331000	1.201173000	-0.160681000
6	1.726390000	-0.974032000	0.016386000	1	-0.111617000	-2.128469000	1.238330000
1	-0.893754000	-2.663628000	0.078033000	1	-1.576876000	2.429935000	0.315084000
4	0.681948000	0.039216000	-1.047044000	1	1.413782000	0.193492000	-2.170251000
6	-0.792659000	-0.064439000	-0.026805000	4	-0.347681000	1.604277000	0.489560000
4	0.944709000	2.015145000	0.011040000	4	0.497788000	-0.849044000	0.782773000
4	-1.161739000	1.641562000	-0.064600000	4	-1.292742000	-1.621534000	0.590207000
4	0.175979000	-1.634432000	0.014892000	6	-0.920087000	-0.039888000	-0.059859000
1	-0.276878000	2.747446000	-0.208785000	4	1.739042000	1.253890000	0.760264000
1	0.937606000	1.527079000	1.429773000	4	0.661914000	0.331819000	-0.822863000
2y				2z			
4	2.255266000	-1.395624000	0.884427000	1	-3.233229000	-0.284510000	-1.545134000
4	3.011419000	0.166249000	0.185563000	4	2.945212000	0.053479000	0.269033000
4	-0.113123000	-1.093888000	-0.124399000	1	-1.008106000	-1.891051000	-0.794275000
4	1.691436000	1.036740000	-0.909726000	4	1.785279000	1.480291000	-0.261364000
4	-0.032673000	0.941358000	0.076537000	4	-2.011223000	-0.867936000	-0.825645000
4	-1.887147000	-1.656171000	-0.585020000	4	-0.081233000	1.045788000	0.032011000
1	0.546254000	1.868028000	-0.990070000	4	-2.950517000	0.806988000	-0.614364000
4	-2.960515000	0.693049000	-0.501005000	1	0.642517000	2.344741000	-0.170600000
4	-1.838310000	1.186891000	0.947638000	4	-0.276193000	-0.992257000	0.239971000
1	-0.727836000	-2.476112000	-0.569250000	1	3.218347000	1.466274000	0.047910000
1	-0.602511000	1.812078000	1.197431000	6	-1.667560000	0.427075000	0.273547000
1	-3.153031000	1.770102000	0.431109000	6	1.241607000	-0.142227000	-0.055567000
6	-1.608125000	-0.126470000	-0.168174000	1	3.516359000	-1.218769000	-0.315183000
6	1.338803000	-0.273940000	0.160664000	4	-1.517110000	-0.325689000	1.694630000
1	3.138535000	1.297266000	-0.711015000	4	2.114818000	-1.381822000	-0.606901000

1	3.650331000	-1.019195000	0.864642000	1	-0.616300000	-1.401146000	1.759918000

2ab				2ac			
1	-3.418649000	0.053984000	-0.103859000	1	-2.666368000	1.382447000	-1.059243000
1	3.020245000	1.169230000	-0.124021000	1	4.382281000	0.004917000	0.021036000
4	-2.294874000	-0.931070000	-0.056231000	1	-2.674925000	-1.254563000	-1.199119000
4	1.790846000	1.825008000	-0.536692000	4	3.202085000	-0.158063000	0.933873000
4	-2.339424000	1.040217000	0.166597000	4	-2.764362000	0.027849000	-0.446106000
4	2.347313000	-0.038120000	0.451900000	4	0.517241000	-0.995384000	0.020354000
1	-1.762527000	-2.257188000	-0.388013000	1	-3.502156000	-0.042011000	0.910738000
1	1.595488000	0.496664000	1.640792000	4	3.207000000	0.156885000	-0.900944000
1	-1.822762000	2.413305000	-0.064522000	1	-0.097812000	2.176408000	-0.580907000
1	2.050644000	-1.898378000	-0.626895000	1	-0.108487000	-2.103096000	-0.822303000
6	-0.923921000	0.084078000	0.207279000	4	-1.332876000	1.447102000	-0.477714000
4	0.425188000	0.127653000	-0.912981000	6	1.884145000	-0.004574000	0.018740000
4	-0.413570000	-1.603732000	-0.227049000	4	-1.341856000	-1.389290000	-0.628862000
6	1.270415000	-1.240329000	-0.228454000	4	0.520781000	0.984161000	0.145727000
4	-0.496337000	1.723817000	-0.066818000	4	-2.192073000	-0.075077000	1.447502000
4	0.545507000	-0.403801000	1.129665000	6	-0.983527000	-0.021566000	0.373673000

2ad				2ae			
4	1.276495000	1.851180000	-0.143791000	1	1.073780000	0.894020000	1.826613000
4	-0.731434000	-1.628133000	0.104362000	1	-3.481159000	-0.399312000	0.207416000
1	-2.264910000	2.188829000	-0.549146000	4	1.347943000	1.470182000	0.485499000
1	-1.984222000	-2.417437000	-0.061614000	1	-1.546506000	-2.364648000	0.598106000
4	0.270960000	0.361338000	0.682272000	1	0.327022000	2.447135000	0.130159000
6	-1.245493000	-0.022253000	0.185197000	4	-2.247397000	-1.198963000	0.108339000
4	-0.903340000	1.689671000	-0.227273000	1	2.991586000	0.544017000	-0.856524000
4	1.595541000	-1.325179000	-0.073906000	4	-2.574612000	0.685838000	-0.175165000
1	0.568754000	-2.312175000	0.055550000	4	1.428106000	-0.366486000	1.202185000
6	2.031511000	0.346710000	0.383266000	4	-0.317421000	-1.568895000	0.319550000
1	-3.712638000	-0.218737000	-0.363230000	4	0.480805000	0.024021000	-1.015431000
1	2.542642000	0.566512000	1.339085000	6	-1.009735000	-0.063021000	-0.328386000
4	-2.585454000	-1.084524000	0.005537000	6	2.095148000	0.098505000	-0.410526000
4	-2.677689000	0.828286000	-0.234183000	1	-2.266936000	2.086641000	0.116142000
4	3.097664000	-0.261310000	-0.715866000	4	1.845285000	-1.528115000	-0.316479000
1	2.687405000	-1.539741000	-1.193178000	4	-0.865275000	1.627228000	-0.005608000

2af				2ag			
1	3.502332000	-0.474101000	0.425848000	1	0.223394000	-1.968919000	1.620380000
1	-2.855224000	-0.849228000	1.391392000	1	-1.658940000	2.072672000	0.959256000
1	1.768685000	-2.325332000	-0.724887000	4	1.347874000	-1.666379000	0.850802000
1	0.322554000	2.742252000	-0.751294000	4	-1.114640000	1.529678000	-0.299898000
4	2.299981000	-1.211476000	0.038510000	4	2.849877000	0.395011000	-0.185764000
4	-0.552749000	-0.143184000	0.793062000	1	0.117297000	2.243267000	-0.664890000
4	2.520623000	0.608596000	0.600245000	4	-0.306229000	-0.555003000	1.098393000
4	1.068527000	1.606809000	-0.234499000	4	-1.890812000	0.652003000	1.261458000
1	2.428915000	2.007870000	0.253165000	6	1.393482000	-0.308336000	-0.017002000
4	-2.389368000	0.965114000	-0.053957000	6	-1.501892000	-0.146305000	-0.189422000
4	0.543074000	-1.474471000	-0.760315000	1	2.690366000	1.785440000	-0.496708000
6	-2.166052000	-0.535636000	0.599884000	4	1.203554000	1.356758000	-0.387373000
1	-0.662019000	-2.114321000	-1.306737000	4	-1.846935000	-1.107870000	-1.428015000
4	-1.102760000	2.442397000	-0.691350000	4	-0.031024000	-0.621796000	-0.986501000
6	0.992168000	-0.067943000	0.124520000	1	-0.658366000	-1.524203000	-2.115896000
4	-1.753232000	-1.630986000	-0.512656000	1	-0.909949000	0.189974000	2.243997000

3a				3b			

1	-4.241171000	-1.861149000	1.362483000	4	-1.235523000	-0.777641000	0.000000000
1	-0.624337000	1.899739000	0.000000000	4	-1.596800000	1.095945000	0.000000000
1	-1.639359000	-1.684456000	2.274627000	4	-3.934409000	1.168349000	0.000000000
4	0.685215000	1.146993000	0.000000000	4	-4.490058000	-0.600474000	0.000000000
4	-2.857220000	-1.364972000	1.543177000	4	-2.952988000	-1.745714000	0.000000000
1	3.253973000	-1.067393000	0.000000000	4	1.225288000	-0.762194000	0.000000000
4	-4.032698000	-1.342091000	0.000000000	4	-0.009825000	2.127784000	0.000000000
4	1.916445000	-0.384281000	0.000000000	1	-1.414032000	2.579506000	0.000000000
4	-0.952021000	-1.220763000	1.026170000	4	1.605524000	1.104721000	0.000000000
6	0.227521000	-0.528156000	0.000000000	1	-1.584350000	-2.231582000	0.000000000
1	-4.241171000	-1.861149000	-1.362483000	4	2.880024000	-1.784143000	0.000000000
4	-1.168560000	0.519401000	0.000000000	4	4.485114000	-0.753259000	0.000000000
6	-2.421467000	-0.743438000	0.000000000	4	4.030935000	1.069170000	0.000000000
4	-2.857220000	-1.364972000	-1.543177000	1	1.518531000	-2.239805000	0.000000000
4	-0.952021000	-1.220763000	-1.026170000	1	1.384568000	2.587595000	0.000000000
1	-1.639359000	-1.684456000	-2.274627000	1	4.298851000	-2.197607000	0.000000000
6	2.411851000	1.373718000	0.000000000	1	5.360880000	0.490844000	0.000000000
4	2.257437000	2.973544000	0.000000000	6	2.896155000	-0.076373000	0.000000000
4	3.935104000	2.181466000	0.000000000	6	0.000000000	0.422628000	0.000000000
4	3.738321000	0.282408000	0.000000000	6	-2.880605000	-0.040403000	0.000000000
1	3.537914000	3.641002000	0.000000000	1	-5.297072000	0.690877000	0.000000000
1	4.940383000	1.132059000	0.000000000	1	-4.389804000	-2.085116000	0.000000000

3c				3d			
4	-0.637257000	-1.204152000	0.213637000	4	2.372306000	-0.387130000	-0.819533000
4	-2.075103000	-0.124285000	1.193238000	1	-0.403722000	1.634173000	1.793615000
4	-2.805133000	-1.384393000	-0.171051000	4	0.368828000	0.051424000	-0.849307000
4	-1.851570000	1.073978000	-0.318791000	4	-0.577457000	-1.616527000	-0.439877000
4	-4.156714000	-0.440973000	-1.140915000	6	-1.342971000	-0.017590000	-0.549510000
4	-0.033014000	1.853192000	-0.122539000	4	0.269858000	1.948693000	0.498497000
1	-1.221116000	2.287424000	-0.886559000	1	-3.802534000	-0.075153000	0.044859000
4	1.034042000	0.170495000	0.888504000	4	0.454498000	0.475380000	1.778497000
1	0.391367000	-2.191924000	-0.150227000	1	-2.190625000	-0.887183000	1.981603000
4	1.724396000	-1.629362000	-0.156948000	1	-0.526690000	2.703206000	-0.450720000
1	1.228831000	2.417845000	-0.580056000	6	1.545918000	0.780263000	0.414378000
4	2.310837000	1.482596000	-0.399255000	4	-1.458960000	1.654198000	-0.829210000
4	3.653964000	-1.345012000	-0.112198000	4	1.245563000	-1.049186000	0.795375000
4	4.006045000	0.526697000	-0.295061000	1	-2.837456000	1.860030000	-1.299123000
1	2.884793000	-2.556495000	-0.341247000	1	3.720382000	0.378127000	-0.901471000
1	3.710851000	1.885691000	-0.729372000	4	-2.936464000	0.426095000	-1.020508000
1	4.872355000	-0.636313000	-0.536919000	1	-1.045798000	-2.428379000	0.684028000
6	2.490251000	-0.123290000	0.155600000	4	-0.845611000	-1.319294000	1.629880000
6	-0.548165000	0.457382000	0.692746000	4	3.050935000	1.225916000	0.028218000
6	-3.399345000	0.274402000	0.115238000	6	1.154245000	-1.513658000	-0.879704000
1	-4.135492000	0.973890000	0.537493000	4	-2.513227000	-0.463434000	0.641074000
1	-3.670008000	-1.746210000	-1.409095000	1	1.222209000	-2.463454000	-1.416197000

3e				3f			
1	-3.795714000	-0.072851000	0.073814000	4	0.534614000	-1.772605000	-0.203929000
1	3.696624000	0.434871000	-0.926549000	4	2.746455000	-1.487775000	-0.133234000
4	-2.946481000	0.424988000	-1.009406000	4	1.151923000	0.394455000	0.062394000
4	3.025205000	1.259325000	0.025653000	4	2.486485000	1.823820000	0.130452000
1	-2.853324000	1.866789000	-1.287255000	4	4.281783000	1.229133000	0.142382000
4	2.375078000	-0.361905000	-0.827230000	4	4.432699000	-0.647778000	0.023733000
1	-2.168539000	-0.917457000	1.978322000	4	-1.649853000	-0.481059000	0.920159000
6	1.536715000	0.778848000	0.433359000	1	3.746344000	2.582104000	0.213611000
6	-1.345605000	-0.018744000	-0.569631000	1	1.723887000	-2.529856000	-0.272082000
4	0.470818000	0.423231000	1.813814000	4	-4.077987000	0.251233000	1.544518000
4	-2.486824000	-0.450663000	0.648218000	1	1.089904000	1.961988000	0.143014000
4	0.248732000	1.935324000	0.538222000	4	-1.642655000	0.108932000	-0.894747000
4	-0.572505000	-1.605697000	-0.460135000	4	-4.824970000	-0.073927000	-0.132716000
1	-0.558555000	2.711016000	-0.413990000	4	-3.491786000	0.642179000	-1.309936000
1	-1.010957000	-2.457475000	0.658789000	1	-5.478767000	0.150845000	1.211750000
1	1.225241000	-2.430772000	-1.467826000	1	-2.295953000	0.672651000	-2.112234000

4	-1.468953000	1.655853000	-0.832268000	1	-4.943861000	0.474469000	-1.474468000
6	1.163484000	-1.494865000	-0.904643000	6	-3.138957000	0.025426000	0.256811000
4	-0.821955000	-1.364495000	1.633520000	6	-0.322941000	-0.463123000	-0.012788000
4	0.363986000	0.067330000	-0.854352000	6	2.923597000	0.173622000	0.040575000
1	-0.422233000	1.572426000	1.836641000	1	5.472190000	0.378780000	0.114694000
4	1.252874000	-1.057786000	0.772351000	1	4.129240000	-2.052972000	-0.128176000

3g				3h			
4	-0.118685000	-1.863085000	-0.059782000	4	1.004013000	-0.605323000	0.000000000
4	0.876869000	-0.378616000	-0.906156000	4	-1.343233000	-2.522114000	0.000000000
4	2.140645000	-1.680734000	-0.107747000	4	-1.081767000	-0.528771000	0.000000000
4	0.840334000	0.322549000	0.900917000	4	-3.234713000	0.235192000	0.000000000
4	1.842128000	1.828341000	0.088835000	4	-4.283042000	-1.374458000	0.000000000
4	3.686265000	1.189652000	-0.143704000	4	-3.203702000	-2.934580000	0.000000000
4	3.853317000	-0.740992000	0.090248000	4	-1.319852000	1.580315000	0.000000000
4	-1.983319000	-1.264645000	0.214023000	1	-4.701928000	0.019666000	0.000000000
4	-0.420531000	1.616511000	0.105666000	4	1.405257000	1.595091000	0.000000000
1	3.148737000	2.536954000	-0.088101000	1	0.023505000	-1.964124000	0.000000000
4	-2.155949000	0.697559000	-0.099968000	4	3.206860000	0.054239000	0.000000000
1	-1.362196000	-2.604051000	0.182361000	1	-2.752017000	1.642899000	0.000000000
1	-1.784848000	2.130661000	-0.068122000	4	3.948051000	3.003283000	0.000000000
4	-4.647238000	0.849714000	-0.202078000	4	4.661098000	1.279540000	0.000000000
1	-3.975795000	-0.651975000	1.063685000	1	2.329433000	-1.121824000	0.000000000
1	-5.415622000	1.893570000	-0.446457000	1	4.680944000	-0.180434000	0.000000000
1	-3.960491000	-1.054117000	-0.689284000	1	5.353270000	2.631479000	0.000000000
6	-3.518905000	-0.403182000	0.087717000	6	3.023567000	1.708368000	0.000000000
6	-0.610437000	-0.152328000	0.015968000	6	0.000000000	0.705470000	0.000000000
6	2.341595000	0.102908000	-0.021438000	6	-2.571202000	-1.338809000	0.000000000
1	4.873667000	0.319701000	-0.029859000	1	-4.659228000	-2.792585000	0.000000000
1	3.547685000	-2.160150000	0.061275000	1	-2.024047000	-3.814913000	0.000000000

3i				3j			
4	1.163439000	0.819615000	0.148753000	4	0.045379000	-1.672255000	0.136581000
4	2.772290000	1.877508000	-0.251933000	4	-1.826653000	-1.077891000	0.338938000
4	1.733816000	-1.097197000	0.223507000	4	-2.042961000	0.654830000	-0.576660000
4	3.662597000	-1.137010000	-0.154397000	4	-3.947390000	1.156631000	-0.332100000
4	4.287031000	0.677268000	-0.450419000	4	-4.756788000	-0.253693000	0.689136000
4	-0.440676000	-2.002748000	0.803156000	4	1.096570000	-0.173148000	-0.579074000
1	2.686667000	-2.262511000	0.077755000	4	0.138249000	1.392823000	0.456320000
4	-1.201868000	0.356392000	0.911451000	1	-2.799651000	1.997256000	-0.533069000
1	1.347220000	2.311366000	-0.079944000	1	-1.182288000	-2.384660000	0.500870000
4	-3.751571000	0.696148000	1.428197000	4	2.287039000	-1.616328000	-0.028501000
1	-1.574155000	-2.480322000	0.128531000	4	2.357833000	1.658665000	0.172753000
4	-1.535957000	-1.008902000	-0.486042000	4	4.104599000	-0.909526000	-0.128395000
4	-4.254021000	0.835975000	-0.367200000	4	4.146018000	1.009725000	-0.044510000
4	-2.871234000	0.087166000	-1.465283000	1	3.620319000	-2.273722000	0.057369000
1	-5.000165000	1.202823000	0.898954000	1	1.123870000	2.395389000	0.629489000
1	-1.916400000	-0.860517000	-1.936581000	1	5.234496000	0.027528000	0.059687000
1	-4.238881000	0.557748000	-1.791862000	1	3.671511000	2.354216000	0.311738000
6	-2.741497000	0.279607000	0.244644000	6	2.733832000	0.082565000	-0.248233000
6	0.070727000	-0.537279000	0.439271000	6	-0.539222000	0.036125000	-0.088459000
6	2.736627000	0.234741000	-0.027599000	6	-3.403813000	-0.491386000	-0.192317000
1	5.013952000	-0.634991000	-0.536135000	1	-5.178009000	1.135854000	0.590693000
1	4.186815000	2.166151000	-0.626734000	1	-3.629532000	-1.302330000	-0.907482000

3k				3l			
4	-1.118577000	2.679842000	-0.652362000	4	-1.343620000	-0.387461000	1.373102000
4	1.192346000	1.455239000	0.227549000	1	-2.903055000	2.398433000	-0.515628000
4	3.054769000	1.215296000	0.788264000	1	1.811941000	-1.799304000	-1.480515000
4	0.722741000	-0.047336000	-0.860423000	1	-0.415847000	1.839036000	-0.092365000
4	2.248209000	-1.660977000	-0.185038000	4	0.987772000	-2.037978000	-0.310358000
4	3.692899000	-0.565832000	0.450251000	4	0.443805000	0.604899000	-0.022782000
4	-2.007341000	1.191500000	0.166311000	1	4.180884000	-0.695354000	-0.804779000
4	0.061931000	-2.143659000	-0.605554000	1	2.345712000	-1.886329000	0.614273000
1	1.319322000	-2.787601000	-0.392734000	4	-1.591837000	-1.049920000	-0.399202000

4	-1.208676000	-0.203082000	-0.959234000	1	-4.362056000	0.363664000	-1.324791000
1	2.155327000	2.369121000	0.927361000	6	-2.631208000	0.118833000	0.472316000
4	-1.969465000	-1.900816000	-0.037410000	1	4.075949000	2.126585000	-0.556955000
4	-3.394528000	-0.521128000	1.512907000	1	-2.556717000	-1.647758000	-1.354174000
1	-2.426947000	2.670176000	-0.069980000	4	2.702178000	2.109215000	-0.100594000
1	-1.001202000	-2.951564000	0.105185000	4	3.838499000	0.632267000	-0.326096000
1	-3.674580000	-0.396699000	-0.623598000	4	-1.825250000	1.547154000	0.062883000
1	-3.744034000	-0.600078000	2.784218000	4	2.732004000	-0.975338000	-0.590766000
6	-2.737423000	-0.409624000	-0.035716000	4	-3.705032000	1.180191000	-0.280685000
6	-0.380297000	1.259539000	-0.540064000	4	-3.504588000	-0.679658000	-0.738077000
6	2.166114000	0.005630000	-0.005039000	4	1.513681000	-0.680736000	1.067705000
1	3.650191000	-2.007649000	0.231804000	6	2.191345000	0.616301000	0.148330000
1	4.334319000	0.574838000	1.141604000	6	-0.088012000	-1.026720000	0.475088000

3m				3n			
1	-1.264254000	-3.023115000	-0.486571000	4	2.080489000	1.693817000	-0.021095000
1	-1.152660000	3.062759000	-1.041577000	1	-3.555282000	2.323890000	-0.246029000
6	-0.651972000	-2.166050000	-0.210484000	4	-3.526760000	-1.006095000	-0.367207000
4	-2.154782000	2.144004000	-0.568229000	6	0.021963000	-1.478220000	0.541695000
1	2.235408000	-2.045429000	-1.483010000	1	5.599472000	1.169132000	-0.487486000
1	-3.580196000	1.827513000	-0.343338000	4	-1.660107000	-1.468774000	-0.051141000
4	-1.798502000	-1.003209000	0.439338000	6	2.799393000	0.254645000	-0.076746000
4	3.503794000	2.298531000	1.061552000	1	1.268693000	2.881057000	-0.094850000
4	1.036344000	-2.053842000	-0.594886000	1	-1.117095000	2.861435000	0.050495000
4	-0.206342000	1.960348000	-0.607682000	4	3.007332000	-1.277037000	-0.397834000
1	-3.271895000	-0.788236000	0.555878000	4	-0.753670000	0.118190000	0.605937000
4	0.015960000	0.365017000	1.131755000	1	0.040802000	-1.941338000	1.549692000
4	-0.271823000	-0.521371000	-0.716085000	4	1.232852000	-0.140301000	0.439417000
6	-1.287356000	0.769752000	-0.000906000	1	-4.740061000	-0.211693000	-0.631822000
4	0.218148000	-1.594876000	1.192545000	4	4.357897000	0.772896000	-0.272071000
4	-2.997270000	0.583099000	0.196006000	1	2.478552000	-2.613688000	-0.644644000
1	-0.473880000	-0.663687000	2.132465000	1	-2.856945000	-2.304742000	-0.407000000
1	1.193466000	2.175461000	-0.687006000	4	-2.155573000	1.818177000	0.008965000
4	2.454070000	-0.736589000	-0.882056000	6	-2.324686000	0.141938000	0.011318000
4	2.053650000	1.070197000	-0.114290000	4	0.075123000	2.099168000	0.255239000
1	3.024433000	0.557605000	-1.181245000	4	-3.816257000	0.894802000	-0.298415000
6	1.252092000	-0.461720000	0.275145000	4	1.120220000	-2.388587000	-0.210623000

4a				4b			
4	-0.030912000	0.949150000	0.000000000	1	-3.018147000	2.313694000	-0.908418000
4	-1.847384000	1.543851000	0.000000000	1	1.412194000	-0.799266000	-1.739807000
4	0.030912000	-0.949150000	0.000000000	1	-0.420121000	3.058548000	-0.606368000
4	-2.324163000	-1.545199000	0.000000000	4	2.296855000	-0.323020000	-0.624479000
4	-3.159435000	0.175382000	0.000000000	4	-1.555095000	2.204380000	-0.930797000
4	2.324163000	1.545199000	0.000000000	1	3.851310000	1.015899000	2.084595000
4	1.847384000	-1.543851000	0.000000000	4	-2.900322000	0.843054000	-0.568392000
1	0.638956000	-2.327096000	0.000000000	4	2.862716000	0.592613000	1.018097000
4	-3.689433000	-2.930558000	0.000000000	4	0.144977000	1.768477000	-0.092390000
4	-5.487618000	-0.451808000	0.000000000	6	1.290634000	0.601187000	0.420182000
4	-5.487618000	-2.303921000	0.000000000	6	-3.841038000	-0.355373000	0.222359000
1	-2.260171000	-3.060206000	0.000000000	4	0.395257000	-0.032352000	-0.947203000
1	-6.641237000	-1.321669000	0.000000000	6	-1.181825000	0.608830000	-0.517073000
1	-4.966224000	-3.665321000	0.000000000	4	-2.029068000	-0.735777000	0.369281000
4	3.159435000	-0.175382000	0.000000000	4	-0.267159000	0.094677000	0.976774000
1	-0.638956000	2.327096000	0.000000000	1	-1.161503000	-0.822461000	1.628650000
1	-3.313656000	1.650012000	0.000000000	6	3.958552000	-0.386651000	-0.080376000
4	3.689433000	2.930558000	0.000000000	4	4.376408000	-1.265267000	-1.351058000
1	3.313656000	-1.650012000	0.000000000	4	5.618615000	-0.802959000	-0.054942000
4	5.487618000	2.303921000	0.000000000	4	4.763816000	0.267273000	1.275705000
4	5.487618000	0.451808000	0.000000000	1	5.778186000	-1.617155000	-1.327114000
1	2.260171000	3.060206000	0.000000000	1	6.164462000	-0.181897000	1.142368000
1	4.966224000	3.665321000	0.000000000	4	-3.500775000	-1.993334000	-0.107425000
1	6.641237000	1.321669000	0.000000000	4	-5.248157000	-1.311282000	0.300929000
6	4.118505000	1.283127000	0.000000000	4	-5.132350000	0.543359000	0.485101000

6	1.457624000	0.093046000	0.000000000
6	-1.457624000	-0.093046000	0.000000000
6	-4.118505000	-1.283127000	0.000000000

1	-4.816195000	-2.681630000	0.064899000
1	-6.337647000	-0.263271000	0.510303000
1	-2.113357000	-2.229786000	-0.116457000

4c

4	-1.569850000	2.525241000	0.390542000	4	0.580628000	2.278788000	0.808431000

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4	-1.569850000	2.525241000	0.390542000	4	0.580628000	2.278788000	0.808431000
4	-0.031638000	1.874037000	-0.549094000	4	0.810407000	-0.097139000	0.547394000
4	2.029492000	2.573635000	0.616525000	4	-0.810407000	0.097139000	-0.547394000
4	0.063709000	0.379618000	0.737772000	4	-0.580628000	-2.278788000	-0.808431000
4	1.910023000	-0.327087000	0.662085000	4	1.287656000	-1.544868000	-2.296105000
4	2.876531000	0.636026000	-0.748379000	4	2.125290000	-0.553611000	-0.839435000
4	-3.191788000	0.865539000	0.219642000	4	-1.287656000	1.544868000	2.296105000
1	0.712986000	-0.884326000	1.309236000	1	-1.505531000	-3.228176000	-0.731425000
4	3.390010000	-2.162568000	1.035806000	4	2.646751000	-2.018265000	-3.601376000
4	4.588824000	-0.241026000	-1.028094000	4	4.372356000	-0.472319000	-1.596052000
4	4.893695000	-1.820861000	0.000338000	4	4.388858000	-1.316326000	-3.251722000
1	4.600464000	-2.949196000	0.977362000	1	1.246722000	-2.345046000	-3.581105000
1	4.049436000	0.925325000	-1.658135000	1	5.514424000	-0.660874000	-2.465294000
1	5.742337000	-1.161785000	-0.975896000	1	3.899810000	-2.107842000	-4.372072000
4	-2.009373000	-0.648674000	-0.276008000	4	-2.125290000	0.553611000	0.839435000
1	-0.534157000	3.337353000	-0.120803000	1	1.505531000	3.228176000	0.731425000
1	2.523494000	3.689977000	1.132031000	1	2.324590000	0.148990000	0.420080000
4	-5.050155000	0.224628000	0.101085000	4	-2.646751000	2.018265000	3.601376000
1	-1.699515000	-2.116884000	-0.634222000	1	-2.324590000	-0.148990000	-0.420080000
4	-5.034077000	-1.664739000	-0.343664000	4	-4.372356000	0.472319000	1.596052000
4	-3.182278000	-2.212131000	-0.565895000	4	-4.388858000	1.316326000	3.251722000
1	-4.505418000	1.597036000	0.424143000	1	-1.246722000	2.345046000	3.581105000
1	-6.184787000	-0.734541000	-0.069064000	1	-5.514424000	0.660874000	2.465294000
1	-4.441613000	-3.000878000	-0.699045000	1	-3.899810000	2.107842000	4.372072000
6	-3.700438000	-0.691828000	-0.172224000	6	-3.036495000	1.096240000	2.223746000
6	-1.431220000	0.959381000	0.126822000	6	-0.454354000	1.009909000	0.921402000
6	1.435858000	1.178532000	-0.048816000	6	0.454354000	-1.009909000	-0.921402000
6	3.462670000	-0.874857000	0.086936000	6	3.036495000	-1.096240000	-2.223746000

4e

4	-0.128160000	-0.290654000	-0.405008000
4	0.063260000	-1.977724000	0.563085000
4	1.574097000	-2.572064000	-0.421514000
4	3.016550000	-0.720025000	-0.755641000
4	2.093220000	0.454391000	0.565925000
4	-1.827629000	0.615402000	0.141839000
4	-2.283246000	-2.098041000	1.377416000
1	0.550339000	-3.421412000	0.059611000
4	4.845932000	-0.011239000	-0.967607000
4	3.343968000	1.914829000	0.995653000
4	4.994513000	1.656025000	0.012088000
1	4.243042000	-1.282497000	-1.479986000
1	4.601537000	2.726022000	0.990219000
1	6.012697000	0.907640000	-0.809333000
4	-3.096128000	-0.969130000	0.098159000
1	-0.671392000	1.004909000	-0.742217000
1	1.990266000	1.646867000	1.535000000
4	-3.300715000	1.822268000	0.726538000
1	-3.675023000	-2.059141000	1.129192000
4	-4.824984000	1.804637000	-0.433230000
4	-4.716650000	0.310605000	-1.539879000
1	-1.973850000	1.768171000	1.188430000
1	-4.402629000	2.820535000	0.513238000
1	-5.749753000	1.328000000	-1.551420000
6	-3.631398000	0.578967000	-0.402504000
6	-1.403877000	-1.129936000	0.481215000
6	1.411714000	-1.027524000	-0.085610000
6	3.633336000	0.712459000	-0.103771000