

## Supporting Information

### Preparation and ESR study of $\text{Sc}_3\text{C}_2@C_{80}$ bis-addition fulleropyrrolidines

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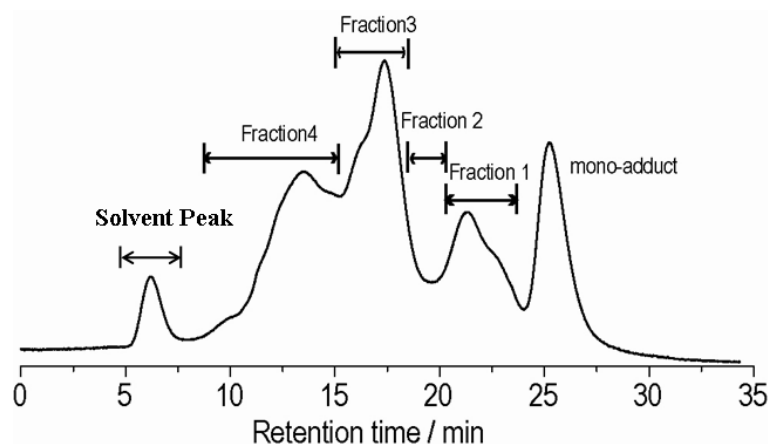
#### Experimental Section:

##### 1. Synthesis of $\text{Sc}_3\text{C}_2@C_{80}$ fulleropyrrolidines

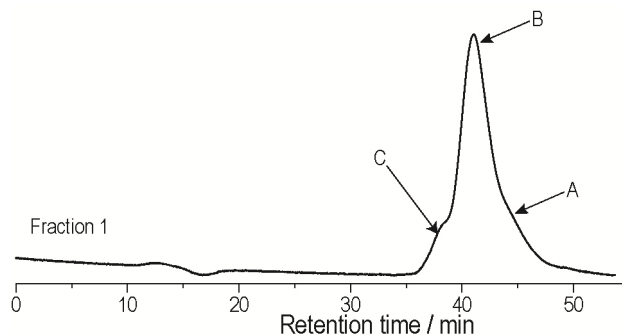
The synthesis of  $\text{Sc}_3\text{C}_2@C_{80}$  fulleropyrrolidine mono-adduct was carried out in *o*-dichlorobenzene solution of  $\text{Sc}_3\text{C}_2@C_{80}$  with an excess of *N*-ethylglycine and paraformaldehyde at 108 °C for 15 min. The product was isolated and purified by HPLC. The bis-adducts of  $\text{Sc}_3\text{C}_2@C_{80}$  fulleropyrrolidine were prepared from  $\text{Sc}_3\text{C}_2@C_{80}$  fulleropyrrolidine mono-adduct (4 mg) in *o*-dichlorobenzene (10 mL) solution with an excess of *N*-ethylglycine (7 mg) and paraformaldehyde (7 mg) at 108 °C for 20 min. The bis-adducts were also isolated and purified by HPLC.

##### 2. HPLC profiles of $\text{Sc}_3\text{C}_2@C_{80}$ fulleropyrrolidines

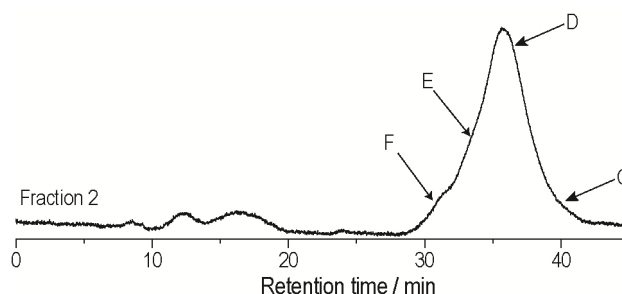
The  $\text{Sc}_3\text{C}_2@C_{80}$  fulleropyrrolidine mono-adduct was isolated easily on a Buckyrep-M column. Only one isomer was obtained for mono-adduct. Due to the numerous isomers of bis-adducts, four fractions (fraction 1, fraction 2, fraction 3 and fraction 4) were collected for further separation. Each fraction was isolated using recycling- HPLC, and finally nine isomers (A, B, C, D, E, F, G, H and I) of bis-adducts were obtained.



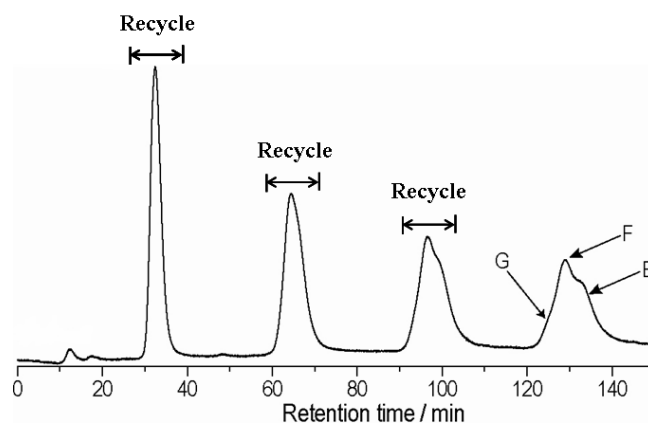
**Figure S1.** The HPLC profile of the reaction mixture treated at 108 °C for 20 min. 20×250 mm Buckyrep-M column; flow rate 12 mL/min; toluene as eluent. Four fractions were collected for further separation.



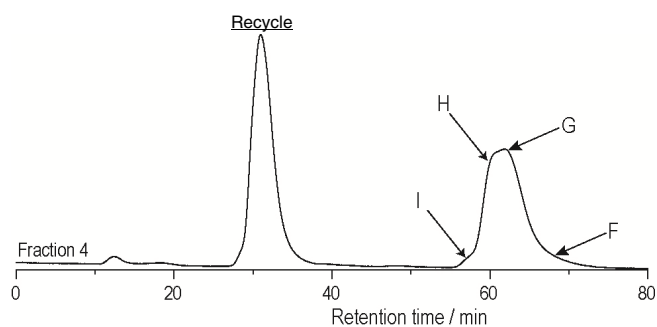
**Figure S2.** The HPLC profile of Fraction 1 for bis-adducts. 20×250 mm Buckyprep-M column; flow rate 6 mL/min; toluene as eluent. The letters of A, B, and C are denoted the three isomers, respectively (similarly hereinafter).



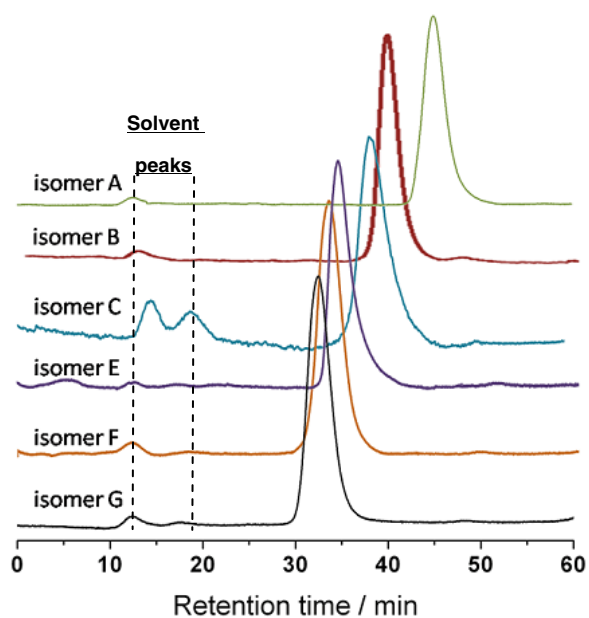
**Figure S3.** The HPLC profile of Fraction 2 for bis-adducts. 20×250 mm Buckyprep-M column; flow rate 6mL/min; toluene as eluent.



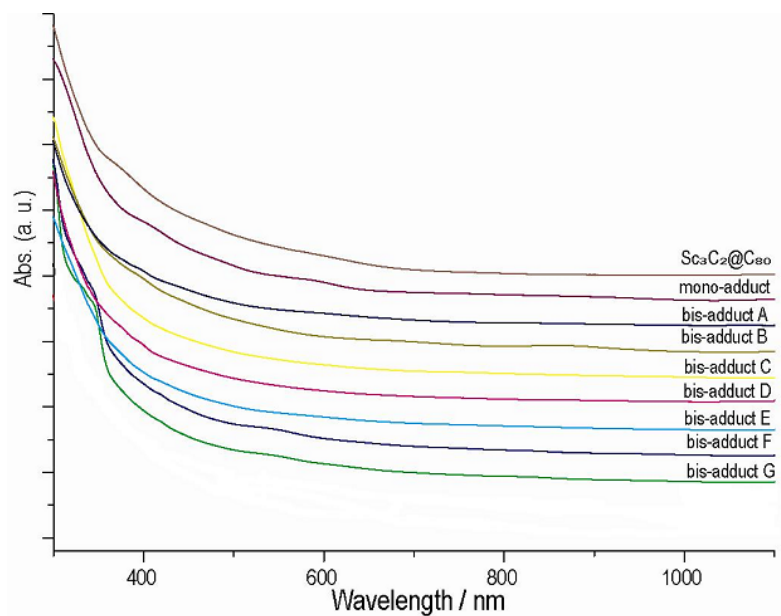
**Figure S4.** The cycling HPLC profile of Fraction 3 for bis-adducts. 20×250 mm Buckyprep-M column; flow rate 6mL/min; toluene as eluent). After three cycles the isomers E, F, and G were well separated and further purification for each isomer underwent the same process. Recycling-HPLC is an useful technique: After passing through the column first time, recycling technique enables the same eluent with the target substances return to the same column again and repeat the cycles until effective separation is made.



**Figure S5.** The cycling HPLC profile of Fraction 4 for bis-adducts. 20×250 mm Buckyprep-M column; flow rate 6mL/min; toluene as eluent. After one cycle the isomers F, G, H, and I were well separated and further purification for each isomer underwent the same process.



**Figure S6.** The HPLC profiles of the purified bis-adducts of  $\text{Sc}_3\text{C}_2@\text{C}_{80}$ . Buckyprep-M column; flow rate 6mL/min; toluene as eluent. Solvent peaks may be caused by trace of dissolved air and water in sample solvent.

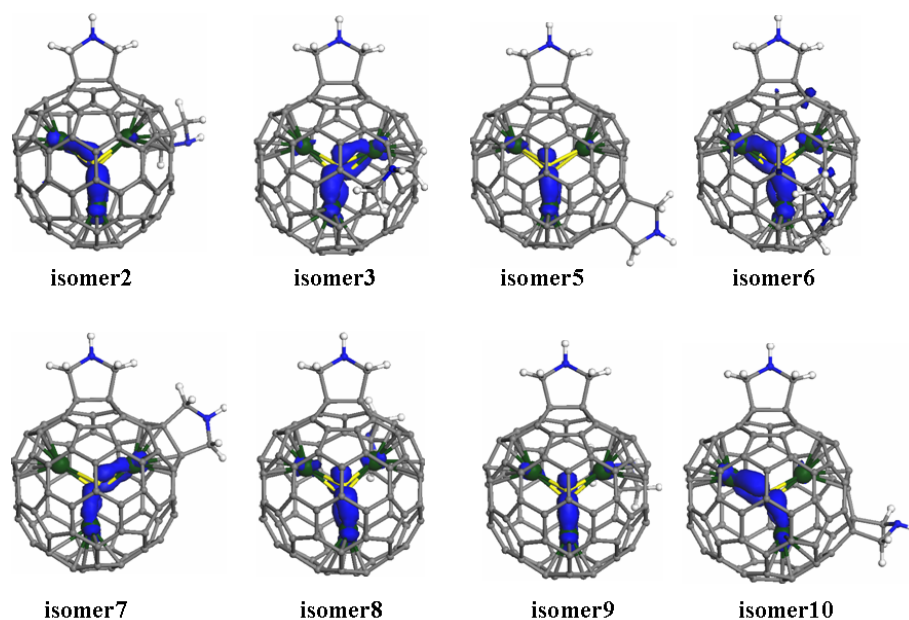


**Figure S7.** UV-Vis absorption spectra of the purified bis-adducts of Sc<sub>3</sub>C<sub>2</sub>@C<sub>80</sub>.

### Calculation Section:

**Table S1** The calculated bis-addition  $\text{Sc}_3\text{C}_2@C_{80}$  fulleropyrrolidines .

Sample	$\Delta E$ (kcal/mol)
Bis-adduct (isomer 1)	0
Bis-adduct (isomer 2)	0.5
Bis-adduct (isomer 3)	0.5
Bis-adduct (isomer 4)	0.5
Bis-adduct (isomer 5)	1.3
Bis-adduct (isomer 6)	2.4
Bis-adduct (isomer 7)	2.5
Bis-adduct (isomer 8)	2.7
Bis-adduct (isomer 9)	3.6
Bis-adduct (isomer 10)	3.8
Bis-adduct (isomer 11)	5.3
Bis-adduct (isomer 12)	5.4
Bis-adduct (isomer 13)	5.8
Bis-adduct (isomer 14)	5.8
Bis-adduct (isomer 15)	6.8
Bis-adduct (isomer 16)	7.2
Bis-adduct (isomer 17)	7.2
Bis-adduct (isomer 18)	7.3
Bis-adduct (isomer 19)	7.4
Bis-adduct (isomer 20)	8.3
Bis-adduct (isomer 21)	8.4
Bis-adduct (isomer 22)	9.1
Bis-adduct (isomer 23)	9.3
Bis-adduct (isomer 24)	10.2
Bis-adduct (isomer 25)	11.2
Bis-adduct (isomer 26)	19.3



**Figure S8.** The calculated spin density distributions of  $\text{Sc}_3\text{C}_2@C_{80}$  and its fulleropyrrolidines. The blue area presents the unpaired spin.

Cartesian coordinates of the ten most stable isomers.

isomer 1

C	-0.467219	-4.907467	3.147697
C	-1.639013	-3.277878	4.306772
H	-2.659556	-3.644711	4.069967
H	-1.693165	-2.636593	5.198695
H	0.406077	-5.574690	3.117867
H	-1.351428	-5.461884	2.767097
N	-0.652940	-4.336651	4.476513
H	-0.928605	-5.027387	5.176411
Sc	0.802246	-2.184229	-0.570877
Sc	0.043049	1.157491	1.402676
Sc	0.057006	1.197060	-2.085267
C	1.053188	0.037415	-0.321907
C	-0.231828	-0.231826	-0.349274
C	-2.413034	3.324163	-1.171780
C	-2.780222	2.005166	-1.815524
C	-2.151627	1.635210	-3.052495
C	4.383460	-1.069554	-1.077554
C	-2.411953	3.324463	0.466112
C	-2.162742	1.639727	2.361440
C	-2.780454	2.007530	1.116988
C	-3.412264	0.996922	0.384603
C	-3.436374	-0.374075	-1.508864
C	-2.759187	-0.783469	-2.681986
C	-2.120242	0.245302	-3.440680
C	-2.169512	-2.086313	-2.714931
C	-3.438417	-1.216372	-0.337605
C	-2.114413	-2.863998	0.893846
C	-2.758623	-2.460025	-0.332010
C	-2.165315	-2.911343	-1.542371
C	-2.146258	0.258642	2.774562
C	-2.755229	-0.785814	2.007063
C	-3.419404	-0.373105	0.818927
C	-2.187637	-2.089127	2.062880
C	1.888972	2.241582	-3.490606
C	1.238950	1.190062	-4.235251
C	-0.925167	0.005142	-4.194308
C	-0.210873	1.260468	-4.339009
C	1.116899	3.249623	-2.774929
C	-0.957874	3.606067	-1.539419
C	-0.332984	3.303263	-2.798821
C	-1.002472	2.316743	-3.661253
C	1.876079	3.579823	0.865312
C	1.229994	3.899599	-0.357388

C	1.873084	3.574483	-1.580405
C	-0.204717	3.879482	-0.356122
C	1.850024	-0.073779	3.500681
C	-0.310583	-1.274895	3.492121
C	1.076144	-1.301513	3.495333
C	-1.108084	-2.496716	3.058106
C	3.068387	-0.324367	2.774787
C	4.385359	0.301952	0.811569
C	3.701557	0.694346	2.003367
C	3.097386	1.993588	2.037114
C	3.040896	-3.117011	0.353532
C	3.669703	-2.058482	1.090624
C	3.053357	-1.685961	2.321764
C	4.380133	-1.064211	0.363879
C	-0.264137	-3.648825	2.256547
C	1.191440	-3.317190	2.009990
C	1.826925	-2.302370	2.742749
C	1.841103	-3.791332	0.814055
C	-0.932495	-3.697043	0.887884
C	-0.958539	-3.712436	-1.542127
C	-0.329059	-4.164814	-0.314467
C	1.138639	-4.340425	-0.351425
C	4.385545	1.143673	-0.356946
C	3.700984	2.393201	-0.355347
C	3.095659	2.825817	0.868335
C	3.090939	2.814126	-1.578891
C	1.115956	3.249523	2.056746
C	-0.333536	3.298076	2.080760
C	-0.958334	3.609713	0.826762
C	-1.006562	2.327068	2.956176
C	1.887693	2.257122	2.780505
C	-0.935435	0.019085	3.512136
C	1.230708	1.213971	3.536462
C	-0.217250	1.280561	3.643510
C	4.389568	0.300773	-1.523646
C	3.106657	-0.338211	-3.504629
C	3.712082	0.687335	-2.718219
C	3.098623	1.982454	-2.747020
C	3.070721	-3.156022	-1.080298
C	3.107851	-1.705375	-3.062928
C	3.701723	-2.076603	-1.817960
C	-3.417772	0.997427	-1.079505
C	-0.201680	-3.338304	-2.713372
C	1.880651	-2.326313	-3.494339
C	1.236763	-3.356629	-2.723630

C	1.902170	-3.891042	-1.545000
C	1.875212	-0.098288	-4.217228
C	1.124064	-1.333378	-4.217302
C	-0.293135	-1.297020	-4.158986
C	-0.955921	-2.331774	-3.436974
C	-3.381262	4.489650	0.805794
C	-3.382092	4.489016	-1.510962
H	-4.399320	4.062456	-1.641133
H	-3.090356	4.998568	-2.440421
H	-3.088319	4.999106	1.734980
H	-4.398408	4.063324	0.936979
N	-3.253559	5.369956	-0.352707
H	-3.947049	6.119524	-0.352569

isomer 2

C	2.150883	3.230903	4.683950
C	4.090944	2.797168	3.495544
H	4.234336	3.827271	3.107118
H	5.052650	2.266949	3.451659
H	1.555383	3.049055	5.590669
H	2.079548	4.308794	4.420775
N	3.518115	2.748402	4.835562
H	4.059190	3.283770	5.516925
Sc	0.391053	-2.161246	0.008846
Sc	-0.384556	1.213952	1.680437
Sc	-0.377017	1.163828	-1.755963
C	0.635888	0.067935	0.014331
C	-0.644964	-0.245997	-0.066703
C	-2.762772	3.356658	-0.808482
C	-3.145500	2.053737	-1.482510
C	-2.516444	1.703609	-2.728854
C	3.992268	-1.092604	-0.719525
C	-2.771776	3.336944	0.830258
C	-2.565597	1.639849	2.693556
C	-3.169206	2.016700	1.452778
C	-3.817318	1.024680	0.693455
C	-3.830389	-0.326528	-1.218152
C	-3.143876	-0.716178	-2.397965
C	-2.494883	0.318867	-3.140569
C	-2.567081	-2.025442	-2.445971
C	-3.875291	-1.189058	-0.072421
C	-2.621416	-2.913300	1.132716
C	-3.222418	-2.456266	-0.081535
C	-2.596476	-2.877012	-1.297886
C	-2.542761	0.242806	3.055186



C	-3.187511	-0.774563	2.282554
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C	1.546070	2.270434	-3.107153
C	0.891085	1.247919	-3.884197
C	-1.289793	0.083226	-3.887939
C	-0.561500	1.333157	-4.008240
C	0.775896	3.254832	-2.380028
C	-1.301156	3.607700	-1.157583
C	-0.668700	3.323083	-2.414095
C	-1.350312	2.381899	-3.315587
C	1.508488	3.436494	1.278361
C	0.877418	3.816176	0.049131
C	1.529055	3.548360	-1.167828
C	-0.549936	3.827709	0.040831
C	1.441478	-0.114433	3.803037
C	-0.730152	-1.305164	3.747031
C	0.685851	-1.338686	3.789983
C	-1.401432	-2.342902	3.031697
C	2.699443	-0.377576	3.116818
C	4.000138	0.249852	1.189347
C	3.344099	0.628118	2.383590
C	2.995981	2.096691	2.621242
C	2.647069	-3.177265	0.677748
C	3.284113	-2.121472	1.434913
C	2.678528	-1.741993	2.667414
C	3.977659	-1.113361	0.716192
C	-0.649050	-3.333294	2.304151
C	0.783426	-3.350511	2.303648
C	1.439141	-2.342721	3.080681
C	1.451253	-3.872785	1.120717
C	-1.408876	-3.708184	1.128510
C	-1.384311	-3.673990	-1.292984
C	-0.761932	-4.157488	-0.085945
C	0.701065	-4.325966	-0.073359
C	4.037361	1.109561	0.027280
C	3.338626	2.357077	0.054425
C	2.750487	2.768244	1.279498
C	2.742860	2.797554	-1.173390
C	0.751362	3.181637	2.477271
C	-0.688723	3.279449	2.483901
C	-1.310888	3.587995	1.215226
C	-1.402032	2.302395	3.315253
C	1.627848	2.408470	3.474620
C	-1.343549	-0.010737	3.798358

C	0.838191	1.166177	3.865604
C	-0.603621	1.233862	3.951505
C	4.020566	0.289661	-1.144040
C	2.735830	-0.306409	-3.148197
C	3.353302	0.698654	-2.346938
C	2.757134	1.995438	-2.360896
C	2.650006	-3.147524	-0.757501
C	2.713288	-1.677818	-2.720904
C	3.299743	-2.073277	-1.478009
C	-3.800497	1.043731	-0.766922
C	-0.611118	-3.280669	-2.456850
C	1.490828	-2.278242	-3.183364
C	0.816190	-3.288153	-2.424560
C	1.458498	-3.820905	-1.234424
C	1.515697	-0.044269	-3.876879
C	0.750888	-1.268476	-3.902440
C	-0.666925	-1.224264	-3.860664
C	-1.348557	-2.271686	-3.171809
C	-3.719540	4.516955	1.177069
C	-3.706491	4.542932	-1.139860
H	-4.731445	4.139050	-1.279561
H	-3.400807	5.056464	-2.062573
H	-3.422801	5.010418	2.113574
H	-4.745993	4.110200	1.296227
N	-3.566959	5.408639	0.029107
H	-4.248356	6.169339	0.034061

isomer 3

C	-3.251443	-2.926941	3.416901
C	-3.225211	-4.298210	1.555209
H	-2.657732	-5.128090	2.028494
H	-3.761831	-4.688424	0.679319
H	-3.806620	-2.203178	4.030783
H	-2.701470	-3.617665	4.090149
N	-4.127206	-3.606725	2.468699
H	-4.789948	-4.237508	2.923138
Sc	0.887403	-2.130934	-0.485175
Sc	0.239177	1.100712	1.666589
Sc	0.182475	1.262043	-1.876016
C	1.246204	0.009479	-0.022468
C	-0.047021	-0.142018	-0.197780
C	-2.284306	3.333020	-0.952232
C	-2.640890	2.006867	-1.589489
C	-2.025133	1.648613	-2.836708
C	4.545213	-0.993180	-0.926613

C	-2.262958	3.334285	0.682850
C	-1.970287	1.650310	2.568269
C	-2.602899	2.012161	1.339010
C	-3.220853	0.988919	0.615644
C	-3.249090	-0.387715	-1.267257
C	-2.594384	-0.778519	-2.461466
C	-1.983527	0.259696	-3.228809
C	-1.992430	-2.065903	-2.497869
C	-3.247287	-1.244049	-0.115673
C	-2.208205	-3.176956	1.164729
C	-2.609751	-2.489155	-0.123640
C	-1.988811	-2.908843	-1.331741
C	-1.932599	0.260281	2.967321
C	-2.574116	-0.771234	2.233494
C	-3.214293	-0.382018	1.060446
C	-2.206600	-2.225715	2.490077
C	1.999868	2.293892	-3.317720
C	1.353338	1.235756	-4.054557
C	-0.798079	0.031624	-3.997876
C	-0.096174	1.294710	-4.141326
C	1.227736	3.297857	-2.596167
C	-0.835693	3.630316	-1.338246
C	-0.224190	3.344074	-2.606947
C	-0.892085	2.345487	-3.461293
C	2.024192	3.628659	1.041521
C	1.360229	3.943598	-0.171579
C	1.991407	3.621516	-1.405059
C	-0.072017	3.915136	-0.157250
C	2.069146	-0.023758	3.680516
C	-0.099700	-1.255230	3.658198
C	1.321608	-1.256559	3.676968
C	-0.770039	-2.311399	2.992350
C	3.301893	-0.259900	2.952601
C	4.568607	0.380796	0.962097
C	3.900885	0.768482	2.166571
C	3.279295	2.057070	2.204236
C	3.244905	-3.045832	0.517379
C	3.883942	-1.987341	1.259289
C	3.305077	-1.620797	2.509348
C	4.563826	-0.986059	0.515217
C	-0.025016	-3.225368	2.206363
C	1.413052	-3.221274	2.176735
C	2.077585	-2.238431	2.951523
C	2.049363	-3.708878	0.976465
C	-0.762677	-3.672397	1.059945

C	-0.797514	-3.735698	-1.371304
C	-0.143434	-4.146156	-0.134315
C	1.325810	-4.259264	-0.171200
C	4.542606	1.220113	-0.206157
C	3.846643	2.461597	-0.195652
C	3.253835	2.887269	1.035448
C	3.214036	2.873202	-1.414334
C	1.278207	3.281378	2.232725
C	-0.165566	3.307533	2.265546
C	-0.811156	3.639719	1.027195
C	-0.822727	2.344077	3.160835
C	2.065680	2.299881	2.957283
C	-0.734944	0.049252	3.739387
C	1.432548	1.262074	3.734839
C	-0.026786	1.311276	3.872228
C	4.535024	0.374523	-1.373391
C	3.238488	-0.277123	-3.343302
C	3.840530	0.753352	-2.560062
C	3.217437	2.043467	-2.583498
C	3.248632	-3.083626	-0.915613
C	3.252455	-1.642239	-2.898456
C	3.864038	-2.005955	-1.661091
C	-3.244503	0.985370	-0.841576
C	-0.038343	-3.328173	-2.541150
C	2.025812	-2.274277	-3.321505
C	1.401697	-3.323333	-2.559969
C	2.081692	-3.831822	-1.371211
C	2.001446	-0.047344	-4.049981
C	1.260917	-1.287277	-4.048520
C	-0.154075	-1.263789	-3.975870
C	-0.795595	-2.308308	-3.243608
C	-3.245601	4.484451	1.035285
C	-3.272248	4.484109	-1.282090
H	-4.284918	4.044053	-1.404134
H	-2.995340	4.998480	-2.213472
H	-2.948613	4.998320	1.960681
H	-4.254776	4.043543	1.179462
N	-3.145432	5.366662	-0.124649
H	-3.850998	6.104872	-0.116518
isomer4			
C	-0.808978	1.767623	5.707256
C	-2.049231	-0.187927	5.599977
H	-1.364620	-0.815593	6.210701
H	-3.043002	-0.657191	5.590946

H	-0.812739	2.864501	5.787199
H	0.026592	1.370237	6.323356
N	-2.115283	1.203678	6.038198
H	-2.333871	1.284155	7.032609
Sc	0.462278	-2.102606	0.344522
Sc	0.153381	1.705297	1.258142
Sc	-0.346618	1.022590	-1.863700
C	0.748697	0.004653	-0.219184
C	-0.521802	-0.146975	0.107164
C	-2.737015	3.340598	-0.792152
C	-3.128205	2.044438	-1.477319
C	-2.511822	1.698597	-2.729872
C	4.021572	-1.047617	-0.767073
C	-2.731005	3.312978	0.843726
C	-2.412894	1.540937	2.631057
C	-3.070338	1.968931	1.436497
C	-3.747227	0.999186	0.697548
C	-3.803110	-0.335080	-1.215797
C	-3.129752	-0.721788	-2.404556
C	-2.493633	0.321484	-3.158662
C	-2.550369	-2.026257	-2.456878
C	-3.816481	-1.196326	-0.060299
C	-2.566483	-2.919429	1.143818
C	-3.168198	-2.461390	-0.078426
C	-2.556250	-2.872750	-1.300056
C	-2.498981	0.208944	3.096329
C	-3.113916	-0.786029	2.304502
C	-3.769552	-0.367892	1.112484
C	-2.564006	-2.116670	2.321611
C	1.546928	2.290150	-3.127386
C	0.891018	1.278195	-3.918578
C	-1.295380	0.094917	-3.928110
C	-0.566684	1.354273	-4.050088
C	0.780298	3.263962	-2.374737
C	-1.285342	3.606410	-1.139188
C	-0.659316	3.294029	-2.384866
C	-1.343656	2.376555	-3.303336
C	1.551329	3.647777	1.284124
C	0.900663	3.929944	0.036610
C	1.544121	3.601108	-1.195405
C	-0.536998	3.913469	0.046814
C	1.471347	-0.116709	3.797172
C	-0.688765	-1.346948	3.780051
C	0.708181	-1.357095	3.788657
C	-1.336069	-2.361437	3.033852

C	2.702480	-0.366496	3.093340
C	4.013557	0.290899	1.136959
C	3.319700	0.657999	2.323682
C	2.699464	1.945496	2.364482
C	2.699818	-3.162947	0.651681
C	3.321814	-2.086832	1.399064
C	2.704311	-1.723808	2.634310
C	4.011911	-1.073596	0.673715
C	-0.586158	-3.366433	2.297950
C	0.850987	-3.404219	2.308593
C	1.471955	-2.344547	3.050291
C	1.529694	-3.906515	1.110951
C	-1.356149	-3.725564	1.126746
C	-1.337788	-3.653223	-1.307372
C	-0.712558	-4.124516	-0.101663
C	0.746883	-4.272926	-0.093018
C	4.031590	1.153871	-0.015093
C	3.356878	2.404784	-0.004351
C	2.727191	2.809301	1.227397
C	2.770032	2.860711	-1.224920
C	0.811524	3.368795	2.527577
C	-0.664156	3.325536	2.503111
C	-1.288462	3.668542	1.232442
C	-1.255880	2.205161	3.184104
C	1.508453	2.232828	3.146450
C	-1.455260	-0.081615	4.161676
C	0.855844	1.155265	3.835198
C	-0.594236	1.309186	4.243949
C	4.042459	0.324594	-1.196690
C	2.742878	-0.273882	-3.181284
C	3.367807	0.735237	-2.384794
C	2.769104	2.034817	-2.400798
C	2.676807	-3.095924	-0.784776
C	2.729276	-1.645157	-2.756285
C	3.321400	-2.033874	-1.519281
C	-3.776065	1.029906	-0.766282
C	-0.586656	-3.269650	-2.485071
C	1.506262	-2.254474	-3.220120
C	0.834985	-3.250233	-2.453373
C	1.471035	-3.734749	-1.243915
C	1.518754	-0.015216	-3.901909
C	0.757891	-1.246382	-3.925110
C	-0.662882	-1.209853	-3.882874
C	-1.335732	-2.266097	-3.192312
C	-3.737363	4.439839	1.205012

C	-3.698365	4.521650	-1.112352
H	-4.709699	4.097579	-1.286821
H	-3.384341	5.065937	-2.014256
H	-3.471125	4.925828	2.154512
H	-4.746121	3.985523	1.305251
N	-3.607887	5.361421	0.078637
H	-4.316606	6.096562	0.092140

isomer5

C	2.810517	-3.698009	4.463841
C	1.614739	-2.084766	5.621488
H	0.754293	-2.728778	5.904750
H	1.642244	-1.217050	6.296105
H	3.792877	-4.123956	4.214002
H	2.088643	-4.530764	4.609582
N	2.895624	-2.785648	5.599266
H	3.089694	-3.273177	6.475196
Sc	1.155415	-2.400674	-0.008960
Sc	0.391774	0.860532	1.728277
Sc	0.372563	0.935922	-1.840848
C	1.375358	-0.175480	-0.057533
C	0.100134	-0.484671	-0.125028
C	-2.074785	3.106108	-0.936002
C	-2.449339	1.790087	-1.581344
C	-1.821200	1.416010	-2.816724
C	4.675826	-1.341787	-0.792608
C	-2.082556	3.109155	0.700661
C	-1.845464	1.425424	2.590950
C	-2.465890	1.795703	1.348742
C	-3.108217	0.793335	0.613639
C	-3.133493	-0.584224	-1.276670
C	-2.452213	-0.999070	-2.450410
C	-1.800017	0.024373	-3.203993
C	-1.877160	-2.309291	-2.484356
C	-3.161629	-1.428664	-0.109616
C	-1.886695	-3.122527	1.108678
C	-2.507427	-2.699117	-0.107063
C	-1.893984	-3.143567	-1.319904
C	-1.822391	0.040612	2.983410
C	-2.465431	-0.980469	2.227976
C	-3.143100	-0.580677	1.047101
C	-1.869985	-2.276780	2.261967
C	2.228094	1.991077	-3.225153
C	1.572348	0.948701	-3.977308
C	-0.603012	-0.221865	-3.956301

C	0.123319	1.028483	-4.093975
C	1.463889	3.000297	-2.512239
C	-0.614833	3.371103	-1.291239
C	0.012299	3.062312	-2.542841
C	-0.662781	2.088460	-3.416266
C	2.207824	3.327124	1.129977
C	1.570846	3.656311	-0.092726
C	2.216740	3.321079	-1.313635
C	0.132977	3.649597	-0.099553
C	2.131940	-0.341345	3.782862
C	-0.017924	-1.497754	3.736801
C	1.427548	-1.646961	4.142349
C	-0.651869	-2.497970	2.988033
C	3.306538	-0.613945	3.012089
C	4.666292	0.022545	1.085692
C	3.971821	0.413813	2.255421
C	3.394486	1.715406	2.294484
C	3.357368	-3.429556	0.642502
C	3.946411	-2.335581	1.391807
C	3.362884	-1.971203	2.631334
C	4.650803	-1.341333	0.645625
C	0.106332	-3.515473	2.257877
C	1.503772	-3.595893	2.281170
C	2.278244	-2.787054	3.319478
C	2.164034	-4.118918	1.101602
C	-0.679472	-3.919670	1.103608
C	-0.685498	-3.941398	-1.316382
C	-0.051697	-4.394276	-0.100349
C	1.404988	-4.570151	-0.093998
C	4.700582	0.873610	-0.082547
C	4.034455	2.128836	-0.082906
C	3.419207	2.560288	1.136476
C	3.429504	2.554837	-1.309867
C	1.436074	2.993478	2.315509
C	-0.011727	3.050971	2.322550
C	-0.630207	3.392308	1.070183
C	-0.695495	2.099336	3.203791
C	2.185206	1.983967	3.037635
C	-0.632750	-0.202917	3.758226
C	1.531622	0.948466	3.812576
C	0.070029	1.062069	3.938777
C	4.704046	0.028847	-1.243451
C	3.418417	-0.598937	-3.226480
C	4.037881	0.421948	-2.444695
C	3.436026	1.721386	-2.475273



C	3.352291	-3.408674	-0.793922
C	3.401908	-1.964944	-2.783823
C	3.987031	-2.338976	-1.536240
C	-3.101710	0.788180	-0.850017
C	0.080432	-3.563558	-2.485025
C	2.178971	-2.577493	-3.239419
C	1.511121	-3.573469	-2.464333
C	2.156615	-4.086208	-1.263038
C	2.195392	-0.346139	-3.952345
C	1.433543	-1.571788	-3.963099
C	0.017263	-1.527060	-3.919966
C	-0.662031	-2.564573	-3.209362
C	-3.050681	4.278583	1.033262
C	-3.032670	4.277576	-1.282732
H	-4.051863	3.858204	-1.421121
H	-2.730203	4.784321	-2.210284
H	-2.763038	4.786263	1.965121
H	-4.071047	3.857095	1.155004
N	-2.907686	5.158238	-0.123787
H	-3.598083	5.910648	-0.128843

isomer6

C	-1.975468	-5.377374	1.851195
C	-3.908180	-4.098050	1.788259
H	-4.342346	-4.562692	0.876678
H	-4.713658	-3.606727	2.352342
H	-1.227134	-5.893740	2.469483
H	-2.189631	-6.001330	0.955790
N	-3.161259	-5.030064	2.628048
H	-3.713674	-5.849991	2.883416
Sc	0.579292	-2.052226	0.330893
Sc	-0.283814	1.348677	1.686200
Sc	-0.320874	1.149086	-1.802091
C	0.756339	0.148747	-0.099090
C	-0.512407	-0.169044	0.031143
C	-2.747999	3.406055	-0.822423
C	-3.124105	2.084816	-1.462166
C	-2.510311	1.714906	-2.708628
C	4.055627	-1.001212	-0.733250
C	-2.746630	3.419473	0.813224
C	-2.479398	1.738104	2.693806
C	-3.108344	2.102701	1.463329
C	-3.760523	1.083105	0.742139
C	-3.787726	-0.290029	-1.143976
C	-3.120886	-0.697143	-2.323188

C	-2.486848	0.326958	-3.099443
C	-2.534439	-1.996257	-2.335816
C	-3.815772	-1.138917	0.019276
C	-2.822024	-3.075150	1.345248
C	-3.180208	-2.401543	0.028210
C	-2.541329	-2.809653	-1.152807
C	-2.450125	0.345919	3.079568
C	-3.100181	-0.696798	2.345991
C	-3.805538	-0.279588	1.180835
C	-2.546877	-2.004286	2.397260
C	1.544267	2.301999	-3.144120
C	0.884735	1.264786	-3.897379
C	-1.291541	0.084246	-3.858982
C	-0.570890	1.339922	-4.018049
C	0.774929	3.295812	-2.418085
C	-1.294672	3.683016	-1.187727
C	-0.669051	3.343673	-2.434756
C	-1.353089	2.387077	-3.314197
C	1.544573	3.653878	1.202750
C	0.899491	3.975504	-0.023526
C	1.542708	3.645528	-1.241256
C	-0.535782	3.957314	-0.015755
C	1.546622	0.000056	3.856923
C	-0.630127	-1.174524	3.759819
C	0.774899	-1.221845	3.822179
C	-1.299173	-2.206551	3.008564
C	2.767682	-0.252913	3.137634
C	4.054528	0.371102	1.151320
C	3.377347	0.764240	2.343445
C	2.765896	2.062333	2.368010
C	2.755962	-3.105348	0.738898
C	3.368878	-2.005804	1.452111
C	2.752402	-1.619925	2.687262
C	4.051438	-1.000548	0.708868
C	-0.563434	-3.255066	2.348987
C	0.861127	-3.284271	2.367044
C	1.520437	-2.226434	3.104154
C	1.574724	-3.840760	1.214286
C	-1.452658	-4.003853	1.359253
C	-1.294525	-3.575772	-1.129494
C	-0.676408	-4.074868	0.043484
C	0.778489	-4.225996	0.032332
C	4.052235	1.211631	-0.018743
C	3.371963	2.463719	-0.024732
C	2.758774	2.889373	1.197828

C	2.765309	2.889138	-1.248209
C	0.793311	3.349570	2.406519
C	-0.661871	3.417814	2.441811
C	-1.288060	3.702415	1.177635
C	-1.327793	2.424879	3.298644
C	1.562513	2.336083	3.117348
C	-1.257268	0.112966	3.822900
C	0.909884	1.288317	3.861362
C	-0.533663	1.366542	3.964174
C	4.059573	0.368920	-1.184472
C	2.751110	-0.268713	-3.146735
C	3.376160	0.756824	-2.375476
C	2.766078	2.052549	-2.410639
C	2.722517	-3.060166	-0.697037
C	2.747690	-1.631568	-2.697648
C	3.356306	-2.001751	-1.457200
C	-3.762139	1.081667	-0.720407
C	-0.563354	-3.218154	-2.321664
C	1.520229	-2.246232	-3.131085
C	0.857655	-3.222709	-2.326303
C	1.506712	-3.707735	-1.133381
C	1.517848	-0.025422	-3.862070
C	0.761421	-1.256338	-3.847615
C	-0.657669	-1.217656	-3.792342
C	-1.322043	-2.245778	-3.060791
C	-3.716219	4.585113	1.144496
C	-3.714395	4.571389	-1.171746
H	-4.732372	4.146709	-1.301512
H	-3.419041	5.073815	-2.103997
H	-3.426041	5.100090	2.071415
H	-4.733400	4.158438	1.276087
N	-3.586296	5.459028	-0.018815
H	-4.278848	6.209439	-0.024675
isomer7			
C	-0.846435	1.738722	5.776099
C	-2.041740	3.351263	4.633912
H	-3.045408	2.965834	4.912642
H	-2.133633	4.406984	4.341832
H	0.025874	1.490039	6.396029
H	-1.732213	1.194837	6.165578
N	-1.031972	3.176621	5.664774
H	-1.291953	3.613163	6.550785
Sc	0.466382	-2.111359	-0.328956
Sc	-0.400308	0.999238	1.920385

Sc	-0.202006	1.266202	-1.747054
C	0.660576	0.127979	0.117918
C	-0.607965	-0.203772	0.045918
C	-2.761846	3.354942	-0.832273
C	-3.122205	2.044447	-1.489283
C	-2.481374	1.683519	-2.713979
C	4.021401	-1.050394	-0.728605
C	-2.774847	3.334907	0.801483
C	-2.557042	1.647066	2.691388
C	-3.145908	2.010486	1.441910
C	-3.791299	1.021741	0.688086
C	-3.789842	-0.335249	-1.209472
C	-3.114183	-0.729694	-2.392904
C	-2.462550	0.302618	-3.130607
C	-2.532384	-2.036499	-2.439421
C	-3.830339	-1.194247	-0.056638
C	-2.571167	-2.903733	1.145021
C	-3.172417	-2.459576	-0.068747
C	-2.557979	-2.888701	-1.289510
C	-2.508799	0.261860	3.094307
C	-3.135430	-0.763433	2.292878
C	-3.805215	-0.355144	1.110825
C	-2.560623	-2.072948	2.312240
C	1.554479	2.300378	-3.134406
C	0.907653	1.256081	-3.897290
C	-1.263180	0.071617	-3.880366
C	-0.539182	1.323786	-4.000505
C	0.781001	3.307609	-2.410455
C	-1.303854	3.640612	-1.183837
C	-0.671079	3.357106	-2.441173
C	-1.328519	2.368865	-3.304465
C	1.499613	3.566451	1.249799
C	0.866728	3.907656	0.031326
C	1.520863	3.598261	-1.198257
C	-0.562555	3.904152	0.010180
C	1.468083	-0.115157	3.841305
C	-0.697518	-1.299211	3.774985
C	0.723547	-1.356906	3.856661
C	-1.356487	-2.337538	3.050494
C	2.699033	-0.353701	3.119712
C	4.019537	0.300661	1.173510
C	3.321461	0.678207	2.363105
C	2.711141	1.968448	2.409939
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isomer9

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