The B_{32} cluster has the most stable bowl structure with a remarkable heptagonal hole

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Supplementary Information. The file contains

- Computational methods
- Model of a particle in circular box
- Shapes and relative energies of the low-lying isomers of B_{32} at neutral and anionic states obtained at the TPSSh/6-311+G(d) level (Figure S1)
- Table of vertical detachment energies (VDEs) of **32a.**1 and **32a.2** obtained using TD-DFT method (Table S1 and S2)
- The relative energies (eV) of the low-lying isomers B_{32} and B_{32}^- calculated using the PBE0 functional in conjugation with the 6-311+G(d) and def2-TZVP basis sets (Table S3)
- The relative energies (eV) of the low-lying isomers B6 obtained at CCSD(T) method (Table S4)
- The T1 diagnostic values of the low-lying isomers B_{32} and B_{32}^- calculated using the CCSD method in conjugation with the basis sets of 6-311G(d) and 6-31G(d) (Table S5)
- Cartesian coordinates of the low-lying isomers (Table S6)

Computational Methods. All electronic structure calculations are carried out by using Gaussian09 package.[1] The initial search for all possible lower-lying isomers of B_{32} cluster is performed using a stochastic search algorithm that was implemented by us.[2] Firstly, the possible structures of the B_{32} are generated by a random kick method, and then rapidly optimized at the TPSSh/3-21G level.[3] In this search procedure, the minimum and maximum distances between atoms are limited to 1.5 and 20 Å, respectively. Geometries of the local minima with relative energies of 0.0 ÷ 5.0 eV and their harmonic vibrational frequencies are further refined using the PBE[4] and PBE0[5], TPSSh[6] functionals, in conjugation with higher 6-311+G(d) basis set.[7]

The model of particle in circular box

The model of particle in circular box describes a free particle moving on a plane encircled by infinite walls. The radius of the disk is denoted by r = R. In polar coordinates, the Schrödinger equation for this problem is written as follows:

$$-\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}+\frac{1}{r^2}\frac{\partial^2}{\partial \varphi^2}\right)\psi(\varphi,r)=E\ \psi(\varphi,r)$$ * MERGEFORMAT (1)

where $\hbar$ is Plank constant and μ is the mass of the particle.

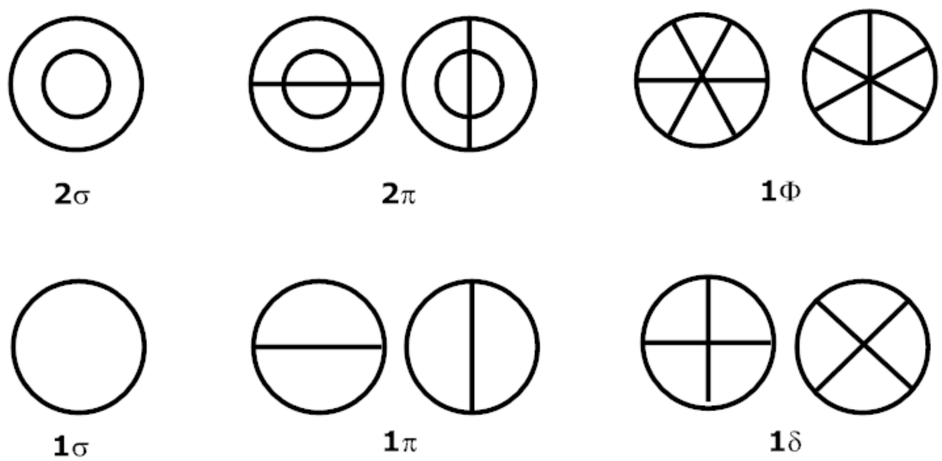


Figure S1. Shapes of the lowest-lying wavefunctions for a particle in a circular box

Because of the circular symmetry, the $\psi(\varphi,r)$ can be written as $R(r)\,\Phi(\varphi)$, with $\Phi(\varphi)=\frac{1}{\sqrt{2\pi}}\exp(im\varphi)$. The cyclic boundary condition requires the angular part to be periodic. As a result the cylindrical quantum number must be integer: $m=0,\pm1,\pm2,...$ Substitution into the Schrödinger equation will give us for the radial part:

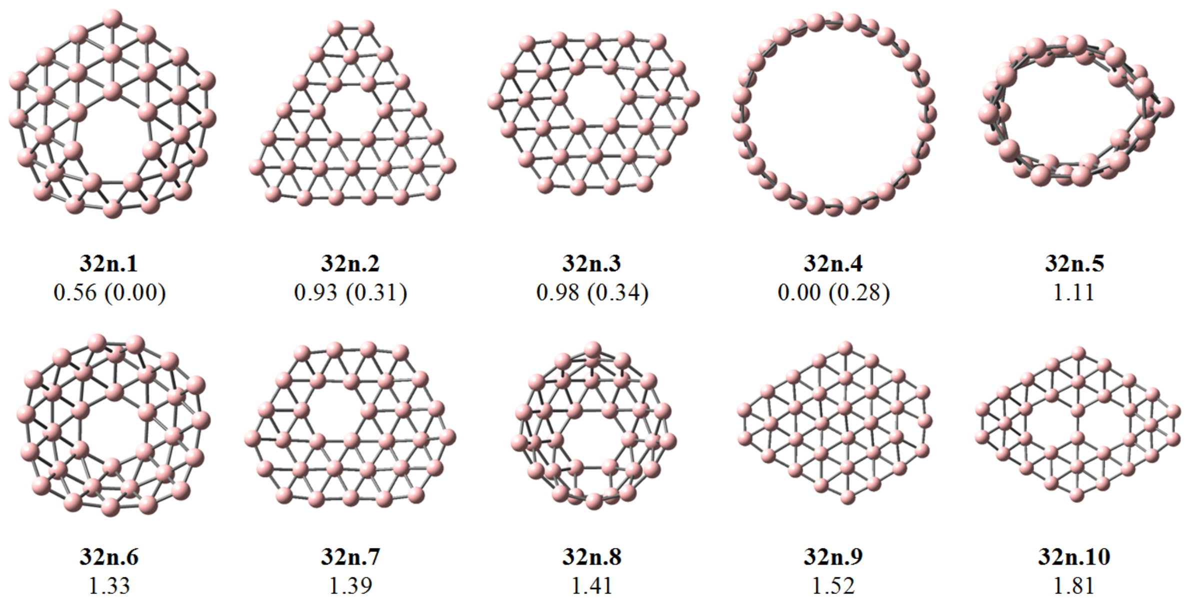
$$\frac{\partial^2 R(r)}{\partial r^2}+\frac{1}{r}\frac{\partial R(r)}{\partial r}+\left(k^2-\frac{m^2}{r^2}\right)R(r)=0$$ * MERGEFORMAT (2)

with $\hbar^2 k^2 = 2\mu E$. This equation is known as Bessel's differential equation,[8] and its solutions are the integer Bessel functions $J_m(kr)$. The potential wall at $r=R$ requires the radial function to vanish at the boundary of the box: $J_m(kR)=0$. The radii that correspond to the zeroes of the Bessel function are denoted as $a_{m,n}$. Here n is a radial quantum number that counts the zeroes.

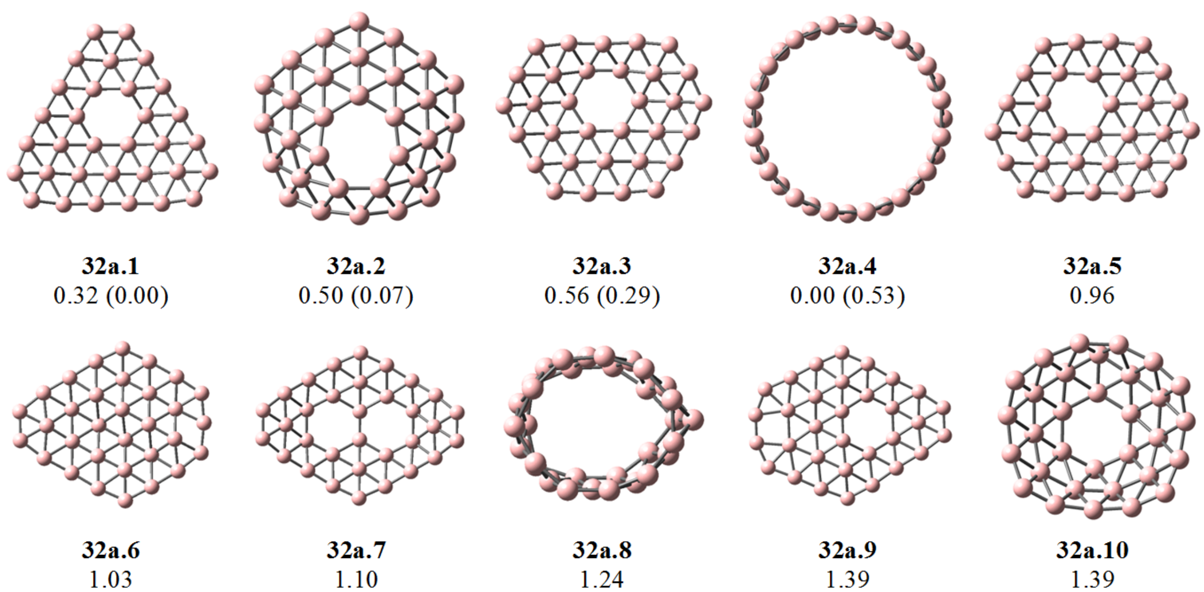
The $a_{m,n}$ quantities are dimensionless. They give rise to a quantisation of the energy as:

$$E = \frac{\hbar^2 \left(a_{m,n}\right)^2}{2\mu R^2} \text{ , with: } n = 1, 2, 3, \ldots \quad m = 0, \pm 1, \pm 2, \pm 3, \ldots \text{ * MERGEFORMAT (3)}$$

The rotational quantum numbers are usually denoted by Greek letters: *m* = σ, π, δ, ϕ, γ, … States with non-zero values for *m* will be twofold degenerate. The lowest eigenstates in ascending order are 1σ, 1π, 1δ, 2σ etc. The lowest eigenstates in ascending order are 1σ, 1π, 1δ, 2σ etc (Figure S1). We consider that the systems containing the number of 2, 6, 10, 12, 16… electrons will exhibit a disk-aromaticity. Oppositely, the systems containing number of 4, 8, 14, 18… electrons will be disk-antiaromatic.



a)



b)

Figure S1. Shapes and relative energies (eV) of the low-lying isomers of a) the neutral B_{32} and b) anion B_{32}^{-} obtained at TPSSh/6-311+G(d) level of theory (values in parenthesis obtained at CCSD(T)/6-311G(d)//TPSSh/6-311+G(d) for the neutral B_{32} and CCSD(T)/6-311G(d)//TPSSh/6-311+G(d) for the anions B_{32}^{-})

Table S1. Vertical detachment energies (VDEs, eV) of **32a.1** obtained at TD-TPSSh/6-311+G(d)//TPSSh/6-311+G(d) level of theory.

32a.1	
Final States and their electronic configurations	**VDE**
^1A {.... $(75a)^2(76a)^2(77a)^2(78a)^2(79a)^2(80a)^2(81a)^0(82a)^0(83a)^0$}	3.77
^3A {.... $(75a)^2(76a)^2(77a)^2(78a)^2(79a)^1(80a)^2(81a)^1(82a)^0(83a)^0$}	4.17
^3A {.... $(75a)^2(76a)^2(77a)^2(78a)^2(79a)^2(80a)^1(81a)^1(82a)^0(83a)^0$}	4.20
^1A {.... $(75a)^2(76a)^2(77a)^2(78a)^2(79a)^2(80a)^1(81a)^1(82a)^0(83a)^0$}	4.36
^1A {.... $(75a)^2(76a)^2(77a)^2(78a)^2(79a)^1(80a)^2(81a)^1(82a)^0(83a)^0$}	4.49
^3A {....$(75a)^2(76a)^2(77a)^1(78a)^2(79a)^2(80a)^2(81a)^1(82a)^0(83a)^0$}	4.78
^3A {....$(75a)^2(76a)^2(77a)^2(78a)^1(79a)^2(80a)^2(81a)^1(82a)^0(83a)^0$}	4.88
^1A {....$(75a)^2(76a)^2(77a)^2(78a)^1(79a)^2(80a)^2(81a)^1(82a)^0(83a)^0$}	5.10
^3A {....$(75a)^2(76a)^1(77a)^2(78a)^2(79a)^2(80a)^2(81a)^1(82a)^0(83a)^0$}	5.11
^3A {....$(75a)^2(76a)^2(77a)^2(78a)^2(79a)^2(80a)^1(81a)^2(82a)^1(83a)^0$}	5.16
^1A {....$(75a)^2(76a)^2(77a)^1(78a)^2(79a)^2(80a)^2(81a)^1(82a)^0(83a)^0$}	5.16
^3A {....$(75a)^2(76a)^2(77a)^2(78a)^2(79a)^2(80a)^1(81a)^0(82a)^0(83a)^1$}	5.21
^3A {....$(75a)^2(76a)^2(77a)^2(78a)^2(79a)^1(80a)^2(81a)^0(82a)^1(83a)^0$}	5.24
^3A {....$(75a)^2(76a)^2(77a)^2(78a)^2(79a)^1(80a)^2(81a)^0(82a)^0(83a)^1$}	5.27
^1A {....$(75a)^2(76a)^2(77a)^2(78a)^2(79a)^2(80a)^1(81a)^0(82a)^1(83a)^0$}	5.27
^1A {....$(75a)^2(76a)^1(77a)^2(78a)^2(79a)^2(80a)^2(81a)^1(82a)^0(83a)^0$}	5.32
^3A {....$(75a)^1(76a)^2(77a)^2(78a)^2(79a)^2(80a)^2(81a)^1(82a)^0(83a)^0$}	5.39
^1A {....$(75a)^2(76a)^2(77a)^2(78a)^2(79a)^2(80a)^1(81a)^0(82a)^0(83a)^1$}	5.39
^1A {....$(75a)^2(76a)^2(77a)^2(78a)^2(79a)^1(80a)^2(81a)^0(82a)^1(83a)^0$}	5.44
^1A {....$(75a)^2(76a)^2(77a)^2(78a)^2(79a)^1(80a)^2(81a)^0(82a)^0(83a)^1$}	5.47
^1A {....$(75a)^1(76a)^2(77a)^2(78a)^2(79a)^2(80a)^2(81a)^1(82a)^0(83a)^0$}	5.58

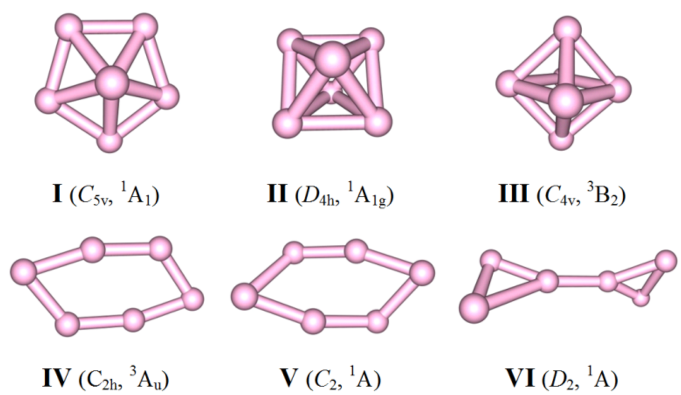
Table S2 Vertical detachment energies (VDEs, eV) of **32a.2** obtained at TD-TPSSh/6-311+G(d) //TPSSh/6-311+G(d) level of theory.

32a.2	
Final States and their electronic configurations	**VDE**
^{1}A’ {…(43a’)^{2}(44a’)^{2}(33a”)^{2}(34a”)^{2}(35a”)^{2}(45a’)^{2}(36a”)^{0}(46a’)^{0}(37a”)^{0}(47a’)^{0}}	3.19
^{3}A” {… (43a’)^{2}(44a’)^{2}(33a”)^{2}(34a”)^{2}(35a”)^{2}(45a’)^{1}(36a”)^{1}(46a’)^{0}(37a”)^{0}(47a’)^{0}}	4.07
^{3}A’ {… (43a’)^{2}(44a’)^{2}(33a”)^{2}(34a”)^{2}(35a”)^{1}(45a’)^{2}(36a”)^{1}(46a’)^{0}(37a”)^{0}(47a’)^{0}}	4.33
^{1}A” {… (43a’)^{2}(44a’)^{2}(33a”)^{2}(34a”)^{2}(35a”)^{2}(45a’)^{1}(36a”)^{1}(46a’)^{0}(37a”)^{0}(47a’)^{0}}	4.52
^{1}A’ {… (43a’)^{2}(44a’)^{2}(33a”)^{2}(34a”)^{2}(35a”)^{1}(45a’)^{2}(36a”)^{1}(46a’)^{0}(37a”)^{0}(47a’)^{0}}	4.54
^{3}A’ {… (43a’)^{2}(44a’)^{2}(33a”)^{2}(34a”)^{2}(35a”)^{2}(45a’)^{1}(36a”)^{0}(46a’)^{1}(37a”)^{0}(47a’)^{0}}	4.55
^{3}A’ {… (43a’)^{2}(44a’)^{2}(33a”)^{2}(34a”)^{1}(35a”)^{2}(45a’)^{2}(36a”)^{1}(46a’)^{0}(37a”)^{0}(47a’)^{0}}	4.63
^{3}A” {… (43a’)^{2}(44a’)^{2}(33a”)^{2}(34a”)^{2}(35a”)^{1}(45a’)^{2}(36a”)^{0}(46a’)^{1}(37a”)^{0}(47a’)^{0}}	4.76
^{3}A’ {… (43a’)^{2}(44a’)^{2}(33a”)^{1}(34a”)^{2}(35a”)^{2}(45a’)^{2}(36a”)^{1}(46a’)^{0}(37a”)^{0}(47a’)^{0}}	4.76
^{1}A’ {… (43a’)^{2}(44a’)^{2}(33a”)^{2}(34a”)^{2}(35a”)^{2}(45a’)^{1}(36a”)^{0}(46a’)^{1}(37a”)^{0}(47a’)^{0}}	4.77
^{1}A” {… (43a’)^{2}(44a’)^{1}(33a”)^{2}(34a”)^{2}(35a”)^{2}(45a’)^{2}(36a”)^{1}(46a’)^{0}(37a”)^{0}(47a’)^{0}}	4.81
^{1}A’ {… (43a’)^{2}(44a’)^{2}(33a”)^{2}(34a”)^{1}(35a”)^{2}(45a’)^{2}(36a”)^{1}(46a’)^{0}(37a”)^{0}(47a’)^{0}}	4.88
^{3}A” {… (43a’)^{2}(44a’)^{2}(33a”)^{2}(34a”)^{2}(35a”)^{2}(45a’)^{1}(36a”)^{0}(46a’)^{0}(37a”)^{1}(47a’)^{0}}	4.93
^{1}A” {… (43a’)^{2}(44a’)^{2}(33a”)^{2}(34a”)^{2}(35a”)^{1}(45a’)^{2}(36a”)^{0}(46a’)^{1}(37a”)^{0}(47a’)^{0}}	4.94
^{3}A” {… (43a’)^{2}(44a’)^{2}(33a”)^{2}(34a”)^{1}(35a”)^{2}(45a’)^{2}(36a”)^{0}(46a’)^{1}(37a”)^{0}(47a’)^{0}}	5.00
^{3}A” {… (43a’)^{1}(44a’)^{2}(33a”)^{2}(34a”)^{2}(35a”)^{2}(45a’)^{2}(36a”)^{1}(46a’)^{0}(37a”)^{0}(47a’)^{0}}	5.06
^{1}A’ {… (43a’)^{2}(44a’)^{1}(33a”)^{2}(34a”)^{2}(35a”)^{2}(45a’)^{2}(36a”)^{0}(46a’)^{1}(37a”)^{0}(47a’)^{0}}	5.14
^{1}A” {… (43a’)^{2}(44a’)^{2}(33a”)^{2}(34a”)^{2}(35a”)^{2}(45a’)^{1}(36a”)^{0}(46a’)^{0}(37a”)^{1}(47a’)^{0}}	5.22
^{1}A” {… (43a’)^{1}(44a’)^{2}(33a”)^{2}(34a”)^{2}(35a”)^{2}(45a’)^{2}(36a”)^{1}(46a’)^{0}(37a”)^{0}(47a’)^{0}}	5.22
^{1}A’ {… (43a’)^{2}(44a’)^{2}(33a”)^{1}(34a”)^{2}(35a”)^{2}(45a’)^{2}(36a”)^{1}(46a’)^{0}(37a”)^{0}(47a’)^{0}}	5.24
^{1}A’ {… (43a’)^{1}(44a’)^{2}(33a”)^{2}(34a”)^{2}(35a”)^{2}(45a’)^{2}(36a”)^{0}(46a’)^{0}(37a”)^{0}(47a’)^{1}}	5.27

Table S3 The relative energies (eV) of the low-lying isomers B_{32} and B_{32}^- calculated using the PBE0 functional in conjugation with the 6-311+G(d) and def2-TZVP basis sets.

Neutral B_{32}		
	PBE0/6-311+G(d)	**PBE0/def2-TZVP**
32n.1	0.08	0.09
32n.2	0.36	0.38
32n.3	0.45	0.43
32n.4	0.00	0.00
Anion B_{32}^-		
	PBE0/6-311+G(d)	**PBE0/def2-TZVP**
32a.1	0.00	0.00
32a.2	0.28	0.26
32a.3	0.38	0.33
32a.4	0.17	0.17

Table S4. The relative energies (eV) of the low-lying isomers B_6 obtained at CCSD(T) in conjugation with several basis sets, including 6-31G(d), 6-311G(d), 6-311+G(d) and aug-cc-pVTZ. The geometries of structures were obtained at the PBE/6-311+G(d) level of theory.



The shapes of low-lying isomers B_6

	6-31G(d)	**6-311G(d)**	**6-311+G(d)**	**Aug-cc-pVTZ**
I	0.00	0.00	0.00	0.00
II	1.81	1.78	1.80	1.68
III	1.97	1.94	1.96	1.84
IV	0.19	0.17	0.17	0.14
V	0.34	0.30	0.29	0.26
VI	2.07	2.10	2.11	2.19

Table S5 The T1 diagnostic values of the low-lying isomers B_{32} and B_{32}^- calculated using the CCSD method in conjugation with the basis sets of 6-311G(d) and 6-31G(d).

	Neutral B_{32}		Anion B_{32}^-	
	6-31G(d)	6-311G(d)		6-31G(d)
32n.1	0.02545143	0.02556658	**32a.1**	0.03334236
32n.2	0.02885683	0.02901858	**32a.2**	0.02329199
32n.3	0.02372617	0.02360387	**32a.3**	0.03489730
32n.4	0.01965435	0.01759936	**32a.4**	0.02804046

Table S6 Coordinates of the lowest-lying isomers B_{32} and B_{32}^- obtained at the TPSSh/6-311+G(d) level of theory.

32n.1			
5	-1.450554000	0.394463000	1.075177000
5	-1.631499000	-1.191902000	1.400432000
5	1.634995000	-1.187130000	1.400370000
5	-0.001800000	1.270744000	1.018829000
5	1.449538000	0.398715000	1.075144000
5	-0.004277000	2.831121000	0.324274000
5	2.752980000	1.096869000	0.127354000
5	2.376754000	-2.080291000	0.160662000
5	-2.370618000	-2.087161000	0.160753000
5	-2.755956000	1.088842000	0.127227000
5	1.442212000	2.038571000	0.607425000
5	2.796638000	-0.530227000	0.471926000
5	-0.839003000	-2.508774000	0.892695000
5	-2.795098000	-0.538322000	0.472084000
5	-1.448261000	2.034503000	0.607589000
5	-0.006090000	4.268667000	-0.512499000
5	3.859912000	1.708164000	-0.958922000
5	2.875032000	-2.863732000	-1.195633000
5	-3.864949000	1.696831000	-0.958883000
5	-2.866724000	-2.872115000	-1.195483000
5	-1.403123000	3.608050000	-0.281704000
5	2.743415000	2.701380000	-0.449611000
5	-2.751423000	2.693395000	-0.449560000
5	1.392533000	3.612134000	-0.281367000
5	3.887898000	0.148467000	-0.777295000
5	3.531741000	-1.462370000	-0.947591000
5	1.557190000	-3.410705000	-0.523704000
5	0.005257000	-3.600964000	-0.034228000
5	-3.527503000	-1.472697000	-0.947447000
5	-3.888367000	0.137067000	-0.777056000
5	0.846389000	-2.506356000	0.892691000
5	-1.547237000	-3.415237000	-0.523652000

32n.2			
5	3.382767000	1.010756000	-0.039262000
5	0.803335000	-3.370334000	0.015343000
5	2.501534000	-0.413454000	0.421023000
5	-0.012846000	-1.880351000	0.231296000
5	2.405743000	-3.406554000	-0.203469000
5	2.556742000	2.396433000	-0.138915000
5	1.734052000	3.821604000	-0.137733000
5	3.226480000	-1.841428000	-0.053931000
5	-1.629290000	-1.877784000	0.399756000
5	-2.451757000	-3.373540000	-0.203576000
5	-0.746000000	5.143763000	-0.225330000
5	-0.844011000	-0.392398000	0.759648000
5	4.189614000	-0.411709000	-0.197130000
5	-0.843813000	2.331491000	-0.156980000
5	0.025318000	3.727271000	0.151674000
5	-1.688744000	1.020361000	0.332694000
5	-4.194778000	-0.354847000	-0.196996000
5	0.815833000	5.133215000	-0.225090000
5	-0.849050000	-3.359148000	0.015504000
5	-3.251542000	-1.797675000	-0.052841000
5	-1.681871000	3.844649000	-0.138177000
5	-2.523819000	2.430803000	-0.139349000
5	1.702518000	0.997458000	0.332901000
5	0.875545000	2.319889000	-0.156751000
5	-3.368682000	1.056587000	-0.039660000
5	0.838547000	-0.403773000	0.759571000
5	-4.034236000	-3.165503000	-0.481106000
5	-4.819106000	-1.810806000	-0.486576000
5	3.990935000	-3.219989000	-0.480834000
5	4.794113000	-1.875999000	-0.486509000

32n.3			
5	2.413454000	3.635326000	-0.383314000
5	-2.414137000	3.634892000	-0.383254000
5	1.662518000	2.303900000	0.225425000
5	1.634252000	-3.410204000	-0.155526000
5	-1.662951000	2.303615000	0.225509000
5	-4.147027000	0.893218000	-0.249246000
5	-0.000220000	2.261515000	0.065077000
5	2.499672000	0.899621000	0.413431000
5	3.172751000	-3.267118000	-0.462873000
5	-2.499836000	0.899160000	0.413417000
5	4.097116000	-1.952975000	-0.496126000
5	-3.344587000	-0.528667000	0.270700000
5	-3.309995000	2.364708000	-0.121006000
5	0.819218000	3.759018000	-0.255598000
5	4.146863000	0.893989000	-0.249262000
5	3.309547000	2.365313000	-0.121048000
5	3.344660000	-0.528042000	0.270660000
5	-3.172126000	-3.267669000	-0.462921000
5	2.397307000	-1.894571000	-0.043316000

5	-0.819949000	3.758889000	-0.255459000
5	-1.633625000	-3.410500000	-0.155482000
5	-2.396933000	-1.894956000	-0.043397000
5	0.000310000	-3.335127000	0.029078000
5	4.761645000	-0.495453000	-0.573013000
5	-4.096722000	-1.953716000	-0.496224000
5	-4.761539000	-0.496328000	-0.573046000
5	0.810188000	0.839617000	0.484224000
5	1.681369000	-0.570020000	0.653605000
5	-0.817444000	-2.038356000	0.645557000
5	-0.810334000	0.839468000	0.484226000
5	-1.681279000	-0.570324000	0.653631000
5	0.817836000	-2.038222000	0.645570000
32n.4			
5	2.289459000	3.426379000	0.737685000
5	2.914377000	2.914432000	-0.737612000
5	1.577170000	3.807617000	-0.737579000
5	0.804127000	4.042718000	0.737545000
5	-0.803987000	4.041607000	0.737666000
5	-2.290135000	3.427401000	0.737497000
5	-2.914432000	2.914377000	-0.737612000
5	-3.426379000	2.289459000	0.737685000
5	-4.042718000	0.804127000	0.737545000
5	-3.807617000	1.577170000	-0.737579000
5	-4.121235000	-0.000023000	-0.737583000
5	-4.041607000	-0.803987000	0.737666000
5	-3.427401000	-2.290135000	0.737497000
5	-0.804127000	-4.042718000	0.737545000
5	-2.914377000	-2.914432000	-0.737612000
5	-3.807793000	-1.577258000	-0.737620000
5	3.427401000	2.290135000	0.737497000
5	4.041607000	0.803987000	0.737666000
5	4.121235000	0.000023000	-0.737583000
5	3.807617000	-1.577170000	-0.737579000
5	3.426379000	-2.289459000	0.737685000
5	2.290135000	-3.427401000	0.737497000
5	0.803987000	-4.041607000	0.737666000
5	0.000023000	-4.121235000	-0.737583000
5	1.577258000	-3.807793000	-0.737620000
5	2.914432000	-2.914377000	-0.737612000
5	3.807793000	1.577258000	-0.737620000
5	-1.577258000	3.807793000	-0.737620000
5	-0.000023000	4.121235000	-0.737583000
5	4.042718000	-0.804127000	0.737545000
5	-1.577170000	-3.807617000	-0.737579000
5	-2.289459000	-3.426379000	0.737685000
32a.1			
5	1.603690000	-1.918872000	0.396481000
5	-2.503014000	-0.380559000	0.370202000
5	3.362810000	0.999646000	-0.025142000

5	0.797740000	-3.395598000	-0.001069000
5	2.497616000	-0.414500000	0.370323000
5	-0.012897000	-1.901180000	0.243382000
5	2.408065000	-3.418264000	-0.197049000
5	2.556409000	2.425698000	-0.069944000
5	1.749634000	3.842262000	-0.147347000
5	3.225041000	-1.861014000	-0.067908000
5	-1.629551000	-1.896901000	0.396169000
5	-2.454357000	-3.385289000	-0.196836000
5	-0.743768000	5.184992000	-0.280591000
5	-0.833954000	-0.420383000	0.746510000
5	4.172581000	-0.411471000	-0.201850000
5	-0.837365000	2.362008000	-0.029070000
5	0.025683000	3.784045000	0.022733000
5	-1.669415000	1.016560000	0.331063000
5	-4.177854000	-0.354792000	-0.201756000
5	0.814152000	5.174458000	-0.280483000
5	-0.843805000	-3.384500000	-0.001022000
5	-3.250046000	-1.817045000	-0.067889000
5	-1.697329000	3.865649000	-0.147608000
5	-2.523169000	2.460085000	-0.070520000
5	1.683276000	0.993985000	0.331815000
5	0.869362000	2.350460000	-0.028812000
5	-3.348819000	1.045135000	-0.025613000
5	0.828293000	-0.431626000	0.746865000
5	-4.039781000	-3.177929000	-0.469938000
5	-4.815388000	-1.818736000	-0.487017000
5	3.996085000	-3.232424000	-0.470510000
5	4.790070000	-1.883896000	-0.487567000
32a.2			
5	-1.478640000	0.402335000	1.077992000
5	-1.666083000	-1.199520000	1.412606000
5	1.669430000	-1.194604000	1.412280000
5	-0.001966000	1.214904000	0.925816000
5	1.477537000	0.406725000	1.078199000
5	-0.004143000	2.803366000	0.314131000
5	2.771447000	1.103704000	0.128332000
5	2.364868000	-2.064938000	0.149797000
5	-2.358744000	-2.071860000	0.150024000
5	-2.774802000	1.095735000	0.128544000
5	1.445318000	2.011632000	0.629254000
5	2.842230000	-0.534109000	0.495852000
5	-0.855507000	-2.490085000	0.899625000
5	-2.840827000	-0.542560000	0.496200000
5	-1.450842000	2.007028000	0.628566000
5	-0.006210000	4.256689000	-0.483640000
5	3.861250000	1.717725000	-0.969427000
5	2.892510000	-2.864129000	-1.187955000
5	-3.866110000	1.706631000	-0.969524000
5	-2.884174000	-2.872661000	-1.187676000
5	-1.410769000	3.601303000	-0.263221000

5	2.755981000	2.709402000	-0.475413000
5	-2.763852000	2.701542000	-0.475559000
5	1.400147000	3.605276000	-0.263314000
5	3.886545000	0.149066000	-0.787992000
5	3.542082000	-1.460261000	-0.954218000
5	1.562128000	-3.401041000	-0.516873000
5	0.005230000	-3.570833000	-0.033485000
5	-3.537837000	-1.470638000	-0.953969000
5	-3.886906000	0.137622000	-0.787899000
5	0.862926000	-2.487809000	0.899629000
5	-1.552217000	-3.405637000	-0.516682000
32a.3			
5	2.396876000	3.613038000	-0.436246000
5	-2.394346000	3.610614000	-0.447046000
5	1.666402000	2.320099000	0.278724000
5	1.630984000	-3.407108000	-0.196606000
5	-1.666756000	2.320823000	0.276557000
5	-4.151342000	0.893791000	-0.257075000
5	0.000463000	2.251378000	0.059143000
5	2.490596000	0.895694000	0.431839000
5	3.172106000	-3.263774000	-0.515430000
5	-2.489820000	0.894745000	0.423100000
5	4.105338000	-1.953360000	-0.495345000
5	-3.334079000	-0.515497000	0.245417000
5	-3.300147000	2.351594000	-0.172752000
5	0.813213000	3.764303000	-0.276945000
5	4.151569000	0.895289000	-0.252705000
5	3.301442000	2.353669000	-0.161170000
5	3.333495000	-0.514584000	0.245864000
5	-3.173718000	-3.267295000	-0.507390000
5	2.439506000	-1.929299000	0.071856000
5	-0.811269000	3.762546000	-0.281522000
5	-1.631725000	-3.409327000	-0.189325000
5	-2.440786000	-1.933320000	0.081660000
5	-0.000143000	-3.355516000	0.000120000
5	4.786113000	-0.497831000	-0.541482000
5	-4.105980000	-1.955207000	-0.487498000
5	-4.788828000	-0.500503000	-0.537596000
5	0.809291000	0.867813000	0.581807000
5	1.692132000	-0.567601000	0.670360000
5	-0.802170000	-2.012094000	0.563164000
5	-0.810366000	0.868613000	0.586378000
5	-1.691956000	-0.566617000	0.670540000
5	0.803905000	-2.015077000	0.569602000
32a.4			
5	2.283162000	3.417497000	0.743091000
5	2.921877000	2.911411000	-0.741029000
5	1.571930000	3.814424000	-0.740917000
5	0.807311000	4.057310000	0.738862000
5	-0.802114000	4.031009000	0.743088000

5	-2.298152000	3.439893000	0.738856000
5	-2.911411000	2.921877000	-0.741029000
5	-3.417497000	2.283162000	0.743091000
5	-4.057310000	0.807311000	0.738862000
5	-3.814424000	1.571930000	-0.740917000
5	-4.124718000	0.007394000	-0.741038000
5	-4.031009000	-0.802114000	0.743088000
5	-3.439893000	-2.298152000	0.738856000
5	-0.807311000	-4.057310000	0.738862000
5	-2.921877000	-2.911411000	-0.741029000
5	-3.808773000	-1.585703000	-0.740913000
5	3.439893000	2.298152000	0.738856000
5	4.031009000	0.802114000	0.743088000
5	4.124718000	-0.007394000	-0.741038000
5	3.814424000	-1.571930000	-0.740917000
5	3.417497000	-2.283162000	0.743091000
5	2.298152000	-3.439893000	0.738856000
5	0.802114000	-4.031009000	0.743088000
5	-0.007394000	-4.124718000	-0.741038000
5	1.585703000	-3.808773000	-0.740913000
5	2.911411000	-2.921877000	-0.741029000
5	3.808773000	1.585703000	-0.740913000
5	-1.585703000	3.808773000	-0.740913000
5	0.007394000	4.124718000	-0.741038000
5	4.057310000	-0.807311000	0.738862000
5	-1.571930000	-3.814424000	-0.740917000
5	-2.283162000	-3.417497000	0.743091000

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