

Supplementary Information

C₇₄ Endohedral Metallofullerenes Violating the Isolated Pentagon Rule: A Density Functional Theory Study

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Table S1: Relative energies [kcal/mol] and HOMO-LUMO gaps [eV] of C_{74} anions.

Sym.(No.) ^a	PA	C_{74}^{4-}			C_{74}^{6-}		
		AM1	B3LYP/6-31G*	gap	AM1	B3LYP/6-31G*	gap
$C_2(13333)$	2	3.69	0.00	1.55	4.39	5.31	1.50
$D_{3h}(14246)$	0	0.00	4.19	0.61	0.00	6.95	1.59
$C_2(13290)$	2	10.44	7.28	1.49	13.54	9.71	1.62
$C_2(13295)$	2	13.09	9.86	1.17	2.94	0.00	2.12
$C_2(13291)$	2	18.41	14.60	1.19	17.96	14.11	1.72
$C_s(13336)$	2	20.20	17.17	1.18	26.11	25.25	1.37
$C_1(13408)$	2	21.43	17.52	1.10	11.64	8.89	2.07
$C_2(13292)$	2	24.47	21.77	0.87	20.83	18.15	1.80
$C_{2v}(14239)$	2	22.81	21.54	0.96	23.95	15.32	1.56

^a Symmetry of the original empty cage. The numbers of cages are spiral numbers.

Table S2. $\Delta E(S-T)$ [kcal/mol] of $M_2@C_{74}$ isomers. Vertical $\Delta E(S-T)$ represents splitting energy without change of geometry structure.

Sym.(No.)	Sc ₂ @C ₇₄	La ₂ @C ₇₄
$D_{3h}(14246)$	12.67	-1.97
$C_2(13295)$	-17.04	0.37
$C_2(13295)$ -vertical	-	-8.56
$C_2(13333)$	-2.75	6.63
$C_2(13333)$ -vertical	-	6.63
$C_1(13408)$	-11.68	-0.11
$C_2(13291)$	-10.35	3.51

5-6	1.426	1.438	2.323	1.442	2.724	1.442	2.356
5-4	1.428	1.431	2.373	1.437	2.725	1.436	2.342
6-7	1.439	1.469	2.345	1.474	2.729	1.470	2.434
7-8	1.464	1.459	2.243	1.463	2.676	1.451	2.415
2-3	1.458	1.460	2.372	1.470	2.676	1.459	2.372
3-4	1.439	1.448	2.485	1.464	2.737	1.462	2.400
average	1.437	1.453	-	1.455	-	1.452	-

^a in triplet state.

b. BV and DV of PAI in $C_2(13295)-C_{74}$ EMFs.

bond	neutral	$Sc_2@C_2(13295)-C_{74}$	$La_2@C_2(13295)-C_{74}$	$Sc_3N@C_2(13295)-C_{74}$			
	BV/Å	BV/Å	DV/Å	BV/Å	DV/Å	BV/Å	DV/Å
1-5	1.451	1.445	2.193	1.435	2.589	1.432	2.299
1-8	1.423	1.45	2.274	1.451	2.661	1.456	2.329
1-2	1.404	1.451	2.300	1.454	2.634	1.457	2.307
5-6	1.420	1.459	2.193	1.456	2.590	1.441	2.356
5-4	1.403	1.465	2.207	1.466	2.553	1.443	2.342
6-7	1.472	1.466	2.260	1.467	2.649	1.453	2.434
7-8	1.453	1.456	2.311	1.463	2.689	1.459	2.415
2-3	1.456	1.456	2.391	1.473	2.632	1.461	2.372
3-4	1.466	1.464	2.328	1.479	2.582	1.451	2.400

c. BV of PAII (in $Sc_3N@C_2(13333)-C_{74}$ and $Sc_3N@C_2(13295)-C_{74}$).

PA II in $Sc_3N@C_2(13333)-C_{74}$		PA II in $Sc_3N@C_2(13295)-C_{74}$	
bond	BV/Å	bond	BV/Å
70-74	1.431	72-73	1.423
70-69	1.421	72-60	1.430
70-71	1.417	72-71	1.434
74-67	1.413	73-62	1.433
74-73	1.432	73-74	1.436
69-68	1.463	62-61	1.456
68-67	1.443	61-60	1.450
71-72	1.476	71-70	1.453
72-73	1.442	70-74	1.453

Table S5: NICS [ppm] values of pentagon rings in PA fragments.

RingA

RingB

	NICS(-1)	NICS(0)	NICS(1)	NICS(-1)	NICS(0)	NICS(1)
$C_2(13333)-C_{74}$	6.14	14.78	3.58	31.12	43.45	17.17
$Sc_2@C_2(13333)-C_{74}$	-42.2	-20.93	-5.91	-43.9	-20.81	-6.43
$La_2@C_2(13333)-C_{74}$	-28.46	-12.54	-4.25	-32.81	-14.05	-4.64
$La_2@C_2(13333)-C_{74-t}$	-28.66	-13.73	-5.07	-29.72	-15.00	-5.37
$Ca_2@C_2(13333)-C_{74}$	-10.16	2.37	0.64	-18.76	-10.48	-4.81
$Sc_3N@C_2(13333)-C_{74}(PAI)$	-39.51	-19.61	-6.07	-38.25	-20.5	-6.41
$Sc_3N@C_2(13333)-C_{74}(PAII)$	-19.85	-9.09	-2.95	-20.38	-8.51	-2.49
$C_2(13295)-C_{74}$	-19.55	-8.39	-3.13	6.07	27.00	12.03
$Sc_2@C_2(13295)-C_{74}$	-46.59	-23.10	-6.41	-35.18	-19.19	-5.50
$La_2@C_2(13295)-C_{74}$	-32.62	-16.42	5.01	-33.50	-15.78	-4.47
$La_2@C_2(13295)-C_{74-t}$	-	-	-	-	-	-
$Ca_2@C_2(13295)-C_{74}$	-3.61	15.59	7.2	-12.81	-5.96	-1.44
$Sc_3N@C_2(13295)-C_{74}(PAI)$	-41.58	-19.33	-5.67	-41.00	-20.05	-6.77
$Sc_3N@C_2(13295)-C_{74}(PAII)$	-23.01	-12.19	-4.37	-21.40	-12.72	-4.74

Table S6: ^{13}C NMR chemical shifts [ppm] of $Sc_2@C_2(13333)-C_{74}$ and $Sc_2@C_2(13295)-C_{74}$ predicted at B3LYP/6-31G*~Lan12DZ and B3LYP/6-311G*~Lan12DZ levels.

$Sc_2@C_2(13333)-C_{74}$		$Sc_2@C_2(13295)-C_{74}$	
B3LYP/6-31G*~lan	B3LYP/6-311G*~lan	B3LYP/6-31G*~lan	B3LYP/6-311G*~lan
128.00	128.72	124.90	125.55
130.30	131.39	130.13	130.77
131.23	132.41	131.05	131.94
133.28	134.47	131.48	132.15
133.60	135.00	131.91	132.61
133.76	135.08	132.28	133.57
134.59	135.87	133.19	134.15
135.04	136.12	133.85	134.49
135.15	136.37	134.32	136.50
135.66	136.86	138.72	139.84
136.76	137.88	139.22	141.39
137.84	139.92	139.95	141.66
137.97	140.00	140.13	142.41
138.09	140.21	141.20	142.54
138.36	140.74	141.42	143.07

139.27	140.75	141.56	143.38
139.40	140.82	141.66	143.44
139.95	142.12	141.87	143.97
140.00	142.15	142.12	144.05
141.59	143.69	142.30	144.90
141.67	144.23	142.96	145.04
141.99	144.96	143.07	145.29
142.62	145.05	145.06	147.49
142.79	145.29	145.27	147.66
144.10	146.63	146.56	149.47
144.19	146.74	147.21	149.94
144.86	147.45	147.53	150.65
145.07	147.46	148.51	151.07
145.51	147.64	149.53	152.57
147.14	149.08	151.31	153.94
147.38	150.80	152.45	156.25
148.31	151.09	153.43	157.00
148.82	151.65	153.45	157.09
149.22	152.62	153.53	157.85
150.51	153.27	155.59	159.47
151.78	154.28	157.04	160.11
156.71	161.50	159.12	164.48

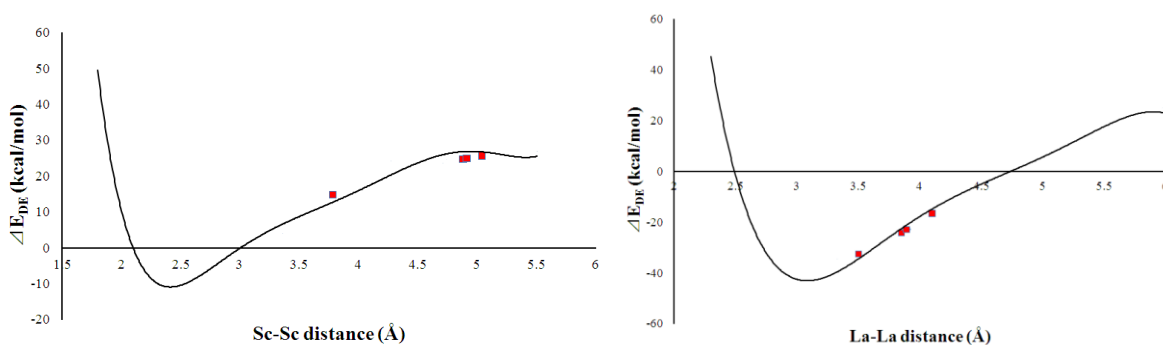


Figure S1: ΔE_{DE} ~M-M distance correlation maps. Red dots represent ΔE_{DE} and M-M distance in $M_2@C_{74}$ isomers.

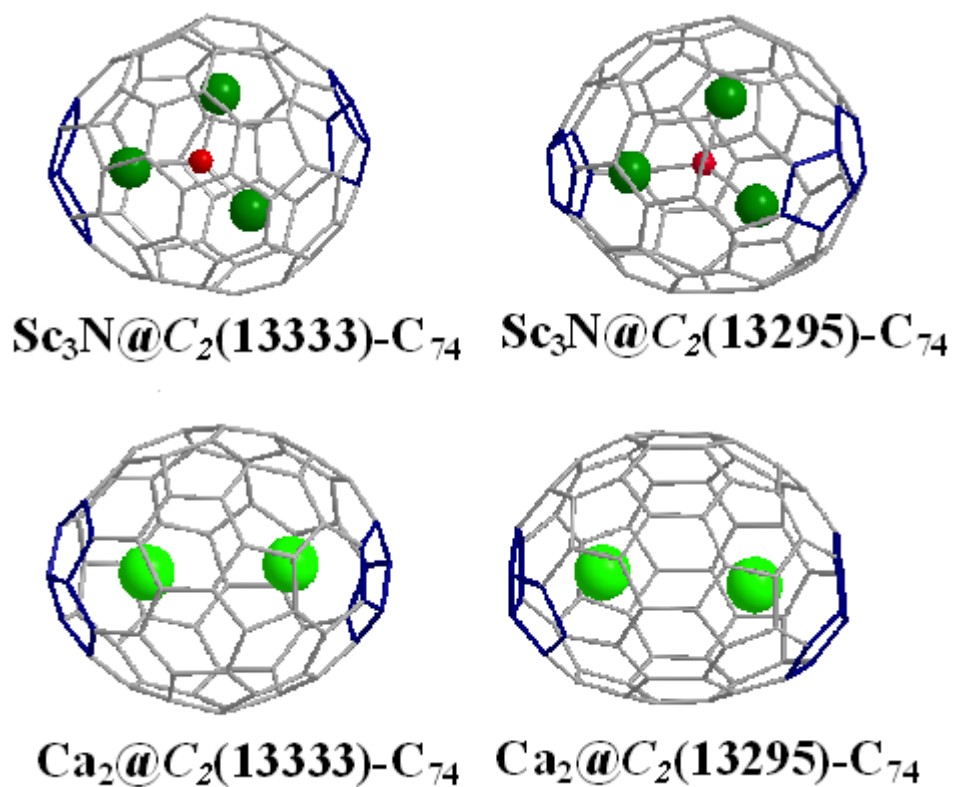
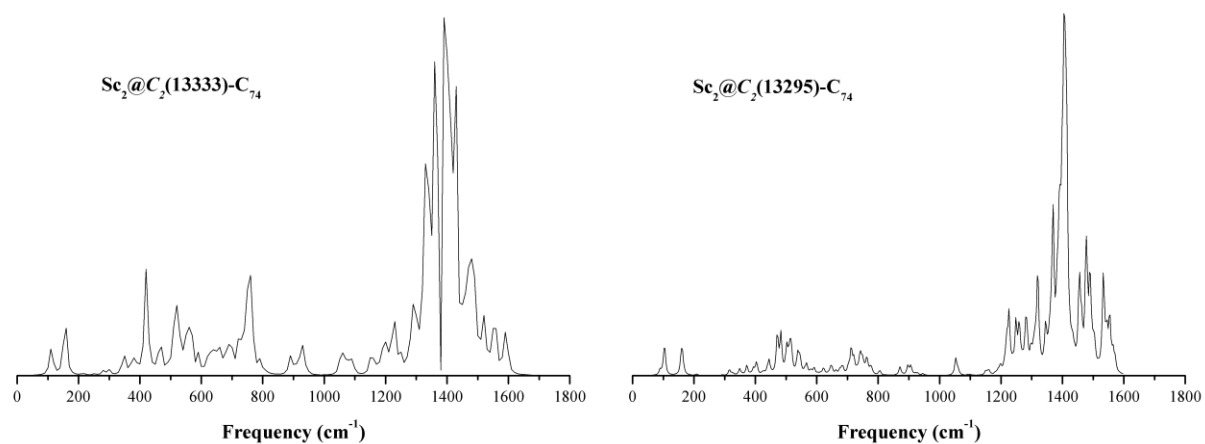


Figure S2: Geometry structures of Sc₃N@C₇₄ and Ca₂@C₇₄ isomers (adjacent pentagons are colored with blue).



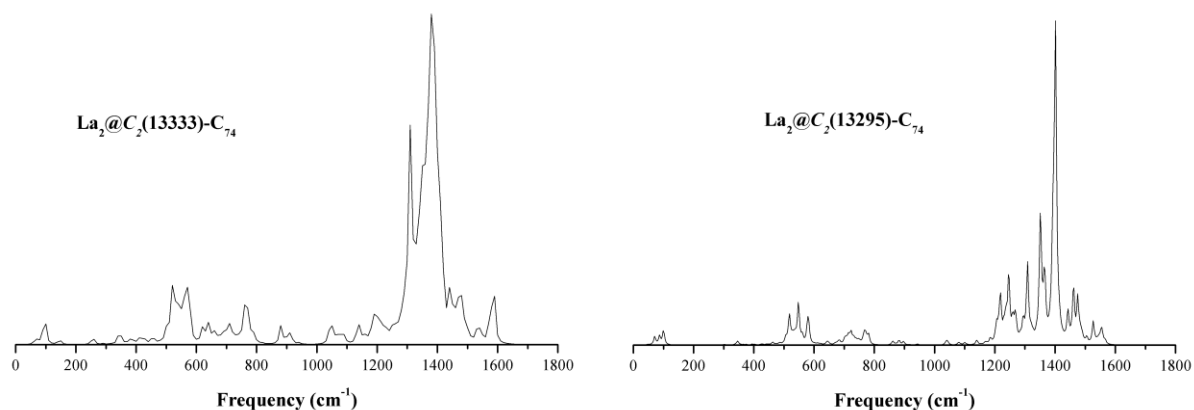


Figure S3: Simulated infrared spectra of $M_2@C_{74}$.

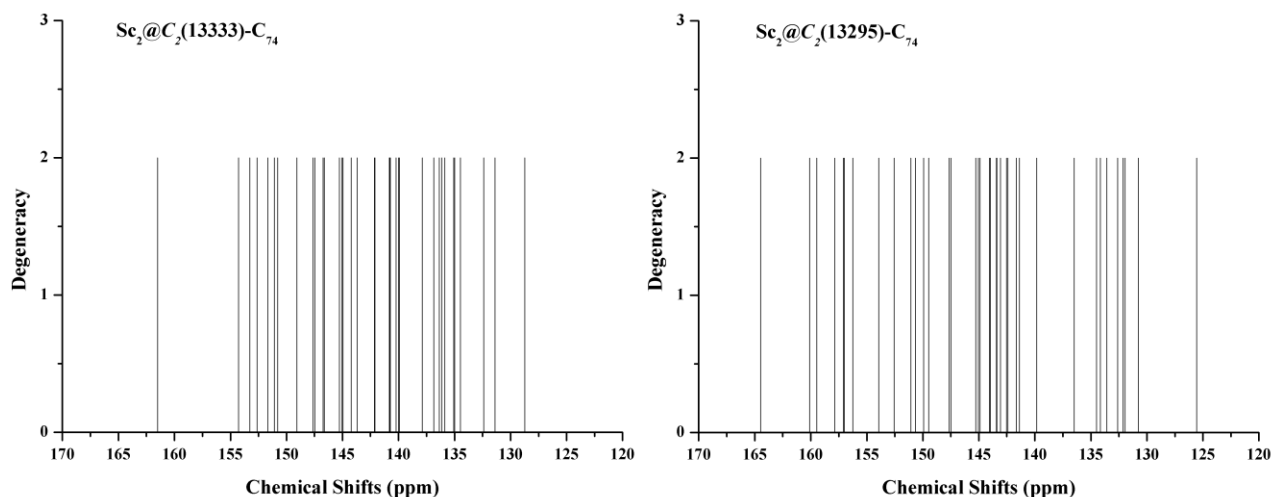


Figure S4: Simulated ^{13}C NMR spectra of $Sc_2@C_{74}$.

Coordinates of main C_{74} EMF isomers predicted at B3LYP/6-31g*~lan level.

$Sc_2@C_{74}$ series:

$Sc_2@C_2(13333)-C_{74}$

76

C	-4.583640	-0.113325	-0.037979
C	-4.103709	-0.946620	1.066883
C	-3.482239	-2.124855	0.469753
C	-3.494058	-1.978639	-0.971118
C	-4.168390	-0.751486	-1.268298
C	-3.568419	0.211493	-2.151127
C	-3.604688	1.501143	-1.448017
C	-4.235856	1.297605	-0.147953

C	-3.590390	1.886497	0.992691
C	-3.253811	1.097412	2.177462
C	-3.440469	-0.339281	2.220535
C	-2.443450	-1.097168	2.889081
C	-1.975260	-2.376581	2.377406
C	-2.426356	-2.861569	1.115468
C	-1.503989	-3.550690	0.278353
C	-1.503548	-3.348424	-1.162285
C	-2.395373	-2.429479	-1.781375
C	-1.903005	-1.541609	-2.846904
C	-2.450663	-0.171270	-2.962614
C	-1.598800	0.884774	-3.400513
C	-1.632985	2.185203	-2.712558
C	-2.520288	2.452184	-1.644732
C	-2.020012	3.204146	-0.478337
C	-2.550740	2.865571	0.819068
C	-1.685187	2.807546	1.965264
C	-2.093209	1.699552	2.778970
C	-1.123637	0.928459	3.506771
C	-1.331315	-0.479079	3.573009
C	-0.219661	-1.385510	3.537945
C	-0.615054	-2.545510	2.776773
C	0.318377	-3.218074	1.925011
C	-0.145802	-3.750721	0.693938
C	0.700732	-3.721575	-0.487939
C	-0.154383	-3.480140	-1.612895
C	0.293975	-2.715091	-2.693749
C	-0.577883	-1.756265	-3.311811
C	0.255473	-0.663714	-3.770546
C	-0.254237	0.641350	-3.774448
C	0.578922	1.736577	-3.321897
C	-0.293106	2.699149	-2.709972
C	0.154948	3.470649	-1.633528
C	-0.700501	3.718644	-0.510245
C	0.145715	3.754741	0.671688
C	-0.318834	3.229496	1.905773
C	0.614356	2.562029	2.761791

C	0.218727	1.406639	3.529805
C	1.330419	0.500420	3.570635
C	1.122751	-0.907480	3.512517
C	2.092483	-1.682908	2.789567
C	1.684716	-2.795823	1.982412
C	2.550505	-2.860544	0.836770
C	2.020261	-3.206885	-0.458738
C	2.520949	-2.461890	-1.629499
C	1.633885	-2.201221	-2.699055
C	1.599913	-0.904882	-3.394851
C	2.451575	0.153737	-2.962693
C	1.903955	1.524725	-2.855391
C	2.396047	2.419023	-1.795105
C	1.504016	3.341647	-1.181780
C	1.503971	3.552239	0.257708
C	2.426119	2.868187	1.099195
C	1.974700	2.390733	2.363913
C	2.442788	1.114481	2.883460
C	3.439679	0.352570	2.219379
C	3.253132	-1.084286	2.184770
C	3.590063	-1.880341	1.004792
C	4.235906	-1.298394	-0.139079
C	3.605533	-1.509804	-1.438271
C	3.569459	-0.224248	-2.149023
C	4.168829	0.744011	-1.271597
C	3.494544	1.972980	-0.981915
C	3.482098	2.127629	0.458090
C	4.102918	0.952808	1.062195
C	4.583251	0.113126	-0.037327
Sc	-2.438870	0.072646	-0.060259
Sc	2.438085	-0.073729	-0.060792

Sc₂@C₂(13295)-C₇₄

76

C	4.328823	-0.765363	-1.306088
C	4.024670	-1.634175	-0.184396
C	4.060687	-0.812593	1.017058

C	4.339863	0.571079	0.627168
C	4.537251	0.581008	-0.824602
C	3.762977	1.476093	-1.677974
C	3.031242	0.669525	-2.659676
C	3.433548	-0.713508	-2.445047
C	2.468363	-1.725651	-2.564544
C	2.343007	-2.782710	-1.584947
C	3.045439	-2.683868	-0.319289
C	2.337656	-3.080986	0.847359
C	2.430968	-2.322315	2.076361
C	3.209452	-1.129760	2.145410
C	2.683569	-0.035942	2.898416
C	2.845599	1.328794	2.436319
C	3.582114	1.636227	1.263104
C	3.037658	2.676651	0.407736
C	3.053488	2.520346	-1.032514
C	1.807980	3.003841	-1.555484
C	1.106896	2.257593	-2.566319
C	1.649020	0.984480	-3.027935
C	0.725214	-0.112326	-3.322779
C	1.169937	-1.457570	-3.128735
C	0.288259	-2.471661	-2.650681
C	1.001251	-3.256337	-1.652863
C	0.325744	-3.716537	-0.483604
C	1.009993	-3.627668	0.765554
C	0.299078	-3.258171	1.959564
C	1.161384	-2.420128	2.747912
C	0.628325	-1.317653	3.482134
C	1.414951	-0.127427	3.559075
C	0.792517	1.173470	3.523813
C	1.653942	2.058750	2.802423
C	1.115319	3.071522	1.950976
C	1.824337	3.364560	0.742022
C	1.096993	3.623296	-0.475617
C	-0.325617	3.716694	-0.485634
C	-1.000813	3.255955	-1.654850
C	-0.287546	2.470734	-2.652070

C	-1.169144	1.456390	-3.129797
C	-0.724401	0.111067	-3.323077
C	-1.648183	-0.985661	-3.027797
C	-1.106214	-2.258503	-2.565407
C	-1.807661	-3.004285	-1.554418
C	-1.096865	-3.623083	-0.474000
C	-1.824493	-3.363758	0.743270
C	-1.115748	-3.070185	1.952243
C	-1.654539	-2.056930	2.802964
C	-0.793343	-1.171312	3.524200
C	-1.415786	0.129598	3.558685
C	-0.629128	1.319801	3.481292
C	-1.162021	2.421853	2.746348
C	-0.299509	3.259439	1.957787
C	-1.010171	3.628436	0.763428
C	-2.337829	3.081827	0.845185
C	-3.045252	2.684057	-0.321488
C	-2.342630	2.782388	-1.587043
C	-2.467680	1.724864	-2.566122
C	-3.432314	0.712466	-2.445662
C	-3.030329	-0.670592	-2.659713
C	-3.762961	-1.476914	-1.678366
C	-3.053549	-2.520901	-1.032130
C	-3.037943	-2.676205	0.408302
C	-3.582798	-1.635406	1.263147
C	-2.846070	-1.327147	2.436079
C	-2.684121	0.037807	2.897664
C	-3.209908	1.131230	2.144018
C	-2.431503	2.323772	2.074546
C	-4.060934	0.813282	1.015719
C	-4.024136	1.634148	-0.186128
C	-4.327875	0.764732	-1.307196
C	-4.537362	-0.581308	-0.825405
C	-4.340808	-0.570649	0.626656
Sc	2.450300	0.115154	-0.508590
Sc	-2.450395	-0.118750	-0.506992

Sc₂@D_{3h}(14246)-C₇₄

76

C	3.999225	-1.334455	0.136598
C	3.841788	-0.404183	1.235406
C	3.719934	0.924905	0.710974
C	3.765711	0.846793	-0.728548
C	3.976308	-0.543948	-1.106190
C	3.234861	-1.026466	-2.252473
C	2.492873	-2.276384	-2.150797
C	2.492632	-3.034945	-0.937880
C	3.262649	-2.573626	0.220607
C	2.463265	-2.852908	1.386078
C	2.446554	-1.982929	2.516683
C	3.134615	-0.738702	2.429921
C	2.367096	0.265189	3.122398
C	2.297239	1.613351	2.648835
C	3.000516	1.961985	1.404546
C	2.522403	3.018080	0.599011
C	2.546311	2.948995	-0.853467
C	3.039231	1.810182	-1.530119
C	2.319678	1.312206	-2.710481
C	2.400084	-0.104271	-2.989419
C	1.233020	-0.808546	-3.434652
C	1.254300	-2.137637	-2.870823
C	0.048280	-2.816003	-2.486004
C	0.054422	-3.578930	-1.244618
C	1.261095	-3.603173	-0.473446
C	1.251761	-3.500231	0.983524
C	0.040709	-3.333566	1.713974
C	0.024657	-2.452376	2.906919
C	1.232827	-1.777797	3.252401
C	1.213932	-0.389558	3.675235
C	-0.018272	0.304158	3.821365
C	-0.036056	1.692108	3.501080
C	1.129609	2.357305	2.976468
C	0.669981	3.437006	2.145870
C	1.360775	3.790831	0.988604

C	0.644715	4.170249	-0.203747
C	1.378030	3.654279	-1.335781
C	0.689643	3.163558	-2.442922
C	1.156619	1.994067	-3.144753
C	-0.003090	1.282513	-3.641146
C	0.016265	-0.126713	-3.722470
C	-1.182699	-0.842434	-3.446984
C	-1.170979	-2.172627	-2.883244
C	-2.406365	-2.340782	-2.165402
C	-2.395708	-3.097367	-0.954563
C	-1.154268	-3.637464	-0.481343
C	-1.159074	-3.535697	0.975194
C	-2.390052	-2.917316	1.366742
C	-2.404747	-2.047555	2.496094
C	-1.205383	-1.810064	3.243303
C	-1.229789	-0.423335	3.666122
C	-2.397556	0.200151	3.104762
C	-2.360787	1.550836	2.630569
C	-1.217697	2.326201	2.966811
C	-0.782596	3.417467	2.140499
C	-1.474689	3.753397	0.977329
C	-0.759398	4.150943	-0.209356
C	-1.469090	3.615828	-1.347692
C	-0.757337	3.143573	-2.448549
C	-1.185662	1.962310	-3.154249
C	-2.331948	1.247728	-2.728025
C	-2.370496	-0.169430	-3.006840
C	-3.181941	-1.112129	-2.271902
C	-3.950870	-0.652485	-1.135656
C	-3.965272	-1.444053	0.106930
C	-3.190109	-2.660670	0.196098
C	-3.840702	-0.508685	1.206307
C	-3.128816	-0.821978	2.404955
C	-3.751253	0.823645	0.682418
C	-3.064314	1.879694	1.381155
C	-2.610277	2.949362	0.579008
C	-2.620758	2.878453	-0.874882

C	-3.075609	1.726162	-1.554271
C	-3.783388	0.744135	-0.757522
Sc	1.906819	-0.743238	-0.411687
Sc	-1.894410	-0.778540	-0.394193

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76

C	4.116691	0.782031	0.932450
C	3.228026	1.106401	2.046651
C	4.403571	-0.607916	0.571977
C	4.064728	1.566708	-0.304680
C	2.636774	0.013953	2.831905
C	2.507649	2.330790	1.951296
C	4.502815	-0.690908	-0.880148
C	3.655776	-1.624467	1.230173
C	4.308799	0.644282	-1.400755
C	3.081729	2.611508	-0.470282
C	2.862413	-1.344417	2.389654
C	1.429767	0.250238	3.541280
C	2.407789	3.072855	0.695147
C	1.277657	2.533083	2.655820
C	3.643190	-1.600724	-1.641883
C	3.001730	-2.701792	0.486930
C	3.376079	0.571749	-2.499753
C	2.367444	2.699059	-1.727093
C	1.820927	-2.328624	2.455535
C	0.756080	1.510112	3.457137
C	0.407377	-0.776155	3.687622
C	1.101020	3.646499	0.629467
C	0.396152	3.331872	1.854517
C	2.902507	-2.632482	-0.949854
C	2.940245	-0.795161	-2.649509
C	1.891909	-3.149008	1.272206
C	2.447551	1.612036	-2.685150
C	1.036878	3.201752	-1.774602
C	0.572008	-2.056854	3.094566
C	-0.659458	1.291511	3.511812

C	-0.870236	-0.134174	3.697971
C	0.390025	3.722381	-0.608156
C	-1.013212	3.131590	1.874345
C	1.682935	-3.068690	-1.534700
C	1.576763	-1.083589	-3.064375
C	0.698579	-3.675276	0.670259
C	1.133679	1.348284	-3.189852
C	0.284925	2.396487	-2.709607
C	-0.585705	-2.728283	2.592939
C	-1.555928	2.080264	2.746651
C	-2.016465	-0.778565	3.157410
C	-1.021672	3.675539	-0.564273
C	-1.734252	3.466835	0.677734
C	0.633013	-3.672233	-0.759785
C	1.056428	-2.323150	-2.608365
C	0.649493	0.009369	-3.351357
C	-0.521465	-3.534178	1.394597
C	-1.110350	2.228013	-2.589633
C	-1.868812	-2.108263	2.645910
C	-2.803608	1.459903	2.380525
C	-3.018916	0.044167	2.563552
C	-1.784298	3.036429	-1.615638
C	-2.981889	2.849096	0.361429
C	-0.611623	-3.437377	-1.433031
C	-0.343232	-2.561802	-2.559412
C	-0.791750	-0.205666	-3.250094
C	-1.774672	-3.402780	0.715392
C	-1.685957	0.940288	-2.986538
C	-2.640255	-2.550769	1.510207
C	-3.543364	1.868366	1.233106
C	-3.887259	-0.433985	1.513585
C	-3.035594	2.627318	-1.056401
C	-1.826647	-3.342320	-0.706272
C	-1.265361	-1.557257	-2.948783
C	-3.063511	0.703959	-2.626897
C	-3.668233	-1.749218	0.933641
C	-4.259849	0.731378	0.701466

C	-3.714651	1.496681	-1.586826
C	-2.869832	-2.542125	-1.282207
C	-2.601518	-1.724634	-2.447450
C	-3.532359	-0.649347	-2.452974
C	-3.905962	-1.887727	-0.496375
C	-4.478762	0.600446	-0.714421
C	-4.377479	-0.740575	-1.278298
Sc	-2.426188	-0.161045	-0.542550
Sc	2.475621	-0.122597	-0.389288

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76

C	4.053103	-1.170133	-0.873573
C	3.147134	-2.192291	-1.300755
C	2.699420	-2.893827	-0.110470
C	3.260548	-2.226856	1.058922
C	4.124287	-1.182970	0.570893
C	4.007981	0.170927	1.051408
C	3.912216	1.021792	-0.129323
C	3.884256	0.185270	-1.312910
C	2.995926	0.492672	-2.415419
C	2.200403	-0.607164	-3.013888
C	2.234786	-1.950224	-2.397554
C	1.082655	-2.779392	-2.431205
C	0.676103	-3.586320	-1.290175
C	1.426784	-3.558389	-0.076191
C	0.755261	-3.574141	1.177882
C	1.253179	-2.783225	2.298175
C	2.428473	-1.991078	2.218218
C	2.436254	-0.648018	2.849063
C	3.191796	0.458125	2.212750
C	2.670766	1.782543	2.297339
C	2.648084	2.671495	1.137832
C	3.206418	2.275204	-0.104306
C	2.586519	2.707593	-1.300028
C	2.506565	1.822307	-2.467924
C	1.294474	2.130533	-3.158416

C	0.580496	1.120058	-3.823259
C	1.038596	-0.247178	-3.756668
C	-0.131911	-1.085834	-3.728463
C	-0.108860	-2.306928	-3.065917
C	-1.251248	-2.755371	-2.332991
C	-0.752809	-3.559751	-1.222598
C	-1.424191	-3.560186	0.031567
C	-0.673466	-3.602828	1.245165
C	-1.080652	-2.810241	2.395997
C	0.110371	-2.345216	3.037023
C	0.132399	-1.131852	3.713496
C	1.303712	-0.291778	3.633412
C	0.850905	1.075948	3.770982
C	1.519977	2.096042	3.084078
C	0.787712	3.152199	2.423439
C	1.461533	3.477405	1.195602
C	0.735134	3.780564	-0.000925
C	1.373312	3.475496	-1.242790
C	0.604100	3.157460	-2.420595
C	-0.790141	3.181493	-2.384441
C	-1.521859	2.133310	-3.058336
C	-0.852023	1.122158	-3.757712
C	-1.303779	-0.247475	-3.637399
C	-2.435849	-0.614243	-2.857341
C	-2.426795	-1.964916	-2.243038
C	-3.258193	-2.215270	-1.086564
C	-2.697231	-2.896870	0.074211
C	-3.145869	-2.210778	1.273200
C	-2.233370	-1.981598	2.372699
C	-2.200100	-0.646146	3.005441
C	-1.038589	-0.294556	3.752572
C	-0.581542	1.071983	3.836507
C	-1.296037	2.090002	3.183877
C	-0.606599	3.126812	2.459273
C	-1.376305	3.459410	1.285729
C	-0.738085	3.779959	0.047622
C	-1.463981	3.490717	-1.152529

C	-2.650165	2.683524	-1.104903
C	-2.672254	1.809219	-2.275492
C	-3.191818	0.483409	-2.207140
C	-4.007238	0.181293	-1.049252
C	-4.122630	-1.178348	-0.585717
C	-4.052515	-1.183823	0.858794
C	-3.885064	0.166320	1.314997
C	-2.996511	0.460537	2.420922
C	-2.507973	1.789733	2.489871
C	-2.588799	2.689829	1.333258
C	-3.208281	2.271683	0.132184
C	-3.913147	1.017550	0.141772
Sc	-2.078793	-0.541420	-0.028967
Sc	2.080004	-0.540683	0.026119

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76

C	-4.018257	0.624943	0.841016
C	-3.969560	1.178903	-0.493109
C	-4.214121	-0.818978	0.757295
C	-3.266663	1.253590	1.902056
C	-4.165953	0.090151	-1.406647
C	-3.112318	2.284819	-0.826443
C	-4.343559	-1.139312	-0.668540
C	-3.368311	-1.662000	1.611201
C	-2.650035	2.488895	1.622725
C	-2.658011	0.394353	2.870688
C	-3.249181	-0.110260	-2.487923
C	-2.615062	3.038890	0.270835
C	-2.327661	2.205935	-2.071972
C	-3.511523	-2.142679	-1.316333
C	-2.676912	-1.046975	2.686805
C	-2.706837	-2.782910	0.981389
C	-1.420421	2.868660	2.289876
C	-1.426934	0.756014	3.500199
C	-2.340071	0.942880	-2.844959
C	-2.817334	-1.506868	-2.429182

C	-1.419199	3.809952	0.149891
C	-1.173971	3.028662	-2.175187
C	-2.734961	-2.997425	-0.471108
C	-1.416387	-1.562545	3.203794
C	-1.421186	-3.240834	1.454962
C	-0.697825	3.731477	1.400723
C	-0.738539	1.968434	3.157505
C	-0.699960	-0.461885	3.755171
C	-1.162438	0.526615	-3.508435
C	-1.450760	-1.859497	-2.798547
C	-0.719007	3.837077	-1.063793
C	-0.000271	2.594804	-2.891986
C	-1.429414	-3.439252	-0.876755
C	-0.729558	-2.635898	2.565345
C	-0.697995	-3.713915	0.323288
C	0.696892	3.731623	1.400729
C	0.737905	1.968591	3.157531
C	0.699770	-0.461789	3.755201
C	-0.715765	-0.864687	-3.484104
C	-0.000204	1.352523	-3.526349
C	-0.729182	-2.852397	-2.005424
C	0.718136	3.837230	-1.063761
C	1.173312	3.028858	-2.175170
C	0.729860	-2.635777	2.565341
C	0.698571	-3.713769	0.323300
C	1.419651	2.868949	2.289915
C	1.418294	3.810328	0.149937
C	1.426532	0.756268	3.500213
C	1.416424	-1.562250	3.203806
C	0.715834	-0.864540	-3.484068
C	1.162217	0.526791	-3.508278
C	0.729647	-2.852264	-2.005430
C	2.327171	2.206391	-2.071904
C	1.421663	-3.240591	1.455021
C	1.429986	-3.438992	-0.876694
C	2.649335	2.489453	1.622807
C	2.614363	3.039515	0.270880

C	2.657686	0.394897	2.870829
C	2.676826	-1.046479	2.686771
C	1.451015	-1.859332	-2.798624
C	2.339670	0.943276	-2.844709
C	3.111901	2.285685	-0.826365
C	2.707343	-2.782582	0.981508
C	2.735495	-2.997039	-0.471021
C	3.266134	1.254245	1.902192
C	3.368580	-1.661504	1.611418
C	2.817253	-1.506373	-2.429039
C	3.249271	-0.109708	-2.488147
C	3.969046	1.179681	-0.492991
C	3.511906	-2.142345	-1.316480
C	4.017484	0.625656	0.841112
C	4.214279	-0.818225	0.757618
C	4.165903	0.090887	-1.406607
C	4.344086	-1.138754	-0.668504
Sc	-2.275457	-0.620931	-0.345261
Sc	2.277144	-0.620575	-0.345110

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76

C	0.082181	1.890690	-3.207694
C	0.611002	0.635777	-3.614661
C	-0.206809	-0.559031	-3.574593
C	0.627530	-1.649393	-3.185341
C	0.132483	-2.692173	-2.353345
C	1.079849	-3.310961	-1.474507
C	0.677719	-3.755057	-0.163750
C	1.663224	-3.389449	0.787742
C	1.295969	-2.693783	1.998760
C	2.174560	-1.649321	2.505748
C	1.581020	-0.518886	3.226950
C	2.153928	0.793189	3.080587
C	1.327140	1.950608	2.968127
C	1.873140	2.793729	1.930466
C	1.004762	3.507446	1.047058

C	1.379635	3.583167	-0.332662
C	0.387451	3.532538	-1.361229
C	0.923203	2.766955	-2.463410
C	-1.327232	1.950589	-2.968046
C	-1.873270	2.793655	-1.930373
C	-1.004927	3.507407	-1.046959
C	-1.379805	3.583089	0.332759
C	-0.387621	3.532494	1.361326
C	-0.923335	2.766865	2.463495
C	-0.082269	1.890625	3.207763
C	-0.611031	0.635673	3.614693
C	0.206839	-0.559092	3.574598
C	-0.627447	-1.649489	3.185329
C	-0.132353	-2.692228	2.353311
C	-1.079684	-3.311056	1.474466
C	-0.677527	-3.755100	0.163695
C	-1.663048	-3.389513	-0.787788
C	-1.295837	-2.693813	-1.998797
C	-2.174476	-1.649378	-2.505766
C	-1.580992	-0.518904	-3.226944
C	-2.153975	0.793140	-3.080550
C	-3.306051	0.996054	-2.231597
C	-3.091932	2.202861	-1.460371
C	-3.460437	2.258949	-0.058522
C	-2.565618	2.919817	0.818930
C	-2.268671	2.393754	2.139570
C	-2.813981	1.150092	2.571221
C	-1.962188	0.268418	3.309679
C	-1.983194	-1.157493	3.074043
C	-2.906562	-1.743412	2.173935
C	-2.431298	-2.837737	1.371998
C	-2.805791	-2.937976	-0.024885
C	-3.782626	-2.112142	-0.593727
C	-3.481723	-1.432219	-1.853712
C	-4.075762	-0.096122	-1.759060
C	-4.653983	0.063057	-0.423156
C	-4.228974	1.146559	0.459174

C	-3.823675	0.546751	1.727992
C	-3.927829	-0.893891	1.602181
C	-4.462817	-1.178594	0.285388
C	3.305959	0.996163	2.231604
C	3.091813	2.202995	1.460437
C	3.460301	2.259104	0.058597
C	2.565481	2.919968	-0.818850
C	2.268563	2.393909	-2.139496
C	2.813930	1.150282	-2.571175
C	1.962173	0.268585	-3.309650
C	1.983251	-1.157330	-3.074041
C	2.906663	-1.743221	-2.173955
C	2.431439	-2.837577	-1.372030
C	2.805946	-2.937829	0.024850
C	3.782801	-2.112012	0.593717
C	3.481806	-1.432103	1.853698
C	4.075701	-0.095953	1.759028
C	4.653939	0.063264	0.423161
C	4.228863	1.146746	-0.459124
C	3.823660	0.546959	-1.727974
C	3.927933	-0.893687	-1.602214
C	4.462940	-1.178404	-0.285405
Sc	-2.509519	-0.226667	-0.213191
Sc	2.509506	-0.226932	0.212986

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76

C	-4.565901	-0.912819	0.005879
C	-3.998343	-1.126959	-1.317157
C	-3.758027	0.183122	-1.901549
C	-4.115803	1.193734	-0.926092
C	-4.638751	0.508948	0.247559
C	-4.077447	0.771006	1.566960
C	-3.602949	-0.492061	2.132998
C	-3.966498	-1.539981	1.173827
C	-3.043286	-2.576061	0.925826
C	-2.678926	-3.001009	-0.416273

C	-3.053099	-2.193969	-1.552834
C	-2.077999	-2.010584	-2.577065
C	-1.895867	-0.731122	-3.224680
C	-2.674547	0.397751	-2.845026
C	-2.039200	1.666176	-2.834496
C	-2.327442	2.638794	-1.795716
C	-3.273226	2.366971	-0.783369
C	-2.925221	2.759267	0.562225
C	-3.235008	1.898163	1.680492
C	-2.112395	1.916613	2.599457
C	-1.595566	0.686501	3.137215
C	-2.311997	-0.559871	2.845705
C	-1.544315	-1.799015	2.754018
C	-1.926435	-2.808516	1.797690
C	-0.947671	-3.534176	1.053083
C	-1.389429	-3.605128	-0.326458
C	-0.438885	-3.462512	-1.383335
C	-0.796085	-2.652048	-2.500959
C	0.174414	-1.796868	-3.136748
C	-0.492799	-0.594922	-3.534549
C	0.170682	0.660609	-3.483469
C	-0.649024	1.803159	-3.193495
C	-0.125230	2.903560	-2.448535
C	-1.098318	3.353735	-1.510986
C	-0.715140	3.686059	-0.171926
C	-1.670113	3.404634	0.853820
C	-1.237988	2.944827	2.147681
C	0.127214	2.901169	2.451374
C	0.650166	1.799610	3.195300
C	-0.170375	0.657372	3.484207
C	0.492240	-0.598650	3.534094
C	-0.175915	-1.799756	3.135199
C	0.793997	-2.655113	2.498630
C	0.436213	-3.464180	1.380185
C	1.386618	-3.606691	0.323204
C	0.944877	-3.534056	-1.056320
C	1.924093	-2.808109	-1.800106

C	1.542846	-1.797505	-2.755467
C	2.311242	-0.558760	-2.845786
C	1.595808	0.688295	-3.136407
C	2.113698	1.917463	-2.597437
C	1.240005	2.945813	-2.144683
C	1.672646	3.404325	-0.850571
C	0.717692	3.685310	0.175359
C	1.100517	3.351207	1.514018
C	2.328978	2.634838	1.797792
C	2.040053	1.661706	2.835845
C	2.674683	0.392917	2.845421
C	1.895237	-0.735721	3.224156
C	2.076390	-2.014729	2.575398
C	3.051086	-2.197695	1.550706
C	2.676489	-3.003518	0.413615
C	3.040895	-2.577167	-0.927948
C	3.964441	-1.541327	-1.174817
C	3.602407	-0.492387	-2.133266
C	4.078882	0.769883	-1.566598
C	3.236452	1.897462	-1.678725
C	2.927610	2.758233	-0.559773
C	3.275054	2.363821	0.785474
C	4.117543	1.190298	0.927683
C	3.758030	0.178690	1.901866
C	3.996839	-1.130924	1.315999
C	4.564839	-0.915881	-0.006610
C	4.640105	0.506120	-0.247002
Sc	-2.533075	-0.090113	0.204426
Sc	2.534287	-0.086563	-0.205491

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C	-4.387175	0.555715	-1.332970
C	-3.945620	1.716309	-0.583307
C	-3.945214	1.355639	0.821452
C	-4.323104	-0.044040	0.940117
C	-4.624533	-0.527122	-0.404930

C	-3.969330	-1.717476	-0.934836
C	-3.280695	-1.354735	-2.177701
C	-3.589446	0.050065	-2.435293
C	-2.560611	0.895923	-2.918675
C	-2.265097	2.180879	-2.326855
C	-2.896893	2.583128	-1.095032
C	-2.106314	3.290806	-0.165920
C	-2.182654	3.016622	1.255875
C	-3.018229	1.978503	1.750131
C	-2.517203	1.169513	2.809382
C	-2.779423	-0.253437	2.846570
C	-3.588725	-0.880350	1.868497
C	-3.148680	-2.171870	1.391315
C	-3.257552	-2.514225	-0.012161
C	-2.071311	-3.252278	-0.401627
C	-1.370770	-2.904002	-1.608691
C	-1.947296	-1.885258	-2.484706
C	-1.042905	-1.037416	-3.261232
C	-1.348579	0.349805	-3.447048
C	-0.331453	1.364825	-3.339834
C	-0.877306	2.458583	-2.588027
C	-0.074657	3.171417	-1.653648
C	-0.732013	3.644157	-0.472790
C	-0.031627	3.720631	0.764395
C	-0.870140	3.241070	1.818119
C	-0.331444	2.399040	2.843019
C	-1.203751	1.395088	3.365729
C	-0.691077	0.122869	3.779545
C	-1.598292	-0.904039	3.385795
C	-1.118411	-2.147285	2.866478
C	-1.946280	-2.789096	1.888006
C	-1.353211	-3.518180	0.800160
C	0.031713	-3.719303	0.770783
C	0.731939	-3.644934	-0.466583
C	0.074485	-3.174249	-1.648207
C	0.877006	-2.463090	-2.583949
C	0.331060	-1.370661	-3.337618

C	1.348185	-0.355759	-3.446562
C	1.042543	1.031756	-3.263045
C	1.947001	1.881022	-2.488224
C	1.370607	2.901270	-1.613865
C	2.071296	3.251595	-0.407444
C	1.353281	3.519530	0.793949
C	1.946480	2.792420	1.883036
C	1.118710	2.152242	2.862669
C	1.598643	0.909864	3.384023
C	0.691451	-0.116345	3.779644
C	1.204068	-1.389285	3.367958
C	0.331724	-2.394127	2.847048
C	0.870355	-3.238012	1.823622
C	2.182832	-3.014543	1.260856
C	2.106317	-3.291081	-0.160449
C	2.896748	-2.584971	-1.090897
C	2.264820	-2.184951	-2.323354
C	2.560238	-0.900995	-2.917351
C	3.589048	-0.054276	-2.435469
C	3.280296	1.350899	-2.180220
C	3.969199	1.715862	-0.938179
C	3.257571	2.514296	-0.016824
C	3.148887	2.174326	1.387295
C	3.588957	0.883616	1.866576
C	2.779686	0.258351	2.845782
C	2.517428	-1.164646	2.811023
C	3.018459	-1.975544	1.753258
C	3.945345	-1.354242	0.823416
C	3.945549	-1.717304	-0.580739
C	4.386890	-0.557987	-1.332398
C	4.624476	0.526433	-0.406291
C	4.323316	0.045676	0.939621
Sc	2.486678	0.123909	-0.444447
Sc	-2.486561	-0.124661	-0.444750

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C	4.546431	-0.072688	0.133288
C	4.141873	-0.969848	-0.959022
C	3.553895	-2.158990	-0.323064
C	3.523650	-1.935188	1.123974
C	4.143576	-0.669516	1.376344
C	3.538583	0.325038	2.220391
C	3.580166	1.596693	1.469898
C	4.213388	1.333713	0.181692
C	3.617832	1.890635	-1.005186
C	3.327959	1.049327	-2.174517
C	3.531123	-0.402395	-2.157775
C	2.514399	-1.193825	-2.796556
C	2.042765	-2.449239	-2.236540
C	2.486767	-2.901942	-0.951628
C	1.539133	-3.557213	-0.106779
C	1.506563	-3.277439	1.320018
C	2.401549	-2.344659	1.929361
C	1.875454	-1.415067	2.949549
C	2.414826	-0.033284	3.034845
C	1.538600	1.036373	3.403480
C	1.571326	2.301908	2.662906
C	2.491014	2.545026	1.605266
C	2.004605	3.246185	0.397949
C	2.563048	2.866406	-0.881873
C	1.709644	2.742999	-2.042067
C	2.148027	1.612655	-2.808049
C	1.181780	0.801846	-3.498544
C	1.401789	-0.608088	-3.512392
C	0.291924	-1.520506	-3.465428
C	0.681539	-2.638869	-2.650107
C	-0.263317	-3.291894	-1.794817
C	0.184097	-3.781890	-0.537326
C	-0.683210	-3.692192	0.622313
C	0.149898	-3.398925	1.753575
C	-0.326107	-2.617099	2.811352
C	0.534861	-1.621454	3.390428

C	-0.311956	-0.512539	3.769028
C	0.181343	0.795112	3.758401
C	-0.656373	1.856876	3.241723
C	0.223417	2.796594	2.604562
C	-0.211265	3.540520	1.503087
C	0.669969	3.740518	0.386931
C	-0.152641	3.701059	-0.804787
C	0.335896	3.146355	-2.017908
C	-0.584722	2.449317	-2.863068
C	-0.167487	1.270422	-3.573362
C	-1.275723	0.354869	-3.602463
C	-1.059626	-1.051102	-3.489251
C	-2.036915	-1.800728	-2.754135
C	-1.629451	-2.878084	-1.892195
C	-2.529347	-2.923685	-0.766139
C	-2.019897	-3.205376	0.555353
C	-2.553497	-2.430743	1.699690
C	-1.675685	-2.121229	2.774794
C	-1.655036	-0.782434	3.378307
C	-2.532975	0.255708	2.933824
C	-1.984804	1.628917	2.774696
C	-2.469527	2.489963	1.674483
C	-1.553278	3.386296	1.036399
C	-1.525593	3.522179	-0.409956
C	-2.443395	2.820178	-1.245596
C	-1.958353	2.288714	-2.484823
C	-2.406215	0.991477	-2.963892
C	-3.428600	0.248058	-2.290169
C	-3.231777	-1.195168	-2.204871
C	-3.576277	-1.958271	-0.999610
C	-4.193004	-1.308512	0.114790
C	-3.639929	-1.489624	1.456608
C	-3.644072	-0.163184	2.120627
C	-4.207052	0.773024	1.181993
C	-3.561077	2.019477	0.859517
C	-3.532712	2.128399	-0.598700
C	-4.105358	0.905496	-1.170706

C	-4.541480	0.095556	-0.043460
La	1.963511	0.027718	-0.047519
La	-1.967193	-0.046770	0.033342

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C	4.569852	0.022141	-0.043578
C	4.148609	0.881744	1.059110
C	3.586780	2.098121	0.453373
C	3.584919	1.922828	-1.000004
C	4.207292	0.658690	-1.279687
C	3.588911	-0.302601	-2.158804
C	3.585221	-1.595803	-1.452184
C	4.183684	-1.371485	-0.135957
C	3.563232	-1.962882	1.006572
C	3.261755	-1.158749	2.192433
C	3.486166	0.282847	2.214083
C	2.476104	1.069823	2.872149
C	2.038666	2.350999	2.351680
C	2.514450	2.830787	1.087187
C	1.590534	3.518784	0.244520
C	1.585681	3.302853	-1.190351
C	2.481655	2.376237	-1.813399
C	1.959599	1.485839	-2.869771
C	2.480125	0.099659	-2.980112
C	1.584385	-0.944257	-3.373163
C	1.590406	-2.241083	-2.706951
C	2.485821	-2.524348	-1.636251
C	1.963787	-3.254731	-0.461983
C	2.500982	-2.928396	0.834768
C	1.629731	-2.832662	1.980662
C	2.069266	-1.728396	2.791902
C	1.108688	-0.930956	3.492927
C	1.348086	0.476772	3.551841
C	0.252705	1.406985	3.512992
C	0.671859	2.547668	2.748260
C	-0.253676	3.233410	1.898172

C	0.224716	3.737622	0.655961
C	-0.618417	3.722942	-0.516834
C	0.236170	3.460317	-1.641914
C	-0.230427	2.699722	-2.715346
C	0.626708	1.719540	-3.323013
C	-0.233164	0.642905	-3.758343
C	0.231266	-0.668826	-3.753940
C	-0.628446	-1.742290	-3.310182
C	0.229010	-2.718111	-2.696002
C	-0.237082	-3.471342	-1.617149
C	0.618053	-3.725894	-0.490526
C	-0.224445	-3.732312	0.682890
C	0.254294	-3.218843	1.921038
C	-0.670771	-2.527024	2.766828
C	-0.251155	-1.380630	3.523075
C	-1.346524	-0.450280	3.555691
C	-1.107258	0.957221	3.486669
C	-2.068201	1.749595	2.780586
C	-1.629107	2.848236	1.961346
C	-2.500803	2.935436	0.815163
C	-1.964193	3.252145	-0.484220
C	-2.486714	2.513421	-1.652868
C	-1.591793	2.222570	-2.722053
C	-1.586200	0.921018	-3.378850
C	-2.481660	-0.119986	-2.978083
C	-1.961118	-1.505496	-2.858083
C	-2.482890	-2.388425	-1.795244
C	-1.586304	-3.310408	-1.165920
C	-1.590524	-3.516002	0.270521
C	-2.514020	-2.822029	1.108779
C	-2.037600	-2.333224	2.369581
C	-2.474788	-1.048089	2.880850
C	-3.484892	-0.265644	2.217613
C	-3.260711	1.175457	2.185652
C	-3.562596	1.970926	0.993970
C	-4.183444	1.371394	-0.143671
C	-3.585865	1.586168	-1.461776

C	-3.590310	0.288070	-2.159112
C	-4.208393	-0.666954	-1.273007
C	-3.585912	-1.929461	-0.984569
C	-3.586885	-2.094121	0.470129
C	-4.148033	-0.872888	1.067162
C	-4.569884	-0.021523	-0.041105
La	1.923343	-0.017813	0.001734
La	-1.922814	0.014156	0.000147

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C	4.313913	-0.759693	-1.278891
C	4.068695	-1.648677	-0.155253
C	4.130385	-0.825201	1.064729
C	4.368505	0.578535	0.665264
C	4.493916	0.579120	-0.794980
C	3.742786	1.478793	-1.659238
C	3.032756	0.677347	-2.661668
C	3.437653	-0.710358	-2.434118
C	2.486763	-1.732385	-2.568688
C	2.367486	-2.784233	-1.575622
C	3.078715	-2.693999	-0.306524
C	2.349452	-3.074864	0.861874
C	2.443264	-2.314939	2.093668
C	3.246324	-1.130581	2.180258
C	2.701016	-0.029487	2.920337
C	2.860088	1.341070	2.461522
C	3.625605	1.665383	1.295923
C	3.060529	2.696497	0.425847
C	3.066554	2.547677	-1.024283
C	1.808299	3.007386	-1.544120
C	1.106619	2.260422	-2.561398
C	1.654084	0.995131	-3.046271
C	0.726417	-0.109104	-3.333240
C	1.180552	-1.456806	-3.124301
C	0.296356	-2.462050	-2.630667
C	1.011447	-3.243082	-1.632801

C	0.333982	-3.707932	-0.468967
C	1.021317	-3.622123	0.781759
C	0.307614	-3.256220	1.974239
C	1.168141	-2.413847	2.760539
C	0.630821	-1.313722	3.493879
C	1.418978	-0.124666	3.569691
C	0.793816	1.170617	3.536258
C	1.657621	2.060964	2.818459
C	1.111082	3.070695	1.965022
C	1.821604	3.361194	0.757366
C	1.089366	3.615489	-0.458030
C	-0.333981	3.707940	-0.468972
C	-1.011442	3.243090	-1.632807
C	-0.296348	2.462058	-2.630671
C	-1.180543	1.456813	-3.124307
C	-0.726407	0.109112	-3.333242
C	-1.654075	-0.995123	-3.046275
C	-1.106612	-2.260414	-2.561399
C	-1.808295	-3.007378	-1.544122
C	-1.089365	-3.615478	-0.458030
C	-1.821607	-3.361183	0.757364
C	-1.111087	-3.070685	1.965022
C	-1.657630	-2.060954	2.818457
C	-0.793826	-1.170606	3.536257
C	-1.418989	0.124677	3.569688
C	-0.630831	1.313733	3.493876
C	-1.168148	2.413857	2.760533
C	-0.307620	3.256229	1.974235
C	-1.021320	3.622131	0.781752
C	-2.349454	3.074873	0.861864
C	-3.078711	2.694004	-0.306535
C	-2.367481	2.784240	-1.575631
C	-2.486755	1.732391	-2.568696
C	-3.437643	0.710364	-2.434126
C	-3.032748	-0.677341	-2.661675
C	-3.742784	-1.478787	-1.659250
C	-3.066553	-2.547671	-1.024290

C	-3.060532	-2.696489	0.425841
C	-3.625614	-1.665376	1.295918
C	-2.860096	-1.341060	2.461516
C	-2.701024	0.029498	2.920330
C	-3.246329	1.130591	2.180247
C	-2.443270	2.314949	2.093659
C	-4.130387	0.825210	1.064715
C	-4.068689	1.648681	-0.155266
C	-4.313907	0.759698	-1.278903
C	-4.493916	-0.579112	-0.794993
C	-4.368512	-0.578528	0.665254
La	2.048955	0.060152	-0.249210
La	-2.048954	-0.060184	-0.249201

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C	4.335845	-0.716916	-1.292132
C	4.077939	-1.600421	-0.177916
C	4.132897	-0.784431	1.045273
C	4.357527	0.615584	0.641383
C	4.508680	0.617745	-0.807271
C	3.725998	1.502933	-1.649229
C	3.019661	0.697952	-2.663078
C	3.440383	-0.674879	-2.439317
C	2.501307	-1.706560	-2.581449
C	2.387568	-2.763524	-1.592668
C	3.089356	-2.661395	-0.329223
C	2.366157	-3.053385	0.842543
C	2.453226	-2.291714	2.073148
C	3.248239	-1.096748	2.157587
C	2.695850	-0.006239	2.904414
C	2.841558	1.365943	2.445267
C	3.605279	1.692606	1.272772
C	3.036808	2.721781	0.419051
C	3.047302	2.567001	-1.034426
C	1.789396	3.023554	-1.557230
C	1.094030	2.273899	-2.570889

C	1.651990	1.007394	-3.049637
C	0.727523	-0.101919	-3.343953
C	1.191217	-1.436160	-3.123582
C	0.308040	-2.458436	-2.632256
C	1.027565	-3.234074	-1.647510
C	0.356792	-3.711687	-0.482829
C	1.044592	-3.617208	0.768314
C	0.330939	-3.263164	1.963868
C	1.183141	-2.403913	2.741703
C	0.636535	-1.307077	3.482048
C	1.415974	-0.112712	3.558294
C	0.783915	1.177106	3.529097
C	1.643329	2.077725	2.806754
C	1.090054	3.087412	1.956049
C	1.801578	3.381954	0.751906
C	1.064520	3.622440	-0.470871
C	-0.356791	3.711687	-0.482834
C	-1.027561	3.234074	-1.647515
C	-0.308033	2.458433	-2.632259
C	-1.191209	1.436158	-3.123587
C	-0.727514	0.101917	-3.343956
C	-1.651983	-1.007397	-3.049642
C	-1.094024	-2.273902	-2.570890
C	-1.789393	-3.023556	-1.557233
C	-1.064518	-3.622441	-0.470870
C	-1.801580	-3.381954	0.751904
C	-1.090058	-3.087410	1.956048
C	-1.643336	-2.077722	2.806751
C	-0.783925	-1.177103	3.529095
C	-1.415983	0.112714	3.558289
C	-0.636544	1.307080	3.482045
C	-1.183148	2.403915	2.741698
C	-0.330944	3.263166	1.963865
C	-1.044594	3.617209	0.768307
C	-2.366159	3.053385	0.842533
C	-3.089355	2.661395	-0.329235
C	-2.387563	2.763523	-1.592677

C	-2.501300	1.706558	-2.581458
C	-3.440378	0.674878	-2.439328
C	-3.019655	-0.697954	-2.663087
C	-3.725994	-1.502935	-1.649239
C	-3.047300	-2.567002	-1.034433
C	-3.036809	-2.721781	0.419044
C	-3.605281	-1.692605	1.272763
C	-2.841564	-1.365941	2.445260
C	-2.695858	0.006241	2.904406
C	-3.248244	1.096750	2.157576
C	-2.453232	2.291716	2.073139
C	-4.132899	0.784432	1.045259
C	-4.077938	1.600421	-0.177929
C	-4.335841	0.716915	-1.292146
C	-4.508678	-0.617746	-0.807283
C	-4.357528	-0.615583	0.641371
La	1.945426	0.007405	-0.201457
La	-1.945425	-0.007405	-0.201465

La₂@D_{3h}(14246)-C₇₄

76

C	3.087427	-2.646806	0.705538
C	2.608535	-3.042591	-0.606965
C	1.286389	-3.587445	-0.455613
C	0.958616	-3.598449	0.972713
C	2.063375	-3.004123	1.666672
C	1.812336	-2.167113	2.787054
C	2.535702	-0.950606	2.962309
C	3.504422	-0.549163	1.985862
C	3.846480	-1.419213	0.871647
C	4.172358	-0.557564	-0.284785
C	3.696683	-0.975644	-1.617193
C	2.896674	-2.190161	-1.738733
C	1.845847	-1.957508	-2.698997
C	0.542134	-2.587697	-2.612637
C	0.256730	-3.432501	-1.441304
C	-1.097549	-3.547256	-0.994705

C	-1.425568	-3.536202	0.432667
C	-0.388810	-3.431345	1.420370
C	-0.642920	-2.585969	2.599260
C	0.456732	-1.968574	3.250615
C	0.366818	-0.613201	3.756612
C	1.628991	0.031645	3.504748
C	1.690992	1.411151	3.129330
C	2.682707	1.823677	2.112642
C	3.567556	0.817955	1.551058
C	3.961657	0.830982	0.134521
C	3.404972	1.860180	-0.753717
C	2.947948	1.443413	-2.104300
C	3.066657	0.032341	-2.470390
C	1.984652	-0.608914	-3.184268
C	0.849850	0.116640	-3.678051
C	-0.390449	-0.571704	-3.757717
C	-0.532726	-1.925579	-3.261594
C	-1.896680	-2.076022	-2.803235
C	-2.179293	-2.908552	-1.685171
C	-3.193707	-2.524800	-0.723114
C	-2.729088	-2.947738	0.589277
C	-2.985786	-2.094953	1.731966
C	-1.923584	-1.908176	2.691326
C	-2.007726	-0.556537	3.182936
C	-0.846018	0.122388	3.680555
C	-0.782235	1.521672	3.504103
C	0.483521	2.166911	3.251586
C	0.239983	3.315224	2.424443
C	1.198650	3.703039	1.469950
C	2.409937	2.952332	1.309961
C	2.754557	2.955674	-0.131486
C	1.729172	3.704848	-0.801776
C	1.286923	3.311312	-2.072124
C	1.884451	2.165535	-2.712745
C	0.839813	1.516206	-3.491947
C	-0.400821	2.207100	-3.235552
C	-1.636340	1.496624	-3.117969

C	-1.628461	0.118709	-3.503488
C	-2.573033	-0.832927	-2.971154
C	-3.526749	-0.402507	-1.989533
C	-3.906351	-1.266768	-0.882550
C	-4.190835	-0.399445	0.282743
C	-3.731522	-0.844955	1.613410
C	-3.060653	0.130602	2.470494
C	-2.887235	1.537735	2.114052
C	-1.800563	2.216014	2.729863
C	-1.160563	3.342984	2.097089
C	-1.587984	3.762225	0.829802
C	-0.605695	4.189629	-0.143029
C	0.764694	4.162988	0.174512
C	-1.056200	3.754818	-1.441340
C	-0.113734	3.338899	-2.399802
C	-2.295473	3.049376	-1.285951
C	-2.610873	1.938067	-2.097218
C	-3.531124	0.961868	-1.542325
C	-3.920071	0.978870	-0.126245
C	-3.326305	1.979305	0.767552
C	-2.640793	3.057899	0.154191
La	-1.749740	-0.407388	0.156628
La	1.739063	-0.414521	-0.166597

La₂@C₁(13408)-C₇₄

76

C	4.146567	0.805586	1.014744
C	3.241801	1.118456	2.126730
C	4.392254	-0.591387	0.635203
C	4.096755	1.599357	-0.235676
C	2.632613	0.007669	2.886545
C	2.496727	2.335696	2.015233
C	4.471206	-0.661007	-0.816720
C	3.684566	-1.641038	1.292902
C	4.310309	0.668645	-1.334124
C	3.109849	2.641682	-0.410699
C	2.863343	-1.351710	2.439141

C	1.395633	0.233254	3.564482
C	2.401574	3.073557	0.755580
C	1.246852	2.523346	2.698758
C	3.669425	-1.586699	-1.613889
C	3.031084	-2.701903	0.520550
C	3.417665	0.596038	-2.471423
C	2.394596	2.716975	-1.676230
C	1.806129	-2.330743	2.473385
C	0.717319	1.489499	3.480348
C	0.374417	-0.794174	3.699838
C	1.087267	3.639332	0.677463
C	0.371052	3.322717	1.892847
C	2.944517	-2.631361	-0.929964
C	2.995531	-0.780021	-2.654087
C	1.893069	-3.141019	1.285848
C	2.484774	1.637210	-2.648619
C	1.050639	3.202109	-1.724207
C	0.548150	-2.068011	3.099658
C	-0.701065	1.263529	3.520203
C	-0.912071	-0.158144	3.705477
C	0.388214	3.719164	-0.567541
C	-1.041575	3.110730	1.889743
C	1.715840	-3.056901	-1.521002
C	1.628386	-1.069730	-3.066413
C	0.707533	-3.673831	0.672841
C	1.169994	1.367883	-3.164943
C	0.309367	2.403222	-2.673482
C	-0.603954	-2.742266	2.581950
C	-1.592500	2.052877	2.748462
C	-2.053578	-0.804469	3.150075
C	-1.026635	3.670059	-0.541711
C	-1.752608	3.447861	0.689160
C	0.658268	-3.665547	-0.759118
C	1.097892	-2.307963	-2.600787
C	0.689555	0.026526	-3.342545
C	-0.524493	-3.540115	1.384231
C	-1.091708	2.239626	-2.582829

C	-1.894572	-2.130139	2.630589
C	-2.840751	1.431649	2.370149
C	-3.070404	0.016229	2.556920
C	-1.779659	3.045774	-1.610320
C	-3.015641	2.848531	0.356774
C	-0.581300	-3.430702	-1.444386
C	-0.304245	-2.548577	-2.561002
C	-0.758584	-0.192485	-3.257945
C	-1.777638	-3.415693	0.693281
C	-1.664732	0.958235	-3.017879
C	-2.660739	-2.575544	1.486510
C	-3.594237	1.859113	1.225821
C	-3.965006	-0.463662	1.512028
C	-3.043947	2.636405	-1.065248
C	-1.813234	-3.350729	-0.732270
C	-1.235490	-1.551613	-2.964383
C	-3.037534	0.711194	-2.651867
C	-3.718221	-1.791986	0.914241
C	-4.330995	0.726197	0.700421
C	-3.715912	1.505448	-1.615663
C	-2.861958	-2.574537	-1.323316
C	-2.575500	-1.737205	-2.483387
C	-3.486316	-0.649247	-2.469859
C	-3.888398	-1.909847	-0.526468
C	-4.455456	0.595108	-0.737172
C	-4.307875	-0.740236	-1.294636
La	2.043430	-0.058015	-0.218844
La	-2.039451	-0.035274	-0.229190

La₂@C_{2v}(14239)-C₇₄

76

C	4.127392	-0.983483	-0.976250
C	3.237569	-1.923149	-1.610762
C	2.750371	-2.825148	-0.568192
C	3.263760	-2.368239	0.719752
C	4.129530	-1.245688	0.445322
C	4.050789	0.001982	1.176272

C	4.024778	1.068647	0.153620
C	4.019013	0.444182	-1.183669
C	3.121736	0.931165	-2.233357
C	2.320885	-0.049091	-3.031306
C	2.345684	-1.484934	-2.669023
C	1.164550	-2.276637	-2.855281
C	0.725868	-3.256890	-1.877386
C	1.462693	-3.461071	-0.672958
C	0.749768	-3.697385	0.540318
C	1.216657	-3.136666	1.796629
C	2.405170	-2.348151	1.888427
C	2.401551	-1.137191	2.752425
C	3.191934	0.064110	2.356833
C	2.629185	1.357144	2.646984
C	2.635210	2.431948	1.668819
C	3.253164	2.276200	0.388536
C	2.625849	2.895740	-0.722494
C	2.578479	2.237773	-2.035657
C	1.373556	2.664881	-2.680308
C	0.675104	1.795719	-3.541445
C	1.141072	0.443617	-3.693768
C	-0.036350	-0.381830	-3.837051
C	-0.020007	-1.705399	-3.419948
C	-1.187707	-2.280739	-2.815722
C	-0.713133	-3.255081	-1.848159
C	-1.425921	-3.482223	-0.633553
C	-0.689190	-3.722780	0.564431
C	-1.135534	-3.170247	1.830546
C	0.044237	-2.831608	2.566312
C	0.048011	-1.751034	3.436796
C	1.223968	-0.920105	3.543952
C	0.754167	0.396320	3.914142
C	1.439815	1.522135	3.439622
C	0.717404	2.674223	2.961656
C	1.420270	3.206949	1.833890
C	0.720211	3.721028	0.697047
C	1.394284	3.635933	-0.561493

C	0.657220	3.533733	-1.787508
C	-0.749754	3.560447	-1.787408
C	-1.461263	2.655025	-2.653612
C	-0.765305	1.785611	-3.504828
C	-1.221144	0.419679	-3.637863
C	-2.394657	-0.081535	-2.981045
C	-2.383434	-1.523503	-2.616089
C	-3.238337	-1.974197	-1.536104
C	-2.718261	-2.862614	-0.502246
C	-3.211974	-2.406403	0.795200
C	-2.323805	-2.375483	1.941608
C	-2.314124	-1.170555	2.802099
C	-1.137973	-0.940919	3.600209
C	-0.685974	0.378295	3.949818
C	-1.394980	1.494352	3.463400
C	-0.688802	2.635780	2.949902
C	-1.428642	3.167877	1.842168
C	-0.758243	3.712126	0.702037
C	-1.456008	3.640888	-0.544803
C	-2.663983	2.847880	-0.674913
C	-2.646973	2.200894	-1.976369
C	-3.198345	0.886110	-2.178600
C	-4.055405	0.390793	-1.102978
C	-4.115767	-1.037889	-0.874739
C	-4.112481	-1.310204	0.544559
C	-4.021622	-0.055513	1.257595
C	-3.126814	0.024486	2.414296
C	-2.597433	1.319056	2.707068
C	-2.652657	2.408145	1.721027
C	-3.278694	2.231056	0.460463
C	-4.039827	1.013584	0.238894
La	-1.816481	-0.237717	-0.068697
La	1.817494	-0.250907	-0.024544

La₂@C_s(13336)-C₇₄

76

C	-4.106557	0.663718	0.885583
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C	-4.034998	1.239879	-0.463061
C	-4.253437	-0.793507	0.772792
C	-3.310681	1.260291	1.945675
C	-4.185254	0.153437	-1.400064
C	-3.147779	2.335275	-0.781373
C	-4.307190	-1.073876	-0.662661
C	-3.407293	-1.671966	1.603795
C	-2.665211	2.490810	1.677630
C	-2.678601	0.373194	2.884526
C	-3.281213	-0.033574	-2.504398
C	-2.628634	3.062441	0.333630
C	-2.345942	2.267513	-2.029120
C	-3.479861	-2.068531	-1.325890
C	-2.696934	-1.063002	2.689856
C	-2.734952	-2.789724	0.961022
C	-1.426090	2.855204	2.345082
C	-1.429739	0.725829	3.517793
C	-2.362970	1.019380	-2.836645
C	-2.825622	-1.440723	-2.460521
C	-1.425690	3.826941	0.226842
C	-1.177412	3.082769	-2.110346
C	-2.731923	-2.959091	-0.502188
C	-1.424465	-1.581504	3.190088
C	-1.430381	-3.242517	1.426388
C	-0.703377	3.730742	1.474049
C	-0.740407	1.942267	3.200350
C	-0.706011	-0.488152	3.750552
C	-1.164362	0.609586	-3.487962
C	-1.460510	-1.789836	-2.832888
C	-0.721755	3.867451	-0.984829
C	-0.001107	2.673065	-2.839739
C	-1.424456	-3.387539	-0.917122
C	-0.732444	-2.649726	2.536201
C	-0.694968	-3.681074	0.285821
C	0.697370	3.731730	1.474383
C	0.736280	1.943384	3.200819
C	0.705220	-0.487144	3.751108

C	-0.714836	-0.780749	-3.500060
C	-0.000027	1.434722	-3.483284
C	-0.730535	-2.791847	-2.046852
C	0.716854	3.868541	-0.984486
C	1.174199	3.084459	-2.109757
C	0.735386	-2.648458	2.536524
C	0.700557	-3.679889	0.286173
C	1.420960	2.857258	2.345770
C	1.420190	3.828977	0.227538
C	1.427260	0.727929	3.518630
C	1.425530	-1.579417	3.190981
C	0.718018	-0.779689	-3.499685
C	1.165505	0.611310	-3.487304
C	0.735918	-2.790640	-2.046484
C	2.343830	2.270810	-2.027835
C	1.434845	-3.240279	1.427087
C	1.430267	-3.385270	-0.916329
C	2.660925	2.494734	1.678882
C	2.624247	3.066320	0.334974
C	2.676810	0.377125	2.885872
C	2.697514	-1.059042	2.691299
C	1.464920	-1.787865	-2.832457
C	2.363214	1.022778	-2.835401
C	3.144710	2.339677	-0.779714
C	2.739210	-2.786047	0.962527
C	2.737382	-2.955697	-0.500865
C	3.307725	1.264992	1.947081
C	3.409333	-1.666939	1.605638
C	2.829608	-1.436937	-2.459589
C	3.282915	-0.028915	-2.502929
C	4.033050	1.245488	-0.461056
C	3.484425	-2.063938	-1.324474
C	4.104515	0.669484	0.887340
C	4.254228	-0.787299	0.774850
C	4.185830	0.159428	-1.397950
C	4.309623	-1.067735	-0.660593
La	-1.901347	-0.349456	-0.180387

La	1.900847	-0.351681	-0.181639
La ₂ @C ₂ (13290)-C ₇₄			
76			
C	-0.091411	1.891449	3.197092
C	-0.622632	0.637175	3.602673
C	0.195085	-0.557198	3.566208
C	-0.641454	-1.647551	3.184397
C	-0.139578	-2.695155	2.354684
C	-1.088573	-3.304877	1.473335
C	-0.678661	-3.744518	0.162401
C	-1.666693	-3.386635	-0.791570
C	-1.296245	-2.706337	-2.018214
C	-2.181396	-1.672506	-2.546802
C	-1.583280	-0.527585	-3.244109
C	-2.155866	0.790870	-3.088409
C	-1.317835	1.948123	-2.958617
C	-1.872835	2.791287	-1.929658
C	-1.002753	3.508616	-1.048341
C	-1.385499	3.588157	0.328175
C	-0.393380	3.536717	1.360726
C	-0.933419	2.770977	2.456064
C	1.317948	1.948075	2.958645
C	1.872979	2.791201	1.929680
C	1.002924	3.508560	1.048357
C	1.385671	3.588058	-0.328165
C	0.393555	3.536679	-1.360715
C	0.933565	2.770949	-2.456078
C	0.091515	1.891462	-3.197112
C	0.622670	0.637160	-3.602683
C	-0.195117	-0.557165	-3.566154
C	0.641368	-1.647559	-3.184338
C	0.139429	-2.695173	-2.354672
C	1.088392	-3.304953	-1.473328
C	0.678478	-3.744606	-0.162396
C	1.666521	-3.386772	0.791580
C	1.296086	-2.706392	2.018185

C	2.181285	-1.672594	2.546774
C	1.583241	-0.527660	3.244114
C	2.155909	0.790769	3.088428
C	3.328700	1.013293	2.270745
C	3.120155	2.219620	1.479707
C	3.504864	2.287686	0.068583
C	2.580551	2.930035	-0.809744
C	2.283958	2.399412	-2.130762
C	2.844002	1.159716	-2.575935
C	1.977718	0.271767	-3.303332
C	1.998429	-1.156209	-3.069521
C	2.940795	-1.751860	-2.184440
C	2.455376	-2.848959	-1.376107
C	2.821393	-2.957294	0.026912
C	3.777487	-2.110668	0.598294
C	3.481203	-1.441511	1.874338
C	4.050009	-0.098052	1.764099
C	4.618101	0.063764	0.420263
C	4.263516	1.168894	-0.468766
C	3.884846	0.563770	-1.759604
C	3.965878	-0.892438	-1.625557
C	4.447531	-1.170859	-0.283233
C	-3.328646	1.013451	-2.270726
C	-3.120029	2.219770	-1.479694
C	-3.504724	2.287836	-0.068579
C	-2.580397	2.930162	0.809745
C	-2.283834	2.399516	2.130756
C	-2.843933	1.159850	2.575920
C	-1.977697	0.271858	3.303318
C	-1.998490	-1.156117	3.069527
C	-2.940898	-1.751718	2.184454
C	-2.455544	-2.848855	1.376121
C	-2.821563	-2.957147	-0.026904
C	-3.777635	-2.110488	-0.598299
C	-3.481299	-1.441348	-1.874336
C	-4.050012	-0.097845	-1.764073
C	-4.618158	0.063982	-0.420256

C	-4.263423	1.169075	0.468757
C	-3.884795	0.563947	1.759590
C	-3.965925	-0.892247	1.625552
C	-4.447662	-1.170648	0.283229
La	2.085384	-0.091750	0.115518
La	-2.085368	-0.091848	-0.115539

La₂@C₂(13291)-C₇₄

76

C	4.563905	-0.900900	0.045817
C	4.001328	-1.123529	1.370523
C	3.773105	0.190045	1.973054
C	4.119124	1.204218	0.986909
C	4.623097	0.507513	-0.187069
C	4.076137	0.775084	-1.512293
C	3.632216	-0.494321	-2.109727
C	3.979542	-1.532341	-1.130054
C	3.079613	-2.595614	-0.902058
C	2.698029	-3.009818	0.441480
C	3.062831	-2.204592	1.588657
C	2.057086	-2.013524	2.594667
C	1.863922	-0.731382	3.235286
C	2.657860	0.402108	2.878429
C	2.007789	1.668247	2.857324
C	2.304247	2.642935	1.820337
C	3.286980	2.382620	0.823096
C	2.952706	2.783475	-0.531033
C	3.278345	1.923896	-1.665183
C	2.148154	1.913872	-2.575928
C	1.645836	0.685394	-3.150417
C	2.368769	-0.566896	-2.875633
C	1.584426	-1.804219	-2.759196
C	1.952532	-2.796866	-1.778439
C	0.955485	-3.518171	-1.035758
C	1.389911	-3.599935	0.338006
C	0.426166	-3.459179	1.382805
C	0.773069	-2.653116	2.506793

C	-0.207793	-1.796520	3.130677
C	0.457470	-0.594500	3.527362
C	-0.212579	0.663145	3.478943
C	0.611757	1.807640	3.207999
C	0.098310	2.913319	2.462396
C	1.086244	3.369529	1.532262
C	0.715022	3.692070	0.187346
C	1.680993	3.397442	-0.824416
C	1.254648	2.932327	-2.122547
C	-0.098084	2.913192	-2.462483
C	-0.611662	1.807501	-3.207965
C	0.212558	0.662900	-3.478851
C	-0.457618	-0.594694	-3.527216
C	0.207478	-1.796790	-3.130585
C	-0.773483	-2.653186	-2.506560
C	-0.426656	-3.459201	-1.382512
C	-1.390454	-3.599760	-0.337714
C	-0.956006	-3.517958	1.036045
C	-1.952984	-2.796530	1.778667
C	-1.584727	-1.803836	2.759335
C	-2.368974	-0.566434	2.875594
C	-1.645826	0.685806	3.150422
C	-2.147971	1.914154	2.575751
C	-1.254379	2.932583	2.122407
C	-1.680714	3.397722	0.824299
C	-0.714701	3.692147	-0.187448
C	-1.085936	3.369534	-1.532361
C	-2.304023	2.643050	-1.820338
C	-2.007719	1.668320	-2.857297
C	-2.657897	0.402227	-2.878206
C	-1.864096	-0.731351	-3.235034
C	-2.057408	-2.013409	-2.594362
C	-3.063304	-2.204343	-1.588405
C	-2.698539	-3.009603	-0.441219
C	-3.080116	-2.595251	0.902346
C	-3.979840	-1.531797	1.130173
C	-3.632250	-0.493725	2.109740

C	-4.076038	0.775615	1.512219
C	-3.278342	1.924454	1.665212
C	-2.952492	2.783868	0.530982
C	-3.286817	2.382916	-0.823066
C	-4.119039	1.204577	-0.986759
C	-3.773258	0.190367	-1.972969
C	-4.001680	-1.123192	-1.370334
C	-4.564508	-0.900458	-0.045651
C	-4.623467	0.508075	0.187187
La	-2.021410	-0.048933	0.141875
La	2.021904	-0.048641	-0.142240

La₂@C₂(13292)-C₇₄

76

C	4.362804	-0.574218	-1.305273
C	3.974497	-1.750679	-0.553857
C	4.008033	-1.387767	0.866810
C	4.363333	0.033156	0.971570
C	4.603103	0.508489	-0.394694
C	3.966211	1.700916	-0.940887
C	3.284962	1.335921	-2.192648
C	3.580458	-0.075029	-2.425079
C	2.571989	-0.933938	-2.927765
C	2.280629	-2.212183	-2.313310
C	2.916472	-2.606613	-1.074009
C	2.100249	-3.284574	-0.130966
C	2.184889	-3.003694	1.290517
C	3.047934	-1.982554	1.788477
C	2.534977	-1.150665	2.833201
C	2.799797	0.273020	2.859467
C	3.644311	0.900833	1.894319
C	3.193675	2.193413	1.392962
C	3.290575	2.534549	-0.023696
C	2.081214	3.233558	-0.422365
C	1.380517	2.897063	-1.646197
C	1.959972	1.886865	-2.527991
C	1.045901	1.013608	-3.269420

C	1.349762	-0.379442	-3.435398
C	0.325119	-1.390479	-3.302531
C	0.875743	-2.478433	-2.551544
C	0.065236	-3.184088	-1.617132
C	0.725924	-3.644733	-0.429721
C	0.028601	-3.710630	0.811862
C	0.869936	-3.224699	1.857963
C	0.332229	-2.367205	2.869560
C	1.209168	-1.362215	3.381623
C	0.700340	-0.089940	3.792395
C	1.613185	0.928607	3.394505
C	1.132264	2.164585	2.854671
C	1.961985	2.793581	1.872217
C	1.358439	3.503429	0.778289
C	-0.025872	3.721891	0.750570
C	-0.727892	3.636147	-0.487273
C	-0.071478	3.156890	-1.669366
C	-0.885534	2.435942	-2.589273
C	-0.337585	1.335011	-3.322790
C	-1.362589	0.322158	-3.435799
C	-1.057985	-1.068469	-3.249158
C	-1.969896	-1.929730	-2.490779
C	-1.386865	-2.924584	-1.593665
C	-2.082613	-3.240793	-0.361943
C	-1.355403	-3.490671	0.840424
C	-1.954844	-2.762078	1.924299
C	-1.122128	-2.117590	2.894059
C	-1.601212	-0.873140	3.415523
C	-0.687185	0.152036	3.793888
C	-1.197323	1.417256	3.363769
C	-0.322287	2.413344	2.831641
C	-0.863592	3.253332	1.807222
C	-2.180580	3.023836	1.248357
C	-2.101413	3.281700	-0.177690
C	-2.921472	2.588818	-1.106677
C	-2.289731	2.173633	-2.341713
C	-2.583555	0.885246	-2.934046

C	-3.591632	0.034518	-2.415027
C	-3.294530	-1.373162	-2.160335
C	-3.969463	-1.716451	-0.898845
C	-3.290143	-2.534557	0.029517
C	-3.187755	-2.170069	1.439493
C	-3.635476	-0.869259	1.920240
C	-2.789189	-0.226329	2.873263
C	-2.524841	1.196453	2.822579
C	-3.041241	2.010467	1.765773
C	-4.004406	1.400967	0.857160
C	-3.977754	1.741458	-0.569254
C	-4.369726	0.552582	-1.300440
C	-4.603777	-0.515005	-0.370261
C	-4.358142	-0.017397	0.986340
La	2.077643	0.073570	-0.212880
La	-2.077362	-0.074857	-0.220352

Sc₃N@C₇₄ isomers:

Sc₃N@C₂(13333)-C₇₄

78

C	-4.528482	-0.068099	0.013367
C	-4.053647	-1.329323	0.556097
C	-3.500774	-2.092416	-0.557411
C	-3.542381	-1.252788	-1.754018
C	-4.191186	-0.023917	-1.393374
C	-3.563999	1.239652	-1.692579
C	-3.534823	2.016548	-0.445393
C	-4.108979	1.185523	0.596714
C	-3.464228	1.167741	1.858391
C	-3.139338	-0.088067	2.503081
C	-3.354500	-1.349077	1.833549
C	-2.370267	-2.368973	2.040028
C	-1.945458	-3.233192	0.962753
C	-2.433729	-3.048052	-0.367048
C	-1.528545	-3.239974	-1.445550
C	-1.543945	-2.354691	-2.605464
C	-2.444012	-1.245683	-2.687085

C	-1.943798	0.049111	-3.192766
C	-2.463313	1.304036	-2.604368
C	-1.590914	2.432952	-2.468687
C	-1.580578	3.241210	-1.242326
C	-2.474512	2.949352	-0.160405
C	-1.952075	3.041586	1.204215
C	-2.442682	2.129985	2.185391
C	-1.565093	1.507606	3.159698
C	-1.975593	0.143011	3.326129
C	-1.010595	-0.890253	3.535827
C	-1.244915	-2.157362	2.909739
C	-0.146891	-2.931853	2.411423
C	-0.568028	-3.585154	1.194838
C	0.352972	-3.847845	0.118066
C	-0.162702	-3.624149	-1.201766
C	0.664719	-3.000975	-2.232579
C	-0.212020	-2.244196	-3.086981
C	0.240247	-1.058282	-3.682489
C	-0.630779	0.086259	-3.729522
C	0.217042	1.250734	-3.608829
C	-0.256935	2.395369	-2.948358
C	0.603518	3.158278	-2.066691
C	-0.252951	3.760491	-1.047500
C	0.254915	3.993308	0.281854
C	-0.586549	3.519252	1.372143
C	0.268068	2.912844	2.365612
C	-0.195473	1.869037	3.246952
C	0.744635	0.873543	3.633359
C	0.341059	-0.499494	3.749152
C	1.443235	-1.320044	3.314084
C	1.215114	-2.530341	2.599123
C	2.172900	-2.925893	1.582345
C	1.770875	-3.613919	0.348405
C	2.607961	-3.043391	-0.737392
C	2.015082	-2.620017	-2.004264
C	2.484722	-1.366086	-2.656184
C	1.580614	-0.619511	-3.472272

C	1.557311	0.839190	-3.419979
C	2.452513	1.567610	-2.565888
C	1.952003	2.736032	-1.799359
C	2.515538	3.032789	-0.456859
C	1.633607	3.622169	0.576465
C	1.618089	2.961574	1.881212
C	2.561226	1.931680	2.273583
C	2.104618	0.910294	3.163845
C	2.542243	-0.446861	2.982447
C	3.496532	-0.787702	1.984700
C	3.275379	-2.042062	1.281822
C	3.566227	-2.161870	-0.126645
C	4.142122	-1.062569	-0.817815
C	3.542119	-0.630174	-2.056820
C	3.548722	0.832853	-2.052308
C	4.185656	1.245031	-0.850808
C	3.572402	2.194235	0.003768
C	3.593894	1.619647	1.363422
C	4.122988	0.281658	1.269311
C	4.531472	0.083971	-0.089073
Sc	-2.244384	-0.061035	-0.158595
Sc	0.447697	1.791828	0.015249
Sc	1.021933	-1.538413	0.036424
N	-0.236582	-0.047344	0.015576

Sc₃N@C₂(13295)-C₇₄

78

C	4.331520	-1.137055	-0.973169
C	4.012907	-1.615261	0.365599
C	3.985393	-0.451745	1.249028
C	4.223853	0.731652	0.443996
C	4.447760	0.289017	-0.910896
C	3.691876	0.870105	-1.991692
C	3.026258	-0.198052	-2.717117
C	3.462085	-1.445284	-2.099035
C	2.493052	-2.449505	-1.914367
C	2.358622	-3.153517	-0.648258

C	3.029241	-2.652626	0.542704
C	2.297606	-2.664314	1.766561
C	2.360944	-1.555574	2.697640
C	3.132629	-0.393713	2.411550
C	2.596383	0.887674	2.773605
C	2.761321	2.035638	1.916272
C	3.502208	1.956262	0.703967
C	2.986344	2.673270	-0.429758
C	3.023974	2.087075	-1.749736
C	1.806064	2.374604	-2.433416
C	1.126047	1.338246	-3.181325
C	1.669116	-0.019454	-3.232938
C	0.759513	-1.159537	-3.203599
C	1.204628	-2.375374	-2.555798
C	0.319612	-3.197714	-1.798339
C	1.020844	-3.637817	-0.591332
C	0.330376	-3.698665	0.650880
C	0.976752	-3.224261	1.831500
C	0.238150	-2.496973	2.832761
C	1.079923	-1.450385	3.341690
C	0.532224	-0.176161	3.680478
C	1.311807	0.990405	3.402460
C	0.682444	2.218398	2.966759
C	1.567863	2.855380	2.012969
C	1.057263	3.620767	0.898364
C	1.758791	3.428092	-0.342408
C	1.066034	3.282966	-1.610320
C	-0.350553	3.367155	-1.677876
C	-1.003809	2.563220	-2.648088
C	-0.262862	1.504603	-3.329422
C	-1.137197	0.387323	-3.477064
C	-0.676609	-0.949277	-3.278619
C	-1.610680	-1.908817	-2.649274
C	-1.093885	-3.015479	-1.837542
C	-1.842791	-3.455802	-0.657009
C	-1.104385	-3.611091	0.592099
C	-1.853628	-2.979075	1.651437

C	-1.172629	-2.322316	2.740519
C	-1.735545	-1.103032	3.224880
C	-0.885952	-0.028883	3.644580
C	-1.510319	1.210739	3.248531
C	-0.748280	2.371099	2.888881
C	-1.281732	3.259512	1.856943
C	-0.386005	3.866356	0.842738
C	-1.052821	3.695613	-0.449838
C	-2.349225	3.116865	-0.238156
C	-3.069144	2.395900	-1.257123
C	-2.355693	2.129772	-2.479687
C	-2.452510	0.820903	-3.077208
C	-3.383677	-0.100757	-2.617112
C	-2.955286	-1.465742	-2.377887
C	-3.705929	-1.927963	-1.218721
C	-3.115156	-2.841042	-0.311540
C	-3.092743	-2.482494	1.105035
C	-3.619071	-1.201138	1.567058
C	-2.921910	-0.539631	2.624840
C	-2.781804	0.890842	2.636237
C	-3.287913	1.688107	1.571106
C	-2.479362	2.819541	1.165565
C	-4.087339	1.055189	0.580421
C	-4.039719	1.450379	-0.816944
C	-4.314913	0.281778	-1.601840
C	-4.492397	-0.831982	-0.734898
C	-4.300369	-0.381561	0.615394
Sc	2.208432	-0.364455	-0.482752
Sc	-1.390085	-1.303058	-0.130350
Sc	-0.237684	1.652318	0.635760
N	0.214367	-0.139026	-0.004283

Ca₂@C₇₄ isomers:

Ca₂@ C₂(13333)-C₇₄

76

C	-4.556664	-0.016245	-0.035885
C	-4.133291	-0.859784	1.057007

C	-3.579937	-2.075207	0.454916
C	-3.587293	-1.897536	-0.987469
C	-4.226499	-0.652533	-1.272803
C	-3.582551	0.305303	-2.134181
C	-3.569490	1.591909	-1.449561
C	-4.153446	1.367551	-0.123413
C	-3.556496	1.967741	1.000457
C	-3.257087	1.173523	2.184710
C	-3.473173	-0.262252	2.195675
C	-2.460516	-1.045257	2.850760
C	-2.027712	-2.326612	2.336699
C	-2.518067	-2.812772	1.080320
C	-1.610070	-3.526137	0.245315
C	-1.605619	-3.300944	-1.179306
C	-2.488361	-2.362603	-1.795058
C	-1.963820	-1.486422	-2.853761
C	-2.478277	-0.101522	-2.950789
C	-1.577682	0.937272	-3.333275
C	-1.585320	2.227457	-2.705762
C	-2.484436	2.515991	-1.636441
C	-1.963918	3.250967	-0.470089
C	-2.497197	2.946460	0.823752
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C	-1.099786	0.943442	3.475255
C	-1.344205	-0.464577	3.546607
C	-0.254917	-1.402222	3.521173
C	-0.673742	-2.542952	2.755846
C	0.247474	-3.229461	1.902921
C	-0.234879	-3.725575	0.658740
C	0.607296	-3.695366	-0.502710
C	-0.250368	-3.446381	-1.634758
C	0.211907	-2.705456	-2.709757
C	-0.645133	-1.732861	-3.330671
C	0.218538	-0.654214	-3.743596
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C	-0.211884	2.705551	-2.709665
C	0.250383	3.446438	-1.634637
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C	0.234874	3.725553	0.658869
C	-0.247488	3.229397	1.903029
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C	1.099760	-0.943560	3.475231
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C	2.497193	-2.946488	0.823672
C	1.963924	-3.250950	-0.470184
C	2.484452	-2.515934	-1.636507
C	1.585342	-2.227361	-2.705825
C	1.577709	-0.937154	-3.333294
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C	2.488378	2.362667	-1.794958
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C	2.518058	2.812735	1.080435
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C	2.460492	1.045160	2.850813
C	3.473151	0.262178	2.195706
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C	3.582573	-0.305227	-2.134166
C	4.226512	0.652579	-1.272749
C	3.587303	1.897572	-0.987376
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C	4.556665	0.016248	-0.035850
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C	0.248185	-2.468657	-2.654863
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C	-2.861842	-1.309951	2.405360
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C	-4.032362	1.655114	-0.217723

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