

*Electronic Supplementary Information (ESI) for*

**20-electron exohedral alkaline-earth-metallofullerenes  $M(C_{60})_3$  ( $M = Ca, Sr, Ba$ )**

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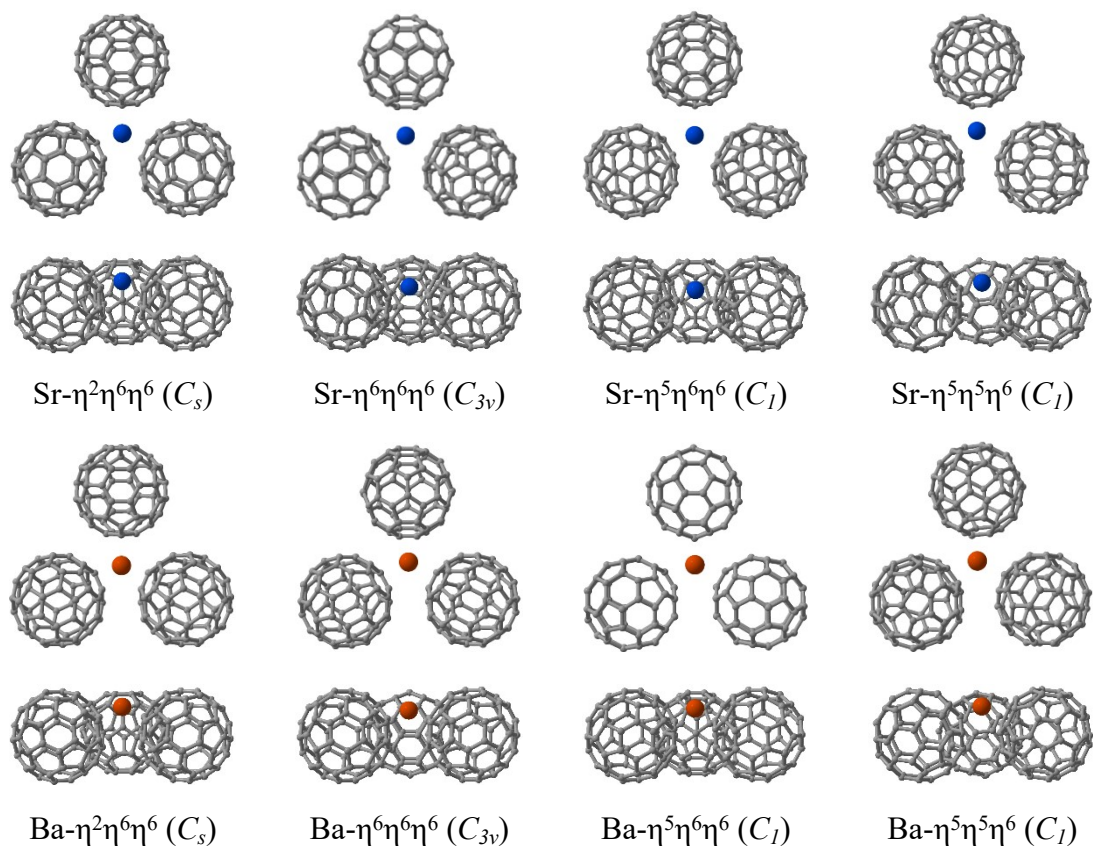
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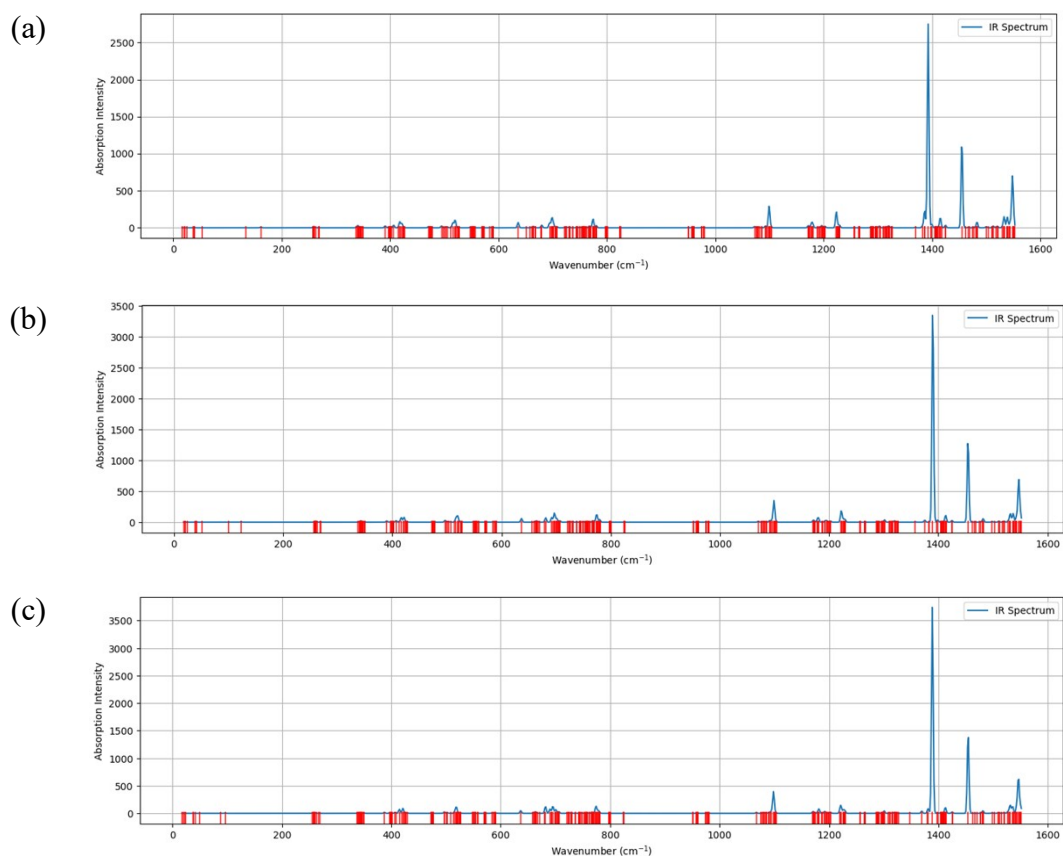
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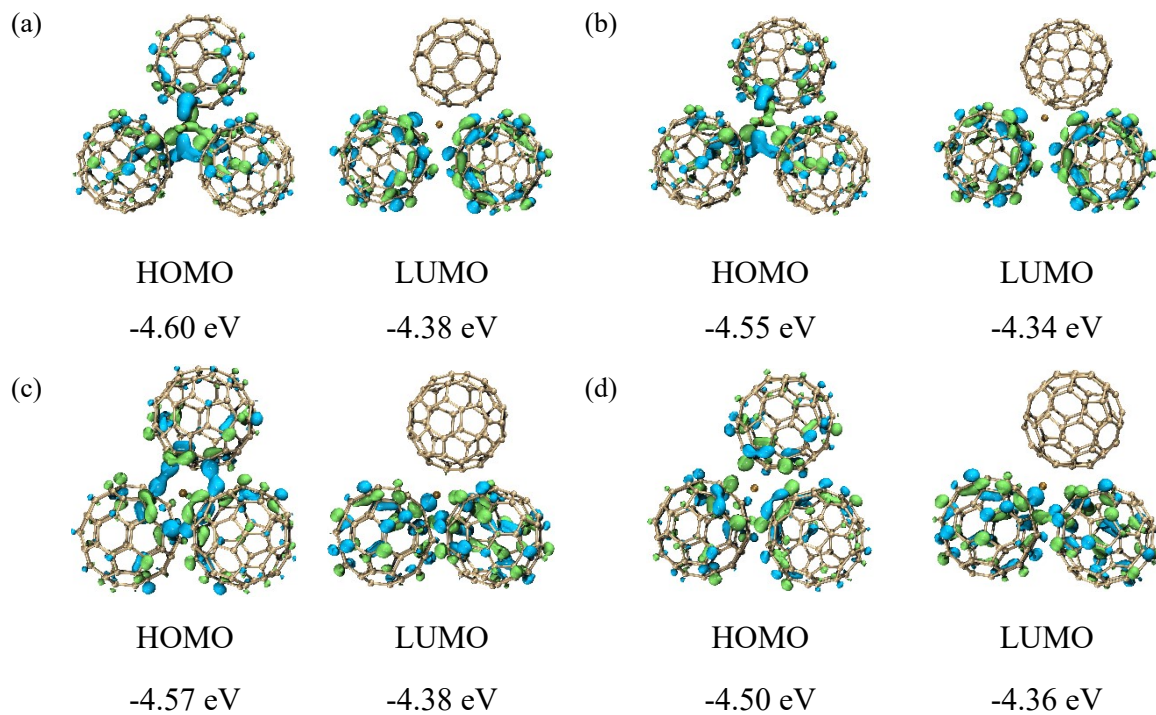
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**Fig. S1** The equilibrium geometric structures of  $M(\text{C}_{60})_3$  ( $M = \text{Sr}, \text{Ba}$ ). The upper panels are the top view and the lower panels are the side view. Calculated at the PBE-D3(BJ)/def2-SVP level.



**Fig. S2** Calculated IR intensity of  $\text{M}(\text{C}_{60})_3$  [ $\text{M} = \text{Ca}$  (a),  $\text{Sr}$  (b),  $\text{Ba}$  (c)] at BP86-D3(BJ)/TZP. The unit of absorption intensity is  $\text{km} \cdot \text{mol}^{-1}$ .



**Fig. S3** The frontier orbitals of (a)  $\text{Sr}(\text{C}_{60})_3$  ( $C_s$ ), (b)  $\text{Sr}(\text{C}_{60})_3$  ( $C_{3v}$ ), (c)  $\text{Ba}(\text{C}_{60})_3$  ( $C_s$ ) and (d)  $\text{Ba}(\text{C}_{60})_3$  ( $C_{3v}$ ) with the isosurface = 0.025 e/bohr<sup>3</sup>. Calculated at the PBE-D3(BJ)/def2-SVP level.

**Table S1.** Calculated HOMO-LUMO gap (eV), binding energy ( $\Delta E_b$ , eV) and root mean square displacement (RMSD, Å) of the two functional optimized structures at B3LYP-D3(BJ)/def2-SVP and PBE-D3(BJ)/def2-SVP levels.  $\Delta E_b$  is defined as  $E[\text{Ca}(\text{C}_{60})_3] - 3E[\text{C}_{60}] - E_{\text{Ca}}$ .

	HOMO-LUMO gap		$\Delta E_b$		RMSD
	B3LYP	PBE	B3LYP	PBE	
$\text{Ca}(\text{C}_{60})_3 (C_s)$	0.80	0.24	-4.06	-4.78	0.052
$\text{Ca}(\text{C}_{60})_3 (C_{3v})$	0.83	0.25	-3.86	-4.65	0.029

**Table S2.** EDA-NOCV calculations on  $M(C_{60})_3$  ( $M = Ca, Sr, Ba$ ) using neutral fragments of metal atoms  $M$  in the singlet state with  $ns^2np^0(n-1)d^0$  electron configuration and  $(C_{60})_3$  (singlet) at BP86-D3 (BJ)/TZ2P (M)~TZP (C) level. All units of energy are kcal mol<sup>-1</sup>.

Term	Interaction	Ca (S, 4s <sup>2</sup> 4p <sup>0</sup> 3d <sup>0</sup> ) + (C <sub>60</sub> ) <sub>3</sub> (S)	Sr (S, 5s <sup>2</sup> 5p <sup>0</sup> 4d <sup>0</sup> ) + (C <sub>60</sub> ) <sub>3</sub> (S)	Ba (S, 6s <sup>2</sup> 6p <sup>0</sup> 5d <sup>0</sup> ) + (C <sub>60</sub> ) <sub>3</sub> (S)
$\Delta E_{\text{int}}$		-91.1	-89.5	-106.0
$\Delta E_{\text{Pauli}}$		470.9	463.4	443.3
$\Delta E_{\text{disp}}^a$		-9.3 (1.7%)	-12.4 (2.3%)	-15.0 (2.7%)
$\Delta E_{\text{elstat}}^a$		-272.0 (48.4%)	-273.8 (49.5%)	-272.4 (49.6%)
$\Delta E_{\text{orb}}^a$		-280.7 (49.9%)	-266.7 (48.2%)	-261.9 (47.7%)
$\Delta E_{\text{orb}(1)}^b$	(C <sub>60</sub> ) <sub>3</sub> ← M(s) backdonation	-219.4 (78.2%)	-204.9 (76.8%)	-195.8 (74.8%)
$\Delta E_{\text{orb}(2)}^b$	(C <sub>60</sub> ) <sub>3</sub> → M(d) donation	-8.6 (3.1%)	-9.4 (3.5%)	-10.5 (4.0%)
$\Delta E_{\text{orb}(3)}^b$	(C <sub>60</sub> ) <sub>3</sub> → M(d) donation	-8.5 (3.0%)	-9.4 (3.5%)	-10.5 (4.0%)
$\Delta E_{\text{orb}(4)}^b$	(C <sub>60</sub> ) <sub>3</sub> → M(d) donation	-9.5 (3.4%)	-8.7 (3.3%)	-8.5 (3.2%)
$\Delta E_{\text{orb}(5)}^b$	(C <sub>60</sub> ) <sub>3</sub> → M(d) donation	-9.5 (3.4%)	-8.7 (3.3%)	-8.5 (3.2%)
$\Delta E_{\text{orb}(6)}^b$		-4.0 (1.4%)	-5.0 (1.9%)	-6.5 (2.5%)
$\Delta E_{\text{orb}(\text{rest})}^b$		-21.2 (7.5%)	-20.6 (7.7%)	-21.6 (8.3%)

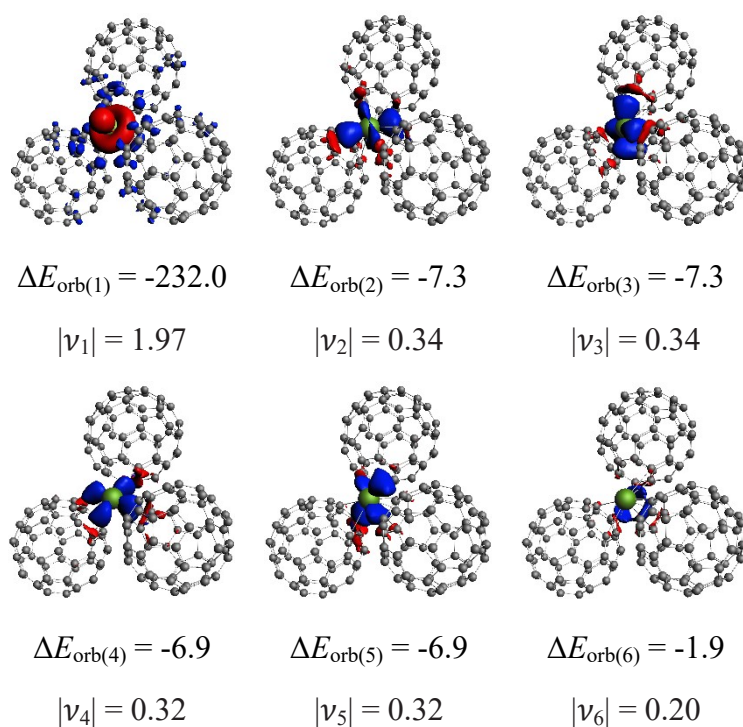
<sup>a</sup> The values in parentheses give the percentage contribution to the total attractive interactions  $\Delta E_{\text{elstat}} + \Delta E_{\text{orb}} + \Delta E_{\text{disp}}$ .

<sup>b</sup> The values in parentheses give the percentage contribution to the total orbital interactions  $\Delta E_{\text{orb}}$ .

The structures of  $Sr(C_{60})_3$  and  $Ba(C_{60})_3$  were re-optimized under  $C_{3v}$  symmetry to accommodate the EDA analysis, which necessitates higher symmetry for the accurate assignment of electron occupations. The molecular orbitals comparison is depicted in Fig. S5 (a), suggesting that the influence of imposing symmetry constraints on orbital characteristics is minimal. Similarly, to accurately specify electron occupations,  $D_3$  symmetry was adopted in the calculations for metal atom fragments, facilitating the distinction between  $d_{z^2}$  and  $p_z$  orbitals, which possess closely related energies.

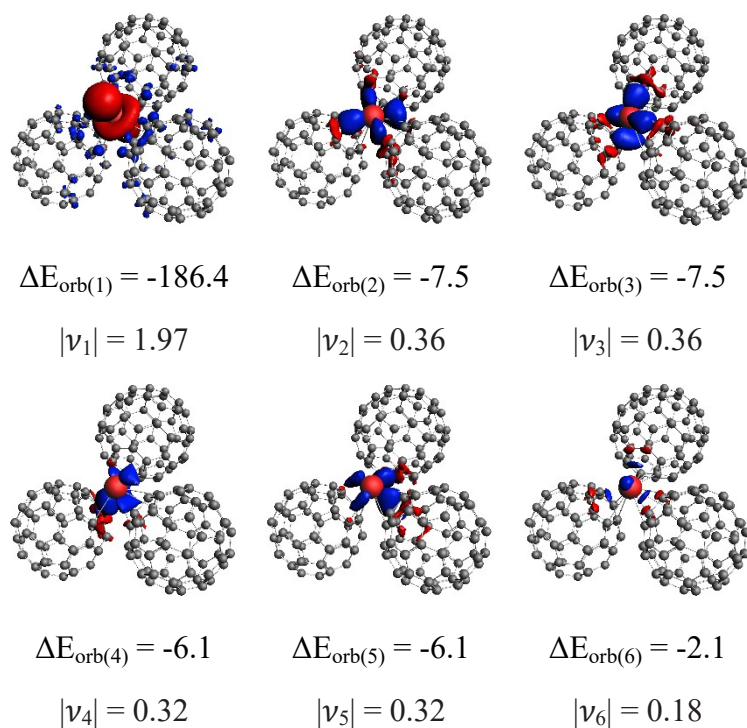
**Table S3.** Calculated singlet–triplet (and singlet–quintet) splitting energy of  $M(C_{60})_3 (C_{3v})$  ( $M = \text{Ca, Sr, Ba}$ ) at BP86-D3(BJ)/TZP level. The splitting energy is defined as  $E_{\text{triplet(quintet)}} - E_{\text{singlet}}$  (eV).

	Singlet–Triplet Splitting Energy	Singlet–Quintet Splitting Energy
$\text{Ca}(C_{60})_3 (C_{3v})$	0.19	1.33
$\text{Sr}(C_{60})_3 (C_{3v})$	0.14	1.34
$\text{Ba}(C_{60})_3 (C_{3v})$	0.11	1.30

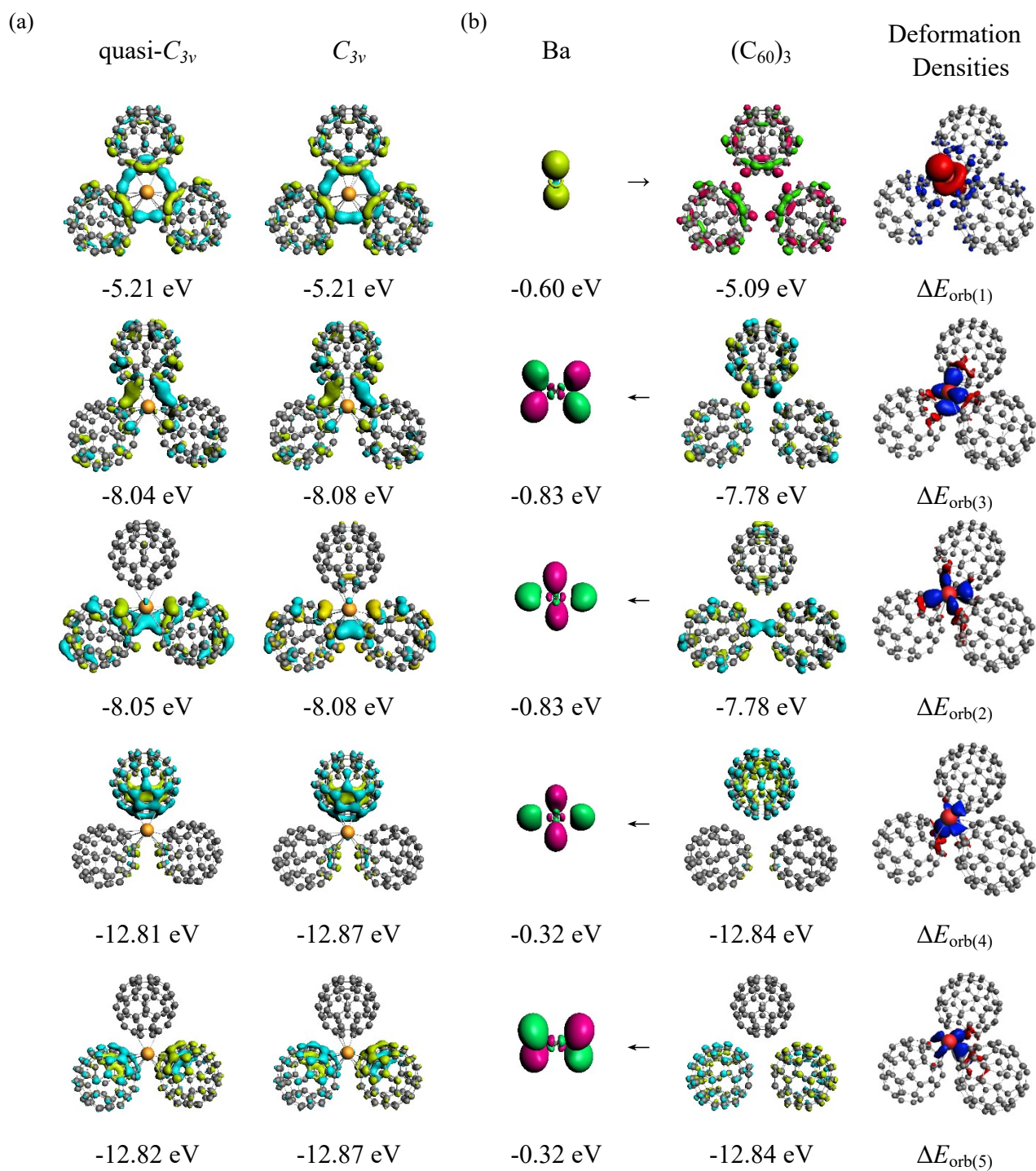


**Fig. S4** Plot of deformation densities  $\Delta\rho_{1-6}$   $\text{Sr}(\text{C}_{60})_3$  with the association interaction energies  $\Delta E$  (in  $\text{kcal mol}^{-1}$ ) and their energy eigenvalues  $\nu$  (in e) which indicates the amount of donated and accepted charges, respectively. The direction of the charge flow is red to blue. The isosurface values are 0.002 for  $\Delta\rho_1$  and 0.0006 e/bohr<sup>3</sup> for  $\Delta\rho_{2-6}$ .



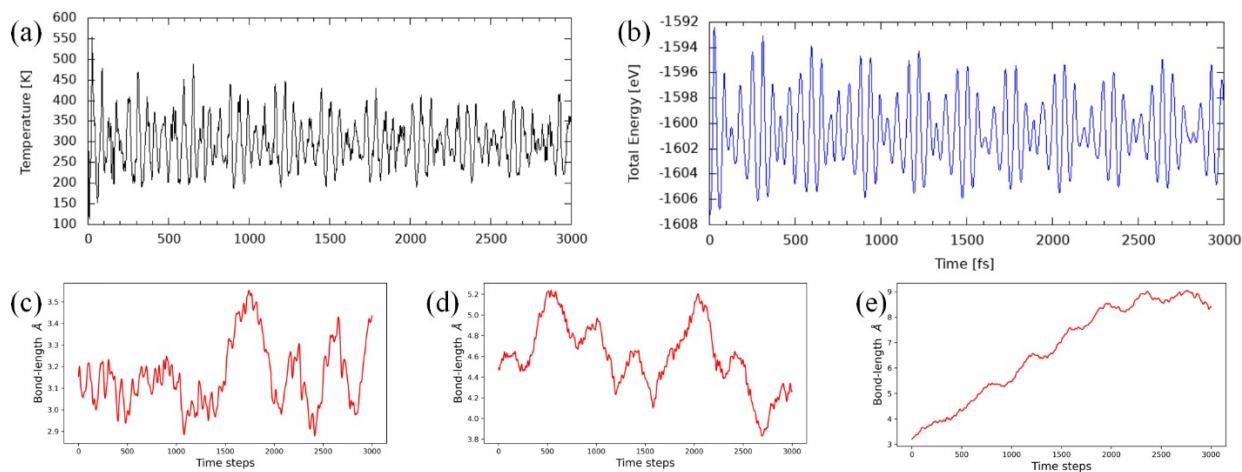


**Fig. S5** Plot of deformation densities  $\Delta\rho_{1-6}$   $\text{Ba}(\text{C}_{60})_3$  with the association interaction energies  $\Delta E$  (in  $\text{kcal mol}^{-1}$ ) and their energy eigenvalues  $\nu$  (in  $e$ ) which indicates the amount of donated and accepted charges, respectively. The direction of the charge flow is red to blue. The isosurface values are 0.002 for  $\Delta\rho_1$  and 0.0006  $e/\text{bohr}^3$  for  $\Delta\rho_{2-6}$ .

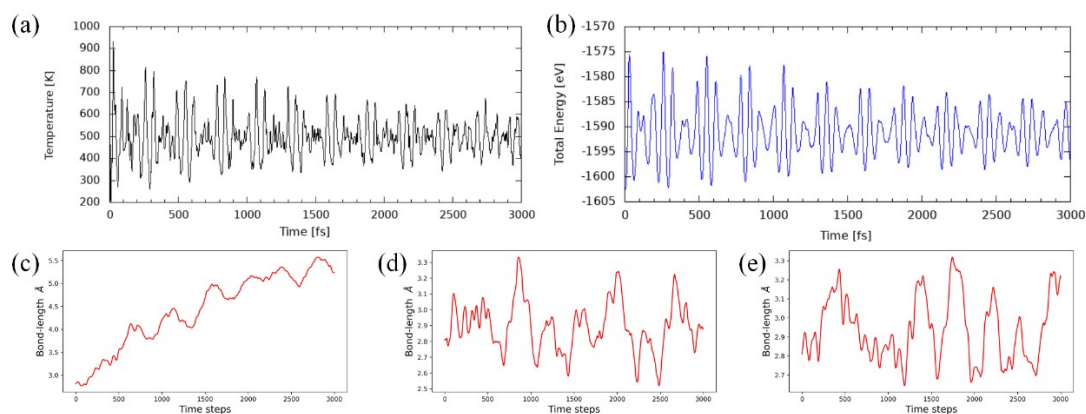


**Fig. S6** (a) Molecular orbital diagrams and energy levels of  $Ba(C_{60})_3$  (quasi- $C_{3v}$ ) and  $Ba(C_{60})_3$  ( $C_{3v}$ ).

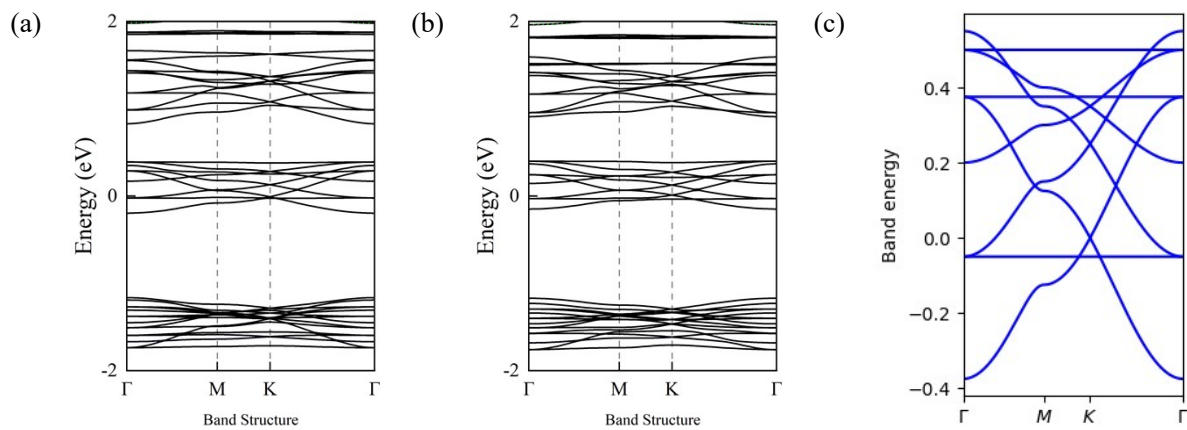
(b) Coordination-related orbital correlation diagrams and corresponding deformation densities of  $Ba(C_{60})_3$  ( $C_{3v}$ ). Calculated at the BP86-D3(BJ)/TZP level.



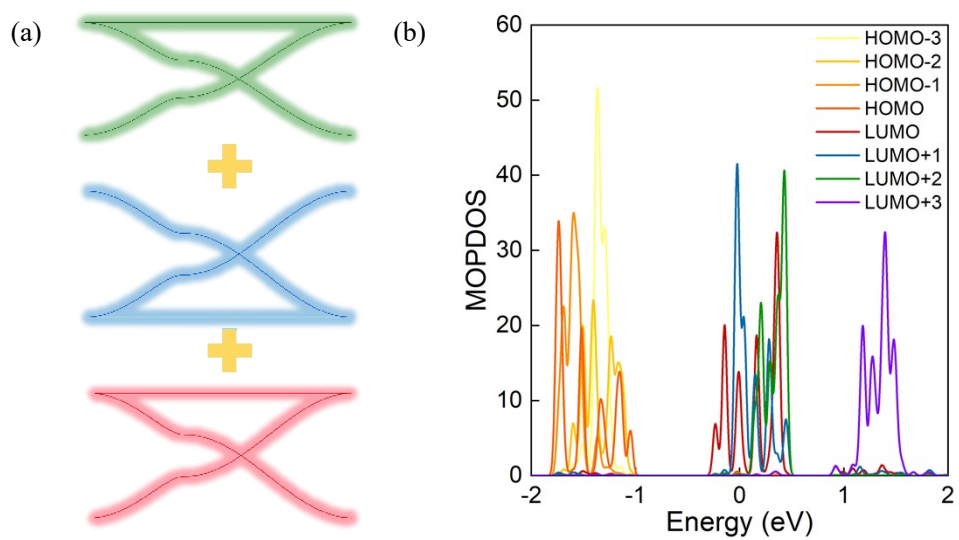
**Fig. S7** Results of the AIMD simulation in 300 K for  $\text{Ba}(\text{C}_{60})_3$ , where represents the temperature (a), energy (b), and changes in distance from metal atoms to the centers of three fullerenes hexagonal rings [(c) to (e)]. The AIMD simulation was conducted with a timestep of 1 fs and a total duration of 3 ps.



**Fig. S8** Results of the AIMD simulation in 500K for  $\text{Ba}(\text{C}_{60})_3$ , where represents the temperature (a), energy (b), and changes in distance from metal atoms to the centers of three fullerenes hexagonal rings [(c) to (e)]. The AIMD simulation was conducted with a timestep of 1 fs and a total duration of 3 ps.



**Fig. S9** (a) and (b) Band structures of  $\text{Sr}_2(\text{C}_{60})_3\text{-HL}$  and  $\text{Ba}_2(\text{C}_{60})_3\text{-HL}$ , respectively. (c) Bands near the fermi level calculated by tight binding model.



**Fig. S10** (a) Schematic diagram of three sets of Kagome lattice bands. (b) Molecular orbital projected density of states (DOS) of  $\text{Ca}_2(\text{C}_{60})_3\text{-HL}$ .

Geometric coordinates of the most stable configuration of  $M(C_{60})_3$  ( $M = Ca, Sr, Ba$ ) (Gaussian format)

(1) $Ca(C_{60})_3 \eta^2\eta^6\eta^6 (C_s)$				C	-3.97374500	-2.79666500	3.09450400
PEB-D3(BJ)/def2-SVP, Singlet				C	-2.22492400	-3.48726000	5.25785200
Ca	-0.40051900	-0.85385700	0.00000000	C	-6.34543800	0.60835500	4.93338000
C	-0.67307100	2.01409600	2.92497500	C	-3.72761300	1.88249500	7.87484400
C	-0.86113500	0.83409700	2.09512000	C	-5.02839100	1.61082700	7.27197000
C	-1.75204700	2.89414400	3.14820500	C	-1.18469100	-0.65017100	8.07916600
C	0.20515400	1.65051600	4.03261600	C	-1.55514000	-2.97663900	6.45112300
C	-2.14143300	0.56204400	1.52611400	C	-2.98520900	0.82930700	8.44494500
C	-0.12644800	-0.26149400	2.72471500	C	-5.63203900	-2.15490800	4.64067800
C	-3.06220000	2.61684400	2.54723300	C	-4.52137900	-3.07340100	4.40937200
C	-1.97569300	3.44747200	4.46939600	C	-3.66228700	-3.41642400	5.47733300
C	0.56548600	0.24924800	3.89447600	C	-6.20642100	-0.21002700	6.06936600
C	-0.00922100	2.19209300	5.31403400	C	-5.53908700	0.30027800	7.26097400
C	-3.25386300	1.48145300	1.74343300	C	-2.40323900	-1.44202100	8.20457700
C	-2.66954200	-0.78662600	1.53659000	C	-2.58347000	-2.58443100	7.40427500
C	-0.61825900	-1.57999600	2.70066300	C	-3.51403000	-0.52671700	8.43423500
C	-4.08886600	3.01120600	3.49924900	C	-5.84452000	-1.61412800	5.92057900
C	-3.41648900	3.51631100	4.69117300	C	-3.88518600	-2.85550200	6.80048500
C	-1.11603000	3.10736100	5.54025200	C	-4.77098500	-0.78918300	7.85208600
C	0.70289800	-0.57869000	5.02795400	C	-4.95794900	-1.97099100	7.02356700
C	0.12948400	1.34017100	6.49420400	C	-3.25386300	1.48145300	-1.74343300
C	-4.46888800	0.68774600	1.87175300	C	-2.14143300	0.56204400	-1.52611400
C	-4.11131900	-0.71651500	1.72987700	C	-3.06220000	2.61684400	-2.54723300
C	-1.91737600	-1.86671800	2.06964000	C	-4.46888800	0.68774600	-1.87175300
C	-0.46816100	-2.43745800	3.86179800	C	-0.86113500	0.83409700	-2.09512000
C	-5.26796100	2.24744900	3.62450300	C	-2.66954200	-0.78662600	-1.53659000
C	-3.94803000	3.24545600	5.96383700	C	-1.75204700	2.89414400	-3.14820500
C	-1.67004400	2.82295000	6.85473600	C	-4.08886600	3.01120600	-3.49924900
C	0.47901600	-0.01596100	6.35390300	C	-4.11131900	-0.71651500	-1.72987700
C	0.17856500	-1.93477400	5.01381900	C	-5.46259300	1.06626100	-2.79591900
C	-0.90025400	1.73201800	7.44619400	C	-0.67307100	2.01409600	-2.92497500
C	-5.46259300	1.06626100	2.79591900	C	-0.12644800	-0.26149400	-2.72471500
C	-4.74389100	-1.69779800	2.51153300	C	-1.91737600	-1.86671800	-2.06964000
C	-2.58036100	-2.87567900	2.87780700	C	-1.97569300	3.44747200	-4.46939600
C	-1.68962900	-3.21994200	3.98315700	C	-3.41648900	3.51631100	-4.69117300
C	-5.81595400	1.96632400	4.94458400	C	-5.26796100	2.24744900	-3.62450300
C	-3.06046000	2.89216200	7.06732700	C	-4.74389100	-1.69779800	-2.51153300
C	-5.16792200	2.45752200	6.09385100	C	-6.12299300	0.04983500	-3.60554200
C	-0.18974700	-1.02939700	7.16120100	C	0.20515400	1.65051600	-4.03261600
C	-0.37749900	-2.21460800	6.33038900	C	0.56548600	0.24924800	-3.89447600
C	-1.54599000	0.75505600	8.22572200	C	-0.61825900	-1.57999600	-2.70066300
C	-6.12299300	0.04983500	3.60554200	C	-2.58036100	-2.87567900	-2.87780700
C	-5.77638900	-1.30809400	3.46213400	C	-1.11603000	3.10736100	-5.54025200

C	-3.94803000	3.24545600	-5.96383700	C	6.06951800	-3.46325800	-0.70336000
C	-5.81595400	1.96632400	-4.94458400	C	2.80708400	-1.76261100	1.18041200
C	-5.77638900	-1.30809400	-3.46213400	C	4.84728600	-3.15233100	1.43622800
C	-3.97374500	-2.79666500	-3.09450400	C	4.37950900	-1.32426000	-3.04471600
C	-6.34543800	0.60835500	-4.93338000	C	2.99492600	0.44351100	-2.31570100
C	-0.00922100	2.19209300	-5.31403400	C	2.09499600	0.32513100	0.00000000
C	0.70289800	-0.57869000	-5.02795400	C	6.65750200	-2.21035100	-2.61336400
C	-0.46816100	-2.43745800	-3.86179800	C	7.19043500	-2.88125700	-1.43254000
C	-1.68962900	-3.21994200	-3.98315700	C	6.06951800	-3.46325800	0.70336000
C	-1.67004400	2.82295000	-6.85473600	C	3.16745200	-1.01111900	2.31261500
C	-5.16792200	2.45752200	-6.09385100	C	5.21086800	-2.38078200	2.61417300
C	-3.06046000	2.89216200	-7.06732700	C	4.96794100	-0.06620300	-3.49291300
C	-5.63203900	-2.15490800	-4.64067800	C	4.10876100	1.02550100	-3.04663800
C	-4.52137900	-3.07340100	-4.40937200	C	2.48102800	1.09415100	-1.17781300
C	-6.20642100	-0.21002700	-6.06936600	C	2.48102800	1.09415100	1.17781300
C	0.12948400	1.34017100	-6.49420400	C	7.22495700	-0.99640500	-3.04543400
C	0.47901600	-0.01596100	-6.35390300	C	8.26922300	-2.31647000	-0.72900700
C	0.17856500	-1.93477400	-5.01381900	C	7.19043500	-2.88125700	1.43254000
C	-2.22492400	-3.48726000	-5.25785200	C	4.37950900	-1.32426000	3.04471600
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C	-3.66228700	-3.41642400	-5.47733300	C	3.06630600	2.34959300	-0.72796500
C	-5.53908700	0.30027800	-7.26097400	C	3.06630600	2.34959300	0.72796500
C	-0.18974700	-1.02939700	-7.16120100	C	8.34196800	-0.41311200	-2.31709500
C	-0.37749900	-2.21460800	-6.33038900	C	8.26922300	-2.31647000	0.72900700
C	-1.55514000	-2.97663900	-6.45112300	C	8.85831300	-1.06070600	-1.17882200
C	-1.54599000	0.75505600	-8.22572200	C	4.96794100	-0.06620300	3.49291300
C	-2.98520900	0.82930700	-8.44494500	C	4.10876100	1.02550100	3.04663800
C	-4.95794900	-1.97099100	-7.02356700	C	7.22495700	-0.99640500	3.04543400
C	-3.88518600	-2.85550200	-6.80048500	C	6.95353300	1.35109400	-3.04643000
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C	-2.40323900	-1.44202100	-8.20457700	C	8.85831300	-1.06070600	1.17882200
C	3.66573200	-2.84850500	-0.72774500	C	9.22257100	-0.28549100	0.00000000
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C	4.84728600	-3.15233100	-1.43622800	C	4.67769200	2.24078700	2.61474300
C	3.66573200	-2.84850500	0.72774500	C	8.34196800	-0.41311200	2.31709500
C	3.16745200	-1.01111900	-2.31261500	C	6.48890800	3.17945000	-1.43417800
C	2.23555100	-1.10483600	0.00000000	C	5.26558600	3.49365400	-0.70387900
C	5.21086800	-2.38078200	-2.61417300	C	5.26558600	3.49365400	0.70387900

C	8.52620600	1.78468800	-1.17788400	C	-3.55055000	2.04991100	3.19863000
C	9.06080400	1.11430200	0.00000000	C	-7.27806000	1.52466600	-2.34661700
C	6.95353300	1.35109400	3.04643000	C	-6.21386200	4.94909400	-2.58072000
C	6.12381500	2.40508600	2.61435600	C	-7.39297200	2.90681500	-2.58072000
C	8.17361000	1.03705100	2.31641300	C	-4.06287100	5.85827400	1.68024100
C	7.66693300	2.87480000	-0.72900000	C	-3.78720900	4.85961300	2.70763300
C	6.48890800	3.17945000	1.43417800	C	-5.71726600	6.31500500	-0.11337300
C	8.52620600	1.78468800	1.17788400	C	-6.83304000	-0.10001900	-0.69288900
C	7.66693300	2.87480000	0.72900000	C	-6.50931400	-0.27949200	0.67111200
				C	-4.88467200	0.15003600	2.32846700
				C	-4.73010000	2.73092400	3.56615200
(2) $\text{Ca}(\text{C}_{60})_3 \eta^6 \eta^6 \eta^6 (C_{3v})$				C	-7.75322100	0.95448300	-1.08814200
PBE-D3(BJ)/def2-SVP, Singlet				C	-7.26271100	5.03300700	-1.57180900
Ca	0.00000000	0.00000000	0.48720300	C	-7.99006700	3.77318900	-1.57180900
C	-1.92141200	2.77283600	-1.95110400	C	-5.38844400	6.12280000	1.29574200
C	-1.67028800	1.77805100	-0.91924900	C	-4.84933100	4.15967200	3.31453700
C	-2.89548400	2.51303100	-2.93747800	C	-7.01529900	5.70541900	-0.35820300
C	-1.84417500	4.08047300	-1.31764800	C	-7.10485000	0.58941300	1.68024100
C	-2.37498100	0.55748600	-0.91924900	C	-6.10215300	0.85001300	2.70763300
C	-1.39206800	2.46797500	0.34022600	C	-6.02704700	2.11980800	3.31453700
C	-3.62409100	1.25104700	-2.93747800	C	-8.32758800	1.79379500	-0.11337300
C	-3.81924400	3.56827000	-3.33279300	C	-8.44868700	3.22271800	-0.35820300
C	-1.51869600	3.89311300	0.09205100	C	-6.48784000	5.39859300	1.92297600
C	-2.73685900	5.09976900	-1.69976500	C	-6.22353600	4.43480500	2.91328600
C	-3.36205200	0.27757400	-1.95110400	C	-7.49137300	5.13733700	0.89801400
C	-2.83336300	-0.02842100	0.34022600	C	-7.99672200	1.60512900	1.29574200
C	-1.85898500	1.90874200	1.56301100	C	-6.95242200	3.17233800	2.91328600
C	-4.99983400	1.52342700	-3.33279300	C	-8.19475100	3.91905100	0.89801400
C	-5.12062400	2.95639300	-3.57739400	C	-7.91923900	2.91933800	1.92297600
C	-3.74243800	4.83577500	-2.72498600	C	-1.44064000	-3.05041000	-1.95110400
C	-2.09138300	4.72980300	1.06860000	C	-0.70469300	-2.33553700	-0.91924900
C	-3.32990100	5.96759600	-0.69288900	C	-0.72860700	-3.76407800	-2.93747800
C	-4.45588100	-0.44313400	-1.31764800	C	-2.61170600	-3.63733900	-1.31764800
C	-4.13088300	-0.63132700	0.09205100	C	0.70469300	-2.33553700	-0.91924900
C	-2.58251200	0.65555700	1.56301100	C	-1.44129500	-2.43955400	0.34022600
C	-2.45312900	2.77725600	2.57827300	C	0.72860700	-3.76407800	-2.93747800
C	-6.05912300	0.82315900	-2.72498600	C	-1.18059000	-5.09169700	-3.33279300
C	-6.29517600	3.63452200	-3.20751300	C	-2.61218700	-3.26178600	0.09205100
C	-4.95942900	5.54065200	-2.34661700	C	-3.04810000	-4.92007400	-1.69976500
C	-3.01261000	5.77697700	0.67111200	C	1.44064000	-3.05041000	-1.95110400
C	-2.57227100	4.15523200	2.32846700	C	1.44129500	-2.43955400	0.34022600
C	-4.70321700	6.23724500	-1.08814200	C	-0.72352700	-2.56429900	1.56301100
C	-5.78495900	-0.17969500	-1.69976500	C	1.18059000	-5.09169700	-3.33279300
C	-5.14182100	-0.55371100	1.06860000	C	0.00000000	-5.91278700	-3.57739400
C	-3.63173900	0.73584400	2.57827300				



C	-2.31668500	-5.65893400	-2.72498600	C	1.43139900	-8.31793100	1.92297600
C	-3.05043800	-4.17609200	1.06860000	C	3.36205200	0.27757400	-1.95110400
C	-3.50313900	-5.86757700	-0.69288900	C	2.37498100	0.55748600	-0.91924900
C	2.61170600	-3.63733900	-1.31764800	C	3.62409100	1.25104700	-2.93747800
C	2.61218700	-3.26178600	0.09205100	C	4.45588100	-0.44313400	-1.31764800
C	0.72352700	-2.56429900	1.56301100	C	1.67028800	1.77805100	-0.91924900
C	-1.17861000	-3.51310000	2.57827300	C	2.83336300	-0.02842100	0.34022600
C	2.31668500	-5.65893400	-2.72498600	C	2.89548400	2.51303100	-2.93747800
C	0.00000000	-7.26904300	-3.20751300	C	4.99983400	1.52342700	-3.33279300
C	-2.31863100	-7.06531700	-2.34661700	C	4.13088300	-0.63132700	0.09205100
C	-3.49670400	-5.49748500	0.67111200	C	5.78495900	-0.17969500	-1.69976500
C	-2.31240100	-4.30526800	2.32846700	C	1.92141200	2.77283600	-1.95110400
C	-3.05000400	-7.19172800	-1.08814200	C	1.39206800	2.46797500	0.34022600
C	3.04810000	-4.92007400	-1.69976500	C	2.58251200	0.65555700	1.56301100
C	3.05043800	-4.17609200	1.06860000	C	3.81924400	3.56827000	-3.33279300
C	1.17861000	-3.51310000	2.57827300	C	5.12062400	2.95639300	-3.57739400
C	0.00000000	-4.09982200	3.19863000	C	6.05912300	0.82315900	-2.72498600
C	2.31863100	-7.06531700	-2.34661700	C	5.14182100	-0.55371100	1.06860000
C	-1.17911000	-7.85590900	-2.58072000	C	6.83304000	-0.10001900	-0.69288900
C	1.17911000	-7.85590900	-2.58072000	C	1.84417500	4.08047300	-1.31764800
C	-3.04197900	-6.44768600	1.68024100	C	1.51869600	3.89311300	0.09205100
C	-2.31494400	-5.70962600	2.70763300	C	1.85898500	1.90874200	1.56301100
C	-2.61032200	-8.10880000	-0.11337300	C	3.63173900	0.73584400	2.57827300
C	3.50313900	-5.86757700	-0.69288900	C	3.74243800	4.83577500	-2.72498600
C	3.49670400	-5.49748500	0.67111200	C	6.29517600	3.63452200	-3.20751300
C	2.31240100	-4.30526800	2.32846700	C	7.27806000	1.52466600	-2.34661700
C	0.00000000	-5.46184900	3.56615200	C	6.50931400	-0.27949200	0.67111200
C	3.05000400	-7.19172800	-1.08814200	C	4.88467200	0.15003600	2.32846700
C	-0.72735600	-8.80619600	-1.57180900	C	7.75322100	0.95448300	-1.08814200
C	0.72735600	-8.80619600	-1.57180900	C	2.73685900	5.09976900	-1.69976500
C	-2.60827800	-7.72792900	1.29574200	C	2.09138300	4.72980300	1.06860000
C	-1.17771600	-6.27948000	3.31453700	C	2.45312900	2.77725600	2.57827300
C	-1.43338800	-8.92813700	-0.35820300	C	3.55055000	2.04991100	3.19863000
C	3.04197900	-6.44768600	1.68024100	C	4.95942900	5.54065200	-2.34661700
C	2.31494400	-5.70962600	2.70763300	C	7.39297200	2.90681500	-2.58072000
C	1.17771600	-6.27948000	3.31453700	C	6.21386200	4.94909400	-2.58072000
C	2.61032200	-8.10880000	-0.11337300	C	7.10485000	0.58941300	1.68024100
C	1.43338800	-8.92813700	-0.35820300	C	6.10215300	0.85001300	2.70763300
C	-1.43139900	-8.31793100	1.92297600	C	8.32758800	1.79379500	-0.11337300
C	-0.72888600	-7.60714300	2.91328600	C	3.32990100	5.96759600	-0.69288900
C	-0.70337800	-9.05638800	0.89801400	C	3.01261000	5.77697700	0.67111200
C	2.60827800	-7.72792900	1.29574200	C	2.57227100	4.15523200	2.32846700
C	0.72888600	-7.60714300	2.91328600	C	4.73010000	2.73092400	3.56615200
C	0.70337800	-9.05638800	0.89801400	C	4.70321700	6.23724500	-1.08814200

C	7.99006700	3.77318900	-1.57180900	C	-3.74367000	3.47635700	5.41367000
C	7.26271100	5.03300700	-1.57180900	C	-1.52381500	3.02949100	6.43132300
C	7.99672200	1.60512900	1.29574200	C	0.41604900	0.00233300	6.42882700
C	6.02704700	2.11980800	3.31453700	C	0.00144300	-2.06991200	5.37902400
C	8.44868700	3.22271800	-0.35820300	C	-0.85149500	1.98888200	7.20378700
C	4.06287100	5.85827400	1.68024100	C	-5.34755100	0.95722900	2.55751900
C	3.78720900	4.85961300	2.70763300	C	-4.83466800	-1.86308600	2.70855300
C	4.84933100	4.15967200	3.31453700	C	-2.77316900	-3.12109000	3.31659200
C	5.71726600	6.31500500	-0.11337300	C	-1.93542000	-3.35883000	4.48970700
C	7.01529900	5.70541900	-0.35820300	C	-5.68130700	2.19471800	4.53439500
C	7.91923900	2.91933800	1.92297600	C	-2.90950400	3.22961900	6.58597700
C	6.95242200	3.17233800	2.91328600	C	-5.02244500	2.80587500	5.61869000
C	8.19475100	3.91905100	0.89801400	C	-0.34593400	-0.82703400	7.35493600
C	5.38844400	6.12280000	1.29574200	C	-0.60358100	-2.10692300	6.70303400
C	6.22353600	4.43480500	2.91328600	C	-1.58600400	1.18968600	8.09877500
C	7.49137300	5.13733700	0.89801400	C	-6.10199900	0.12411600	3.48590500
C	6.48784000	5.39859300	1.92297600	C	-5.85487900	-1.26050600	3.55722200
(3) Sr(C <sub>60</sub> ) <sub>3</sub> η <sup>2</sup> η <sup>6</sup> η <sup>6</sup> (C <sub>s</sub> )				C	-4.16188100	-2.91123700	3.47420400
PBE-D3(BJ)/def2-SVP, Singlet				C	-2.51751900	-3.39079600	5.77143700
Sr	-0.32422000	-1.68830600	0.00000000	C	-6.31133700	0.89129500	4.70796500
C	-0.50712900	1.56744800	2.70375600	C	-3.66860300	2.40394800	7.51202000
C	-0.76247900	0.29306600	2.05162200	C	-4.97291300	2.13837100	6.91309600
C	-1.51903000	2.54853800	2.75627600	C	-1.32913300	-0.24393000	8.17304900
C	0.31898900	1.31314000	3.87836500	C	-1.83792900	-2.75573800	6.89701000
C	-2.04659500	0.03102300	1.48863300	C	-3.02034100	1.39847700	8.25674100
C	-0.11826900	-0.74820400	2.85243900	C	-5.80000500	-1.92711300	4.85243000
C	-2.83299600	2.27849800	2.16118900	C	-4.75703000	-2.94654200	4.79671600
C	-1.72881100	3.31021000	3.97120100	C	-3.95014400	-3.18634200	5.93134600
C	0.58020600	-0.11597700	3.95908900	C	-6.26016800	0.24619400	5.95728700
C	0.11678100	2.05555600	5.05679800	C	-5.58104900	0.88101600	7.08077900
C	-3.09055700	1.04806500	1.53704700	C	-2.60616000	-0.91882000	8.37566300
C	-2.67441500	-1.26348400	1.67065200	C	-2.85411800	-2.15382900	7.74859900
C	-0.71106000	-2.01687300	3.00887500	C	-3.64951700	0.09714700	8.42879900
C	-3.84787700	2.88369300	3.00892100	C	-6.00080300	-1.18694300	6.03036800
C	-3.16521100	3.51391300	4.13320900	C	-4.15904700	-2.41885500	7.14861900
C	-0.92148500	3.07178400	5.10827800	C	-4.90929500	-0.15943400	7.85061300
C	0.62719100	-0.76880400	5.20870100	C	-5.16608900	-1.43567600	7.20117000
C	0.16572900	1.38466700	6.35440200	C	-3.09055700	1.04806500	-1.53704700
C	-4.36442900	0.37260900	1.73592700	C	-2.04659500	0.03102300	-1.48863300
C	-4.11171400	-1.05940800	1.81052300	C	-2.83299600	2.27849800	-2.16118900
C	-2.01746100	-2.29784600	2.38953800	C	-4.36442900	0.37260900	-1.73592700
C	-0.65505000	-2.69359200	4.29221800	C	-0.76247900	0.29306600	-2.05162200
C	-5.08433300	2.23358100	3.20641500	C	-2.67441500	-1.26348400	-1.67065200
				C	-1.51903000	2.54853800	-2.75627600

C	-3.84787700	2.88369300	-3.00892100	C	-1.58600400	1.18968600	-8.09877500
C	-4.11171400	-1.05940800	-1.81052300	C	-3.02034100	1.39847700	-8.25674100
C	-5.34755100	0.95722900	-2.55751900	C	-5.16608900	-1.43567600	-7.20117000
C	-0.50712900	1.56744800	-2.70375600	C	-4.15904700	-2.41885500	-7.14861900
C	-0.11826900	-0.74820400	-2.85243900	C	-4.90929500	-0.15943400	-7.85061300
C	-2.01746100	-2.29784600	-2.38953800	C	-1.32913300	-0.24393000	-8.17304900
C	-1.72881100	3.31021000	-3.97120100	C	-2.85411800	-2.15382900	-7.74859900
C	-3.16521100	3.51391300	-4.13320900	C	-3.64951700	0.09714700	-8.42879900
C	-5.08433300	2.23358100	-3.20641500	C	-2.60616000	-0.91882000	-8.37566300
C	-4.83466800	-1.86308600	-2.70855300	C	4.13727700	-3.06349400	-0.72807800
C	-6.10199900	0.12411600	-3.48590500	C	3.13396800	-2.10846900	-1.18198300
C	0.31898900	1.31314000	-3.87836500	C	5.35049900	-3.19635600	-1.43539600
C	0.58020600	-0.11597700	-3.95908900	C	4.13727700	-3.06349400	0.72807800
C	-0.71106000	-2.01687300	-3.00887500	C	3.38521300	-1.31313100	-2.31584700
C	-2.77316900	-3.12109000	-3.31659200	C	2.48313200	-1.53419300	0.00000000
C	-0.92148500	3.07178400	-5.10827800	C	5.60253700	-2.38190500	-2.61358000
C	-3.74367000	3.47635700	-5.41367000	C	6.60451000	-3.33349900	-0.70318700
C	-5.68130700	2.19471800	-4.53439500	C	3.13396800	-2.10846900	1.18198300
C	-5.85487900	-1.26050600	-3.55722200	C	5.35049900	-3.19635600	1.43539600
C	-4.16188100	-2.91123700	-3.47420400	C	4.63126100	-1.45273400	-3.04594800
C	-6.31133700	0.89129500	-4.70796500	C	3.01319300	0.10406600	-2.31738200
C	0.11678100	2.05555600	-5.05679800	C	2.14820100	-0.13895900	0.00000000
C	0.62719100	-0.76880400	-5.20870100	C	7.01064900	-2.00967100	-2.61227100
C	-0.65505000	-2.69359200	-4.29221800	C	7.63271100	-2.60004100	-1.43278800
C	-1.93542000	-3.35883000	-4.48970700	C	6.60451000	-3.33349900	0.70318700
C	-1.52381500	3.02949100	-6.43132300	C	3.38521300	-1.31313100	2.31584700
C	-5.02244500	2.80587500	-5.61869000	C	5.60253700	-2.38190500	2.61358000
C	-2.90950400	3.22961900	-6.58597700	C	5.03858200	-0.12455300	-3.49329500
C	-5.80000500	-1.92711300	-4.85243000	C	4.03521700	0.83622200	-3.04711200
C	-4.75703000	-2.94654200	-4.79671600	C	2.41884200	0.67631600	-1.17699200
C	-6.26016800	0.24619400	-5.95728700	C	2.41884200	0.67631600	1.17699200
C	0.16572900	1.38466700	-6.35440200	C	7.40359400	-0.72880200	-3.04497300
C	0.41604900	0.00233300	-6.42882700	C	8.62269200	-1.89121200	-0.72928700
C	0.00144300	-2.06991200	-5.37902400	C	7.63271100	-2.60004100	1.43278800
C	-2.51751900	-3.39079600	-5.77143700	C	4.63126100	-1.45273400	3.04594800
C	-0.85149500	1.98888200	-7.20378700	C	3.01319300	0.10406600	2.31738200
C	-4.97291300	2.13837100	-6.91309600	C	7.01064900	-2.00967100	2.61227100
C	-3.66860300	2.40394800	-7.51202000	C	6.39840400	0.23092800	-3.49330100
C	-6.00080300	-1.18694300	-6.03036800	C	4.42911600	2.11917900	-2.61493000
C	-3.95014400	-3.18634200	-5.93134600	C	2.81900100	2.00279100	-0.72816300
C	-5.58104900	0.88101600	-7.08077900	C	2.81900100	2.00279100	0.72816300
C	-0.34593400	-0.82703400	-7.35493600	C	8.42837900	0.00469500	-2.31717200
C	-0.60358100	-2.10692300	-6.70303400	C	8.62269200	-1.89121200	0.72928700
C	-1.83792900	-2.75573800	-6.89701000	C	9.02926300	-0.56477600	-1.17839300

C	5.03858200	-0.12455300	3.49329500	C	1.00075800	5.71937300	2.84388100
C	4.03521700	0.83622200	3.04711200	C	-0.33276300	5.32295100	-1.05467200
C	7.40359400	-0.72880200	3.04497300	C	0.14105100	6.76780900	0.90871000
C	6.80667800	1.55754600	-3.04733700	C	4.15346900	1.60157300	0.97858700
C	5.83757400	2.48491300	-2.61440300	C	3.98318900	1.45601200	-0.46459000
C	3.80914400	2.71089200	-1.43495300	C	2.03823500	2.04280500	-1.91439100
C	3.80914400	2.71089200	1.43495300	C	0.94064400	3.96830800	-2.71793800
C	8.05858200	1.41718100	-2.31689000	C	4.93870700	3.28798400	2.62020600
C	9.02926300	-0.56477600	1.17839300	C	3.80903100	5.80175300	3.39551700
C	9.28172300	0.25358200	0.00000000	C	1.74801600	6.94996800	2.62837300
C	6.39840400	0.23092800	3.49330100	C	-0.02491600	6.62219000	-0.48784900
C	4.42911600	2.11917900	2.61493000	C	0.38838300	5.19970700	-2.32432800
C	8.42837900	0.00469500	2.31717200	C	1.21678400	7.59534100	1.43053000
C	6.09124900	3.30205000	-1.43354500	C	5.19184800	2.40685500	1.48323000
C	4.83595500	3.44271200	-0.70385900	C	4.85512800	2.11890500	-1.35006200
C	4.83595500	3.44271200	0.70385900	C	2.94362800	2.73018300	-2.83214100
C	8.30413200	2.20694100	-1.17841200	C	2.26239100	3.91888400	-3.32544400
C	8.92475700	1.61666200	0.00000000	C	5.68656800	4.51851300	2.40369000
C	6.80667800	1.55754600	3.04733700	C	3.12819000	6.99180500	2.89786000
C	5.83757400	2.48491300	2.61440300	C	5.13206600	5.75401800	2.78388000
C	8.05858200	1.41718100	2.31689000	C	0.88337000	7.30739500	-1.40120600
C	7.30060000	3.16624500	-0.72910600	C	1.13326300	6.43069000	-2.54027600
C	6.09124900	3.30205000	1.43354500	C	2.09216700	8.25792400	0.54766700
C	8.30413200	2.20694100	1.17841200	C	6.09644000	3.08992600	0.57006300
C	7.30060000	3.16624500	0.72910600	C	5.92436300	2.94773200	-0.82630800
				C	4.32005700	2.77147000	-2.54918800
				C	2.98716600	5.11094600	-3.53160400
				C	6.39939500	4.39513600	1.13471500
				C	4.03206400	7.67997300	1.98476900
				C	5.26841200	6.91630400	1.91429300
				C	1.91980000	8.11016700	-0.89445700
				C	2.41183200	6.38711800	-3.13137800
				C	3.51882200	8.30237000	0.82808700
				C	6.05645700	4.11195400	-1.69562400
				C	5.06898200	3.99919600	-2.76418000
				C	4.41404700	5.15094300	-3.24609000
				C	6.52757900	5.51846100	0.29468900
				C	5.95517800	6.79616600	0.68903700
				C	3.24258700	8.06619100	-1.50615600
				C	3.48521200	7.22058200	-2.60429400
				C	4.23022100	8.17937200	-0.43915800
				C	6.35307800	5.37170000	-1.14697700
				C	4.72396200	6.45558200	-2.67536700
				C	5.42449200	7.43997300	-0.50731900
(4) Sr(C <sub>60</sub> ) <sub>3</sub> η <sup>6</sup> η <sup>6</sup> η <sup>6</sup> (quasi-C <sub>3v</sub> )							
PBE-D3(BJ)/def2-SVP, Singlet.							
Sr	-0.00747500	0.00013200	-1.13873500				
C	0.38583100	3.15849300	1.73501700				
C	0.65632900	2.29829500	0.59353100				
C	1.34837500	3.26422600	2.76137200				
C	-0.28989300	4.34450500	1.23090100				
C	1.85580700	1.56121800	0.52451100				
C	0.10852900	2.92822500	-0.60926900				
C	2.58677400	2.50076200	2.69000200				
C	1.65632800	4.57085800	3.32704200				
C	-0.46287500	4.20127600	-0.21206200				
C	0.00869700	5.60699000	1.77752100				
C	2.83695800	1.64755100	1.59578300				
C	2.56010600	1.41153200	-0.74834300				
C	0.80746200	2.80593600	-1.84250100				
C	3.66261900	3.33300500	3.21303100				
C	3.08735500	4.61383400	3.60691500				

C	5.67624400	6.56338500	-1.64456400	C	4.76047700	-7.26125900	1.94034100
C	2.65351000	-1.85360800	1.63365000	C	3.47902900	-7.95020200	1.96874000
C	1.70649000	-1.69483800	0.54041800	C	6.01253600	-5.74554000	-1.07147000
C	2.32540800	-2.70372300	2.70981100	C	4.14463100	-5.38356600	-3.21498100
C	3.98585500	-1.87911400	1.05023200	C	5.48418000	-7.16664200	0.73412400
C	0.46483300	-2.36166600	0.56844500	C	0.44599200	-7.34810900	-1.48840400
C	2.45179300	-1.57281100	-0.71273700	C	0.77663200	-6.47382800	-2.60853500
C	1.04288500	-3.39344200	2.73916700	C	2.07033000	-6.49975500	-3.16717300
C	3.33610100	-3.60507000	3.24770000	C	1.54561400	-8.39371900	0.47616300
C	3.86206600	-1.70509700	-0.39417400	C	2.95989300	-8.52647000	0.79141400
C	4.96160200	-2.75057300	1.56957600	C	5.27935200	-6.88831700	-1.60238300
C	0.11474500	-3.21823000	1.69125000	C	4.36172100	-6.71139300	-2.65490200
C	-0.08993500	-2.94060800	-0.65570400	C	4.94729300	-7.76249900	-0.48384100
C	1.92380800	-2.15847900	-1.89868800	C	1.41994600	-8.21710300	-0.96732200
C	1.25802600	-4.72303800	3.29491000	C	3.07846100	-7.40196800	-2.62517100
C	2.67623300	-4.85412000	3.60960400	C	3.70980200	-8.43002000	-0.45583400
C	4.62751300	-3.62901300	2.68762900	C	2.75816100	-8.24521000	-1.54498000
C	4.71631900	-2.40684500	-1.26687900	C	-2.96246100	-1.42538800	1.61238600
C	5.84825900	-3.47389100	0.67014400	C	-2.34196900	-0.67540100	0.53066900
C	-0.61757800	-4.35487600	1.15421700	C	-3.52745900	-0.72594000	2.69883600
C	-0.74571800	-4.18298600	-0.29058200	C	-3.66399500	-2.54870900	1.01036400
C	0.64717100	-2.84512700	-1.86981200	C	-2.28052200	0.73184100	0.58194700
C	2.81008700	-2.88589200	-2.80346500	C	-2.61580800	-1.35841400	-0.73328400
C	0.54812700	-5.82414900	2.77976100	C	-3.46514500	0.72832300	2.75161000
C	3.33183500	-6.08009300	3.39941500	C	-4.81881700	-1.14296600	3.22903300
C	5.30755800	-4.89866100	2.47373000	C	-3.45007400	-2.50800600	-0.43357100
C	5.72052700	-3.30471700	-0.72823000	C	-4.91265300	-2.94997300	1.52196400
C	4.17426800	-3.01120800	-2.48809600	C	-2.83997900	1.45218300	1.71470500
C	6.05847000	-4.80198700	1.22414900	C	-2.49753700	1.52411300	-0.63029800
C	-0.40753600	-5.63955200	1.69032000	C	-2.84880700	-0.58739400	-1.90820300
C	-0.65960300	-5.29996800	-1.14485200	C	-4.71836000	1.21407100	3.31369000
C	0.73449100	-4.00286700	-2.75642900	C	-5.55582400	0.05691000	3.60950300
C	2.07212600	-4.02511000	-3.33031100	C	-5.49817800	-2.23201500	2.65082200
C	1.22621800	-7.09480600	2.56634900	C	-4.49043600	-2.86864300	-1.31193200
C	4.67043600	-6.10361700	2.82155800	C	-5.98765800	-3.32681600	0.61569300
C	2.59438500	-7.22082000	2.86834800	C	-3.44279900	2.67077200	1.19613500
C	5.80474300	-4.46383800	-1.60950700	C	-3.22986600	2.71637600	-0.24767600
C	4.85417600	-4.27917400	-2.70121900	C	-2.79098900	0.86078000	-1.85429800
C	6.14142800	-5.92033400	0.37210400	C	-3.92743300	-0.96295400	-2.81977700
C	-0.32255400	-6.79479100	0.80954300	C	-5.30206000	2.39482000	2.81583400
C	-0.44433200	-6.62252200	-0.58878900	C	-6.94423200	0.12345100	3.39881300
C	0.09947400	-5.20393900	-2.39524700	C	-6.93731400	-2.16362700	2.43664700
C	2.73019100	-5.25532000	-3.53516600	C	-5.77606100	-3.28181700	-0.78126800
C	0.68850700	-7.69210600	1.34623800	C	-4.73282100	-2.07566300	-2.52089800

C	-7.23734700	-2.83928900	1.17711200	C	-3.352429	3.449779	3.253646
C	-4.65440300	3.13835400	1.73859600	C	-3.908397	1.555668	-0.372573
C	-4.23227600	3.22712300	-1.09635400	C	-4.984901	2.553756	1.617099
C	-3.82868900	1.39091300	-2.73542900	C	-0.171764	3.168070	1.621149
C	-4.52996200	0.26141800	-3.32789200	C	-0.019783	2.906311	-0.724389
C	-6.74027300	2.46400400	2.60093000	C	-2.029479	2.071119	-1.913118
C	-7.64786900	-1.00616700	2.80216900	C	-1.311382	4.628178	3.253646
C	-7.54808000	1.34828300	2.88645200	C	-2.722256	4.715086	3.603806
C	-6.81529400	-2.74863900	-1.65579600	C	-4.650229	3.436592	2.729130
C	-6.16974500	-2.00936500	-2.73519600	C	-4.800068	2.230229	-1.215503
C	-8.24049700	-2.32583900	0.33137800	C	-5.911375	3.253806	0.744295
C	-5.69073900	3.66964300	0.86443000	C	0.511561	4.325231	1.072501
C	-5.47977100	3.70744000	-0.53281900	C	0.606951	4.162605	-0.372573
C	-4.53698100	2.54450300	-2.35658000	C	-0.778903	2.793140	-1.913118
C	-5.92370900	0.32788500	-3.53347800	C	-2.957733	2.770092	-2.792898
C	-6.97865300	3.24995500	1.39311300	C	-0.651061	5.745512	2.729130
C	-8.68771800	-0.47850400	1.92745100	C	-3.414785	5.914582	3.415596
C	-8.62651300	0.97424100	1.97996900	C	-5.370704	4.684352	2.537094
C	-8.02375300	-2.28117300	-1.11125100	C	-5.815369	3.093537	-0.649781
C	-6.75643600	-0.82737000	-3.23175200	C	-4.308657	2.852766	-2.445802
C	-8.97650900	-1.13038900	0.71139900	C	-6.148207	4.570124	1.308328
C	-6.55824700	3.32865900	-1.43939200	C	0.280833	5.593929	1.617099
C	-5.97463100	2.61570400	-2.57043000	C	0.468599	5.272095	-1.215503
C	-6.65661600	1.52527100	-3.14679600	C	-0.920104	3.946518	-2.792898
C	-8.02011700	2.88587700	0.51726200	C	-2.269131	3.930250	-3.331898
C	-8.85657000	1.73344900	0.81417100	C	-1.371416	6.993342	2.537094
C	-8.63083000	-1.05849100	-1.62339100	C	-4.765682	5.899846	2.872349
C	-8.00931000	-0.34443100	-2.66465000	C	-2.726576	7.077125	2.872349
C	-9.21498500	-0.34490600	-0.49462400	C	-5.957470	4.250450	-1.522804
C	-7.80343700	2.92706400	-0.92554400	C	-5.030713	4.098221	-2.636467
C	-7.94772400	1.11092700	-2.61241500	C	-6.285380	5.681937	0.467509
C	-9.15599100	1.05929600	-0.44415300	C	0.137809	6.746304	0.744295
C	-8.51018000	1.79972900	-1.52179400	C	0.228603	6.583026	-0.649781

(5)  $\text{Sr}(\text{C}_{60})_3 \eta^6 \eta^6 \eta^6 (\text{C}_{3v})$  (for EDA-NOCV)

BP86-D3(BJ)/TZP, Singlet

Sr	0.000000	0.000000	-1.190176
C	-2.657747	1.732787	1.621149
C	-1.737352	1.609331	0.506673
C	-2.330511	2.583174	2.686998
C	-4.001541	1.719590	1.072501
C	-0.525046	2.309257	0.506673
C	-2.507047	1.470288	-0.724389
C	-1.071839	3.309869	2.686998

C	-3.352429	3.449779	3.253646
C	-3.908397	1.555668	-0.372573
C	-4.984901	2.553756	1.617099
C	-0.171764	3.168070	1.621149
C	-0.019783	2.906311	-0.724389
C	-2.029479	2.071119	-1.913118
C	-1.311382	4.628178	3.253646
C	-2.722256	4.715086	3.603806
C	-4.650229	3.436592	2.729130
C	-4.800068	2.230229	-1.215503
C	-5.911375	3.253806	0.744295
C	0.511561	4.325231	1.072501
C	0.606951	4.162605	-0.372573
C	-0.778903	2.793140	-1.913118
C	-2.957733	2.770092	-2.792898
C	-0.651061	5.745512	2.729130
C	-3.414785	5.914582	3.415596
C	-5.370704	4.684352	2.537094
C	-5.815369	3.093537	-0.649781
C	-4.308657	2.852766	-2.445802
C	-6.148207	4.570124	1.308328
C	0.280833	5.593929	1.617099
C	0.468599	5.272095	-1.215503
C	-0.920104	3.946518	-2.792898
C	-2.269131	3.930250	-3.331898
C	-1.371416	6.993342	2.537094
C	-4.765682	5.899846	2.872349
C	-2.726576	7.077125	2.872349
C	-5.957470	4.250450	-1.522804
C	-5.030713	4.098221	-2.636467
C	-6.285380	5.681937	0.467509
C	0.137809	6.746304	0.744295
C	0.228603	6.583026	-0.649781
C	-0.316240	5.157789	-2.445802
C	-2.964374	5.134446	-3.513958
C	-0.883740	7.609566	1.308328
C	-4.911189	7.054581	1.998404
C	-3.653852	7.780505	1.998404
C	-6.188683	5.516084	-0.977123
C	-4.370937	5.218952	-3.158903
C	-5.658971	6.944293	0.817539
C	-0.702262	7.284546	-1.522804
C	-1.033807	6.405836	-2.636467
C	-2.334276	6.394819	-3.158903

C	-1.778011	8.284267	0.467509	C	6.659733	3.034096	-1.522804
C	-3.184448	8.372959	0.817539	C	6.064520	2.307615	-2.636467
C	-5.504088	6.680340	-1.519940	C	8.063391	2.602330	0.467509
C	-4.613162	6.535269	-2.588858	C	5.773566	-3.492498	0.744295
C	-5.172362	7.560234	-0.408813	C	5.586766	-3.489489	-0.649781
C	-1.682727	8.117599	-0.977123	C	4.624896	-2.305023	-2.445802
C	-3.353128	7.262750	-2.588858	C	5.928748	0.000000	-3.513958
C	-3.961174	8.259514	-0.408813	C	7.031947	-3.039442	1.308328
C	-3.033301	8.106850	-1.519940	C	8.565041	0.725924	1.998404
C	2.829511	1.435283	1.621149	C	8.565041	-0.725924	1.998404
C	2.262398	0.699925	0.506673	C	7.871410	2.601515	-0.977123
C	3.402350	0.726695	2.686998	C	6.705214	1.175867	-3.158903
C	3.489979	2.605641	1.072501	C	8.843419	1.428666	0.817539
C	2.262398	-0.699925	0.506673	C	6.659733	-3.034096	-1.522804
C	2.526830	1.436023	-0.724389	C	6.064520	-2.307615	-2.636467
C	3.402350	-0.726695	2.686998	C	6.705214	-1.175867	-3.158903
C	4.663811	1.178399	3.253646	C	8.063391	-2.602330	0.467509
C	3.301446	2.606937	-0.372573	C	8.843419	-1.428666	0.817539
C	4.704068	3.040173	1.617099	C	8.537388	1.426510	-1.519940
C	2.829511	-1.435283	1.621149	C	7.966290	0.727481	-2.588858
C	2.526830	-1.436023	-0.724389	C	9.133536	0.699280	-0.408813
C	2.808381	0.722020	-1.913118	C	7.871410	-2.601515	-0.977123
C	4.663811	-1.178399	3.253646	C	7.966290	-0.727481	-2.588858
C	5.444512	0.000000	3.603806	C	9.133536	-0.699280	-0.408813
C	5.301290	2.308921	2.729130	C	8.537388	-1.426510	-1.519940
C	4.331469	3.041866	-1.215503	C	-0.171764	-3.168070	1.621149
C	5.773566	3.492498	0.744295	C	-0.525046	-2.309257	0.506673
C	3.489979	-2.605641	1.072501	C	-1.071839	-3.309869	2.686998
C	3.301446	-2.606937	-0.372573	C	0.511561	-4.325231	1.072501
C	2.808381	-0.722020	-1.913118	C	-1.737352	-1.609331	0.506673
C	3.877836	1.176426	-2.792898	C	-0.019783	-2.906311	-0.724389
C	5.301290	-2.308921	2.729130	C	-2.330511	-2.583174	2.686998
C	6.829570	0.000000	3.415596	C	-1.311382	-4.628178	3.253646
C	6.742119	2.308990	2.537094	C	0.606951	-4.162605	-0.372573
C	5.586766	3.489489	-0.649781	C	0.280833	-5.593929	1.617099
C	4.624896	2.305023	-2.445802	C	-2.657747	-1.732787	1.621149
C	7.031947	3.039442	1.308328	C	-2.507047	-1.470288	-0.724389
C	4.704068	-3.040173	1.617099	C	-0.778903	-2.793140	-1.913118
C	4.331469	-3.041866	-1.215503	C	-3.352429	-3.449779	3.253646
C	3.877836	-1.176426	-2.792898	C	-2.722256	-4.715086	3.603806
C	4.538262	0.000000	-3.331898	C	-0.651061	-5.745512	2.729130
C	6.742119	-2.308990	2.537094	C	0.468599	-5.272095	-1.215503
C	7.492257	1.177279	2.872349	C	0.137809	-6.746304	0.744295
C	7.492257	-1.177279	2.872349	C	-4.001541	-1.719590	1.072501

C	-3.908397	-1.555668	-0.372573	Ba	-0.32937600	-2.13295100	0.00000000
C	-2.029479	-2.071119	-1.913118	C	-0.39383100	1.35552700	2.71474400
C	-0.920104	-3.946518	-2.792898	C	-0.73461900	0.07652900	2.11349400
C	-4.650229	-3.436592	2.729130	C	-1.33332200	2.40717800	2.71668000
C	-3.414785	-5.914582	3.415596	C	0.40435600	1.09400900	3.90729800
C	-1.371416	-6.993342	2.537094	C	-2.02722400	-0.11836700	1.54359300
C	0.228603	-6.583026	-0.649781	C	-0.16833400	-0.97232900	2.96274100
C	-0.316240	-5.157789	-2.445802	C	-2.65754900	2.20527500	2.11985800
C	-0.883740	-7.609566	1.308328	C	-1.49689400	3.23381800	3.89607000
C	-4.984901	-2.553756	1.617099	C	0.56411300	-0.34490600	4.04966100
C	-4.800068	-2.230229	-1.215503	C	0.24731300	1.89823500	5.05148100
C	-2.957733	-2.770092	-2.792898	C	-2.99655800	0.97179300	1.54148500
C	-2.269131	-3.930250	-3.331898	C	-2.74722600	-1.35653900	1.77264000
C	-5.370704	-4.684352	2.537094	C	-0.85487600	-2.18587000	3.16824100
C	-2.726576	-7.077125	2.872349	C	-3.63306400	2.91744400	2.92987900
C	-4.765682	-5.899846	2.872349	C	-2.91615100	3.54587000	4.03426600
C	-0.702262	-7.284546	-1.522804	C	-0.71729200	2.98605100	5.05015200
C	-1.033807	-6.405836	-2.636467	C	0.55464500	-0.94607100	5.32650000
C	-1.778011	-8.284267	0.467509	C	0.23831200	1.28049300	6.37633200
C	-5.911375	-3.253806	0.744295	C	-4.31755000	0.39752900	1.75509400
C	-5.815369	-3.093537	-0.649781	C	-4.16727300	-1.04483100	1.89215200
C	-4.308657	-2.852766	-2.445802	C	-2.17245000	-2.39929700	2.54834800
C	-2.964374	-5.134446	-3.513958	C	-0.85592200	-2.81065300	4.47864900
C	-6.148207	-4.570124	1.308328	C	-4.91356200	2.36528900	3.14129800
C	-3.653852	-7.780505	1.998404	C	-3.50468100	3.60296400	5.30956600
C	-4.911189	-7.054581	1.998404	C	-1.32934600	3.04370600	6.36799100
C	-1.682727	-8.117599	-0.977123	C	0.39006600	-0.11142600	6.51141000
C	-2.334276	-6.394819	-3.158903	C	-0.16419900	-2.19017100	5.54494100
C	-3.184448	-8.372959	0.817539	C	-0.73887500	1.99087300	7.18967100
C	-5.957470	-4.250450	-1.522804	C	-5.26235100	1.08453600	2.54263600
C	-5.030713	-4.098221	-2.636467	C	-4.95232800	-1.75585700	2.81650900
C	-4.370937	-5.218952	-3.158903	C	-2.99084700	-3.12845700	3.49932900
C	-6.285380	-5.681937	0.467509	C	-2.18093700	-3.37615200	4.69003600
C	-5.658971	-6.944293	0.817539	C	-5.52090500	2.42414700	4.46387300
C	-3.033301	-8.106850	-1.519940	C	-2.69866200	3.34771100	6.49980900
C	-3.353128	-7.262750	-2.588858	C	-4.82883300	3.03287900	5.52864500
C	-3.961174	-8.259514	-0.408813	C	-0.43472300	-0.84534200	7.46396500
C	-6.188683	-5.516084	-0.977123	C	-0.77875800	-2.13004400	6.86345300
C	-4.613162	-6.535269	-2.588858	C	-1.53496100	1.28362500	8.10903400
C	-5.172362	-7.560234	-0.408813	C	-6.08003200	0.34699200	3.49765000
C	-5.504088	-6.680340	-1.519940	C	-5.93250100	-1.04710900	3.62923100
				C	-4.36278200	-2.81616300	3.63275600
				C	-2.77258000	-3.31419700	5.96586600
				C	-6.24327100	1.17769900	4.68467800

(6) Ba(C<sub>60</sub>)<sub>3</sub> η<sup>2</sup>η<sup>6</sup>η<sup>6</sup> (C<sub>s</sub>)  
PBE-D3(BJ)/def2-SVP, Singlet



C	-3.52111800	2.61614500	7.45084300	C	-6.24327100	1.17769900	-4.68467800
C	-4.83633900	2.41836300	6.84995900	C	0.24731300	1.89823500	-5.05148100
C	-1.38028500	-0.16022400	8.24713400	C	0.55464500	-0.94607100	-5.32650000
C	-2.05772600	-2.68118400	7.07106800	C	-0.85592200	-2.81065300	-4.47864900
C	-2.95160200	1.59946600	8.24287200	C	-2.18093700	-3.37615200	-4.69003600
C	-5.93590300	-1.66132300	4.95165400	C	-1.32934600	3.04370600	-6.36799100
C	-4.96768100	-2.75314700	4.94947800	C	-4.82883300	3.03287900	-5.52864500
C	-4.18836800	-3.00182800	6.10169000	C	-2.69866200	3.34771100	-6.49980900
C	-6.24737100	0.58331100	5.96021700	C	-5.93590300	-1.66132300	-4.95165400
C	-5.53339500	1.21538300	7.06310700	C	-4.96768100	-2.75314700	-4.94947800
C	-2.70412200	-0.73386100	8.46312600	C	-6.24737100	0.58331100	-5.96021700
C	-3.03498600	-1.97295000	7.88490300	C	0.23831200	1.28049300	-6.37633200
C	-3.67288900	0.35483100	8.46379600	C	0.39006600	-0.11142600	-6.51141000
C	-6.09177800	-0.85972100	6.09579100	C	-0.16419900	-2.19017100	-5.54494100
C	-4.35113300	-2.17054600	7.28340200	C	-2.77258000	-3.31419700	-5.96586600
C	-4.94365300	0.16369800	7.88365000	C	-0.73887500	1.99087300	-7.18967100
C	-5.28623800	-1.11737700	7.28514500	C	-4.83633900	2.41836300	-6.84995900
C	-2.99655800	0.97179300	-1.54148500	C	-3.52111800	2.61614500	-7.45084300
C	-2.02722400	-0.11836700	-1.54359300	C	-6.09177800	-0.85972100	-6.09579100
C	-2.65754900	2.20527500	-2.11985800	C	-4.18836800	-3.00182800	-6.10169000
C	-4.31755000	0.39752900	-1.75509400	C	-5.53339500	1.21538300	-7.06310700
C	-0.73461900	0.07652900	-2.11349400	C	-0.43472300	-0.84534200	-7.46396500
C	-2.74722600	-1.35653900	-1.77264000	C	-0.77875800	-2.13004400	-6.86345300
C	-1.33332200	2.40717800	-2.71668000	C	-2.05772600	-2.68118400	-7.07106800
C	-3.63306400	2.91744400	-2.92987900	C	-1.53496100	1.28362500	-8.10903400
C	-4.16727300	-1.04483100	-1.89215200	C	-2.95160200	1.59946600	-8.24287200
C	-5.26235100	1.08453600	-2.54263600	C	-5.28623800	-1.11737700	-7.28514500
C	-0.39383100	1.35552700	-2.71474400	C	-4.35113300	-2.17054600	-7.28340200
C	-0.16833400	-0.97232900	-2.96274100	C	-4.94365300	0.16369800	-7.88365000
C	-2.17245000	-2.39929700	-2.54834800	C	-1.38028500	-0.16022400	-8.24713400
C	-1.49689400	3.23381800	-3.89607000	C	-3.03498600	-1.97295000	-7.88490300
C	-2.91615100	3.54587000	-4.03426600	C	-3.67288900	0.35483100	-8.46379600
C	-4.91356200	2.36528900	-3.14129800	C	-2.70412200	-0.73386100	-8.46312600
C	-4.95232800	-1.75585700	-2.81650900	C	4.47273000	-3.15866700	-0.72807900
C	-6.08003200	0.34699200	-3.49765000	C	3.38031800	-2.30601700	-1.18171000
C	0.40435600	1.09400900	-3.90729800	C	5.69253600	-3.17277400	-1.43594500
C	0.56411300	-0.34490600	-4.04966100	C	4.47273000	-3.15866700	0.72807900
C	-0.85487600	-2.18587000	-3.16824100	C	3.55036900	-1.49063200	-2.31772600
C	-2.99084700	-3.12845700	-3.49932900	C	2.68471800	-1.79396200	0.00000000
C	-0.71729200	2.98605100	-5.05015200	C	5.86320300	-2.33682700	-2.61450300
C	-3.50468100	3.60296400	-5.30956600	C	6.95366600	-3.18582100	-0.70331700
C	-5.52090500	2.42414700	-4.46387300	C	3.38031800	-2.30601700	1.18171000
C	-5.93250100	-1.04710900	-3.62923100	C	5.69253600	-3.17277400	1.43594500
C	-4.36278200	-2.81616300	-3.63275600	C	4.80587100	-1.50661700	-3.04625800

C	3.04234500	-0.11619200	-2.31965300	C	7.93640200	1.68443000	2.31711100
C	2.21392600	-0.44242900	0.00000000	C	7.00998900	3.34983800	-0.72897400
C	7.22857300	-1.82956000	-2.61362300	C	5.79344200	3.36793800	1.43433100
C	7.90496000	-2.35580100	-1.43303200	C	8.10310700	2.49415200	1.17827100
C	6.95366600	-3.18582100	0.70331700	C	7.00998900	3.34983800	0.72897400
C	3.55036900	-1.49063200	2.31772600				
C	5.86320300	-2.33682700	2.61450300	(7) Ba(C <sub>60</sub> ) <sub>3</sub> η <sup>6</sup> η <sup>6</sup> η <sup>6</sup> (quasi-C <sub>3v</sub> )			
C	5.08096500	-0.14547000	-3.49391100	PBE-D3(BJ)/def2-SVP, Singlet			
C	3.98809800	0.71303600	-3.04863300	Ba	0.01442500	-1.85958700	0.00000000
C	2.39808900	0.39499500	-1.17772800	C	2.85342300	1.14573200	1.56766300
C	2.39808900	0.39499500	1.17772800	C	1.89196500	0.05284900	1.58346100
C	7.49419100	-0.51590000	-3.04519300	C	2.53665600	2.35019500	2.22870200
C	8.81904100	-1.55250500	-0.72897100	C	4.17673400	0.55733800	1.69349500
C	7.90496000	-2.35580100	1.43303200	C	0.64562000	0.20822600	2.22528200
C	4.80587100	-1.50661700	3.04625800	C	2.61766500	-1.21244000	1.66647800
C	3.04234500	-0.11619200	2.31965300	C	1.25197400	2.51023700	2.89441500
C	7.22857300	-1.82956000	2.61362300	C	3.55148200	3.01566600	3.03534400
C	6.40002100	0.34125400	-3.49310400	C	4.03279700	-0.89591200	1.75260100
C	4.25440400	2.02906800	-2.61732300	C	5.15600100	1.19873800	2.47578900
C	2.66684500	1.75425600	-0.72781000	C	0.30918300	1.46025600	2.88615200
C	2.66684500	1.75425600	0.72781000	C	0.07180300	-0.89722200	2.99550900
C	8.44215800	0.31456000	-2.31710200	C	2.06976900	-2.28010000	2.43534500
C	8.81904100	-1.55250500	0.72897100	C	1.46950200	3.27211600	4.11668800
C	9.09525300	-0.19301800	-1.17827100	C	2.89132300	3.58600400	4.20421300
C	5.08096500	-0.14547000	3.49391100	C	4.83468200	2.45041500	3.15803900
C	3.98809800	0.71303600	3.04863300	C	4.86894800	-1.65058400	2.59962800
C	7.49419100	-0.51590000	3.04519300	C	6.02320700	0.41795800	3.34406100
C	6.67619600	1.70094700	-3.04683300	C	-0.43461500	1.12634900	4.09036000
C	5.62096700	2.52977000	-2.61556400	C	-0.58487400	-0.32513400	4.15601600
C	3.58060100	2.55667200	-1.43571200	C	0.79148400	-2.11937300	3.10337700
C	3.58060100	2.55667200	1.43571200	C	2.93950300	-3.06407500	3.30775200
C	7.93640200	1.68443000	-2.31711100	C	0.74690100	2.95508700	5.28236900
C	9.09525300	-0.19301800	1.17827100	C	3.53764400	3.57111700	5.45248600
C	9.26756300	0.64592600	0.00000000	C	5.50411000	2.43693700	4.45111900
C	6.40002100	0.34125400	3.49310400	C	5.87810200	-0.98749100	3.40403500
C	4.25440400	2.02906800	2.61732300	C	4.30771000	-2.74966100	3.39079900
C	8.44215800	0.31456000	2.31710200	C	6.23701000	1.17914400	4.56494700
C	5.79344200	3.36793800	-1.43433100	C	-0.22372400	1.86268200	5.27154400
C	4.53100800	3.38444300	-0.70406400	C	-0.51457200	-0.98685900	5.39882200
C	4.53100800	3.38444300	0.70406400	C	0.85976000	-2.80728700	4.39005900
C	8.10310700	2.49415200	-1.17827100	C	2.18951600	-3.38782100	4.51441900
C	8.77937000	1.96803600	0.00000000	C	1.41609500	2.94277400	6.57487400
C	6.67619600	1.70094700	3.04683300	C	4.86815700	2.98700900	5.57890200
C	5.62096700	2.52977000	2.61556400	C	2.78799200	3.24413000	6.66008600

C	5.94444100	-1.66833100	4.69158200	C	-3.38921800	-0.55463700	-2.61678700
C	4.97885600	-2.76263600	4.68095800	C	-3.04945100	-2.14457500	-0.72573200
C	6.30404500	0.51987400	5.80804000	C	-4.20534900	-2.91474900	1.17843800
C	-0.15592800	1.18094700	6.55481500	C	-5.08509600	2.73591900	-2.31628800
C	-0.29776100	-0.22504100	6.61397500	C	-6.54420500	3.57190400	0.00000000
C	0.22664700	-2.24463700	5.51243800	C	-6.54026700	2.68591900	2.31655700
C	2.83815400	-3.39602700	5.76533200	C	-5.70178500	-0.60938200	3.50065100
C	0.85912500	1.84300100	7.35881900	C	-4.91965000	-2.49268000	2.31325500
C	4.93956700	2.30384700	6.86478000	C	-6.94965100	1.49007200	3.04891900
C	3.65639900	2.46364100	7.53231300	C	-4.59889500	1.56875600	-3.04771700
C	6.15446500	-0.93122300	5.87010100	C	-4.50553600	-1.29667500	-3.05196800
C	4.25654700	-3.07760200	5.84949400	C	-4.20534900	-2.91474900	-1.17843800
C	5.64755200	1.08975300	6.97473700	C	-4.91723100	-3.38829000	0.00000000
C	0.57467300	-1.00539700	7.48353300	C	-6.54026700	2.68591900	-2.31655700
C	0.89287700	-2.25839900	6.80603200	C	-7.25866600	3.09530500	1.17862900
C	2.17833900	-2.82157200	6.93007700	C	-7.25866600	3.09530500	-1.17862900
C	1.69981100	1.08905200	8.20015000	C	-6.85683900	-1.37405300	3.04386300
C	3.11746600	1.40236900	8.28861400	C	-6.37339600	-2.54295300	2.31623300
C	5.40853300	-1.25793800	7.07875900	C	-8.06559800	0.75028700	2.61020900
C	4.47610900	-2.31290000	7.06977700	C	-5.75097900	0.80381700	-3.50256300
C	5.09024800	-0.00779200	7.75800500	C	-5.70178500	-0.60938200	-3.50065100
C	1.55299900	-0.36286100	8.26222200	C	-4.91965000	-2.49268000	-2.31325500
C	3.19092800	-2.15380800	7.73794700	C	-6.32653600	-3.43381200	0.00000000
C	3.84898500	0.14624200	8.40165400	C	-6.94965100	1.49007200	-3.04891900
C	2.88240400	-0.94571000	8.39143100	C	-8.41486800	2.33023200	0.72743500
C	-2.72129600	1.38739900	1.44066100	C	-8.41486800	2.33023200	-0.72743500
C	-2.26020200	0.21927800	0.70511800	C	-8.01588200	-0.70861000	2.60872800
C	-3.19237000	2.51018300	0.72775500	C	-7.06586200	-3.00317500	1.17810400
C	-3.43704000	0.90507400	2.61217800	C	-8.80897900	1.17574700	1.43463900
C	-2.26020200	0.21927800	-0.70511800	C	-6.85683900	-1.37405300	-3.04386300
C	-2.64890400	-0.98206600	1.44373200	C	-6.37339600	-2.54295300	-2.31623300
C	-3.19237000	2.51018300	-0.72775500	C	-7.06586200	-3.00317500	-1.17810400
C	-4.39466900	3.19785900	1.17984900	C	-8.06559800	0.75028700	-2.61020900
C	-3.38921800	-0.55463700	2.61678700	C	-8.80897900	1.17574700	-1.43463900
C	-4.59889500	1.56875600	3.04771700	C	-8.73318000	-1.18479700	1.43183800
C	-2.72129600	1.38739900	-1.44066100	C	-8.26730600	-2.31148200	0.72864400
C	-2.64890400	-0.98206600	-1.44373200	C	-9.21724500	-0.01835200	0.70328300
C	-3.04945100	-2.14457500	0.72573200	C	-8.01588200	-0.70861000	-2.60872800
C	-4.39466900	3.19785900	-1.17984900	C	-8.26730600	-2.31148200	-0.72864400
C	-5.13913100	3.62332000	0.00000000	C	-9.21724500	-0.01835200	-0.70328300
C	-5.08509600	2.73591900	2.31628800	C	-8.73318000	-1.18479700	-1.43183800
C	-4.50553600	-1.29667500	3.05196800	C	0.30918300	1.46025600	-2.88615200
C	-5.75097900	0.80381700	3.50256300	C	0.64562000	0.20822600	-2.22528200
C	-3.43704000	0.90507400	-2.61217800	C	1.25197400	2.51023700	-2.89441500

C	-0.43461500	1.12634900	-4.09036000
C	1.89196500	0.05284900	-1.58346100
C	0.07180300	-0.89722200	-2.99550900
C	2.53665600	2.35019500	-2.22870200
C	1.46950200	3.27211600	-4.11668800
C	-0.58487400	-0.32513400	-4.15601600
C	-0.22372400	1.86268200	-5.27154400
C	2.85342300	1.14573200	-1.56766300
C	2.61766500	-1.21244000	-1.66647800
C	0.79148400	-2.11937300	-3.10337700
C	3.55148200	3.01566600	-3.03534400
C	2.89132300	3.58600400	-4.20421300
C	0.74690100	2.95508700	-5.28236900
C	-0.51457200	-0.98685900	-5.39882200
C	-0.15592800	1.18094700	-6.55481500
C	4.17673400	0.55733800	-1.69349500
C	4.03279700	-0.89591200	-1.75260100
C	2.06976900	-2.28010000	-2.43534500
C	0.85976000	-2.80728700	-4.39005900
C	4.83468200	2.45041500	-3.15803900
C	3.53764400	3.57111700	-5.45248600
C	1.41609500	2.94277400	-6.57487400
C	-0.29776100	-0.22504100	-6.61397500
C	0.22664700	-2.24463700	-5.51243800
C	0.85912500	1.84300100	-7.35881900
C	5.15600100	1.19873800	-2.47578900
C	4.86894800	-1.65058400	-2.59962800
C	2.93950300	-3.06407500	-3.30775200
C	2.18951600	-3.38782100	-4.51441900
C	5.50411000	2.43693700	-4.45111900
C	2.78799200	3.24413000	-6.66008600
C	4.86815700	2.98700900	-5.57890200
C	0.57467300	-1.00539700	-7.48353300
C	0.89287700	-2.25839900	-6.80603200
C	1.69981100	1.08905200	-8.20015000
C	6.02320700	0.41795800	-3.34406100
C	5.87810200	-0.98749100	-3.40403500
C	4.30771000	-2.74966100	-3.39079900
C	2.83815400	-3.39602700	-5.76533200
C	6.23701000	1.17914400	-4.56494700
C	3.65639900	2.46364100	-7.53231300
C	4.93956700	2.30384700	-6.86478000
C	1.55299900	-0.36286100	-8.26222200
C	2.17833900	-2.82157200	-6.93007700

C	3.11746600	1.40236900	-8.28861400
C	5.94444100	-1.66833100	-4.69158200
C	4.97885600	-2.76263600	-4.68095800
C	4.25654700	-3.07760200	-5.84949400
C	6.30404500	0.51987400	-5.80804000
C	5.64755200	1.08975300	-6.97473700
C	2.88240400	-0.94571000	-8.39143100
C	3.19092800	-2.15380800	-7.73794700
C	3.84898500	0.14624200	-8.40165400
C	6.15446500	-0.93122300	-5.87010100
C	4.47610900	-2.31290000	-7.06977700
C	5.09024800	-0.00779200	-7.75800500
C	5.40853300	-1.25793800	-7.07875900

(8) Ba(C<sub>60</sub>)<sub>3</sub> η<sup>6</sup>η<sup>6</sup> (C<sub>3v</sub>) (for EDA-NOCV)

BP86-D3(BJ)/TZP, Singlet

Ba	0.000000	0.000000	1.817288
C	2.572035	1.585419	-1.349176
C	1.718703	1.577023	-0.175422
C	2.180456	2.324055	-2.475065
C	3.944957	1.623746	-0.881899
C	0.506391	2.276952	-0.175422
C	2.558796	1.559023	1.015597
C	0.922462	3.050358	-2.475065
C	3.165556	3.126363	-3.183795
C	3.937310	1.603433	0.576174
C	4.893449	2.394614	-1.563460
C	0.086996	3.020157	-1.349176
C	0.070755	2.995494	1.015597
C	2.149237	2.278069	2.163049
C	1.124732	4.304633	-3.183795
C	2.512479	4.351742	-3.622667
C	4.492006	3.162277	-2.737587
C	4.874668	2.357838	1.292930
C	5.867143	3.175457	-0.820875
C	-0.566274	4.228306	-0.881899
C	-0.580041	4.211527	0.576174
C	0.898247	3.000329	2.163049
C	3.124637	3.058532	2.912575
C	0.492609	5.471330	-2.737587
C	3.211296	5.562128	-3.596857
C	5.218259	4.420459	-2.713805
C	5.853862	3.156381	0.585892
C	4.453187	3.102362	2.480471

C	6.066029	4.428159	-1.526899	C	-2.629551	-1.436471	1.015597
C	-0.372928	5.435158	-1.563460	C	-3.047484	0.722259	2.163049
C	-0.395386	5.400506	1.292930	C	-4.290288	-1.178270	-3.183795
C	1.086448	4.235282	2.912575	C	-5.024959	0.000000	-3.622667
C	2.464728	4.269034	3.372757	C	-4.984615	2.309053	-2.737587
C	1.219101	6.729374	-2.713805	C	-4.479282	3.042667	1.292930
C	4.591197	5.598080	-3.134037	C	-5.683598	3.493366	-0.820875
C	2.552481	6.775134	-3.134037	C	-3.378684	-2.604560	-0.881899
C	6.041958	4.394838	1.327693	C	-3.357269	-2.608094	0.576174
C	5.181177	4.358022	2.502742	C	-3.047484	-0.722259	2.163049
C	6.249028	5.618750	-0.812227	C	-4.211085	1.176749	2.912575
C	-0.183545	6.668823	-0.820875	C	-4.984615	-2.309053	-2.737587
C	-0.193425	6.647784	0.585892	C	-6.422592	0.000000	-3.596857
C	0.460131	5.407754	2.480471	C	-6.437359	2.308915	-2.713805
C	3.165482	5.482775	3.390175	C	-5.660437	3.491403	0.585892
C	0.801883	7.467415	-1.526899	C	-4.913318	2.305392	2.480471
C	4.783941	6.834213	-2.390822	C	-6.867913	3.039256	-1.526899
C	3.526631	7.560121	-2.390822	C	-4.520521	-3.040544	-1.563460
C	6.236558	5.599297	0.645694	C	-4.479282	-3.042667	1.292930
C	4.549199	5.527262	2.947101	C	-4.211085	-1.176749	2.912575
C	5.599562	6.841261	-1.250463	C	-4.929456	0.000000	3.372757
C	0.785063	7.429908	1.327693	C	-6.437359	-2.308915	-2.713805
C	1.183569	6.666042	2.502742	C	-7.143678	1.177054	-3.134037
C	2.512150	6.703353	2.947101	C	-7.143678	-1.177054	-3.134037
C	1.741466	8.221192	-0.812227	C	-6.827020	3.035070	1.327693
C	3.124925	8.269994	-1.250463	C	-6.364747	2.308020	2.502742
C	5.581322	6.813618	1.107282	C	-7.990494	2.602442	-0.812227
C	4.753770	6.779355	2.235454	C	-5.683598	-3.493366	-0.820875
C	5.182403	7.577817	-0.065828	C	-5.660437	-3.491403	0.585892
C	1.730854	8.200666	0.645694	C	-4.913318	-2.305392	2.480471
C	3.494209	7.506563	2.235454	C	-6.330964	0.000000	3.390175
C	3.971381	8.277001	-0.065828	C	-6.867913	-3.039256	-1.526899
C	3.110105	8.240376	1.107282	C	-8.310572	0.725909	-2.390822
C	-2.659031	1.434738	-1.349176	C	-8.310572	-0.725909	-2.390822
C	-2.225093	0.699929	-0.175422	C	-7.967412	2.601369	0.645694
C	-3.102918	0.726303	-2.475065	C	-7.061348	1.176091	2.947101
C	-3.378684	2.604560	-0.881899	C	-8.724487	1.428732	-1.250463
C	-2.225093	-0.699929	-0.175422	C	-6.827020	-3.035070	1.327693
C	-2.629551	1.436471	1.015597	C	-6.364747	-2.308020	2.502742
C	-3.102918	-0.726303	-2.475065	C	-7.061348	-1.176091	2.947101
C	-4.290288	1.178270	-3.183795	C	-7.990494	-2.602442	-0.812227
C	-3.357269	2.608094	0.576174	C	-8.724487	-1.428732	-1.250463
C	-4.520521	3.040544	-1.563460	C	-8.691427	1.426758	1.107282
C	-2.659031	-1.434738	-1.349176	C	-8.247979	0.727208	2.235454

C	-9.153784	0.699184	-0.065828	C	4.893449	-2.394614	-1.563460
C	-7.967412	-2.601369	0.645694	C	4.874668	-2.357838	1.292930
C	-8.247979	-0.727208	2.235454	C	3.124637	-3.058532	2.912575
C	-9.153784	-0.699184	-0.065828	C	2.464728	-4.269034	3.372757
C	-8.691427	-1.426758	1.107282	C	5.218259	-4.420459	-2.713805
C	0.086996	-3.020157	-1.349176	C	2.552481	-6.775134	-3.134037
C	0.506391	-2.276952	-0.175422	C	4.591197	-5.598080	-3.134037
C	0.922462	-3.050358	-2.475065	C	0.785063	-7.429908	1.327693
C	-0.566274	-4.228306	-0.881899	C	1.183569	-6.666042	2.502742
C	1.718703	-1.577023	-0.175422	C	1.741466	-8.221192	-0.812227
C	0.070755	-2.995494	1.015597	C	5.867143	-3.175457	-0.820875
C	2.180456	-2.324055	-2.475065	C	5.853862	-3.156381	0.585892
C	1.124732	-4.304633	-3.183795	C	4.453187	-3.102362	2.480471
C	-0.580041	-4.211527	0.576174	C	3.165482	-5.482775	3.390175
C	-0.372928	-5.435158	-1.563460	C	6.066029	-4.428159	-1.526899
C	2.572035	-1.585419	-1.349176	C	3.526631	-7.560121	-2.390822
C	2.558796	-1.559023	1.015597	C	4.783941	-6.834213	-2.390822
C	0.898247	-3.000329	2.163049	C	1.730854	-8.200666	0.645694
C	3.165556	-3.126363	-3.183795	C	2.512150	-6.703353	2.947101
C	2.512479	-4.351742	-3.622667	C	3.124925	-8.269994	-1.250463
C	0.492609	-5.471330	-2.737587	C	6.041958	-4.394838	1.327693
C	-0.395386	-5.400506	1.292930	C	5.181177	-4.358022	2.502742
C	-0.183545	-6.668823	-0.820875	C	4.549199	-5.527262	2.947101
C	3.944957	-1.623746	-0.881899	C	6.249028	-5.618750	-0.812227
C	3.937310	-1.603433	0.576174	C	5.599562	-6.841261	-1.250463
C	2.149237	-2.278069	2.163049	C	3.110105	-8.240376	1.107282
C	1.086448	-4.235282	2.912575	C	3.494209	-7.506563	2.235454
C	4.492006	-3.162277	-2.737587	C	3.971381	-8.277001	-0.065828
C	3.211296	-5.562128	-3.596857	C	6.236558	-5.599297	0.645694
C	1.219101	-6.729374	-2.713805	C	4.753770	-6.779355	2.235454
C	-0.193425	-6.647784	0.585892	C	5.182403	-7.577817	-0.065828
C	0.460131	-5.407754	2.480471	C	5.581322	-6.813618	1.107282
C	0.801883	-7.467415	-1.526899				

Geometric coordinates of the most stable configuration of  $M_2(C_{60})_3$ -HL (M = Ca, Sr, Ba) (VASP format)

(1) $Ca_2(C_{60})_3$ -HL- $P\bar{3}m1$				0.6194463357184700	0.5017768091569398	0.4246930797243478
PBE-D3(BJ)/PAW, 0 $\mu_B$				0.5415556490672102	0.4598389999558337	0.4052264175124345
Lattice constants				0.5795152393010320	0.6524063389593802	0.5949698327311697
19.7000007629000002	0.0000000000000000	0.0000000000000000	-	0.3798831475821906	0.4968918138006359	0.6039729682984487
9.8500003814999992	17.0607011152999988	0.0000000000000000		0.4991179873172650	0.6170325550651038	0.6043474372494432
0.0000000000000000	0.0000000000000000	30.0000000000000000		0.3210164399750479	0.3696962763144394	0.4592580325393216
Ca	C			0.3779395247613664	0.3872656228385462	0.4238827680106150
2	180			0.2969264434241221	0.4359834742955886	0.5219867256105089
Direct				0.6719754511367889	0.6813684364386492	0.5378073867935321
0.6665014785402609	0.3326993979981424	0.4917952241706071		0.6808255763757567	0.6733408494352253	0.4918956405809082
0.3330153217688083	0.6668406516932593	0.5365694645487228		0.6538374065549247	0.5819730606986361	0.4343814707355826
0.5074729731463450	0.3468584437954988	0.5733534325337227		0.5009942786769160	0.4996383313814322	0.3957540768839299
0.5641502380288388	0.3651300472453310	0.5380112193032268		0.6107809842843966	0.6955750924183944	0.5534640586256666
0.5235712130508601	0.4013919740828562	0.6075061738130085		0.3735427441086053	0.5489206338977372	0.5722792490807264
0.4300374315100429	0.3054659138111235	0.5533861621374532		0.4470124312967265	0.6230169765091409	0.5725315494254094
0.6354881396107024	0.4369537675392250	0.5382262372306155		0.3059465867316831	0.4279409372140426	0.4745500243856438
0.5219254670372528	0.3344667577858066	0.4964282419018058		0.4176661175751969	0.4627948591506625	0.4051466606105060
0.5973617670263240	0.4757330963960584	0.6077273744749807		0.3330040524083936	0.5187425286406154	0.5318622909338170
0.4625171040272365	0.4158577808487173	0.6232063218294895		0.6284108976461785	0.6793480049112839	0.4601472495769335
0.4389643246538922	0.2973849192449833	0.5059485435860148		0.6120088322718381	0.6230736050082351	0.4245579052328541
0.3708917527622400	0.3192854480243718	0.5685456950299990		0.5367893540242586	0.5827787221539030	0.4054993643756140
0.6525301998814448	0.4929605418092266	0.5737775289881074		0.5603714693685774	0.7013066321140008	0.5227509072608147
0.6662642991465163	0.4799371901282602	0.4968408873755659		0.4774144667873680	0.6642221693693499	0.5322822989302182
0.5523298552300234	0.3756747133894583	0.4561721010054154		0.3467725484884008	0.5057176819726332	0.4549418280190399
0.5816469279419897	0.5358714838625649	0.6235517786291109		0.4019773504998086	0.5229286501146179	0.4210213696125394
0.4983052888152086	0.4990066519793201	0.6329370112341767		0.3637651614160428	0.5617314740098907	0.4904883168836089
0.3873106563351021	0.3755778176352113	0.6041286723198949		0.5692861019961606	0.6931961641900763	0.4753196442710096
0.3885733898601754	0.3030863621554795	0.4752269667722321		0.4757671239331939	0.5972658799262882	0.4212330822278447
0.3185152489487821	0.3253245264397518	0.5367889215531984		0.4351221774936100	0.6336191740452118	0.4906910812212796
0.6933493354410255	0.5707222356889228	0.5541562839913433		0.4918423935324136	0.6518170842572619	0.4553634408645692
0.7023371019959898	0.5626626728336689	0.5067136191508426		0.8396024040728982	0.4929823279532186	0.5735903132649183
0.6257646400977245	0.4497472731883481	0.4564125488345828		0.8009360229095860	0.4361224388404756	0.5383819808408957
0.5002162529404470	0.3816466481307336	0.4243541026010864		0.8782096325187518	0.4770058528981167	0.6077100907677383
0.6213953858941562	0.6113909400950920	0.6048100824357261		0.8756027801649109	0.5703054314999820	0.5534574320942232
0.4577666964632134	0.5388159808495807	0.6234562279241886		0.8014048195598096	0.3647968337268397	0.5386703925061714
0.3455026563294371	0.4166903940867092	0.5942837799039198		0.8123261556725323	0.4781287619723238	0.4967126574116465
0.3273994477528394	0.3173280186669351	0.4908857505620057		0.8786273182457780	0.4031520910424419	0.6080260845805381
0.4198128356672089	0.3462409133939839	0.4337093439977140		0.9538765828192558	0.5380695821937719	0.6231996562373963
0.3030615691456128	0.3856275987952866	0.5525815383373150		0.8582746273589041	0.5611123430281165	0.5060490774386330
0.6783514753822101	0.6290077373155949	0.5694419305365878		0.9487221005382744	0.6294480601673109	0.5684147938282631
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0.0012009972223964	0.5022356973161999	0.6329139217201617	0.1979047890723352	0.5642472981774255	0.4902604425727727
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0.8231564930972545	0.373844808999869	0.4567833843817565	0.5632499325987631	0.1984368934069088	0.5398362817011992
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0.9504714143597891	0.321713377662473	0.5697173109209718	0.6266707417637707	0.1776583879145046	0.4583144967071684
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0.1856562298817932	0.6667476234220686	0.5313125700627811	0.5438553628814289	0.0837833052605466	0.4064864700953851
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0.4211126249498807	0.0738419099194088	0.4345891233740665	0.5523918777456306	0.3768407623038916	0.4597744707654211
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0.3752695199848466	0.8233817744726040	0.5720535282487461	0.3915659474646536	0.3070450957818424	0.4770930751083245
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0.4055284803873028	0.8804204424772993	0.4210388632698246	0.6942959898186399	0.6098221616582128	0.4777886450544420
0.3670179623179232	0.8023248419197319	0.4901093119971742	0.6197158753595648	0.4994218079593303	0.4271475463039974
0.3499562283572454	0.8414962329501253	0.4546566622112289	0.5439486281548932	0.4581419511168694	0.4069966222485559
			0.5773379384543855	0.6529298022544858	0.5935346451273295
			0.3811367001920855	0.5016163322785095	0.6017690872079514
			0.4983514455382062	0.6188643801890129	0.6020404801914013
			0.3265095205663584	0.3726077544356757	0.4585711635334041
			0.3831734537810620	0.3884443543374452	0.4239528711694500
			0.3015446553885246	0.4397695546303262	0.5194782393192646
			0.6693034860452935	0.6790242969444683	0.5376385196660667
			0.6791483473498247	0.6696646401744690	0.4920882594780194
			0.6536801606122864	0.5783103950706397	0.4359141972310073
			0.5049224431185177	0.4972358032446533	0.3959608889938176
			0.6092822927429309	0.6939850094369182	0.5518322396262964
			0.3761089846373041	0.5518434165172814	0.5689822190765064
			0.4484649721166858	0.6242062085104417	0.5691434131726447
			0.3116990682461949	0.4303998236289220	0.4723981712642533
			0.4230428320764298	0.4618425185624820	0.4044957141008354
			0.3370709926758749	0.5212013307430622	0.5283916460346235
			0.6288581018700555	0.6750136496038818	0.4592661126726229
			0.6134265916776617	0.6187265088085748	0.4244752892760329
			0.5402172919301214	0.5790289171854117	0.4047709798621801
			0.5610355468393998	0.6993333292573337	0.5200792198169071
			0.4795142602317191	0.6636888198787394	0.5287219241281182
			0.3527704103271939	0.5060670656868000	0.4520920500601046
			0.4077453944164459	0.5215981322365175	0.4188945952033296

(2)  $\text{Sr}_2(\text{C}_{60})_3\text{-HL-}P\bar{3}m1$

PBE-D3(BJ)/PAW, 0  $\mu_B$

Lattice constants

20.1000003814999992 0.0000000000000000 0.0000000000000000

-10.0500001907000005 17.4071109463999996 0.0000000000000000

0.0000000000000000 0.0000000000000000 30.0000000000000000

Sr C

2 180

Direct

0.6666083225010079 0.3333542186185519 0.4921212400437679

0.3333052044618148 0.6665764688485567 0.5371378619859105

0.5053969887784298 0.3522657172058818 0.5765018061762012

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0.5931077129802763 0.4794399610420173 0.6100452180719913

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0.6480647843491169 0.4949558226462050 0.5768324043207054

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0.0753500281492402	0.4215852060020171	0.5929710075501831	0.6932124239742193	0.0846535607193184	0.4777764334258557
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0.6522673303717280	0.0752871131126765	0.4359984448153463
0.6089654632842959	0.9158150811277658	0.5520747958434716
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0.3902225833755810	0.0841849106083321	0.4776993597132198
0.5008268973899912	0.1199295834217626	0.4272451057156033
0.5422514598657044	0.0854298183691787	0.4072927508715464
0.3469003049451974	0.9246731675559621	0.5937696660259582
0.4983350922829064	0.8800379178202763	0.6025228548335292
0.3810078327338457	0.8798531107963303	0.6024849073345289
0.6278444972360214	0.9539585663243575	0.4594512668702581
0.6120643843004601	0.9945814749978479	0.4246802646051606
0.5605501459600890	0.8620487544515385	0.5204447868290074
0.3208834431213087	0.9902125028332938	0.5376230635112862
0.3303756312357014	0.0092165120649416	0.4920504587844660
0.4219159718125695	0.0749445222111455	0.4359358606592490
0.5032747160075687	0.0072579173036409	0.3963667292228515
0.3059724666335745	0.9153187280985802	0.5519885533534995
0.4482617794518694	0.8246100258749551	0.5697578857904175
0.3758328821013645	0.8244916248087851	0.5697374932928227
0.5700782170775749	0.8813849131836163	0.4733356358068594
0.5387364702114193	0.9608861371309484	0.4051178857798658
0.4790719123420996	0.8161143971409678	0.5292721261009197
0.3252113816647421	0.9534700617180639	0.4593635378291029
0.3816251457611126	0.9942263579645850	0.4246169870137744
0.4214441216045522	0.9607018965921479	0.4050884309908508
0.3008068275712804	0.8616250472435057	0.5203730240120977
0.3364922014021227	0.8158311696765029	0.5292352172435590
0.4944823078274841	0.8466357553347721	0.4529226660780193
0.4790005320668123	0.8858672590396672	0.4195690681473722
0.4382917299215111	0.8066900265485401	0.4876099002698940
0.3106037147911103	0.8809654470162381	0.4732633585513931
0.4063691081321149	0.8857557512987750	0.4195567883493742
0.3679939390782667	0.8065523488513221	0.4875919837970196
0.3516537943485576	0.8464055300254973	0.4528857911454712

(3)  $\text{Ba}_2(\text{C}_{60})_3\text{-HL-}P\bar{3}m1$

PBE-D3(BJ)/PAW, 0  $\mu\text{B}$

Lattice constants

20.1000003814999992	0.0000000000000000	0.0000000000000000
-10.0500001907000005	17.4071109463999996	0.0000000000000000
0.0000000000000000	0.0000000000000000	30.0000000000000000

Ba C

2 180

Direct

0.6666705589900715	0.3332440068633530	0.4599921351481079
0.3333676783043308	0.6666081175651682	0.5691237992768662
0.5120603832199021	0.3431586334602779	0.5605367093975704
0.5634034775515122	0.3649075689015318	0.5226529590613118
0.5321569191315453	0.3924625318036365	0.5973529513324226
0.4339636085494579	0.3050345965753074	0.5435224461207595
0.6337046158562345	0.4351185592246771	0.5229704869725282
0.5172008726942270	0.3396969972431622	0.4823364032923443
0.6047986523801594	0.4650082245211808	0.5976873706728479
0.4747659373019110	0.4048996425681373	0.6186659855923209
0.4371107403085794	0.3024390330107133	0.4951977122017032
0.3784029343287289	0.3170926924639640	0.5640544678477969
0.6548075077708136	0.4857205262142375	0.5611756691420626
0.6597733723724235	0.4821236979579185	0.4829702643673147
0.5426377814121386	0.3850894814400942	0.4433679818120249
0.5920925948283331	0.5220662054588324	0.6192120603958932
0.5116412359055005	0.4850919843590710	0.6319759173259253
0.3990019239671059	0.3679147833451740	0.6023858275588525
0.3848304446830382	0.3121930778130976	0.4690687876562707
0.3239124146000736	0.3268999411318509	0.5370615332152476
0.6934109960957736	0.5641486370290675	0.5446815767702023
0.6969606921109124	0.5619499749286141	0.4963559809894568
0.6151478084392081	0.4575202358475668	0.4436957519773196
0.4885768027558418	0.3949728412648780	0.4163097500834169
0.6295540832061063	0.5981582742655880	0.6034402797658083
0.4716702931293175	0.5253004219690048	0.6287534814494488
0.3577397218645358	0.4094599694285848	0.5989764293869304
0.3272385472843427	0.3244968581344890	0.4903088040783778
0.4110021677012529	0.3593585385763532	0.4289257754001676
0.3113680876954911	0.3841757672635995	0.5585100138644384
0.6811203150735839	0.6194003620281325	0.5654254117427756
0.6878869721434248	0.6148408174558542	0.4704122286785608
0.6059750158570690	0.5122112201786094	0.4168266020638354
0.5275648987403897	0.4737019603518196	0.4001921487459236
0.5882397120313063	0.6396391140051652	0.6000117299334043
0.3932669798810802	0.4867807512238027	0.6121016937879593
0.5106599180949131	0.6040274378156405	0.6126394269132560
0.3181075850098570	0.3796057601829733	0.4635147729862232
0.3696804403061658	0.4008397621677697	0.4255058679092334
0.3022759346244153	0.4370679223285659	0.5325726673970224
0.6719859458239141	0.6744933423988841	0.5386189908288164
0.6753182325361803	0.6721012982796288	0.4918620430119960

0.6415036229492500	0.5895334253046515	0.4299530183175043	0.0520853015520659	0.6425878262241753	0.5988021381084681
0.4875812693185730	0.5138941240023199	0.3969558745535520	0.9974106931145795	0.6727025265663504	0.4901166476862345
0.6143862719316528	0.6867603375280016	0.5598593650318284	0.9483754539535744	0.5887264532052535	0.4288389552278659
0.3840866428030299	0.5414588587110342	0.5852249606898524	0.0731081106257078	0.6888325283186716	0.5582863139875771
0.4566052974651899	0.6138779627296760	0.5855533116600297	0.9385044710484707	0.3190625247185996	0.5656406088507120
0.3058134249027688	0.4348700096584622	0.4842483038395349	0.9269888055926512	0.3119731288417071	0.4706344430914722
0.4071354839794021	0.4769290138961452	0.4097281004904190	0.9062018918579109	0.3937170258963635	0.4169588478346928
0.3394500219734335	0.5168989279308092	0.5459560818359631	0.9460749432615690	0.4720681259816069	0.4002264232204519
0.6208420705237468	0.6819107259926790	0.4648639248346370	0.0517035412340669	0.4120768532032319	0.6001039627004645
0.6002418561778613	0.6310770295738856	0.4265376475287347	0.0938836060898347	0.6070933551719332	0.6119627769985376
0.5244806972083462	0.5940918764985894	0.4102600215075824	0.0937085404749136	0.4896901834191433	0.6126434360460004
0.5621130509710696	0.6965230003369359	0.5337231303866034	0.0615974118685382	0.6817406304005607	0.4632995558847177
0.4820441715590245	0.6592820363561909	0.5465887470304274	0.0311772458584350	0.6300293281801009	0.4253566213927309
0.3444215398122866	0.5133020863908277	0.467756540533030	0.1350226001286663	0.6978084036418754	0.5323269223094125
0.3944331865863091	0.5339978019139630	0.4312370354838752	0.0026817658679116	0.3281048933859214	0.5388144775914673
0.3655264398012270	0.5638955860751657	0.5059611554426464	0.9968520404029017	0.3246023752452059	0.4920615622647590
0.5652648505366983	0.6939421285073134	0.4854008604748630	0.9480035832975575	0.3582252641222495	0.4301210281234785
0.4670846416303049	0.6065411126759153	0.4315604431012590	0.0262507952683907	0.5120257806169805	0.3969341873042619
0.4358306953666363	0.6340860183945858	0.5062732124112619	0.0725986910718865	0.3857687588029113	0.5599823215688349
0.4871712701949730	0.6558325681725166	0.4683889140769700	0.1576712771695283	0.6161548748757857	0.5850646073050854
0.8313528594502315	0.4881435684804655	0.5605747120474435	0.1575685633227112	0.5436377276864103	0.5854851409763352
0.8016601755355049	0.4366594172338615	0.5227532394307438	0.1291961975510208	0.6941057485763681	0.4840081163237993
0.8606362502352176	0.4681744174809175	0.5974101299466917	0.0697687386801444	0.5925183281602413	0.4096164934468502
0.8713114486003807	0.5661890371998460	0.5434654435164261	0.1776676031706013	0.6606418414652115	0.5457435957897991
0.8015743412239302	0.3663634536586230	0.5231479278494542	0.0610965878075583	0.3789729767899146	0.4649901110891349
0.8226076943288234	0.4827325007642055	0.4823838631585551	0.0308026524617330	0.3994558496956579	0.4266443409298474
0.8605138580838703	0.3955168176979919	0.5978279423507730	0.0695618376110305	0.4751555628070137	0.4102688003480771
0.9305261263178767	0.5256433571444288	0.6186411088433523	0.1345800903352266	0.4379344984385009	0.5337763489387639
0.8654732720180132	0.5628688312319629	0.4951468203759317	0.1774332835857113	0.5180514347644399	0.5465426415921792
0.9389909474046835	0.6218159173097321	0.5639215691968787	0.1689889127701331	0.6554297779889638	0.4675555529974029
0.8311222544152446	0.3453680636494410	0.5613765107861345	0.1395872302828747	0.6052870434792571	0.4310962070336050
0.8224417926866070	0.3401695441234760	0.4831781693056197	0.1985296695177101	0.6344374839661923	0.5057819425102665
0.8424789452473901	0.4571580581963762	0.4434413552386826	0.1287535256636998	0.4346122310207344	0.4854584321002355
0.9303239184306367	0.4082925790153408	0.6193295639698998	0.1394513795464841	0.5326198782146533	0.4315040738042425
0.9738425827836747	0.4887962727906458	0.6319964053676864	0.1983872830164099	0.5641226791068757	0.5061751191248831
0.9692860885254695	0.6013413218209209	0.6022652947724548	0.1687186205198705	0.5126497326351956	0.4683533795893320
0.9274682285457685	0.6150494023436283	0.4689525305605576	0.6546184608798032	0.1692861466715195	0.5621375893492180
0.0032439505530637	0.6762106166337130	0.5368620686002449	0.6337570882275637	0.1987443301088281	0.5238023517805729
0.8709136082448626	0.3066975062332624	0.5449203873574214	0.6041786695119000	0.1396651871706118	0.5984447654867785
0.8650866146917191	0.3030058812821086	0.4965980646052305	0.6936767736763305	0.1297677317785000	0.5458659197285565
0.8423930516664352	0.3846493661229204	0.4438480645050858	0.5633188214046719	0.1983520060046533	0.5231740778909795
0.9063787891015832	0.5111213871456152	0.4163087334717287	0.6604287501722624	0.1780891508884120	0.4839543363873569
0.9689092711973345	0.3707676233056475	0.6035912496683867	0.5313719331020337	0.1392422688626469	0.5977922404234894
0.0540192887221236	0.5287537933570613	0.6287154504768053	0.5914951944082032	0.0699034052181627	0.6199707791138476

0.6977362207810525	0.1356652047224120	0.4975491195669616	0.3402983568408252	0.8221969238623972	0.5458332031893725
0.6814123770568419	0.0622180288223360	0.5666096438275389	0.4891876654560388	0.8318652730113421	0.4689287015906919
0.5115356846243648	0.1684365643426592	0.5608572901506172	0.4693531986587681	0.8610620623256718	0.4319897194896988
0.5175575657983521	0.1773247240879611	0.4826800128582748	0.4374351955831942	0.8019923023900056	0.5066121694688382
0.6162599329113182	0.1580448460744573	0.4445031447624740	0.3070628950737600	0.8705388974001265	0.4839403799433780
0.4739141896170163	0.0692232832073459	0.6189106322733114	0.3965431174279902	0.8606337010842757	0.4313312817907506
0.5109124586062354	0.0261269133666312	0.6324295555114314	0.3669912286248298	0.8015844275895359	0.5059769910968277
0.6294009117715639	0.0315889102024858	0.6044160107553265	0.3461294229676131	0.8310411399358076	0.4676535852490372
0.6892212927001971	0.0738936132259002	0.4716281708750517			
0.6728451574350405	0.9981833018652908	0.5398321030319916			
0.4336337837632612	0.1282647535462873	0.5435433801916993			
0.4373321546987959	0.1342075934790497	0.4952274887836330			
0.5435996192659713	0.1576561416012213	0.4438514575631465			
0.6076783953400690	0.0944022047759293	0.4176489484516979			
0.3983466372901912	0.0302469074314516	0.6023424337017254			
0.4712445113308473	0.9459601445452818	0.6291089724870546			
0.5883850402677960	0.9487940474626181	0.6008869689965199			
0.6766981861852909	0.0040902266392279	0.4930838861169499			
0.6433148967225892	0.0528156747622831	0.4309808697547379			
0.6151858282129030	0.9281202462313684	0.5608842325073115			
0.3780082594740841	0.0604566306858535	0.5638962990317276			
0.3855223288961095	0.0721778284661008	0.4689205484844817			
0.4900375318837094	0.0937424025059126	0.4165998538359302			
0.5294827122689029	0.0543285773678569	0.4006968969725329			
0.3574014608442681	0.9474618470924907	0.5988281342775705			
0.5106799484505151	0.9065368113936085	0.6132047164307312			
0.3930445448773542	0.9058809488938667	0.6121480086780967			
0.6227093820938813	0.9398080040329974	0.4659047246145371			
0.6023831014401347	0.9700288865659198	0.4274493134031023			
0.5633875504864605	0.8660802429727311	0.5345755542238000			
0.3240036898062456	0.9961691603603279	0.5367233084510623			
0.3278746513933148	0.0021078543692934	0.4899759996227530			
0.4123314406802693	0.0515004598688283	0.4289142512925420			
0.4898130806812538	0.9741662314995198	0.3973564231900106			
0.3114759937669482	0.9263667981431668	0.5581783543023674			
0.4571149425986357	0.8426309604790641	0.5859391571745500			
0.3844569912139251	0.8422299295641789	0.5852882754887836			
0.5670754514282155	0.8720198535249062	0.4862563161504657			
0.5268125964388379	0.9310703665040743	0.4108663761948463			
0.4831570412766337	0.8229598568438538	0.5471160667406068			
0.3193335158037353	0.9380808012447326	0.4632012177548328			
0.3713285600911501	0.9687120597051362	0.4253892486720123			
0.4092293657645685	0.9303987938987537	0.4098172347215739			
0.3029782480998906	0.8646080097900430	0.5322533083444739			