

Supplementary Information. The file contains

- Computational methods;
- Shapes of selected molecular orbitals and Cartesian coordinates of molecules **1**, **2a**, **2b** and **2c**

Computational Methods. All electronic structure calculations are carried out by using Gaussian09 package.¹ The optimization of geometries and calculations of harmonic vibrational frequencies are performed using the B3LYP functional^{2,3,4} in conjugation with 6-31G(d) basis set.⁵ Calculations of the nucleus independent chemical shift (NICS) are carried out at the B3LYP/6-31G(d) level of theory.

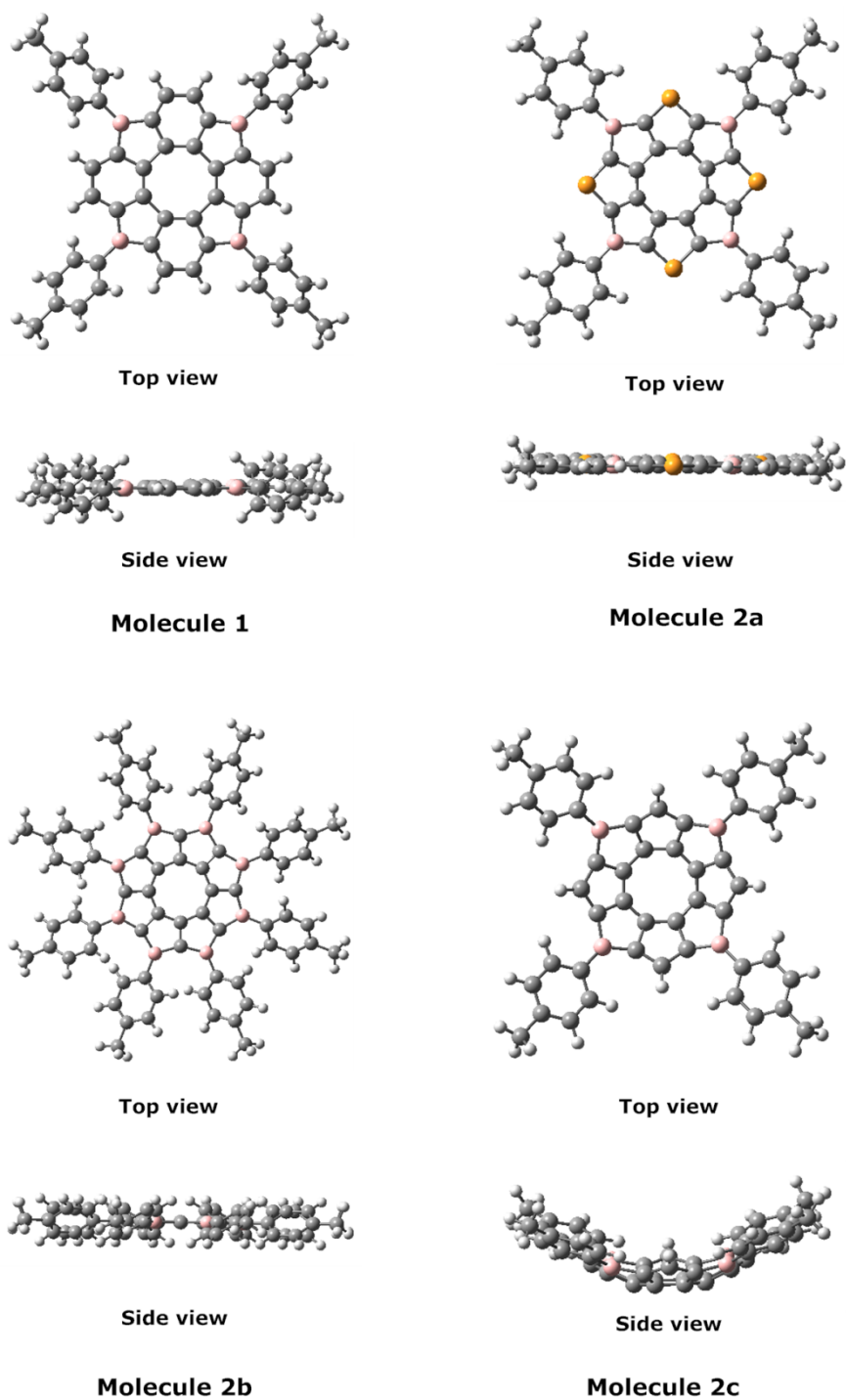


Figure S1. Shapes of molecules 1 and 2a-2c obtained at the B3LYP/6-31G* level of theory

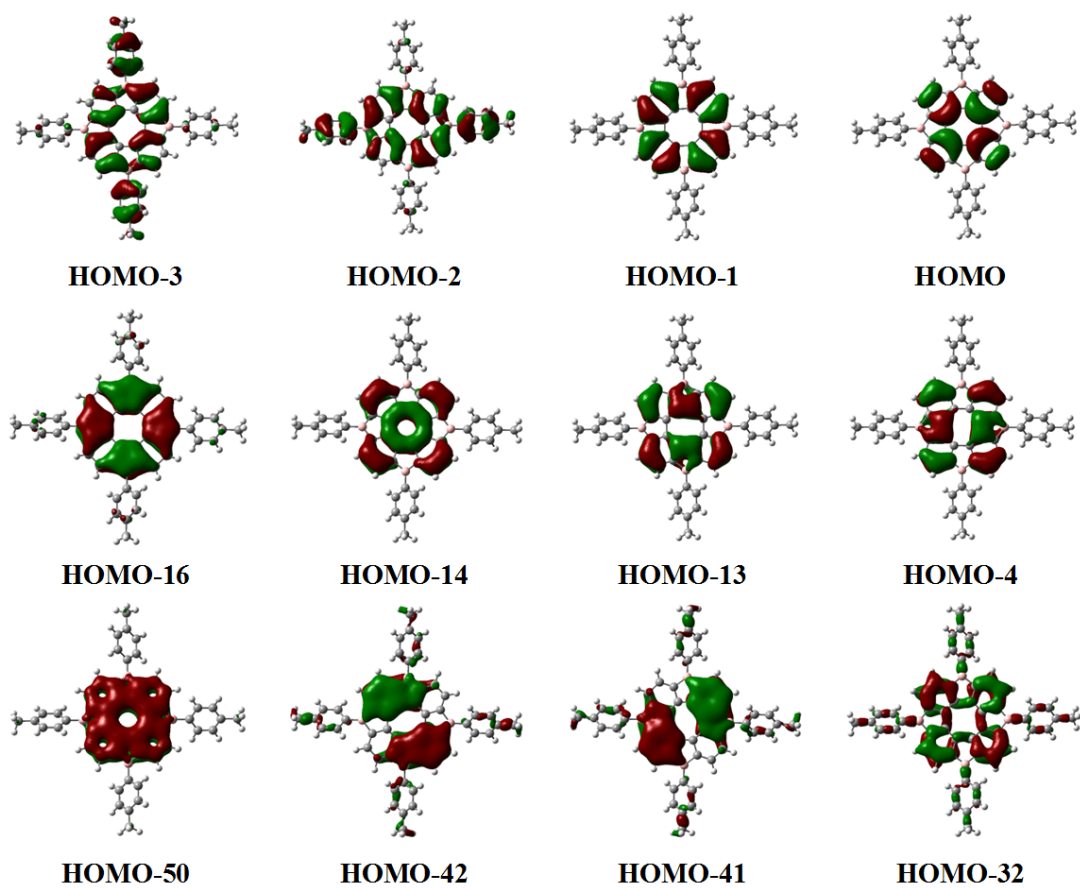


Figure S2. Shapes of π molecular orbitals of compound **1** obtained at the B3LYP/6-31G(d) level of theory

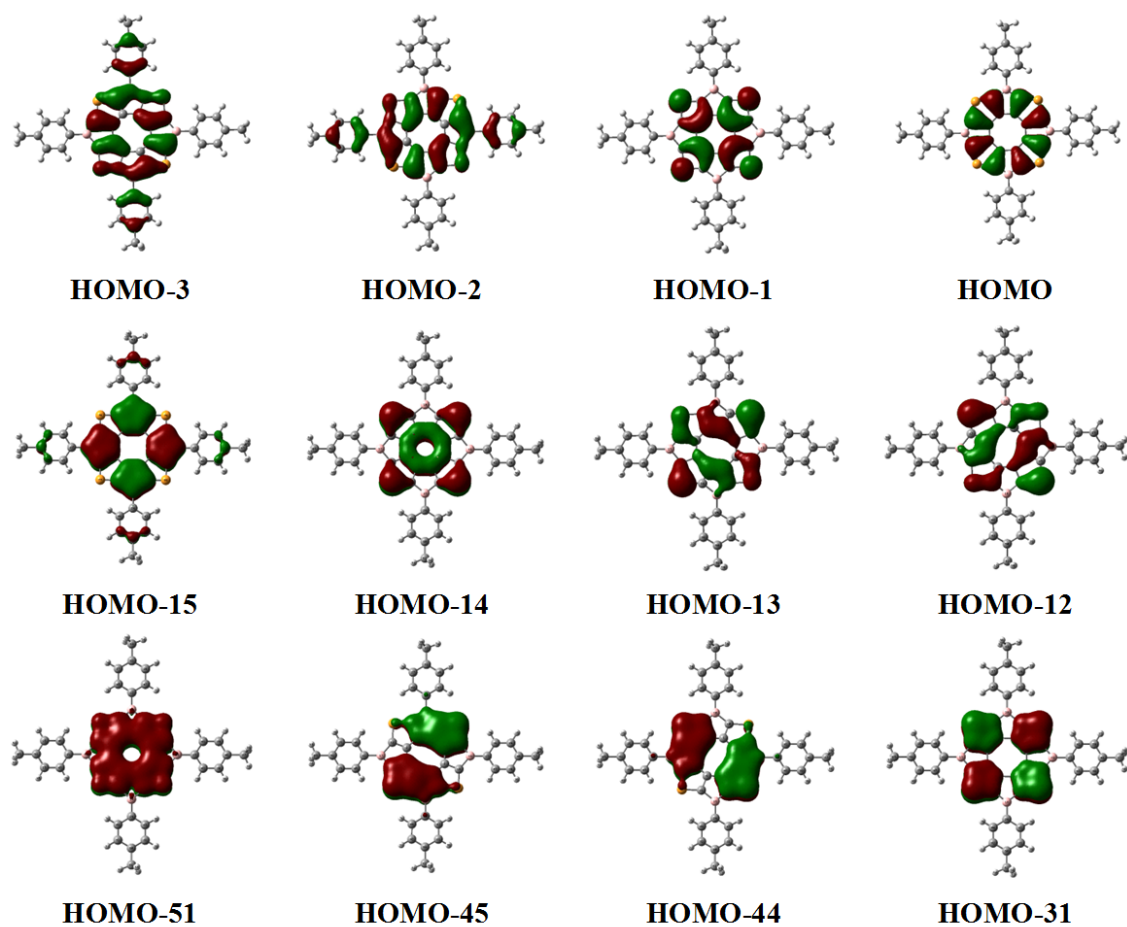


Figure S3. Shapes of π molecular orbitals of compound **2a** obtained at the B3LYP/6-31G(d) level of theory

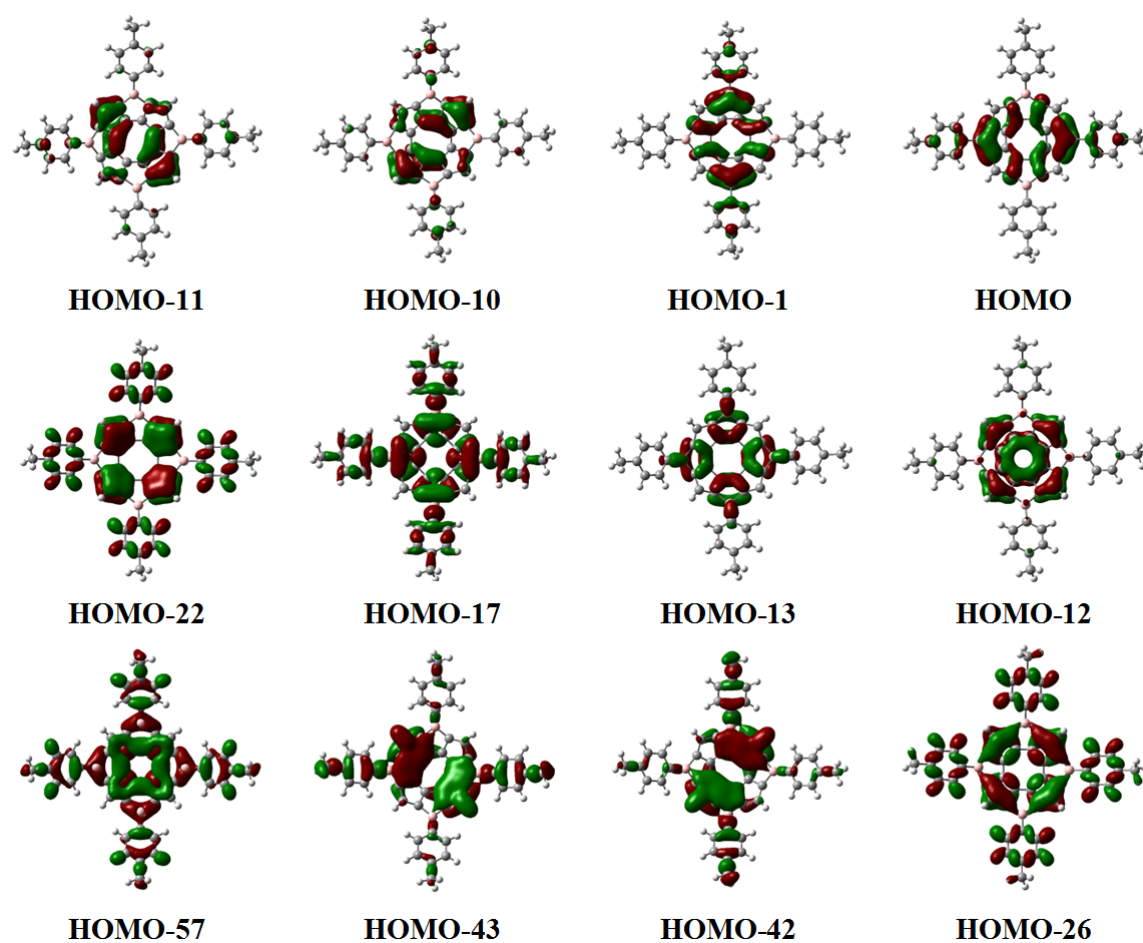


Figure S4. Shapes of π molecular orbitals of compound **2c** obtained at the B3LYP/6-31G(d) level of theory

Table S1. The Cartesian coordinates of the molecules **1**, **2a-2c** obtained at the B3LYP/6-31G(d) level of theory.

Cartesian Coordinates				
Compound 1				
C	-0.25703800	-1.89681200	0.01226209	
C	1.10589400	-1.56247500	0.00057209	
C	-1.10589400	1.56247500	0.00057209	
C	1.89681200	-0.25703800	0.01226209	
C	0.25703800	1.89681200	0.01226209	
C	1.56247500	1.10589400	0.00057209	
C	-1.56247500	-1.10589400	0.00057209	
C	-1.89681200	0.25703800	0.01226209	
C	-3.30588300	0.59300600	0.02918009	
C	-2.65611300	-2.05583000	-0.01675691	
C	-0.59300600	-3.30588300	0.02918009	
C	2.05583000	-2.65611300	-0.01675691	
C	3.30588300	-0.59300600	0.02918009	
C	2.65611300	2.05583000	-0.01675691	
C	0.59300600	3.30588300	0.02918009	
C	-2.05583000	2.65611300	-0.01675691	
B	3.50260800	-2.12250500	0.00538609	
B	2.12250500	3.50260800	0.00538609	
B	-3.50260800	2.12250500	0.00538609	
B	-2.12250500	-3.50260800	0.00538609	
C	4.83182600	-2.92612200	0.00234109	
C	-2.92612200	-4.83182600	0.00234109	
C	-4.83182600	2.92612200	0.00234109	
C	2.92612200	4.83182600	0.00234109	
C	7.09884600	-3.30588300	0.84891309	
C	6.22106900	-4.75189700	-0.85575891	
C	-3.30588300	-7.09884600	0.84891309	
C	-4.75189700	-6.22106900	-0.85575891	
C	-7.09884600	3.30588300	0.84891309	
C	-6.22106900	4.75189700	-0.85575891	
C	3.30588300	7.09884600	0.84891309	
C	4.75189700	6.22106900	-0.85575891	
H	-5.59744400	-6.33645600	-1.53020991	
H	-3.01895600	-7.90155100	1.52601809	
H	-7.90155100	3.01895600	1.52601809	
H	-6.33645600	5.59744400	-1.53020991	
H	5.59744400	6.33645600	-1.53020991	
H	3.01895600	7.90155100	1.52601809	
H	6.33645600	-5.59744400	-1.53020991	
H	7.90155100	-3.01895600	1.52601809	
C	-5.91245600	2.57817000	0.84234909	
C	-5.02233000	4.04056400	-0.84036291	
C	2.57817000	5.91245600	0.84234909	
C	4.04056400	5.02233000	-0.84036291	
C	5.91245600	-2.57817000	0.84234909	

C	5.02233000	-4.04056400	-0.84036291
C	-4.04056400	-5.02233000	-0.84036291
C	-2.57817000	-5.91245600	0.84234909
C	-7.27935300	4.40150300	-0.00827691
C	4.40150300	7.27935300	-0.00827691
C	7.27935300	-4.40150300	-0.00827691
C	-4.40150300	-7.27935300	-0.00827691
C	-5.16582100	-8.58176900	-0.02140391
H	-6.10003000	-8.49254400	-0.58487091
H	-4.57611800	-9.38384600	-0.48463391
H	-5.41336500	-8.91222600	0.99413809
C	-8.58176900	5.16582100	-0.02140391
H	-9.38384600	4.57611800	-0.48463391
H	-8.91222600	5.41336500	0.99413809
H	-8.49254400	6.10003000	-0.58487091
C	5.16582100	8.58176900	-0.02140391
H	6.10003000	8.49254400	-0.58487091
H	4.57611800	9.38384600	-0.48463391
H	5.41336500	8.91222600	0.99413809
C	8.58176900	-5.16582100	-0.02140391
H	9.38384600	-4.57611800	-0.48463391
H	8.91222600	-5.41336500	0.99413809
H	8.49254400	-6.10003000	-0.58487091
H	4.22423700	-4.34355000	-1.51353491
H	5.80979200	-1.73605700	1.52227709
H	-1.73605700	-5.80979200	1.52227709
H	-4.34355000	-4.22423700	-1.51353491
H	-4.22423700	4.34355000	-1.51353491
H	-5.80979200	1.73605700	1.52227709
H	1.73605700	5.80979200	1.52227709
H	4.34355000	4.22423700	-1.51353491
C	4.32436200	0.34372600	0.01140009
C	3.99249300	1.69672100	0.00085009
C	1.69672100	-3.99249300	0.00085009
C	0.34372600	-4.32436200	0.01140009
C	-3.99249300	-1.69672100	0.00085009
C	-4.32436200	-0.34372600	0.01140009
C	-1.69672100	3.99249300	0.00085009
C	-0.34372600	4.32436200	0.01140009
H	-2.46589000	4.75966300	0.01195009
H	-0.01688200	5.36034000	0.00008709
H	5.36034000	0.01688200	0.00008709
H	4.75966300	2.46589000	0.01195009
H	2.46589000	-4.75966300	0.01195009
H	0.01688200	-5.36034000	0.00008709
H	-4.75966300	-2.46589000	0.01195009
H	-5.36034000	-0.01688200	0.00008709

Compound 2a			
C	0.85588900	-1.65834100	-0.00511609
C	1.76559100	-0.60446100	-0.00506109
C	-1.76559100	0.60446100	-0.00506109
C	1.65834100	0.85588900	-0.00511609
C	-0.85588900	1.65834100	-0.00511609
C	0.60446100	1.76559100	-0.00506109
C	-0.60446100	-1.76559100	-0.00506109
C	-1.65834100	-0.85588900	-0.00511609
C	-2.92541300	-1.44600700	-0.00509809
C	-1.00326700	-3.10529000	-0.00488109
C	1.44600700	-2.92541300	-0.00509809
C	3.10529000	-1.00326700	-0.00488109
C	2.92541300	1.44600700	-0.00509809
C	1.00326700	3.10529000	-0.00488109
C	-1.44600700	2.92541300	-0.00509809
C	-3.10529000	1.00326700	-0.00488109
B	4.01880100	0.29530300	-0.00446209
B	-0.29530300	4.01880100	-0.00446209
B	-4.01880100	-0.29530300	-0.00446209
B	0.29530300	-4.01880100	-0.00446209
C	5.55333100	0.40794200	-0.00179809
C	0.40794200	-5.55333100	-0.00179809
C	-5.55333100	-0.40794200	-0.00179809
C	-0.40794200	5.55333100	-0.00179809
C	7.59097200	1.76559100	0.00272891
C	7.76831000	-0.63545200	0.00333891
C	1.76559100	-7.59097200	0.00272891
C	-0.63545200	-7.76831000	0.00333891
C	-7.59097200	-1.76559100	0.00272891
C	-7.76831000	0.63545200	0.00333891
C	-1.76559100	7.59097200	0.00272891
C	0.63545200	7.76831000	0.00333891
H	-1.53795600	-8.37536800	0.00397191
H	2.74754900	-8.05968900	0.00292991
H	-8.05968900	-2.74754900	0.00292991
H	-8.37536800	1.53795600	0.00397191
H	1.53795600	8.37536800	0.00397191
H	-2.74754900	8.05968900	0.00292991
H	8.37536800	-1.53795600	0.00397191
H	8.05968900	2.74754900	0.00292991
C	-6.20591500	-1.66194100	-0.00055409
C	-6.38017900	0.73535700	-0.00013409
C	-1.66194100	6.20591500	-0.00055409
C	0.73535700	6.38017900	-0.00013409
C	6.20591500	1.66194100	-0.00055409
C	6.38017900	-0.73535700	-0.00013409
C	-0.73535700	-6.38017900	-0.00013409
C	1.66194100	-6.20591500	-0.00055409
C	-8.39865000	-0.61630200	0.00587991

C	-0.61630200	8.39865000	0.00587991
C	8.39865000	0.61630200	0.00587991
C	0.61630200	-8.39865000	0.00587991
C	0.73535800	-9.90331300	0.01674991
H	-0.24535900	-10.38447400	-0.04518209
H	1.34123200	-10.26080600	-0.82493609
H	1.22438500	-10.25528400	0.93401891
C	-9.90331300	-0.73535800	0.01674991
H	-10.26080600	-1.34123200	-0.82493609
H	-10.25528400	-1.22438500	0.93401891
H	-10.38447400	0.24535900	-0.04518209
C	-0.73535800	9.90331300	0.01674991
H	0.24535900	10.38447400	-0.04518209
H	-1.34123200	10.26080600	-0.82493609
H	-1.22438500	10.25528400	0.93401891
C	9.90331300	0.73535800	0.01674991
H	10.26080600	1.34123200	-0.82493609
H	10.25528400	1.22438500	0.93401891
H	10.38447400	-0.24535900	-0.04518209
H	5.92650100	-1.72333900	-0.00244809
H	5.61189900	2.57249000	-0.00246909
H	2.57249000	-5.61189900	-0.00246909
H	-1.72333900	-5.92650100	-0.00244809
H	-5.92650100	1.72333900	-0.00244809
H	-5.61189900	-2.57249000	-0.00246909
H	-2.57249000	5.61189900	-0.00246909
H	1.72333900	5.92650100	-0.00244809
S	2.74285000	3.17758100	-0.00499409
S	3.17758100	-2.74285000	-0.00499409
S	-2.74285000	-3.17758100	-0.00499409
S	-3.17758100	2.74285000	-0.00499409
Compound 2b			
C	1.51322000	-1.10468400	-0.01831494
C	1.85113700	0.28887900	-0.01831494
C	-1.85113700	-0.28887900	-0.01831494
C	1.10468400	1.51322000	-0.01831494
C	-1.51322000	1.10468400	-0.01831494
C	-0.28887900	1.85113700	-0.01831494
C	0.28887900	-1.85113700	-0.01831494
C	-1.10468400	-1.51322000	-0.01831494
C	-1.93662000	-2.65173800	-0.01430194
C	0.50566500	-3.24445900	-0.01430194
C	2.65173800	-1.93662000	-0.01430194
C	3.24445900	0.50566500	-0.01430194
C	1.93662000	2.65173800	-0.01430194
C	-0.50566500	3.24445900	-0.01430194
C	-2.65173800	1.93662000	-0.01430194
C	-3.24445900	-0.50566500	-0.01430194
B	3.41994600	2.08425800	-0.01138794

B	0.94447400	3.89206000	-0.01138794
B	-2.08425800	3.41994600	-0.01138794
B	-3.89206000	0.94447400	-0.01138794
B	-3.41994600	-2.08425800	-0.01138794
B	-0.94447400	-3.89206000	-0.01138794
B	2.08425800	-3.41994600	-0.01138794
B	3.89206000	-0.94447400	-0.01138794
C	4.74498200	2.89136200	-0.00415894
C	5.39971000	-1.31070700	-0.00415894
C	2.89136200	-4.74498200	-0.00415894
C	-1.31070700	-5.39971000	-0.00415894
C	-4.74498200	-2.89136200	-0.00415894
C	-5.39971000	1.31070700	-0.00415894
C	-2.89136200	4.74498200	-0.00415894
C	1.31070700	5.39971000	-0.00415894
C	2.76004900	7.24711900	-0.69978494
C	0.87012600	7.69886200	0.71749106
C	6.05919000	4.82864500	0.71749106
C	7.07613600	3.17283800	-0.69978494
C	7.24711900	-2.76004900	-0.69978494
C	7.69886200	-0.87012600	0.71749106
C	4.82864500	-6.05919000	0.71749106
C	3.17283800	-7.07613600	-0.69978494
C	-2.76004900	-7.24711900	-0.69978494
C	-0.87012600	-7.69886200	0.71749106
C	-6.05919000	-4.82864500	0.71749106
C	-7.07613600	-3.17283800	-0.69978494
C	-7.69886200	0.87012600	0.71749106
C	-7.24711900	2.76004900	-0.69978494
C	-4.82864500	6.05919000	0.71749106
C	-3.17283800	7.07613600	-0.69978494
H	2.80128100	-7.93362600	-1.25742194
H	5.75789100	-6.12027700	1.27948106
H	-3.62911600	-7.59072600	-1.25742194
H	-0.25624600	-8.39913300	1.27948106
H	-6.12027700	-5.75789100	1.27948106
H	-7.93362600	-2.80128100	-1.25742194
H	-7.59072600	3.62911600	-1.25742194
H	-8.39913300	0.25624600	1.27948106
H	-2.80128100	7.93362600	-1.25742194
H	-5.75789100	6.12027700	1.27948106
H	3.62911600	7.59072600	-1.25742194
H	0.25624600	8.39913300	1.27948106
H	7.93362600	2.80128100	-1.25742194
H	6.12027700	5.75789100	1.27948106
H	7.59072600	-3.62911600	-1.25742194
H	8.39913300	-0.25624600	1.27948106
C	-4.86542800	-4.11497800	0.69252106
C	-5.89076100	-2.44003300	-0.69256394
C	-6.35010600	0.53064800	0.69252106
C	-5.89076100	2.44003300	-0.69256394

C	-4.11497800	4.86542800	0.69252106
C	-2.44003300	5.89076100	-0.69256394
C	0.53064800	6.35010600	0.69252106
C	2.44003300	5.89076100	-0.69256394
C	4.86542800	4.11497800	0.69252106
C	5.89076100	2.44003300	-0.69256394
C	6.35010600	-0.53064800	0.69252106
C	5.89076100	-2.44003300	-0.69256394
C	2.44003300	-5.89076100	-0.69256394
C	4.11497800	-4.86542800	0.69252106
C	-2.44003300	-5.89076100	-0.69256394
C	-0.53064800	-6.35010600	0.69252106
C	-7.18380900	-4.37611400	0.00926406
C	-8.17410000	1.98534000	0.00926406
C	-4.37611400	7.18380900	0.00926406
C	1.98534000	8.17410000	0.00926406
C	7.18380900	4.37611400	0.00926406
C	8.17410000	-1.98534000	0.00926406
C	4.37611400	-7.18380900	0.00926406
C	-1.98534000	-8.17410000	0.00926406
C	-2.32915500	-9.64444600	0.01035006
H	-1.59573900	-10.22445800	-0.56578794
H	-2.33042100	-10.05385800	1.02764906
H	-3.31395900	-9.82740500	-0.43007294
C	5.17269200	-8.46661400	0.01035006
H	4.60570200	-9.29234700	-0.43007294
H	6.10142500	-8.35814100	-0.56578794
H	5.46129500	-8.75700800	1.02764906
C	-8.46661400	-5.17269200	0.01035006
H	-8.35814100	-6.10142500	-0.56578794
H	-8.75700800	-5.46129500	1.02764906
H	-9.29234700	-4.60570200	-0.43007294
C	-9.64444600	2.32915500	0.01035006
H	-10.22445800	1.59573900	-0.56578794
H	-10.05385800	2.33042100	1.02764906
H	-9.82740500	3.31395900	-0.43007294
C	-5.17269200	8.46661400	0.01035006
H	-4.60570200	9.29234700	-0.43007294
H	-6.10142500	8.35814100	-0.56578794
H	-5.46129500	8.75700800	1.02764906
C	2.32915500	9.64444600	0.01035006
H	1.59573900	10.22445800	-0.56578794
H	2.33042100	10.05385800	1.02764906
H	3.31395900	9.82740500	-0.43007294
C	8.46661400	5.17269200	0.01035006
H	8.35814100	6.10142500	-0.56578794
H	8.75700800	5.46129500	1.02764906
H	9.29234700	4.60570200	-0.43007294
C	9.64444600	-2.32915500	0.01035006
H	9.82740500	-3.31395900	-0.43007294
H	10.22445800	-1.59573900	-0.56578794

H	10.05385800	-2.33042100	1.02764906
H	3.07417800	5.19790500	-1.23669394
H	-0.34846200	6.01834000	1.23677706
H	5.84924600	1.50170200	-1.23669394
H	4.00920900	4.50200900	1.23677706
H	5.19790500	-3.07417800	-1.23669394
H	6.01834000	0.34846200	1.23677706
H	4.50200900	-4.00920900	1.23677706
H	1.50170200	-5.84924600	-1.23669394
H	0.34846200	-6.01834000	1.23677706
H	-3.07417800	-5.19790500	-1.23669394
H	-5.84924600	-1.50170200	-1.23669394
H	-4.00920900	-4.50200900	1.23677706
H	-5.19790500	3.07417800	-1.23669394
H	-6.01834000	-0.34846200	1.23677706
H	-4.50200900	4.00920900	1.23677706
H	-1.50170200	5.84924600	-1.23669394
Compound 2c			
C	1.68647600	0.69284000	-1.58557699
C	0.69284000	1.68649000	-1.58544899
C	-0.69284000	-1.68649000	-1.58544899
C	-0.69284000	1.68647600	-1.58557699
C	-1.68647600	-0.69284000	-1.58557699
C	-1.68649000	0.69284000	-1.58544899
C	1.68649000	-0.69284000	-1.58544899
C	0.69284000	-1.68647600	-1.58557699
C	1.22697200	-2.89143600	-0.96320799
C	2.89136300	-1.22697200	-0.96279299
C	2.89143600	1.22697200	-0.96320799
C	1.22697200	2.89136300	-0.96279299
C	-1.22697200	2.89143600	-0.96320799
C	-2.89136300	1.22697200	-0.96279299
C	-2.89143600	-1.22697200	-0.96320799
C	-1.22697200	-2.89136300	-0.96279299
B	-0.00001800	3.82588700	-0.62574799
B	-3.82588700	-0.00001800	-0.62574799
B	0.00001800	-3.82588700	-0.62574799
B	3.82588700	0.00001800	-0.62574799
C	-0.00098800	5.24912400	-0.01781399
C	5.24912400	0.00098800	-0.01781399
C	0.00098800	-5.24912400	-0.01781399
C	-5.24912400	-0.00098800	-0.01781399
C	-1.20648600	7.21361100	0.81281601
C	1.19785300	7.20980200	0.83064401
C	7.21361100	1.20648600	0.81281601
C	7.20980200	-1.19785300	0.83064401
C	1.20648600	-7.21361100	0.81281601
C	-1.19785300	-7.20980200	0.83064401
C	-7.21361100	-1.20648600	0.81281601

C	-7.20980200	1.19785300	0.83064401
H	7.70361700	-2.14247300	1.04892801
H	7.71100300	2.15269300	1.01716001
H	2.15269300	-7.71100300	1.01716001
H	-2.14247300	-7.70361700	1.04892801
H	-7.70361700	2.14247300	1.04892801
H	-7.71100300	-2.15269300	1.01716001
H	2.14247300	7.70361700	1.04892801
H	-2.15269300	7.71100300	1.01716001
C	1.20196800	-5.93709500	0.26201801
C	-1.19670000	-5.93129300	0.27841101
C	-5.93709500	-1.20196800	0.26201801
C	-5.93129300	1.19670000	0.27841101
C	-1.20196800	5.93709500	0.26201801
C	1.19670000	5.93129300	0.27841101
C	5.93129300	-1.19670000	0.27841101
C	5.93709500	1.20196800	0.26201801
C	0.00381800	-7.87453400	1.10842201
C	-7.87453400	-0.00381800	1.10842201
C	-0.00381800	7.87453400	1.10842201
C	7.87453400	0.00381800	1.10842201
C	9.26814600	0.01212700	1.68952401
H	9.56772300	-0.98448800	2.02865201
H	10.00588500	0.34508200	0.94755401
H	9.34201800	0.69660400	2.54297201
C	0.01212700	-9.26814600	1.68952401
H	0.34508200	-10.00588500	0.94755401
H	0.69660400	-9.34201800	2.54297201
H	-0.98448800	-9.56772300	2.02865201
C	-9.26814600	-0.01212700	1.68952401
H	-9.56772300	0.98448800	2.02865201
H	-10.00588500	-0.34508200	0.94755401
H	-9.34201800	-0.69660400	2.54297201
C	-0.01212700	9.26814600	1.68952401
H	-0.34508200	10.00588500	0.94755401
H	-0.69660400	9.34201800	2.54297201
H	0.98448800	9.56772300	2.02865201
H	2.14863200	5.45066800	0.06675301
H	-2.15208300	5.45926600	0.03598901
H	5.45926600	2.15208300	0.03598901
H	5.45066800	-2.14863200	0.06675301
H	-2.14863200	-5.45066800	0.06675301
H	2.15208300	-5.45926600	0.03598901
H	-5.45926600	-2.15208300	0.03598901
H	-5.45066800	2.14863200	0.06675301
C	2.57200300	-2.57221800	-0.61669099
C	-2.57221800	-2.57200300	-0.61669099
C	-2.57200300	2.57221800	-0.61669099
C	2.57221800	2.57200300	-0.61669099
H	-3.23161000	3.23201300	-0.06108699
H	3.23201300	3.23161000	-0.06108699

H	3.23161000	-3.23201300	-0.06108699
H	-3.23201300	-3.23161000	-0.06108699

References

-
- [1] Gaussian 09, Revision C.01, Gaussian, Inc., Wallingford CT, **2009**, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, Jr. J. A. Montgomery, T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, J. A. Pople.
- [2] C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* **1988**, 37, 785
- [3] A. D. Becke, *Phys. Rev. A.*, **1988**, 38, 3098
- [4] P. J. Stephens, F. J. Devlin, C. F. Chabalowski, M. J. Frisch, *J. Phys. Chem.* **1994**, 98, 11623
- [5] J. A. Pople, *J. Chem. Phys.*, **1980**, 72, 650