Electronic supplementary information

Be atoms in fullerenes: strong metal-cage covalency with formation of Be-Be banana bonds, multicenter bonds and trapped superatoms

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†Electronic supplementary information (ESI) available.

Table S1 Relative energies (ΔE, kcal/mol) of $Be@C_{2n}$ ($2n$ = 24, 32, 60, 74) with different spin multiplicities (M) at the M06-2X/6-31G* level of theory.

species	*M*	Δ*E*
$Be@C_{24}$	1	**0.0**
	3	14.6
$Be@C_{32}$	1	**0.0**
	3	14.8
$Be@C_{60}$	1	**0.0**
	3	45.7
$Be@C_{74}$	1	**0.0**
	3	15.4

Table S2 Encapsulation energies (E_e, kcal/mol) and HOMO-LUMO gaps (eV) of Be-based EMFs at the M06-2X/6-31G* level of theory.

species	E_e	gap	species	E_e	gap
$Be@C_{24}$	-38.7	3.74	$Be_7@C_{60}$	-372.1	2.97
$Be@C_{32}$	-34.2	3.71	$Be_8@C_{60}$	-441.7	2.31
$Be@C_{60}$	-18.9	4.21	$Be_9@C_{60}$	-490.2	2.60
$Be@C_{74}$	-31.7	2.89	$Be_{10}@C_{60}$	-521.9	3.57
$Be_2@C_{60}$	-62.8	2.53	$Be_{11}@C_{60}$	-540.6	3.40
$Be_2@C_{74}$	-123.0	2.78	$Be_{12}@C_{60}$	-564.1	3.25
$Be_3@C_{60}$	-126.9	2.61	$Be_{13}@C_{60}$	-583.7	3.05
$Be_4@C_{60}$	-164.5	2.52	$Be_{14}@C_{60}$	-552.9	2.63
$Be_5@C_{60}$	-220.0	2.31	$(Be_{13}@C_{60})^{4-}$	-446.6	2.65
$Be_6@C_{60}$	-304.9	2.98			

Table S3 Interatomic distances (d, Å), Mayer bond orders (MBOs) and density descriptors (a.u.) at the BCPs for the Be-Be and Be-cage bondings in Be-based EMFs.

species	atom pair	MBO	d	ρ	$\nabla^2\rho$	H	$\lvert V\rvert/G$	G/ρ
$Be@C_{24}$	Be-C1	0.31	1.73	0.08	0.44	-0.02	1.15	1.63
$Be@C_{32}$	Be-C1	0.31	1.71	0.09	0.46	-0.02	1.14	1.75
	Be-C2	0.31	1.71	0.09	0.46	-0.02	1.14	1.75
$Be@C_{60}$	Be-C1	0.00	3.54	0.01	0.01	0.00	1.00	0.30
$Be@C_{74}$	Be-C1	0.39	1.71	0.08	0.40	-0.02	1.15	1.63
$Be_2@C_{60}$	Be1-Be2	1.01	2.01	0.07	-0.05	-0.04	3.50	0.29
	Be1-C1	0.19	1.91	0.05	0.24	-0.01	1.14	1.40
	Be1-C2	0.19	1.91	0.05	0.24	-0.01	1.16	1.32
	Be2-C3	0.19	1.91	0.05	0.24	-0.01	1.14	1.40
	Be2-C4	0.19	1.91	0.05	0.24	-0.01	1.16	1.32
$Be_2@C_{74}$	Be1-Be2	1.01	2.13	0.06	-0.04	-0.03	1.83	0.36
	Be1-C1	0.20	2.01	0.04	0.18	-0.01	1.20	1.25
	Be2-C2	0.22	1.95	0.05	0.24	-0.01	1.14	1.40
$Be_3@C_{60}$	Be1-Be2	0.49	2.08	0.06	-0.01	-0.03	2.07	0.47
	Be1-Be3	0.49	2.08	0.06	-0.01	-0.03	2.07	0.47
	Be2-Be3	0.49	2.08	0.06	-0.01	-0.03	2.07	0.47
	Be1-C1	0.23	1.83	0.06	0.27	-0.01	1.14	1.32
	Be1-C2	0.25	1.82	0.06	0.27	-0.01	1.16	1.35
	Be1-C3	0.23	1.83	0.06	0.27	-0.01	1.15	1.32
	Be2-C4	0.23	1.83	0.06	0.27	-0.01	1.13	1.31
	Be2-C5	0.25	1.82	0.06	0.27	-0.01	1.15	1.35
	Be2-C6	0.23	1.83	0.06	0.27	-0.01	1.14	1.32
	Be3-C7	0.23	1.83	0.06	0.27	-0.01	1.15	1.32
	Be3-C8	0.25	1.82	0.06	0.27	-0.01	1.16	1.34
	Be3-C9	0.23	1.83	0.06	0.27	-0.01	1.14	1.33
$Be_4@C_{60}$	Be1-Be2	0.28	2.05	0.06	-0.02	-0.03	1.84	0.55
	Be1-Be3	0.85	2.12	0.07	-0.06	-0.04	2.52	0.37
	Be2-Be3	0.46	2.05	0.07	-0.09	-0.03	2.05	0.48
	Be3-Be4	0.74	1.95	0.08	-0.11	-0.05	3.50	0.10
	Be1-C1	0.26	1.82	0.07	0.33	-0.02	1.12	1.40
	Be2-C2	0.29	1.80	0.07	0.34	-0.01	1.12	1.39
	Be2-C3	0.27	1.81	0.07	0.34	-0.01	1.12	1.39
	Be2-C4	0.27	1.81	0.07	0.33	-0.01	1.12	1.40
	Be4-C5	0.17	1.87	0.06	0.27	-0.01	1.14	1.32
	Be4-C6	0.17	1.87	0.06	0.27	-0.01	1.14	1.32
	Be4-C7	0.19	1.88	0.06	0.27	-0.01	1.14	1.32
$Be_5@C_{60}$	Be1-Be2	0.67	1.90	0.07	-0.01	-0.04	2.12	0.47
	Be2-Be3	0.67	1.90	0.07	-0.01	-0.04	2.09	0.47
	Be2-Be4	0.75	1.92	0.07	-0.02	-0.04	2.16	0.46
	Be2-Be5	0.75	1.92	0.07	-0.02	-0.04	2.14	0.46
	Be1-C1	0.18	1.89	0.05	0.26	-0.01	1.13	1.52
	Be1-C2	0.15	1.89	0.05	0.26	-0.01	1.12	1.50
	Be1-C3	0.18	1.89	0.05	0.26	-0.01	1.13	1.52
	Be3-C4	0.18	1.89	0.05	0.26	-0.01	1.13	1.52
	Be3-C5	0.18	1.89	0.03	0.26	-0.01	1.13	1.52
	Be3-C6	0.15	1.89	0.05	0.26	-0.01	1.10	1.49
	Be4-C7	0.21	1.95	0.05	0.21	-0.01	1.16	1.26

	Be4-C8	0.21	1.95	0.05	0.21	-0.01	1.16	1.26
	Be5-C9	0.21	1.95	0.05	0.21	-0.01	1.16	1.26
	Be5-C10	0.21	1.95	0.05	0.21	-0.01	1.15	1.24
	Be1-Be2	0.29	1.99	0.06	-0.01	-0.03	2.12	0.55
	Be1-Be3	0.29	1.99	0.06	-0.01	-0.03	2.12	0.55
	Be1-Be4	0.29	1.99	0.06	-0.01	-0.03	2.12	0.55
	Be1-Be5	0.29	1.99	0.06	-0.01	-0.03	2.12	0.55
	Be1-Be6	0.29	1.99	0.06	-0.01	-0.03	2.12	0.55
	Be2-Be3	0.44	2.17	0.06	-0.01	-0.03	3.96	0.22
	Be2-Be4	0.44	2.17	0.06	-0.01	-0.03	3.96	0.22
	Be3-Be5	0.44	2.17	0.06	-0.01	-0.03	3.96	0.22
	Be4-Be6	0.44	2.17	0.06	-0.01	-0.03	3.96	0.22
	Be5-Be6	0.44	2.17	0.06	-0.01	-0.03	3.96	0.22
$Be_6@C_{60}$	Be2-C1	0.20	1.81	0.07	0.34	-0.01	1.22	1.29
	Be2-C2	0.20	1.81	0.07	0.34	-0.01	1.21	1.28
	Be3-C3	0.20	1.81	0.07	0.34	-0.01	1.22	1.29
	Be3-C4	0.20	1.81	0.07	0.34	-0.01	1.21	1.28
	Be4-C5	0.20	1.81	0.07	0.34	-0.01	1.22	1.29
	Be4-C6	0.20	1.81	0.07	0.34	-0.01	1.21	1.28
	Be5-C7	0.20	1.81	0.07	0.34	-0.01	1.22	1.29
	Be5-C8	0.20	1.81	0.07	0.34	-0.01	1.21	1.28
	Be6-C9	0.20	1.81	0.07	0.34	-0.01	1.22	1.29
	Be6-C10	0.20	1.81	0.07	0.34	-0.01	1.21	1.28

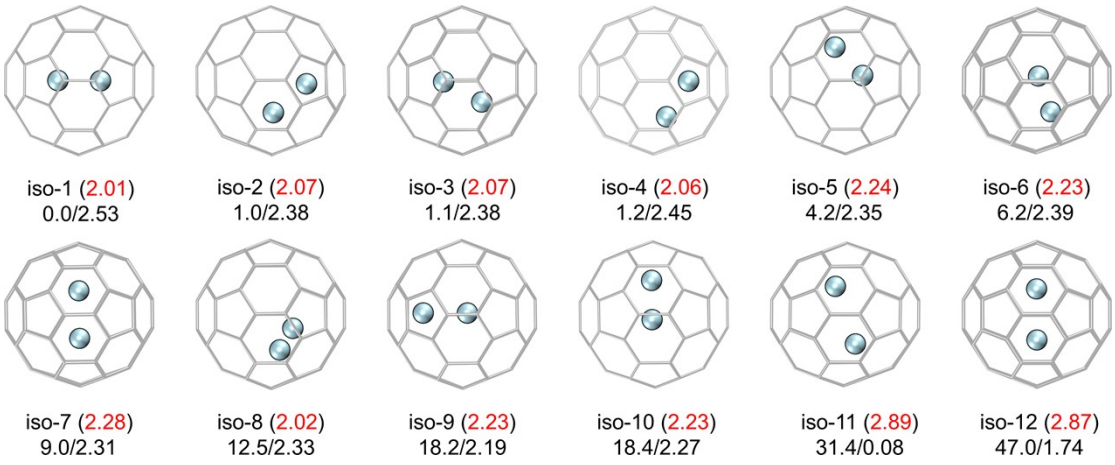

Fig. S1 Optimized structures of 12 $Be_2@C_{60}$ isomers. For each isomer, the Be-Be distance (Å) is given in red and the relative energy (kcal/mol)/HOMO-LUMO gap (eV) are given in black.

Table S4 Relative energies (ΔE, kcal/mol) of $Be_2@C_{60}$ and $Be_2@C_{74}$ isomers with different spin multiplicities (M) at the M06-2X/6-31G* level of theory.

$Be_2@C_{60}$	***M***	**ΔE**	**$Be_2@C_{74}$**	***M***	**ΔE**
iso-1	**1**	**0.0**	iso-1	**1**	**0.0**
	3	4.8		3	13.3

iso-2	1	1.0	iso-2	1	0.9
	3	4.1		3	11.0
iso-3	1	1.1	iso-3	1	2.0
	3	4.1		3	12.7
iso-4	1	1.2	iso-4	1	4.0
	3	5.5		3	14.1
iso-5	1	4.2	iso-5	1	8.3
	3	8.6		3	20.3
iso-6	1	6.2	iso-6	1	8.7
	3	11.0		3	21.5
iso-7	1	9.0	iso-7	1	12.1
	3	12.7		3	32.5
iso-8	1	12.5	iso-8	1	32.8
	3	13.1		3	20.1
iso-9	1	18.2	iso-9	1	52.8
	3	19.8		3	22.2
iso-10	1	18.4	iso-10	1	84.1
	3	14.5		3	33.9
iso-11	1	31.4			
	3	32.8			
iso-12	1	47.0			
	3	38.8			

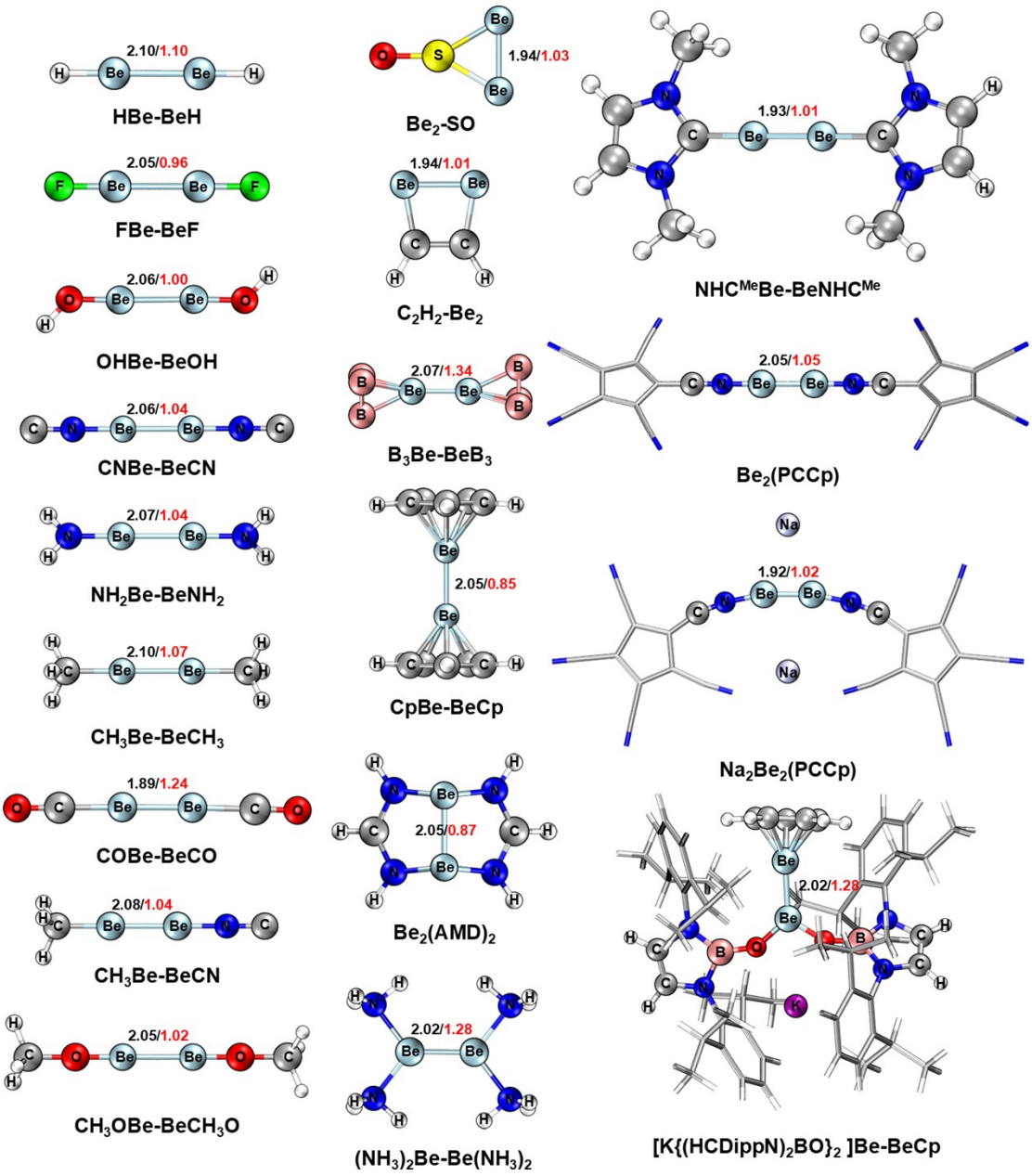

Fig. S2 Optimized structures of various reported compounds containing a Be-Be single bond (M06-2X/6-31G* level). Be-Be bond lengths (Å, in black) and MBOs (in red) are given.

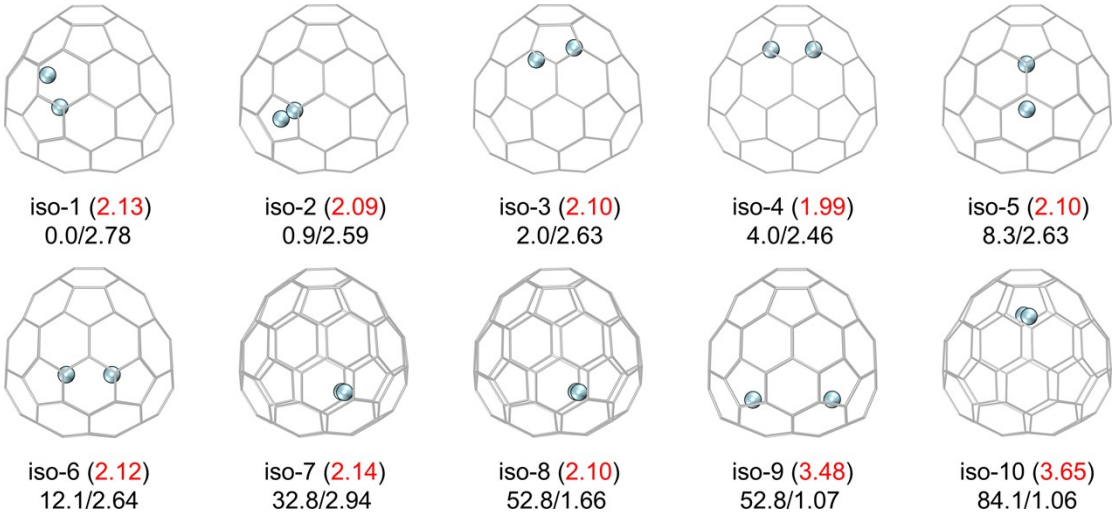

Fig. S3 Optimized structures of 10 $Be_2@C_{74}$ isomers. For each isomer, the Be-Be distance (Å) is given in red and the relative energy (kcal/mol)/HOMO-LUMO gap (eV) are given in black.

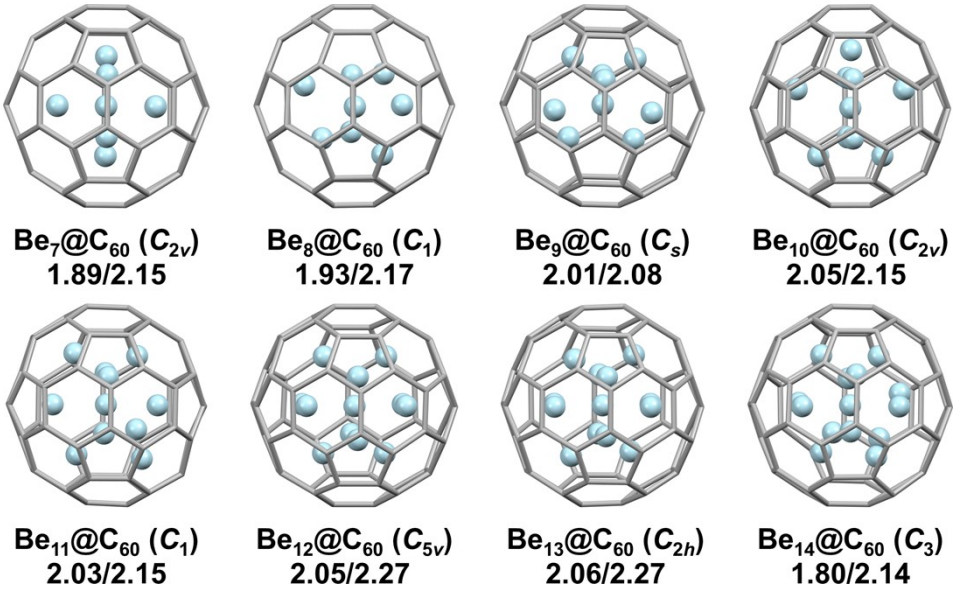

Fig. S4 Optimized structures and molecular symmetries of $Be_x@C_{60}$ (x = 7-14). C: gray; Be: blue. For clarity, the shortest and longest Be-Be distances are given in Å.

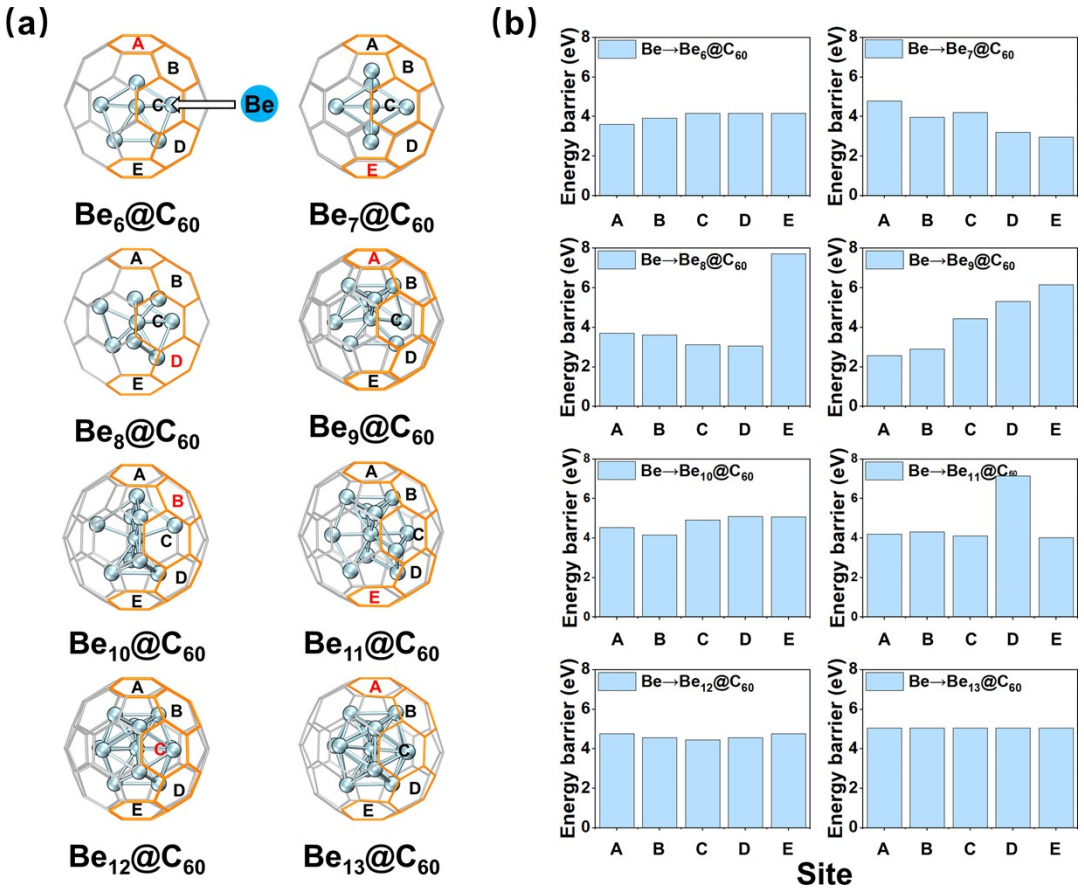

Fig. S5 (a) The penetration of a Be atom into $Be_{x-1}@C_{60}$ (x = 7-14) through a hexagon center on the cage surface. For each cage, five different hexagons (A-E) are selected with the one featuring the lowest energy barrier marked in red. (b) Energy barriers for Be atom located at different hexagon centers on $Be_{x-1}@C_{60}$ (x = 7-14).

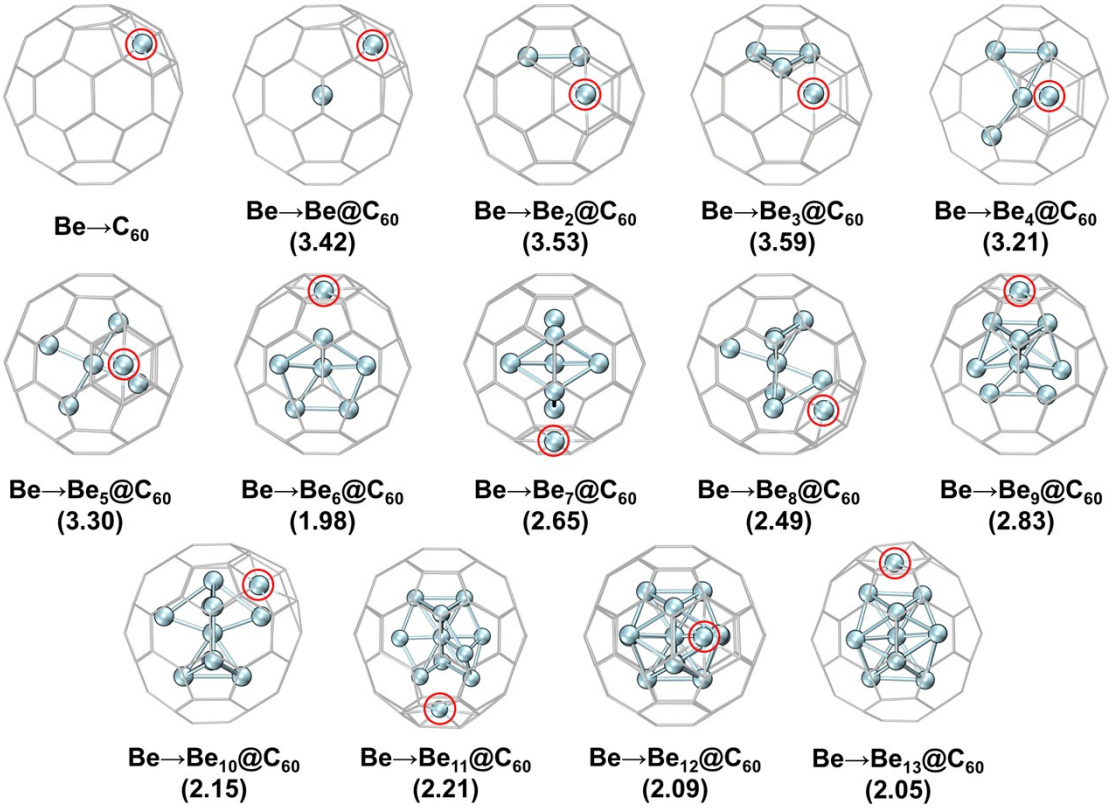

Fig. S6 Optimized structures corresponding to the lowest energy barriers for Be→Be$_x$@C$_{60}$ (x = 0-13) with the shortest distances (in parentheses; Å) between the injected atom (highlighted by red circles) and the encapsulated metals.

Table S5 IQA interaction energy (V_{Int}, kcal/mol) and interatomic exchange-correlation (V_{XC}) and Coulombic energy (V_C) components between the injected Be and the nearest interior Be atom for the Be$_7$@C$_{60}$ formation (Be→Be$_6$@C$_{60}$).

Insertion process	atom pair	V_{Int}	V_{XC}	V_C
Be→Be$_6$@C$_{60}$	Be$_{inject}$-Be$_{interior}$	224.6	-25.2	249.8

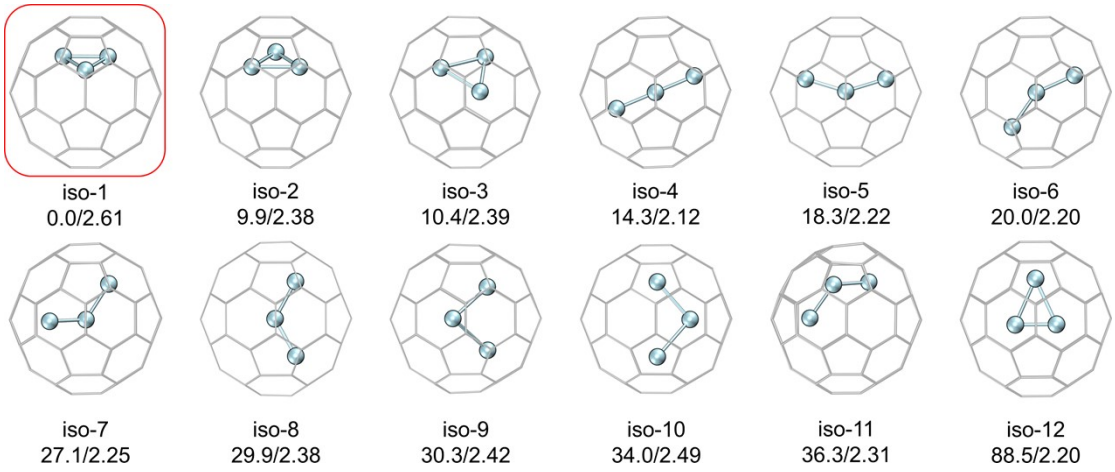

Fig. S7 Optimized structures of 12 $Be_3@C_{60}$ isomers. For each structure, the isomer number *n* is given, followed by its relative energy (kcal/mol)/HOMO-LUMO gap energy (eV). The isomer with internal metal cluster configuration similar to the reported isolated cluster is highlighted by red circle. Be: blue; C: gray.

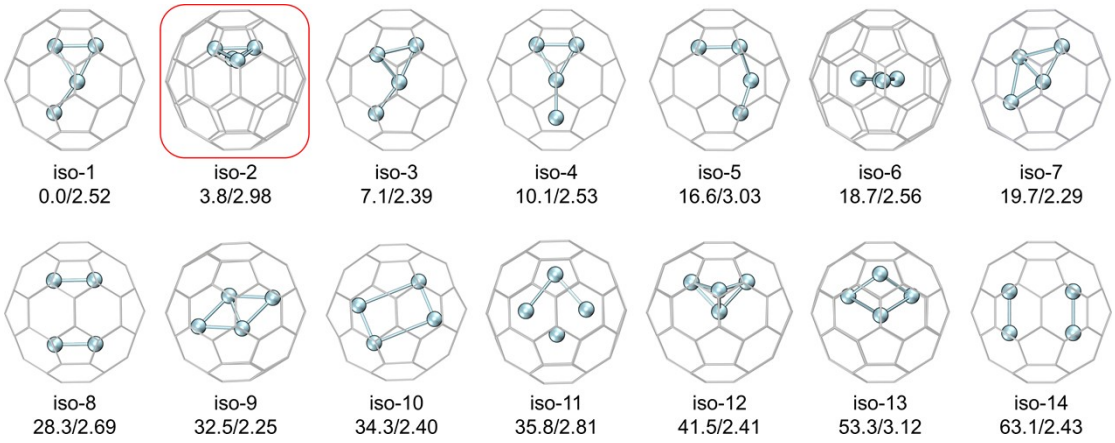

Fig. S8 Optimized structures of 14 $Be_4@C_{60}$ isomers. For each structure, the isomer number *n* is given, followed by its relative energy (kcal/mol)/HOMO-LUMO gap energy (eV). The isomer with internal metal cluster configuration similar to the reported isolated cluster is highlighted by red circle. Be: blue; C: gray.

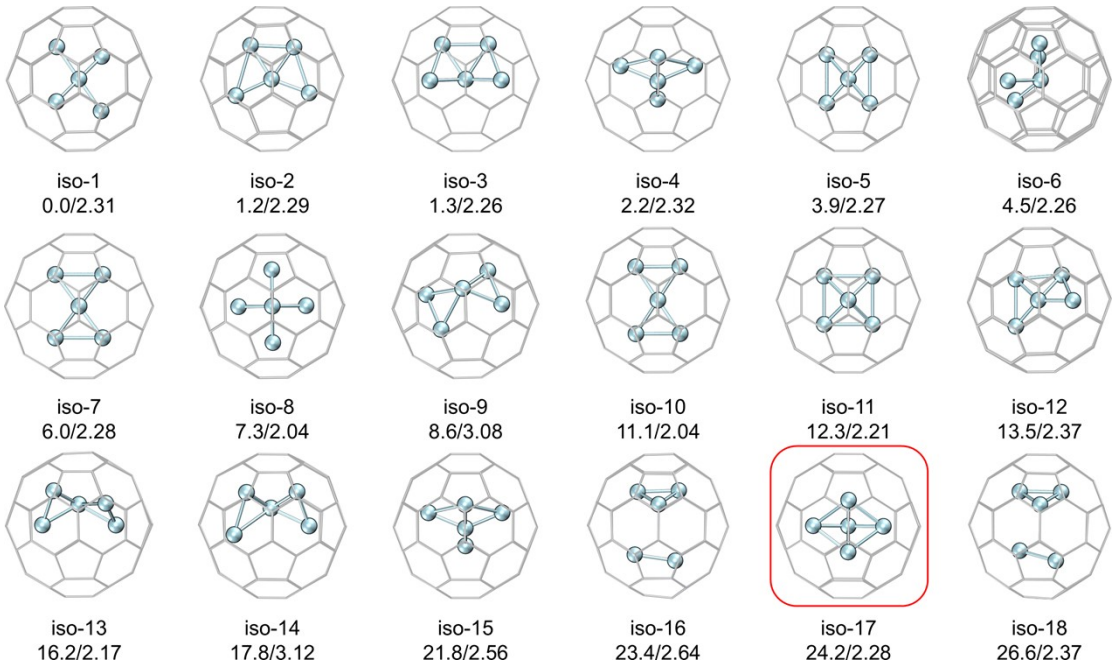

Fig. S9 Optimized structures of 18 $Be_5@C_{60}$ isomers. For each structure, the isomer number *n* is given, followed by its relative energy (kcal/mol)/HOMO-LUMO gap energy (eV). The isomer with internal metal cluster configuration similar to the reported isolated cluster is highlighted by red circle. Be: blue; C: gray.

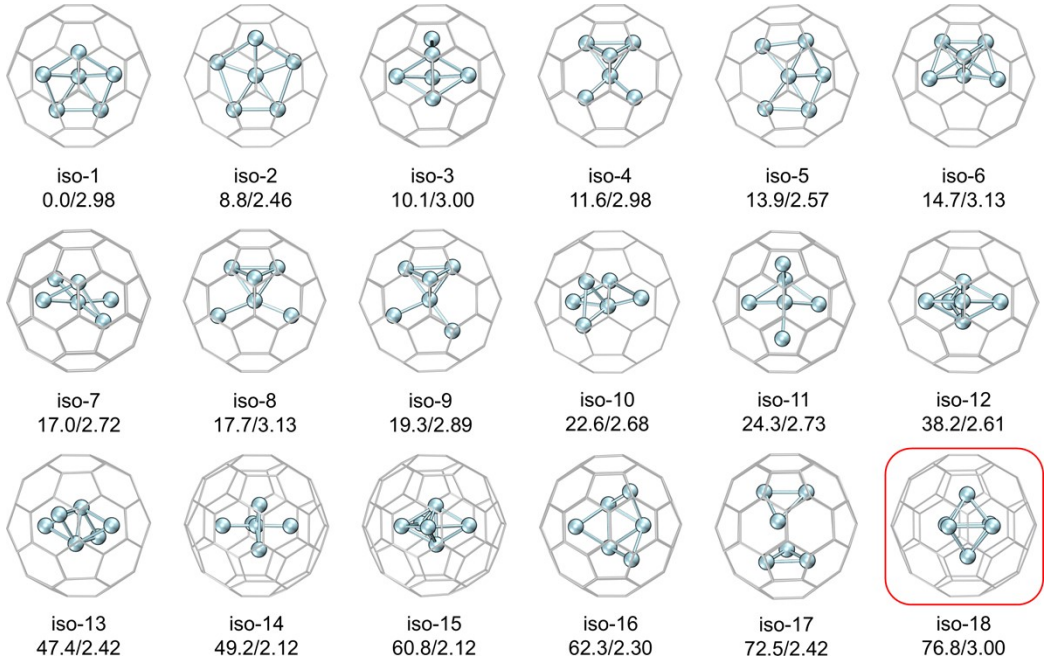

Fig. S10 Optimized structures of 18 $Be_6@C_{60}$ isomers. For each structure, the isomer number *n* is given, followed by its relative energy (kcal/mol)/HOMO-LUMO gap energy (eV). The isomer with internal metal cluster configuration similar to the reported isolated cluster is highlighted by red circle. Be: blue; C: gray.

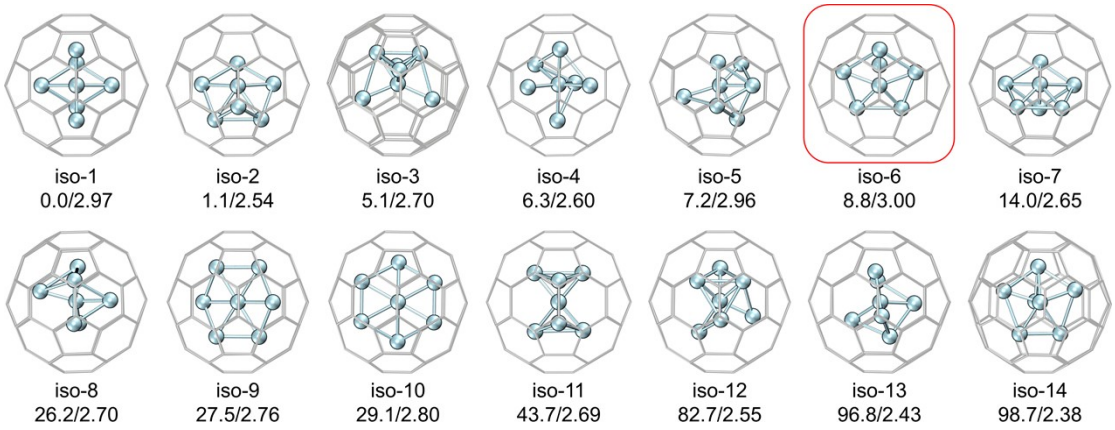

Fig. S11 Optimized structures of 14 $Be_7@C_{60}$ isomers. For each structure, the isomer number *n* is given, followed by its relative energy (kcal/mol)/HOMO-LUMO gap energy (eV). The isomer with internal metal cluster configuration similar to the reported isolated cluster is highlighted by red circle. Be: blue; C: gray.

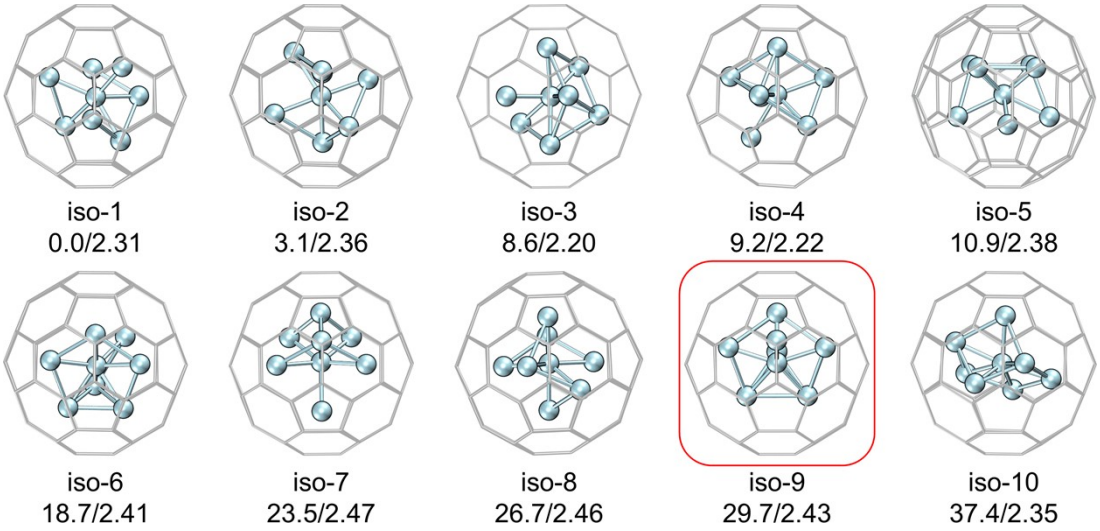

Fig. S12 Optimized structures of 10 $Be_8@C_{60}$ isomers. For each structure, the isomer number *n* is given, followed by its relative energy (kcal/mol)/HOMO-LUMO gap energy (eV). The isomer with internal metal cluster configuration similar to the reported isolated cluster is highlighted by red circle. Be: blue; C: gray.

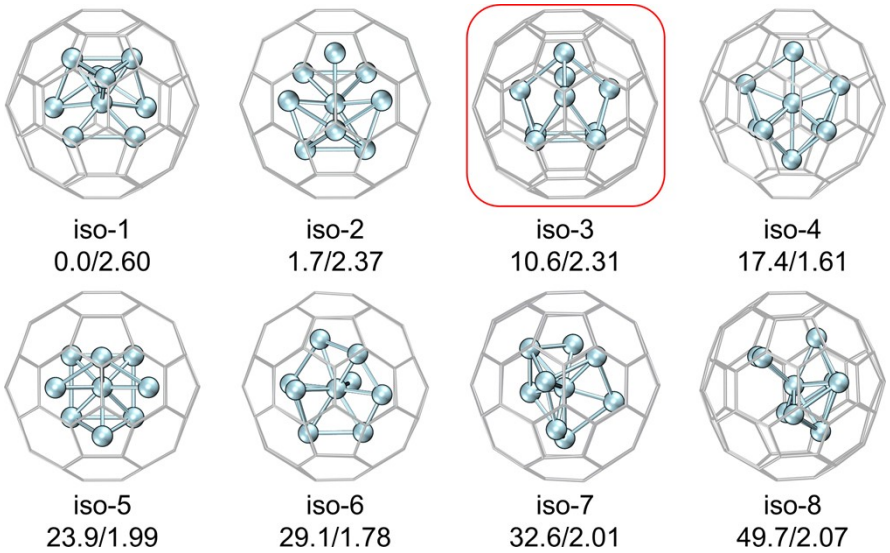

Fig. S13 Optimized structures of 8 $Be_9@C_{60}$ isomers. For each structure, the isomer number *n* is given, followed by its relative energy (kcal/mol)/HOMO-LUMO gap energy (eV). The isomer with internal metal cluster configuration similar to the reported isolated cluster is highlighted by red circle. Be: blue; C: gray.

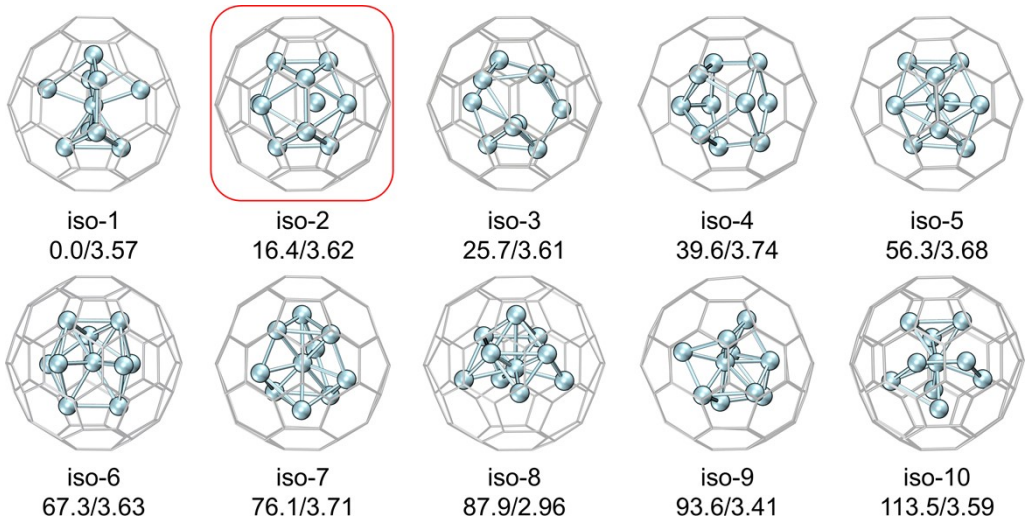

Fig. S14 Optimized structures of 10 $Be_{10}@C_{60}$ isomers. For each structure, the isomer number *n* is given, followed by its relative energy (kcal/mol)/HOMO-LUMO gap energy (eV). The isomer with internal metal cluster configuration similar to the reported isolated cluster is highlighted by red circle. Be: blue; C: gray.

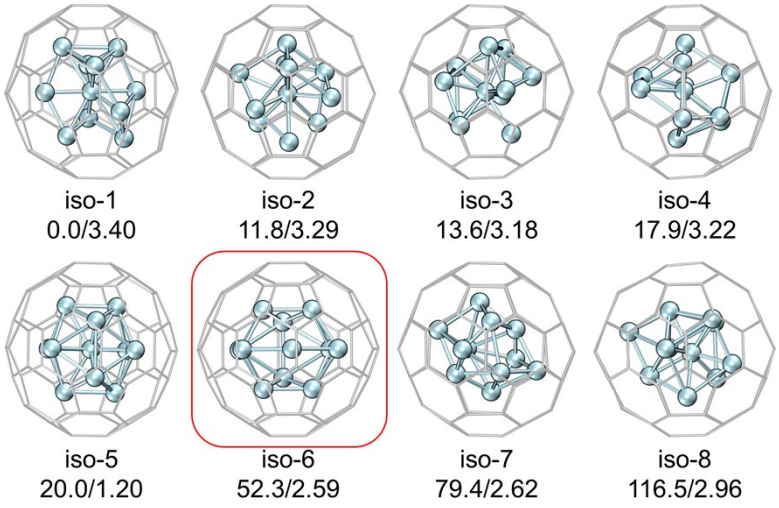

Fig. S15 Optimized structures of 8 $Be_{11}@C_{60}$ isomers. For each structure, the isomer number *n* is given, followed by its relative energy (kcal/mol)/HOMO-LUMO gap energy (eV). The isomer with internal metal cluster configuration similar to the reported isolated cluster is highlighted by red circle. Be: blue; C: gray.

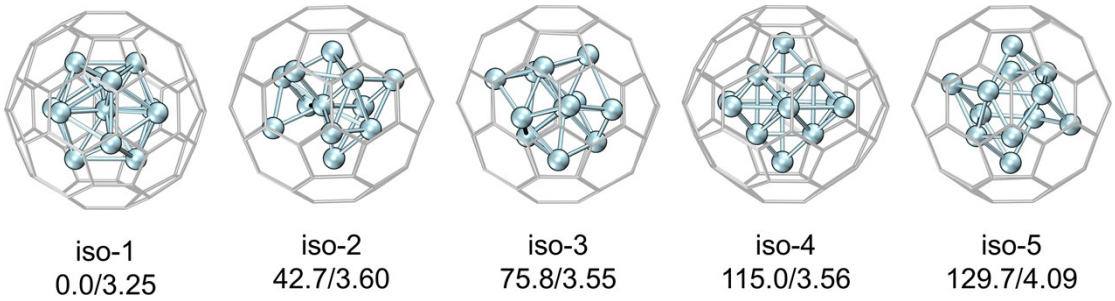

Fig. S16 Optimized structures of 5 $Be_{12}@C_{60}$ isomers. For each structure, the isomer number *n* is given, followed by its relative energy (kcal/mol)/HOMO-LUMO gap energy (eV). Be: blue; C: gray.

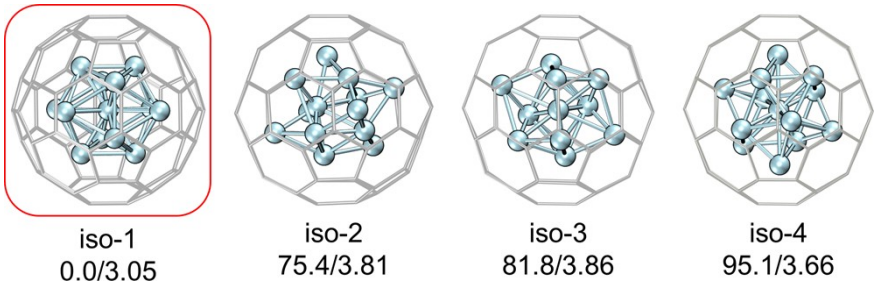

Fig. S17 Optimized structures of 4 $Be_{13}@C_{60}$ isomers. For each structure, the isomer number *n* is given, followed by its relative energy (kcal/mol)/HOMO-LUMO gap energy (eV). The isomer with internal metal cluster configuration similar to the reported isolated cluster is highlighted by red circle. Be: blue; C: gray.

Table S6 Relative energies (ΔE, kcal/mol) of $Be_x@C_{60}$ (x = 3-6) isomers with different spin multiplicities (M) at the M06-2X/6-31G* level of theory.

$Be_3@C_6$			**$Be_4@C_6$**			**$Be_5@C_6$**			**$Be_6@C$**		
0	***M***	**ΔE**	**0**	***M***	**ΔE**	**0**	***M***	**ΔE**	**60**	***M***	**ΔE**
iso-1	**1**	**0.0**	iso-1	**1**	**0.0**	iso-1	**1**	**0.0**	iso-1	**1**	**0.0**
	3	8.2		3	5.3		3	2.1		3	18.1
iso-2	1	9.9	iso-2	1	3.8	iso-2	1	1.2	iso-2	1	8.8
	3	12.3		3	12.7		3	1.9		3	12.8
iso-3	1	10.6	iso-3	1	7.1	iso-3	1	1.3	iso-3	1	10.1
	3	14.9		3	10.7		3	2.3		3	17.3
iso-4	1	14.3	iso-4	1	10.1	iso-4	1	2.2	iso-4	1	11.6
	3	14.8		3	18.3		3	4.5		3	17.8
iso-5	1	18.3	iso-5	1	16.6	iso-5	1	3.9	iso-5	1	13.9
	3	21.4		3	29.9		3	8.2		3	20.2
iso-6	1	20.0	iso-6	1	18.7	iso-6	1	4.5	iso-6	1	14.7
	3	21.2		3	29.3		3	5.5		3	21.0
iso-7	1	27.1	iso-	1	19.7	iso-	1	6.0	iso-	1	17.0

	3	29.6	7	3	10.74	7	3	6.1	7	3	25.5
iso-8	1	29.9	iso-8	1	28.3	iso-8	1	7.3	iso-8	1	17.7
	3	29.6		3	41.6		3	15.3		3	35.8
iso-9	1	30.3	iso-9	1	32.5	iso-9	1	8.6	iso-9	1	19.3
	3	32.0		3	35.8		3	24.9		3	29.3
iso-10	1	34.0	iso-10	1	34.3	iso-10	1	11.1	iso-10	1	22.6
	3	37.8		3	41.0		3	15.9		3	37.6
iso-11	1	36.3	iso-11	1	35.8	iso-11	1	12.3	iso-11	1	24.3
	3	46.7		3	41.0		3	12.6		3	26.8
iso-12	1	88.5	iso-12	1	41.5	iso-12	1	13.5	iso-12	1	38.2
	3	89.7		3	23.6		3	16.7		3	36.3
			iso-13	1	53.3	iso-13	1	16.2	iso-13	1	47.4
				3	36.7		3	35.9		3	38.2
			iso-14	1	63.1	iso-14	1	17.8	iso-14	1	49.2
				3	68.4		3	18.9		3	50.4
						iso-15	1	21.8	iso-15	1	60.8
							3	14.5		3	60.2
						iso-16	1	23.4	iso-16	1	62.3
							3	27.4		3	64.8
						iso-17	1	24.2	iso-17	1	64.2
							3	24.6		3	66.3
						iso-18	1	26.6	iso-18	1	72.5
							3	31.0		3	77.8

Table S7 Relative energies (ΔE, kcal/mol) for the most stable structures of $Be_x@C_{60}$ (x = 7-14) with different spin multiplicities (M) at the M06-2X/6-31G* level of theory. For clarity, the results for all high-energy isomers are omitted.

species	*M*	Δ*E*	species	*M*	Δ*E*
$Be_7@C_{60}$	**1**	**0.0**	**$Be_{11}@C_{60}$**	**1**	**0.0**
	3	2.8		3	3.3

$Be_8@C_{60}$	**1**	**0.0**	**$Be_{12}@C_{60}$**	**1**	**0.0**
	3	3.1		3	6.5
$Be_9@C_{60}$	**1**	**0.0**	**$Be_{13}@C_{60}$**	**1**	**0.0**
	3	4.6		3	4.9
$Be_{10}@C_{60}$	**1**	**0.0**	**$Be_{14}@C_{60}$**	**1**	**0.0**
	3	5.8		3	8.3

Table S8 Encapsulation energies (kcal/mol) defined as $E_e = E_{EMF} - (E_{cage} + E_{cluster})$ for $Be_x@C_{60}$ (x = 3-14).

species	E_e	species	E_e
$Be_3@C_{60}$	-97.8	$Be_9@C_{60}$	-149.2
$Be_4@C_{60}$	-76.1	$Be_{10}@C_{60}$	-96.1
$Be_5@C_{60}$	-107.2	$Be_{11}@C_{60}$	-132.0
$Be_6@C_{60}$	-189.7	$Be_{12}@C_{60}$	-34.3
$Be_7@C_{60}$	-202.4	$Be_{13}@C_{60}$	-15.9
$Be_8@C_{60}$	-218.7	$Be_{14}@C_{60}$	110.5

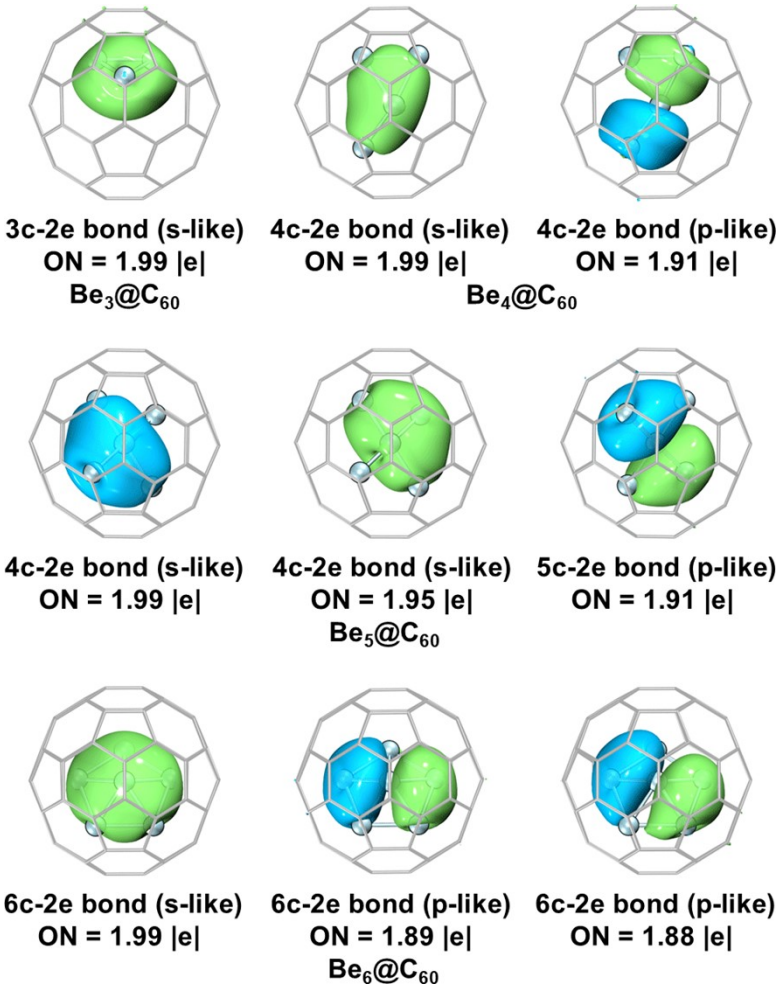

Fig. S18 AdNDP analyses results (isovalue: ±0.03 a.u.) for $Be_x@C_{60}$ (x = 3-6) (ON =

occupation number).

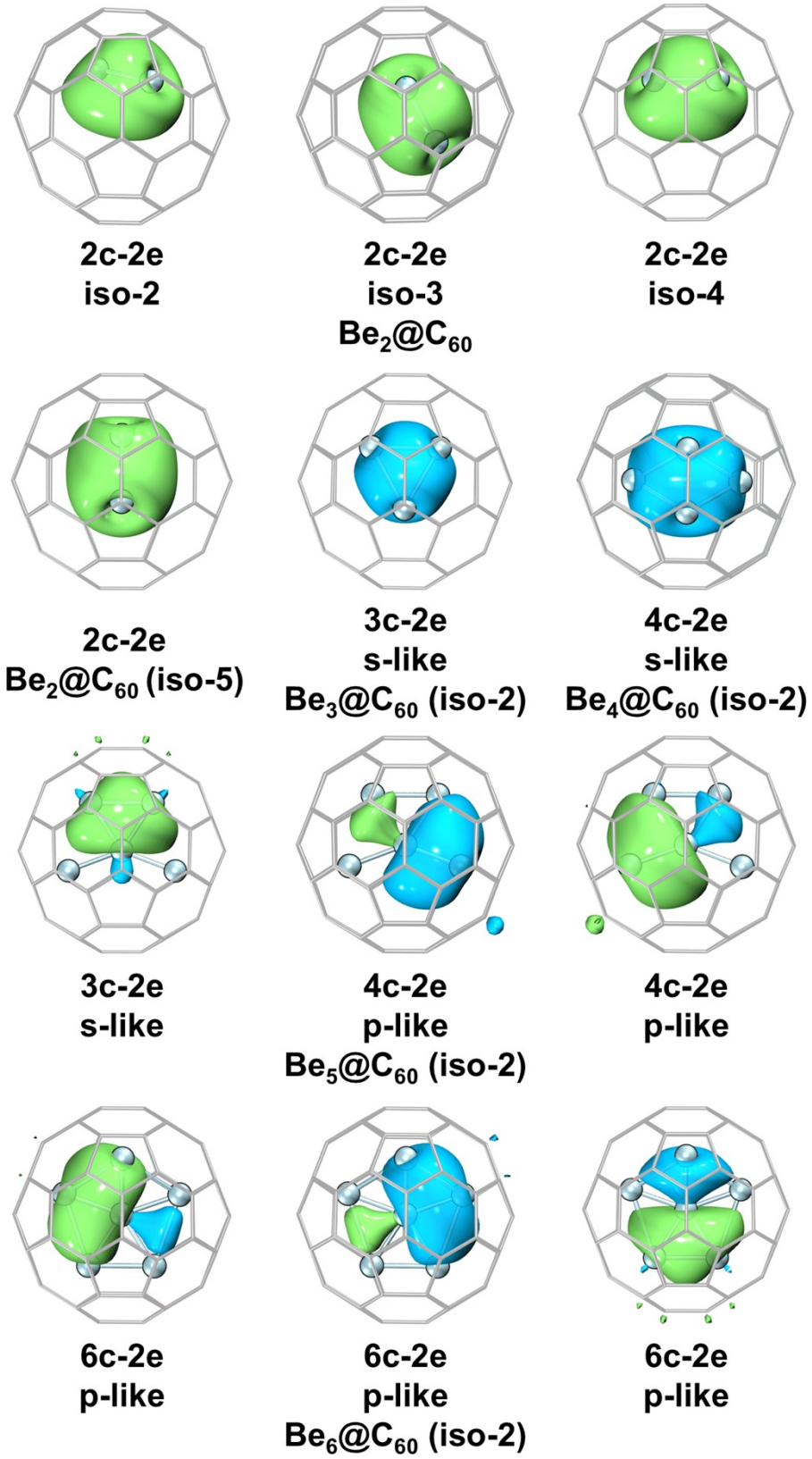

Fig. S19 LMOs (isovalue: ±0.03 a.u.) of some higher-energy $Be_x@C_{2n}$ (x = 2-6) isomers.

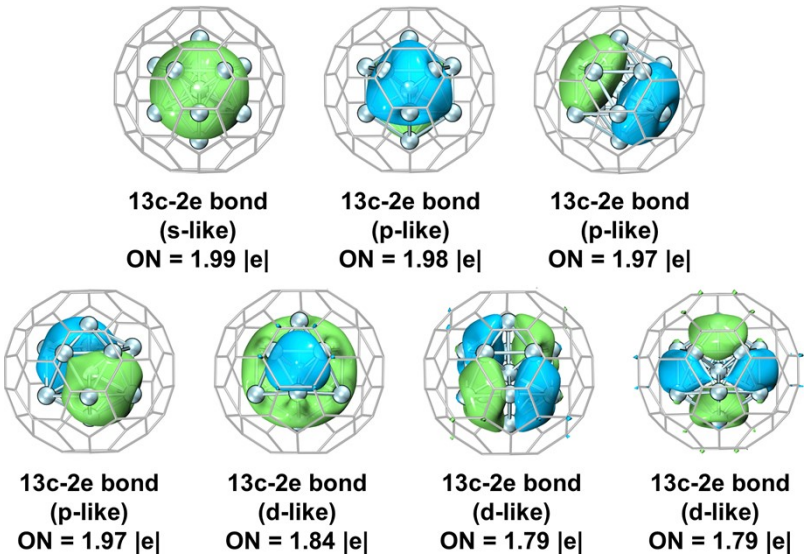

Fig. S20 AdNDP analyses results (isovalue: ±0.03 a.u.) for the internal B_{13} cluster of $Be_{13}@C_{60}$ (ON = occupation number).

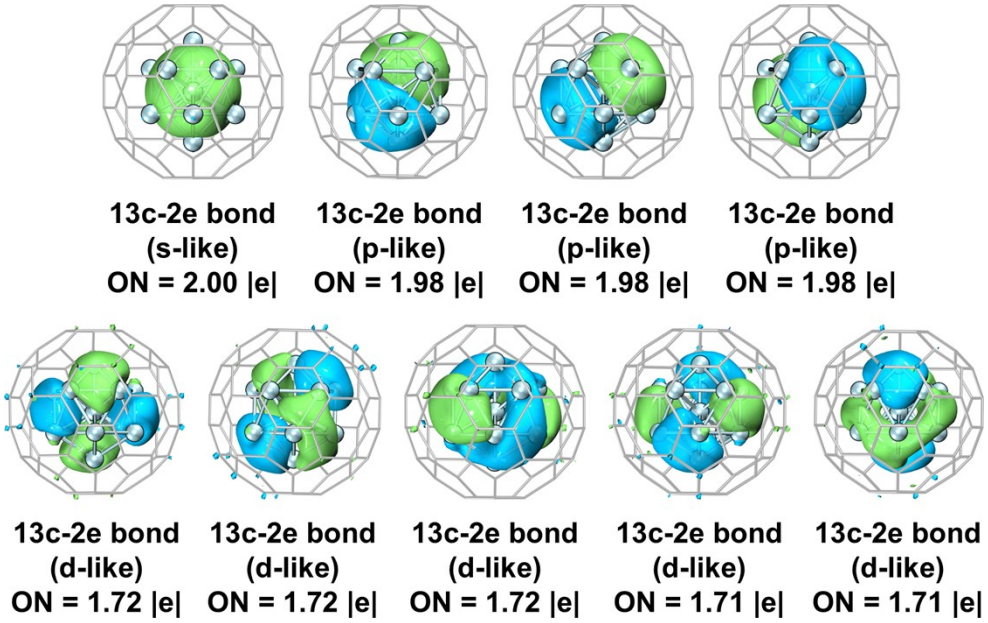

Fig. S21 AdNDP analyses results (isovalue: ±0.03 a.u.) for the internal B_{13} cluster of the $(Be_{13}@C_{60})^{4-}$ anion (ON = occupation number).

Optimized Cartesian coordinates and the lowest vibrational frequencies

$Be@C_{24}$ (100.26 cm^{-1})

C	2.09172261	1.13420857	-0.27938968
C	1.17236632	2.02901912	0.36635580
C	2.29957402	0.01395233	0.50989620

C	0.61288258	1.30791338	1.59022008
C	1.30408048	0.07797545	1.68447584
C	2.07396486	-1.19826328	-0.19121009
C	1.14032420	-1.98520285	0.50874108
C	0.59290433	-1.15131316	1.67403183
C	1.38705372	-0.79995883	-1.47613196
C	1.39754639	0.62594696	-1.53128034
C	0.17754003	1.35403781	-1.63464917
C	0.14982274	-1.51724432	-1.52480144
C	-1.09255682	-0.78697849	-1.64735313
C	-1.07483299	0.65252244	-1.70265042
C	0.05444834	-2.37667187	-0.29550697
C	-1.14932541	2.03971818	0.22029038
C	0.09731693	2.31754362	-0.45805349
C	-1.96502010	1.17260556	-0.54555351
C	-2.40074637	0.03225694	0.23714478
C	-1.98896113	-1.18947506	-0.46754643
C	-1.16655478	-1.98682251	0.35694979
C	-0.82142160	1.32032547	1.48636303
C	-1.60189857	0.08087657	1.53015763
C	-0.83066268	-1.16142531	1.58049213
Be	-0.68935062	-0.00832010	0.01351209

Be@C_{32} (167.03 cm^{-1})

C	2.93620620	-0.02591946	-0.01352789
C	2.37400041	-1.35726705	-0.35009868
C	1.72968971	-0.81897071	1.79624786
C	2.43653505	0.31808430	1.24935284
C	-0.31782829	-2.35849764	-0.63956800
C	0.31789133	-2.35847107	0.63966729
C	1.68379834	-1.87204974	0.74497271
C	1.66854389	1.54594145	1.12826148
C	0.46166056	-0.68201273	2.31732238
C	-0.29344165	0.57085996	2.28094929
C	0.32796196	1.73764833	1.65483123
C	-0.40745456	-1.74781190	1.74118833
C	1.70513870	1.97128881	-0.24737270
C	2.38732539	0.91459350	-0.96781569
C	1.63882590	0.21266468	-1.93289189
C	0.41887159	2.51220673	-0.62314124
C	-0.32812690	1.73754058	-1.65486346
C	0.29334859	0.57075866	-2.28091706
C	-0.41900662	2.51207701	0.62299930
C	0.40749350	-1.74788647	-1.74111720

C	1.68489808	-1.24690405	-1.59860876
C	-1.72967801	-0.81910754	-1.79621097
C	-0.46167240	-0.68214532	-2.31731007
C	-2.43653216	0.31796046	-1.24934925
C	-1.66868943	1.54591051	-1.12834663
C	-2.93619843	-0.02602362	0.01352890
C	-2.38733110	0.91457818	0.96775786
C	-1.70528252	1.97126998	0.24727144
C	-1.63886746	0.21272265	1.93290985
C	-1.68375651	-1.87213498	-0.74490763
C	-2.37395738	-1.35730094	0.35014705
C	-1.68486010	-1.24686008	1.59865503
Be	0.00074147	0.97988626	-0.00002365

Be@C_{60} (259.74 cm^{-1})

C	-0.72590798	-0.99912708	3.31828168
C	0.72590842	-0.99912676	3.31828168
C	1.41988832	-1.95430773	2.58858823
C	0.69398034	-2.95343481	1.82532318
C	-0.69397906	-2.95343510	1.82532318
C	-1.41988748	-1.95430834	2.58858823
C	-1.17454422	0.38163227	3.31828168
C	-0.00000027	1.23498879	3.31828168
C	1.17454406	0.38163278	3.31828168
C	2.29742672	0.74647974	2.58858823
C	2.59443238	-1.57267495	1.82532318
C	1.41988859	-3.18929652	0.59033439
C	0.72590894	-3.41478434	-0.59033439
C	-0.72590746	-3.41478466	-0.59033439
C	-1.41988721	-3.18929713	0.59033439
C	-2.59443153	-2.33594112	0.59033439
C	-2.59443170	-1.57267607	1.82532318
C	-3.02333503	-0.25264833	1.82532318
C	-2.29742704	0.74647875	2.58858823
C	-0.00000052	2.41565758	2.58858823
C	-1.17454475	2.79728985	1.82532318
C	-2.29742731	1.98146754	1.82532318
C	-3.02333545	1.74560551	0.59033439
C	-3.47197110	0.36484597	0.59033439
C	-3.47197094	-0.36484747	-0.59033439
C	-3.02333470	-1.74560682	-0.59033439
C	-2.29742645	-1.98146853	-1.82532318
C	-1.17454353	-2.79729035	-1.82532318
C	2.59443254	-2.33594000	0.59033439

C	1.17454422	-0.38163227	-3.31828168
C	2.29742704	-0.74647875	-2.58858823
C	3.02333503	0.25264833	-1.82532318
C	2.59443170	1.57267607	-1.82532318
C	1.41988748	1.95430834	-2.58858823
C	-0.72590842	0.99912676	-3.31828168
C	-1.17454406	-0.38163278	-3.31828168
C	0.00000027	-1.23498879	-3.31828168
C	0.00000052	-2.41565758	-2.58858823
C	1.17454475	-2.79728985	-1.82532318
C	2.29742731	-1.98146754	-1.82532318
C	3.47197110	-0.36484597	-0.59033439
C	3.47197094	0.36484747	0.59033439
C	3.02333470	1.74560682	0.59033439
C	2.59443153	2.33594112	-0.59033439
C	1.41988721	3.18929713	-0.59033439
C	0.69397906	2.95343510	-1.82532318
C	-0.69398034	2.95343481	-1.82532318
C	-1.41988832	1.95430773	-2.58858823
C	-2.29742672	-0.74647974	-2.58858823
C	-3.02333514	0.25264702	-1.82532318
C	-2.59443238	1.57267495	-1.82532318
C	-2.59443254	2.33594000	-0.59033439
C	-1.41988859	3.18929652	-0.59033439
C	-0.72590894	3.41478434	0.59033439
C	0.72590746	3.41478466	0.59033439
C	1.17454353	2.79729035	1.82532318
C	2.29742645	1.98146853	1.82532318
C	3.02333545	-1.74560551	-0.59033439
C	3.02333514	-0.25264702	1.82532318
C	0.72590798	0.99912708	-3.31828168
Be	0.00000000	-0.00000000	-0.00000000

Be@C_{74} (156.05 cm^{-1})

C	0.22870711	3.87239825	1.15628846
C	-0.29520855	3.27770959	2.28251752
C	0.48878172	2.32576678	3.04098040
C	-0.39989028	1.34315754	3.53572519
C	0.03271617	0.00804673	3.74014236
C	-0.90022956	-1.04017148	3.52439420
C	-0.48829771	-2.31840627	3.06781487
C	-1.58361138	-2.85669782	2.31692166
C	-1.33990351	-3.56200112	1.15108384
C	-2.18891927	-3.43499426	-0.00032287

C	-1.33970937	-3.56188734	-1.15160640
C	-1.58325329	-2.85648885	-2.31742306
C	-0.48783498	-2.31812856	-3.06810165
C	-0.89968929	-1.03984456	-3.52461119
C	0.03328540	0.00839623	-3.74012931
C	-0.39935801	1.34348426	-3.53566130
C	0.48923678	2.32604235	-3.04067636
C	-0.29486860	3.27792693	-2.28225447
C	0.22888159	3.87250278	-1.15588535
C	-0.59819255	4.10457561	0.00015036
C	1.56978332	3.51385888	0.71020810
C	1.56989123	3.51392701	-0.70963950
C	2.38265947	2.62097723	-1.45374544
C	1.82620050	1.99778648	-2.66406292
C	2.29881460	0.72089480	-3.03862603
C	1.40202224	-0.28119718	-3.53163183
C	1.81792107	-1.57200646	-3.03721169
C	0.87609851	-2.54940814	-2.67556212
C	1.13321639	-3.33610908	-1.45992344
C	0.02708426	-3.81566332	-0.70667795
C	0.02696784	-3.81571524	0.70633505
C	1.13298955	-3.33623879	1.45979175
C	0.87568924	-2.54964935	2.67546806
C	1.81746426	-1.57228889	3.03736015
C	1.40148594	-0.28152723	3.53182165
C	2.29835872	0.72061615	3.03905095
C	1.82580004	1.99753982	2.66453385
C	2.38243972	2.62084142	1.45435551
C	3.36876248	1.92430623	0.71407322
C	3.36887060	1.92437349	-0.71338023
C	3.87462201	0.63713458	-1.15791868
C	3.32592149	0.04692519	-2.27877317
C	3.02846340	-1.36802651	-2.27739057
C	3.30099925	-2.13359251	-1.16006473
C	2.31233644	-3.09717523	-0.71760663
C	2.31222139	-3.09723528	0.71767455
C	3.30082721	-2.13369926	1.16037756
C	3.02811417	-1.36823556	2.27772992
C	3.32557276	0.04671708	2.27928777
C	3.87445172	0.63702862	1.15857169
C	4.18599230	-0.16141992	0.00031501
C	3.90187574	-1.52682980	0.00023172
C	-1.67447073	2.83882899	2.29159673
C	-1.74783784	1.63334925	3.05290271

C	-2.61482933	0.59450730	2.67471475
C	-2.23584536	-0.75274007	3.02587488
C	-2.67242094	-1.88311641	2.31254867
C	-3.54916069	-1.75824374	1.17960956
C	-3.38339379	-2.60850288	-0.00037913
C	-3.54914572	-1.75818489	-1.18035228
C	-2.67205917	-1.88288863	-2.31307435
C	-2.23535030	-0.75244234	-3.02622029
C	-2.61443851	0.59478117	-2.67506025
C	-1.74738001	1.63363935	-3.05301893
C	-1.67412596	2.83905730	-2.29159128
C	-2.47225933	3.02825196	-1.16494757
C	-1.92546751	3.67769118	0.00002205
C	-2.47244150	3.02815360	1.16485960
C	-3.33574197	1.96700573	0.73351915
C	-3.43021478	0.78068474	1.47626936
C	-3.78836691	-0.40080170	0.72294682
C	-3.78836861	-0.40074375	-0.72360871
C	-3.43003736	0.78082764	-1.47673572
C	-3.33564362	1.96707015	-0.73384736
Be	-2.29134061	-1.29671995	-0.00052034

$Be_2@C_{60}$ (215.41 cm^{-1})

C	-1.42479116	3.02395274	1.11106835
C	-0.71381470	3.48177066	-0.02375780
C	-0.73416502	2.57777742	2.26855788
C	0.71381470	3.48177066	-0.02375780
C	1.43054862	3.01726309	-1.19937601
C	-1.43054862	3.01726309	-1.19937601
C	-0.73157037	2.57993736	-2.31296989
C	0.73157037	2.57993736	-2.31296989
C	-2.36433973	0.69979694	2.58522503
C	-3.05604283	1.16658950	1.37856523
C	-1.18658628	1.42482561	3.00923350
C	-2.61712515	2.27979552	0.67791355
C	-2.61354974	2.29070911	-0.76636601
C	-3.50738085	-0.00000000	0.64689367
C	-3.49184464	-0.00000000	-0.74401295
C	-3.04163126	1.17050651	-1.46899833
C	-0.00000000	-0.71492994	3.44982194
C	-1.18658628	-1.42482561	3.00923350
C	-0.00000000	0.71492994	3.44982194
C	-2.36433973	-0.69979694	2.58522503
C	-3.05604283	-1.16658950	1.37856523

C	-0.73416502	-2.57777742	2.26855788
C	-1.42479116	-3.02395274	1.11106835
C	-2.61712515	-2.27979552	0.67791355
C	2.36433973	0.69979694	2.58522503
C	2.36433973	-0.69979694	2.58522503
C	1.18658628	1.42482561	3.00923350
C	1.18658628	-1.42482561	3.00923350
C	0.73416502	-2.57777742	2.26855788
C	3.05604283	-1.16658950	1.37856523
C	2.61712515	-2.27979552	0.67791355
C	1.42479116	-3.02395274	1.11106835
C	1.42479116	3.02395274	1.11106835
C	2.61712515	2.27979552	0.67791355
C	0.73416502	2.57777742	2.26855788
C	3.05604283	1.16658950	1.37856523
C	3.50738085	0.00000000	0.64689367
C	2.61354974	2.29070911	-0.76636601
C	3.04163126	1.17050651	-1.46899833
C	3.49184464	0.00000000	-0.74401295
C	1.43054862	-3.01726309	-1.19937601
C	2.61354974	-2.29070911	-0.76636601
C	3.04163126	-1.17050651	-1.46899833
C	0.73157037	-2.57993736	-2.31296989
C	-1.43054862	-3.01726309	-1.19937601
C	-0.71381470	-3.48177066	-0.02375780
C	0.71381470	-3.48177066	-0.02375780
C	-0.73157037	-2.57993736	-2.31296989
C	-2.31221048	-0.72356774	-2.63658396
C	-3.04163126	-1.17050651	-1.46899833
C	-2.61354974	-2.29070911	-0.76636601
C	-1.17765570	-1.41835122	-3.04646426
C	0.00000000	0.69315635	-3.48558954
C	-1.17765570	1.41835122	-3.04646426
C	-2.31221048	0.72356774	-2.63658396
C	0.00000000	-0.69315635	-3.48558954
C	2.31221048	-0.72356774	-2.63658396
C	2.31221048	0.72356774	-2.63658396
C	1.17765570	1.41835122	-3.04646426
C	1.17765570	-1.41835122	-3.04646426
Be	0.00000000	1.00660817	1.47118846
Be	0.00000000	-1.00660817	1.47118846

$Be_2@C_{74}$ (217.47 cm^{-1})

C	3.09029035	2.29217310	0.86952882

C	1.98542025	2.89570382	1.51904299
C	1.14182441	3.68151958	0.69605307
C	-0.26134639	3.90316509	1.03575233
C	-0.79966315	3.28216468	2.14856944
C	3.70041317	1.07462915	1.38051263
C	3.13905850	0.45266887	2.47749150
C	1.99140107	1.03038754	3.14358294
C	1.40854123	2.24396261	2.70520715
C	0.02553871	2.44279677	2.98786385
C	-2.29716933	3.45101065	-0.24775787
C	-2.83937486	2.77325323	0.89781165
C	-1.01876483	4.02315038	-0.17300826
C	-2.11811624	2.70155524	2.08397638
C	-2.13746423	1.50997155	2.88899381
C	-2.87691425	0.37895262	2.50275953
C	-2.37994690	-0.92006448	2.91320759
C	1.17707209	-0.04418746	3.60476214
C	-0.22252882	0.12103723	3.71838492
C	-0.79299949	1.38718076	3.46544919
C	-1.03399896	-1.02421108	3.44262624
C	-0.46210076	3.16903072	-2.40483089
C	-1.78208007	2.57389316	-2.48952486
C	-0.09432068	3.84637843	-1.26298639
C	-2.67285295	2.71639126	-1.42074367
C	-3.40369694	1.55851272	-1.00409148
C	-3.33440963	0.32499817	-1.70847026
C	-3.68805976	-0.84904528	-0.96309828
C	-3.63550563	0.40679962	1.22197895
C	-3.53707737	1.59398857	0.44665385
C	-3.84446488	-0.81730556	0.47945334
C	2.43364037	0.90047674	-2.90885337
C	1.80142943	2.12389026	-2.60730670
C	0.47008347	2.30273775	-3.08803480
C	-0.27479167	1.20969509	-3.59498016
C	-0.52234764	-1.21550828	-3.54993565
C	0.30768107	-0.07720900	-3.73378661
C	1.68129034	-0.21112425	-3.42442856
C	-2.43647012	0.21669825	-2.86976038
C	-1.67280260	1.35798221	-3.21447006
C	-1.92296793	-1.07001885	-3.17425152
C	2.19797834	2.83129634	-1.37817503
C	1.24571123	3.64829626	-0.71777353
C	3.46363366	0.35763334	-2.05952160
C	3.87287416	1.02774176	-0.92276678

C	3.19565883	2.26168826	-0.55180898
C	3.32041074	-1.08314474	-2.04202742
C	4.18064015	0.29341446	0.27254383
C	4.04169284	-1.10035835	0.28916876
C	3.59600984	-1.79256628	-0.88960532
C	-0.00796630	-2.42006410	-3.01366540
C	1.33820805	-2.49897057	-2.54586734
C	2.20095784	-1.43548974	-2.87989220
C	-1.09161647	-3.05536166	-2.30220026
C	-0.87001268	-3.77944803	-1.15777685
C	0.49385182	-3.83364788	-0.62199468
C	1.59372892	-3.23964656	-1.30076110
C	2.68955649	-2.85817415	-0.49260190
C	-2.98115236	-2.91701947	-0.15184247
C	-3.18639901	-2.14603044	-1.34191340
C	-2.27356229	-2.20478985	-2.40390739
C	-1.81666973	-3.74591342	-0.06632315
C	-1.42895032	-2.93282486	2.19910561
C	-2.62500753	-2.12046228	2.14975767
C	-3.38625180	-2.11445676	0.95440109
C	-1.03788938	-3.72656310	1.10657274
C	1.77027495	-1.30123169	3.17368455
C	0.97806877	-2.36941097	2.74410391
C	-0.43964624	-2.23948581	2.97968794
C	2.58992743	-2.82724649	0.93381178
C	3.42440396	-1.74123766	1.41719605
C	3.00166500	-0.98382892	2.49734142
C	0.39214430	-3.80074233	0.78479863
C	1.38824614	-3.17667959	1.58936356
Be	-1.08452412	-1.08339914	1.46900555
Be	-2.09842744	0.04336461	-0.02968845

$Be_3@C_{60}$ (204.91 cm^{-1})

C	-2.70488000	1.79380600	1.51120700
C	-3.37666400	0.72222800	0.82647000
C	-3.38734500	0.71028300	-0.59778300
C	-2.72141300	1.77357900	-1.35274700
C	-2.06428300	2.84778700	-0.64867100
C	-2.05109000	2.81086100	0.77743400
C	-2.06492900	1.20874400	2.66352000
C	-2.36663100	-0.21793800	2.67786700
C	-3.19320900	-0.51589300	1.53424300
C	-3.01008400	-1.72453100	0.82268300
C	-3.21227100	-0.54590600	-1.32973100

C	-2.17228300	1.17046200	-2.55426800
C	-0.84812400	1.64472200	-3.03118200
C	-0.17950700	2.68406900	-2.26824300
C	-0.77552800	3.30862300	-1.11254200
C	0.05458900	3.56503900	0.01922200
C	-0.73521300	3.26669400	1.20678100
C	-0.13204600	2.69167200	2.30985800
C	-0.80694300	1.64566600	3.06426600
C	-1.39175900	-1.11907400	3.09209200
C	-0.09346500	-0.65712100	3.51686600
C	0.19481400	0.70564000	3.50286700
C	1.48939800	1.16921200	3.03665900
C	1.29377000	2.39782900	2.30744600
C	2.05524700	2.68421600	1.17985900
C	1.43954000	3.27798000	0.01846800
C	2.05363900	2.66763300	-1.12946300
C	1.25102400	2.37142600	-2.26823100
C	-2.47081000	-0.23965300	-2.54035300
C	2.16426000	-1.22198700	-2.57145400
C	0.85380000	-1.66730400	-2.97838300
C	0.17472400	-2.71769300	-2.21740000
C	0.79342800	-3.29142300	-1.06975000
C	2.09415900	-2.82496200	-0.67081400
C	3.41652000	-0.72921600	-0.68094500
C	3.22845200	0.51006100	-1.42399300
C	2.46310300	0.19157100	-2.58539000
C	1.44362000	1.12147000	-3.00609300
C	0.13869300	0.69487200	-3.47950300
C	-0.16858600	-0.75797400	-3.46538800
C	-1.25983100	-2.42423900	-2.21703600
C	-2.05302800	-2.73246500	-1.05235700
C	-1.39314200	-3.28092200	0.08744800
C	-0.01046400	-3.57892500	0.08696000
C	0.79752200	-3.26312900	1.23928400
C	2.09784400	-2.79743000	0.77118200
C	2.74174200	-1.76940900	1.45123500
C	3.40613000	-0.71325200	0.70144000
C	3.05571000	1.72231600	-0.71642900
C	3.05386800	1.72327800	0.72585300
C	3.22926000	0.53577300	1.42800300
C	2.44340100	0.25144300	2.60340200
C	2.14281800	-1.16909100	2.61762000
C	0.90076800	-1.61398300	3.06478700
C	0.22159200	-2.67199700	2.35844500

C	-1.20116700	-2.36318900	2.36047900
C	-1.98966200	-2.66565400	1.26599600
C	-1.45363400	-1.21820100	-3.00261100
C	-3.04283000	-1.78028600	-0.60235800
C	2.74010500	-1.80046000	-1.40098200
Be	0.21151600	1.00437900	-1.65681100
Be	-0.21884300	-1.03508500	-1.63776400
Be	-1.64675400	0.33723000	-0.98918900

$Be_4@C_{60}$ (178.02 cm^{-1})

C	3.47958700	0.87341100	-0.00101200
C	3.36872000	0.02890300	1.18605000
C	2.83236300	2.20386500	-0.00139500
C	2.63232700	0.47419000	2.34664100
C	1.79069300	-0.45440400	3.03316600
C	3.20128900	-1.35457000	0.73551600
C	2.36016100	-2.26531300	1.45404600
C	1.66120300	-1.80558600	2.61621100
C	2.01662100	1.78101700	-2.36908800
C	2.63137800	0.47247400	-2.34800900
C	2.09665100	2.61840900	-1.18429700
C	3.36821400	0.02802500	-1.18737200
C	3.20098000	-1.35507300	-0.73577400
C	1.78949600	-0.45667000	-3.03353300
C	1.66019100	-1.80752400	-2.61550000
C	2.35962500	-2.26641900	-1.45328200
C	-0.33105800	3.22360300	-1.43989100
C	-0.39509800	2.37995900	-2.63051700
C	0.90539400	3.31853300	-0.73795900
C	0.75965800	1.66468700	-3.02401800
C	0.61223000	0.27374600	-3.45611500
C	-1.67229200	1.75040700	-2.62885000
C	-1.81768500	0.40922600	-3.05220400
C	-0.63792900	-0.32412500	-3.46471600
C	-0.33051000	3.22463100	1.43762700
C	-1.55238500	3.14683000	0.71894300
C	0.90568600	3.31913400	0.73519100
C	-1.55262400	3.14629700	-0.72069800
C	-2.37651300	2.20631400	-1.43499800
C	-2.37600500	2.20743600	1.43426400
C	-3.23650500	1.32413700	0.73981800
C	-3.23679900	1.32359200	-0.73954600
C	2.01750800	1.78277600	2.36695100
C	0.76086100	1.66695300	3.02247900

C	2.09714600	2.61927400	1.18158200
C	-0.39408300	2.38194100	2.62890800
C	-1.67126100	1.75239000	2.62817700
C	0.61360400	0.27633900	3.45563800
C	-0.63654000	-0.32150400	3.46516400
C	-1.81647100	0.41152700	3.05258800
C	-3.45861800	-0.91439200	0.00102600
C	-3.37429700	-0.05695300	1.18739600
C	-2.65074600	-0.50034200	2.33386700
C	-2.83245500	-2.18705600	0.00138300
C	-2.02404700	-1.81048900	-2.30847700
C	-2.65168800	-0.50209300	-2.33244400
C	-3.37480300	-0.05785800	-1.18604000
C	-2.12246900	-2.63532000	-1.17536900
C	0.25401700	-3.25338600	-1.41358800
C	0.35052000	-2.41177200	-2.59944700
C	-0.77624800	-1.70672000	-3.01815900
C	-0.95245700	-3.35462700	-0.72762300
C	0.25457300	-3.25235900	1.41590500
C	1.50902300	-3.15785100	0.70387000
C	1.50875600	-3.15834600	-0.70211000
C	-0.95217300	-3.35407000	0.73048800
C	-2.02310700	-1.80874900	2.31061400
C	-0.77505400	-1.70447100	3.01970800
C	0.35154900	-2.40983700	2.60109200
C	-2.12200100	-2.63444200	1.17816000
Be	2.02442900	-0.18873300	-0.00028300
Be	1.09939900	1.63933400	-0.00073400
Be	-0.02341100	-0.16136400	0.00019600
Be	-1.93956700	0.19920900	0.00016000

$Be_5@C_{60}$ (178.30 cm^{-1})

C	0.12736400	-2.41404500	2.60995500
C	-1.27137000	-2.02809800	2.60340400
C	1.08806000	-1.47554800	3.04675500
C	-1.67754800	-0.77050900	3.02991300
C	-2.73525100	-0.04798300	2.32959600
C	-1.90089200	-2.63357000	1.42536200
C	-2.93463300	-1.92942500	0.73369300
C	-3.34081100	-0.62726000	1.18422700
C	2.59955500	-2.14242500	1.18239000
C	1.59679500	-3.09082100	0.72831500
C	2.34623200	-1.32302000	2.32392900
C	0.36554200	-3.23228400	1.45725500

C	-0.87267800	-3.37116800	0.72236300
C	1.59764100	-3.09033200	-0.72755700
C	0.36744600	-3.23187800	-1.45827600
C	-0.87163200	-3.37091200	-0.72521200
C	3.33914000	0.62667300	1.18891900
C	3.56384200	-0.17641300	0.00228000
C	2.73195300	0.04687800	2.33309300
C	3.23999700	-1.55495700	0.00184000
C	2.60087000	-2.14169300	-1.17975600
C	3.34083400	0.62715400	-1.18414800
C	2.73519800	0.04786000	-2.32947000
C	2.34948700	-1.32194400	-2.32137400
C	1.26792900	2.02706800	2.60614300
C	1.89911300	2.63312200	1.42926200
C	1.67327300	0.76926000	3.03245800
C	2.93375600	1.92934800	0.73859400
C	2.93463100	1.92964200	-0.73370500
C	0.87161100	3.37044100	0.72504800
C	0.87255000	3.37092500	-0.72226900
C	1.90110100	2.63370900	-1.42542200
C	-0.68459100	0.18228900	3.49020900
C	-1.09220200	1.47427100	3.04589200
C	0.67977600	-0.18378400	3.49110500
C	-0.13093300	2.41295600	2.61081900
C	-0.36753700	3.23180100	1.45841300
C	-2.34934200	1.32198500	2.32114300
C	-2.60156300	2.14224700	1.18000900
C	-1.59738000	3.08988600	0.72751200
C	-0.12732800	2.41418300	-2.60967500
C	-0.36543900	3.23276000	-1.45726300
C	-1.59621600	3.09004500	-0.72804700
C	-1.08798800	1.47584100	-3.04647000
C	0.68453100	-0.18209000	-3.49021200
C	1.67751200	0.77067800	-3.02990100
C	1.27154500	2.02827100	-2.60344600
C	-0.67981700	0.18401800	-3.49100300
C	-1.26787000	-2.02677300	-2.60608200
C	0.13088500	-2.41274700	-2.61081300
C	1.09211200	-1.47414100	-3.04585900
C	-1.67339700	-0.76900300	-3.03259900
C	-3.33918400	-0.62654300	-1.18901000
C	-2.93344000	-1.92897700	-0.73853100
C	-1.89891100	-2.63269300	-1.42910000
C	-2.73208800	-0.04669500	-2.33327500

C	-2.59957100	2.14255600	-1.18223900
C	-3.24092000	1.55561700	-0.00180500
C	-3.56350000	0.17659900	-0.00238800
C	-2.34627900	1.32318200	-2.32371300
Be	1.36822000	-1.32421700	0.00191200
Be	0.00047700	0.00042600	-0.00652800
Be	-1.37188100	1.31984400	0.00112300
Be	1.13720000	1.54882900	0.00174700
Be	-1.13397400	-1.55017300	-0.00016800

$Be_6@C_{60}$ (240.53 cm^{-1})

C	-0.53362000	-1.12768200	3.36372200
C	0.88867700	-0.86852900	3.36563400
C	-1.04557400	-2.18913200	2.62237900
C	1.74427300	-1.68057900	2.62602900
C	2.83728400	-1.09827000	1.87446800
C	1.08152300	0.56414400	3.37364900
C	2.12234100	1.12945700	2.64190300
C	3.02360300	0.28741000	1.88221600
C	-2.93528600	-0.79887100	1.87433800
C	-2.39128100	0.30677800	2.63604500
C	-2.27178200	-2.02966200	1.86760500
C	-1.21972400	0.14471300	3.37063400
C	-0.22148900	1.19025100	3.37694700
C	-2.62232600	1.52540800	1.88759200
C	-1.65699400	2.53690100	1.89389500
C	-0.43341100	2.35777600	2.64843900
C	-2.72499200	-2.29860000	-0.56929000
C	-3.42051500	-1.00856500	-0.56229500
C	-2.14032800	-2.82393400	0.65215100
C	-3.53230700	-0.24185500	0.66634700
C	-3.34324100	1.15960200	0.67430200
C	-3.06664200	-0.31895900	-1.79646100
C	-2.87029900	1.13905200	-1.78825300
C	-3.03055100	1.88319900	-0.54568000
C	-0.09470000	-3.56179700	-0.57555800
C	-0.63402900	-3.00794400	-1.81067700
C	-0.86551100	-3.43611600	0.64891600
C	-1.96001800	-2.37113000	-1.80756700
C	-2.15132600	-1.14570600	-2.55282400
C	0.43920900	-2.39032800	-2.55922900
C	0.21918400	-1.17766900	-3.34611800
C	-1.07021500	-0.55822600	-3.34269800
C	1.21778500	-2.79441300	1.86417700

C	2.02081600	-2.90993500	0.65269600
C	-0.15789100	-3.04494700	1.86230400
C	1.34714800	-3.29915800	-0.57389200
C	1.65949500	-2.58979900	-1.80787500
C	2.99749400	-1.88731600	0.65874400
C	3.36179700	-1.18871500	-0.56146400
C	2.67565600	-1.52611100	-1.80188600
C	0.52811600	1.11599100	-3.33307900
C	1.20697600	-0.14301800	-3.33996000
C	2.42399800	-0.31168000	-2.54728500
C	1.06007100	2.21861800	-2.53368200
C	-1.26058500	2.82589500	-1.77852500
C	-1.76820600	1.70311000	-2.53744900
C	-0.87930200	0.85948400	-3.33500700
C	0.18700300	3.08915900	-1.77645300
C	0.07344200	3.53484400	0.68877900
C	-1.31785700	3.28153500	0.68705800
C	-2.01867400	2.94322100	-0.53939200
C	0.85165600	3.46613300	-0.53558600
C	2.71738900	2.26452900	0.68236600
C	1.91046600	2.35152700	1.89362600
C	0.65026300	2.95691500	1.89656000
C	2.17244600	2.83138400	-0.53867800
C	2.98642200	0.78440800	-1.78847000
C	3.55714500	0.26351600	-0.55310500
C	3.38860100	1.01971500	0.67541500
C	2.28849400	2.07944400	-1.78152000
Be	-0.00015000	0.00043000	-0.03051100
Be	-1.62792400	-0.87409600	-0.77435100
Be	0.33185500	-1.81443600	-0.78047600
Be	-1.33749100	1.28147000	-0.76533100
Be	1.83300800	-0.24273900	-0.77199500
Be	0.80054300	1.67116200	-0.76079900

$Be_7@C_{60}$ (252.52 cm^{-1})

C	2.22690300	-2.51046700	1.27405200
C	2.22134200	-2.81644400	-0.13876300
C	1.08526900	-2.75809600	2.03239700
C	1.07451700	-3.35387200	-0.71826900
C	0.63754900	-2.87563900	-2.02181400
C	2.99297600	-1.78150800	-0.82152100
C	2.58939000	-1.32169600	-2.09329500
C	1.38705700	-1.86859100	-2.69383500
C	1.41066000	-0.58969000	3.21541400

C	2.60732600	-0.34183100	2.43237300
C	0.65750500	-1.78295100	3.02422400
C	3.00159200	-1.28699800	1.46187400
C	3.48732000	-0.87418400	0.17507100
C	2.65050400	1.08213700	2.16678300
C	3.12604600	1.51479600	0.86696200
C	3.56060600	0.53740900	-0.13062300
C	-1.46407900	-0.49856700	3.20716200
C	-0.70635500	0.73282200	3.41221200
C	-0.78686300	-1.73706700	3.01997600
C	0.73165900	0.68683300	3.41610500
C	1.53083100	1.71130200	2.78027800
C	-1.43483700	1.80583900	2.77238200
C	-0.64675000	2.82993000	2.08931400
C	0.81337700	2.78335900	2.09342900
C	-2.38906700	-2.36440800	1.26061700
C	-3.08570900	-1.09403100	1.44418800
C	-1.26985300	-2.68368100	2.02554800
C	-2.63785500	-0.17542900	2.41768200
C	-2.58859800	1.24827700	2.15179900
C	-3.53644200	-0.65139600	0.15512500
C	-3.51825400	0.76200300	-0.15082300
C	-3.02795500	1.70993300	0.84956600
C	-0.11469600	-3.61270000	0.07140000
C	-1.28069400	-3.27929800	-0.72518400
C	-0.10939200	-3.31818500	1.42919000
C	-2.39490900	-2.67071400	-0.15221300
C	-3.09487700	-1.58872700	-0.83921800
C	-0.80696200	-2.83034600	-2.02621000
C	-1.48740000	-1.77776700	-2.70286700
C	-2.65573800	-1.15529000	-2.10815900
C	-2.27319000	2.42742900	-1.24954300
C	-3.03820400	1.21098400	-1.45750800
C	-2.60717600	0.25110200	-2.45541200
C	-1.07752500	2.68737400	-2.07187800
C	0.11277300	3.54786400	-0.01178400
C	-1.06564900	3.30510300	0.78351400
C	-2.26726900	2.73064100	0.15159100
C	0.10687200	3.23633500	-1.45759200
C	2.43040700	2.27868400	-1.23673000
C	2.43544700	2.58163400	0.16474100
C	1.26880900	3.23086700	0.79001700
C	1.25747400	2.61342200	-2.06556000
C	1.50633500	0.40595300	-3.25134400

C	2.63128700	0.08472700	-2.43998800
C	3.11770500	1.01579500	-1.44036400
C	0.79218300	1.66701200	-3.06265300
C	-1.45935700	0.50005400	-3.25970600
C	-0.73354600	-0.74251500	-3.40369000
C	0.70430400	-0.78771800	-3.39918900
C	-0.66764900	1.71323400	-3.06667500
Be	0.05322400	1.76577100	0.73132000
Be	-1.70705400	0.87519800	-0.18523100
Be	-0.01661900	-0.33240100	1.86255500
Be	0.04554600	1.31720100	-1.39267400
Be	0.00311500	0.03735900	-0.00915700
Be	1.76121700	0.77079200	-0.17731800
Be	-0.03319500	-1.07849300	-1.55336500

$Be_8@C_{60}$ (217.46 cm^{-1})

C	-0.64959500	-2.96651500	1.92298700
C	0.73387400	-2.77502200	2.19123900
C	-1.08434700	-3.35950700	0.58199700
C	1.72678300	-2.94753500	1.12671800
C	2.83254700	-2.00358600	0.98539300
C	0.86333900	-1.61927100	3.04284300
C	1.95414300	-0.68823100	2.90069600
C	2.95922100	-0.86325900	1.90129100
C	-3.01267000	-1.75605200	0.73653200
C	-2.57827100	-1.37208500	2.03589300
C	-2.27419800	-2.78316500	-0.01766900
C	-1.40905600	-1.98177100	2.64390300
C	-0.48648200	-1.13191200	3.33521100
C	-2.85187500	0.06582900	2.18685100
C	-1.90662100	0.88615700	2.88137500
C	-0.72858100	0.28750400	3.47131200
C	-2.59221200	-1.41527700	-2.11263500
C	-3.30231300	-0.43574600	-1.37011600
C	-2.04683200	-2.59938200	-1.43461600
C	-3.53916300	-0.58598000	0.04312500
C	-3.45330100	0.53983400	0.94868000
C	-2.92377500	0.89374700	-1.83656300
C	-2.85425300	1.99512900	-0.94155300
C	-3.13431100	1.87268500	0.44387000
C	0.15108200	-2.37414600	-2.69327600
C	-0.38405200	-1.18887900	-3.32324700
C	-0.69683600	-3.07944600	-1.72660000
C	-1.72161000	-0.71745500	-3.03965000

C	-1.95387100	0.71279700	-2.88473600
C	0.72424200	-0.23115100	-3.45609000
C	0.49631900	1.19037200	-3.32086000
C	-0.85411800	1.65083700	-3.03269800
C	1.31400400	-3.34245100	-0.20064400
C	2.12786400	-2.63982600	-1.17365800
C	-0.12581800	-3.55536100	-0.48300000
C	1.53215300	-2.14988800	-2.42051000
C	1.89658200	-0.84577200	-2.89863100
C	3.07714200	-1.83373400	-0.42968900
C	3.41586500	-0.48486700	-0.93515300
C	2.82596300	-0.01431600	-2.15635000
C	0.68731100	2.97934100	-1.86212400
C	1.43594500	2.03954400	-2.64258600
C	2.60222300	1.42395500	-2.01773400
C	1.08999600	3.36319100	-0.54891800
C	-1.31008000	3.34901800	0.21432300
C	-1.71938500	2.93397100	-1.08653900
C	-0.74703000	2.74645100	-2.11894000
C	0.10378800	3.56830100	0.49191900
C	-0.14740000	2.40344900	2.63312500
C	-1.56635900	2.19428800	2.37606400
C	-2.15417900	2.64348100	1.17528200
C	0.67672000	3.06604800	1.71307200
C	2.53823600	1.44809200	2.10315600
C	1.69309500	0.75797300	3.03585300
C	0.36432200	1.22468500	3.31518500
C	2.04539900	2.61231600	1.42708200
C	3.03365300	1.82125900	-0.69915500
C	3.53582300	0.62808500	-0.01596300
C	3.28182400	0.44004000	1.38777900
C	2.31245200	2.83495600	0.06265000
Be	-1.79273100	-0.23813800	0.70355800
Be	-0.76079300	-1.82501000	-0.41573100
Be	-0.41789100	0.12464000	-1.88766400
Be	1.34323400	-1.52229200	0.05976500
Be	0.01248100	-0.05677900	-0.01884300
Be	-0.25422200	1.87875000	-0.33410800
Be	0.34619900	-0.08016500	1.88926000
Be	1.78874300	0.47138000	-0.64949400

$Be_9@C_{60}$ (203.06 cm^{-1})

C	1.90300600	0.71104900	2.95005900
C	1.90705300	-0.73289900	2.94208700

C	0.62952200	1.44927400	3.19433100
C	0.63766300	-1.48071100	3.17756000
C	0.32547700	-2.65133200	2.38668200
C	2.83974000	-1.16923400	1.92373000
C	2.48723100	-2.34885200	1.08746600
C	1.25846800	-3.07176300	1.31375400
C	1.24107800	3.06430100	1.34737600
C	2.47381500	2.35044000	1.11296900
C	0.31061600	2.62634800	2.41540600
C	2.83330200	1.16403100	1.93658800
C	3.40688400	0.00252600	1.27967100
C	2.73242200	2.33723900	-0.31304600
C	3.30242900	1.16069800	-0.94375000
C	3.67474400	0.01133800	-0.17355300
C	-1.64552500	3.09772900	0.86979700
C	-0.74233200	3.54791300	-0.13723500
C	-1.12744100	2.63835900	2.17175500
C	0.71764000	3.52151100	0.08236300
C	1.64406900	3.08122600	-0.95893700
C	-1.22461200	3.06925600	-1.40321800
C	-0.31417400	2.60188700	-2.43473000
C	1.15981700	2.62514700	-2.25039300
C	-2.78476700	0.70665200	2.16601700
C	-3.29425600	1.16653000	0.89261200
C	-1.68708700	1.46704200	2.83310000
C	-2.72434500	2.37298500	0.25553900
C	-2.47694100	2.33173300	-1.14556100
C	-3.62203000	-0.01048500	0.09799900
C	-3.42549000	-0.00214200	-1.36411200
C	-2.82221000	1.16148300	-1.94878500
C	-0.59657300	-0.76892800	3.43845000
C	-1.67892900	-1.50780100	2.81710300
C	-0.60102300	0.72772900	3.44771500
C	-2.78018500	-0.74547900	2.15770500
C	-3.28690600	-1.19406400	0.87942100
C	-1.11276900	-2.66912800	2.14341600
C	-1.62808500	-3.11603300	0.83591300
C	-2.71081400	-2.39048600	0.22959700
C	-1.87596100	-0.71005400	-2.97349700
C	-2.81577400	-1.15596300	-1.96144600
C	-2.46350800	-2.33232900	-1.17065400
C	-0.63152700	-1.42505800	-3.22481500
C	0.61170700	0.71208900	-3.43423500
C	-0.63955900	1.45658500	-3.20891400

C	-1.87980500	0.73186600	-2.96523500
C	0.61567000	-0.67113000	-3.44181700
C	2.78465600	-0.69270000	-2.22638400
C	2.78058300	0.73231700	-2.21862800
C	1.70772600	1.47342200	-2.83461400
C	1.71590800	-1.43284000	-2.85049900
C	1.66157900	-3.06150500	-0.99263800
C	2.74563100	-2.31832600	-0.33835200
C	3.30858500	-1.13186200	-0.95622400
C	1.17452500	-2.59365900	-2.27858300
C	-1.20702900	-3.05955800	-1.43606600
C	-0.72232400	-3.55010200	-0.17590600
C	0.73741600	-3.51777800	0.04381300
C	-0.29955300	-2.57631800	-2.46249500
Be	-0.34243600	-1.12765100	1.66098000
Be	-0.94166500	-1.15133700	-1.38577700
Be	-1.94109600	-0.00864600	0.69534400
Be	-0.01038300	-0.00081200	0.05608900
Be	1.07088400	1.73023700	0.04462000
Be	-0.34584200	1.10450900	1.67537800
Be	-0.94938600	1.16218100	-1.37149400
Be	1.61790000	-0.00186800	1.28962800
Be	1.08087700	-1.72489400	0.02673000

$Be_{10}@C_{60}$ (58.81 cm^{-1})

C	2.31903800	2.67099800	-0.74421400
C	2.32258800	2.68009900	0.71173400
C	1.08960400	3.10636300	-1.45491100
C	1.09342000	3.12001800	1.41793500
C	0.67400400	2.35976100	2.56573300
C	3.07037800	1.52718800	1.17459300
C	2.64192400	0.77524300	2.37085300
C	1.44459900	1.20299700	3.04134600
C	1.43622600	1.16813900	-3.05727700
C	2.63462400	0.74798000	-2.38361500
C	0.66739700	2.32888200	-2.59218000
C	3.06446600	1.51243300	-1.19651200
C	3.56051400	0.83211000	-0.00840900
C	2.67238600	-0.67737500	-2.40453300
C	3.11906300	-1.38544500	-1.18367600
C	3.55640100	-0.65876800	-0.00042300
C	-1.49517400	1.10371100	-3.05341000
C	-0.74302900	-0.05653200	-3.50930700
C	-0.77766900	2.29780900	-2.59070400

C	0.73491300	-0.02408100	-3.51107500
C	1.51640300	-1.15664000	-3.10259300
C	-1.47271300	-1.22234200	-3.09882800
C	-0.68404100	-2.38249800	-2.64367600
C	0.78050600	-2.35031200	-2.64575600
C	-2.43830000	2.56916900	-0.73797800
C	-3.13068300	1.37695100	-1.18784800
C	-1.23043600	3.05604000	-1.45239400
C	-2.67178400	0.63153700	-2.37635100
C	-2.64660700	-0.79402400	-2.39717900
C	-3.58998900	0.67466400	0.00129600
C	-3.52403400	-0.81412400	0.00927200
C	-3.05823300	-1.52075000	-1.17519900
C	-0.07995400	3.63717100	0.73749400
C	-1.22688800	3.06979600	1.42174700
C	-0.08218600	3.64000400	-0.78176100
C	-2.43765600	2.57776800	0.71811100
C	-3.12993200	1.39127400	1.18248700
C	-0.77139500	2.32858300	2.56807100
C	-1.48830400	1.13848800	3.04541700
C	-2.66701400	0.65865700	2.37787900
C	-2.31130500	-2.66346700	0.74506500
C	-3.05466500	-1.50712800	1.19998200
C	-2.64079700	-0.76702200	2.41296800
C	-1.09722200	-3.09768500	1.49689800
C	0.07615100	-3.51637300	-0.72784800
C	-1.10095900	-3.11340700	-1.45944500
C	-2.31381200	-2.67206000	-0.70955500
C	0.07803600	-3.50941000	0.76728200
C	2.42784700	-2.55966500	0.73872300
C	2.42681900	-2.56831200	-0.71619600
C	1.23235300	-3.06231300	-1.46288800
C	1.23599300	-3.04645300	1.49384200
C	1.52330300	-1.12131700	3.10981300
C	2.67863000	-0.65029500	2.40579600
C	3.12127200	-1.37176900	1.19150000
C	0.78698800	-2.32088800	2.66959600
C	-1.46418300	-1.18705300	3.11432500
C	-0.73420000	-0.01618100	3.51031700
C	0.74352900	0.01630600	3.50804600
C	-0.67725800	-2.35317100	2.67164500
Be	0.03627400	-1.73770900	-1.15202600
Be	-1.76011400	-1.12391600	0.00739400
Be	-0.01762200	0.65827600	-1.94369300

Be	0.03891200	-1.72490600	1.17147200
Be	0.00064400	0.00140700	-0.00090400
Be	1.80768600	-1.04764300	0.00212700
Be	-0.01282300	0.68454400	1.93555200
Be	-0.03584300	2.08925800	-0.03997200
Be	1.80542900	1.09693200	-0.00213400
Be	-1.84597200	1.02384500	0.00114700

$Be_{11}@C_{60}$ (164.97 cm^{-1})

C	-3.29529700	-0.36972900	1.46159400
C	-3.18206800	-1.62856800	0.74541000
C	-3.47264700	0.93070200	0.72432400
C	-3.18206800	-1.62856800	-0.74541000
C	-2.20241400	-2.45620300	-1.44514700
C	-2.20241400	-2.45620300	1.44514700
C	-1.26507600	-3.32704300	0.71576800
C	-1.26507600	-3.32704300	-0.71576800
C	-1.82893200	2.01718200	2.36400400
C	-1.70603300	0.78247400	3.12213900
C	-2.72112700	2.09878200	1.16982100
C	-2.42987300	-0.43372700	2.62232600
C	-1.78079700	-1.73291500	2.63188900
C	-0.33922900	0.67633800	3.59254500
C	0.33922900	-0.67633800	3.59254500
C	-0.38058000	-1.86090900	3.12974700
C	-0.93569600	3.49226800	0.00000000
C	-0.09227700	3.42732500	1.15984600
C	-2.23581700	2.82026800	0.00000000
C	-0.53686200	2.68327200	2.34419800
C	0.38058000	1.86090900	3.12974700
C	1.26507600	3.32704300	0.71576800
C	2.20241400	2.45620300	1.44514700
C	1.78079700	1.73291500	2.63188900
C	-1.82893200	2.01718200	-2.36400400
C	-0.53686200	2.68327200	-2.34419800
C	-2.72112700	2.09878200	-1.16982100
C	-0.09227700	3.42732500	-1.15984600
C	1.26507600	3.32704300	-0.71576800
C	0.38058000	1.86090900	-3.12974700
C	1.78079700	1.73291500	-2.63188900
C	2.20241400	2.45620300	-1.44514700
C	-3.29529700	-0.36972900	-1.46159400
C	-2.42987300	-0.43372700	-2.62232600
C	-3.47264700	0.93070200	-0.72432400

C	-1.70603300	0.78247400	-3.12213900
C	-0.33922900	0.67633800	-3.59254500
C	-1.78079700	-1.73291500	-2.63188900
C	-0.38058000	-1.86090900	-3.12974700
C	0.33922900	-0.67633800	-3.59254500
C	3.29529700	0.36972900	-1.46159400
C	2.42987300	0.43372700	-2.62232600
C	1.70603300	-0.78247400	-3.12213900
C	3.47264700	-0.93070200	-0.72432400
C	3.29529700	0.36972900	1.46159400
C	3.18206800	1.62856800	0.74541000
C	3.18206800	1.62856800	-0.74541000
C	3.47264700	-0.93070200	0.72432400
C	1.82893200	-2.01718200	2.36400400
C	1.70603300	-0.78247400	3.12213900
C	2.42987300	0.43372700	2.62232600
C	2.72112700	-2.09878200	1.16982100
C	0.93569600	-3.49226800	0.00000000
C	0.09227700	-3.42732500	1.15984600
C	0.53686200	-2.68327200	2.34419800
C	2.23581700	-2.82026800	0.00000000
C	1.82893200	-2.01718200	-2.36400400
C	0.53686200	-2.68327200	-2.34419800
C	0.09227700	-3.42732500	-1.15984600
C	2.72112700	-2.09878200	-1.16982100
Be	1.55349900	0.79657800	1.04892300
Be	1.55349900	0.79657800	-1.04892300
Be	-0.46662400	0.95627800	1.82857100
Be	1.84969400	-1.06161900	0.00000000
Be	0.00000000	0.00000000	0.00000000
Be	0.46662400	-0.95627800	1.82857100
Be	0.46662400	-0.95627800	-1.82857100
Be	-1.55349900	-0.79657800	-1.04892300
Be	-1.84969400	1.06161900	0.00000000
Be	-0.46662400	0.95627800	-1.82857100
Be	-1.55349900	-0.79657800	1.04892300

$Be_{12}@C_{60}$ (112.39 cm^{-1})

C	-3.54716600	0.66874400	0.61506400
C	-3.14520800	0.01023600	1.84465300
C	-3.61824500	-0.12751700	-0.66543600
C	-2.79155300	-1.44683600	1.84554900
C	-1.61237500	-1.89324300	2.57589600
C	-2.30156900	0.94844900	2.57378400

C	-1.14702200	0.47381000	3.38125400
C	-0.80386000	-0.94123300	3.38234700
C	-2.52158800	1.84407200	-1.88715200
C	-2.48007800	2.63519300	-0.66637900
C	-3.09055200	0.46284200	-1.88686100
C	-2.99073000	2.02171700	0.61458500
C	-2.24098500	2.20799100	1.84371000
C	-1.23848000	3.40117000	-0.66669400
C	-0.46077700	3.57993300	0.61440800
C	-0.96416700	2.99405500	1.84334600
C	-1.18271800	-0.28969500	-3.40458600
C	-0.63754100	1.03530400	-3.40547100
C	-2.38305400	-0.58018100	-2.62285300
C	-1.28566500	2.08715600	-2.62436100
C	-0.51307400	3.08268400	-1.88773200
C	0.79097700	0.92609700	-3.40467600
C	1.59040900	1.86759100	-2.62297900
C	0.97681000	2.96843000	-1.88678400
C	-1.39575500	-2.79731600	-1.88337700
C	-0.18560800	-2.44850000	-2.62092100
C	-2.53446900	-1.83043500	-1.88510200
C	-0.09115500	-1.21777400	-3.40391500
C	1.12861600	-0.46618300	-3.40371200
C	0.95702600	-2.97818300	-1.88288400
C	2.22930700	-2.19412100	-1.88283200
C	2.27050400	-0.93553100	-2.62086000
C	-2.84685000	-2.21862100	0.61738900
C	-1.73264800	-3.16658800	0.61892300
C	-3.27433600	-1.54555400	-0.66432700
C	-0.99674700	-3.47919600	-0.66121400
C	0.45773500	-3.59138300	-0.66085800
C	-0.98118700	-2.98625000	1.84793400
C	0.51397300	-3.09982500	1.84826100
C	1.23061900	-3.39235700	0.62029300
C	3.55676800	-0.67505200	-0.66142900
C	3.00136200	-2.02415600	-0.66079900
C	2.47640100	-2.62554000	0.62035000
C	3.60698000	0.12264500	0.61892300
C	2.85224400	2.22841600	-0.66379500
C	2.77496400	1.44039700	-1.88490200
C	3.12734600	-0.01186700	-1.88375700
C	3.26227100	1.54438900	0.61777200
C	1.40543500	2.81329000	1.84459400
C	0.99792500	3.46928500	0.61528500

C	1.74051300	3.17309400	-0.66500200
C	2.54827900	1.84225900	1.84617500
C	1.20246500	0.29447300	3.38407000
C	0.09271500	1.23784200	3.38244100
C	0.18816000	2.48160800	2.57336700
C	2.41599400	0.58798900	2.57607300
C	2.53775700	-1.85410900	1.84855500
C	1.30320000	-2.11555500	2.57712800
C	0.64810800	-1.05241600	3.38418400
C	3.10829400	-0.46746000	1.84793100
Be	1.23695700	1.45285400	-0.88044900
Be	1.76601200	-0.72679100	-0.87873800
Be	-0.99854200	1.62577100	-0.88240400
Be	1.83328300	0.44587500	0.81868700
Be	-0.00266300	-0.00064100	0.02180000
Be	0.14460600	1.88162600	0.81581300
Be	0.98977400	-1.60483800	0.81842200
Be	-1.22190600	-1.43934300	0.81767500
Be	-1.85689300	-0.45116300	-0.87936800
Be	-0.14180400	-1.90303000	-0.87970200
Be	-1.74698900	0.71968500	0.81626400
Be	0.00117300	0.00227200	2.08811300

$Be_{13}@C_{60}$ (153.51 cm^{-1})

C	-0.70504600	-0.27050100	3.58485400
C	-1.81014200	0.57468800	3.13870500
C	0.70504600	0.27050100	3.58485400
C	-1.51014100	1.94122600	2.62540900
C	-2.19056500	2.47632300	1.45380400
C	-2.75204600	-0.26475300	2.40175900
C	-3.45523100	0.28223900	1.18226400
C	-3.20371400	1.64549500	0.73099300
C	1.51014100	-1.94122600	2.62540900
C	0.15344000	-2.47158600	2.63079200
C	1.81014200	-0.57468800	3.13870500
C	-0.97574600	-1.63384700	3.14457800
C	-2.24167500	-1.63028700	2.41322200
C	0.00093000	-3.33501800	1.47361600
C	-1.29058100	-3.33155500	0.72787000
C	-2.36492100	-2.46420300	1.17654700
C	3.45523100	-0.28223900	1.18226400
C	3.20371400	-1.64549500	0.73099300
C	2.75204600	0.26475300	2.40175900
C	2.19056500	-2.47632300	1.45380400

C	1.26141000	-3.33808400	0.74552000
C	3.20371400	-1.64549500	-0.73099300
C	2.19056500	-2.47632300	-1.45380400
C	1.26141000	-3.33808400	-0.74552000
C	2.36492100	2.46420300	1.17654700
C	3.03604500	1.92801400	0.00000000
C	2.24167500	1.63028700	2.41322200
C	3.62547300	0.55908600	0.00000000
C	3.45523100	-0.28223900	-1.18226400
C	2.36492100	2.46420300	-1.17654700
C	2.24167500	1.63028700	-2.41322200
C	2.75204600	0.26475300	-2.40175900
C	-0.15344000	2.47158600	2.63079200
C	-0.00093000	3.33501800	1.47361600
C	0.97574600	1.63384700	3.14457800
C	1.29058100	3.33155500	0.72787000
C	1.29058100	3.33155500	-0.72787000
C	-1.26141000	3.33808400	0.74552000
C	-1.26141000	3.33808400	-0.74552000
C	-0.00093000	3.33501800	-1.47361600
C	0.70504600	0.27050100	-3.58485400
C	0.97574600	1.63384700	-3.14457800
C	-0.15344000	2.47158600	-2.63079200
C	-0.70504600	-0.27050100	-3.58485400
C	0.15344000	-2.47158600	-2.63079200
C	1.51014100	-1.94122600	-2.62540900
C	1.81014200	-0.57468800	-3.13870500
C	-0.97574600	-1.63384700	-3.14457800
C	-2.36492100	-2.46420300	-1.17654700
C	-1.29058100	-3.33155500	-0.72787000
C	0.00093000	-3.33501800	-1.47361600
C	-2.24167500	-1.63028700	-2.41322200
C	-3.45523100	0.28223900	-1.18226400
C	-3.62547300	-0.55908600	0.00000000
C	-3.03604500	-1.92801400	0.00000000
C	-2.75204600	-0.26475300	-2.40175900
C	-1.51014100	1.94122600	-2.62540900
C	-2.19056500	2.47632300	-1.45380400
C	-3.20371400	1.64549500	-0.73099300
C	-1.81014200	0.57468800	-3.13870500
Be	0.59372400	-1.55254200	-1.03784600
Be	1.05640100	0.41028800	-1.83076400
Be	0.59372400	-1.55254200	1.03784600
Be	-1.05640100	-0.41028800	-1.83076400

Be	0.00000000	0.00000000	0.00000000
Be	-1.20207500	-1.54907100	0.00000000
Be	-0.59372400	1.55254200	-1.03784600
Be	-0.59372400	1.55254200	1.03784600
Be	1.05640100	0.41028800	1.83076400
Be	1.20207500	1.54907100	0.00000000
Be	-1.05640100	-0.41028800	1.83076400
Be	-2.11258300	0.41822300	0.00000000
Be	2.11258300	-0.41822300	0.00000000

$(Be_{13}@C_{60})^{4-}$ (26.45 cm^{-1})

C	0.03977600	2.80330600	-2.33779800
C	1.42892900	2.35058400	-2.43301600
C	-0.46743400	3.46715500	-1.09756100
C	2.32714000	2.50883300	-1.24773700
C	3.25887100	1.45114300	-0.85942900
C	1.45124800	1.10287400	-3.18847900
C	2.37160500	0.00330100	-2.76346800
C	3.28069800	0.17431100	-1.63125400
C	-2.66697700	2.13777600	-1.32095700
C	-2.18100500	1.50313000	-2.54876500
C	-1.80179900	3.11652600	-0.59079700
C	-0.80314300	1.82591100	-3.04160900
C	0.07656400	0.77245600	-3.56801900
C	-2.63155700	0.10918600	-2.54956600
C	-1.72753400	-0.96815100	-3.06189600
C	-0.39300000	-0.64692800	-3.58720400
C	-2.52228300	2.08074600	1.65282300
C	-3.35911800	1.11010500	0.93324300
C	-1.73047900	3.08903600	0.88124300
C	-3.43259000	1.13910300	-0.56263000
C	-3.40955400	-0.12047600	-1.32504100
C	-3.26510500	-0.17772400	1.64236500
C	-3.24170300	-1.45877300	0.86708500
C	-3.31233600	-1.42995100	-0.60437000
C	0.26966500	2.71007200	2.42676400
C	-0.50256000	1.70545400	3.17082000
C	-0.35375600	3.42348000	1.26976200
C	-1.92296500	1.40051800	2.80344900
C	-2.37353500	0.00745400	2.79449700
C	0.42165300	0.63605900	3.57108600
C	-0.04649700	-0.78363200	3.58160700
C	-1.42509800	-1.08618400	3.17409000
C	1.82460000	3.14113500	-0.02681300

C	2.44343700	2.46548800	1.11461900
C	0.41885600	3.65194500	0.05039500
C	1.66115000	2.25766000	2.37169200
C	1.75365000	0.98274400	3.07430900
C	3.33055400	1.42469800	0.59868700
C	3.42158400	0.11876100	1.31469600
C	2.62742800	-0.09797400	2.52235300
C	-0.01015600	-2.81114300	2.35535900
C	0.81910900	-1.84488700	3.07178000
C	2.16176900	-1.48460100	2.51583100
C	0.49500900	-3.44543500	1.09923100
C	-1.84041300	-3.18394500	0.02888400
C	-2.32666100	-2.54157300	1.25144100
C	-1.40229300	-2.34661800	2.41189100
C	-0.40646700	-3.61212300	-0.04826700
C	-0.24297800	-2.72084300	-2.44930600
C	-1.63349100	-2.25750900	-2.35443000
C	-2.43963600	-2.49576400	-1.11669900
C	0.37991600	-3.39819800	-1.27058600
C	2.52549600	-2.06591200	-1.62811000
C	1.90639000	-1.38423000	-2.76530700
C	0.51580300	-1.72589600	-3.20366600
C	1.75765000	-3.10297900	-0.87352400
C	2.66499900	-2.12086600	1.29869400
C	3.44541400	-1.13083700	0.55932600
C	3.37616300	-1.10347500	-0.93084500
C	1.82796300	-3.13205600	0.58320100
Be	-1.58529700	-1.31552400	0.05009300
Be	-0.27435800	-1.04029000	1.71066700
Be	-1.72318600	0.56545400	-0.98595300
Be	0.43863100	-1.93899700	-0.05972800
Be	-0.07614500	0.00130400	-0.00080700
Be	-0.43964800	-0.97717400	-1.72259500
Be	1.58662600	-0.53978600	0.94177200
Be	1.46275600	1.26316400	-0.04842800
Be	-0.49323000	1.97015300	0.06011400
Be	0.38734700	0.96602400	1.69996500
Be	0.22554100	1.03427000	-1.69945900
Be	1.49274700	-0.50153700	-1.11625600
Be	-1.61823100	0.52453500	1.16450300

$Be_{14}@C_{60}$ (119.08 cm^{-1})

C	-0.18678913	-3.45021146	1.14895394
C	-1.05187593	-3.47371634	-0.02679239

C	-0.64174630	-2.70236531	2.36217069
C	-2.42499580	-2.82562117	-0.01975553
C	-2.85017857	-2.06099227	-1.19557225
C	-0.18970499	-3.43148451	-1.20414542
C	-0.64756650	-2.66404518	-2.40372877
C	-1.94050226	-1.98563270	-2.40393202
C	1.72761371	-1.73724697	2.53449310
C	2.19091362	-2.49227336	1.39336093
C	0.32084090	-1.84779091	3.05088242
C	1.20792011	-3.37498990	0.69040705
C	1.20610872	-3.36322882	-0.74763246
C	3.29453606	-1.77798158	0.74181714
C	3.29282079	-1.76570235	-0.77828619
C	2.18716308	-2.46890413	-1.43824611
C	0.35122951	0.62636025	3.57326633
C	1.73570069	0.72638123	3.10978003
C	-0.36804756	-0.68354969	3.57334963
C	2.43438335	-0.47853664	2.55816659
C	3.46186512	-0.45672012	1.51364582
C	1.90478392	1.98224131	2.40697272
C	2.77725535	1.99198348	1.18115068
C	3.62349297	0.86180527	0.76431137
C	-2.46682897	0.46235424	2.64512555
C	-1.77148147	1.74806735	2.64622360
C	-1.76455527	-0.76300542	3.12055477
C	-0.34474363	1.82015647	3.10139525
C	0.61531054	2.66999269	2.40433561
C	-2.22752929	2.52316083	1.50322555
C	-1.23200104	3.36719251	0.76142023
C	0.15714708	3.45335089	1.20289760
C	-2.84778372	-2.08051749	1.16927573
C	-3.53554891	-0.86755133	0.72802100
C	-1.93462257	-2.02425241	2.37628242
C	-3.35804620	0.42793881	1.48752464
C	-3.19390629	1.69939521	0.76221782
C	-3.53735385	-0.85574610	-0.73327306
C	-3.36156653	0.45223419	-1.47255572
C	-3.19564843	1.71144240	-0.72727509
C	0.15415574	3.47203663	-1.14712230
C	-1.23372644	3.37906031	-0.70383820
C	-2.23196234	2.54771394	-1.45753638
C	0.60944215	2.70855514	-2.36248192
C	2.77472212	2.01124615	-1.15583898
C	2.32894827	2.73321420	0.01915337

C	1.01680503	3.49562975	0.02723633
C	1.89910526	2.02112782	-2.37948353
C	2.42800646	-0.43674665	-2.57109194
C	3.45841984	-0.43202587	-1.52932073
C	3.62174421	0.87428196	-0.75925725
C	1.72809459	0.77674427	-3.10164107
C	-0.37683947	-0.62544517	-3.58276208
C	0.31317976	-1.79783766	-3.08010172
C	1.72092460	-1.69539403	-2.56544149
C	0.34241854	0.68412286	-3.56353806
C	-1.77878704	1.79155183	-2.61444380
C	-2.47364975	0.50545226	-2.63165146
C	-1.77215865	-0.71233083	-3.12807019
C	-0.35245427	1.87023443	-3.07093379
Be	1.47757115	1.09533108	0.00699803
Be	-0.15757089	2.09449877	0.01672571
Be	1.16653499	-0.75308599	1.04592689
Be	0.52234490	1.01182973	-1.74456747
Be	-0.28789728	0.00734735	0.00024406
Be	1.16258525	-0.73470990	-1.05992210
Be	-1.64932055	0.85901612	-1.05574194
Be	-1.91052924	-1.12956624	-0.00638519
Be	-0.64089618	-0.99366064	1.75143281
Be	-1.64734179	0.84010093	1.07083255
Be	0.06251828	-2.04985150	-0.01629538
Be	-0.64663172	-0.96479062	-1.76539883
Be	0.52763707	0.98274093	1.75977823
Be	2.63231957	-0.35997351	-0.00642937