

Supporting information

A bottom-up approach from medium-sized bilayer boron nanoclusters to bilayer borophene nanomaterials

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Fig. S2 Top and side views of the optimized BL *D*₂ B₈₂₈ (**XIII**).

Fig. S3 AdNDP bonding patterns of *C*_{2v} B₈₆ (**II**).

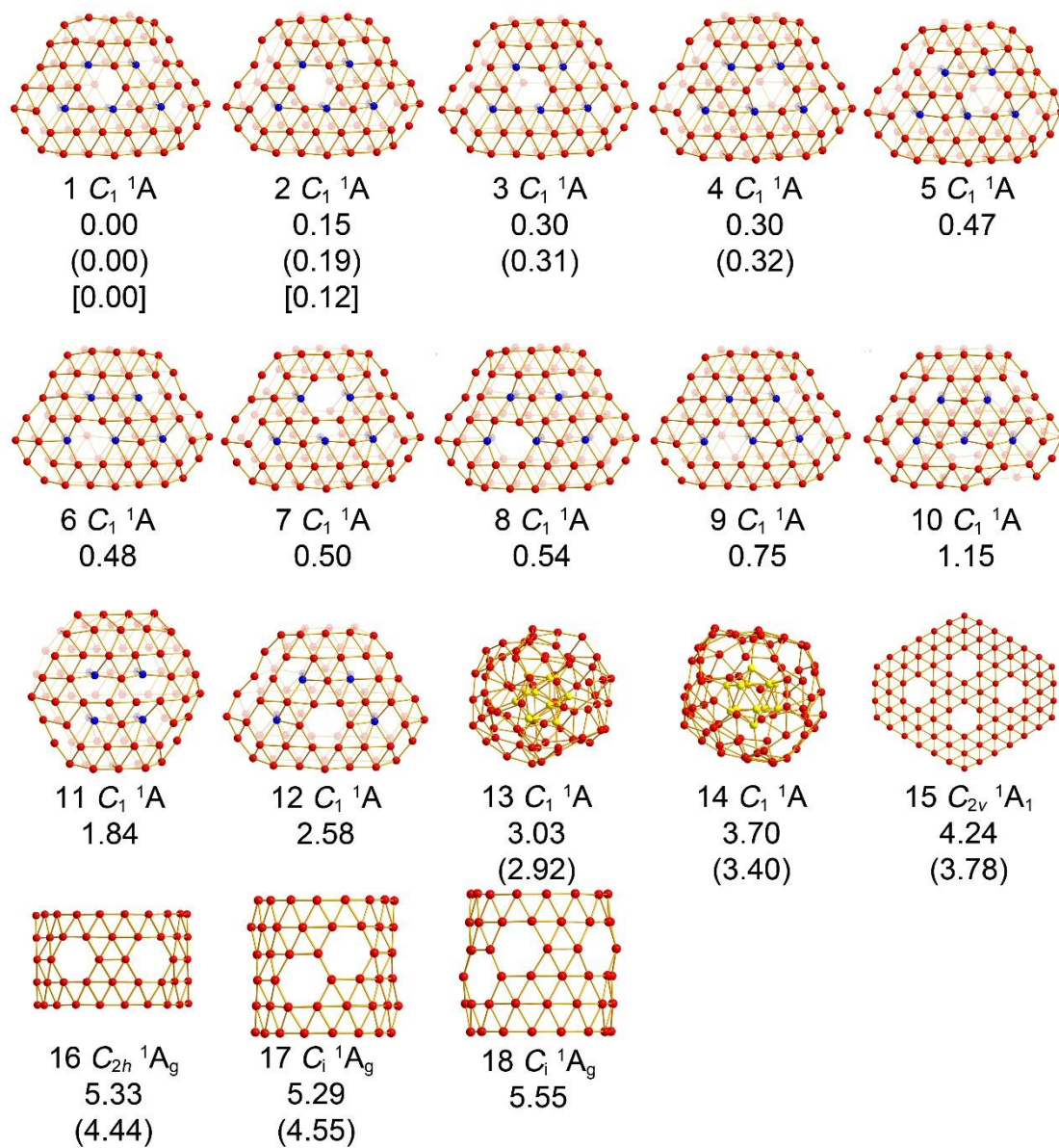
Fig.S4 Born-Oppenheimer molecular dynamics simulations of *C*_{2v} B₈₆ (**II**) and *C*_{2v} B₉₆ (**VII**).

Fig. S5 Simulated IR, Raman, and UV-Vis of *C*_{2v} B₈₆ (**II**) and *C*_{2v} B₉₆ (**VII**)

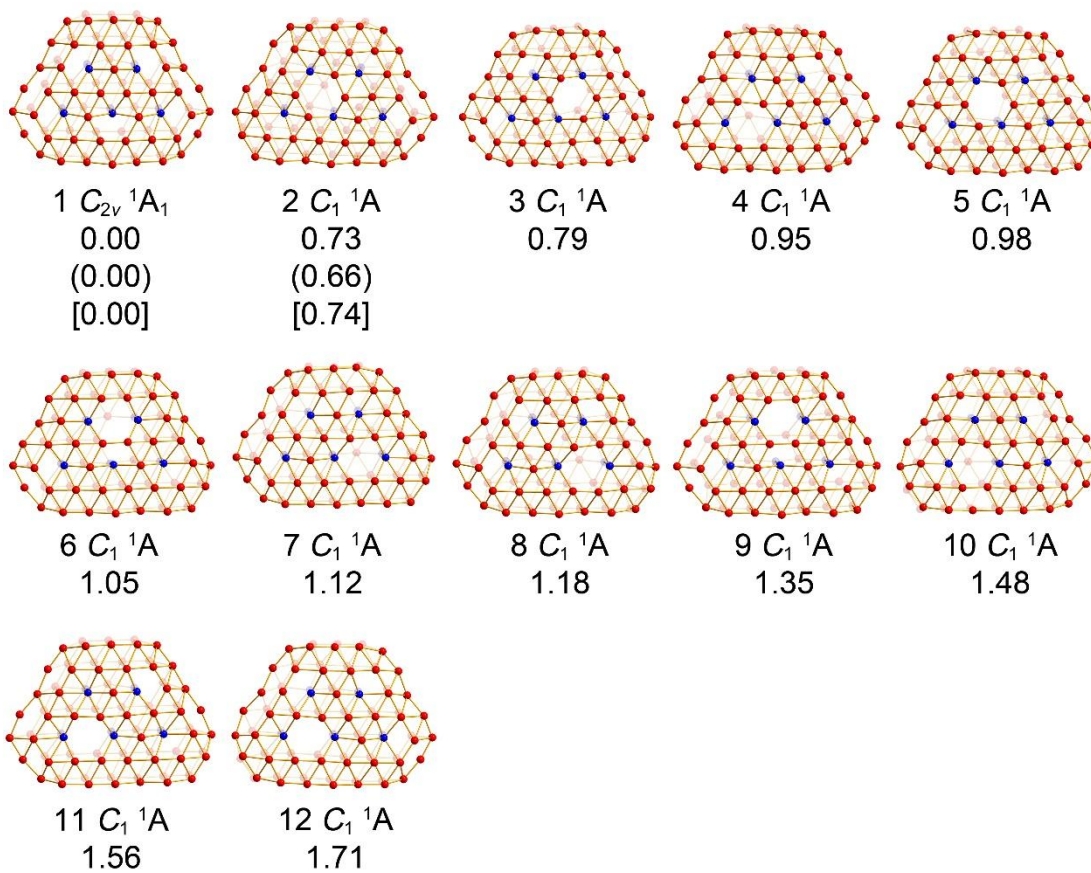
Table S1 Optimized cartesian coordinates of *C*₁ B₈₄ (**I**), *C*_{2v} B₈₆ (**II**), *C*₁ B₈₈ (**III**), *C*₁ B₉₀ (**IV**), *C*₁ B₉₂ (**V**), *C*₁ B₉₄ (**VI**), *C*_{2v} B₉₆ (**VII**), *C*₁ B₉₈ (**VIII**), *C*₂ B₁₂₈ (**IX**), *D*_{2h} B₂₁₄ (**X**), *C*_{2v} B₂₆₀ (**XI**), *D*_{2h} B₃₇₂ (**XII**), and *D*₂ B₈₂₈ (**XIII**).

Fig. S1 Low-lying isomers of (a) B₈₄, (b) B₈₆ (c) B₈₈, (d) B₉₀, (e) B₉₂, (f) B₉₄, (g) B₉₆, (h) B₉₈ and (i) B₁₂₈ with their relative energies indicated in eV at PBE0/6-31G(d), PBE0/6-311+G(d) (in parentheses), and TPSSh/6-31G(d) (in square brackets) levels, respectively.

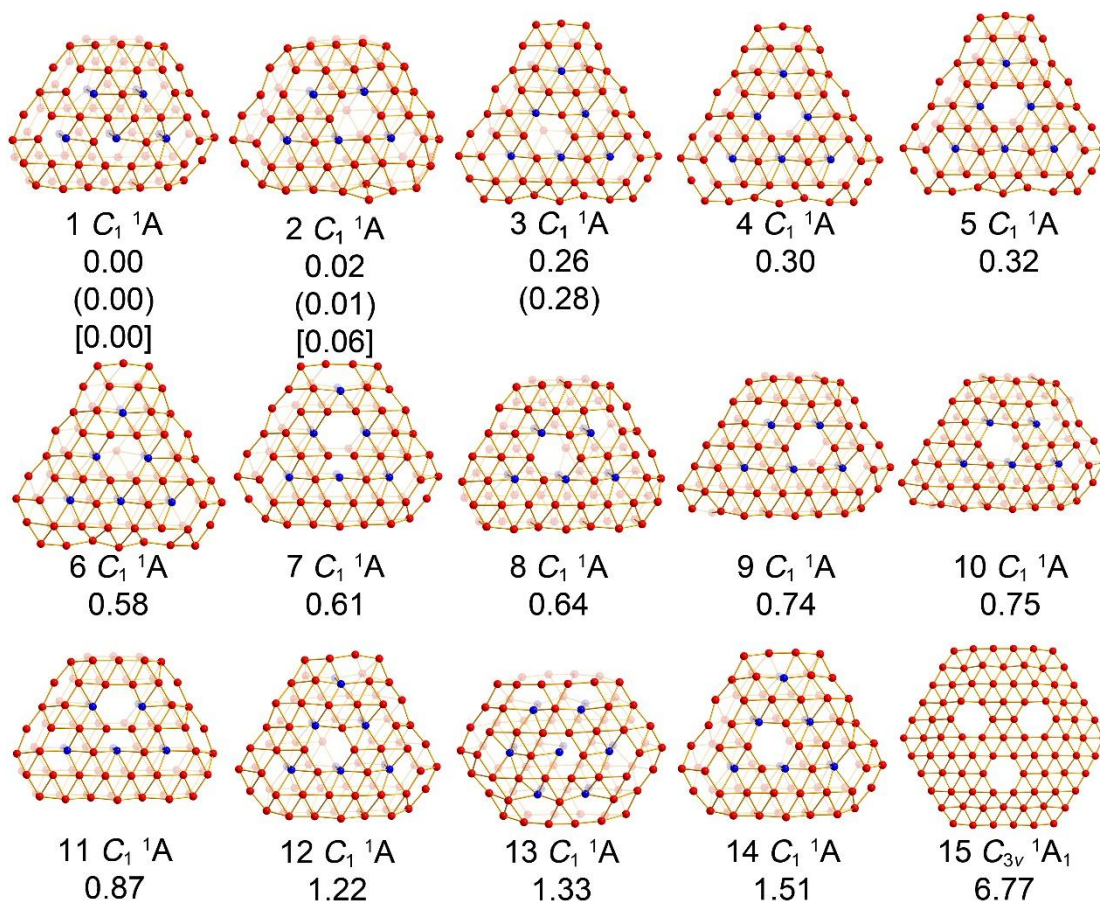
(a) B₈₄



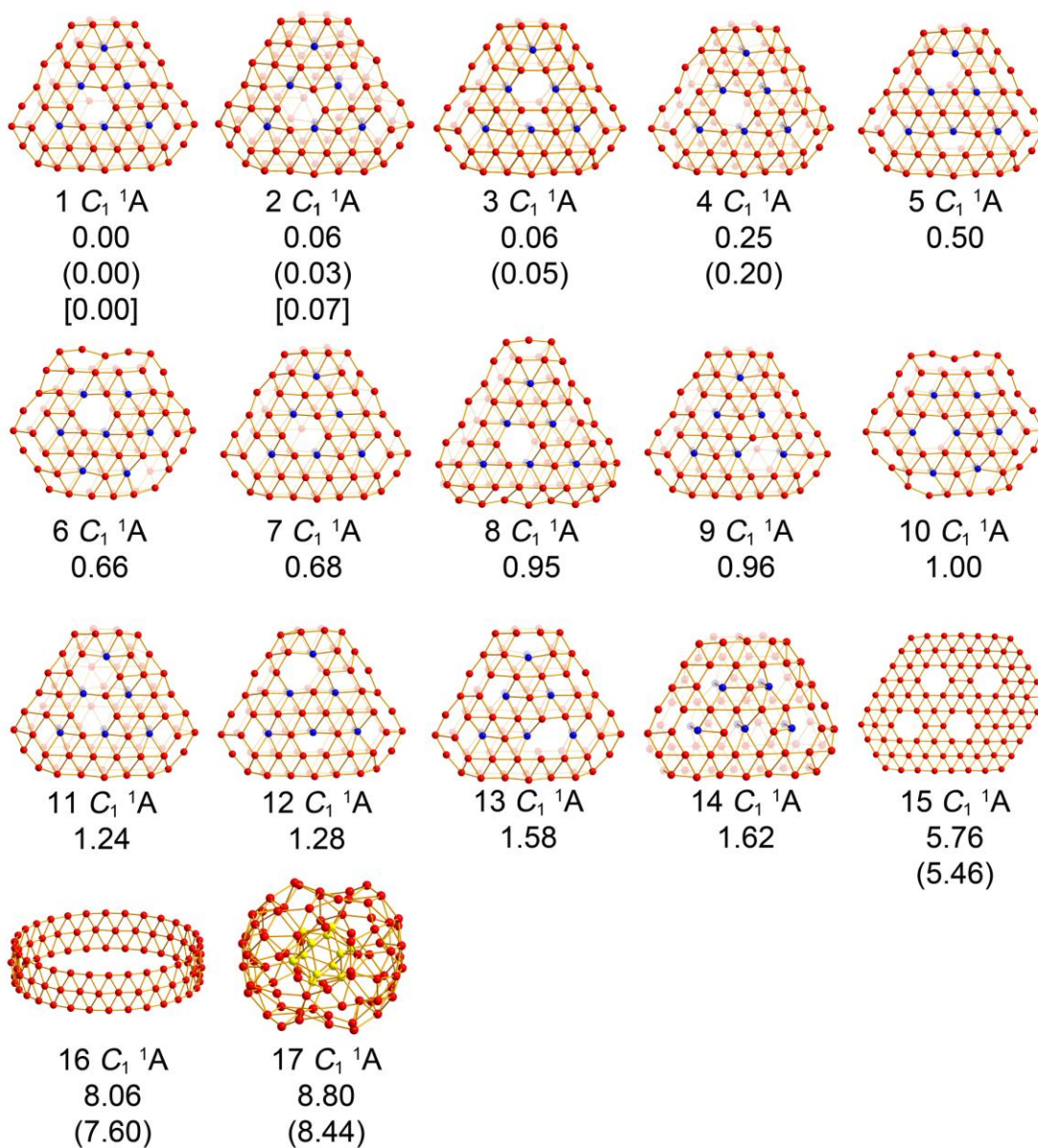
(b) B₈₆



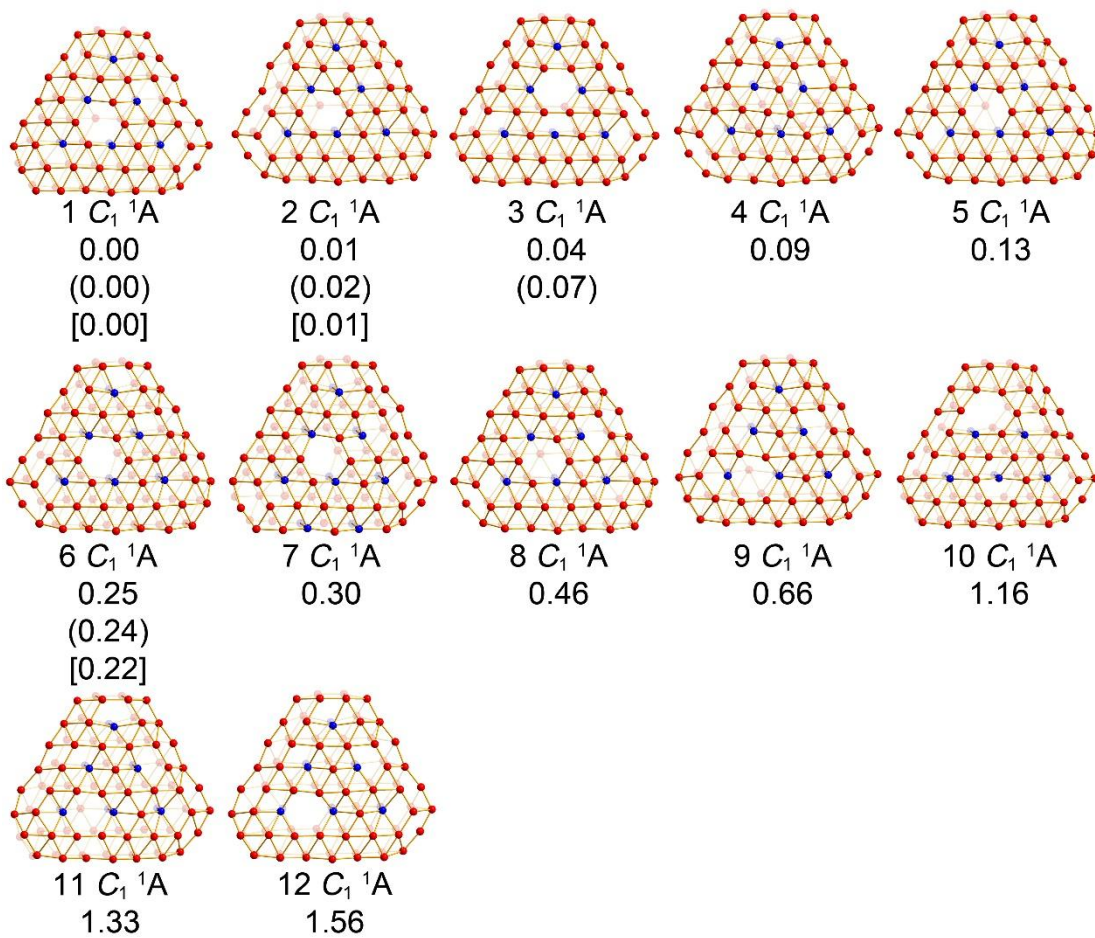
(c) B₈₈



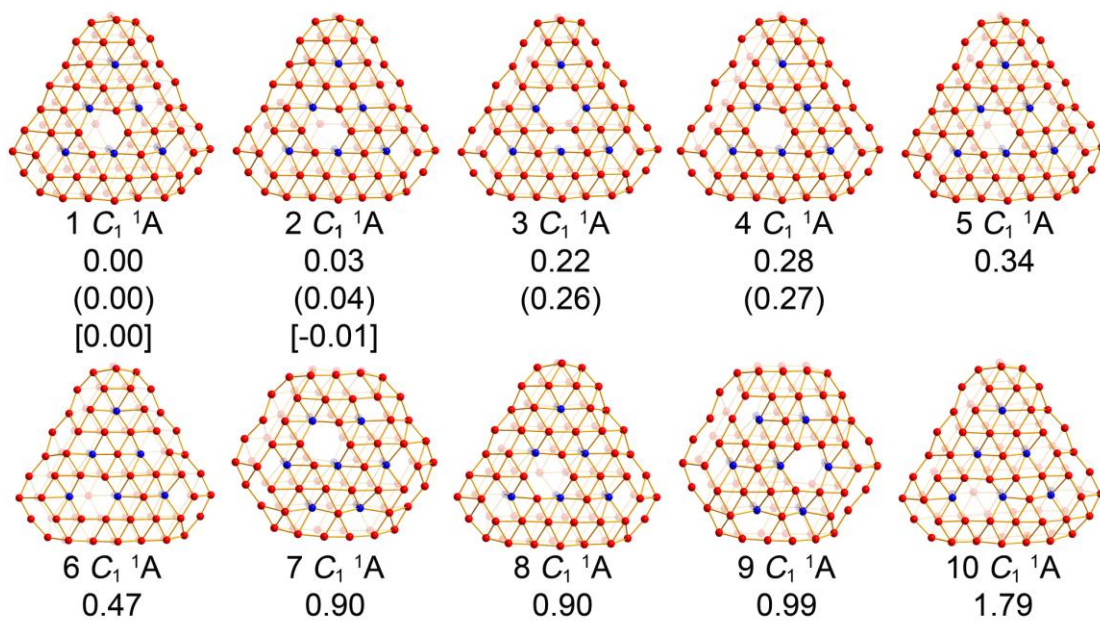
(d) B₉₀



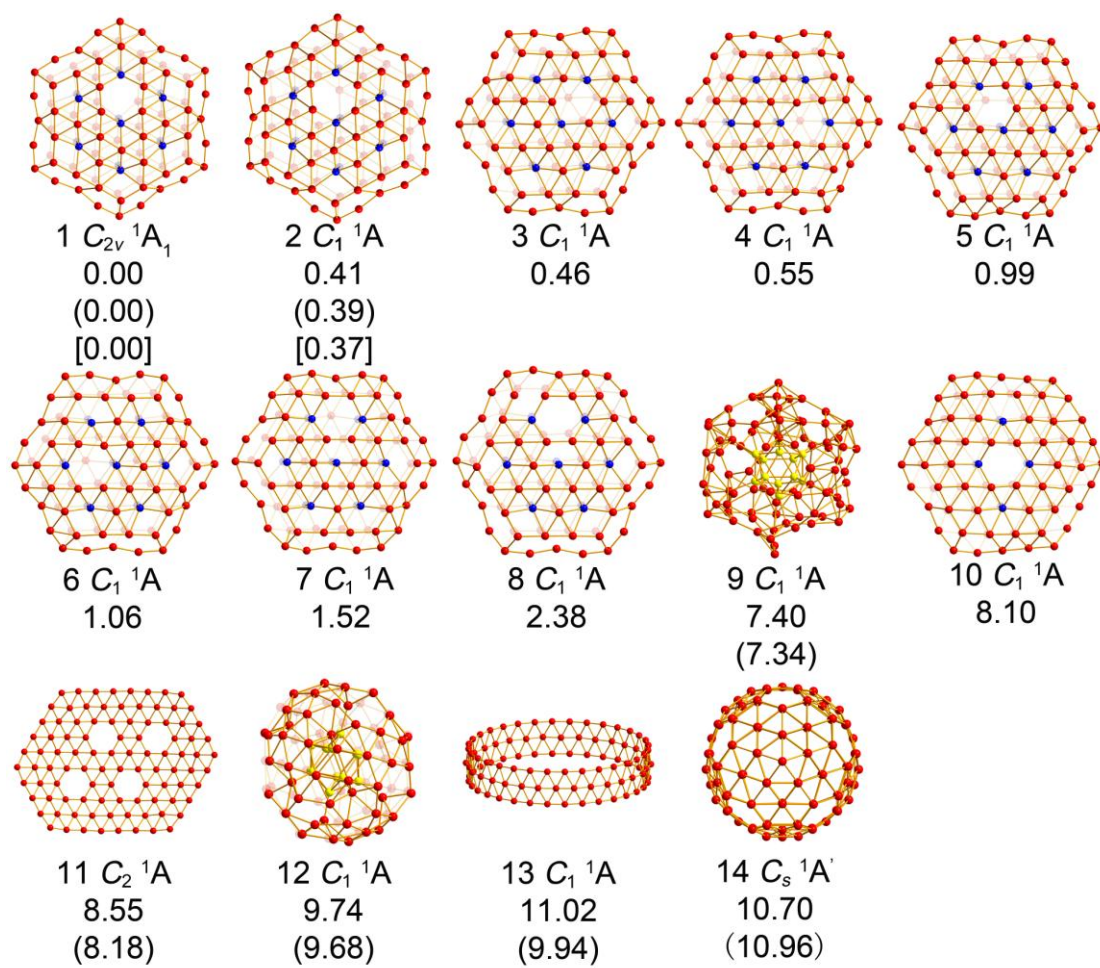
(e) B₉₂



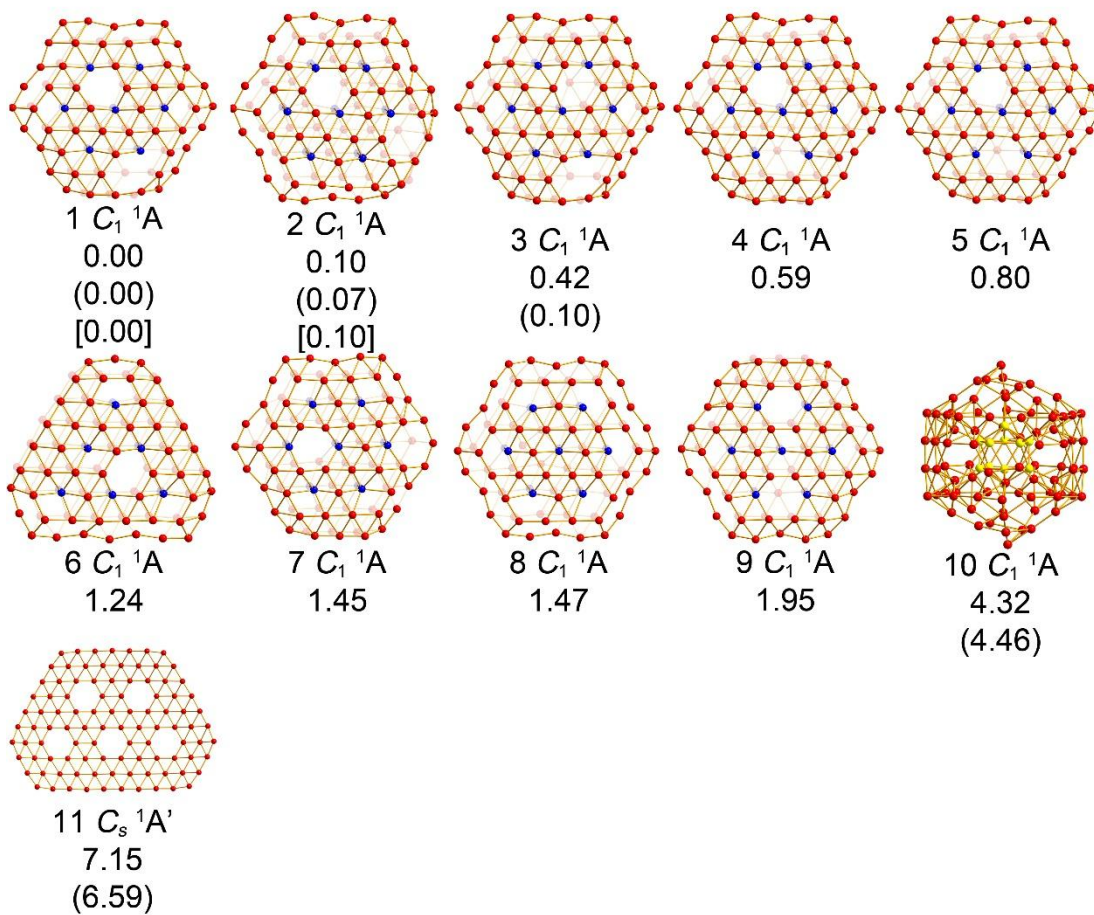
(f) B₉₄



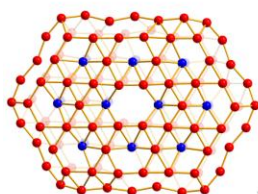
(g) B₉₆



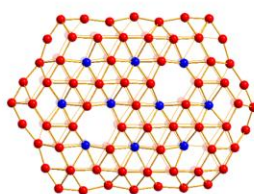
(h) B₉₈



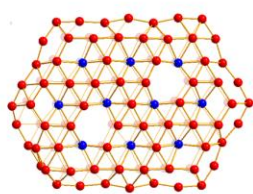
(i) B_{128}



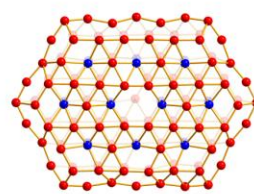
1 C_2 $1A$
0.00



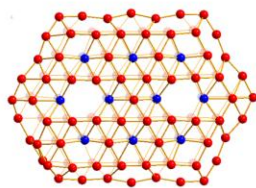
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-0.17



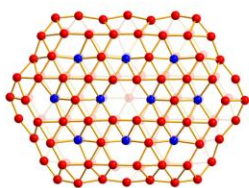
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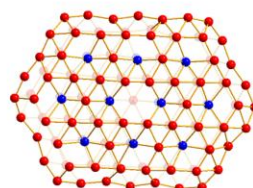
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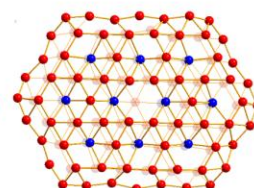
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-0.04



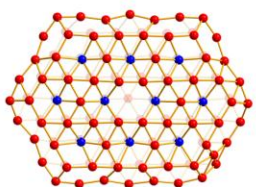
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0.07



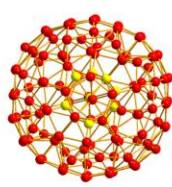
7 C_1 $1A$
0.15



8 C_1 $1A$
0.22



9 C_1 $1A$
0.38



10 C_{2h} $1A_g$
1.99

Fig. S2 Top and side views of the optimized BL D_{2h} B_{372} (**XIII**), with the inward-buckled B atoms interconnected by interlayer B-B σ bonds colored in blue, the B_{72} BL hexagonal prisms at the center of highlighted in a purple dotted circle.

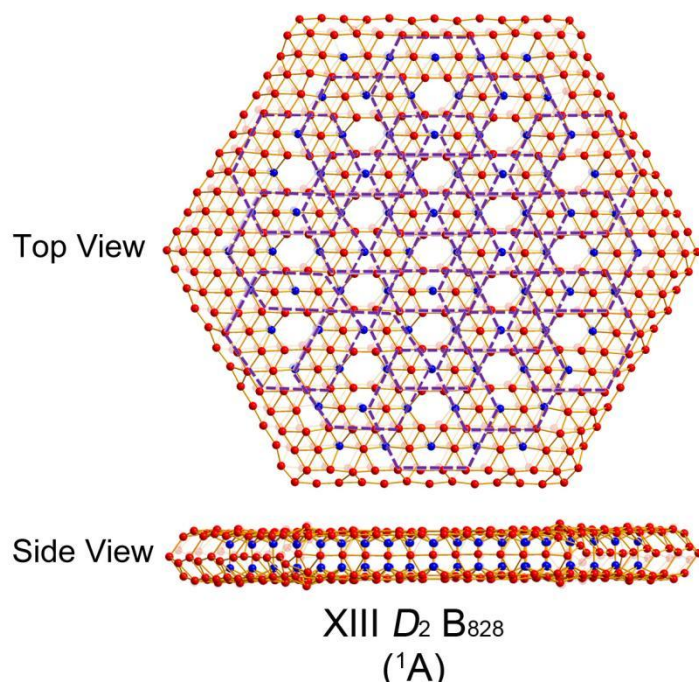


Fig. S3 AdNDP bonding patterns of C_{2v} B_{86} (**II**)

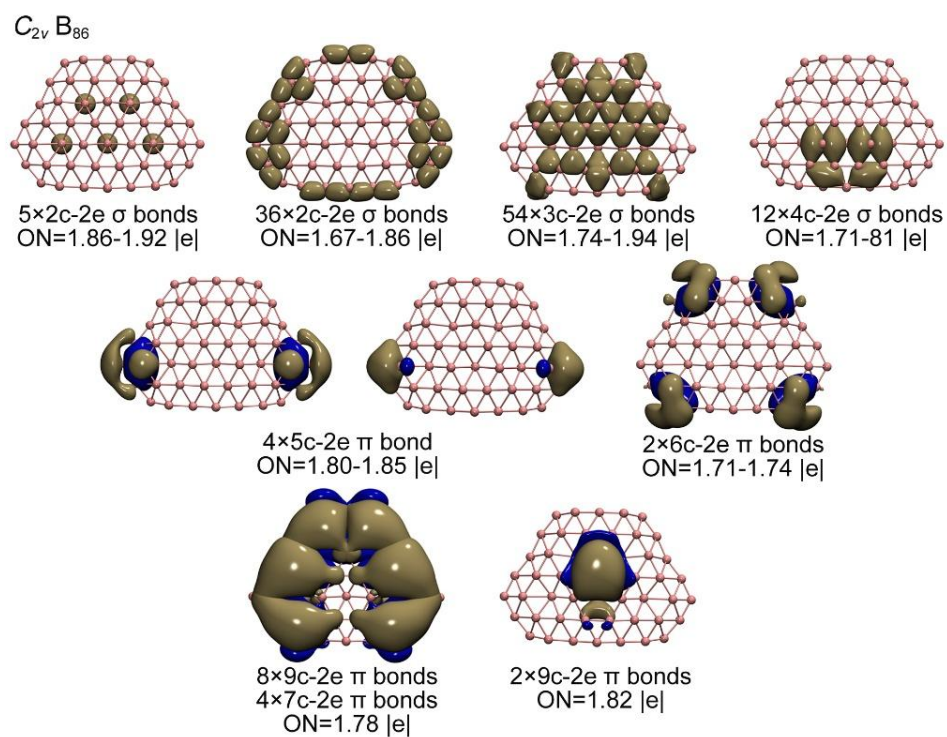


Fig. S4 Born-Oppenheimer molecular dynamics (BOMD) simulations of (a) $C_{2v} B_{86}$ (II) and (b) $C_{2v} B_{96}$ (VII).

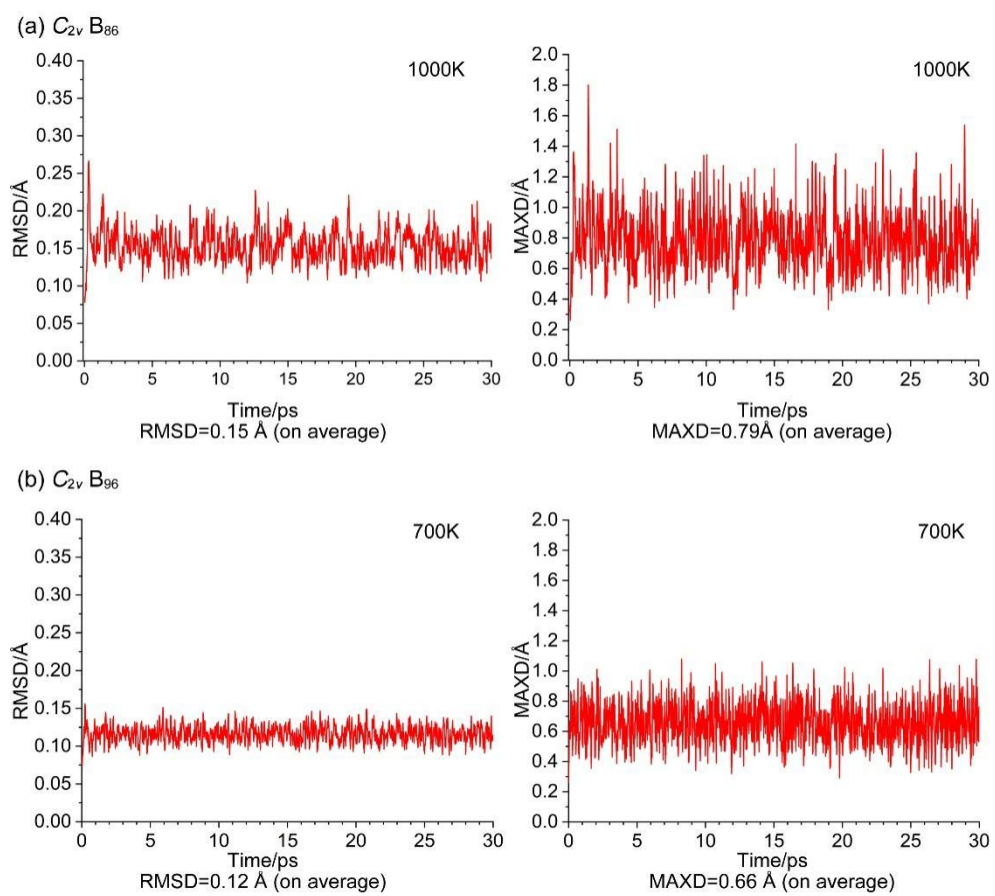


Fig. S5 Simulated IR, Raman, and UV-Vis of (a) $C_{2v} B_{86}$ (**II**) and (b) $C_{2v} B_{96}$ (**VII**) at PBE0/6-31G(d) level.

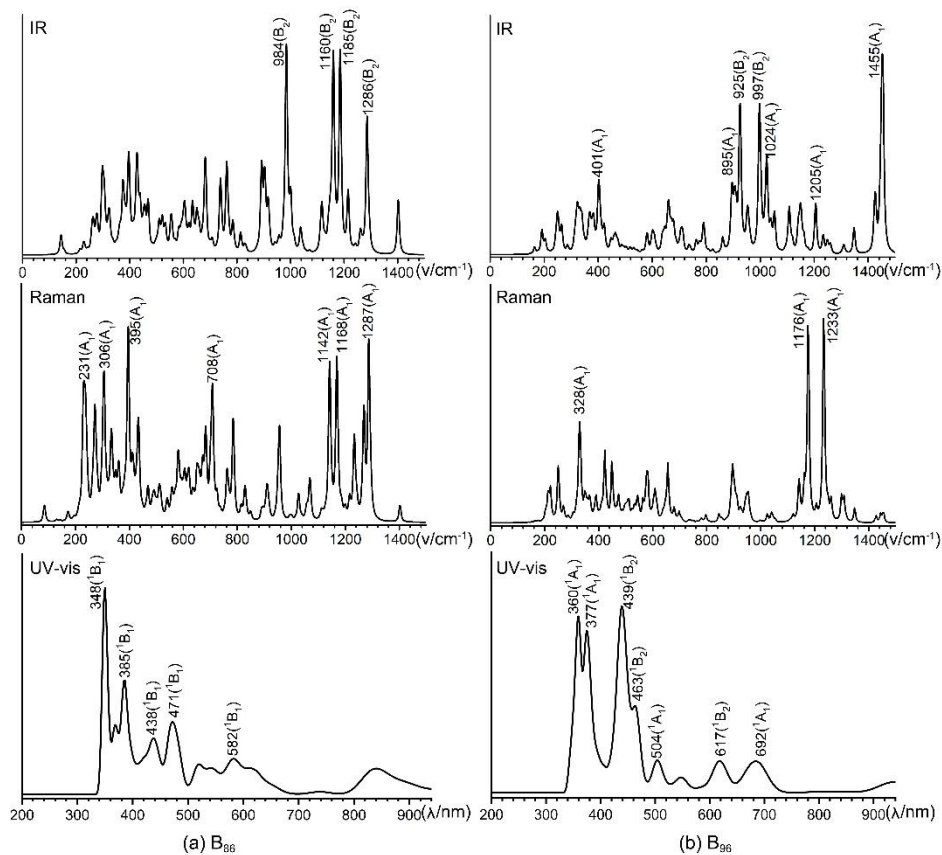


Table S1 Optimized cartesian coordinates of (a) $C_1 B_{84}$ (**I**), (b) $C_{2v} B_{86}$ (**II**), (c) $C_1 B_{88}$ (**III**), (d) $C_1 B_{90}$ (**IV**), (e) $C_1 B_{92}$ (**V**), (f) $C_1 B_{94}$ (**VI**), (g) $C_{2v} B_{96}$ (**VII**) and (h) $C_1 B_{98}$ (**VIII**) at PBE0/6-311+G(d), (i) $C_2 B_{128}$ (**IX**) at PBE0/6-31G(d), (j) $D_{2h} B_{214}$ (**X**), (k) $C_{2v} B_{260}$ (**XI**), (l) $D_{2h} B_{372}$ (**XII**) at PBE0/6-31G, and (m) $D_2 B_{828}$ (**XIII**) at PBE.

(a) $C_1 B_{84}$ (**I**)

B	1.54459600	-0.92758500	-1.81133200
B	-0.02072600	-1.04637900	-0.88448100
B	-0.73550400	0.37476100	-1.80091300
B	2.45182700	-2.37317600	-1.63117000
B	-0.83223500	-2.49817100	-1.70107600
B	-2.44213600	0.42591100	-1.64086600
B	-2.47692900	-2.46387800	-1.64003300
B	-4.11001200	-2.44923300	-1.41380300
B	-1.58634400	-1.01917100	-1.75772600
B	-4.98455400	-1.03569400	-1.36448500
B	-4.13341800	0.38278800	-1.47402300
B	-3.11048200	-0.97722300	-0.85589900
B	1.58637400	-1.01915100	1.75773100
B	0.02074200	-1.04637300	0.88454000
B	0.73553300	0.37479200	1.80095500
B	2.47696600	-2.46385300	1.64003000
B	-2.37981400	0.45356900	1.72408600
B	-2.45180600	-2.37319100	1.63118800
B	-4.10158500	-2.40602200	1.39919900
B	-1.54459900	-0.92760600	1.81136200
B	-4.97483700	-1.02084900	1.24030700
B	-4.04509200	0.41187900	1.38130200
B	-3.05785300	-0.93335500	0.81311500
B	-3.39280000	1.83194400	-1.44506500
B	-0.86494000	3.21169200	-1.73164300
B	-1.53344100	1.73129300	-0.84267100
B	0.81604000	3.20848800	-1.70418400
B	-2.58594300	3.21947900	-1.46788400
B	1.52339900	1.80936400	-0.87593300
B	2.37980800	0.45359300	-1.72407600
B	2.40883300	3.36414300	-1.38122400
B	4.04509800	0.41194300	-1.38132100
B	-0.00259400	1.77941200	-1.88027200
B	4.97483700	-1.02079000	-1.24030200
B	3.22263000	1.86555700	-1.41382600
B	4.10161900	-2.40598800	-1.39922400
B	3.05791500	-0.93334200	-0.81316600

B	-3.22266000	1.86552800	1.41380000
B	-0.81605800	3.20846800	1.70410900
B	-1.52343000	1.80932300	0.87595300
B	0.86490300	3.21170900	1.73159900
B	-2.40886300	3.36408600	1.38113000
B	1.53340800	1.73128900	0.84268400
B	2.44215100	0.42593600	1.64088900
B	2.58591400	3.21950700	1.46778300
B	4.13342800	0.38286000	1.47395000
B	0.00256300	1.77941400	1.88033100
B	4.98457200	-1.03562500	1.36442500
B	3.39277000	1.83198200	1.44507600
B	4.11003900	-2.44915900	1.41379700
B	3.11047000	-0.97718200	0.85584800
B	4.49586200	1.69012200	-0.10709300
B	3.90846200	3.19187800	-0.57832700
B	-3.90858600	3.19186800	0.57843500
B	-4.49587700	1.69009100	0.10709800
B	5.55450800	0.44342300	-0.47635900
B	-5.55449400	0.44336100	0.47639300
B	-0.80811600	-2.41780000	1.77082900
B	0.83226600	-2.49815100	1.70109600
B	0.80814500	-2.41779200	-1.77079400
B	-6.16922100	-0.90841700	-0.04817400
B	6.16926900	-0.90836800	0.04813200
B	5.52282100	-2.32233800	0.06702300
B	-5.52275900	-2.32238300	-0.06705700
B	4.48589200	-3.57691600	-0.01524400
B	3.24159100	-3.80100500	-1.13659200
B	1.57230700	-3.89322600	0.88568800
B	-0.01290100	-3.95962800	1.44203900
B	-1.57227100	-3.89325500	-0.88566000
B	-3.24153000	-3.80103000	1.13656700
B	-4.48584200	-3.57696700	0.01523700
B	2.88491200	4.32718400	0.02782900
B	1.38806600	4.82708400	-0.50061300
B	-0.14362000	4.61366500	-0.90341600
B	-1.77370800	4.59823900	-1.20339200
B	-2.88501200	4.32711100	-0.02784600
B	1.77366500	4.59829500	1.20343600
B	0.14355600	4.61362600	0.90333100
B	-1.38822700	4.82701900	0.50079100
B	1.58800400	-3.86485600	-0.94956400

B	0.01295200	-3.95964000	-1.44196700
B	-1.58794500	-3.86486400	0.94959400
B	-3.23443000	-3.86705100	-1.05251200
B	3.23448300	-3.86699300	1.05250000

(b) $C_1 B_{88}$ (III)

B	-1.80907800	1.62318400	-1.04832400
B	-0.87773100	0.00000000	-0.96526900
B	-1.83903500	-0.83350400	0.40344400
B	-1.66474000	2.48618400	-2.44827300
B	-1.69105200	-0.81022100	-2.52415900
B	-1.64335700	-2.48222600	0.42639900
B	-1.83903500	0.83350400	0.40344400
B	-1.66474000	-2.48618400	-2.44827300
B	-1.39355900	-4.10797500	-2.42465000
B	-1.80907800	-1.62318400	-1.04832400
B	-1.28034000	-5.01097400	-1.01425900
B	-1.42060100	-4.13766600	0.41458000
B	-0.83565500	-3.07631800	-0.97326400
B	1.80907800	1.62318400	-1.04832400
B	0.87773100	0.00000000	-0.96526900
B	1.83903500	-0.83350400	0.40344400
B	1.66474000	2.48618400	-2.44827300
B	1.64335700	-2.48222600	0.42639900
B	1.83903500	0.83350400	0.40344400
B	1.66474000	-2.48618400	-2.44827300
B	1.39355900	-4.10797500	-2.42465000
B	1.80907800	-1.62318400	-1.04832400
B	1.28034000	-5.01097400	-1.01425900
B	1.42060100	-4.13766600	0.41458000
B	0.83565500	-3.07631800	-0.97326400
B	-1.36197700	-3.34600000	1.89052000
B	-1.64199100	-0.87886600	3.27793000
B	-0.85603200	-1.50921300	1.70757600
B	-1.64199100	0.87886600	3.27793000
B	-1.33583100	-2.51380600	3.28023800
B	-0.85603200	1.50921300	1.70757600
B	-1.64335700	2.48222600	0.42639900
B	-1.33583100	2.51380600	3.28023800
B	-1.42060100	4.13766600	0.41458000
B	-1.88936700	0.00000000	1.86150600
B	-1.28034000	5.01097400	-1.01425900
B	-1.36197700	3.34600000	1.89052000
B	-1.39355900	4.10797500	-2.42465000
B	-0.83565500	3.07631800	-0.97326400
B	1.36197700	-3.34600000	1.89052000
B	1.64199100	-0.87886600	3.27793000
B	0.85603200	-1.50921300	1.70757600

B	1.64199100	0.87886600	3.27793000
B	1.33583100	-2.51380600	3.28023800
B	0.85603200	1.50921300	1.70757600
B	1.64335700	2.48222600	0.42639900
B	1.33583100	2.51380600	3.28023800
B	1.42060100	4.13766600	0.41458000
B	1.88936700	0.00000000	1.86150600
B	1.28034000	5.01097400	-1.01425900
B	1.36197700	3.34600000	1.89052000
B	1.39355900	4.10797500	-2.42465000
B	0.83565500	3.07631800	-0.97326400
B	0.00000000	4.56158400	1.64875900
B	0.00000000	3.86775400	3.17184200
B	0.00000000	-3.86775400	3.17184200
B	0.00000000	-4.56158400	1.64875900
B	0.00000000	5.57636300	0.37608800
B	0.00000000	-5.57636300	0.37608800
B	1.69105200	-0.81022100	-2.52415900
B	1.69105200	0.81022100	-2.52415900
B	-1.69105200	0.81022100	-2.52415900
B	0.00000000	-6.24579300	-1.01805700
B	0.00000000	6.24579300	-1.01805700
B	0.00000000	5.52362900	-2.38218300
B	0.00000000	-5.52362900	-2.38218300
B	0.00000000	4.48322200	-3.62727300
B	-1.09614600	3.24113300	-3.85474400
B	0.94141900	1.58352600	-3.93146500
B	1.47547800	0.00000000	-3.98472700
B	-0.94141900	-1.58352600	-3.93146500
B	1.09614600	-3.24113300	-3.85474400
B	0.00000000	-4.48322200	-3.62727300
B	0.00000000	2.87363900	4.45898300
B	-1.14554200	1.62483900	4.68946700
B	-0.95951700	0.00000000	4.71829600
B	-1.14554200	-1.62483900	4.68946700
B	0.00000000	-2.87363900	4.45898300
B	1.14554200	1.62483900	4.68946700
B	0.95951700	0.00000000	4.71829600
B	1.14554200	-1.62483900	4.68946700
B	-0.94141900	1.58352600	-3.93146500
B	-1.47547800	0.00000000	-3.98472700
B	0.94141900	-1.58352600	-3.93146500
B	-1.09614600	-3.24113300	-3.85474400

B	1.09614600	3.24113300	-3.85474400
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(c) $C_1 B_{88}$ (III)

B	1.63956000	-0.72420900	-1.86181600
B	0.00899800	-0.89046700	-0.88141600
B	-1.01609500	0.33571000	-1.79630100
B	2.66263600	-2.00604700	-1.74762500
B	-0.56973800	-2.55402500	-1.71114300
B	-2.65754100	0.12069100	-1.65028100
B	0.62910400	0.58937800	-1.84923000
B	-2.23950400	-2.71993700	-1.66068500
B	-3.85021800	-2.93583400	-1.39746900
B	-1.59552300	-1.20777300	-1.83137800
B	-4.95612200	-1.67544200	-1.27024200
B	-4.29667300	-0.12843600	-1.41379600
B	-3.03870200	-1.35059300	-0.83896900
B	1.63944000	-0.72428600	1.86084800
B	0.00898300	-0.89058900	0.88081200
B	-1.01640600	0.33548300	1.79733300
B	2.66290500	-2.00616000	1.74659500
B	-2.65737800	0.12036700	1.65051500
B	0.62883500	0.58876000	1.84774900
B	-2.23873100	-2.72066300	1.65968200
B	-3.84942800	-2.93730100	1.39686300
B	-1.59543100	-1.20815500	1.83073300
B	-4.95501300	-1.67520900	1.27362500
B	-4.29769700	-0.12917900	1.41726800
B	-3.03919400	-1.35088000	0.83982300
B	-3.72881400	1.44114900	-1.37582100
B	-1.48150200	3.17741300	-1.65720400
B	-1.89022500	1.53498800	-0.86116600
B	0.26392000	3.42585500	-1.62530800
B	-3.09863500	2.93652100	-1.32579000
B	1.11162200	1.96610100	-0.85909600
B	2.26701900	0.84753700	-1.58681400
B	1.89182900	3.68573000	-1.35170800
B	3.94326000	1.10819500	-1.38505200
B	-0.40126100	1.90641100	-1.90224100
B	4.90027300	-0.18740000	-1.34140400
B	2.90807400	2.42962800	-1.35928100
B	4.27526500	-1.75224000	-1.59963700
B	3.07358000	-0.48421300	-0.84503800
B	-3.73092200	1.44001900	1.37904800
B	-1.48221800	3.17678900	1.65845600
B	-1.89026800	1.53490900	0.86175900

B	0.26337000	3.42512200	1.62430500
B	-3.09899300	2.93415900	1.32601000
B	1.11149800	1.96577700	0.85896700
B	2.26678600	0.84763100	1.58723400
B	1.89191100	3.68690200	1.35324300
B	3.94313200	1.10827100	1.38536800
B	-0.40161900	1.90589300	1.90142200
B	4.89944700	-0.18788100	1.34084500
B	2.90732800	2.42950500	1.36001400
B	4.27597700	-1.75268000	1.60101800
B	3.07361400	-0.48412600	0.84506500
B	4.17931400	2.33939300	0.00044900
B	3.21642300	3.70586200	0.00008800
B	-4.43869000	2.64193200	-0.00267800
B	-4.88548900	1.02405400	0.00086500
B	5.28501500	1.11799100	0.00079000
B	-5.71189600	-0.37724500	-0.01095600
B	-0.56954000	-2.55422000	1.71026200
B	1.02525100	-2.29019000	1.63732500
B	1.02475500	-2.28983000	-1.63697900
B	-6.18360700	-1.85603700	0.00268000
B	6.13939400	-0.30149800	-0.00009800
B	3.66513900	-3.38063400	-1.38652200
B	2.03748200	-3.56888100	0.96232900
B	0.45510300	-3.87437100	1.47453600
B	-1.12556500	-4.04189700	-0.94139400
B	-2.78018900	-4.22206800	1.09292000
B	2.07988900	4.87492000	0.00070400
B	0.79169400	4.93435900	-1.11124600
B	-0.82152800	4.71604700	-0.95726200
B	-2.42589100	4.46169700	-1.15078800
B	-3.63123400	4.05377000	0.00020400
B	0.79093200	4.93422300	1.11274500
B	-0.82236400	4.71555500	0.95779500
B	-2.42708300	4.46058700	1.15192300
B	2.03720800	-3.56890900	-0.96321800
B	0.45443000	-3.87362200	-1.47566500
B	-1.12473700	-4.04212300	0.94003300
B	-2.78120700	-4.22131500	-1.09420900
B	3.66552300	-3.38070700	1.38617900
B	5.86339500	-1.55722800	-1.10703900
B	5.18564400	-3.03842700	-0.87353500
B	5.86371900	-1.55763700	1.10533200

B	5.18581500	-3.03912500	0.87397300
B	-4.04221500	-4.17757600	0.00004300
B	-5.24940600	-3.08801800	0.00172500

(d) $C_1 B_{90}$ (IV)

B	1.55177200	-1.35808400	-1.78530300
B	-0.03101800	-1.43845900	-0.88992100
B	-0.69715000	0.00617400	-1.79397700
B	2.43091400	-2.82190300	-1.62855800
B	-0.86124700	-2.87029900	-1.72354000
B	-2.41446000	0.08712800	-1.65115300
B	-2.51136300	-2.79431900	-1.65069100
B	-4.14502800	-2.75050300	-1.38637900
B	-1.58055600	-1.37573700	-1.76496700
B	-5.01605600	-1.34331000	-1.22983200
B	-4.07867000	0.07630400	-1.34069400
B	-3.08018000	-1.30515200	-0.81465600
B	1.54998400	-1.36624500	1.78036800
B	-0.03043700	-1.44564500	0.88806000
B	-0.69809000	-0.00629000	1.78897600
B	2.43152400	-2.82894200	1.61254700
B	-2.41192800	0.09012800	1.66089000
B	-2.50285000	-2.80297800	1.65671600
B	-4.13234000	-2.76411800	1.39717500
B	-1.58448500	-1.38008900	1.77448100
B	-4.99226500	-1.32660100	1.33774300
B	-4.10663600	0.07922200	1.46245400
B	-3.09513400	-1.30851200	0.85512800
B	-3.27066800	1.52095000	-1.32843200
B	-0.79162300	2.83582300	-1.73677100
B	-1.49983000	1.40529900	-0.84675900
B	0.95668200	2.80245400	-1.66654900
B	-2.48783900	2.95661700	-1.36379100
B	1.62946500	1.39893300	-0.92014100
B	2.43437700	0.01031700	-1.70104500
B	2.65502400	2.85924800	-1.44015600
B	4.13085100	-0.05312800	-1.43135800
B	5.00095500	-1.48090400	-1.26723700
B	3.38186100	1.39170700	-1.49606700
B	4.06919000	-2.87194300	-1.39253900
B	3.08150600	-1.39350100	-0.84554700
B	-3.33165100	1.52243400	1.46234600
B	-0.81217200	2.81763900	1.70274500
B	-1.50226000	1.40228900	0.86410100
B	0.94087400	2.78830700	1.70647100
B	-2.53434400	2.93365700	1.41966600
B	1.62351500	1.40224900	0.86827500

B	2.42133900	0.00330900	1.67931700
B	2.62289400	2.87283200	1.38112900
B	4.11101700	-0.07837900	1.34390500
B	5.00317000	-1.51693900	1.21927100
B	3.35379800	1.37026700	1.36769300
B	4.07167300	-2.88180900	1.38183800
B	3.06295200	-1.40222000	0.80896900
B	4.57513400	1.18550500	0.00256800
B	4.08396400	2.72959700	0.33048300
B	-3.95967600	2.87934400	-0.31890600
B	-4.50719500	1.32735200	-0.01113000
B	5.58243800	-0.12719800	0.15198700
B	-5.58571900	0.09769000	-0.29601100
B	-0.85892000	-2.88034300	1.73832200
B	0.78246700	-2.83243700	1.75870900
B	0.78372400	-2.82491900	-1.77426200
B	-6.23287500	-1.26951900	0.05810500
B	6.26655500	-1.51065800	-0.02301400
B	5.49794700	-2.86302900	-0.03430400
B	-5.55794400	-2.66375600	0.06822600
B	4.41366700	-4.07077200	-0.01274600
B	3.17790000	-4.25826300	-1.13659400
B	1.52098600	-4.29338800	0.90918100
B	-0.03910600	-4.35185100	1.44036400
B	-1.64052800	-4.25011900	-0.91577000
B	-3.27847400	-4.20188100	1.07851800
B	-4.53718400	-3.91672500	0.01042800
B	3.06898100	3.99405600	0.00673400
B	1.81628600	4.27870700	-1.37806900
B	0.11360300	4.00175800	-0.83128200
B	-1.54415500	4.32050900	-1.30055400
B	-2.92408800	4.10425100	-0.00947700
B	1.75392500	4.27948200	1.37963600
B	0.09172800	3.99818000	0.85460900
B	-1.60295400	4.30217000	1.34238800
B	1.51984200	-4.29095700	-0.92925200
B	-0.04476700	-4.34276600	-1.44686700
B	-1.63195200	-4.25748000	0.91751700
B	-3.29688400	-4.19201800	-1.07931000
B	3.18275600	-4.26457400	1.11507300
B	2.25914500	5.41545900	0.03498900
B	-2.09118700	5.54308100	-0.03716300
B	0.08778500	1.37541600	1.82954700

B	0.07873100	1.39331700	-1.85585900
B	0.93863800	5.66308200	-0.97351400
B	-0.70014000	5.73157100	-0.93838100
B	0.88097600	5.65928400	0.97512800
B	-0.75848500	5.71556600	0.97575100

(e) $C_1 B_{92}$ (V)

B	-0.91739000	-1.88546500	1.76407800
B	0.52717500	-1.24929900	0.88354600
B	0.47218900	0.33163200	1.80164100
B	-1.04971000	-3.58479900	1.62154300
B	1.90884700	-2.16654900	1.69746200
B	1.97257000	1.17358700	1.62284900
B	3.33577700	-1.38850200	1.71131700
B	4.75124400	-0.60382600	1.60193100
B	1.88180400	-0.49669200	1.76338100
B	4.83106400	1.08995200	1.36302800
B	3.49627400	1.98381000	1.45342900
B	3.22789200	0.21539400	0.86389200
B	-0.93089700	-1.88236500	-1.76796400
B	0.51992600	-1.24683000	-0.88292800
B	0.46369300	0.33922600	-1.79346000
B	-1.06527300	-3.58312800	-1.63479300
B	1.96177300	1.16431300	-1.59657400
B	3.33367200	-1.38441800	-1.71077700
B	4.79824300	-0.64843600	-1.64712000
B	1.87960200	-0.50031500	-1.74666500
B	4.81807100	1.00437900	-1.29236700
B	3.48169200	1.93153200	-1.33743300
B	3.20655200	0.20947200	-0.81653200
B	2.13755100	2.87463400	1.43214400
B	-0.68042100	2.91373800	1.70798100
B	0.57066600	1.95131600	0.86411700
B	-2.22877000	2.10608100	1.69796500
B	0.80888500	3.79368100	1.41749200
B	-2.22546500	0.56115200	0.87062300
B	-2.31390000	-1.04839100	1.66468300
B	-3.77603900	1.43058400	1.37932700
B	-3.79430600	-1.87960100	1.36730200
B	-0.83830500	1.22398600	1.84518700
B	-3.94729700	-3.55808400	1.24157600
B	-3.76282800	-0.24414900	1.37473300
B	-2.49673900	-4.35789900	1.38726800
B	-2.26134100	-2.59475000	0.81486400
B	2.11071500	2.84478200	-1.33495700
B	-0.69859500	2.91539400	-1.72990900
B	0.56647300	1.94953600	-0.84028600
B	-2.24369800	2.10639100	-1.66439900
B	0.78217000	3.78633100	-1.36085800

B	-2.23081000	0.55277100	-0.91951900
B	-2.33527900	-1.05220400	-1.68398800
B	-3.79467800	1.40556100	-1.44007300
B	-3.82952200	-1.86588100	-1.43419000
B	-0.83702800	1.24023800	-1.87227600
B	-3.97018000	-3.52912200	-1.26148100
B	-3.79595800	-0.23648800	-1.48972200
B	-2.51123500	-4.35061200	-1.38686700
B	-2.28630000	-2.59750200	-0.84350600
B	-4.77731200	-0.95189000	0.00529000
B	-5.01587900	0.64519800	0.31372900
B	2.13221100	4.33202300	-0.27381200
B	3.34111800	3.20884200	0.00384000
B	-5.06664200	-2.58436100	0.12286300
B	4.84872600	2.48462600	-0.27080900
B	1.89697700	-2.16217300	-1.68482400
B	0.41316000	-2.85538700	-1.76172500
B	0.43001300	-2.85852300	1.74665600
B	6.03293000	1.38872300	-0.01058800
B	-5.07650400	-4.12692000	-0.00522700
B	-1.07767800	-5.20460700	1.12030800
B	0.40527000	-4.50109000	-0.92792900
B	1.83764900	-3.85268200	-1.43700800
B	3.26683900	-3.04874500	0.95599200
B	4.73229700	-2.39472900	-1.36451300
B	-4.66829800	2.23779600	0.00025700
B	-3.62791800	3.07885400	1.38285900
B	-2.00973200	3.56891800	0.84977300
B	-0.63106500	4.59544900	1.34472400
B	0.64971300	5.00020700	-0.00756400
B	-3.67720800	3.04902300	-1.39426600
B	-2.02354400	3.56248100	-0.83488300
B	-0.67244800	4.58273000	-1.31371900
B	0.41936900	-4.49745500	0.90518600
B	1.85956000	-3.85661700	1.43255400
B	3.24407200	-3.05458000	-0.94383300
B	4.75598500	-2.34573000	1.38480400
B	-1.09094200	-5.20229300	-1.14007300
B	-0.73065500	5.92213600	-0.05329700
B	-2.06291800	5.47029000	-0.94908100
B	-3.49781800	4.67432700	-0.99068700
B	-4.57316800	3.86375600	0.02624900
B	-2.01059300	5.48304500	0.96334600

B	-3.45234800	4.70021600	0.97391600
B	-3.78369800	-4.99136600	-0.01666200
B	-2.27283200	-5.58139200	-0.00562700
B	6.17893500	0.12087500	1.14171200
B	6.05860900	-1.58627100	-0.87764700
B	6.06922200	-1.50414600	0.87481000
B	6.20399000	0.02728000	-1.00981000

(f) $C_1 B_{94}$ (VI)

B	-1.64008500	-1.56765100	-1.80777300
B	-1.73596900	0.00218600	-0.88856300
B	-0.29449100	0.71602500	-1.74472200
B	-3.08203600	-2.46892800	-1.60217300
B	-3.17747600	0.81719500	-1.71565900
B	-0.23701500	2.42282000	-1.63797400
B	-3.13402100	2.46498900	-1.65574400
B	-3.11582400	4.08994500	-1.41935200
B	-1.69195200	1.56682800	-1.75896400
B	-1.68904100	4.98154000	-1.34561000
B	-0.26472000	4.12107700	-1.45917800
B	-1.65005600	3.09222000	-0.86319800
B	-1.69195500	-1.56682200	1.75895400
B	-1.73596900	-0.00218000	0.88856600
B	-3.13403400	-2.46497300	1.65573300
B	-0.26333200	2.41265500	1.72248500
B	-3.08203100	2.46893200	1.60217800
B	-3.11429800	4.11851700	1.35905100
B	-1.64008200	1.56765100	1.80776900
B	-1.74333100	5.01991300	1.18667100
B	-0.31580300	4.09230200	1.33167900
B	-1.64365300	3.06584900	0.79953600
B	1.18654800	3.35434200	-1.44034600
B	2.52969400	0.84141800	-1.64454900
B	1.08766100	1.54997300	-0.81759500
B	2.52179500	-0.86211200	-1.63822500
B	2.59757000	2.56061800	-1.45438100
B	1.12677100	-1.60528100	-0.91148100
B	-0.26333800	-2.41265900	-1.72249500
B	2.58613300	-2.55168700	-1.41143300
B	-0.31580700	-4.09230100	-1.33166600
B	-1.74334200	-5.01991300	-1.18666400
B	1.12566900	-3.32319000	-1.41960100
B	-3.11430300	-4.11851300	-1.35905000
B	-1.64365500	-3.06584800	-0.79953200
B	1.12567400	3.32319200	1.41959900
B	2.52179700	0.86211000	1.63822600
B	1.12677700	1.60527900	0.91147800
B	2.52969000	-0.84142200	1.64454200
B	2.58613700	2.55168500	1.41142900
B	1.08765300	-1.54997200	0.81759000
B	-0.23701700	-2.42282300	1.63798600

B	2.59756500	-2.56061700	1.45438000
B	-0.26472500	-4.12108000	1.45918500
B	-1.68904900	-4.98153700	1.34563000
B	1.18654400	-3.35434400	1.44034000
B	-3.11582200	-4.08993800	1.41936700
B	-1.65005800	-3.09221900	0.86320200
B	0.96029700	-4.53627900	-0.03527000
B	2.51325800	-4.05704300	-0.37735500
B	2.51326400	4.05704000	0.37734400
B	0.96030200	4.53627500	0.03526900
B	-0.30770700	-5.59163900	-0.25776200
B	-0.30770600	5.59163300	0.25772200
B	-3.11610600	0.82191700	1.76187400
B	-3.17747800	-0.81718500	1.71564800
B	-3.11610300	-0.82191200	-1.76186000
B	-1.67770000	6.24555400	-0.08779000
B	-1.67769900	-6.24554500	0.08780000
B	-3.05817500	-5.53362600	0.09809300
B	-3.05817200	5.53362500	-0.09807500
B	-4.29053800	-4.47831600	0.04438700
B	-4.50597400	-3.24262100	-1.10012600
B	-4.58145100	-1.56694900	0.91606300
B	-4.64794500	0.01917800	1.44378000
B	-4.58145400	1.56694700	-0.91606100
B	-4.50597200	3.24262600	1.10013500
B	-4.29053900	4.47831800	-0.04438000
B	3.73707000	-2.99254200	-0.03979400
B	4.01084200	-1.76284300	-1.41434500
B	3.86610300	-0.00929700	-0.85251700
B	3.99797400	1.74816100	-1.49319700
B	3.73707500	2.99253500	0.03978800
B	3.99797100	-1.74816200	1.49319000
B	3.86610200	0.00929400	0.85251300
B	4.01084400	1.76283600	1.41434000
B	-4.56382600	-1.59192200	-0.92012100
B	-4.64794000	-0.01917300	-1.44378700
B	-4.56382400	1.59192800	0.92012300
B	-4.54996900	3.22992100	-1.11196200
B	-4.54997200	-3.22993100	1.11197800
B	5.28110700	-2.43334700	-0.39863400
B	5.28111200	2.43334600	0.39863400
B	1.10132300	0.04327800	1.78306500
B	1.10132600	-0.04327500	-1.78306600

B	5.38506300	-0.87211400	-1.36317800
B	5.38404900	0.88289000	-1.42429900
B	5.38404900	-0.88289700	1.42428600
B	5.38506600	0.87211000	1.36316700
B	6.39153100	1.40563900	-0.00923200
B	6.70204500	-0.03234100	0.84038800
B	6.39153100	-1.40564300	0.00922500
B	6.70204400	0.03233700	-0.84039500
B	-0.29448800	-0.71603200	1.74474400

(g) C_{2v} B₉₆ (VII)

B	-1.42685200	1.42713300	-4.11996200
B	-1.67408200	1.43479500	-2.44574700
B	-0.84999200	2.68207900	-1.51909100
B	-1.79220700	0.00000000	-1.62935900
B	-0.84679000	0.00000000	-3.09412600
B	-1.41784300	4.27752100	-0.79354300
B	-1.67408200	-1.43479500	-2.44574700
B	-0.90400500	0.00000000	-0.03847100
B	-1.77707500	1.31290400	0.89560700
B	-1.77707500	-1.31290400	0.89560700
B	-1.70930400	1.41699200	2.49169700
B	-1.42692500	4.29178100	0.88291900
B	-0.84112300	2.69904400	1.58655300
B	-1.43420700	2.88438900	-3.26605800
B	-1.80939800	-1.38221600	-0.73744500
B	-1.65622700	2.82702800	0.06585700
B	-1.80939800	1.38221600	-0.73744500
B	1.42685200	1.42713300	-4.11996200
B	1.67408200	1.43479500	-2.44574700
B	0.84999200	2.68207900	-1.51909100
B	1.79220700	0.00000000	-1.62935900
B	0.84679000	0.00000000	-3.09412600
B	1.41784300	4.27752100	-0.79354300
B	1.67408200	-1.43479500	-2.44574700
B	0.90400500	0.00000000	-0.03847100
B	1.77707500	1.31290400	0.89560700
B	1.77707500	-1.31290400	0.89560700
B	1.70930400	1.41699200	2.49169700
B	1.42692500	4.29178100	0.88291900
B	0.84112300	2.69904400	1.58655300
B	1.43420700	2.88438900	-3.26605800
B	1.80939800	-1.38221600	-0.73744500
B	1.65622700	2.82702800	0.06585700
B	1.80939800	1.38221600	-0.73744500
B	0.00000000	5.43666400	-3.09213200
B	0.00000000	5.54942100	-1.56123800
B	0.00000000	5.23091600	0.03360400
B	0.00000000	4.15299700	-3.92585100
B	0.00000000	2.62183800	-4.50762900
B	1.31041200	4.34227700	-2.47267100
B	-1.31041200	4.34227700	-2.47267100
B	-1.65622700	-2.82702800	0.06585700

B	-0.84999200	-2.68207900	-1.51909100
B	-1.41784300	-4.27752100	-0.79354300
B	-0.84112300	-2.69904400	1.58655300
B	-1.70930400	-1.41699200	2.49169700
B	-1.40447200	-2.87773800	3.30871800
B	-1.28086500	-4.38812000	2.54333000
B	-1.29757400	-1.43119900	4.09527100
B	-0.84608100	0.00000000	3.10342000
B	-1.42692500	-4.29178100	0.88291900
B	1.65622700	-2.82702800	0.06585700
B	0.84999200	-2.68207900	-1.51909100
B	1.41784300	-4.27752100	-0.79354300
B	0.84112300	-2.69904400	1.58655300
B	1.70930400	-1.41699200	2.49169700
B	1.40447200	-2.87773800	3.30871800
B	1.28086500	-4.38812000	2.54333000
B	1.29757400	-1.43119900	4.09527100
B	0.84608100	0.00000000	3.10342000
B	1.42692500	-4.29178100	0.88291900
B	0.00000000	-5.46804700	3.17761400
B	0.00000000	-4.17034100	4.01022500
B	0.00000000	-2.64521800	4.59986500
B	0.00000000	-5.52495500	1.64366600
B	0.00000000	-5.23091600	0.03360400
B	1.01752800	0.00000000	4.98872000
B	1.29757400	1.43119900	4.09527100
B	1.40447200	2.87773800	3.30871800
B	1.28086500	4.38812000	2.54333000
B	-1.28086500	4.38812000	2.54333000
B	-1.40447200	2.87773800	3.30871800
B	-1.29757400	1.43119900	4.09527100
B	-1.01752800	0.00000000	4.98872000
B	0.00000000	-1.41562500	5.73076400
B	0.00000000	5.52495500	1.64366600
B	1.31308700	0.00000000	-4.99147800
B	1.42685200	-1.42713300	-4.11996200
B	1.43420700	-2.88438900	-3.26605800
B	1.31041200	-4.34227700	-2.47267100
B	-1.31041200	-4.34227700	-2.47267100
B	-1.43420700	-2.88438900	-3.26605800
B	-1.42685200	-1.42713300	-4.11996200
B	-1.31308700	0.00000000	-4.99147800
B	0.00000000	1.38366200	-5.57342400

B	0.00000000	-5.54942100	-1.56123800
B	0.00000000	-2.62183800	-4.50762900
B	0.00000000	-1.38366200	-5.57342400
B	0.00000000	-4.15299700	-3.92585100
B	0.00000000	0.00000000	-6.23688800
B	0.00000000	-5.43666400	-3.09213200
B	0.00000000	2.64521800	4.59986500
B	0.00000000	4.17034100	4.01022500
B	0.00000000	1.41562500	5.73076400
B	0.00000000	0.00000000	6.42680700
B	0.00000000	5.46804700	3.17761400

(h) $C_1 B_{98}$ (VIII)

B	-0.70082500	-4.33120800	1.46378700
B	-0.93930400	-2.65675400	1.63543100
B	-2.37565000	-1.92928100	0.98586100
B	0.36668600	-1.56449300	1.85119900
B	0.55803600	-3.08231300	0.84629200
B	1.89147400	-2.22291200	1.66473900
B	0.07735700	-0.03610300	0.93992400
B	-1.32345800	0.64746300	1.85938700
B	0.04690800	1.56637600	1.77860800
B	-1.51316100	2.29410400	1.63648500
B	-4.14211800	0.35578000	1.72215800
B	-2.71413100	1.22297400	0.84718000
B	-2.24065200	-3.77746800	1.51061000
B	1.62686400	-0.51203600	1.78717600
B	-2.72245700	-0.35120200	1.87547000
B	-1.20837200	-1.02094100	1.82653600
B	-0.76057200	-4.25405700	-1.46377500
B	-0.97842900	-2.58605100	-1.58806400
B	-2.38517900	-1.82494300	-0.72290400
B	0.35289500	-1.53537300	-1.75623100
B	0.54162400	-3.07313500	-0.85151400
B	-4.09668100	-1.34024700	-1.64987700
B	1.87352700	-2.20301300	-1.66560400
B	0.07934500	-0.00845600	-0.85869300
B	-1.30625500	0.68149200	-1.77164100
B	0.04407900	1.59257600	-1.75747000
B	-1.51435600	2.32425500	-1.63665100
B	-4.20208600	0.37475400	-1.63344400
B	-2.74109400	1.24302000	-0.85832500
B	-2.30822400	-3.57105900	-1.37340000
B	1.61260200	-0.49808400	-1.76376900
B	-2.70098400	-0.32880700	-1.72436400
B	-1.20149400	-0.96854600	-1.69400900
B	-4.77656900	-3.43793000	0.06620500
B	-3.48528000	-4.33670100	-0.25400300
B	-1.92117400	-4.84206200	-0.09638300
B	-3.83534800	-2.94058400	-1.36953800
B	-3.73714500	-3.25307200	1.50644400
B	2.96987900	0.36416400	1.70125300
B	3.01217300	-1.19547200	0.82472700
B	4.50977100	-0.29717700	1.40187200
B	2.60615400	1.86472500	0.84810100

B	1.26270300	2.61986500	1.71275600
B	2.54145700	3.60468900	1.29195200
B	4.11612600	2.99752300	1.00127100
B	1.05337500	4.28107900	1.41624800
B	-0.21761000	3.10111100	0.83597200
B	4.26641500	1.31900700	1.27974500
B	2.95523000	0.38013900	-1.70920800
B	3.01290400	-1.19281200	-0.85553500
B	4.48988000	-0.30271500	-1.41793400
B	2.61166700	1.88128200	-0.84219300
B	1.26313800	2.64003000	-1.69015500
B	2.54421200	3.62050900	-1.30668300
B	4.11415100	3.01573200	-1.03261400
B	1.04935200	4.30321700	-1.39431000
B	-0.22231300	3.12368100	-0.83768900
B	4.25274700	1.33001700	-1.31227400
B	5.26598000	3.86884900	-0.00905200
B	3.86011800	4.58398300	0.00699000
B	2.21659500	4.88717100	0.00658000
B	5.56003500	2.31924000	-0.05183700
B	5.39062400	0.65824800	-0.02875500
B	-0.46843300	5.06630700	-1.24325200
B	-1.74212300	3.98855300	-1.41068200
B	-3.06955300	3.03330600	-1.46863100
B	-4.36084900	2.06309700	-1.40862800
B	-4.36185000	1.96090800	1.34571800
B	-3.04649400	2.97486200	1.36024700
B	-1.70829400	3.96289800	1.39818400
B	-0.44532200	5.05414900	1.27590700
B	0.82837300	5.76201200	-0.01567700
B	0.74866900	-4.91308400	-1.44395700
B	2.07010800	-3.89127000	-1.48875300
B	3.40407700	-2.91163200	-1.45995200
B	4.78480300	-1.97646500	-1.29616800
B	4.82659000	-1.94306000	1.25458800
B	3.43039200	-2.85988300	1.37174600
B	2.10404900	-3.89344200	1.36244200
B	0.78421900	-4.99568100	1.25746200
B	-0.47887300	-5.65860900	-0.31762100
B	5.83908300	-0.91588200	-0.08118600
B	3.30440900	-4.16195100	0.02598600
B	2.27171100	-5.39781900	0.42516100
B	4.76970700	-3.42743300	0.13446900

B	0.97988600	-6.10050900	-0.11269300
B	5.95004600	-2.45267400	-0.03740400
B	-3.01687900	4.21227100	0.03566200
B	-4.46714700	3.43949000	0.35915800
B	-1.89136200	5.41203600	0.15732100
B	-0.62379300	6.29137200	0.01414000
B	-5.51826700	2.26655200	0.00235400
B	-5.54489100	-0.49695300	-0.90932000
B	-5.39237600	-1.98199200	-0.32175000
B	-5.68334100	1.09421400	-1.18961500
B	-5.59245900	0.83308500	0.97701600
B	-5.43277400	-0.73682800	0.97688800
B	-4.97620200	-2.29199000	1.31777600

(i) $C_2 B_{128}$ (IX)

B	4.30429900	-4.05656500	-1.53613400
B	4.36096000	-4.17351000	1.24219600
B	-1.40253300	-5.81987200	1.51239800
B	-1.49370800	-5.77837600	-1.40628400
B	1.36320700	-5.76492800	-1.48525300
B	-0.08303900	-6.65591100	-1.32455800
B	0.00710100	-6.66009700	1.34886100
B	1.51080400	-5.84792500	1.33133700
B	2.67878600	-3.18798400	-0.92634800
B	-0.02949600	-1.69174700	-0.88885700
B	1.49161200	-4.13490300	1.56451800
B	1.34680800	-0.80516000	1.76854300
B	0.03378400	-1.70516900	0.89296400
B	2.73589100	-3.18046400	0.79727800
B	1.35969300	-0.77684400	-1.80953200
B	1.37897000	-4.09727700	-1.70866100
B	-0.04656100	-3.27615300	-1.77865200
B	4.62481300	-0.91754300	-1.31457900
B	2.82203400	-1.61543900	-1.74221900
B	-1.49348900	-4.09942000	-1.62443900
B	2.86498100	-1.58002100	1.64662700
B	-1.39309800	-4.11986200	1.66772300
B	0.05181300	-3.31669800	1.76946900
B	4.38432800	-0.78218100	1.57581000
B	4.24664700	-2.42114700	-1.88207300
B	0.02320100	-4.80035600	0.84805800
B	4.32737100	-2.46743700	1.37246300
B	-0.02928600	-4.76539300	-0.85260200
B	1.34735100	-2.39797100	-1.75607700
B	1.43887800	-2.44403200	1.76042600
B	2.73589100	3.16754200	-0.79613600
B	4.28521600	0.83223600	1.58197600
B	4.31413400	4.13675100	1.42598700
B	2.67068900	3.18923700	0.89553100
B	4.40919200	4.13844800	-1.17266400
B	4.39170500	0.74851300	-1.31577100
B	2.90617300	1.57029200	-1.59281900
B	1.36170600	0.79767300	-1.73146500
B	1.28200900	0.78901300	1.77876600
B	2.77799600	1.60499800	1.64145300
B	2.72547400	0.00413400	0.85616800
B	2.75588400	-0.01817000	-0.85924200

B	4.34399100	2.44285300	-1.29530100
B	4.25260800	2.47951900	1.55608100
B	-2.73589100	-3.16754200	-0.79613600
B	-4.31413400	-4.13675100	1.42598700
B	-4.28521600	-0.83223600	1.58197600
B	-2.67068900	-3.18923700	0.89553100
B	-4.39170500	-0.74851300	-1.31577100
B	-4.40919200	-4.13844800	-1.17266400
B	-1.36170600	-0.79767300	-1.73146500
B	-2.90617300	-1.57029200	-1.59281900
B	-2.77799600	-1.60499800	1.64145300
B	-1.28200900	-0.78901300	1.77876600
B	-1.44787100	-2.41575500	-1.75373000
B	-1.33735700	-2.41974200	1.79329600
B	-4.34399100	-2.44285300	-1.29530100
B	-4.25260800	-2.47951900	1.55608100
B	0.02949600	1.69174700	-0.88885700
B	-2.67878600	3.18798400	-0.92634800
B	-1.34680800	0.80516000	1.76854300
B	-1.49161200	4.13490300	1.56451800
B	-2.73589100	3.18046400	0.79727800
B	-0.03378400	1.70516900	0.89296400
B	-1.37897000	4.09727700	-1.70866100
B	-1.35969300	0.77684400	-1.80953200
B	-2.82203400	1.61543900	-1.74221900
B	1.49348900	4.09942000	-1.62443900
B	0.04656100	3.27615300	-1.77865200
B	-4.62481300	0.91754300	-1.31457900
B	-0.05181300	3.31669800	1.76946900
B	-4.38432800	0.78218100	1.57581000
B	-2.86498100	1.58002100	1.64662700
B	1.39309800	4.11986200	1.66772300
B	1.44787100	2.41575500	-1.75373000
B	-2.72547400	-0.00413400	0.85616800
B	1.33735700	2.41974200	1.79329600
B	-2.75588400	0.01817000	-0.85924200
B	-1.34735100	2.39797100	-1.75607700
B	-1.43887800	2.44403200	1.76042600
B	1.40253300	5.81987200	1.51239800
B	1.49370800	5.77837600	-1.40628400
B	0.08303900	6.65591100	-1.32455800
B	-1.36320700	5.76492800	-1.48525300
B	-1.51080400	5.84792500	1.33133700

B	-0.00710100	6.66009700	1.34886100
B	-0.02320100	4.80035600	0.84805800
B	0.02928600	4.76539300	-0.85260200
B	-4.30429900	4.05656500	-1.53613400
B	-4.36096000	4.17351000	1.24219600
B	-4.24664700	2.42114700	-1.88207300
B	-4.32737100	2.46743700	1.37246300
B	-2.83689600	4.89296500	-1.52613500
B	-2.93065800	4.99716300	1.41070700
B	2.94534100	4.93477500	-1.34551000
B	2.83926400	4.94020500	1.48307000
B	2.83689600	-4.89296500	-1.52613500
B	2.93065800	-4.99716300	1.41070700
B	-2.83926400	-4.94020500	1.48307000
B	-2.94534100	-4.93477500	-1.34551000
B	-5.50181400	-3.22185800	0.07108100
B	-5.24590400	-1.60226600	0.16650500
B	-5.35791500	1.58390500	0.26977700
B	-5.58034400	3.22649300	0.45926300
B	-5.31802200	4.62396100	-0.16903500
B	-4.16505400	5.56842500	-0.64651800
B	-2.64399900	6.17102600	-0.22912100
B	-1.43414000	7.24612700	-0.53781300
B	-0.07744400	7.82976900	0.00576500
B	1.32957400	7.21481000	0.05184100
B	2.62687000	6.18974300	0.07765300
B	4.16970800	5.63377900	0.09419000
B	5.43826700	4.75755100	0.17220400
B	5.24590400	1.60226600	0.16650500
B	5.50181400	3.22185800	0.07108100
B	5.35791500	-1.58390500	0.26977700
B	5.58034400	-3.22649300	0.45926300
B	4.16505400	-5.56842500	-0.64651800
B	-4.16970800	-5.63377900	0.09419000
B	-5.43826700	-4.75755100	0.17220400
B	-2.62687000	-6.18974300	0.07765300
B	-1.32957400	-7.21481000	0.05184100
B	0.07744400	-7.82976900	0.00576500
B	1.43414000	-7.24612700	-0.53781300
B	2.64399900	-6.17102600	-0.22912100
B	5.31802200	-4.62396100	-0.16903500
B	-5.54280100	0.01030800	0.11754400
B	5.54280100	-0.01030800	0.11754400

(j) $D_{2h} B_{214} (\mathbf{X})$

B	-2.47515800	7.17544900	1.46737400
B	2.47515800	7.17544900	-1.46737400
B	1.60377500	5.67781500	-1.59516100
B	-1.60377500	5.67781500	-1.59516100
B	-2.47515800	7.17544900	-1.46737400
B	-2.43536500	4.23442400	-1.73285200
B	0.00000000	5.58304000	-0.84733100
B	-0.82937800	7.22697400	-1.47086000
B	-3.20615800	5.54286400	-0.84195900
B	-0.79684000	4.16792200	-1.77246400
B	0.79684000	4.16792200	-1.77246400
B	3.20615800	5.54286400	-0.84195900
B	0.82937800	7.22697400	-1.47086000
B	1.60377500	5.67781500	1.59516100
B	-1.60377500	5.67781500	1.59516100
B	2.43536500	4.23442400	1.73285200
B	2.47515800	7.17544900	1.46737400
B	0.00000000	5.58304000	0.84733100
B	-3.20615800	5.54286400	0.84195900
B	-0.79684000	4.16792200	1.77246400
B	-0.82937800	7.22697400	1.47086000
B	3.20615800	5.54286400	0.84195900
B	0.82937800	7.22697400	1.47086000
B	0.79684000	4.16792200	1.77246400
B	-3.32650200	2.84717000	-1.69196000
B	-6.74367400	2.94924900	-1.47315500
B	-4.87001800	2.79344500	-0.85191900
B	-5.89596500	4.34990900	-1.48479100
B	-5.80019000	1.45134300	-1.63945000
B	-4.13955800	1.43081400	-1.84222600
B	-1.70670700	2.81854300	-0.87983600
B	-4.14698600	4.28972800	-1.62803000
B	-3.32650200	2.84717000	1.69196000
B	-6.74367400	2.94924900	1.47315500
B	-2.42308600	1.43533000	1.80107400
B	-2.43536500	4.23442400	1.73285200
B	-4.87001800	2.79344500	0.85191900
B	-5.80019000	1.45134300	1.63945000
B	-5.89596500	4.34990900	1.48479100
B	-1.70670700	2.81854300	0.87983600
B	-4.14698600	4.28972800	1.62803000
B	-4.13955800	1.43081400	1.84222600

B	6.74367400	2.94924900	-1.47315500
B	3.32650200	2.84717000	-1.69196000
B	2.43536500	4.23442400	-1.73285200
B	2.42308600	1.43533000	-1.80107400
B	4.87001800	2.79344500	-0.85191900
B	4.14698600	4.28972800	-1.62803000
B	1.70670700	2.81854300	-0.87983600
B	4.13955800	1.43081400	-1.84222600
B	5.80019000	1.45134300	-1.63945000
B	5.89596500	4.34990900	-1.48479100
B	6.74367400	2.94924900	1.47315500
B	3.32650200	2.84717000	1.69196000
B	4.87001800	2.79344500	0.85191900
B	1.70670700	2.81854300	0.87983600
B	4.13955800	1.43081400	1.84222600
B	4.14698600	4.28972800	1.62803000
B	5.89596500	4.34990900	1.48479100
B	5.80019000	1.45134300	1.63945000
B	1.59703500	0.00000000	-1.64267600
B	-1.59703500	0.00000000	-1.64267600
B	-2.42308600	1.43533000	-1.80107400
B	-2.42308600	-1.43533000	-1.80107400
B	0.00000000	0.00000000	-0.84155900
B	-0.80201300	1.51698000	-1.73880500
B	-3.27201100	0.00000000	-0.86656800
B	-0.80201300	-1.51698000	-1.73880500
B	0.80201300	-1.51698000	-1.73880500
B	3.27201100	0.00000000	-0.86656800
B	0.80201300	1.51698000	-1.73880500
B	1.59703500	0.00000000	1.64267600
B	-1.59703500	0.00000000	1.64267600
B	2.42308600	-1.43533000	1.80107400
B	2.42308600	1.43533000	1.80107400
B	0.00000000	0.00000000	0.84155900
B	-3.27201100	0.00000000	0.86656800
B	-0.80201300	-1.51698000	1.73880500
B	-0.80201300	1.51698000	1.73880500
B	3.27201100	0.00000000	0.86656800
B	0.80201300	1.51698000	1.73880500
B	0.80201300	-1.51698000	1.73880500
B	-3.32650200	-2.84717000	-1.69196000
B	-6.74367400	-2.94924900	-1.47315500
B	-4.87001800	-2.79344500	-0.85191900

B	-5.80019000	-1.45134300	-1.63945000
B	-5.89596500	-4.34990900	-1.48479100
B	-4.14698600	-4.28972800	-1.62803000
B	-1.70670700	-2.81854300	-0.87983600
B	-4.13955800	-1.43081400	-1.84222600
B	-3.32650200	-2.84717000	1.69196000
B	-6.74367400	-2.94924900	1.47315500
B	-2.43536500	-4.23442400	1.73285200
B	-2.42308600	-1.43533000	1.80107400
B	-4.87001800	-2.79344500	0.85191900
B	-5.89596500	-4.34990900	1.48479100
B	-5.80019000	-1.45134300	1.63945000
B	-1.70670700	-2.81854300	0.87983600
B	-4.13955800	-1.43081400	1.84222600
B	-4.14698600	-4.28972800	1.62803000
B	6.74367400	-2.94924900	-1.47315500
B	3.32650200	-2.84717000	-1.69196000
B	2.42308600	-1.43533000	-1.80107400
B	2.43536500	-4.23442400	-1.73285200
B	4.87001800	-2.79344500	-0.85191900
B	4.13955800	-1.43081400	-1.84222600
B	1.70670700	-2.81854300	-0.87983600
B	4.14698600	-4.28972800	-1.62803000
B	5.89596500	-4.34990900	-1.48479100
B	5.80019000	-1.45134300	-1.63945000
B	6.74367400	-2.94924900	1.47315500
B	3.32650200	-2.84717000	1.69196000
B	4.87001800	-2.79344500	0.85191900
B	1.70670700	-2.81854300	0.87983600
B	4.14698600	-4.28972800	1.62803000
B	4.13955800	-1.43081400	1.84222600
B	5.80019000	-1.45134300	1.63945000
B	5.89596500	-4.34990900	1.48479100
B	1.60377500	-5.67781500	-1.59516100
B	-1.60377500	-5.67781500	-1.59516100
B	-2.43536500	-4.23442400	-1.73285200
B	-2.47515800	-7.17544900	-1.46737400
B	0.00000000	-5.58304000	-0.84733100
B	-0.79684000	-4.16792200	-1.77246400
B	-3.20615800	-5.54286400	-0.84195900
B	-0.82937800	-7.22697400	-1.47086000
B	0.82937800	-7.22697400	-1.47086000
B	3.20615800	-5.54286400	-0.84195900

B	0.79684000	-4.16792200	-1.77246400
B	1.60377500	-5.67781500	1.59516100
B	-1.60377500	-5.67781500	1.59516100
B	2.47515800	-7.17544900	1.46737400
B	2.43536500	-4.23442400	1.73285200
B	0.00000000	-5.58304000	0.84733100
B	-3.20615800	-5.54286400	0.84195900
B	-0.82937800	-7.22697400	1.47086000
B	-0.79684000	-4.16792200	1.77246400
B	3.20615800	-5.54286400	0.84195900
B	0.79684000	-4.16792200	1.77246400
B	0.82937800	-7.22697400	1.47086000
B	-4.15722300	-7.23093600	-1.32562000
B	-2.47515800	-7.17544900	1.46737400
B	-4.15722300	-7.23093600	1.32562000
B	2.47515800	-7.17544900	-1.46737400
B	4.15722300	-7.23093600	-1.32562000
B	4.15722300	-7.23093600	1.32562000
B	4.97556200	-5.75960600	1.47930000
B	4.97556200	-5.75960600	-1.47930000
B	-4.97556200	-5.75960600	1.47930000
B	-4.97556200	-5.75960600	-1.47930000
B	-4.92040800	0.00000000	1.67076600
B	-4.92040800	0.00000000	-1.67076600
B	4.92040800	0.00000000	1.67076600
B	4.92040800	0.00000000	-1.67076600
B	4.97556200	5.75960600	1.47930000
B	4.97556200	5.75960600	-1.47930000
B	4.15722300	7.23093600	-1.32562000
B	4.15722300	7.23093600	1.32562000
B	-4.15722300	7.23093600	1.32562000
B	-4.15722300	7.23093600	-1.32562000
B	-4.97556200	5.75960600	1.47930000
B	-4.97556200	5.75960600	-1.47930000
B	5.70596100	-7.03842900	0.00000000
B	6.26635300	-5.50117600	0.00000000
B	7.26227000	-4.18660600	0.00000000
B	7.26227000	4.18660600	0.00000000
B	6.26635300	5.50117600	0.00000000
B	5.70596100	7.03842900	0.00000000
B	-5.70596100	7.03842900	0.00000000
B	-6.26635300	5.50117600	0.00000000
B	-7.26227000	4.18660600	0.00000000

B	-7.26227000	-4.18660600	0.00000000
B	-6.26635300	-5.50117600	0.00000000
B	-5.70596100	-7.03842900	0.00000000
B	-3.24716800	-8.39684900	0.00000000
B	-1.60468800	-8.15197300	0.00000000
B	0.00000000	-8.50308100	0.00000000
B	1.60468800	-8.15197300	0.00000000
B	3.24716800	-8.39684900	0.00000000
B	4.79089900	-8.29957400	0.00000000
B	-4.79089900	8.29957400	0.00000000
B	-3.24716800	8.39684900	0.00000000
B	-1.60468800	8.15197300	0.00000000
B	0.00000000	8.50308100	0.00000000
B	1.60468800	8.15197300	0.00000000
B	3.24716800	8.39684900	0.00000000
B	-4.79089900	-8.29957400	0.00000000
B	4.79089900	8.29957400	0.00000000
B	-7.49633700	1.42368700	1.47687100
B	-7.49633700	1.42368700	-1.47687100
B	-6.43086500	0.00000000	-0.85598000
B	-6.43086500	0.00000000	0.85598000
B	-7.49633700	-1.42368700	1.47687100
B	-7.49633700	-1.42368700	-1.47687100
B	-8.42089100	0.00000000	1.34089100
B	-8.42089100	0.00000000	-1.34089100
B	6.43086500	0.00000000	0.85598000
B	6.43086500	0.00000000	-0.85598000
B	7.49633700	1.42368700	1.47687100
B	7.49633700	1.42368700	-1.47687100
B	7.49633700	-1.42368700	1.47687100
B	7.49633700	-1.42368700	-1.47687100
B	8.42089100	0.00000000	1.34089100
B	8.42089100	0.00000000	-1.34089100
B	7.91275200	2.70911400	0.00000000
B	8.85593700	1.37212300	0.00000000
B	9.60366600	0.00000000	0.00000000
B	8.85593700	-1.37212300	0.00000000
B	7.91275200	-2.70911400	0.00000000
B	-7.91275200	2.70911400	0.00000000
B	-8.85593700	1.37212300	0.00000000
B	-9.60366600	0.00000000	0.00000000
B	-8.85593700	-1.37212300	0.00000000
B	-7.91275200	-2.70911400	0.00000000

(k) C_{2v} B_{260} (XI)

B	1.33244500	7.23551300	-5.80771300
B	-1.47743400	7.16710000	-4.12135100
B	-1.33244500	7.23551300	-5.80771300
B	1.47487700	7.28049100	0.82117200
B	1.46280000	7.28810900	2.45631500
B	-1.46280000	7.28810900	2.45631500
B	1.58184100	5.70388300	-0.03296400
B	1.58643600	5.67521700	-3.25017200
B	1.47743400	7.16710000	-4.12135100
B	1.72469500	4.23441100	-4.07635000
B	0.85127600	5.60459200	-1.63323600
B	1.50701000	7.24587600	-2.47620700
B	0.84499900	5.53900300	-4.86103900
B	1.75684700	4.16504100	-2.43944700
B	1.72844800	4.18964800	-0.83872400
B	0.85367500	5.58564900	1.62933300
B	1.51321500	7.25372800	-0.83102400
B	-1.58184100	5.70388300	-0.03296400
B	-1.58643600	5.67521700	-3.25017200
B	-1.73702800	4.23989500	0.79608300
B	-1.47487700	7.28049100	0.82117200
B	-0.85127600	5.60459200	-1.63323600
B	-0.84499900	5.53900300	-4.86103900
B	-1.75684700	4.16504100	-2.43944700
B	-1.50701000	7.24587600	-2.47620700
B	-0.85367500	5.58564900	1.62933300
B	-1.51321500	7.25372800	-0.83102400
B	-1.72844800	4.18964800	-0.83872400
B	1.71484000	2.84636700	-4.97080700
B	1.48200100	2.95624200	-8.40775300
B	0.85479800	2.79415900	-6.51451100
B	1.49416800	4.33906600	-7.54224000
B	1.64103600	1.44232000	-7.43712000
B	1.86235000	1.43698100	-5.80041300
B	0.88012400	2.81167300	-3.36064400
B	-1.71484000	2.84636700	-4.97080700
B	-1.48200100	2.95624200	-8.40775300
B	-1.78869400	1.43288600	-4.07312600
B	-1.72469500	4.23441100	-4.07635000
B	-0.85479800	2.79415900	-6.51451100
B	-1.64103600	1.44232000	-7.43712000
B	-1.49416800	4.33906600	-7.54224000

B	-0.88012400	2.81167300	-3.36064400
B	-1.64360400	4.29279300	-5.79877800
B	-1.86235000	1.43698100	-5.80041300
B	1.58387100	4.26786100	5.78456800
B	1.46177000	4.35668800	7.53950200
B	-1.46177000	4.35668800	7.53950200
B	1.73668600	2.82163100	4.91152400
B	1.71679900	2.80558900	1.69788000
B	1.73702800	4.23989500	0.79608300
B	1.73164600	1.40729600	0.79710000
B	0.84762000	2.83169200	3.27935000
B	1.77277900	4.27627200	2.47160600
B	0.88006200	2.83016600	0.07625100
B	1.74239400	1.31346400	2.49272900
B	1.78129100	1.31507200	4.08170400
B	0.85050700	2.78451000	6.49513100
B	1.70762000	4.26515300	4.10876100
B	-1.73668600	2.82163100	4.91152400
B	-1.71679900	2.80558900	1.69788000
B	-1.75159200	1.39453700	5.74508300
B	-1.58387100	4.26786100	5.78456800
B	-0.84762000	2.83169200	3.27935000
B	-0.88006200	2.83016600	0.07625100
B	-1.74239400	1.31346400	2.49272900
B	-1.77277900	4.27627200	2.47160600
B	-0.85050700	2.78451000	6.49513100
B	-1.70762000	4.26515300	4.10876100
B	-1.78129100	1.31507200	4.08170400
B	1.61574400	0.00000000	-0.08025600
B	1.67395000	0.00000000	-3.23931400
B	1.78869400	1.43288600	-4.07312600
B	1.78869400	-1.43288600	-4.07312600
B	0.84236500	0.00000000	-1.65674200
B	1.76717100	1.53596700	-2.44565400
B	0.86459800	0.00000000	-4.88711400
B	1.76717100	-1.53596700	-2.44565400
B	1.72560500	-1.51644100	-0.84950700
B	0.88075100	0.00000000	1.59103600
B	1.72560500	1.51644100	-0.84950700
B	-1.61574400	0.00000000	-0.08025600
B	-1.67395000	0.00000000	-3.23931400
B	-1.73164600	-1.40729600	0.79710000
B	-1.73164600	1.40729600	0.79710000

B	-0.84236500	0.00000000	-1.65674200
B	-0.86459800	0.00000000	-4.88711400
B	-1.76717100	-1.53596700	-2.44565400
B	-1.76717100	1.53596700	-2.44565400
B	-0.88075100	0.00000000	1.59103600
B	-1.72560500	1.51644100	-0.84950700
B	-1.72560500	-1.51644100	-0.84950700
B	1.71484000	-2.84636700	-4.97080700
B	1.48200100	-2.95624200	-8.40775300
B	0.85479800	-2.79415900	-6.51451100
B	1.64103600	-1.44232000	-7.43712000
B	1.49416800	-4.33906600	-7.54224000
B	1.64360400	-4.29279300	-5.79877800
B	0.88012400	-2.81167300	-3.36064400
B	1.86235000	-1.43698100	-5.80041300
B	-1.71484000	-2.84636700	-4.97080700
B	-1.48200100	-2.95624200	-8.40775300
B	-1.72469500	-4.23441100	-4.07635000
B	-1.78869400	-1.43288600	-4.07312600
B	-0.85479800	-2.79415900	-6.51451100
B	-1.49416800	-4.33906600	-7.54224000
B	-1.64103600	-1.44232000	-7.43712000
B	-0.88012400	-2.81167300	-3.36064400
B	-1.86235000	-1.43698100	-5.80041300
B	1.62814100	0.00000000	6.60796500
B	1.75159200	1.39453700	5.74508300
B	1.75159200	-1.39453700	5.74508300
B	0.84526700	0.00000000	8.11949400
B	1.61927400	1.44884300	7.44949100
B	0.87377000	0.00000000	4.97260600
B	1.61927400	-1.44884300	7.44949100
B	1.50102000	-1.44270000	9.15004500
B	1.50102000	1.44270000	9.15004500
B	-1.62814100	0.00000000	6.60796500
B	-0.84526700	0.00000000	8.11949400
B	-0.87377000	0.00000000	4.97260600
B	-1.61927400	-1.44884300	7.44949100
B	-1.61927400	1.44884300	7.44949100
B	-1.50102000	1.44270000	9.15004500
B	-1.50102000	-1.44270000	9.15004500
B	1.73668600	-2.82163100	4.91152400
B	1.71679900	-2.80558900	1.69788000
B	1.73164600	-1.40729600	0.79710000

B	1.73702800	-4.23989500	0.79608300
B	0.84762000	-2.83169200	3.27935000
B	1.74239400	-1.31346400	2.49272900
B	0.88006200	-2.83016600	0.07625100
B	1.77277900	-4.27627200	2.47160600
B	1.70762000	-4.26515300	4.10876100
B	0.85050700	-2.78451000	6.49513100
B	1.78129100	-1.31507200	4.08170400
B	-1.73668600	-2.82163100	4.91152400
B	-1.71679900	-2.80558900	1.69788000
B	-1.58387100	-4.26786100	5.78456800
B	-1.75159200	-1.39453700	5.74508300
B	-0.84762000	-2.83169200	3.27935000
B	-0.88006200	-2.83016600	0.07625100
B	-1.77277900	-4.27627200	2.47160600
B	-1.74239400	-1.31346400	2.49272900
B	-0.85050700	-2.78451000	6.49513100
B	-1.78129100	-1.31507200	4.08170400
B	-1.70762000	-4.26515300	4.10876100
B	1.58184100	-5.70388300	-0.03296400
B	1.58643600	-5.67521700	-3.25017200
B	1.72469500	-4.23441100	-4.07635000
B	1.47743400	-7.16710000	-4.12135100
B	0.85127600	-5.60459200	-1.63323600
B	1.75684700	-4.16504100	-2.43944700
B	0.84499900	-5.53900300	-4.86103900
B	1.50701000	-7.24587600	-2.47620700
B	1.51321500	-7.25372800	-0.83102400
B	0.85367500	-5.58564900	1.62933300
B	1.72844800	-4.18964800	-0.83872400
B	-1.58184100	-5.70388300	-0.03296400
B	-1.58643600	-5.67521700	-3.25017200
B	-1.47487700	-7.28049100	0.82117200
B	-1.73702800	-4.23989500	0.79608300
B	-0.85127600	-5.60459200	-1.63323600
B	-0.84499900	-5.53900300	-4.86103900
B	-1.50701000	-7.24587600	-2.47620700
B	-1.75684700	-4.16504100	-2.43944700
B	-0.85367500	-5.58564900	1.62933300
B	-1.72844800	-4.18964800	-0.83872400
B	-1.51321500	-7.25372800	-0.83102400
B	1.33244500	-7.23551300	-5.80771300
B	-1.47743400	-7.16710000	-4.12135100

B	-1.33244500	-7.23551300	-5.80771300
B	1.58387100	-4.26786100	5.78456800
B	1.46177000	-4.35668800	7.53950200
B	-1.46177000	-4.35668800	7.53950200
B	1.47487700	-7.28049100	0.82117200
B	1.46280000	-7.28810900	2.45631500
B	-1.46280000	-7.28810900	2.45631500
B	1.45168300	-2.92696000	8.36424400
B	-1.45168300	-2.92696000	8.36424400
B	-1.45168300	2.92696000	8.36424400
B	1.45168300	2.92696000	8.36424400
B	-1.56268700	5.74063300	3.27917700
B	1.56268700	5.74063300	3.27917700
B	1.56268700	-5.74063300	3.27917700
B	-1.56268700	-5.74063300	3.27917700
B	-1.47068400	-5.76247200	-6.62099700
B	1.47068400	-5.76247200	-6.62099700
B	-1.62289000	0.00000000	-6.54980400
B	1.62289000	0.00000000	-6.54980400
B	1.47068400	5.76247200	-6.62099700
B	-1.47068400	5.76247200	-6.62099700
B	1.50840800	-7.21061100	4.13762500
B	-0.84808800	-5.57287600	4.85997000
B	0.00000000	-4.19573800	8.90768700
B	0.00000000	-2.69886900	9.56892200
B	0.00000000	2.69886900	9.56892200
B	0.00000000	4.19573800	8.90768700
B	0.00000000	7.00511200	-7.28646400
B	0.00000000	5.48234700	-7.90250300
B	0.00000000	4.18827500	-8.90958500
B	0.00000000	2.69359300	-9.53641000
B	-1.51198400	1.42549300	-9.13283100
B	0.85426100	0.00000000	-8.08096700
B	0.00000000	-2.69359300	-9.53641000
B	0.00000000	-4.18827500	-8.90958500
B	0.00000000	-5.48234700	-7.90250300
B	0.00000000	-7.00511200	-7.28646400
B	0.00000000	-8.34344700	1.62622800
B	0.00000000	-8.19915000	-0.02229000
B	0.00000000	-8.43547400	-1.63314600
B	0.00000000	-8.14266100	-3.25245400
B	0.00000000	-8.42257600	-4.87640200
B	0.00000000	-8.30330100	-6.42470300

B	0.00000000	-8.21465500	3.24732900
B	0.00000000	-5.50284400	7.92491600
B	0.00000000	5.50284400	7.92491600
B	-1.48588300	5.75768000	6.62728100
B	0.00000000	8.21465500	3.24732900
B	0.00000000	8.34344700	1.62622800
B	0.00000000	8.19915000	-0.02229000
B	0.00000000	8.43547400	-1.63314600
B	0.00000000	8.14266100	-3.25245400
B	0.00000000	8.42257600	-4.87640200
B	0.00000000	8.30330100	-6.42470300
B	-1.48588300	-5.75768000	6.62728100
B	1.48588300	-5.75768000	6.62728100
B	0.84808800	-5.57287600	4.85997000
B	-1.50840800	-7.21061100	4.13762500
B	1.34539400	-7.25090800	5.81978900
B	-1.34539400	-7.25090800	5.81978900
B	1.51198400	-1.42549300	-9.13283100
B	-1.51198400	-1.42549300	-9.13283100
B	-0.85426100	0.00000000	-8.08096700
B	1.51198400	1.42549300	-9.13283100
B	-1.35388300	0.00000000	-10.05048800
B	1.35388300	0.00000000	-10.05048800
B	1.48588300	5.75768000	6.62728100
B	-0.84808800	5.57287600	4.85997000
B	0.84808800	5.57287600	4.85997000
B	1.50840800	7.21061100	4.13762500
B	-1.50840800	7.21061100	4.13762500
B	1.34539400	7.25090800	5.81978900
B	-1.34539400	7.25090800	5.81978900
B	0.00000000	-8.37388300	4.87690100
B	0.00000000	-8.29927600	6.42935700
B	0.00000000	-7.01734400	7.31433700
B	0.00000000	-1.38085900	-10.51409000
B	0.00000000	1.38085900	-10.51409000
B	0.00000000	7.01734400	7.31433700
B	0.00000000	8.29927600	6.42935700
B	0.00000000	8.37388300	4.87690100
B	0.00000000	-1.40733700	10.58001200
B	0.00000000	0.00000000	11.24013200
B	0.00000000	1.40733700	10.58001200
B	0.00000000	0.00000000	-11.23576500
B	-1.64360400	-4.29279300	-5.79877800

B	1.64360400	4.29279300	-5.79877800
B	1.34107400	0.00000000	10.03554000
B	-1.34107400	0.00000000	10.03554000

(I) D_{2h} B₃₇₂ (XII)

B	-2.44841000	10.02677900	1.48786700
B	-7.55765400	7.14860100	1.75413300
B	2.44841000	10.02677900	-1.48786700
B	1.61260200	8.46071000	-1.54549900
B	-1.61260200	8.46071000	-1.54549900
B	-2.44841000	10.02677900	-1.48786700
B	-2.44113600	7.02684600	-1.80792700
B	0.00000000	8.36842100	-0.84530800
B	-0.82846800	10.00394300	-1.47965300
B	-3.28898100	8.37026400	-0.84906300
B	-0.81513500	6.96155600	-1.73531200
B	0.81513500	6.96155600	-1.73531200
B	3.28898100	8.37026400	-0.84906300
B	0.82846800	10.00394300	-1.47965300
B	1.61260200	8.46071000	1.54549900
B	-1.61260200	8.46071000	1.54549900
B	2.44113600	7.02684600	1.80792700
B	2.44841000	10.02677900	1.48786700
B	0.00000000	8.36842100	0.84530800
B	-3.28898100	8.37026400	0.84906300
B	-0.81513500	6.96155600	1.73531200
B	-0.82846800	10.00394300	1.47965300
B	3.28898100	8.37026400	0.84906300
B	0.82846800	10.00394300	1.47965300
B	0.81513500	6.96155600	1.73531200
B	-3.36891200	5.61406900	-1.69176400
B	-6.58934600	5.64445500	-1.72026600
B	-7.55765400	7.14860100	-1.75413300
B	-7.43435700	4.23261200	-1.69853200
B	-4.93048400	5.67867300	-0.84868200
B	-5.80888500	7.09594300	-1.75758500
B	-8.44867400	5.77411100	-1.51127100
B	-5.77322200	4.15613600	-1.77520700
B	-4.16549900	4.11999100	-1.73060100
B	-1.74277100	5.63149900	-0.88490900
B	-4.14036700	7.09798600	-1.80062300
B	-3.36891200	5.61406900	1.69176400
B	-6.58934600	5.64445500	1.72026600
B	-2.47050000	4.21181200	1.72974000
B	-2.44113600	7.02684600	1.80792700
B	-4.93048400	5.67867300	0.84868200
B	-8.44867400	5.77411100	1.51127100

B	-5.77322200	4.15613600	1.77520700
B	-5.80888500	7.09594300	1.75758500
B	-1.74277100	5.63149900	0.88490900
B	-4.14036700	7.09798600	1.80062300
B	-4.16549900	4.11999100	1.73060100
B	-8.30740700	2.84711400	-1.57739800
B	-10.08823700	2.92953400	-1.48218800
B	-9.09306300	1.40901000	-1.75683700
B	-6.63555500	2.81413300	-0.87518500
B	-9.23772400	4.33239200	-1.75636000
B	-8.30740700	2.84711400	1.57739800
B	-7.41577300	1.43577400	1.76821000
B	-7.43435700	4.23261200	1.69853200
B	-10.08823700	2.92953400	1.48218800
B	-6.63555500	2.81413300	0.87518500
B	-9.23772400	4.33239200	1.75636000
B	-9.09306300	1.40901000	1.75683700
B	7.55765400	7.14860100	-1.75413300
B	6.58934600	5.64445500	-1.72026600
B	3.36891200	5.61406900	-1.69176400
B	2.44113600	7.02684600	-1.80792700
B	2.47050000	4.21181200	-1.72974000
B	4.93048400	5.67867300	-0.84868200
B	4.14036700	7.09798600	-1.80062300
B	1.74277100	5.63149900	-0.88490900
B	4.16549900	4.11999100	-1.73060100
B	5.77322200	4.15613600	-1.77520700
B	8.44867400	5.77411100	-1.51127100
B	5.80888500	7.09594300	-1.75758500
B	6.58934600	5.64445500	1.72026600
B	3.36891200	5.61406900	1.69176400
B	7.43435700	4.23261200	1.69853200
B	7.55765400	7.14860100	1.75413300
B	4.93048400	5.67867300	0.84868200
B	1.74277100	5.63149900	0.88490900
B	4.16549900	4.11999100	1.73060100
B	4.14036700	7.09798600	1.80062300
B	8.44867400	5.77411100	1.51127100
B	5.80888500	7.09594300	1.75758500
B	5.77322200	4.15613600	1.77520700
B	1.57312400	2.81174400	-1.68037600
B	-1.57312400	2.81174400	-1.68037600
B	-2.47050000	4.21181200	-1.72974000

B	-2.48144100	1.40581200	-1.71840500
B	0.00000000	2.82111500	-0.84569600
B	-0.79539300	4.33420000	-1.73420500
B	-3.23109400	2.82520900	-0.87831500
B	-0.79724400	1.29218400	-1.71979900
B	0.79724400	1.29218400	-1.71979900
B	3.23109400	2.82520900	-0.87831500
B	0.79539300	4.33420000	-1.73420500
B	1.57312400	2.81174400	1.68037600
B	-1.57312400	2.81174400	1.68037600
B	2.48144100	1.40581200	1.71840500
B	2.47050000	4.21181200	1.72974000
B	0.00000000	2.82111500	0.84569600
B	-3.23109400	2.82520900	0.87831500
B	-0.79724400	1.29218400	1.71979900
B	-0.79539300	4.33420000	1.73420500
B	3.23109400	2.82520900	0.87831500
B	0.79539300	4.33420000	1.73420500
B	0.79724400	1.29218400	1.71979900
B	-3.37923400	0.00000000	-1.65688700
B	-6.53852000	0.00000000	-1.74538500
B	-7.41577300	1.43577400	-1.76821000
B	-7.41577300	-1.43577400	-1.76821000
B	-4.96525000	0.00000000	-0.84984000
B	-5.74654700	1.51455600	-1.74444300
B	-8.13492500	0.00000000	-0.83835500
B	-5.74654700	-1.51455600	-1.74444300
B	-4.15912000	-1.52051200	-1.72045800
B	-1.73249600	0.00000000	-0.87482400
B	-4.15912000	1.52051200	-1.72045800
B	-3.37923400	0.00000000	1.65688700
B	-6.53852000	0.00000000	1.74538500
B	-2.48144100	-1.40581200	1.71840500
B	-2.48144100	1.40581200	1.71840500
B	-4.96525000	0.00000000	0.84984000
B	-8.13492500	0.00000000	0.83835500
B	-5.74654700	-1.51455600	1.74444300
B	-5.74654700	1.51455600	1.74444300
B	-1.73249600	0.00000000	0.87482400
B	-4.15912000	1.52051200	1.72045800
B	-4.15912000	-1.52051200	1.72045800
B	-8.30740700	-2.84711400	-1.57739800
B	-10.08823700	-2.92953400	-1.48218800

B	-9.23772400	-4.33239200	-1.75636000
B	-6.63555500	-2.81413300	-0.87518500
B	-9.09306300	-1.40901000	-1.75683700
B	-8.30740700	-2.84711400	1.57739800
B	-7.43435700	-4.23261200	1.69853200
B	-7.41577300	-1.43577400	1.76821000
B	-10.08823700	-2.92953400	1.48218800
B	-6.63555500	-2.81413300	0.87518500
B	-9.09306300	-1.40901000	1.75683700
B	-9.23772400	-4.33239200	1.75636000
B	8.30740700	2.84711400	-1.57739800
B	7.43435700	4.23261200	-1.69853200
B	7.41577300	1.43577400	-1.76821000
B	10.08823700	2.92953400	-1.48218800
B	9.23772400	4.33239200	-1.75636000
B	6.63555500	2.81413300	-0.87518500
B	9.09306300	1.40901000	-1.75683700
B	8.30740700	2.84711400	1.57739800
B	10.08823700	2.92953400	1.48218800
B	6.63555500	2.81413300	0.87518500
B	9.09306300	1.40901000	1.75683700
B	9.23772400	4.33239200	1.75636000
B	6.53852000	0.00000000	-1.74538500
B	3.37923400	0.00000000	-1.65688700
B	2.48144100	1.40581200	-1.71840500
B	2.48144100	-1.40581200	-1.71840500
B	4.96525000	0.00000000	-0.84984000
B	4.15912000	1.52051200	-1.72045800
B	1.73249600	0.00000000	-0.87482400
B	4.15912000	-1.52051200	-1.72045800
B	5.74654700	-1.51455600	-1.74444300
B	8.13492500	0.00000000	-0.83835500
B	5.74654700	1.51455600	-1.74444300
B	6.53852000	0.00000000	1.74538500
B	3.37923400	0.00000000	1.65688700
B	7.41577300	-1.43577400	1.76821000
B	7.41577300	1.43577400	1.76821000
B	4.96525000	0.00000000	0.84984000
B	1.73249600	0.00000000	0.87482400
B	4.15912000	-1.52051200	1.72045800
B	4.15912000	1.52051200	1.72045800
B	8.13492500	0.00000000	0.83835500
B	5.74654700	1.51455600	1.74444300

B	5.74654700	-1.51455600	1.74444300
B	1.57312400	-2.81174400	-1.68037600
B	-1.57312400	-2.81174400	-1.68037600
B	-2.48144100	-1.40581200	-1.71840500
B	-2.47050000	-4.21181200	-1.72974000
B	0.00000000	-2.82111500	-0.84569600
B	-0.79724400	-1.29218400	-1.71979900
B	-3.23109400	-2.82520900	-0.87831500
B	-0.79539300	-4.33420000	-1.73420500
B	0.79539300	-4.33420000	-1.73420500
B	3.23109400	-2.82520900	-0.87831500
B	0.79724400	-1.29218400	-1.71979900
B	1.57312400	-2.81174400	1.68037600
B	-1.57312400	-2.81174400	1.68037600
B	2.47050000	-4.21181200	1.72974000
B	2.48144100	-1.40581200	1.71840500
B	0.00000000	-2.82111500	0.84569600
B	-3.23109400	-2.82520900	0.87831500
B	-0.79539300	-4.33420000	1.73420500
B	-0.79724400	-1.29218400	1.71979900
B	3.23109400	-2.82520900	0.87831500
B	0.79724400	-1.29218400	1.71979900
B	0.79539300	-4.33420000	1.73420500
B	-3.36891200	-5.61406900	-1.69176400
B	-6.58934600	-5.64445500	-1.72026600
B	-7.43435700	-4.23261200	-1.69853200
B	-7.55765400	-7.14860100	-1.75413300
B	-4.93048400	-5.67867300	-0.84868200
B	-5.77322200	-4.15613600	-1.77520700
B	-8.44867400	-5.77411100	-1.51127100
B	-5.80888500	-7.09594300	-1.75758500
B	-4.14036700	-7.09798600	-1.80062300
B	-1.74277100	-5.63149900	-0.88490900
B	-4.16549900	-4.11999100	-1.73060100
B	-3.36891200	-5.61406900	1.69176400
B	-6.58934600	-5.64445500	1.72026600
B	-2.44113600	-7.02684600	1.80792700
B	-2.47050000	-4.21181200	1.72974000
B	-4.93048400	-5.67867300	0.84868200
B	-8.44867400	-5.77411100	1.51127100
B	-5.80888500	-7.09594300	1.75758500
B	-5.77322200	-4.15613600	1.77520700
B	-1.74277100	-5.63149900	0.88490900

B	-4.16549900	-4.11999100	1.73060100
B	-4.14036700	-7.09798600	1.80062300
B	8.30740700	-2.84711400	-1.57739800
B	7.41577300	-1.43577400	-1.76821000
B	7.43435700	-4.23261200	-1.69853200
B	10.08823700	-2.92953400	-1.48218800
B	9.09306300	-1.40901000	-1.75683700
B	6.63555500	-2.81413300	-0.87518500
B	9.23772400	-4.33239200	-1.75636000
B	8.30740700	-2.84711400	1.57739800
B	10.08823700	-2.92953400	1.48218800
B	6.63555500	-2.81413300	0.87518500
B	9.23772400	-4.33239200	1.75636000
B	9.09306300	-1.40901000	1.75683700
B	6.58934600	-5.64445500	-1.72026600
B	3.36891200	-5.61406900	-1.69176400
B	2.47050000	-4.21181200	-1.72974000
B	2.44113600	-7.02684600	-1.80792700
B	4.93048400	-5.67867300	-0.84868200
B	4.16549900	-4.11999100	-1.73060100
B	1.74277100	-5.63149900	-0.88490900
B	4.14036700	-7.09798600	-1.80062300
B	5.80888500	-7.09594300	-1.75758500
B	8.44867400	-5.77411100	-1.51127100
B	5.77322200	-4.15613600	-1.77520700
B	6.58934600	-5.64445500	1.72026600
B	3.36891200	-5.61406900	1.69176400
B	7.55765400	-7.14860100	1.75413300
B	7.43435700	-4.23261200	1.69853200
B	4.93048400	-5.67867300	0.84868200
B	1.74277100	-5.63149900	0.88490900
B	4.14036700	-7.09798600	1.80062300
B	4.16549900	-4.11999100	1.73060100
B	8.44867400	-5.77411100	1.51127100
B	5.77322200	-4.15613600	1.77520700
B	5.80888500	-7.09594300	1.75758500
B	1.61260200	-8.46071000	-1.54549900
B	-1.61260200	-8.46071000	-1.54549900
B	-2.44113600	-7.02684600	-1.80792700
B	-2.44841000	-10.02677900	-1.48786700
B	0.00000000	-8.36842100	-0.84530800
B	-0.81513500	-6.96155600	-1.73531200
B	-3.28898100	-8.37026400	-0.84906300

B	-0.82846800	-10.00394300	-1.47965300
B	0.82846800	-10.00394300	-1.47965300
B	3.28898100	-8.37026400	-0.84906300
B	0.81513500	-6.96155600	-1.73531200
B	1.61260200	-8.46071000	1.54549900
B	-1.61260200	-8.46071000	1.54549900
B	2.44841000	-10.02677900	1.48786700
B	2.44113600	-7.02684600	1.80792700
B	0.00000000	-8.36842100	0.84530800
B	-3.28898100	-8.37026400	0.84906300
B	-0.82846800	-10.00394300	1.47965300
B	-0.81513500	-6.96155600	1.73531200
B	3.28898100	-8.37026400	0.84906300
B	0.81513500	-6.96155600	1.73531200
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B	-7.55765400	-7.14860100	1.75413300
B	2.44841000	-10.02677900	-1.48786700
B	7.55765400	-7.14860100	-1.75413300
B	-2.44841000	-10.02677900	1.48786700
B	4.95150500	-8.58400900	-1.69721900
B	6.71793800	-8.54365700	-1.46127600
B	6.71793800	-8.54365700	1.46127600
B	4.07524900	-10.01585200	-1.39380900
B	5.84346400	-10.00905300	-1.31025200
B	4.07524900	-10.01585200	1.39380900
B	4.95150500	-8.58400900	1.69721900
B	5.84346400	-10.00905300	1.31025200
B	-4.95150500	-8.58400900	-1.69721900
B	-4.07524900	-10.01585200	-1.39380900
B	-4.07524900	-10.01585200	1.39380900
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B	-5.84346400	-10.00905300	-1.31025200
B	-6.71793800	-8.54365700	1.46127600
B	-4.95150500	-8.58400900	1.69721900
B	-5.84346400	-10.00905300	1.31025200
B	-5.84346400	10.00905300	-1.31025200
B	-4.07524900	10.01585200	-1.39380900
B	-4.07524900	10.01585200	1.39380900
B	-6.71793800	8.54365700	-1.46127600
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B	5.84346400	10.00905300	-1.31025200
B	6.71793800	8.54365700	-1.46127600
B	6.71793800	8.54365700	1.46127600
B	4.07524900	10.01585200	-1.39380900
B	4.95150500	8.58400900	-1.69721900
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B	5.84346400	10.00905300	1.31025200
B	4.95150500	8.58400900	1.69721900
B	9.88425500	0.00000000	-1.58465800
B	10.83098100	1.44824800	-1.62642500
B	10.83098100	1.44824800	1.62642500
B	10.83098100	-1.44824800	-1.62642500
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B	4.81752100	11.12533400	0.00000000
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B	8.82845300	6.88714300	0.00000000
B	9.61193000	5.51773800	0.00000000
B	10.49516600	4.12418900	0.00000000
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(m) $D_2 B_{822}$ (XIII)

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B	4.13787386	9.73998005	-1.73545182
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B	4.14829776	12.69674516	-1.76277230
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B	3.38334443	5.61441510	1.66920398
B	8.20284776	5.62835560	0.87946148
B	3.36959312	5.61142465	-1.66892169
B	8.17909202	5.62370117	-0.89153849
B	6.51567951	5.60582122	-1.67163276
B	1.72297083	5.61166293	-0.88136551

B	2.48444581	7.02277327	1.69717157
B	7.40887498	6.99692134	-1.73548272
B	2.46734334	7.01916448	-1.69653960
B	7.43731984	7.00549958	1.71606619
B	4.95863514	5.61729393	0.85298610
B	4.94519274	5.61460415	-0.85279425
B	-0.79361756	4.31223099	1.72198383
B	0.80181867	1.29392995	1.72266930
B	0.79361756	4.31223099	-1.72198383
B	-0.80181867	1.29392995	-1.72266930
B	0.79805474	1.29045647	-1.72398772
B	-0.80515868	4.31483721	-1.72648987
B	-0.79805474	1.29045647	1.72398772
B	0.80515868	4.31483721	1.72648987
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B	-3.22082940	2.80262811	0.88349251
B	-1.57145577	2.80298274	1.67686773
B	3.22739760	2.80453925	0.88096804
B	-1.57908610	2.80519090	-1.67863095
B	3.22082940	2.80262811	-0.88349251
B	1.57145577	2.80298274	-1.67686773
B	-3.22739760	2.80453925	-0.88096804
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B	2.47020166	4.20773768	-1.69683391
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B	-0.00283266	2.80343262	-0.85356579
B	-5.75209715	1.50372200	1.72289465
B	-4.15956427	-1.51402028	1.72345949
B	-4.15956427	1.51402028	-1.72345949
B	-5.75209715	-1.50372200	-1.72289465
B	-4.15294214	-1.51058420	-1.72677630
B	-5.75938153	1.51261332	-1.72898161
B	-5.75938153	-1.51261332	1.72898161
B	-4.15294214	1.51058420	1.72677630
B	-3.38138371	-0.00278349	1.67823735
B	-8.18338752	-0.00328421	0.88349755
B	-6.53087419	-0.00444118	1.68030724
B	-1.73288383	-0.00242603	0.88190295
B	-6.53087419	0.00444118	-1.68030724
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B	-7.43440126	1.41027186	-1.69659927
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B	-10.69306614	-1.33648354	1.72351268
B	-9.12914167	-4.32384763	1.70532636
B	-9.09227959	-1.30397892	-1.71405045
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B	-7.43440126	-1.41027186	1.69659927
B	-9.92310443	-2.83029797	0.85466460
B	-9.91260670	-2.82534999	-0.85815825
B	-15.83230271	-4.35192457	1.61934643
B	-14.15089243	-7.20052466	1.70576086
B	-14.02148669	-4.32960247	-1.93054507
B	-14.15241304	-7.25516373	-1.63299434
B	-15.73030877	-4.36642706	-1.65390503
B	-14.13263663	-4.35521122	1.96123948
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B	-12.41948536	-4.26354740	1.73287491
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B	6.68997082	2.81006985	0.88337295
B	8.34146517	2.82022681	1.66461573
B	13.14689484	2.77584242	0.83683803
B	8.32717520	2.81306321	-1.66962521
B	13.13010954	2.80372303	-0.88535122
B	11.47695318	2.84152815	-1.74180352
B	6.67967412	2.80363905	-0.88106109
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B	4.15956427	1.51402028	1.72345949
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B	1.73288383	0.00242603	0.88190295
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B	8.18338752	0.00328421	0.88349755
B	3.38138371	-0.00278349	-1.67823735
B	8.18338752	-0.00328421	-0.88349755
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B	7.42499283	1.40333140	-1.69441437
B	2.47549779	1.40003752	-1.69548352
B	7.43440126	1.41027186	1.69659927
B	4.95862804	0.00382884	0.85409711
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B	-0.80181867	-1.29392995	1.72266930
B	0.79361756	-4.31223099	1.72198383
B	0.80181867	-1.29392995	-1.72266930
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B	0.80515868	-4.31483721	-1.72648987
B	-0.79805474	-1.29045647	-1.72398772
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B	-6.53768240	-5.61353412	1.67416427
B	-1.73262119	-5.61391028	0.88317979
B	-6.51567951	-5.60582122	-1.67163276
B	-1.72297083	-5.61166293	-0.88136551
B	-3.36959312	-5.61142465	-1.66892169
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B	-7.44588618	-4.21776776	1.69065385
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B	13.13010954	-2.80372303	0.88535122
B	8.34146517	-2.82022681	-1.66461573
B	13.14689484	-2.77584242	-0.83683803
B	11.51305116	-2.84656116	-1.71776031
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B	5.73901287	-7.11252327	1.73631890
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B	3.38334443	-5.61441510	-1.66920398
B	8.20284776	-5.62835560	-0.87946148
B	6.53768240	-5.61353412	-1.67416427
B	1.73262119	-5.61391028	-0.88317979
B	2.47020166	-4.20773768	1.69683391
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B	-0.81011277	-6.91725911	1.70860940
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