Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

On the gas-phase dimerization of negatively charged *closo*-dodecaborates: a theoretical study

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Table of Contents

Table S1 Relative energies (E), dimerization energies (ΔE), dimerization free enthalpies (ΔG) and vertical detachment energies (VDE) calculated for all modeled isomers of the type $B_{24}I_{18}^{2-}$. The respective structures are depicted in Fig. S2.

$B_{24}I_{18}^{2-}$ isomers	Multiplicity, M	Relative energy, E[a] (kJ mol^{-1})	Dimerization energy[b] (kJ mol^{-1}) ΔE	ΔG	VDE[c] (eV)
1	1	0	−400.6	−318.9	3.0
2	3	263.2	−137.3	−50.8	2.1
3	3	303.1	−97.5	−18.0	2.7
4	3	663.3	262.7	---	---
5	3	716.6	316.0	---	---

[a] Values calculated w.r.t. the most stable isomer of $B_{24}I_{18}^{2-}$ (with M = 1)

[b] Values calculated w.r.t. two monomers of the type $B_{12}I_9^-$ (with M = 1)

[c] Values calculated only for the $B_{24}I_{18}^{2-}$ isomers resulting from exothermic dimerization

Table S2 Relative energies (E), dimerization energies (ΔE) and vertical detachment energies (VDE) calculated for all modeled isomers of the type $B_{24}I_{16}^{2-}$. The respective structures are depicted in Fig. S4.

$B_{24}I_{16}^{2-}$ isomers	Multiplicity, M	Relative energy, E[a] (kJ mol^{-1})	Dimerization energy, ΔE[b] (kJ mol^{-1})	VDE[c] (eV)
1[d]	3	0	-387.9	2.2
2	1	191.2	-196.7	2.4
3	1	302.3	-85.6	1.2
4	1	319.3	-68.6	1
5	1	333.6	48.8	---
6	1	436.6	68.3	---
7	1	458.2	70.4	---
8	1	508.3	120.4	---
9	1	508.6	120.7	---
10	1	535.3	147.4	---
11	1	545.3	157.4	---
12	1	546.8	158.9	---
13	1	559.9	172.0	---
14	1	560	172.1	---
15	1	560.1	172.2	---
16	1	571	183.1	---
17	1	578.7	190.8	---
18	1	599.8	211.9	---
19	1	608.8	220.9	---
20	1	613.7	225.8	---

[a] Values calculated w.r.t. the most stable isomer of $B_{24}I_{16}^{2-}$ (with M = 3)

[b] Values calculated w.r.t. two monomers of the type $B_{12}I_8^-$ (with M = 2). The

dimerization free enthalpies (ΔG) for the exothermic dimerization processes are given in the main paper.

[c] Values calculated only for the $B_{24}I_{16}^{2-}$ isomers resulting from exothermic dimerization

[d] For isomer **1**, we found a local minimum structure with M = 1, which lies by 103 kJ mol^{-1} higher in energy w.r.t. the triplet ground state (the respective dimerization energy is ΔE = -284.9 kJ mol^{-1}, and calculated VDE = 1.1 eV). The structure in terms of configuration, bond lengths and angles was found to be the same for both species.

Table S3 Detailed list of the NPA charges calculated for the most stable isomers of the $B_{12}I_n^-$ (n = 9, 8) monomers and the $B_{24}I_{2n}^{2-}$ dimers. The atom number corresponds to the numbering of the fragments in the output of the NPA calculation (with the ADF software).

$B_{12}I_9^-$ (M = 1)

Atom number	Natural charge	Remarks
B 1	0.035	bare center (B**1** in Fig. 1a)
B 2	0.035	bare center (B**2** in Fig. 1a)
B 3	0.035	bare center (B**3** in Fig. 1a)
B 5	-0.115	
B 7	-0.115	
B 9	-0.116	
B 10	-0.132	
B 11	-0.134	
B 12	-0.135	
B 8	-0.152	
B 6	-0.153	
B 4	-0.154	
I 18	0.013	
I 15	0.013	
I 16	0.013	
I 17	0.031	
I 13	0.032	
I 19	0.031	
I 20	-0.012	
I 21	-0.011	
I 14	-0.011	

Total charge -1.000

$B_{24}I_{18}^{2-}$ (M = 1)

Atom number	Natural charge	Remarks
B 8	-0.023	bridging center from the 3c-2e bond (Fig. 1c)
B 20	-0.023	bridging center from the 3c-2e bond (Fig. 1c)
B 1	-0.027	bridging center from the 3c-2e bond (B**1** in Fig. 1c)
B 13	-0.027	bridging center from the 3c-2e bond (B**1'** in Fig. 1c)
B 10	-0.119	
B 11	-0.119	
B 22	-0.119	
B 23	-0.119	
B 16	-0.150	
B 17	-0.150	
B 19	-0.150	
B 4	-0.150	
B 5	-0.151	
B 7	-0.151	
B 9	-0.151	
B 12	-0.152	
B 14	-0.152	
B 18	-0.152	
B 21	-0.152	
B 2	-0.152	bridging center from the 2c-2e bond (B**2** in Fig. 1c)
B 6	-0.152	bridging center from the 2c-2e bond (B**3'** in Fig. 1c)
B 15	-0.153	
B 24	-0.153	bridging center from the 2c-2e bond (B**2'** in Fig. 1c)
B 3	-0.153	bridging center from the 2c-2e bond (B**3** in Fig. 1c)
I 32	0.527	bridging center from the 3c-2e bond
I 41	0.527	bridging center from the 3c-2e bond
I 30	0.0007	
I 39	0.0007	
I 26	0.0005	
I 35	0.0005	
I 28	0.0005	
I 37	0.0004	
I 33	0.0002	
I 42	0.0003	
I 29	-0.004	
I 31	-0.004	
I 38	-0.004	
I 40	-0.004	
I 25	-0.010	

I 27	-0.010
I 34	-0.010
I 36	-0.010
==========	
Total charge	-2.000

$B_{12}I_8^-$ (M = 2)

Atom number	Natural charge	Natural spin density	Remarks
B 10	0.159	0.731	bare center (B**4** in Fig. 1b)
B 1	0.046	-0.058	bare center from the deiodinated face (B**1** in Fig.1b)
B 3	0.047	-0.057	bare center from the deiodinated face (B**3** in Fig.1b)
B 2	0.008	0.317	bare center from the deiodinated face (B**2** in Fig.1b)
B 7	-0.098	-0.001	
B 6	-0.135	0.005	
B 8	-0.135	0.005	
B 9	-0.153	-0.009	
B 5	-0.154	-0.009	
B 4	-0.181	-0.007	
B 11	-0.184	-0.008	
B 12	-0.184	-0.008	
I 16	0.007	0.005	
I 13	0.020	0.019	
I 17	0.020	0.019	
I 15	-0.007	0.016	
I 18	-0.007	0.016	
I 14	-0.016	0.006	
I 20	-0.016	0.006	
I 19	-0.036	0.013	coordinated to the B center with 3 bare neighbors
==========			
Total	-1.000	1.000	

$B_{24}I_{16}^{2-}$ (M = 3)

Atom number	Natural charge	Natural spin density	Remarks
B 1	0.006	0.010	bridging center from the 3c-2e bond (B**1** in Fig. 1d)
B 8	0.005	0.010	bridging center from the 3c-2e bond (Fig. 1d)
B 15	0.005	0.010	bridging center from the 3c-2e bond (Fig. 1d)

B 18	0.006	0.010	bridging center from the 3c-2e bond (B**1'** in Fig. 1d)
B 10	0.100	0.804	bare center in monomer 1 (B**4** in Fig. 1d)
B 22	0.100	0.804	bare center in monomer 2 (B**4'** in Fig. 1d)
B 3	-0.100	0.012	bridging center from the 2c-2e bond (B**3** in Fig. 1d)
B 13	-0.100	0.012	bridging center from the 2c-2e bond (B**3'** in Fig. 1d)
B 19	-0.121	0.011	
B 20	-0.121	0.011	
B 6	-0.121	0.011	
B 7	-0.121	0.011	
B 11	-0.158	-0.011	
B 24	-0.158	-0.011	
B 16	-0.187	-0.013	
B 17	-0.187	-0.013	
B 4	-0.187	-0.013	
B 9	-0.187	-0.013	
B 5	-0.191	-0.012	
B 12	-0.191	-0.012	
B 21	-0.192	-0.012	
B 23	-0.191	-0.012	
B 14	-0.197	0.005	bridging center from the 2c-2e bond (B**2'** in Fig. 1d)
B 2	-0.197	0.005	bridging center from the 2c-2e bond (B**2** in Fig. 1d)
I 26	0.507	0.026	bridging center from the 3c-2e bond
I 40	0.507	0.025	bridging center from the 3c-2e bond
I 28	-0.007	0.011	
I 34	-0.007	0.011	
I 36	-0.007	0.011	
I 32	-0.007	0.011	
I 30	-0.025	0.030	
I 31	-0.025	0.030	
I 35	-0.025	0.030	
I 39	-0.025	0.030	
I 33	-0.029	0.032	
I 29	-0.029	0.032	
I 25	-0.035	0.030	
I 27	-0.035	0.030	
I 37	-0.035	0.030	
I 38	-0.035	0.030	
==========	==========	==========	
Total	-2.000	2.000	

Table S4 Energies of the frontier molecular orbitals (FMOs) as calculated for: (A) the closed-shell systems (with M =1), (B) the open-shell $B_{12}I_8^-$ monomer (with M = 2), (C) the open-shell $B_{24}I_{16}^{2-}$ dimer (with M = 3, the ground spin state), and (D) the hypothetical $B_{36}I_{24}^{3-}$ trimer (with M = 2).

(A)	**Orbital energies (in eV) for species with M = 1**		
Orbital notation	**$B_{12}I_9^-$**	**$B_{24}I_{18}^{2-}$**	**$B_{24}I_{16}^{2-}$[a]**
LUMO+1	-0.55	2.11	
LUMO	-0.55	1.40	0.18
HOMO	-3.78	-1.90	-0.29
HOMO-1	-3.85	-1.96	
HOMO-LUMO gap	**3.23**	**3.3**	**0.47**

[a] The high-spin state of the lowest-energy structure for $B_{24}I_{16}^{2-}$.

(B) **$B_{12}I_8^-$ (M = 2)**	**Orbital number, symmetry and spin component**	**Orbital energy, eV**
LUMO+2	244A_*alpha*	-0.40
LUMO+1	244A_*beta*	-0.53
LUMO	243A_*beta*	-0.72
SOMO	243A_*alpha*	-3.36
HOMO-1	242A_(*alpha* + *beta*)	-3.78
SOMO-LUMO gap	**|243A_(*alpha* – *beta*)|**	**2.64**

(C) **$B_{24}I_{16}^{2-}$ (M = 3)**	**Orbital number, symmetry and spin component**	**Orbital energy, eV**
LUMO+1	486A_*beta*	1.36
LUMO	485A_*beta*	1.07
SOMO	486A_*alpha*	-1.13
SOMO-1	485A_*alpha*	-1.34
SOMO-LUMO gap	**|486A_*alpha* – 485A_*beta*|**	**2.2**

(D) **$B_{36}I_{24}^{3-}$ (M = 2)**	**Orbital number, symmetry and spin component**	**Orbital energy, eV**
LUMO+1	729A_*alpha*	2.57
LUMO	728A_*beta*	2.13
SOMO	727A_*beta*	1.61

SOMO-LUMO gap	**|727A_*beta* – 728A_*beta*|**	**0.51**

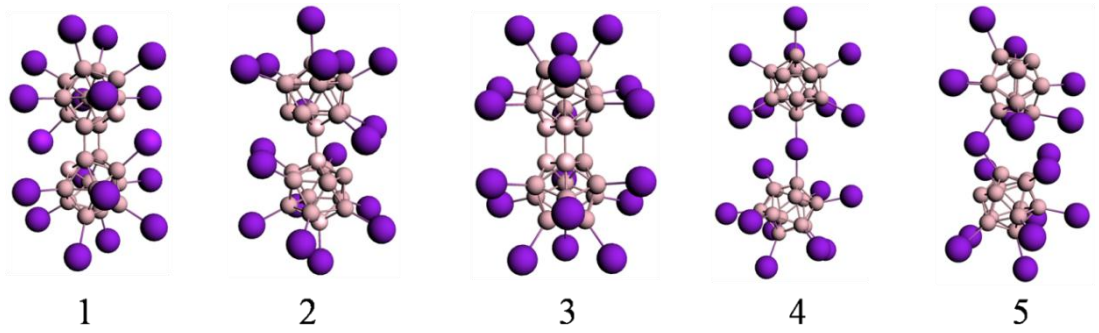


Fig. S1 Ball-and-stick representation of the initial (prior to optimization) structures of all $B_{24}I_{18}^{2-}$ isomers. The numbering of the isomers is the same as the one shown in Table S1. Color legend: B pink, I violet.

The initial structures were constructed by placing two equal $B_{12}I_9^-$ monomers close to each other, such that the following types and numbers of bonds are created: 1) two B–B bonds in isomer **1**, 2) one B–B bond in isomer **2**, 3) three B–B bonds in isomer **3**, and 4) one B–I–B bond in isomers **4** and **5**.

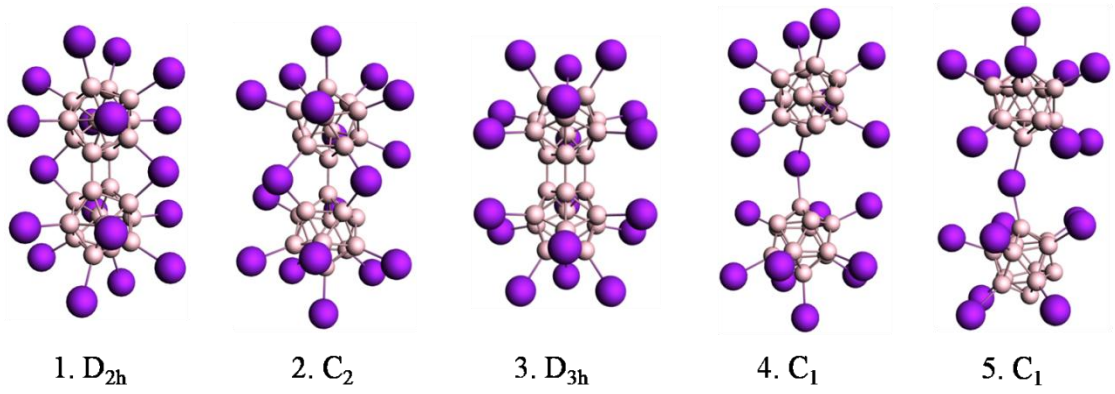


Fig. S2 Ball-and-stick representation of the optimized structures of all $B_{24}I_{18}^{2-}$ isomers. The numbering of the isomers is the same as the one shown in Table S1. The symmetry of each isomer is shown. Color legend: B pink, I violet.

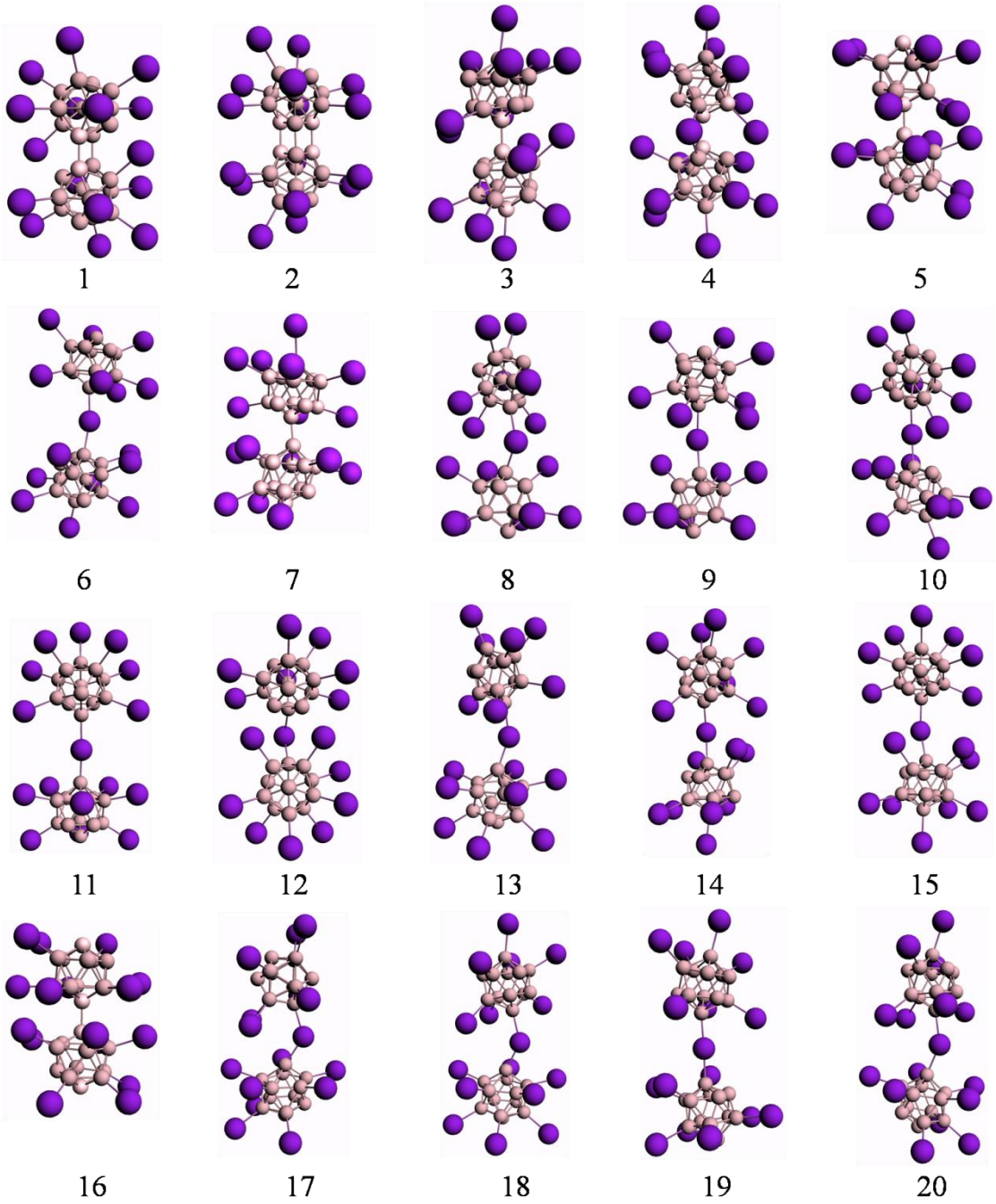


Fig. S3 Ball-and-stick representation of the initial (prior to optimization) structures of all $B_{24}I_{16}^{2-}$ isomers. The numbering of the isomers is the same as the one shown in Table S2. Color legend: B pink, I violet.

The initial structures were constructed by placing two equal $B_{12}I_8^-$ monomers close to each other, such that the following types and numbers of bonds are created: 1) two B–B bonds in isomer **1**, 2) three B–B bonds in isomer **2**, 3) one B–B bond in isomers **3**, **4**, **5**, **7** and **16**, 4) one B–I–B bond in other isomers **6**, **8**-**15** and **17**-**20**.

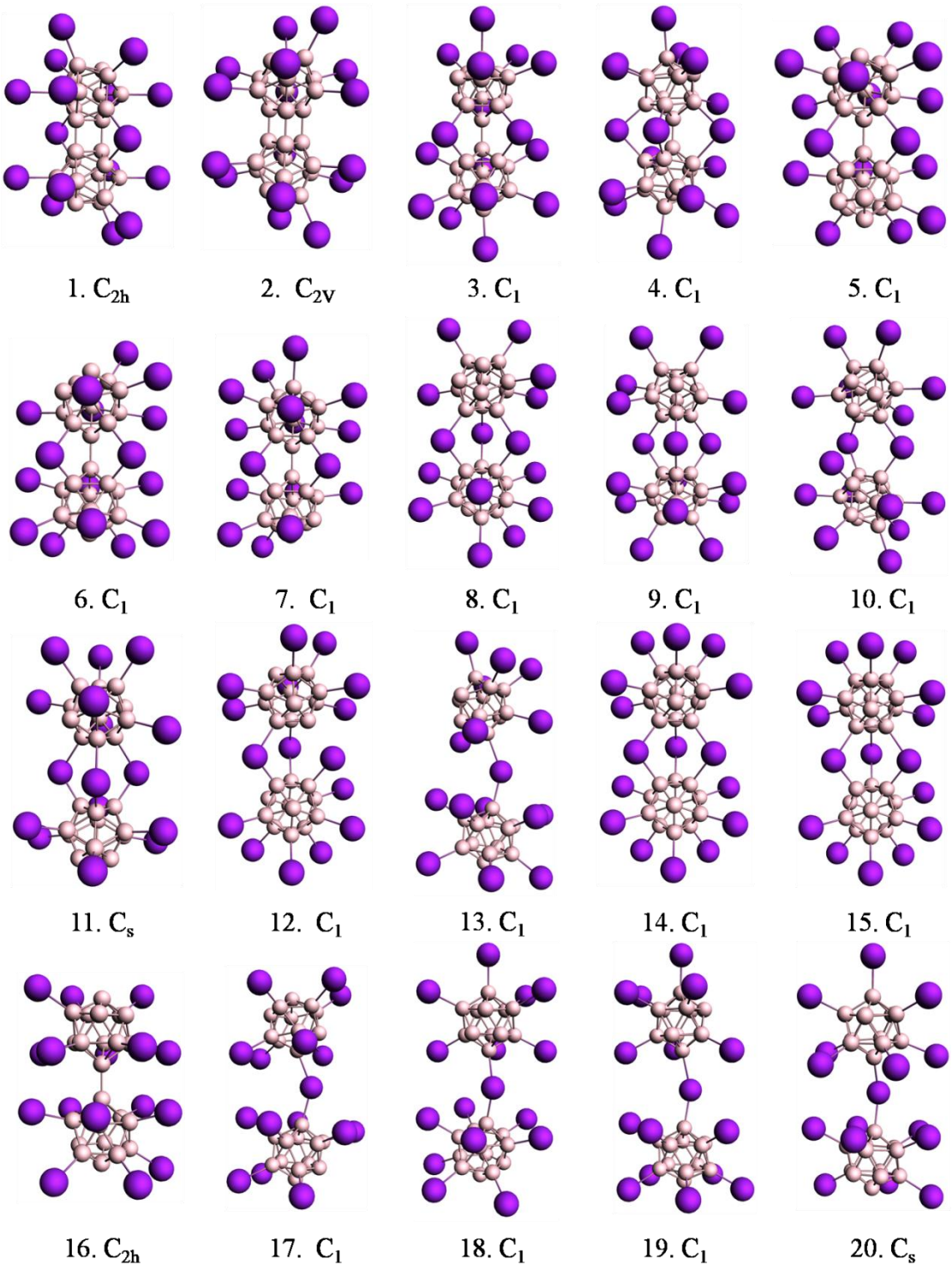
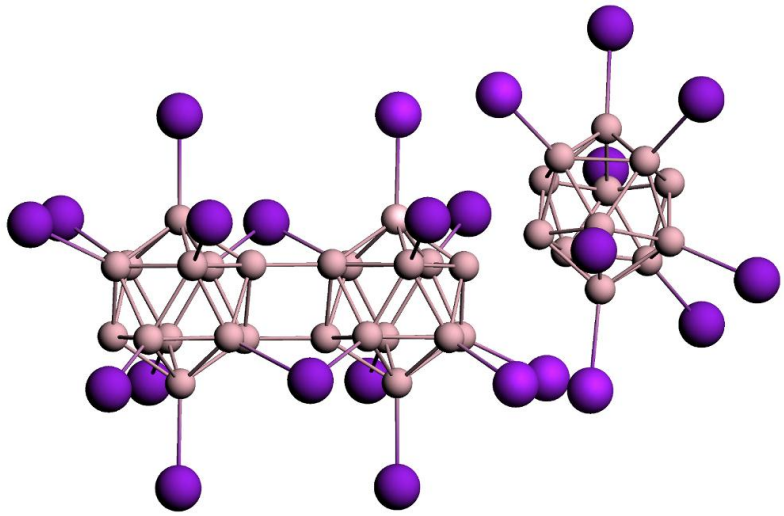
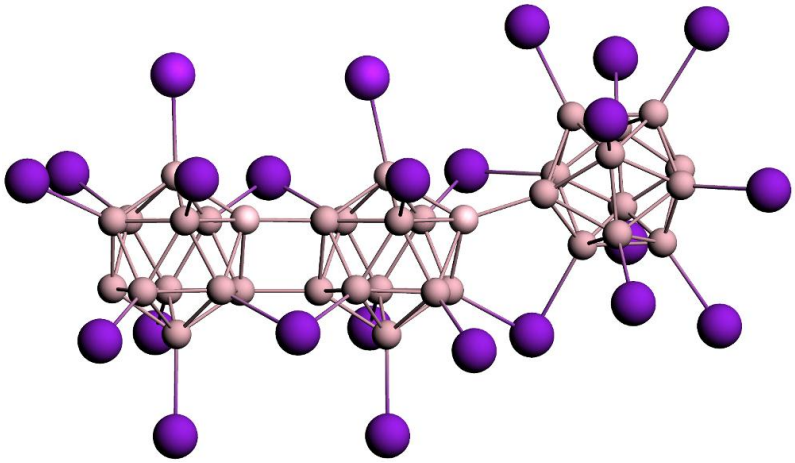


Fig. S4 Ball-and-stick representation of the optimized structures of all $B_{24}I_{16}^{2-}$ isomers. The numbering of the isomers is the same as the one shown in Table S2. The symmetry of each isomer is shown. Color legend: B pink, I violet.



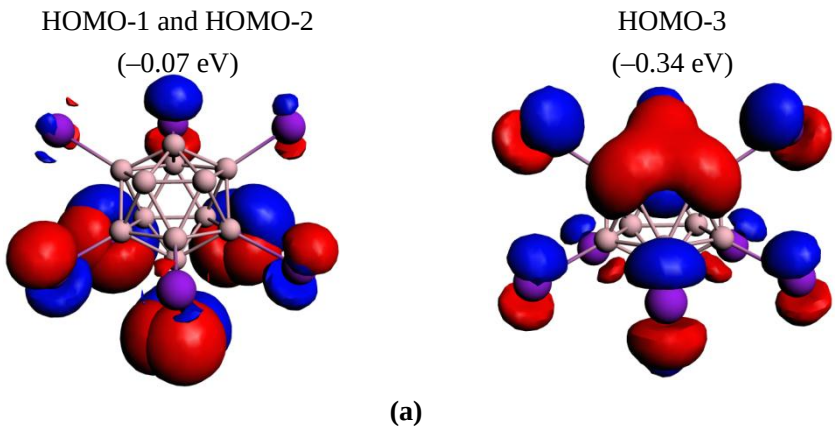
(a)



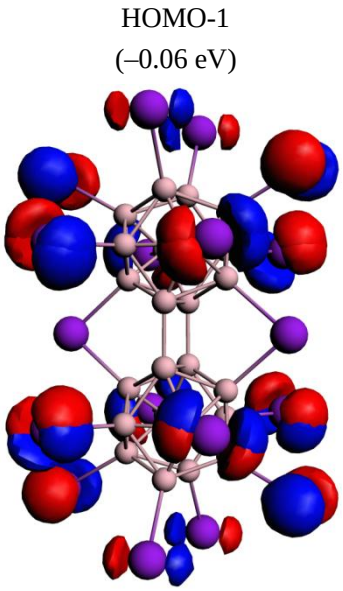
(b)

Fig. S5 Ball-and-stick representation of (a) the initial and (b) the optimized structures of a hypothetical $B_{36}I_{24}^{3-}$ trimer species. Color legend: B pink, I violet.

The trimer $B_{36}I_{24}^{3-}$ species shown in Fig. S5b is found to be less stable than the separate $B_{24}I_{16}^{2-}$ and $B_{12}I_8^{-}$ clusters (ΔE = 115.3 kJ mol^{-1}, as calculated at the B3LYP/ZORA scalar/TZP level of theory).



(a)



(b)

Fig. S6 The lower-lying doubly-occupied MOs of (**a**) the most stable $B_{12}I_9^-$ monomer (M = 1, C_{3V} symmetry), and (**b**) the most stable $B_{24}I_{18}^{2-}$ dimer (M = 1, D_{2h} symmetry). HOMO–m (m = 1, 2 and 3) are shown for $B_{12}I_9^-$; HOMO-1 is shown for $B_{24}I_{18}^{2-}$. The energies of the orbitals are given in parenthesis with respect to the HOMO levels shifted to zero. The unscaled values of E(HOMO) are -3.78 eV for $B_{12}I_9^-$, and -1.9 eV for $B_{24}I_{18}^{2-}$.

Fig. S6a shows that, similarly to the respective HOMO (see paper), the main contributions to the doubly degenerate HOMO-1 and HOMO-2 of the $B_{12}I_9^-$ monomer come from the 4*p*-orbitals of the I substituents only, whereas HOMO-3 includes considerable contributions also from the 2*p*- and 2*s*-orbitals of the three bare B neighbors. Figure S6b shows that the HOMO-1 of the $B_{24}I_{18}^{2-}$ dimer lies very closely to the respective HOMO (only 0.06 eV below) and is localized on all I substituents (with contributions from the respective 4*p*-atomic orbitals), excluding the two bridging iodines.

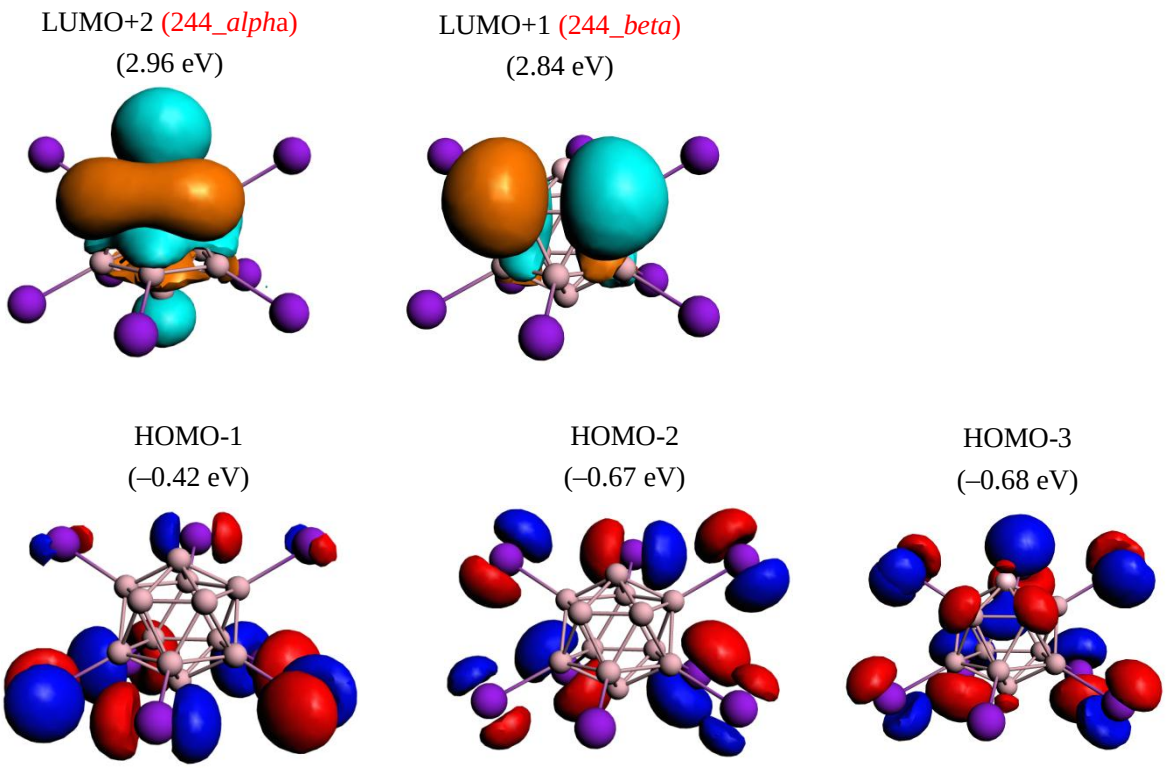


Fig. S7 LUMO+2 (*alpha*-spin), LUMO+1 (*beta*-spin) and HOMO–*m* (*m* = 1, 2, 3) of the most stable $B_{12}I_8^-$ monomer (*M* = 2, C_S symmetry). The numbers of LUMO+2 and LUMO+1, as defined in the ADF output, are shown in parenthesis. The energies of the orbitals are shown in parenthesis, with respect to the SOMO (*alpha*-spin) shifted to zero. The unscaled value of *E*(SOMO_ *alpha*-spin) = -3.36 eV.

Fig. S7 shows that the LUMO+2 and LUMO+1 are the spatially different (by 0.1 eV in terms of energy) *alpha* and *beta* spin components of one and the same orbital, with major contributions from all four bare B atoms. The doubly occupied MOs accommodating the paired electrons of the $B_{12}I_8^-$ monomer are either localized exclusively on the I substituents (HOMO-1 and HOMO-2), or contain also contributions from the bare boron face (HOMO-3 and lower MOs).

Movie S1. Molecular dynamics of the lowest-energy structure of $B_{24}I_{18}^{2-}$ at 300 K.
File to download: B24I18_MD_final.mpg

Movie S2. Molecular dynamics of the lowest-energy structure of $B_{24}I_{16}^{2-}$ at 300 K.
File to download: B24I16_MD_final.mpg

Cartesian coordinates [in Å] of all studied isomers of $B_{24}I_{18}^{2-}$ and $B_{24}I_{16}^{2-}$.

The most stable isomer of $B_{24}I_{18}^{2-}$ (Fig.S2. Isomer **1)**

B	0.91504536	-1.72461099	8.18520694
B	1.40266398	-1.01188208	9.73428344
B	2.04039887	-0.35265021	8.12926345
B	0.73714440	-0.51331658	6.90285607
B	-0.70580393	-1.26820819	7.73240453
B	-0.28629486	-1.56436822	9.48309171
B	0.02332379	0.01718911	10.25005434
B	1.39358878	0.72665789	9.37778959
B	1.04739504	1.06827589	7.66984458
B	-0.65102415	0.50956822	7.42846865
B	-1.27833358	-0.13141377	9.01258402
B	-0.19704173	1.31257640	8.98087492
I	-0.83069116	3.34265845	9.53134573
I	-1.11758774	-3.27806377	10.57799725
I	-2.04853746	-2.64250477	6.66613527
I	-0.39489701	0.41664573	12.36917243
I	-3.40009700	0.05656911	9.53455783
I	1.90612071	2.76942454	6.57610426
I	-2.00639348	1.45216405	5.98450790
I	3.04615541	1.78854238	10.49377111
I	1.17442172	-0.92009632	4.78863151
B	4.12540876	-0.16095321	10.12036128
B	3.00520053	-1.53514753	10.15613577
B	3.64592919	-0.85867462	8.55952797
B	5.33108941	-0.29734669	8.82790181
B	5.74398054	-0.61890718	10.57895638
B	4.30274664	-1.39147694	11.38810239
B	4.00322873	-2.96229996	10.59666339
B	3.66024061	-2.59913643	8.89570726
B	5.03195737	-1.86935098	8.03572488
B	6.32886860	-1.72850502	9.28136236
B	5.69790956	-2.40267104	10.85008251
B	5.25456129	-3.18097212	9.28462082
I	5.90734647	-5.19283705	8.69144058
I	3.85285263	-1.02135205	13.50626271
I	7.05914132	0.72894177	11.71147193
I	3.15294577	-4.68785712	11.65742882
I	7.05140598	-3.39610352	12.26057929
I	5.46006765	-2.22540491	5.91021838
I	8.45957721	-1.85594192	8.77794432

I	2.00036054	-3.66826494	7.79685861
I	6.15976731	1.43869036	7.76669012

Fig.S2. Isomer **2**

B	2.00848000	-1.73399000	9.26787000
B	1.04206000	-2.46793000	10.57210000
B	1.81823000	-0.98047400	10.88640000
B	1.63127000	0.01541970	9.46950000
B	0.75274600	-0.90861400	8.23992000
B	0.37592300	-2.50129000	8.96145000
B	-0.67551800	-2.21778000	10.40390000
B	0.25590700	-1.28789000	11.60610000
B	0.61908100	0.32748500	10.90770000
B	-0.07479340	0.36598400	9.24321000
B	-0.88631700	-1.20261000	8.93607000
B	-0.96324300	-0.44704100	10.58710000
I	-2.82449000	0.36177800	11.42290000
I	0.08237300	-4.33234000	7.78743000
I	1.13084000	-0.64158400	6.09220000
I	-2.15957000	-3.70589000	11.07470000
I	-2.67021000	-1.31503000	7.66434000
I	0.89335200	2.13833000	12.13470000
I	-0.71511900	2.27318000	8.35865000
I	0.08494070	-1.57750000	13.79700000
I	3.29121000	1.40314000	8.85512000
B	4.60521000	-0.44999300	8.77986000
B	3.69391000	-1.99443000	8.87067000
B	4.60495000	-1.49047000	7.42529000
B	6.04735000	-0.56335700	7.79767000
B	6.18316000	-0.52625500	9.58948000
B	4.77969000	-1.44636000	10.19940000
B	4.83833000	-3.14261000	9.69852000
B	4.73162000	-3.15948000	7.91307000
B	6.16181000	-2.26258000	7.26738000
B	7.16960000	-1.68496000	8.64561000
B	6.34893000	-2.23067000	10.15550000
B	6.34575000	-3.30294000	8.72146000
I	7.50260000	-5.16481000	8.72795000
I	3.73308000	-0.87380800	12.10220000
I	6.99760000	1.19056000	10.70600000
I	4.01747000	-4.75366000	10.94580000
I	7.42631000	-2.67724000	12.01830000
I	7.05726000	-2.74572000	5.31016000

I	9.35080000	-1.48868000	8.50699000
I	3.93574000	-4.84361000	6.75215000
I	6.68781000	1.16411000	6.56609000

Fig.S2. Isomer **3**

B	1.84042000	0.42999900	8.58724000
B	1.70322000	-1.00914000	9.71395000
B	1.70143000	0.69110400	10.39590000
B	0.78016100	1.71054000	9.25436000
B	0.24258800	0.72652100	7.86014000
B	0.78394700	-0.95058400	8.17596000
B	0.02186230	-1.59446000	9.66094000
B	0.56559400	-0.55009600	11.01140000
B	0.01682080	1.13584000	10.76950000
B	-0.89849700	1.14480000	9.20596000
B	-0.89582700	-0.51137600	8.53165000
B	-1.03281000	-0.26538800	10.29800000
I	-2.89381000	-0.72734300	11.38550000
I	1.02961000	-2.31922000	6.44038000
I	0.00399721	1.55489000	5.82715000
I	-0.49689000	-3.72521000	9.91707000
I	-2.57927000	-1.26558000	7.32533000
I	-0.51407200	2.47984000	12.43930000
I	-2.58220000	2.53298000	8.88853000
I	0.52118100	-1.38960000	13.07000000
I	1.02050000	3.90287000	8.96735000
B	3.43560000	0.64343900	10.53140000
B	3.43527000	-1.06350000	9.86053000
B	3.57269000	0.36765400	8.72338000
B	4.59193000	1.58657000	9.53994000
B	5.06439000	0.99540500	11.16120000
B	4.37684000	-0.64991200	11.32730000
B	5.06204000	-1.75056000	10.09340000
B	4.59020000	-1.08913000	8.49768000
B	5.28167000	0.54394200	8.25763000
B	6.21727000	0.91573700	9.76348000
B	6.08329000	-0.47570200	10.88010000
B	6.21583000	-0.75154300	9.11761000
I	8.01426000	-1.65798000	8.22070000
I	4.03639000	-1.44292000	13.37700000
I	5.41002000	2.34362000	12.87600000
I	5.40020000	-3.90225000	10.45620000
I	7.70634000	-1.00865000	12.27410000

I	5.89315000	1.31232000	6.27992000
I	8.02196000	2.17834000	9.68254000
I	4.53787000	-2.47775000	6.76066000
I	4.54401000	3.78310000	9.19114000

Fig.S2. Isomer **4**

B	-0.72801300	-1.48022000	9.12312000
B	-1.02244000	-0.66261200	10.50930000
B	0.34763100	-1.46741000	10.33590000
B	0.98609800	-1.45503000	8.74377000
B	-0.24648200	-0.41757400	7.87136000
B	-1.56929000	0.05465100	9.03711000
B	-0.80808200	1.05413000	10.38950000
B	0.40161400	-0.00390673	11.23850000
B	1.73184000	-0.45315000	10.07790000
B	1.31069000	0.29317000	8.47266000
B	-0.24504700	1.22097000	8.66751000
B	0.96905000	1.18830000	10.02210000
I	2.13520000	2.93909000	10.61850000
I	-3.67070000	0.26954000	8.44653000
I	-0.55836800	-0.48172000	5.58869000
I	-1.93517000	2.58547000	11.47670000
I	-0.63637500	3.05548000	7.54213000
I	3.78153000	-0.81081400	10.75940000
I	2.85511000	0.94227900	7.06363000
I	0.75365200	0.05830950	13.41810000
I	2.16906000	-3.12027000	7.98166000
B	-1.84319000	-2.16791000	4.55838000
B	-2.59212000	-3.53265000	5.28102000
B	-3.57342000	-2.24043000	4.63459000
B	-2.84851000	-1.63291000	3.16657000
B	-1.35799000	-2.61592000	2.88846000
B	-1.20984000	-3.81456000	4.22652000
B	-2.64090000	-4.89758000	4.19222000
B	-4.10915000	-3.89235000	4.48011000
B	-4.26939000	-2.73650000	3.10550000
B	-2.88098000	-2.99614000	1.99089000
B	-1.88318000	-4.33736000	2.65199000
B	-3.67924000	-4.40847000	2.80495000
I	-4.87695000	-5.88130000	1.71217000
I	0.73693300	-4.57626000	4.84956000
I	0.41524000	-1.74111000	1.93047000
I	-2.51603000	-6.95324000	4.96483000

I	-0.78171600	-5.70547000	1.33577000
I	-6.24013000	-2.03615000	2.41738000
I	-3.03368000	-2.67204000	-0.17316400
I	-5.85254000	-4.62027000	5.61884000
I	-3.00877000	0.48691300	2.57916000

Fig.S2. Isomer **5**

B	-1.63487000	-1.42618000	9.97006000
B	-2.27900000	-0.05075680	10.88830000
B	-0.90869800	-0.88964900	11.33580000
B	0.10041000	-1.48631000	10.07820000
B	-0.71266800	-0.88497100	8.59680000
B	-2.23516000	-0.02224890	9.12971000
B	-1.73685000	1.42602000	10.11480000
B	-0.92112400	0.81261900	11.58730000
B	0.59727300	-0.06975790	11.09760000
B	0.69139100	0.00841836	9.31195000
B	-0.74833400	0.91848600	8.69548000
B	0.07539500	1.43727000	10.22720000
I	1.22256000	3.28463000	10.40220000
I	-4.10389000	-0.09072950	7.96153000
I	-0.63570700	-2.00155000	6.70142000
I	-2.95739000	3.25299000	10.15480000
I	-0.68464400	2.14096000	6.87887000
I	2.31108000	-0.20473700	12.44820000
I	2.60477000	0.01522920	8.01474000
I	-1.12454000	1.73225000	13.58480000
I	1.10483000	-3.44906000	10.21610000
B	5.07655000	0.18149500	8.09752000
B	5.70583000	-0.93169600	7.02791000
B	5.58592000	0.59172100	6.56272000
B	5.91914000	1.71647000	7.83381000
B	6.33528000	0.62841800	9.24254000
B	6.13342000	-1.10312000	8.69650000
B	7.32954000	-1.42673000	7.33675000
B	6.90953000	-0.32893200	5.95861000
B	7.11416000	1.39313000	6.47952000
B	7.63971000	1.35714000	8.20523000
B	7.77224000	-0.36890700	8.73155000
B	8.26034000	0.10371300	7.04691000
I	10.34470000	0.06554020	6.37684000
I	5.45918000	-2.69785000	10.04370000
I	6.02823000	1.26402000	11.31440000

I	8.13803000	-3.44066000	6.99350000
I	9.26614000	-1.02349000	10.19520000
I	7.67084000	2.97061000	5.05489000
I	8.96051000	2.91134000	9.00651000
I	7.08959000	-0.96101400	3.84150000
I	4.96686000	3.68021000	8.06353000

The most stable isomer of $B_{24}I_{16}^{2-}$ in its ground state (*M* = 3, **Fig.S4** Isomer **1**)

B	22.16777951	12.78351581	15.81465913
B	21.24961737	12.41073802	14.34470763
B	21.73531492	14.14527284	14.74929300
B	23.34254324	14.07878174	15.55041702
B	23.84069332	12.32934126	15.65877118
B	22.53807585	11.29579562	14.90800314
B	22.42747055	11.73088045	13.17390303
B	21.99601776	13.45849031	13.12523580
B	23.23228502	14.51171564	13.82462470
B	24.43037832	13.36452617	14.38107412
B	24.03252345	11.69320172	13.98722067
B	23.66132628	13.03459154	12.84769902
I	24.64858085	13.23455915	10.87753688
I	20.46450032	14.25147072	11.65157029
I	25.06062337	11.60893280	17.35847241
I	21.83532703	10.29610274	11.61636137
I	25.60113952	10.21014860	13.51575872
I	23.72615976	16.53333074	13.08066649
I	23.98185097	15.52856323	17.09091858
I	22.09286637	9.28088120	15.66755988
B	19.57842874	12.84643051	14.56053990
B	20.06358695	14.58053031	14.96666941
B	19.14534942	14.20939609	13.49658103
B	17.97128404	12.91336752	13.75912506
B	18.08180857	12.47794356	15.48442178
B	19.31768038	13.53104327	16.18526151
B	18.88557227	15.25828735	16.13886778
B	18.77426370	15.69587090	14.40566755
B	17.47209536	14.66256886	13.65349406
B	16.88322106	13.62526099	14.92969527
B	17.65230476	13.95353616	16.46347231
B	17.28024222	15.29615288	15.32603744
I	15.70961345	16.77576297	15.80160786
I	19.21676090	17.71450176	13.65435846
I	17.59052600	10.45426201	16.22454810

I	19.47822162	16.69150655	17.69765029
I	16.66540110	13.74958932	18.43341185
I	16.24990748	15.38400121	11.95588960
I	17.33344023	11.46764107	12.21415771
I	20.84916641	12.74000217	17.65987643

Isomer 1 of $B_{24}I_{16}^{2-}$ in the singlet spin state (*M* = 1, **Fig.S4** Isomer **1**)

B	22.16880000	12.78310000	15.81250000
B	21.24920000	12.41200000	14.34250000
B	21.73590000	14.13940000	14.74440000
B	23.34970000	14.07560000	15.54540000
B	23.84580000	12.33140000	15.65610000
B	22.53460000	11.29420000	14.90800000
B	22.42630000	11.72820000	13.17210000
B	21.99890000	13.45520000	13.12140000
B	23.24130000	14.50650000	13.82370000
B	24.41300000	13.35600000	14.38090000
B	24.03810000	11.69420000	13.98860000
B	23.67060000	13.03390000	12.85080000
I	24.65200000	13.23180000	10.87160000
I	20.46580000	14.25060000	11.65770000
I	25.05500000	11.60630000	17.36830000
I	21.83820000	10.29490000	11.61330000
I	25.59160000	10.18760000	13.51540000
I	23.71270000	16.53750000	13.07420000
I	23.96500000	15.53110000	17.09850000
I	22.08950000	9.28080000	15.66850000
B	19.57950000	12.85820000	14.56040000
B	20.06400000	14.58370000	14.96460000
B	19.14380000	14.21710000	13.49610000
B	17.96550000	12.91970000	13.76130000
B	18.07650000	12.48410000	15.48200000
B	19.31730000	13.53580000	16.18400000
B	18.88670000	15.26330000	16.13840000
B	18.77290000	15.70150000	14.40520000
B	17.46360000	14.66150000	13.65620000
B	16.90200000	13.63230000	14.92970000
B	17.64660000	13.95400000	16.45990000
B	17.27140000	15.29350000	15.32640000
I	15.70060000	16.77780000	15.81790000
I	19.21250000	17.71810000	13.65010000
I	17.61170000	10.45030000	16.22710000
I	19.48010000	16.69630000	17.69610000

I	16.67640000	13.74890000	18.44370000
I	16.25040000	15.39070000	11.94830000
I	17.35330000	11.47020000	12.20140000
I	20.84910000	12.74600000	17.65040000

Fig.S4. Isomer **2**

B	20.58050000	13.91500000	13.30560000
B	21.22100000	14.23530000	14.97660000
B	20.71340000	12.54500000	14.53510000
B	21.16260000	12.27900000	12.80780000
B	21.94280000	13.81170000	12.18530000
B	22.01730000	14.99520000	13.53750000
B	23.02270000	14.32870000	14.88840000
B	22.22700000	12.81970000	15.49350000
B	22.15730000	11.59220000	14.18130000
B	22.83570000	12.48260000	12.85500000
B	23.48280000	14.04070000	13.15240000
B	23.61290000	12.68900000	14.36820000
I	25.58370000	11.81720000	14.80510000
I	22.69500000	12.12500000	17.53360000
I	21.91680000	14.32120000	10.04340000
I	24.28810000	15.59480000	16.15900000
I	25.30150000	14.76820000	12.15370000
I	22.38950000	9.41935000	14.45260000
I	20.43640000	10.83860000	11.28500000
I	22.21180000	17.13140000	13.02130000
B	19.08290000	12.87180000	15.07550000
B	19.55160000	14.56760000	15.53240000
B	18.94890000	14.24620000	13.84750000
B	17.66100000	12.98270000	13.96500000
B	17.47860000	12.52570000	15.72700000
B	18.61260000	13.53730000	16.69110000
B	18.20320000	15.28940000	16.49150000
B	18.39890000	15.72010000	14.74310000
B	17.25830000	14.75250000	13.74180000
B	16.52390000	13.74710000	14.94900000
B	16.89480000	14.03070000	16.59730000
B	16.76220000	15.38630000	15.38860000
I	15.10010000	16.81530000	15.56070000
I	18.71260000	17.83520000	14.20310000
I	16.70510000	10.55220000	16.32290000
I	18.44380000	16.75570000	18.10680000
I	15.39020000	13.86210000	18.19150000

I	16.19050000	15.47150000	11.95440000
I	16.83690000	11.56980000	12.46790000
I	19.19740000	12.80650000	18.68770000

Fig.S4. Isomer **3**

B	21.21070000	13.67480000	13.87820000
B	20.77210000	12.44590000	12.64490000
B	21.11480000	14.09710000	12.11770000
B	22.51200000	14.65020000	13.08890000
B	22.94010000	13.34810000	14.24520000
B	21.87890000	11.99680000	13.92190000
B	22.11790000	11.32920000	12.29260000
B	21.64950000	12.64770000	11.13530000
B	22.75340000	14.01720000	11.41220000
B	23.75150000	13.51550000	12.72740000
B	23.50110000	11.91350000	13.28350000
B	23.36980000	12.32680000	11.53510000
I	24.82890000	11.51520000	10.07540000
I	20.73170000	12.17070000	9.18912000
I	23.63570000	13.77510000	16.32210000
I	21.77770000	9.18715000	11.86380000
I	25.04930000	10.53820000	14.09680000
I	23.41890000	15.32830000	9.75743000
I	23.07200000	16.74640000	13.49310000
I	21.13400000	10.69420000	15.64260000
B	19.65930000	12.38430000	16.01100000
B	20.08330000	13.83420000	16.80880000
B	19.97200000	13.89200000	15.07690000
B	18.52010000	12.86250000	14.80760000
B	17.89510000	12.10170000	16.25140000
B	18.95740000	12.73290000	17.57920000
B	18.73900000	14.50600000	17.70390000
B	19.33510000	15.25810000	16.15560000
B	18.31510000	14.50390000	14.97200000
B	17.17740000	13.52790000	15.56650000
B	17.30640000	13.42700000	17.30920000
B	17.55350000	14.96990000	16.43410000
I	16.13670000	16.67550000	16.62780000
I	20.13720000	17.30400000	16.16380000
I	17.04680000	10.04630000	16.23240000
I	18.95480000	15.52670000	19.64260000
I	15.64560000	13.09750000	18.73200000
I	19.52800000	15.47470000	11.46360000

I	18.65910000	11.72320000	12.73240000
I	19.51110000	11.47790000	19.30620000

Fig.S4. Isomer **4**

B	22.69570000	13.93410000	15.64180000
B	22.24850000	12.55400000	14.71500000
B	21.51830000	14.16740000	14.33950000
B	22.89840000	15.31150000	14.57950000
B	24.32670000	14.36570000	15.14360000
B	23.90640000	12.64120000	15.24280000
B	23.48880000	12.06820000	13.57840000
B	22.05900000	13.04770000	13.07700000
B	22.45900000	14.73820000	12.93520000
B	24.09350000	14.74610000	13.48650000
B	24.81330000	13.21290000	13.82560000
B	23.63690000	13.45240000	12.46220000
I	24.21160000	13.17110000	10.32680000
I	20.05070000	12.22710000	11.98660000
I	25.84270000	15.24320000	16.52380000
I	23.69990000	9.94380000	12.94140000
I	26.95140000	12.68060000	13.44550000
I	21.49190000	16.08490000	11.43930000
I	22.81580000	17.46380000	15.12420000
I	24.68500000	11.25980000	16.80580000
B	18.37290000	14.63960000	13.94040000
B	18.85660000	13.01470000	13.75100000
B	19.85990000	14.14910000	14.71330000
B	18.66000000	15.33360000	15.47510000
B	16.98040000	14.87310000	14.91060000
B	17.12340000	13.43640000	13.80750000
B	17.72850000	12.04680000	14.76700000
B	19.35260000	12.52660000	15.33330000
B	19.30710000	13.92680000	16.36000000
B	17.62650000	14.32150000	16.39950000
B	16.59110000	13.21330000	15.51190000
B	18.02130000	12.65980000	16.43910000
I	17.87200000	11.38710000	18.24120000
I	20.94220000	10.95000000	15.58740000
I	15.40950000	16.40790000	14.57470000
I	17.26730000	9.93816000	14.31050000
I	14.52790000	12.63970000	16.09610000
I	21.25000000	14.17600000	17.70190000
I	18.99520000	17.43740000	16.06250000

I	15.87190000	13.15380000	12.00640000

Fig.S4. Isomer **5**

B	24.82160000	11.98800000	14.01880000
B	25.80180000	12.76120000	12.98450000
B	24.51730000	11.98150000	12.43620000
B	23.18360000	12.07620000	13.49240000
B	23.78710000	13.09600000	14.84070000
B	25.51000000	13.49470000	14.51340000
B	25.56270000	14.47270000	12.96660000
B	24.95480000	13.44140000	11.63700000
B	23.21380000	12.98760000	11.94260000
B	22.63440000	13.80710000	13.61290000
B	24.19950000	14.70930000	14.14130000
B	23.80140000	14.63730000	12.37920000
I	23.19170000	16.37960000	11.21790000
I	25.88540000	13.53130000	9.63280000
I	23.00820000	12.78870000	16.91270000
I	27.19960000	15.88900000	12.60040000
I	24.37340000	16.62760000	15.16570000
I	22.25940000	12.21980000	10.10710000
I	21.60580000	10.49980000	13.72790000
I	26.98680000	13.64110000	16.15190000
B	20.87390000	13.13000000	15.97580000
B	20.94580000	13.91170000	14.35970000
B	20.29490000	12.26750000	14.59080000
B	19.53580000	12.00180000	16.13760000
B	19.53070000	13.57870000	16.96900000
B	20.34680000	14.81090000	15.92140000
B	19.41870000	14.96040000	14.39140000
B	19.37780000	13.37300000	13.54770000
B	18.57280000	12.16030000	14.63340000
B	18.19600000	13.03370000	16.05040000
B	18.57030000	14.71040000	15.97900000
B	17.98940000	13.84730000	14.54690000
I	15.97420000	14.28740000	13.71320000
I	18.98710000	13.31310000	11.37700000
I	19.67050000	13.63580000	19.21380000
I	19.29750000	16.87630000	13.31490000
I	17.28930000	16.24530000	16.95040000
I	17.46750000	10.38850000	13.79560000
I	19.72450000	10.03500000	17.26380000
I	21.19760000	16.54140000	17.00730000

Fig.S4. Isomer **6**

B	22.24820000	14.66590000	14.36070000
B	21.10810000	13.33400000	13.87310000
B	21.50320000	14.70260000	12.76140000
B	23.15550000	15.33420000	12.98450000
B	23.94970000	14.27420000	14.18910000
B	22.75560000	13.01050000	14.72840000
B	22.30520000	12.01780000	13.30690000
B	21.53860000	13.06150000	12.06770000
B	22.73630000	14.33220000	11.56390000
B	24.18210000	14.03250000	12.48520000
B	24.01420000	12.62500000	13.51220000
B	23.27800000	12.65940000	11.90090000
I	24.11020000	11.41120000	10.28060000
I	20.28970000	12.22460000	10.47320000
I	25.49270000	15.12540000	15.53190000
I	21.84120000	9.88524000	13.48860000
I	25.74950000	11.32630000	13.93110000
I	22.72530000	15.25380000	9.54982000
I	23.63300000	17.49520000	12.80730000
I	23.05960000	12.16810000	16.72310000
B	17.30180000	13.80150000	16.53030000
B	16.69920000	15.24820000	16.03960000
B	18.22850000	15.10160000	16.86620000
B	18.98410000	13.56120000	16.46830000
B	17.91840000	12.71730000	15.28180000
B	16.43900000	13.81650000	15.07460000
B	16.96250000	15.34540000	14.32240000
B	18.07140000	16.16000000	15.49470000
B	19.48290000	15.07440000	15.71840000
B	19.45970000	13.58730000	14.65430000
B	17.71580000	13.73970000	13.82650000
B	18.72000000	15.18080000	14.13160000
I	19.78260000	16.11120000	12.39300000
I	18.29800000	18.38230000	15.62750000
I	17.68320000	10.53370000	15.26200000
I	15.77480000	16.58720000	12.91620000
I	16.98370000	12.95040000	11.90860000
I	21.53820000	16.00020000	16.00440000
I	19.69220000	12.47430000	18.29650000
I	14.38020000	12.99110000	14.89430000

Fig.S4. Isomer **7**

B	25.57970000	12.70300000	13.34220000
B	25.49590000	13.90850000	12.07220000
B	24.46910000	12.66300000	12.11720000
B	23.97280000	12.17270000	13.71060000
B	24.79810000	13.31100000	14.80550000
B	25.86450000	14.36420000	13.70810000
B	24.74800000	15.35780000	12.64450000
B	23.87540000	14.19840000	11.60200000
B	22.92240000	13.13080000	12.65360000
B	22.98340000	13.61940000	14.40720000
B	24.30350000	14.98120000	14.37750000
B	23.10320000	14.84310000	13.05920000
I	21.29280000	16.23290000	12.95060000
I	23.19610000	14.64810000	9.50376000
I	25.47880000	12.73370000	16.81350000
I	25.18210000	17.41150000	11.92940000
I	24.59340000	16.63910000	15.78290000
I	20.91600000	12.32320000	11.97640000
I	23.91120000	9.95694000	13.97240000
I	27.88490000	15.07550000	14.26870000
B	21.30030000	13.63260000	15.13550000
B	20.20980000	14.82400000	14.30310000
B	20.07640000	13.11080000	13.89790000
B	20.14600000	12.17760000	15.39220000
B	20.33770000	13.35600000	16.70980000
B	20.36000000	15.00970000	16.05930000
B	18.77010000	15.31380000	15.20930000
B	18.61510000	14.14500000	13.84830000
B	18.56940000	12.49600000	14.54960000
B	18.75050000	12.71160000	16.26390000
B	18.82250000	14.36610000	16.72930000
B	17.75550000	13.84810000	15.37730000
I	15.55250000	13.92170000	15.52410000
I	17.64150000	14.67150000	11.94050000
I	21.32010000	12.81690000	18.60550000
I	17.91940000	17.33560000	15.00980000
I	17.90890000	15.06090000	18.61790000
I	17.44120000	10.88420000	13.52310000
I	20.60200000	10.04960000	15.75660000
I	21.16890000	16.71760000	17.16820000

Fig.S4. Isomer **8**

B	22.37940000	14.09160000	15.04940000
B	22.12310000	12.82180000	13.87720000
B	21.92700000	14.49360000	13.41130000
B	23.12090000	15.46840000	14.24340000
B	24.09380000	14.33950000	15.24250000
B	23.46820000	12.67340000	15.03500000
B	23.66980000	12.21540000	13.28640000
B	22.68220000	13.35340000	12.27150000
B	23.32600000	15.00830000	12.51820000
B	24.58080000	14.81030000	13.66620000
B	24.90970000	13.18620000	14.13470000
B	24.43060000	13.59920000	12.44810000
I	25.83670000	13.32650000	10.74700000
I	21.67780000	12.69990000	10.40460000
I	24.95820000	15.00040000	17.20290000
I	23.89700000	10.09240000	12.69680000
I	26.93030000	12.38370000	14.59530000
I	23.16590000	16.54630000	10.88730000
I	22.76570000	17.59750000	14.86830000
I	23.49470000	11.16090000	16.64910000
B	16.03120000	13.11530000	14.77070000
B	17.33300000	13.05900000	13.75180000
B	16.75680000	14.47900000	14.38510000
B	16.03950000	14.37760000	15.97680000
B	16.28240000	12.65440000	16.42960000
B	17.10940000	11.80400000	14.95930000
B	18.68110000	12.59820000	14.75280000
B	18.43780000	14.28620000	14.29910000
B	17.63010000	15.15450000	15.73890000
B	17.38230000	13.91980000	16.97140000
B	18.03000000	12.37150000	16.45420000
B	18.83110000	13.88970000	16.02440000
I	20.87020000	14.39980000	16.84560000
I	19.80990000	15.41610000	12.91100000
I	14.81540000	11.53770000	17.65230000
I	20.41810000	11.34580000	14.01750000
I	18.94500000	10.89590000	17.81220000
I	17.97130000	17.31440000	16.07880000
I	14.19990000	15.52330000	16.52580000
I	16.78530000	9.67306000	14.46300000

Fig.S4. Isomer **9**

B	22.31190000	14.53470000	14.51750000

B	22.01440000	12.81490000	14.55840000
B	21.66650000	13.72900000	13.11050000
B	22.87580000	14.98890000	12.92240000
B	24.01070000	14.82220000	14.30400000
B	23.47050000	13.46960000	15.35140000
B	23.53330000	11.94380000	14.36680000
B	22.38770000	12.10500000	12.96600000
B	22.94350000	13.47860000	11.95570000
B	24.31260000	14.09000000	12.78610000
B	24.78610000	13.20990000	14.18980000
B	24.12620000	12.37860000	12.73570000
I	25.38340000	11.00090000	11.52570000
I	21.29130000	10.36630000	12.14920000
I	25.01000000	16.62740000	15.19410000
I	23.82980000	9.98511000	15.35280000
I	26.88900000	12.89930000	14.84210000
I	22.54370000	13.51110000	9.74735000
I	22.41880000	16.98890000	11.98260000
I	23.73680000	13.45410000	17.54820000
B	16.25770000	15.37110000	15.70110000
B	17.61160000	15.79360000	14.85940000
B	17.58160000	15.70920000	16.51470000
B	16.49790000	14.51870000	17.20030000
B	15.82150000	13.68520000	15.75590000
B	16.53760000	14.55130000	14.23050000
B	18.29820000	14.30020000	14.28610000
B	18.95910000	15.11050000	15.72310000
B	18.26230000	14.27700000	17.24520000
B	17.18210000	13.02000000	16.65150000
B	17.18430000	12.96050000	14.89070000
B	18.64970000	13.33860000	15.79920000
I	20.38260000	11.88020000	15.82900000
I	21.01140000	16.04580000	15.79650000
I	13.74530000	12.92740000	15.69940000
I	19.44700000	14.06380000	12.36730000
I	16.96150000	11.10100000	13.73090000
I	19.41440000	14.23790000	19.13530000
I	15.28430000	14.93520000	19.03070000
I	15.41170000	14.74140000	12.34140000

Fig.S4. Isomer **10**

B	23.44210000	13.65060000	14.51110000
B	22.26490000	12.80120000	13.61360000

B	22.38260000	14.54820000	13.50890000
B	24.09120000	15.01580000	13.72790000
B	25.04330000	13.47110000	13.96260000
B	23.87730000	12.08460000	13.90000000
B	23.10860000	12.02160000	12.25500000
B	22.14810000	13.57930000	12.01430000
B	23.31090000	14.96520000	12.07690000
B	24.82870000	14.19710000	12.43110000
B	24.84650000	12.45800000	12.46470000
B	23.78860000	13.39080000	11.32390000
I	24.16810000	13.30160000	9.16027000
I	20.30980000	13.63680000	10.82350000
I	26.88710000	13.44850000	15.19830000
I	22.45450000	10.13520000	11.33660000
I	26.50080000	11.19290000	11.72950000
I	23.05250000	16.80360000	10.87620000
I	24.69060000	16.93740000	14.69090000
I	24.10720000	10.27780000	15.16670000
B	17.24210000	12.77750000	14.17520000
B	18.07060000	13.97200000	13.38570000
B	16.45460000	14.07930000	13.72010000
B	15.91880000	13.30000000	15.18270000
B	17.43150000	12.71960000	15.91800000
B	18.78650000	13.16410000	14.74290000
B	18.87290000	14.90540000	14.61450000
B	17.37490000	15.51140000	13.86160000
B	15.98580000	15.08660000	15.06190000
B	16.70350000	14.23030000	16.42130000
B	18.43700000	14.14160000	16.24160000
B	17.56070000	15.58530000	15.70390000
I	17.89530000	17.55580000	16.64920000
I	17.27340000	17.28060000	12.54790000
I	17.60680000	10.80370000	17.04500000
I	20.80690000	16.04510000	14.36080000
I	19.89800000	14.18370000	17.89740000
I	14.15820000	16.33870000	15.11180000
I	13.99520000	12.15410000	15.30110000
I	20.55650000	11.72610000	14.67350000

Fig.S4. Isomer **11**

B	25.01780000	12.76130000	14.19130000
B	25.00170000	14.02120000	13.12760000
B	24.54510000	12.49720000	12.69520000

B	23.76030000	11.59890000	13.94810000
B	23.71750000	12.76970000	15.33510000
B	24.55360000	14.31890000	14.77750000
B	23.60750000	15.02730000	13.39080000
B	23.68140000	13.83140000	12.01790000
B	22.83450000	12.27610000	12.54070000
B	22.28220000	12.53910000	14.24900000
B	22.75930000	14.19990000	14.76380000
B	22.22390000	13.90030000	13.06920000
I	20.32060000	14.68840000	12.21710000
I	23.72640000	14.44830000	9.90020000
I	23.80300000	12.10670000	17.41820000
I	23.51240000	17.19000000	13.03850000
I	21.59360000	15.39960000	16.23610000
I	21.80740000	10.99120000	11.09890000
I	23.99410000	9.41857000	14.25930000
I	25.71110000	15.55920000	16.18790000
B	19.19950000	14.88850000	15.70920000
B	18.20460000	15.97520000	14.93840000
B	18.69670000	14.60880000	14.12700000
B	18.72030000	13.30820000	15.24520000
B	18.28030000	13.89590000	16.83300000
B	17.94630000	15.66050000	16.62240000
B	16.56950000	15.81960000	15.48600000
B	17.07680000	15.17730000	13.89160000
B	17.40730000	13.41090000	14.09400000
B	17.16880000	13.06370000	15.78280000
B	16.59740000	14.44650000	16.68040000
B	16.05780000	14.14640000	14.98460000
I	13.95240000	13.66310000	14.50350000
I	16.42060000	16.01940000	11.93000000
I	19.10070000	13.01840000	18.72170000
I	15.13940000	17.50120000	15.64420000
I	15.18740000	14.35210000	18.38350000
I	17.10480000	11.91100000	12.46060000
I	20.41820000	11.54470000	15.01400000
I	18.42940000	17.13410000	18.22890000

Fig.S4. Isomer **12**

B	23.77330000	12.83500000	14.70710000
B	23.78740000	11.61820000	13.65350000
B	22.34400000	12.50510000	13.84780000
B	22.84230000	14.16580000	14.14940000

B	24.64110000	14.22670000	14.14620000
B	25.23280000	12.55640000	13.83610000
B	24.67860000	12.02090000	12.21200000
B	22.85150000	11.97000000	12.22750000
B	22.26510000	13.66650000	12.52790000
B	23.70630000	14.64490000	12.72960000
B	25.19530000	13.74490000	12.49610000
B	23.71920000	13.38270000	11.51960000
I	23.63830000	13.83450000	9.36949000
I	21.72440000	10.49660000	11.04310000
I	25.69500000	15.71830000	15.40350000
I	25.84930000	10.62840000	10.97270000
I	26.98760000	14.63710000	11.58440000
I	20.36510000	14.44240000	11.61980000
I	21.74020000	15.63690000	15.49860000
I	27.08690000	11.78190000	14.78510000
B	18.35020000	15.98280000	14.35080000
B	18.81830000	14.56460000	13.65310000
B	19.44020000	15.02210000	15.17450000
B	18.20120000	15.87590000	16.07000000
B	16.75570000	15.91550000	15.01270000
B	17.16830000	15.09260000	13.46700000
B	17.52910000	13.37000000	13.81580000
B	18.96810000	13.37770000	14.89980000
B	18.56970000	14.17340000	16.46630000
B	16.90890000	14.71290000	16.28470000
B	16.22350000	14.22880000	14.72690000
B	17.35950000	13.16290000	15.60730000
I	16.74670000	11.21850000	16.46160000
I	20.44450000	11.60300000	14.84490000
I	15.31950000	17.61230000	15.11450000
I	17.12780000	11.73670000	12.38910000
I	14.09250000	13.69810000	14.49960000
I	19.46730000	13.56230000	18.40260000
I	18.72490000	17.53780000	17.48170000
I	16.36290000	15.73640000	11.48880000

Fig.S4. Isomer **13**

B	24.98760000	12.29970000	14.56860000
B	25.70410000	12.90870000	13.26260000
B	24.65680000	11.68900000	13.12860000
B	23.38100000	11.72920000	14.29310000
B	23.71590000	13.27990000	15.22020000

B	25.27090000	13.99790000	14.54010000
B	25.01890000	14.42410000	12.77810000
B	24.66620000	12.87300000	11.87480000
B	23.10230000	12.14440000	12.52490000
B	22.53520000	13.24340000	13.85220000
B	23.67920000	14.63860000	14.00390000
B	23.30700000	13.94570000	12.36260000
I	22.16540000	15.06280000	10.87530000
I	25.38130000	12.48620000	9.82388000
I	23.17600000	13.49600000	17.32200000
I	26.09300000	16.08220000	11.83350000
I	23.01950000	16.62420000	14.60070000
I	21.80290000	10.92280000	11.25220000
I	22.55870000	9.92107000	15.23990000
I	26.74630000	15.02120000	15.81930000
B	17.00540000	14.48330000	17.82530000
B	16.99080000	15.98030000	17.20290000
B	18.28920000	14.99450000	17.01940000
B	17.91330000	13.31080000	16.91690000
B	16.11100000	13.26630000	16.91570000
B	15.53630000	15.01410000	17.13750000
B	16.06560000	16.00880000	15.72370000
B	17.87980000	16.01880000	15.69400000
B	18.39690000	14.24770000	15.49670000
B	17.04110000	13.28990000	15.41590000
B	15.56190000	14.22370000	15.49540000
B	16.99270000	14.85700000	14.62800000
I	16.97340000	15.13900000	12.43670000
I	19.03390000	17.75760000	14.99820000
I	14.99380000	11.56550000	17.76470000
I	14.87200000	17.68480000	14.96010000
I	13.68610000	13.71640000	14.46460000
I	20.24660000	13.27510000	14.13040000
I	19.11560000	11.70040000	17.86780000
I	13.70670000	15.45900000	18.30030000

Fig.S4. Isomer **14**

B	22.45360000	13.88210000	14.42600000
B	23.17210000	12.65040000	13.53690000
B	22.06790000	13.64770000	12.76820000
B	22.31670000	15.23850000	13.37290000
B	23.60730000	15.20290000	14.59330000
B	24.13790000	13.49040000	14.70480000

B	24.80480000	13.00310000	13.10250000
B	23.47550000	13.09380000	11.89060000
B	22.94260000	14.80330000	11.76680000
B	23.90590000	15.66220000	12.93830000
B	25.08860000	14.66210000	13.74160000
B	24.67940000	14.41530000	11.99280000
I	26.15460000	14.83230000	10.40170000
I	23.27140000	11.66870000	10.18690000
I	23.66000000	16.64950000	16.28880000
I	26.40560000	11.48460000	12.94180000
I	27.08130000	15.39000000	14.35780000
I	22.17220000	15.74960000	9.90644000
I	20.52980000	16.80370000	13.56730000
I	24.79530000	12.58110000	16.63230000
B	18.01950000	15.50940000	15.70850000
B	17.17280000	16.11920000	14.48110000
B	18.72470000	15.48660000	14.15900000
B	18.90970000	14.11360000	15.25210000
B	17.41770000	13.97650000	16.24980000
B	16.30950000	15.29860000	15.73950000
B	15.86370000	15.06930000	14.01270000
B	17.38740000	15.20580000	13.01390000
B	18.48970000	13.85960000	13.53390000
B	17.65240000	13.00880000	14.81560000
B	16.04360000	13.63770000	15.12540000
B	16.72390000	13.58650000	13.45340000
I	15.92650000	12.19910000	11.94610000
I	17.36840000	16.02740000	10.97250000
I	17.54170000	13.16310000	18.30780000
I	13.91770000	15.69950000	13.20150000
I	14.36500000	12.34910000	15.72420000
I	19.85800000	12.82560000	12.06730000
I	20.87500000	13.43220000	16.18950000
I	14.98370000	16.33230000	17.19260000

Fig.S4. Isomer **15**

B	23.75190000	13.47990000	14.74280000
B	23.87280000	12.40730000	13.54710000
B	22.34810000	13.10530000	13.85780000
B	22.68040000	14.76470000	14.35530000
B	24.46330000	15.01120000	14.35170000
B	25.21680000	13.46130000	13.83610000
B	24.69290000	13.07070000	12.16150000

B	22.88160000	12.83070000	12.17930000
B	22.13730000	14.40540000	12.69230000
B	23.46960000	15.49880000	13.00150000
B	25.03800000	14.79220000	12.65150000
B	23.58940000	14.40170000	11.64620000
I	23.41200000	15.10720000	9.57023000
I	21.88260000	11.41510000	10.82250000
I	25.37910000	16.44080000	15.77730000
I	25.97020000	11.95040000	10.76160000
I	26.71310000	15.96990000	11.84910000
I	20.15020000	15.09700000	11.87340000
I	21.44780000	15.95460000	15.86280000
I	27.15600000	12.77380000	14.67540000
B	19.20890000	15.17710000	15.41070000
B	18.06510000	16.14870000	14.65520000
B	18.67070000	14.83110000	13.81640000
B	18.86080000	13.55340000	14.95200000
B	18.38540000	14.12880000	16.56330000
B	17.88980000	15.84260000	16.35220000
B	16.46530000	15.88390000	15.24790000
B	16.98280000	15.25480000	13.64140000
B	17.47310000	13.53940000	13.84100000
B	17.30260000	13.21520000	15.54570000
B	16.64840000	14.55550000	16.45070000
B	16.08260000	14.19160000	14.76700000
I	14.02580000	13.48420000	14.37860000
I	16.19600000	16.03730000	11.70650000
I	19.29850000	13.30420000	18.42150000
I	14.92160000	17.45840000	15.42450000
I	15.30710000	14.30200000	18.18840000
I	17.23080000	11.96960000	12.28240000
I	20.57230000	11.91240000	14.73180000
I	18.26700000	17.38110000	17.92150000

Fig.S4. Isomer **16**

B	24.75100000	12.10470000	14.37580000
B	25.52090000	12.80090000	13.16610000
B	24.27340000	11.85030000	12.87800000
B	23.07380000	11.84450000	14.10760000
B	23.70050000	13.10990000	15.28970000
B	25.32940000	13.68690000	14.62930000
B	25.09650000	14.46190000	13.01760000
B	24.45730000	13.21770000	11.87980000

B	22.79890000	12.62870000	12.46580000
B	22.28920000	13.52310000	14.07360000
B	23.83460000	14.66360000	14.35160000
B	23.29020000	14.37110000	12.63960000
I	22.64280000	15.98120000	11.30300000
I	25.12480000	13.11510000	9.76943000
I	23.73940000	12.81690000	17.47070000
I	26.47860000	16.02330000	12.31170000
I	23.90190000	16.65630000	15.25990000
I	21.62590000	11.69770000	10.85460000
I	22.48010000	9.76598000	14.64320000
I	27.07420000	14.17220000	15.90670000
B	18.52880000	15.57260000	15.78260000
B	17.28000000	14.62500000	15.49420000
B	18.04870000	15.32430000	14.28480000
B	19.72630000	15.58200000	14.55030000
B	20.00310000	14.79140000	16.18900000
B	18.34820000	14.20010000	16.77500000
B	17.70240000	12.96290000	15.63400000
B	17.46520000	13.74530000	14.02720000
B	19.09710000	14.32190000	13.36480000
B	20.50900000	13.90130000	14.57710000
B	19.51120000	13.04890000	16.00560000
B	18.96170000	12.76560000	14.29510000
I	18.88710000	10.77680000	13.37900000
I	15.71380000	13.27890000	12.75230000
I	21.17560000	15.72370000	17.80080000
I	16.31800000	11.40190000	16.33520000
I	20.15610000	11.43180000	17.33580000
I	19.05680000	14.61760000	11.18520000
I	20.31640000	17.66010000	14.00900000
I	17.68690000	14.28590000	18.88780000

Fig.S4. Isomer **17**

B	25.12230000	11.92380000	14.28990000
B	25.75810000	12.61290000	12.97710000
B	24.58830000	11.50780000	12.84190000
B	23.44660000	11.53130000	14.13960000
B	24.02510000	12.92850000	15.17560000
B	25.56160000	13.58490000	14.39990000
B	25.16490000	14.22400000	12.73160000
B	24.58140000	12.81770000	11.72150000
B	23.03080000	12.15520000	12.46410000

B	22.71480000	13.14800000	13.94800000
B	23.98690000	14.41220000	14.11740000
B	23.38230000	13.93810000	12.46340000
I	22.19710000	15.29450000	11.23780000
I	25.03900000	12.61090000	9.57359000
I	23.73120000	12.93720000	17.33730000
I	26.27870000	15.88850000	11.84500000
I	23.59020000	16.37080000	14.97560000
I	21.50220000	11.18690000	11.23020000
I	22.54020000	9.70886000	14.99380000
I	27.24770000	14.34290000	15.60160000
B	16.02220000	15.76850000	16.60800000
B	17.32800000	16.71800000	16.59310000
B	17.24710000	15.41560000	17.57030000
B	16.35020000	14.07840000	16.92370000
B	15.89180000	14.65700000	15.26700000
B	16.51220000	16.40800000	15.09620000
B	18.33370000	16.37430000	15.20360000
B	18.78080000	15.77820000	16.87970000
B	18.14760000	14.03840000	17.06250000
B	17.34340000	13.69080000	15.54950000
B	17.41550000	15.00650000	14.39810000
B	18.73470000	14.61980000	15.50480000
I	20.46190000	13.22890000	14.56580000
I	20.50030000	16.53130000	18.02810000
I	14.01350000	14.01060000	14.30090000
I	19.57390000	17.80300000	14.10960000
I	17.51770000	14.72940000	12.21270000
I	19.14870000	12.58850000	18.40240000
I	15.00360000	12.79580000	18.15440000
I	15.40040000	17.93530000	13.95280000

Fig.S4. Isomer **18**

B	24.91330000	12.11020000	14.21690000
B	25.76850000	12.84090000	13.05510000
B	24.59010000	11.79770000	12.68570000
B	23.26610000	11.79030000	13.80210000
B	23.73890000	13.10850000	15.00320000
B	25.39970000	13.74020000	14.49300000
B	25.27550000	14.48840000	12.83190000
B	24.78990000	13.16930000	11.66150000
B	23.12780000	12.53230000	12.13030000
B	22.63350000	13.44400000	13.62070000

B	23.91560000	14.65150000	14.04230000
B	23.54200000	14.29630000	12.29850000
I	22.61200000	15.78320000	10.98750000
I	25.54240000	13.07390000	9.58888000
I	23.15440000	13.00290000	17.09330000
I	26.56540000	16.14920000	12.21660000
I	23.45200000	16.57980000	14.94950000
I	21.75930000	11.72040000	10.62310000
I	22.16630000	9.98580000	14.39930000
I	26.91690000	14.34920000	15.97010000
B	16.28860000	15.50680000	15.03710000
B	17.29090000	14.44380000	14.22130000
B	17.86170000	15.61820000	15.26090000
B	16.84830000	16.00980000	16.61490000
B	15.47360000	14.86520000	16.41060000
B	15.75230000	13.88050000	14.84110000
B	17.25590000	12.91070000	15.07700000
B	18.58030000	14.09750000	15.25590000
B	18.38280000	15.07070000	16.81970000
B	16.84630000	14.51050000	17.45230000
B	16.14940000	13.20830000	16.49950000
B	17.93100000	13.32140000	16.74750000
I	19.02090000	11.82120000	17.91910000
I	20.35040000	13.95080000	13.66320000
I	13.42730000	15.39860000	17.07190000
I	17.52040000	10.93840000	14.15170000
I	14.96990000	11.56430000	17.36610000
I	20.07360000	15.87160000	17.97650000
I	16.60000000	18.09060000	17.38940000
I	14.05640000	13.25140000	13.57940000

Fig.S4. Isomer **19**

B	23.75790000	15.05640000	14.27700000
B	22.44740000	14.00380000	14.04970000
B	23.23340000	14.80570000	12.77950000
B	24.90750000	15.14700000	12.99500000
B	25.28090000	14.33170000	14.60350000
B	23.70540000	13.62710000	15.27250000
B	23.08080000	12.34720000	14.10330000
B	22.72280000	13.16570000	12.48910000
B	24.30020000	13.86860000	11.81450000
B	25.44140000	13.52240000	13.07530000
B	24.85960000	12.56970000	14.41220000

B	24.26230000	12.28940000	12.72130000
I	24.77030000	10.44500000	11.64360000
I	21.11730000	12.54530000	11.15020000
I	26.91120000	15.06710000	15.88800000
I	21.95710000	10.61350000	14.78920000
I	26.10350000	11.06640000	15.41840000
I	24.71160000	14.03300000	9.65909000
I	25.98590000	16.96190000	12.31130000
I	23.32640000	13.57980000	17.42330000
B	16.19940000	15.64260000	17.14680000
B	15.74340000	16.23370000	15.71020000
B	17.32600000	15.98910000	16.06700000
B	17.65210000	14.66590000	17.11750000
B	16.02860000	13.90320000	17.33690000
B	14.80490000	14.95550000	16.43370000
B	15.19030000	14.94500000	14.66480000
B	16.82500000	15.68220000	14.44550000
B	18.02220000	14.60110000	15.37720000
B	17.15820000	13.36850000	16.08730000
B	15.45230000	13.42160000	15.69860000
B	16.68750000	13.88000000	14.48020000
I	17.00090000	12.68930000	12.65900000
I	17.36780000	16.91230000	12.69640000
I	15.50820000	12.82400000	19.18400000
I	13.63110000	15.08630000	13.13060000
I	14.18640000	11.64660000	15.44620000
I	20.39920000	14.95710000	14.65200000
I	19.17280000	14.72010000	18.73430000
I	12.75030000	15.20010000	17.21760000

Fig.S4. Isomer **20**

B	24.82540000	12.12270000	14.37530000
B	25.68910000	12.79170000	13.18440000
B	24.37290000	11.91260000	12.85820000
B	23.12920000	12.00780000	14.05640000
B	23.82370000	13.22040000	15.25930000
B	25.51400000	13.67170000	14.66840000
B	25.38070000	14.49210000	13.03960000
B	24.67940000	13.28160000	11.86270000
B	22.97400000	12.82400000	12.40800000
B	22.67810000	13.72300000	13.95010000
B	24.12400000	14.75970000	14.33460000
B	23.60970000	14.51960000	12.60400000

I	22.79780000	16.15790000	11.40280000
I	25.29450000	13.17090000	9.74862000
I	23.33250000	13.13190000	17.38040000
I	26.82120000	16.01470000	12.39870000
I	23.96510000	16.70400000	15.32650000
I	21.43180000	12.24340000	10.98330000
I	21.93260000	10.27410000	14.65530000
I	27.17550000	14.05010000	16.06770000
B	16.05200000	15.32800000	14.78220000
B	17.64400000	15.66420000	15.13580000
B	16.47360000	15.52280000	16.31190000
B	15.19560000	14.41170000	15.97030000
B	15.67200000	13.66980000	14.40070000
B	17.23390000	14.52340000	13.84770000
B	18.46930000	14.18420000	15.09450000
B	18.01480000	14.88560000	16.67930000
B	16.44520000	14.02790000	17.20910000
B	16.06010000	12.91000000	15.92510000
B	17.26860000	12.88670000	14.65130000
B	17.74620000	13.11070000	16.37890000
I	18.91730000	11.60370000	17.45960000
I	19.40640000	15.72760000	18.17100000
I	14.17360000	12.98880000	12.92020000
I	20.65480000	14.78090000	14.42550000
I	17.82410000	11.09690000	13.51420000
I	15.94710000	13.81310000	19.35480000
I	13.05130000	14.77930000	16.51500000
I	17.62910000	14.89630000	11.70980000