Electronic Supplementary Information (ESI)

Covalent interactions depended on the distances between metal and fullerenes for thermodynamically stable M@C_{78} (M = La, Ce, and Sm)

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Table S1 The relative energy (ΔE) in kcal/mol and HOMO-LUMO gap (Gap) in eV for M@C_{78} (M = La, Ce, and Sm).

Molecules	PA	B3LYP/6-31G*-SDD		LC-M06L/6-31G*-SDD
		ΔE	Gap	ΔE
La@C_{2v}(24107)-C_{78}	0	0.0	1.29	0.0
La@D_{3h}(24109)-C_{78}	0	0.0	0.80	4.4
La@C_1(22595)-C_{78}	1	3.7	1.67	-0.7
La@C_1(23349)-C_{78}	1	12.4	1.38	10.8
La@C_{2v}(24106)-C_{78}	1	18.0	0.95	19.0
La@C_1(23863)-C_{78}	1	18.7	1.14	15.4
La@C_1(22618)-C_{78}	1	19.5	1.35	17.6
La@C_s(24099)-C_{78}	1	21.3	1.50	28.6
La@C_1(23318)-C_{78}	1	23.6	1.12	24.4
La@C_1(23474)-C_{78}	1	24.3	1.32	19.4
La@C_1(24060)-C_{78}	1	25.0	1.14	24.0
La@C_1(24003)-C_{78}	1	25.6	1.15	28.3
La@C_s(21882)-C_{78}	2	30.4	1.77	21.1
Ce@D_{3h}(24109)-C_{78}	0	0.0	1.24	0.0
Ce@C_1(22595)-C_{78}	1	22.6	1.24	28.8
Ce@C_{2v}(24107)-C_{78}	0	31.4	1.03	41.6
Ce@C_1(23349)-C_{78}	1	32.8	0.95	45.3
Ce@C_{2v}(24106)-C_{78}	0	33.1	1.55	43.2
Ce@C_1(23863)-C_{78}	1	33.2	1.22	37.7
Sm@D_{3h}(24109)-C_{78}	0	0.0	1.08	0.0
Sm@C_{2v}(24107)-C_{78}	0	3.2	0.81	1.7
Sm@C_1(23349)-C_{78}	1	13.4	0.95	9.9
Sm@C_1(23863)-C_{78}	1	13.5	1.22	3.9
Sm@D_3(24105)-C_{78}	0	14.3	1.20	11.3
Sm@C_1(23318)-C_{78}	1	15.8	1.18	10.0
Sm@C_1(24060)-C_{78}	1	15.8	1.47	4.5
Sm@C_1(24003)-C_{78}	1	20.1	1.24	13.3
Sm@C_1(23474)-C_{78}	1	20.1	1.28	9.0
Sm@C_s(24099)-C_{78}	1	22.8	0.71	28.2
Sm@C_1(22595)-C_{78}	1	24.2	0.99	24.9
Sm@C_s(23222)-C_{78}	1	28.0	1.39	18.3
Sm@C_1(21971)-C_{78}	2	28.1	1.16	22.9

Sm@C_1(22618)-C_{78}	1	34.9	1.29	28.8

2. The relative energy for thermodynamically stable M@C78 (M = La, Ce, and Sm) isomers with different spin multiplicity Table S2 and S3.

Table S2 The relative energy in kcal·mol^{-1} for thermodynamically stable M@C_{78} (M = La, Ce, and Sm) isomers with different spin multiplicity on the B3LYP/6-31G(d)~SDD.

	Singlet	Doublet	Triplet	Quartet	Quintet	Sextet	Septet	Nonet
La@C_1(22595)-C_{78}		0.0		30.5		71.3		
La@C_{2v}(24107)-C_{78}		0.0		28.1		62.8		
La@D_{3h}(24109)-C_{78}		0.0		18.3		51.9		
Ce@D_{3h}(24109)-C_{78}	25.8		0.0		12.4			
Sm@C_{2v}(24107)-C_{78}	121.7		82.4		0.0		1.5	1.2
Sm@D_{3h}(24109)-C_{78}	120.8		74.1		9.8		0.0	10.7

Table S3 The relative energy in kcal·mol^{-1} for thermodynamically stable Sm@C_{78} isomers with different spin multiplicity on the M06-2X/6-31G(d)~SDD.

	Singlet	Triplet	Quintet	Septet	Nonet
Sm@C_{2v}(24107)-C_{78}	173.6	68.3	0.0	0.5	0.5
Sm@D_{3h}(24109)-C_{78}	173.5	97.3	11.1	0.0	11.5

3. The populations of spin electron for thermodynamically stable M@C_{78} (M = La, Ce, and Sm).

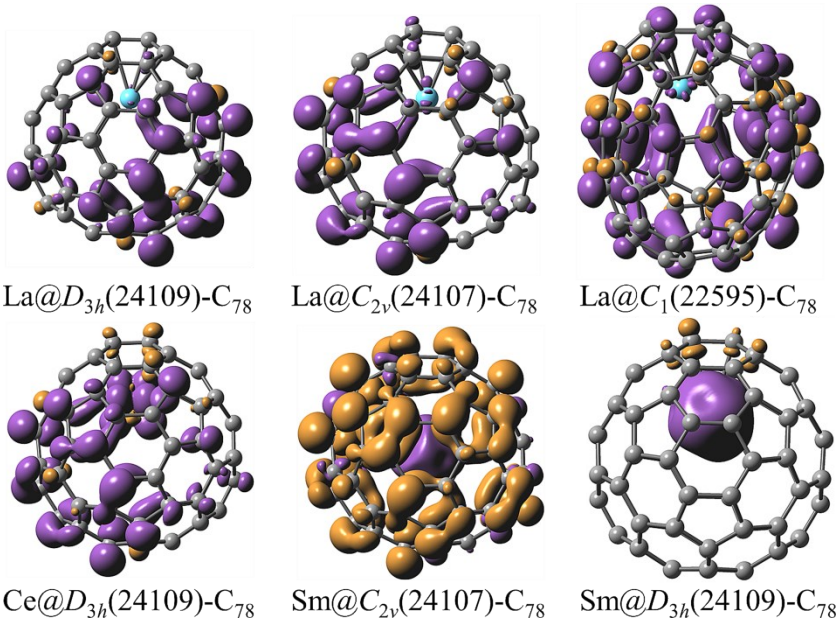

Figure S1 The populations of spin electron for thermodynamically stable M@C_{78} (M = La, Ce, and Sm) based on the B3LYP/6-31G(d)~SDD

4. The frontier molecular orbitals, including the α(β)-HOMO and α(β)-LUMO of thermodynamically stable M@C_{78} (M = La, Ce, and Sm).

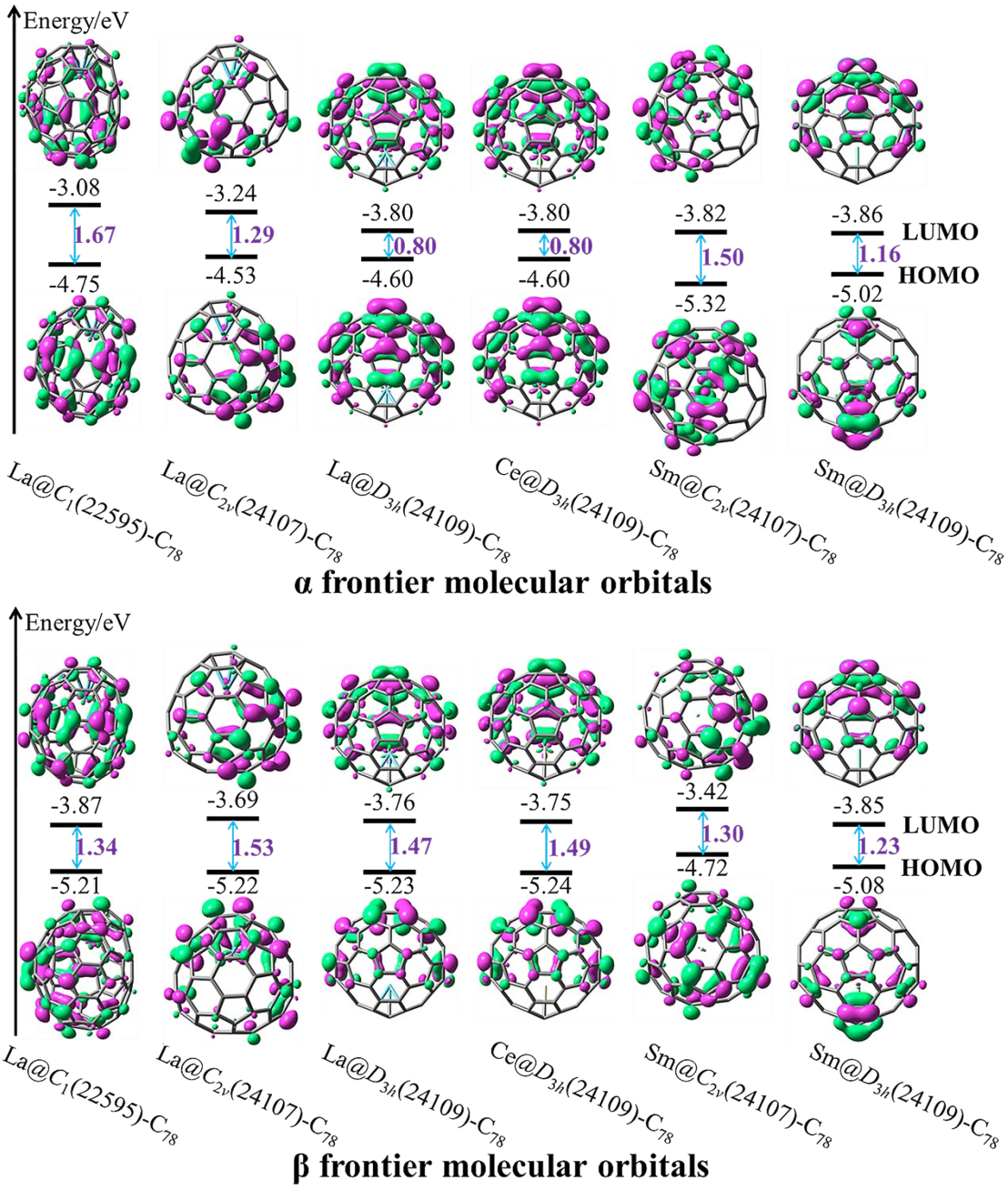

Figure S2 The frontier molecular orbitals for La@C_{78} with doublet, Ce@C_{78} with triplet, Sm@C_{2v}(24107)-C_{78} with quintet, and Sm@D_{3h}(24109)-C_{78} with septet, including their the α(β)-HOMO and α(β)-LUMO, energy level of these orbitals, and the HOMO-LUMO gaps.

5. The geometries of thermodynamically stable $M@C_{78}$ (M = La, Ce, and Sm) with ground state.

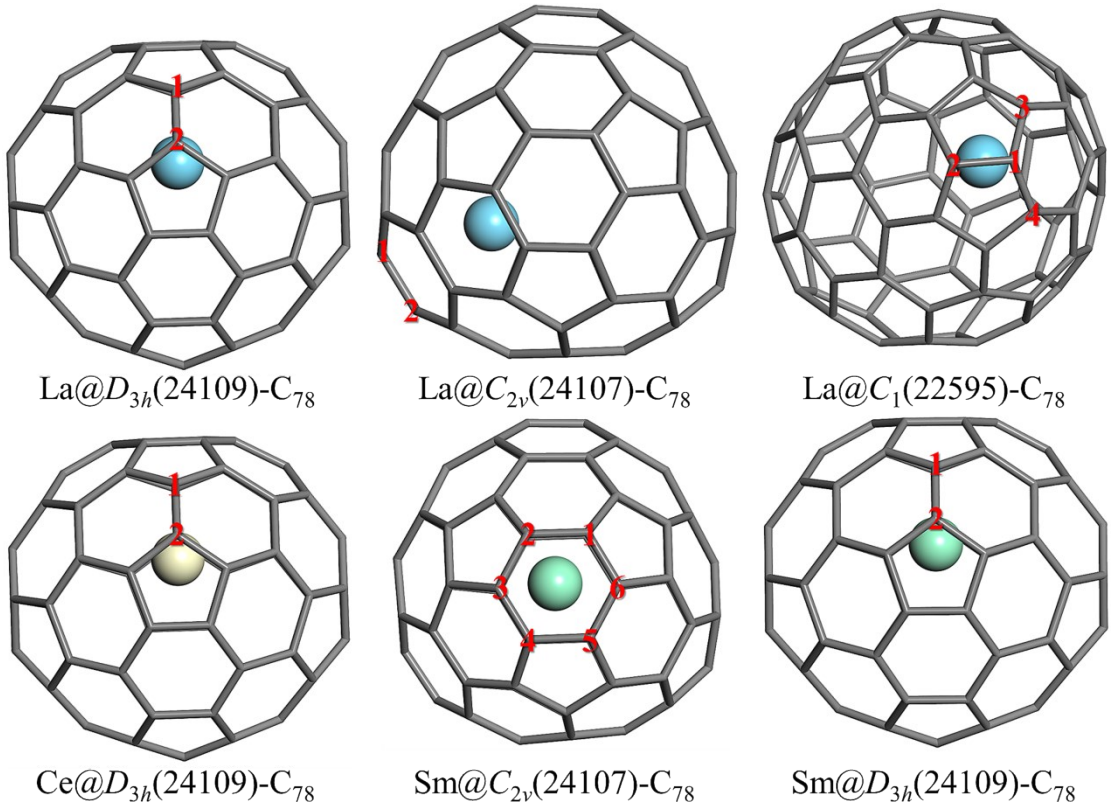

Figure S3 The geometries of thermodynamically stable $M@C_{78}$ (M = La, Ce, and Sm) with ground state on the B3LYP/6-31G(d)~SDD. The marked carbons in C_{78} are close to the inner metal atoms.

6. The distances d_{M-C} (Å) between the marked carbon atoms in Figure S2 and inner metal atoms Table S4.

Table S4 The distances d_{M-C} (Å) between inner metal atoms and the marked carbon in Figure S2 in thermodynamically stable M@C_{78} (M = La, Ce, and Sm) with ground state on the B3LYP/6-31G(d)~SDD. All of these marked carbons are much closer to inner metal atoms than other carbons.

	d_{M-C1}	d_{M-C2}	d_{M-C3}	d_{M-C4}	d_{M-C5}	d_{M-C6}
La@D_{3h}(24109)-C_{78}	2.46	2.48				
La@C_{2v}(24107)-C_{78}	2.47	2.49				
La@C_1(22595)-C_{78}	2.57	2.67	2.53	2.60		
Ce@D_{3h}(24109)-C_{78}	2.43	2.45				
Sm@D_{3h}(24109)-C_{78}	2.56	2.56				
Sm@C_{2v}(24107)-C_{78}	2.67	2.60	2.61	2.69	2.79	2.78

7. The β-HOMO and β-(HOMO-1) for Sm@C_{2v}(24107)-C_{78}.

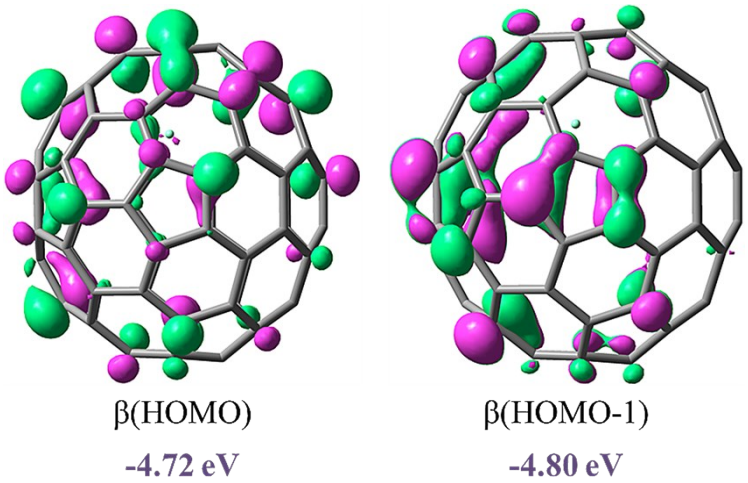

Figure S4 The β-HOMO and β-(HOMO-1) for Sm@C_{2v}(24107)-C_{78}, and these two orbitals are occupied by the electrons, with opposite spin states compared remaining electrons on Sm, transferred from Sm to C_{2v}(24107)-C_{78}.

8. The 234 α orbital for Ce@D_{3h}(24109)-C_{78}.

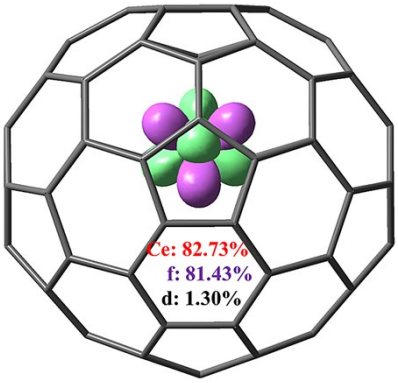

Figure S5 The 234 α molecular orbital for Ce@D_{3h}(24109)-C_{78}. The numbers in picture mean the contribution of Ce, f, and d orbitals in Ce to the 234 α molecular orbital. The α HOMO for Ce@ C_{78} is 250 molecular orbital.

9. The percentage of Sm atom and f orbitals of Sm atom in α molecular orbitals for Sm@C_{78} Table S5.

Table S5 The percentage of Sm atom and f orbitals of Sm atom in α molecular orbitals for Sm@C_{2v}(24107)-C_{78} and Sm@D_{3h}(24109)-C_{78}, respectively.

	Sm/%	f/%
Sm@C_{2v}(24107)-C_{78}		
250	88.30	87.52
249	79.07	78.51
248	48.57	48.28
244	62.89	62.62
243	75.58	75.06
240	51.58	51.49
Sm@D_{3h}(24109)-C_{78}		
250	94.05	93.22
249	61.68	61.26
248	84.81	84.40
247	87.66	86.98
246	88.41	88.1
245	79.29	78.33

10. The α orbitals for Sm@C_{78}.

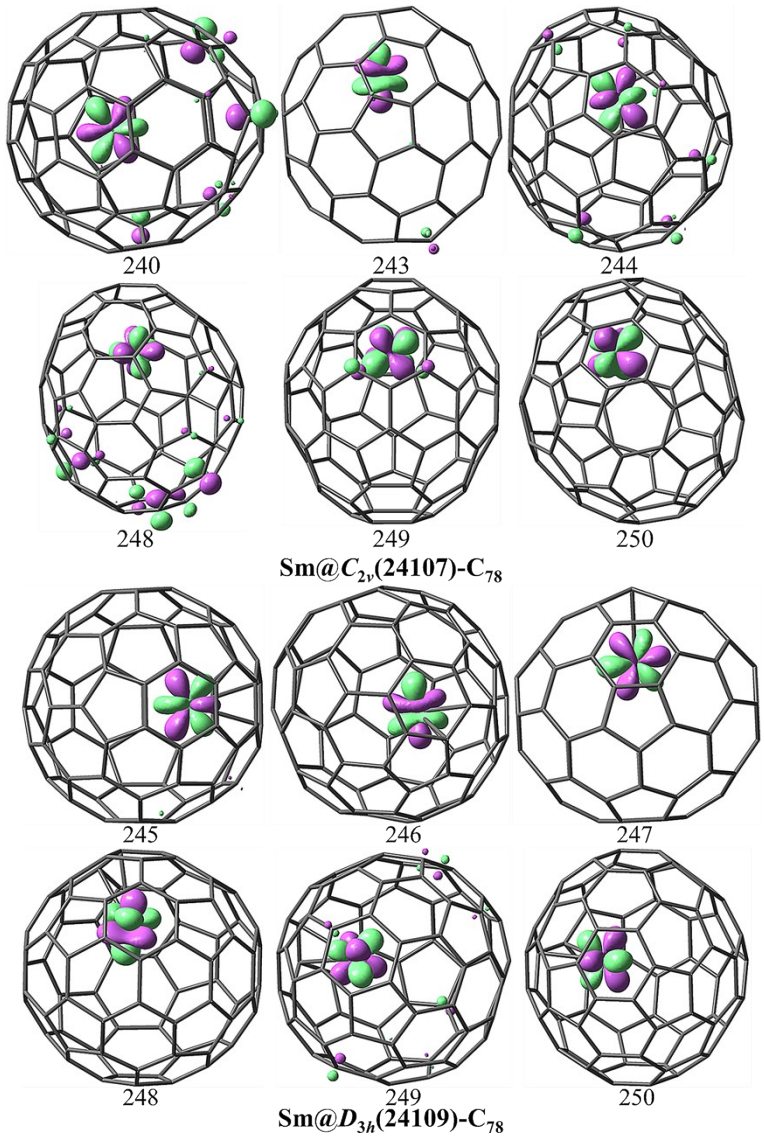

Figure S6 The α molecular orbitals for Sm@C_{2v}(24107)-C_{78} and Sm@D_{3h}(24109)-C_{78}, respectively.

11. The parameters for BCPs of thermodynamically stable M@C_{78} (M = La, Ce, and Sm) Table S6.

Table S6 The average values of electronic density (ρ_{BCP}) of BCPs, absolute energy density (|H|) of BCPs, ratios of absolute potential energy density to Lagrangian kinetic energy (|V|/G) of BCPs, and MBOs for M@C_{78} (M = La, Ce, and Sm).

Isomers	D/Å	ρ_{BCP}	|H|	|V|/G	MBO
Ce@D_{3h}(24109)-C_{78}	2.441	0.068	0.017	1.293	0.326
La@D_{3h}(24109)-C_{78}	2.471	0.065	0.015	1.274	0.309
La@C_{2v}(24107)-C_{78}	2.477	0.064	0.014	1.271	0.306
Sm@D_{3h}(24109)-C_{78}	2.563	0.045	0.004	1.104	0.187
La@C_1(22595)-C_{78}	2.565	0.054	0.008	1.188	0.247
Sm@C_{2v}(24107)-C_{78}	2.604	0.042	0.003	1.084	0.170

12. The coordinates for thermodynamically stable M@C_{78} (M = La, Ce, and Sm) with spin ground states based on B3LYP/6-31G(d)~SDD.

La@C_1(22595)-C_{78} with doublet

C	3.49758300	0.18722000	-2.42795600
C	3.06852600	-1.11717900	-2.63739700
C	1.72958200	-1.37469400	-3.13362200
C	1.26524300	-2.59739200	-2.53408700
C	-0.10339000	-2.82752900	-2.28539400
C	-0.49104000	-3.59530900	-1.09295600
C	-1.83112100	-3.43163000	-0.54210100
C	-2.01967600	-3.40702200	0.86662700
C	-2.95622200	-2.48182600	1.48182500
C	-2.29962100	-1.93602300	2.65141700
C	-2.49670400	-0.57614700	3.01815100
C	-1.40100400	0.10419300	3.61416500
C	-1.18910400	1.50936600	3.39910400
C	0.22465400	1.75573000	3.43404000
C	0.81088200	2.77455900	2.62632200
C	2.14494200	2.57139600	2.19751500
C	2.59646600	3.04559300	0.91754900
C	3.66894100	2.18120300	0.48640100
C	3.82867800	1.86526600	-0.85822800
C	4.24606900	0.53495500	-1.24158400
C	2.62244100	1.28668800	-2.76279500
C	2.84920000	2.34468900	-1.81315600
C	1.80548800	3.22754800	-1.42340400
C	1.68246500	3.61736600	-0.01382300
C	0.38763300	3.95937900	0.48441100
C	-0.04347000	3.55112700	1.78675500
C	-1.46221700	3.28642300	1.73493700
C	-2.03278600	2.24452600	2.51897500
C	-3.17534500	1.57360200	1.97079800
C	-3.43446000	0.19023300	2.24155300
C	-4.18368400	-0.36992000	1.14023500
C	-3.90174800	-1.73998300	0.71443600
C	-3.91519800	-2.00152000	-0.70962400
C	-2.80965400	-2.73510200	-1.32054100
C	-2.41981000	-2.04412900	-2.53136300
C	-1.04213400	-1.89249300	-2.89281200
C	-0.58811600	-0.60137000	-3.40527000
C	0.83860100	-0.32178200	-3.45036900

C	1.33200700	1.05256300	-3.30947700
C	0.39127000	2.09715600	-3.12712800
C	0.62408200	3.17858200	-2.21752500
C	-0.65984500	3.58276100	-1.70423300
C	-0.77818200	3.95967000	-0.36888200
C	-1.92728900	3.54441800	0.39302300
C	-2.98526600	2.79640200	-0.20237100
C	-3.70140300	1.88660100	0.66778700
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C	-1.01479800	1.84840500	-3.19398500
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C	-2.88316300	2.44326200	-1.62041900
C	-3.57744200	1.26439400	-2.09687800
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C	-1.01399500	-2.56064800	2.80353500
C	0.13401000	-1.83238100	3.25901900
C	-0.10711000	-0.52056600	3.73457600
C	0.89123800	0.50420100	3.63776900
C	2.18815200	0.24258300	3.10758800
C	2.85726900	1.34709400	2.51065300
C	3.84543800	1.15013500	1.49119400
C	4.22491700	-0.13563200	1.12967200
C	4.48007700	-0.44301200	-0.26382000
C	4.06709000	-1.80442100	-0.49544300
C	3.40357500	-2.14522600	-1.67831500
C	2.29736700	-3.07661300	-1.64400000
C	1.92637300	-3.68443600	-0.45659500
C	0.54405000	-3.96754000	-0.18674500
C	0.35712900	-3.82676800	1.23156500
C	1.55071000	-3.23677100	1.80351800
C	1.46500700	-2.15793600	2.72393100
C	2.51090900	-1.12161600	2.67468000
C	3.58008600	-1.27722600	1.74788000
C	3.57409800	-2.33566500	0.76780400
C	2.56531700	-3.28022000	0.78580800
La	-2.07004700	-0.18233200	-0.51018700

La@D_{3h}(24109)-C_{78} with doublet

C	-0.00105000	3.07560100	-2.60317000
C	-1.18618400	2.35009400	-3.01835900
C	-2.36796400	2.32135100	-2.21633700
C	-3.17616300	1.14529800	-2.32170700
C	-4.00375100	0.69309100	-1.21894700
C	-4.00402900	-0.75321300	-1.20681900
C	-4.00560300	-1.44034600	0.01534600
C	-3.17164500	-2.60277600	0.17668400
C	-2.70887200	-2.61707100	1.55992000
C	-1.45894300	-3.18326800	1.89900900
C	-0.72736300	-2.60288400	2.96772700
C	0.72405500	-2.60306900	2.96769800
C	1.17432800	-1.39062000	3.58434000
C	2.35699000	-0.71898200	3.13930200
C	2.35644700	0.75502900	3.11628100
C	3.17685000	1.41821900	2.16524100
C	2.70253500	2.60902700	1.47728500
C	3.16915300	2.58032100	0.12244400
C	2.36558300	3.06250700	-0.95029600
C	2.36569000	2.32075600	-2.21643400
C	1.18388400	2.34979400	-3.01840600
C	0.73027800	1.19656500	-3.71865200
C	-0.73289700	1.19674900	-3.71862200
C	-1.45800600	-0.02013800	-3.66588000

C	-2.70776400	-0.01801000	-3.00212500
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C	-0.00093800	3.77061100	-1.41663500
C	1.18360100	3.78240900	-0.58110300
C	0.73107400	3.83461300	0.76359100
C	1.45322700	3.20382000	1.81490000
C	0.72333500	2.63908200	2.90159300
C	1.17414300	1.44513200	3.54608400
C	-0.00121200	0.72877500	3.96432400
C	-0.00138800	-0.66233500	3.98255600
C	-1.17730400	-1.39032400	3.58438700
C	-2.35981600	-0.71838700	3.13939700
C	-3.17646300	-1.41667400	2.20272400
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C	-3.99172500	1.39381900	-0.02185800
C	-3.17126600	2.58111900	0.12257300
C	-2.36761700	3.06310300	-0.95020000
C	-1.18544000	3.78270800	-0.58105400
C	-0.73284500	3.83479800	0.76362100
C	-1.45511400	3.20418600	1.81495900
C	-0.72532100	2.63926500	2.90162200
C	-1.17640300	1.44542800	3.54613100
C	-2.35890100	0.75562300	3.11637600
C	-3.17917300	1.41902000	2.16537000
C	-2.70458600	2.60970900	1.47739500
C	-2.38645500	-2.38257400	-2.17071500
C	-2.38612600	-3.11331200	-0.89434100
C	-1.17477900	-3.84899400	-0.52830400
C	-0.71523900	-3.82263600	0.84150600
C	0.71154000	-3.82282400	0.84147800
C	1.45544400	-3.18363600	1.89895000
C	2.70550200	-2.61775200	1.55981000
C	3.17342300	-1.41747500	2.20259500
C	4.00543500	-0.71178100	1.25576400
C	3.99617400	0.68596800	1.24156900
C	3.98930500	1.39281300	-0.02202000
C	4.00110600	0.69208200	-1.21911000
C	3.17358900	1.14449800	-2.32183600
C	2.70486600	-0.01869100	-3.00223400
C	1.45508300	-0.02050600	-3.66594100
C	0.71019300	-1.25382600	-3.66600100
C	-0.71342300	-1.25364300	-3.66596600
C	-1.17216800	-2.43987500	-2.98234200
C	-0.00184500	-3.21545700	-2.62643300
C	-0.00191000	-3.93966500	-1.37717000
C	1.17102400	-3.84931500	-0.52835400
C	2.38254000	-3.11393000	-0.89444300
C	3.16821900	-2.60357300	0.17655400
C	4.00246600	-1.44135500	0.01518500
C	4.00101500	-0.75422200	-1.20698000
C	3.17950800	-1.21173400	-2.28629600
C	2.38300000	-2.38318800	-2.17082200
C	1.16866800	-2.44018100	-2.98240500
La	-0.00150600	-1.54674000	-0.79268300

La@C_{2v}(24107)-C_{78} with doublet

C	0.00001400	-1.29743000	3.75054500
C	-0.00180100	-2.52781900	3.10342900
C	1.17372900	-2.97388500	2.39896200
C	0.71981200	-3.71855200	1.25861600
C	1.45187100	-3.69048400	0.04205500
C	0.70710300	-3.70777500	-1.19491700
C	1.16600800	-3.01939800	-2.38423400
C	-0.00610200	-2.64414300	-3.15159600
C	-0.00508500	-1.35680000	-3.81541200
C	-1.17041600	-0.51006300	-3.68964400

C	-0.71142600	0.85705200	-3.57286600
C	-1.46952300	1.88813500	-2.91921300
C	-0.73697500	2.94613900	-2.22248400
C	-1.41373100	3.58699300	-1.15187500
C	-0.68122900	3.99706700	0.02636200
C	-1.40512300	3.58532200	1.19767500
C	-0.73304400	2.95494200	2.27514100
C	-1.46356000	1.89836100	2.98496800
C	-0.71989100	0.89475600	3.65327500
C	-1.17151700	-0.46453600	3.70760900
C	1.17335400	-0.46716700	3.70605400
C	0.72470100	0.89313600	3.65230900
C	1.46972300	1.89507600	2.98301500
C	0.74063600	2.95330800	2.27417300
C	1.41270400	3.58219800	1.19581200
C	0.68817600	3.99555800	0.02544900
C	1.41819100	3.58385500	-1.15377200
C	0.73857000	2.94450900	-2.22349100
C	1.46781500	1.88486000	-2.92119800
C	0.70655300	0.85547400	-3.57386500
C	1.16235300	-0.51268700	-3.69132400
C	2.38705100	-0.91923800	-3.02320500
C	2.38289300	-2.21237400	-2.32098400
C	3.18107400	-2.34059900	-1.15258800
C	2.70897400	-3.04386200	0.03598000
C	3.18955100	-2.34198800	1.19470900
C	2.36210100	-2.18631400	2.34956600
C	2.36504900	-0.88938200	3.04266500
C	3.21458200	0.14516900	2.57022100
C	2.78037800	1.52304400	2.55795300
C	3.40482500	2.16357400	1.42574600
C	2.71773200	3.15205900	0.73981900
C	2.71690700	3.15804000	-0.71302700
C	3.41034500	2.16619300	-1.40884400
C	2.77553900	1.52631000	-2.52621500
C	3.21716900	0.12493400	-2.54600700
C	4.08238000	-0.06733000	-1.41297600
C	4.03943400	-1.27592400	-0.70713200
C	4.04515000	-1.27544900	0.73872800
C	4.08580500	-0.06189500	1.43229500
C	4.18913500	1.17802400	0.70614500
C	4.19362000	1.18126600	-0.69533000
C	-1.17926600	-2.97124100	2.40052300
C	-0.72855100	-3.71690900	1.25957300
C	-1.46217400	-3.68723500	0.04398800
C	-0.71906600	-3.70614600	-1.19396300
C	-1.17798100	-3.01669100	-2.38261600
C	-2.39296700	-2.20697500	-2.31771900
C	-2.39514600	-0.91386300	-3.01993300
C	-3.22231900	0.13215800	-2.54171500
C	-2.77752200	1.53251800	-2.52251500
C	-3.40938300	2.17381500	-1.40429700
C	-2.71279300	3.16407400	-0.70940800
C	-2.71170500	3.15811100	0.74342800
C	-3.40008700	2.17118300	1.43026500
C	-2.77559400	1.52926900	2.56165700
C	-3.21285700	0.15238300	2.57450000
C	-2.36504200	-0.88407100	3.04582200
C	-2.36592800	-2.18100400	2.35271600
C	-3.19521300	-2.33479600	1.19894800
C	-2.71780600	-3.03777700	0.03960100
C	-3.18989900	-2.33344500	-1.14832300
C	-4.04522700	-1.26682500	-0.70173500
C	-4.08643500	-0.05816500	-1.40752700
C	-4.19389700	1.19065800	-0.68973300
C	-4.18754300	1.18740800	0.71171700
C	-4.08603100	-0.05272200	1.43773200
C	-4.04898100	-1.26632500	0.74411000
La	-0.00265800	-0.94649800	-1.36217100

Ce@D_{3h}(24109)-C_{78} with triplet

C	-0.00105000	3.14115200	-2.71485500
C	-1.17536700	2.35742600	-3.05644600
C	-2.38593300	2.30731400	-2.23678600
C	-3.17351100	1.12438600	-2.32918900
C	-4.00671400	0.68459300	-1.24080300
C	-4.01063700	-0.75539200	-1.22660600
C	-4.00172100	-1.43922500	-0.00657200
C	-3.17903600	-2.60402000	0.16794400
C	-2.70763000	-2.60629100	1.54433400
C	-1.45808100	-3.19364100	1.89030700
C	-0.73454400	-2.59606100	2.96030200
C	0.73125000	-2.59624400	2.96027100
C	1.18330300	-1.40558700	3.58362100
C	2.36669100	-0.72597400	3.14357700
C	2.36692400	0.74143400	3.13102900
C	3.17710400	1.41934800	2.16530500
C	2.70599000	2.58765500	1.49366500
C	3.18328900	2.56571800	0.10474200
C	2.38475200	3.04830700	-0.96891800
C	2.38364600	2.30672300	-2.23688900
C	1.17306000	2.35713800	-3.05650200
C	0.71203400	1.15530600	-3.71117700
C	-0.71467100	1.15548300	-3.71114500
C	-1.45843600	-0.07996600	-3.68593700
C	-2.70861600	-0.06733400	-3.02644400
C	-3.17981000	-1.22423600	-2.30908400
C	-0.00093400	3.86242200	-1.46611000
C	1.17087400	3.78050900	-0.61527800
C	0.71084900	3.77560200	0.75237500
C	1.45591500	3.16304600	1.82284600
C	0.73088300	2.60212700	2.90352500
C	1.18493400	1.42120800	3.55458000
C	-0.00121400	0.69815700	3.97418100
C	-0.00138600	-0.67555300	3.99117300
C	-1.18627400	-1.40529200	3.58367100
C	-2.36951000	-0.72538300	3.14367600
C	-3.17143900	-1.41432600	2.19133800
C	-3.99455700	-0.69712500	1.23410900
C	-4.00594900	0.69054900	1.22454600
C	-4.00424000	1.40126600	-0.03636500
C	-3.18541600	2.56651300	0.10487600
C	-2.38680100	3.04889900	-0.96881700
C	-1.17272400	3.78079400	-0.61522800
C	-0.71264400	3.77577700	0.75240400
C	-1.45781900	3.16340900	1.82290700
C	-0.73288100	2.60230900	2.90355500
C	-1.18719900	1.42150400	3.55462900
C	-2.36937700	0.74202400	3.13112700
C	-3.17942800	1.42014100	2.16543800
C	-2.70805200	2.58833100	1.49377900
C	-2.36072900	-2.38305400	-2.16924700
C	-2.36042600	-3.09855600	-0.88027600
C	-1.17730500	-3.81615000	-0.49561600
C	-0.72702100	-3.85316500	0.85918100
C	0.72332600	-3.85334600	0.85915100
C	1.45459400	-3.19400400	1.89024600
C	2.70427400	-2.60696600	1.54422100
C	3.16840800	-1.41511700	2.19120600
C	3.99166500	-0.69812100	1.23394200
C	4.00340400	0.68955000	1.22437900
C	4.00181800	1.40026800	-0.03653200
C	4.00406200	0.68359400	-1.24097000
C	3.17092200	1.12359600	-2.32932200
C	2.70570200	-0.06800900	-3.02655600
C	1.45549000	-0.08032900	-3.68599800

C	0.72414600	-1.29563400	-3.71594400
C	-0.72739600	-1.29545300	-3.71591300
C	-1.17829800	-2.43398300	-2.97209600
C	-0.00183000	-3.14046900	-2.53657000
C	-0.00189000	-3.82360400	-1.32573100
C	1.17356200	-3.81644400	-0.49566500
C	2.35684500	-3.09914200	-0.88037400
C	3.17562400	-2.60481200	0.16781100
C	3.99859200	-1.44022200	-0.00673900
C	4.00762700	-0.75639200	-1.22677400
C	3.17663700	-1.22502800	-2.30921600
C	2.35727300	-2.38364100	-2.16934500
C	1.17479600	-2.43427600	-2.97214500
Ce	-0.00119200	1.46960500	-0.94572700

Sm@C_{2v}(24107)-C_{78} with quintet

C	-0.01761900	-1.27340300	3.70905800
C	-0.02404200	-2.50003700	3.05817700
C	1.14940600	-2.95094200	2.35281400
C	0.69837400	-3.68969000	1.21417300
C	1.43338700	-3.66790300	-0.00873700
C	0.70587000	-3.68755500	-1.23634900
C	1.16364700	-2.94697900	-2.37102500
C	-0.00567200	-2.49493100	-3.08281700
C	0.00472200	-1.26705500	-3.73135200
C	-1.16390800	-0.42996200	-3.70231700
C	-0.70127800	0.93185300	-3.64356700
C	-1.43657900	1.93666500	-2.97352500
C	-0.70394100	2.99169500	-2.25863600
C	-1.37799600	3.62758700	-1.18476100
C	-0.65381500	4.03517200	-0.00762500
C	-1.38488600	3.62569100	1.16443000
C	-0.71761400	2.98798500	2.24140100
C	-1.45498700	1.93213300	2.95011500
C	-0.72312900	0.92567600	3.62196900
C	-1.18581300	-0.43605500	3.67474400
C	1.16102600	-0.44580800	3.67510000
C	0.72187800	0.91281800	3.62443600
C	1.47492300	1.91699700	2.96158000
C	0.75636400	2.97792200	2.24876200
C	1.43658900	3.60278500	1.17335400
C	0.71748700	4.01565500	-0.00369300
C	1.44376700	3.60505100	-1.17713400
C	0.76992500	2.98175800	-2.25751700
C	1.49259200	1.92216500	-2.96812500
C	0.74371000	0.91902500	-3.63747000
C	1.18313500	-0.43939700	-3.68863100
C	2.37343600	-0.86897400	-3.02594200
C	2.35957900	-2.16152200	-2.32602100
C	3.17638500	-2.31386600	-1.17305700
C	2.69153100	-3.00983700	-0.00433800
C	3.16963600	-2.31605200	1.16853100
C	2.34568600	-2.16561100	2.31660900
C	2.35527000	-0.87430900	3.01897000
C	3.21039200	0.15807500	2.55799600
C	2.78234600	1.53644000	2.54250500
C	3.42218000	2.17964300	1.41766000
C	2.74113700	3.17011300	0.72868500
C	2.74544300	3.17137400	-0.72550400
C	3.43079200	2.18223100	-1.41227100
C	2.79748300	1.54083700	-2.54196800
C	3.22566900	0.16257900	-2.55781900
C	4.09934900	-0.04542200	-1.41887700
C	4.04167800	-1.25043700	-0.72260400
C	4.03740100	-1.25180000	0.72529400
C	4.09108500	-0.04793300	1.42415000
C	4.20937200	1.19561700	0.70433300

C	4.21352000	1.19697700	-0.69609800
C	-1.20332000	-2.94152500	2.35401500
C	-0.74686200	-3.68590500	1.20908700
C	-1.46955600	-3.64929100	-0.01740400
C	-0.73916400	-3.68312000	-1.23978300
C	-1.18908600	-2.93760400	-2.38671800
C	-2.36842600	-2.14190800	-2.34929600
C	-2.36015400	-0.84508900	-3.04745200
C	-3.21652200	0.19765400	-2.57610400
C	-2.75827500	1.57471100	-2.55249900
C	-3.39062800	2.22188400	-1.43427700
C	-2.68905600	3.21084700	-0.73649800
C	-2.69306500	3.20878000	0.70726800
C	-3.40035600	2.22051500	1.39987500
C	-2.77424100	1.57131700	2.52104600
C	-3.23080200	0.19402500	2.53781600
C	-2.37738700	-0.84931600	3.01052200
C	-2.38182800	-2.14545300	2.31053000
C	-3.22415500	-2.28684400	1.15051000
C	-2.72903000	-2.97371000	-0.02091000
C	-3.21889500	-2.28578800	-1.19470900
C	-4.10800200	-1.23534800	-0.75357000
C	-4.12930100	0.00208300	-1.46353500
C	-4.20458000	1.24703300	-0.73148500
C	-4.20923600	1.24682600	0.68989500
C	-4.13374700	0.00040500	1.41772700
C	-4.10888000	-1.23504700	0.70550600
Sm	-1.87721800	-0.10746300	-0.03748300

Sm@D_{3h}(24109)-C_{78} with septet

C	-0.00081300	3.05479700	-2.58801100
C	-1.18500000	2.33870800	-3.01622000
C	-2.36679600	2.30806000	-2.21458000
C	-3.17507900	1.13893600	-2.32477900
C	-4.00580100	0.68810200	-1.22463700
C	-4.00570800	-0.75651300	-1.21389900
C	-4.00489400	-1.44403500	0.00409600
C	-3.17633400	-2.60499000	0.17194400
C	-2.70385400	-2.60353700	1.55431100
C	-1.45343300	-3.18281500	1.89961200
C	-0.73221500	-2.59010500	2.96968900
C	0.72900000	-2.59041000	2.96955500
C	1.18233300	-1.38859500	3.58602400
C	2.36377300	-0.71852300	3.14546200
C	2.36490600	0.75393100	3.12350600
C	3.17059500	1.41649200	2.16408700
C	2.70357200	2.60032300	1.48492300
C	3.17083900	2.57004200	0.12047800
C	2.36564800	3.04960000	-0.94269800
C	2.36472700	2.30779000	-2.21463000
C	1.18305300	2.33894100	-3.01634500
C	0.72977600	1.19059500	-3.72644000
C	-0.73215900	1.19054900	-3.72631600
C	-1.45384600	-0.03219400	-3.68241100
C	-2.70448900	-0.02863400	-3.00838300
C	-3.17682200	-1.21259000	-2.29508800
C	-0.00090200	3.76272100	-1.40566600
C	1.18080400	3.77295300	-0.57076700
C	0.73094900	3.83093400	0.77270800
C	1.45557200	3.19847200	1.82243600
C	0.73051900	2.62710000	2.90629000
C	1.18011400	1.44622200	3.55071600
C	-0.00119100	0.72669500	3.97351700
C	-0.00140300	-0.65187500	3.97754100
C	-1.18530900	-1.38809900	3.58634100

C	-2.36669500	-0.71780100	3.14592200
C	-3.17543400	-1.41629500	2.20162000
C	-4.00532500	-0.70706500	1.24705100
C	-4.00159200	0.68107800	1.23071900
C	-4.00134000	1.39118300	-0.02752500
C	-3.17288000	2.57078800	0.12040100
C	-2.36754300	3.05001900	-0.94272500
C	-1.18256600	3.77328200	-0.57090200
C	-0.73264600	3.83088900	0.77259000
C	-1.45746800	3.19873100	1.82241400
C	-0.73251500	2.62726300	2.90630300
C	-1.18239400	1.44654600	3.55083400
C	-2.36741100	0.75461700	3.12381700
C	-3.17297700	1.41728600	2.16427900
C	-2.70555800	2.60085300	1.48486800
C	-2.36888100	-2.37687800	-2.17378200
C	-2.36814300	-3.10263000	-0.88789900
C	-1.17110700	-3.83493600	-0.51599800
C	-0.71561200	-3.83922200	0.85685000
C	0.71238500	-3.84049200	0.85716700
C	1.45009900	-3.18397600	1.89949300
C	2.70059700	-2.60460300	1.55397300
C	3.17215900	-1.41722500	2.20102200
C	4.00238500	-0.70806500	1.24660900
C	3.99922500	0.68020800	1.23044500
C	3.99934700	1.39041800	-0.02746700
C	4.00333600	0.68734600	-1.22474400
C	3.17293900	1.13853200	-2.32483400
C	2.70144100	-0.02897000	-3.00793600
C	1.45084600	-0.03198600	-3.68174200
C	0.71234400	-1.26331300	-3.70442700
C	-0.71609400	-1.26346600	-3.70578000
C	-1.17087200	-2.43574200	-2.99167700
C	-0.00224800	-3.18372700	-2.60382300
C	-0.00186400	-3.88945200	-1.35658300
C	1.16730600	-3.83494000	-0.51617800
C	2.36497600	-3.10353100	-0.88786600
C	3.17309600	-2.60618800	0.17158000
C	4.00186600	-1.44483400	0.00381400
C	4.00281300	-0.75723800	-1.21397400
C	3.17349700	-1.21318700	-2.29503300
C	2.36504100	-2.37694600	-2.17340100
C	1.16698700	-2.43561000	-2.99117500
Sm	-0.00332000	-1.39649200	-0.76587400