

Supporting Information for

Endohedrally Stabilized C₇₀ Isomer with Fused Pentagons Characterized by Crystallography

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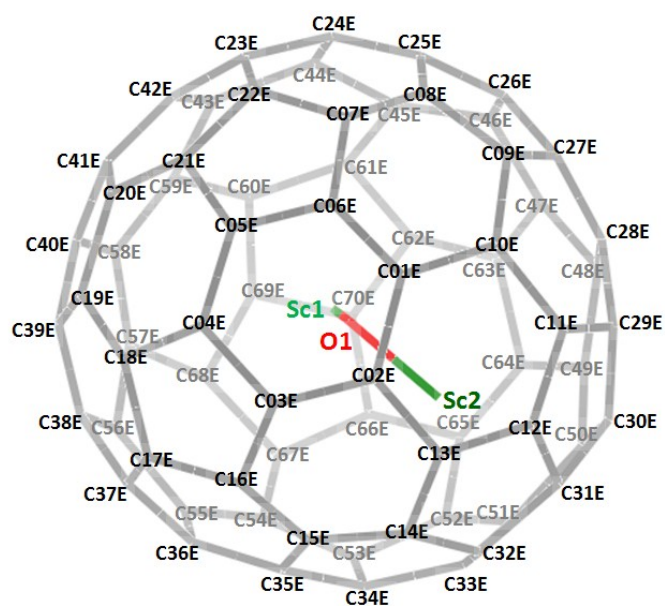


Figure S1. Three-dimensional diagrams of the $C_2(7892)-C_{70}$ cage with enantiomeric systematic numbering schemes, showing a ^{13}C configuration.



Figure S2. View of the structure of $\text{Sc}_2\text{O}@C_2(7892)\text{-C}_{70}\cdot[\text{Ni}^{\text{II}}(\text{OEP})]\cdot 0.5\text{C}_6\text{H}_6\cdot 1.5\text{CHCl}_3$ showing the close contact between the adjacent C_{70} cages in the unit cell.

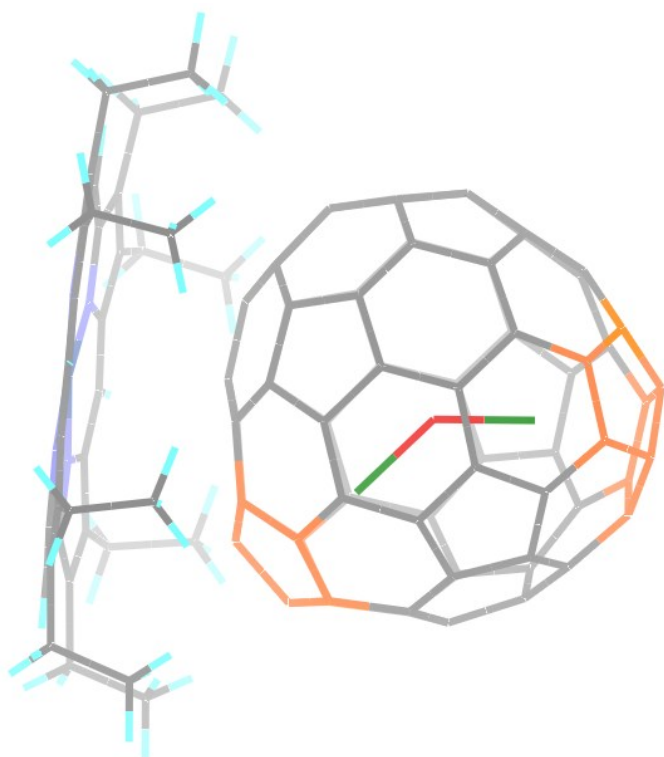


Figure S3. DFT-optimized structure of $\text{Sc}_2\text{O}@C_2(7892)\text{-C}_{70}\cdot[\text{Ni}^{\text{II}}(\text{OEP})]$ complex.

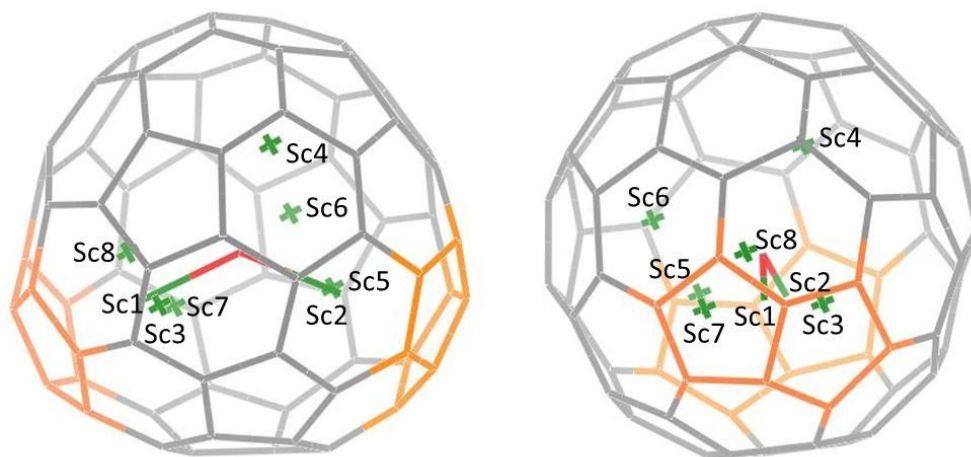


Figure S4. Two views of the X-ray structure of $\text{Sc}_2\text{O}@C_2(7892)\text{-C}_{70}$, showing all the identified Sc sites (Sc1-Sc8) inside the C_{70} cage.

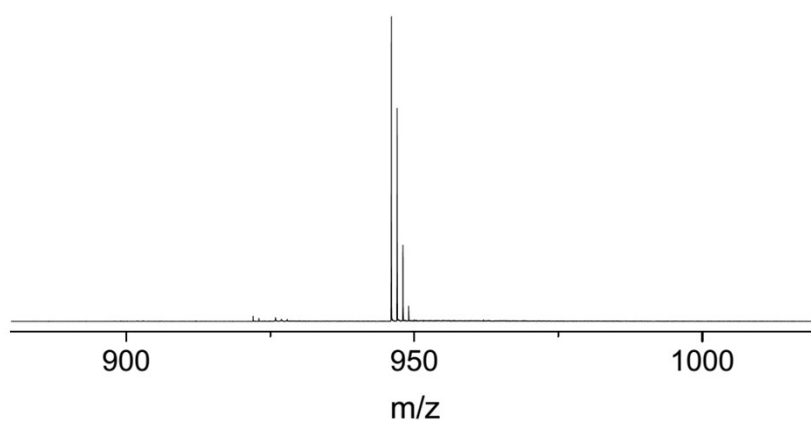


Figure S5. MALDI-TOF mass spectrum of the purified sample $\text{Sc}_2\text{O}@C_{70}$ in a positive-ion reflection mode.

Table S1. Crystal and structure data of $\text{Sc}_2\text{O}@C_2(7892)\text{-}C_{70}\cdot[\text{Ni}^{\text{II}}(\text{OEP})]\cdot 0.5C_6H_6\cdot 1.5CHCl_3$ at 120 K.

Temperature	T=120(2) K	Crystal size	0.20×0.15×0.15 mm ³
Empirical formula	$\text{Sc}_2\text{O}@C_2(7892)\text{-}C_{70}\cdot[\text{Ni}^{\text{II}}(\text{OEP})]\cdot 0.5C_6H_6\cdot 1.5CHCl_3$	Theta range for data collection	2.624° to 25.510°
Formula weight	1756.19	Index ranges	-17≤h≤17
Wavelength	0.71073 Å		-17≤k≤17
Crystal system	triclinic		-22≤l≤22
Space group	P -1 (No. 2)	Reflections collected	99396
Unit cell dimensions	a= 14.452(3) b=14.462(3) c = 18.805(4) α= 86.30(3), β= 87.93(3), γ= 62.15(3)	Independent reflections	12764 (>2sigma(I))
Volume	3467.8(15) Å ³	Completeness to θ	0.988 (θ= 25.510°)
Z	2	Absorption correction	Multi-scan
Density	1.682 gcm ⁻³	Max. and min. transmission	0.986 and 0.972
Absorption coefficient	0.701 mm ⁻¹	Refinement method	Full-matrix least-squares on F ²
F(000)	1788.0	Data/ parameters / restraints	12764/1220/925
		Goodness-of-fit on F ²	1.052
		Final R indices [I>2sigma(I)]	R1= 0.1086, wR2= 0.2953
		R indices (all data)	R1= 0.1227, wR2= 0.3091
		Largest diff. peak hole	2.237 and -1.753e/Å ⁻³

Coordinates of DFT-optimized Sc₂O@C₂(7892)-C₇₀[Ni^{II}(OEP)] complex

H	-2.213851	-2.361763	-6.268533
H	-2.121320	2.530945	-6.260755
C	-2.364033	-2.275117	-5.188365
H	-4.134147	-3.516646	-5.129407
H	-4.473444	-1.811679	-5.353510
H	-1.716073	-3.003854	-4.690271
H	-2.036933	-1.278424	-4.872170
H	-4.370965	2.107962	-5.283558
C	-3.832191	-2.514170	-4.807944
C	-2.235530	2.453916	-5.175537
H	-3.932565	3.786116	-5.038061
H	-1.943662	1.442826	-4.867779
C	-3.676054	2.762673	-4.744556
H	-1.536249	3.152202	-4.704994
H	-3.960532	0.125963	-4.328494
H	-4.329755	-5.108596	-3.576885
C	-4.054699	-2.375434	-3.333050
C	2.829125	-0.531731	-3.695053
H	-1.897897	-4.857766	-3.005764
C	2.245788	0.767205	-3.817700
H	-2.518792	-6.411576	-2.412892
C	-4.027217	0.114692	-3.245471
C	2.048613	-1.642201	-3.300888
H	-3.908465	5.337225	-3.456294
C	-4.026829	-4.835138	-2.560542
C	0.891803	0.969976	-3.564009
C	4.187563	-0.356460	-3.214763
C	-3.866564	2.603190	-3.266953
C	3.210838	1.738647	-3.364533
C	-2.594832	-5.325712	-2.302747
C	0.617904	-1.435190	-3.025665
C	0.086146	-0.132047	-3.121239
C	4.398521	1.047275	-2.960545
C	-4.140828	-3.351783	-2.386869
C	-4.107201	-1.115682	-2.620914
C	2.731634	-2.689735	-2.588592
H	-4.721436	-5.348941	-1.885852
H	-1.503393	4.879224	-2.790042
C	4.807158	-1.334375	-2.415914
C	-3.999563	1.331771	-2.587770
C	0.470792	2.162676	-2.875159
C	4.074906	-2.520418	-2.117216

C	2.803684	2.872941	-2.683231
C	-3.646949	5.032229	-2.437458
C	-3.862299	3.556611	-2.293486
H	-2.037194	6.501818	-2.300735
H	-2.269094	-5.056243	-1.291978
C	-0.061196	-2.328742	-2.103969
C	-2.194240	5.430899	-2.142314
C	1.398625	3.116953	-2.469498
C	-0.848498	0.385455	-2.121188
C	2.044746	-3.504293	-1.637033
C	5.165407	1.498035	-1.855498
C	5.779896	-0.888713	-1.453751
H	-4.322354	5.581531	-1.770842
C	0.631252	-3.438884	-1.479408
C	-0.612535	1.791088	-1.990395
C	-4.227612	-2.672469	-1.110596
N	-4.206068	-1.314491	-1.270542
C	6.007343	0.518820	-1.226960
C	3.536599	3.318648	-1.518142
C	4.199711	-3.159417	-0.839292
N	-4.059930	1.498224	-1.232470
H	-1.928291	5.193284	-1.107217
C	-1.018741	-1.814810	-1.134921
C	-3.984084	2.850493	-1.034609
C	4.673381	2.626764	-1.046375
C	2.918542	-3.720446	-0.507232
C	-1.232469	-0.394453	-1.013290
C	1.256407	3.761051	-1.182159
C	5.999015	-1.596691	-0.204122
H	-4.223153	-4.419912	0.086174
C	-4.213141	-3.334897	0.103015
C	0.101070	-3.614448	-0.153446
C	-0.739190	2.399572	-0.751960
C	2.584734	3.911093	-0.616168
Sc	1.125304	-1.568291	-0.192588
C	5.057808	-2.621521	0.170641
C	6.435810	0.676395	0.138029
C	-0.916931	-2.617724	0.047778
Ni	-4.129298	0.072228	0.154679
O	2.407701	-0.177444	-0.047656
C	0.193138	3.439516	-0.352543
Sc	4.261736	-0.086497	0.326157
C	-3.954847	3.474546	0.199611
H	-3.896778	4.558345	0.214153

C	4.909224	2.620863	0.413135
C	6.440558	-0.615568	0.770019
C	2.405157	-3.678572	0.835068
C	-1.261875	0.222498	0.327175
H	-2.095185	-5.106952	1.198344
C	-1.064782	1.616417	0.407035
C	5.762780	1.610504	0.991006
C	0.976668	-3.607879	1.003905
C	-4.072489	-2.712342	1.330400
C	2.767568	3.809890	0.753541
C	4.557610	-2.608634	1.518616
N	-4.043448	-1.360101	1.531306
H	-4.449776	-5.419793	2.077214
C	-0.700723	-1.994598	1.328030
C	-3.916211	2.812417	1.414966
C	3.926941	3.151789	1.272235
C	3.238645	-3.084267	1.834666
H	-2.189947	-6.473789	2.328077
N	-3.971132	1.456180	1.577744
C	0.387298	3.327222	1.075971
C	-2.289542	-5.387917	2.239085
C	-0.909194	-0.585623	1.504120
C	5.773431	-0.484591	2.037935
H	-1.872419	5.164012	1.445180
C	0.442087	-2.632734	1.939428
C	-3.683293	-4.916960	2.678431
C	-0.421437	2.227918	1.544996
C	1.647195	3.533127	1.624901
C	5.352660	0.893216	2.190699
C	-3.829610	-3.430371	2.563887
C	4.841011	-1.499253	2.400169
H	-1.515233	-4.918694	2.855362
H	-4.257692	5.499153	2.235368
C	-3.801278	-1.202369	2.869161
C	-2.107837	5.419236	2.484310
C	2.688211	-2.209113	2.827865
C	3.530755	2.459573	2.500501
C	-3.701749	3.483045	2.681149
H	-1.995393	6.500272	2.608486
H	-3.861229	-5.221197	3.715340
C	-3.769204	1.248145	2.914062
C	1.293758	-1.912779	2.850276
C	-0.221251	0.027303	2.582529
C	-3.526063	4.961539	2.849973

C	0.028618	1.437820	2.589175
C	4.123580	1.238434	2.880482
C	2.130310	2.696643	2.693545
C	3.658117	-1.199910	3.141460
C	-3.646834	-2.482762	3.526283
H	-1.367152	4.918612	3.116338
C	-3.690346	0.009562	3.525447
C	0.899806	-0.613852	3.222655
C	1.323945	1.671092	3.181338
C	3.267444	0.160673	3.401896
C	-3.600414	2.500887	3.620237
C	1.883407	0.406300	3.542299
H	-3.740211	5.235880	3.888492
H	-3.507800	-0.012442	4.595002
C	-3.245300	-2.665291	4.957674
H	-1.151765	-3.106277	4.561945
H	-3.488693	-3.683669	5.278733
H	-1.478397	-1.394462	4.839450
H	-3.825550	-1.994045	5.601841
C	-3.297557	2.627570	5.082604
C	-1.745337	-2.407183	5.160710
H	-1.171691	3.036726	4.866489
H	-1.544275	1.328159	5.091669
H	-3.550384	3.639354	5.417377
H	-3.938160	1.947640	5.656829
C	-1.824201	2.340687	5.402981
H	-1.458970	-2.523968	6.210077
H	-1.628426	2.439080	6.474719

Coordinates of DFT-optimized $[C_2(7892)-C_{70}]^{4-}$

C	-0.000455	3.698662	-0.121201
C	0.000455	3.574750	1.306914
C	-1.143822	3.315455	-0.887158
C	-1.132068	3.125705	2.001146
C	1.348602	3.366574	-0.587020
C	1.322665	3.122842	1.720638
C	-2.344318	2.822970	-0.166968
C	-2.298039	2.710911	1.251064
C	2.144467	2.974494	0.546114
C	-0.926420	2.868688	-2.226505
C	1.555835	2.759728	-1.855296
C	-0.967307	2.241289	3.131090
C	0.418118	2.542660	-2.690365
C	1.472863	2.259456	2.797747
C	-3.257239	1.965890	-0.846446
C	0.306126	1.834640	3.546831
C	-2.867205	1.547152	1.920609
C	-1.826023	1.937862	-2.847901
C	3.107334	1.911570	0.446694
C	2.689590	1.913054	-2.016601
C	-3.031372	1.567090	-2.216907
C	-2.053650	1.264516	3.073977
C	3.493521	1.525899	-0.862507
C	2.411128	1.141842	2.705275
C	0.336710	1.376214	-3.521229
C	-3.856760	0.812750	-0.158322
C	3.170225	0.909345	1.530904
C	-1.055420	0.973141	-3.601437
C	-3.478070	0.499112	1.173915
C	0.524944	0.456201	3.962148
C	2.647359	0.785016	-2.927049
C	-3.508770	0.233667	-2.382694
C	-1.844244	-0.048478	3.471013
C	1.844244	0.048478	3.471013
C	1.410820	0.420723	-3.547690
C	4.029208	0.222728	-1.122788
C	-4.029208	-0.222728	-1.122788
C	-0.524944	-0.456201	3.962148
C	3.478070	-0.499112	1.173915
C	3.508770	-0.233667	-2.382694
C	-1.410820	-0.420723	-3.547690
C	-3.170225	-0.909345	1.530904

C	-2.411128	-1.141842	2.705275
C	3.856760	-0.812750	-0.158322
C	-2.647359	-0.785016	-2.927049
C	2.053650	-1.264516	3.073977
C	1.055420	-0.973141	-3.601437
C	-3.493521	-1.525899	-0.862507
C	2.867205	-1.547152	1.920609
C	-0.336710	-1.376214	-3.521229
C	-0.306126	-1.834640	3.546831
C	-3.107334	-1.911570	0.446694
C	3.031372	-1.567090	-2.216907
C	-2.689590	-1.913054	-2.016601
C	-1.472863	-2.259456	2.797747
C	0.967307	-2.241289	3.131090
C	3.257239	-1.965890	-0.846446
C	1.826023	-1.937862	-2.847901
C	-0.418118	-2.542660	-2.690365
C	2.298039	-2.710911	1.251064
C	-1.555835	-2.759728	-1.855296
C	-2.144467	-2.974494	0.546114
C	-1.322665	-3.122842	1.720638
C	2.344318	-2.822970	-0.166968
C	1.132068	-3.125705	2.001146
C	0.926420	-2.868688	-2.226505
C	-1.348602	-3.366574	-0.587020
C	-0.000455	-3.574750	1.306914
C	1.143822	-3.315455	-0.887158
C	0.000455	-3.698662	-0.121201