Electronic Supplementary Material

Highly efficient synthesis of [60]fullerene oxides by plasma jet

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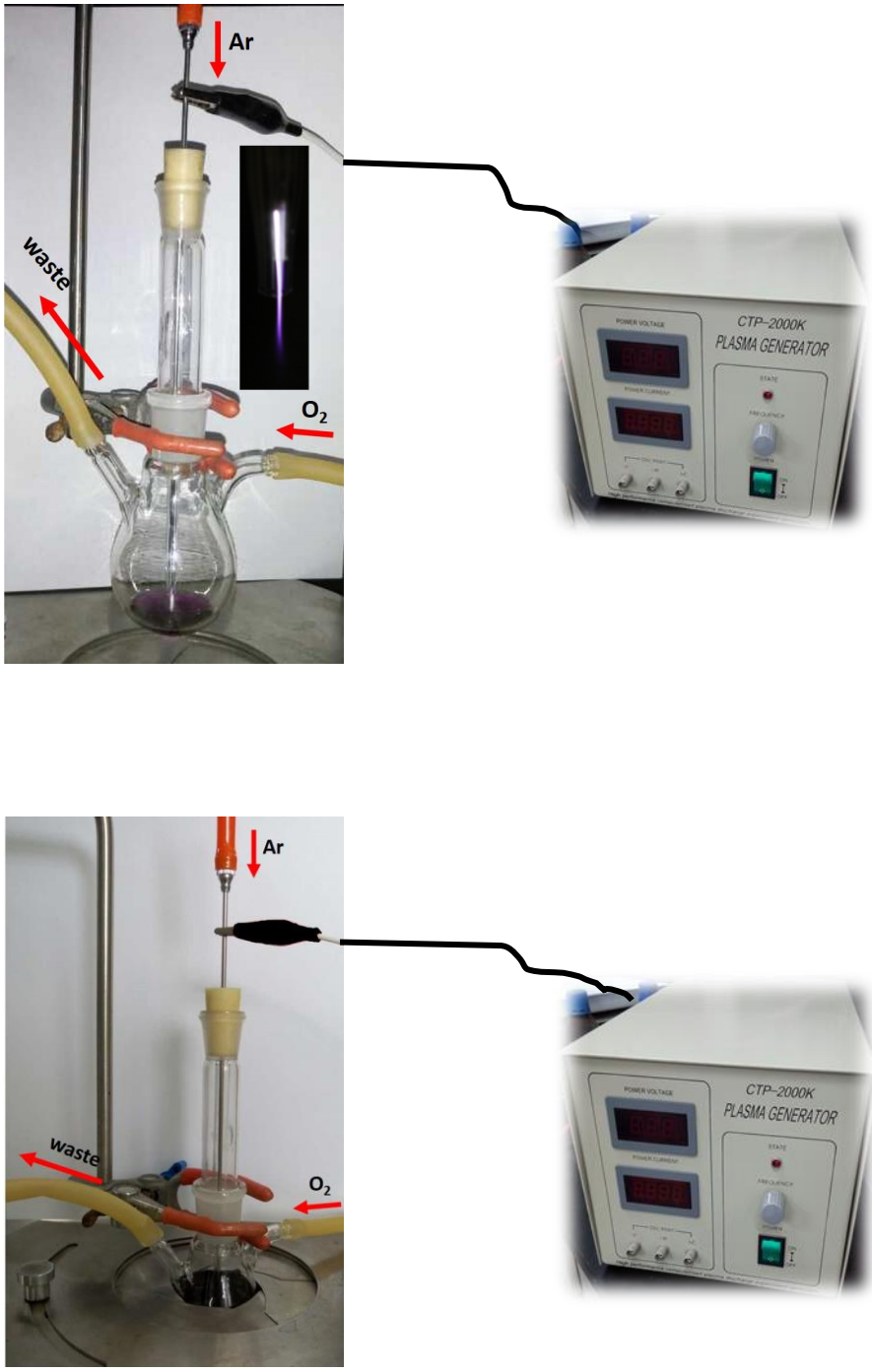

Figure S1. Schematic view of the experimental setup

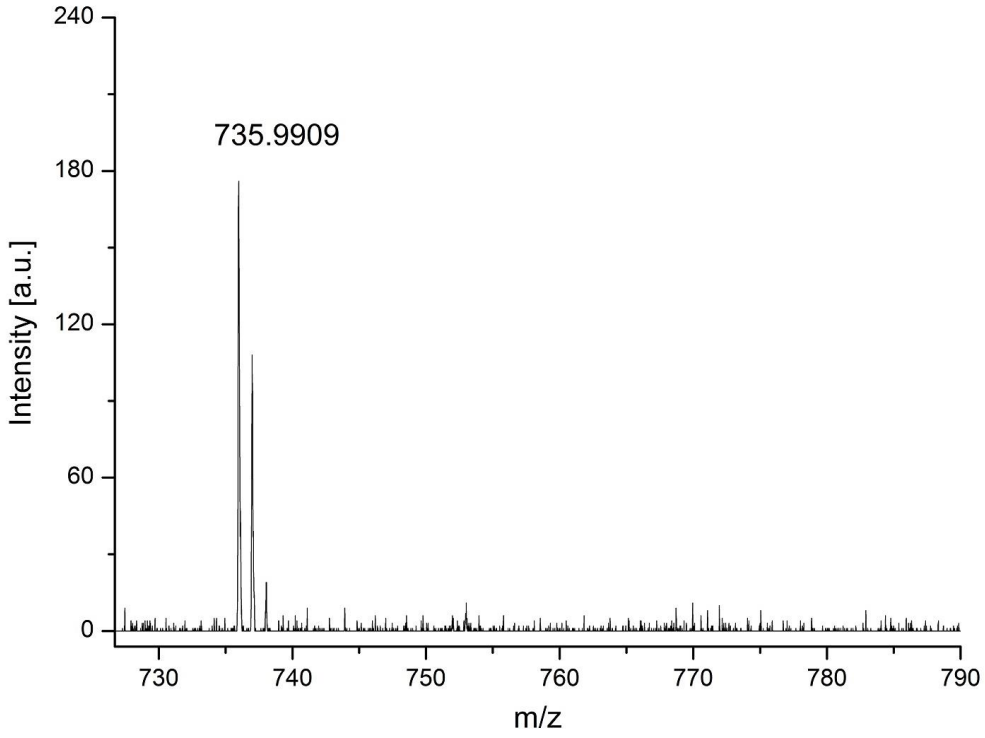

Figure S2. The HR-MS (MALDI-TOF) spectrum of $C_{60}O$

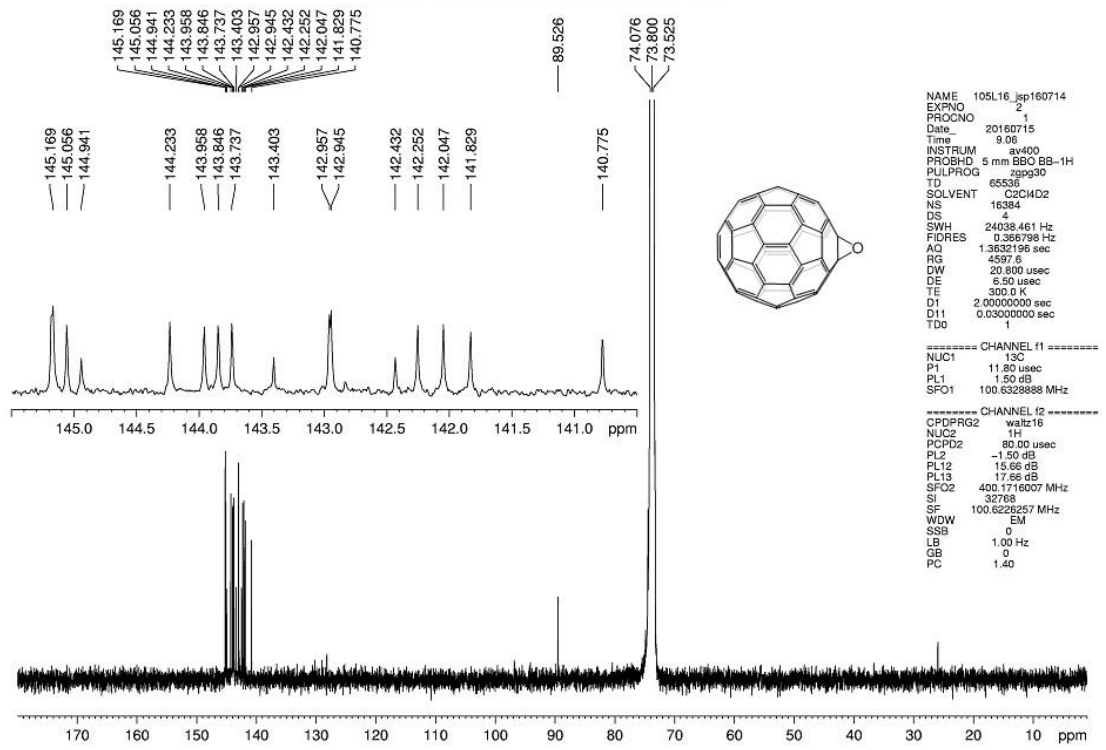

Figure S3. The ^{13}C NMR (100 MHz, $C_2D_2Cl_4$ with $Cr(acac)_3$ as a relaxation reagent)

spectrum of $C_{60}O$

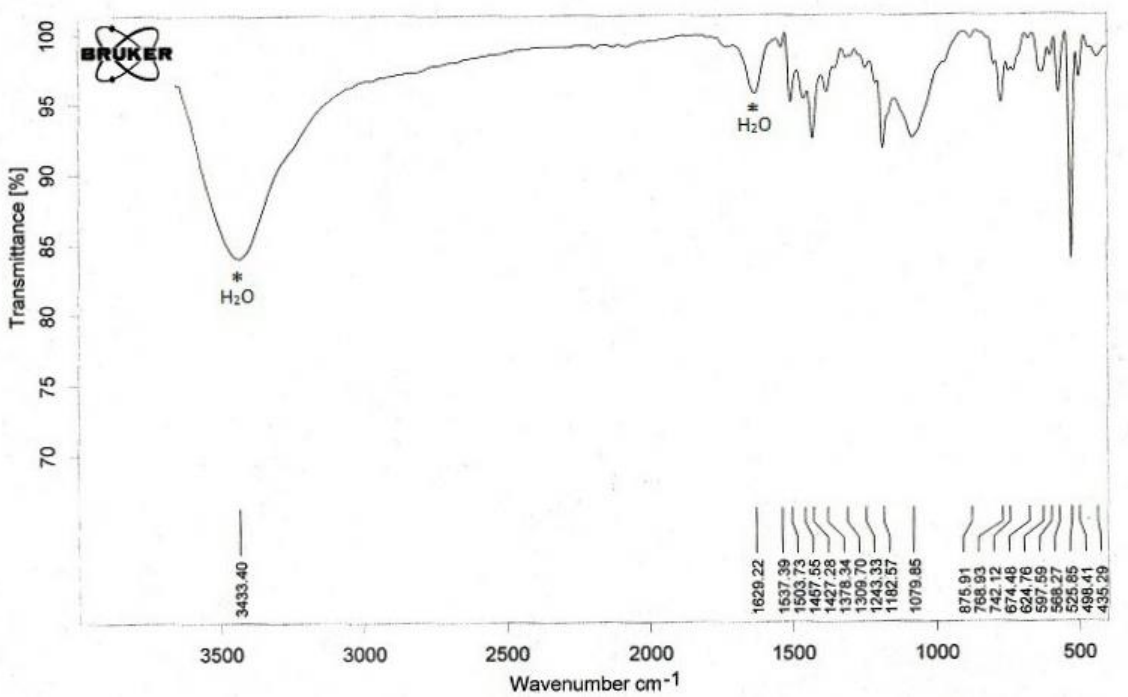

Figure S4. The IR spectrum of $C_{60}O$

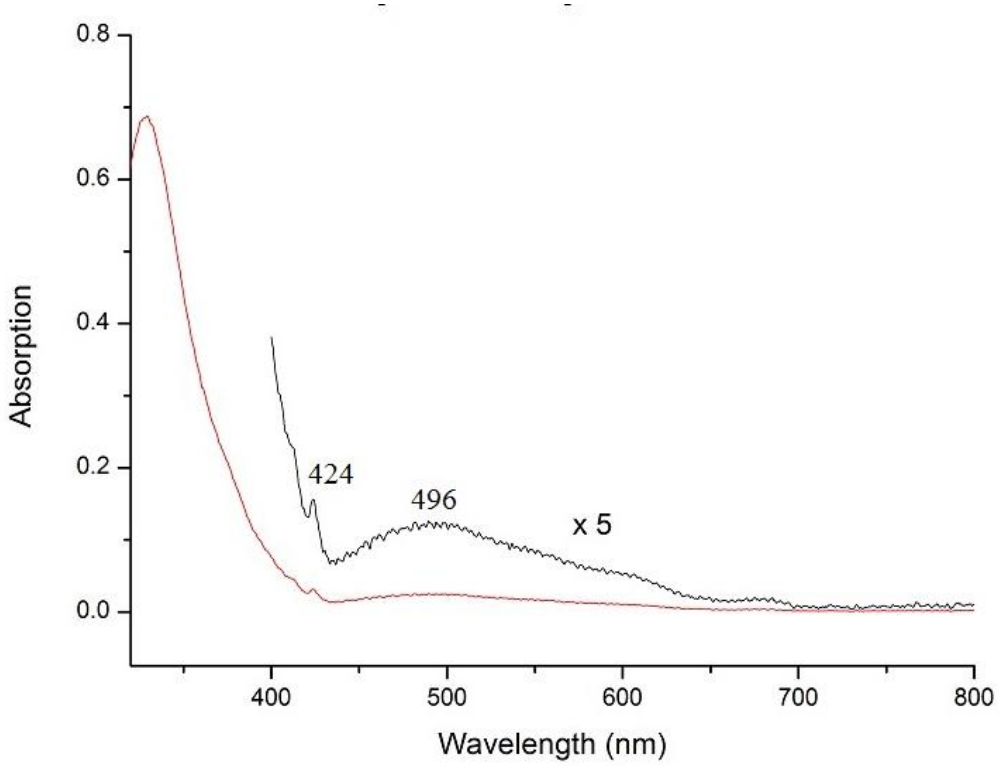

Figure S5. The UV-vis spectrum of $C_{60}O$ in toluene

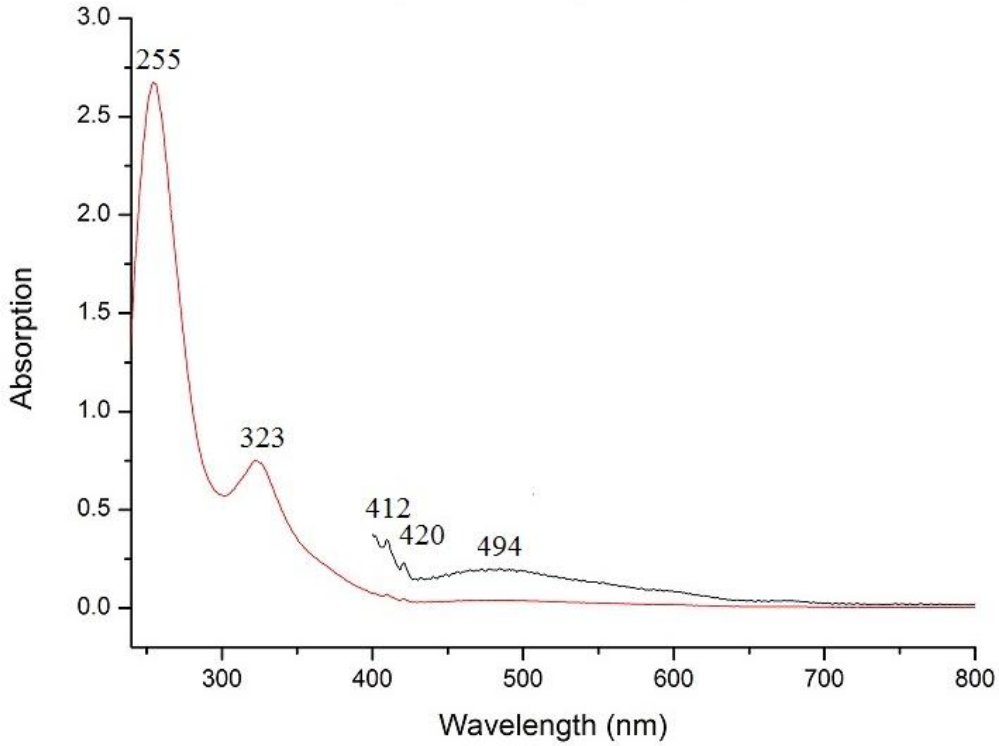

Figure S6. The UV-vis spectrum of $C_{60}O$ in $CHCl_3$

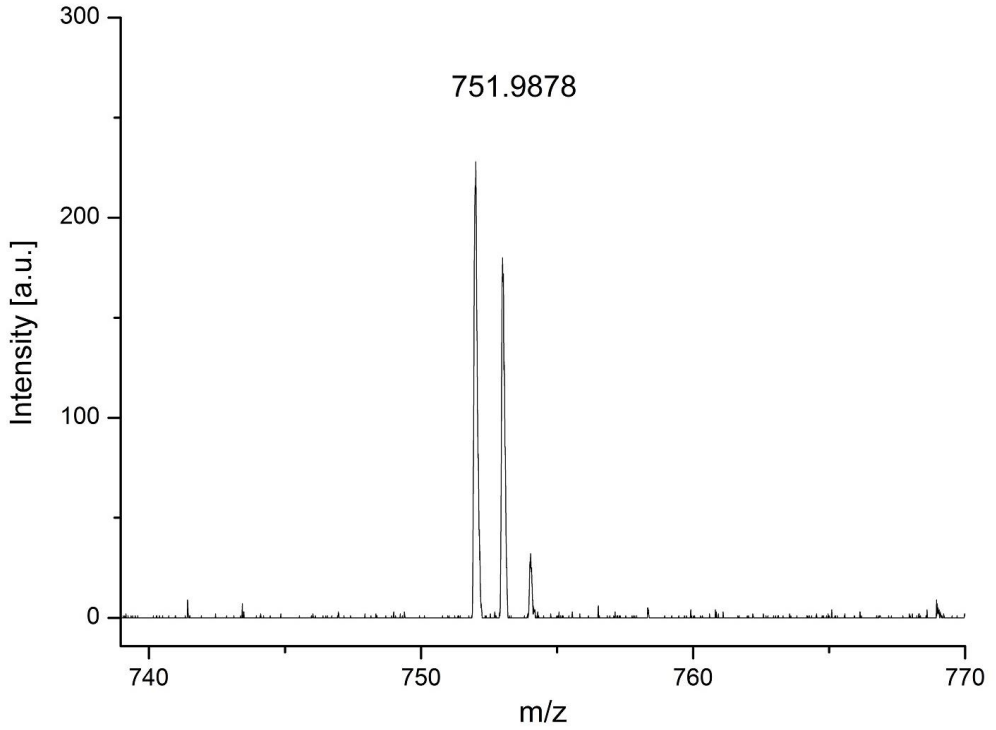

Figure S7. The HR-MS (MALDI-TOF) spectrum of $C_{60}O_2$

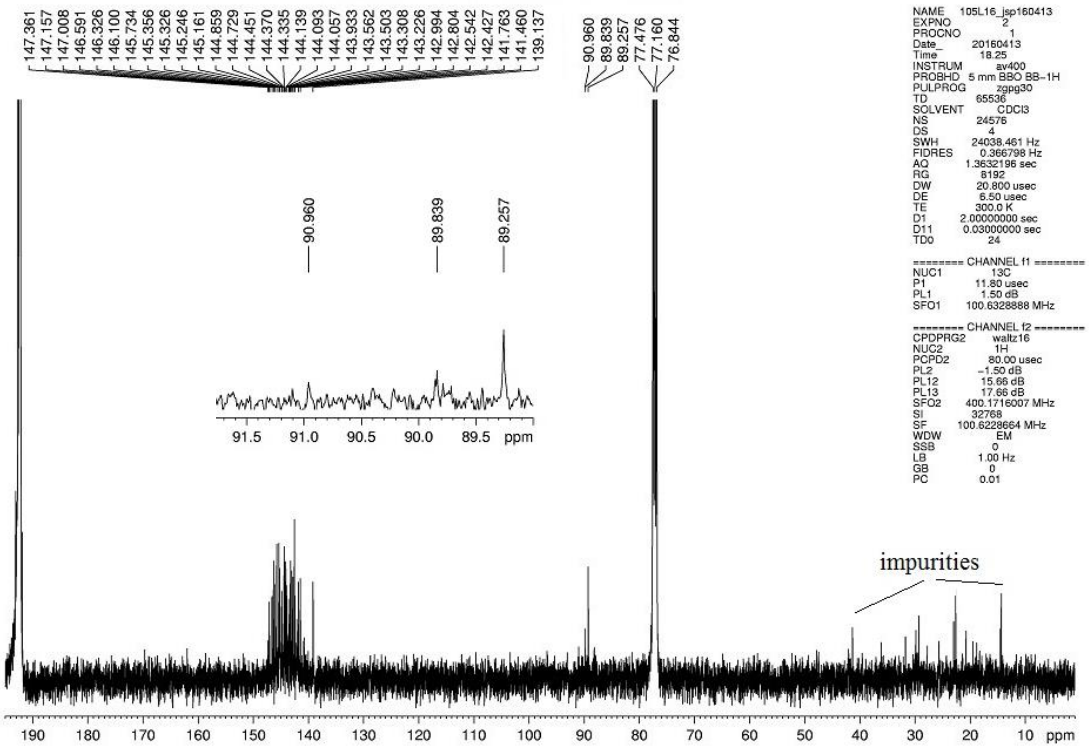

Figure S8. The ^{13}C NMR (100 MHz, $CS_2/CDCl_3$ with $Cr(acac)_3$ as a relaxation reagent) spectrum of $C_{60}O_2$

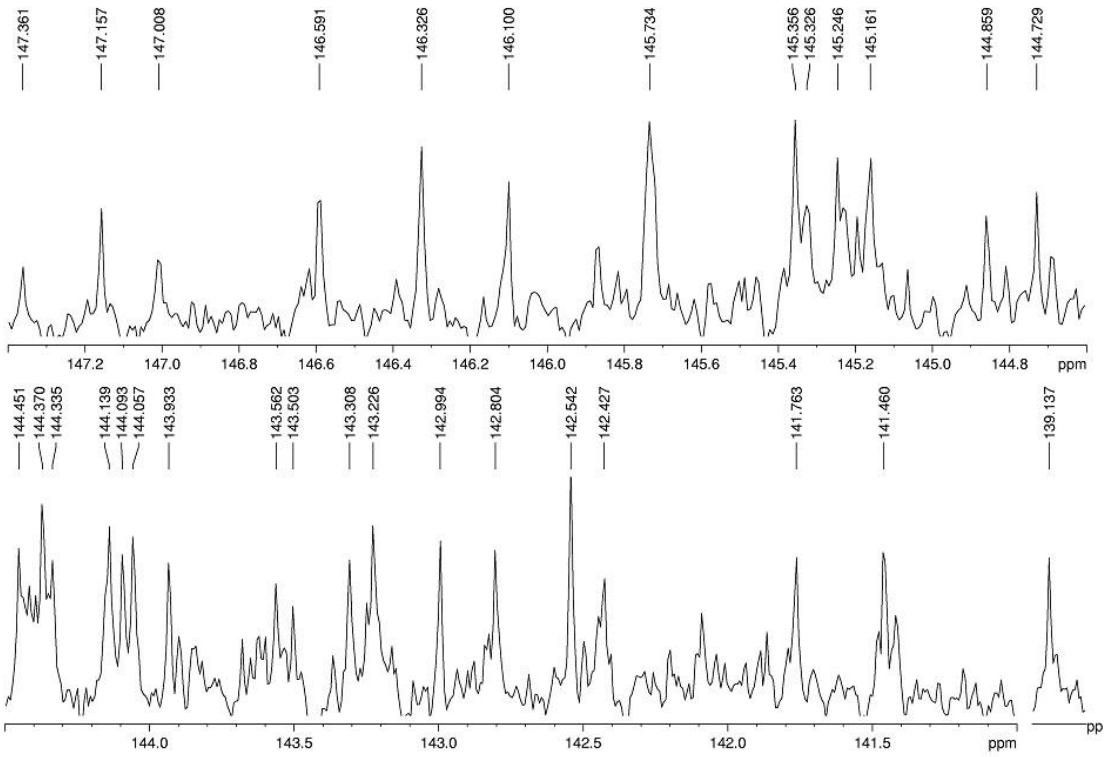

Figure S9. The expanded ^{13}C NMR (100 MHz, $CS_2/CDCl_3$ with $Cr(acac)_3$ as a relaxation reagent) spectrum of $C_{60}O_2$

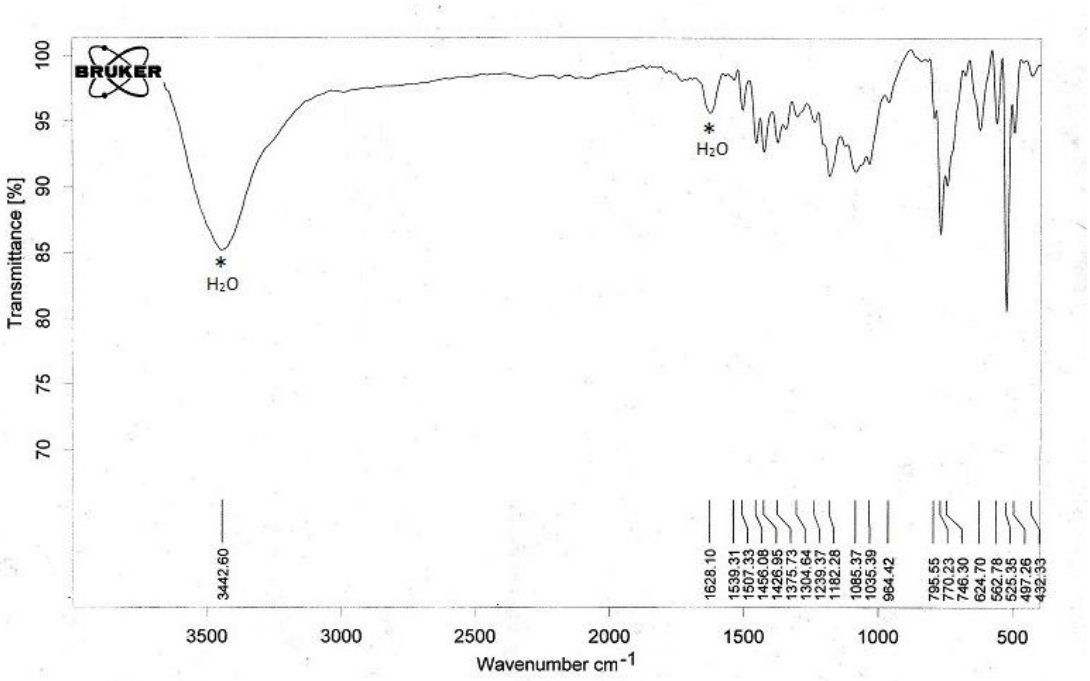

Figure S10. The IR spectrum of $C_{60}O_2$

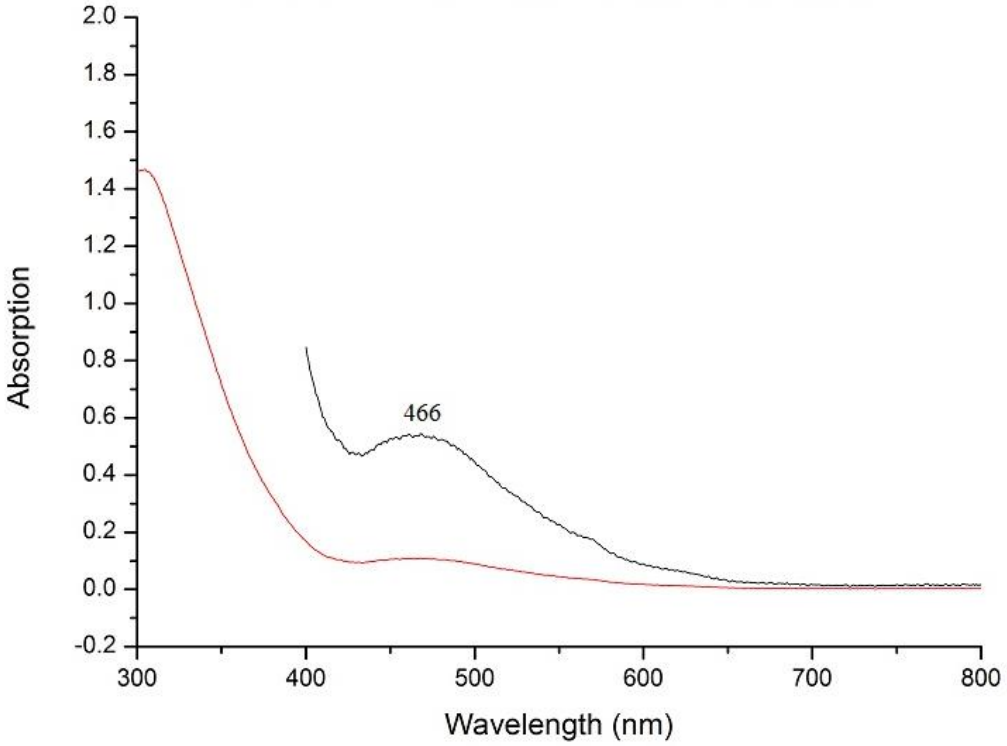

Figure S11. The UV-vis spectrum of $C_{60}O_2$ in toluene

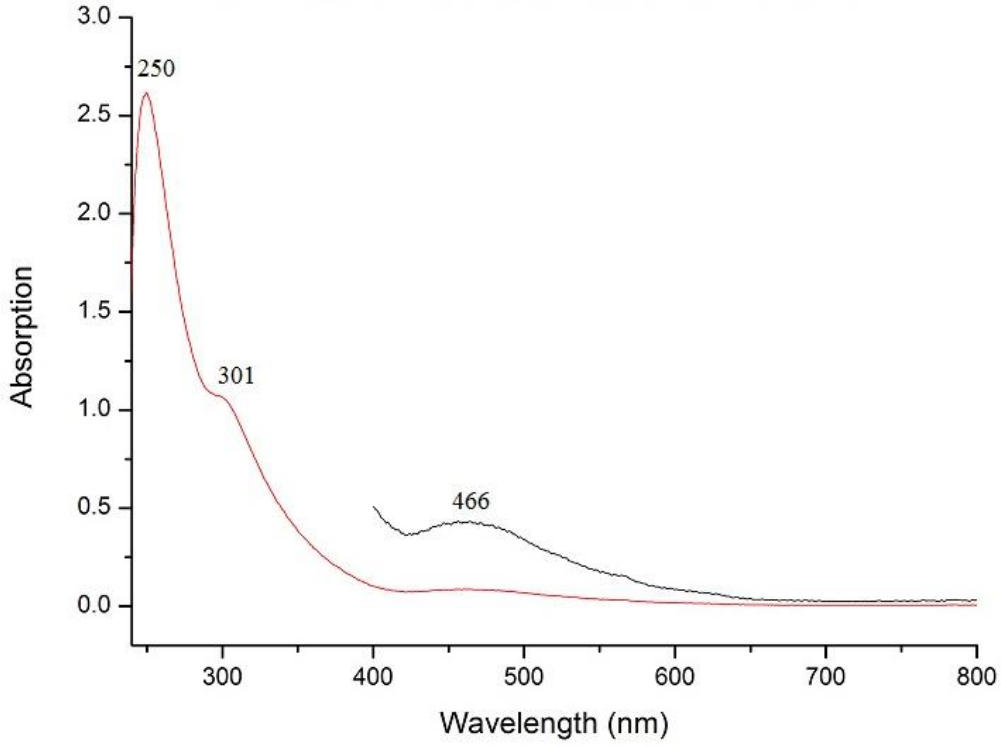

Figure S12. The UV-vis spectrum of $C_{60}O_2$ in $CHCl_3$

Recycling separation of $C_{60}O_2$

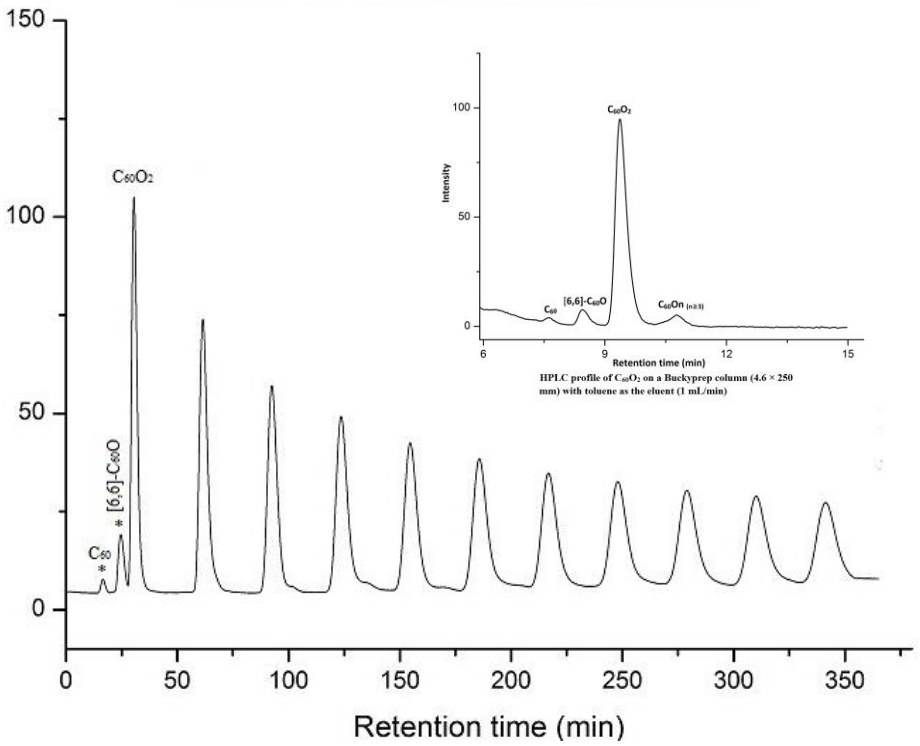

Figure S13. Recycling HPLC profile of $C_{60}O_2$ on a Buckyprep column (10 × 250 mm) with toluene as the eluent (5 mL/min)

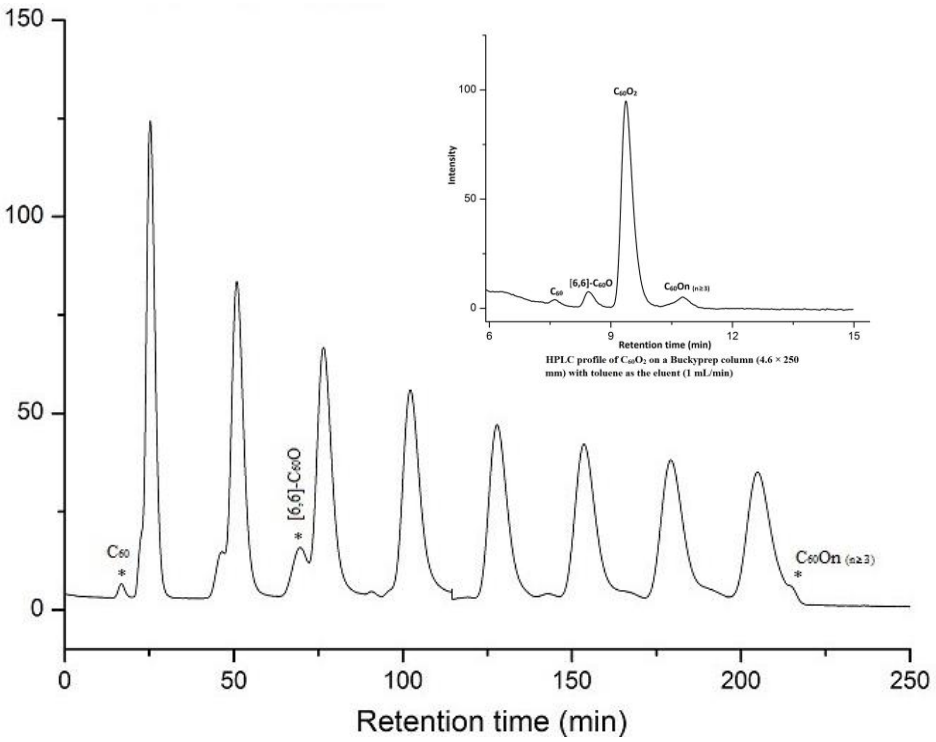

Figure S14. Recycling HPLC profile of $C_{60}O_2$ on a Buckyprep-M column (10 × 250 mm) with toluene as the eluent (5 mL/min)

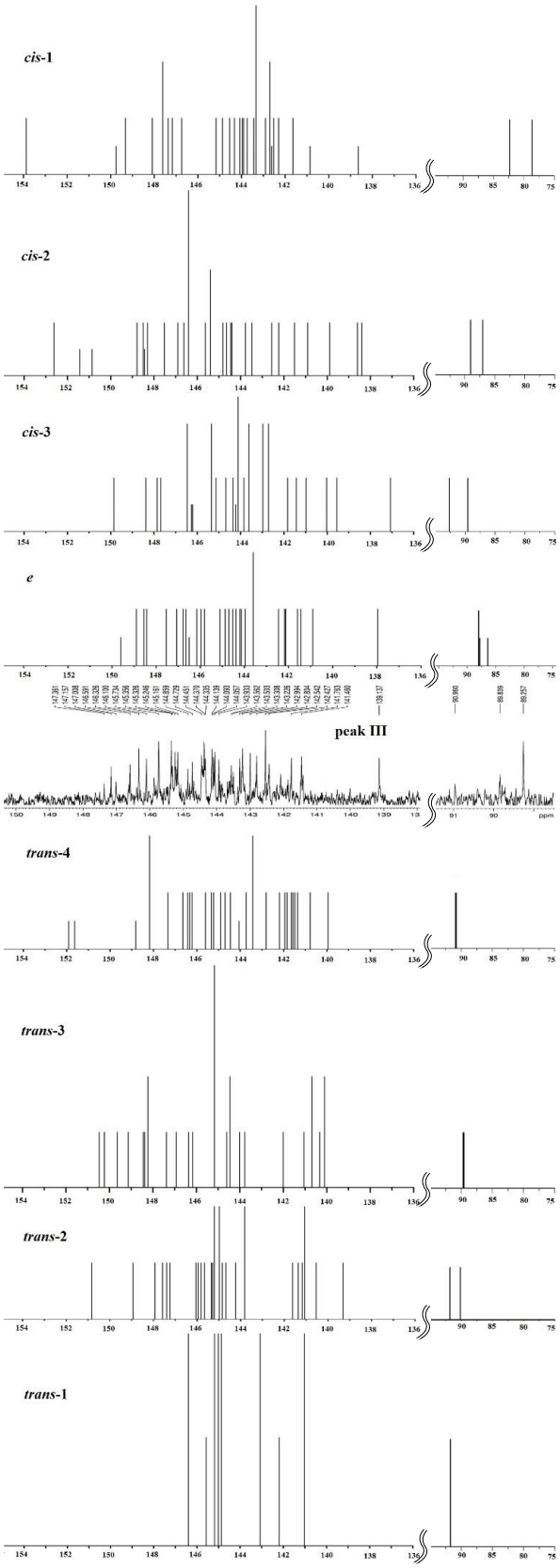

Figure S15. Comparison between calculated ^{13}C NMR spectra of $C_{60}O_2$ isomers and experimental ^{13}C NMR spectrum for peak **III**

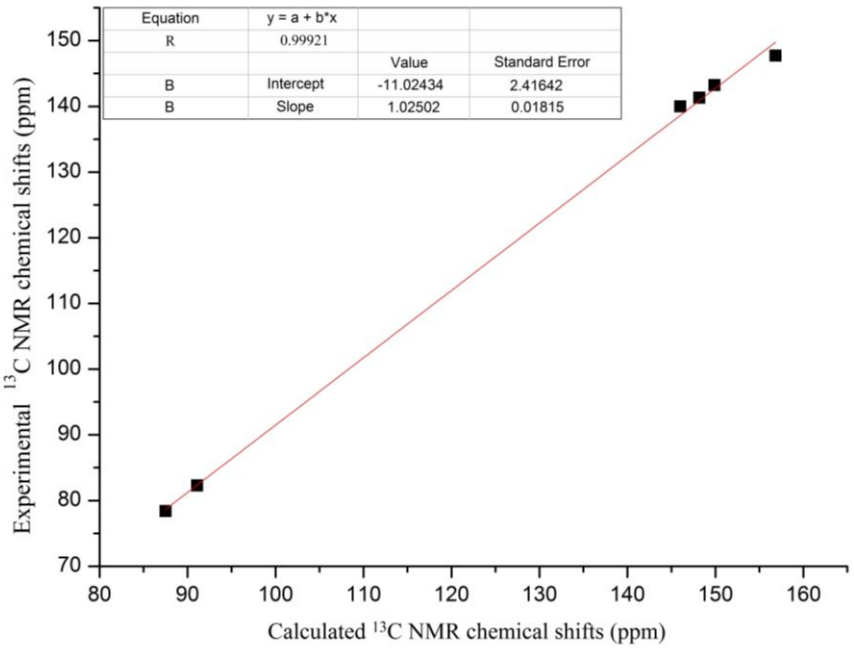

Figure S16. Linear correlation between experimental[1] and GIAO (B3LYP/6-311+ G (2df, 2pd)) calculated ^{13}C NMR data for *cis*-1 isomer of $C_{60}O_2$: $\delta_{(exp)}$ = 1.02502$\delta_{(cal)}$-11.02434 (R = 0.99921)

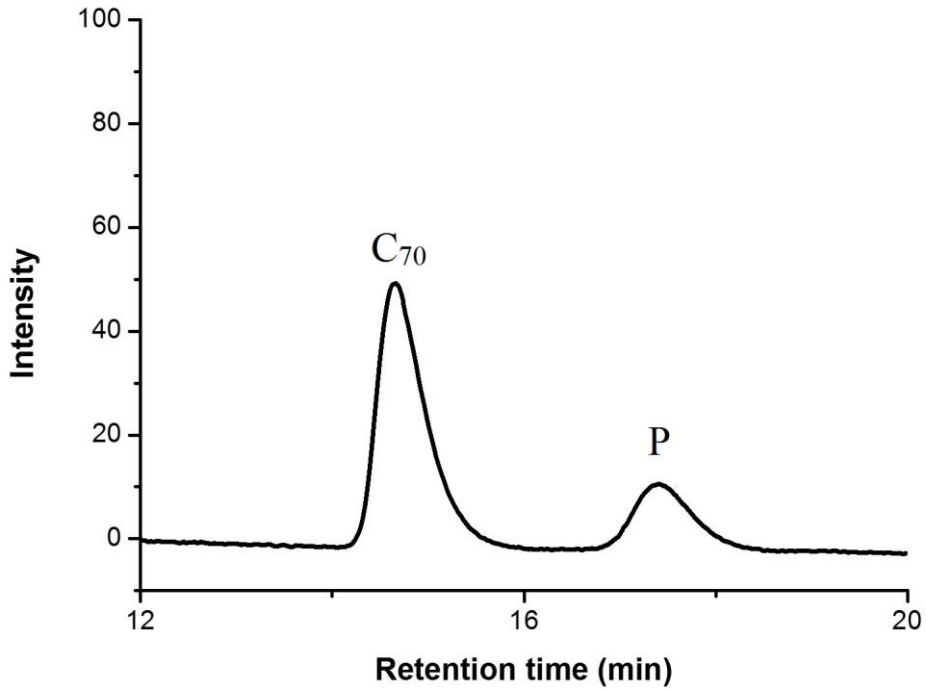

Figure S17. HPLC profile of C_{70} treated with plasma jet (Ar: 200 mL/min, O_2: 400 mL/min, 3.5 kV, 0 ºC, 15 min) on a Buckyprep column (4.6 × 250 mm) with toluene as the eluent (1 mL/min)

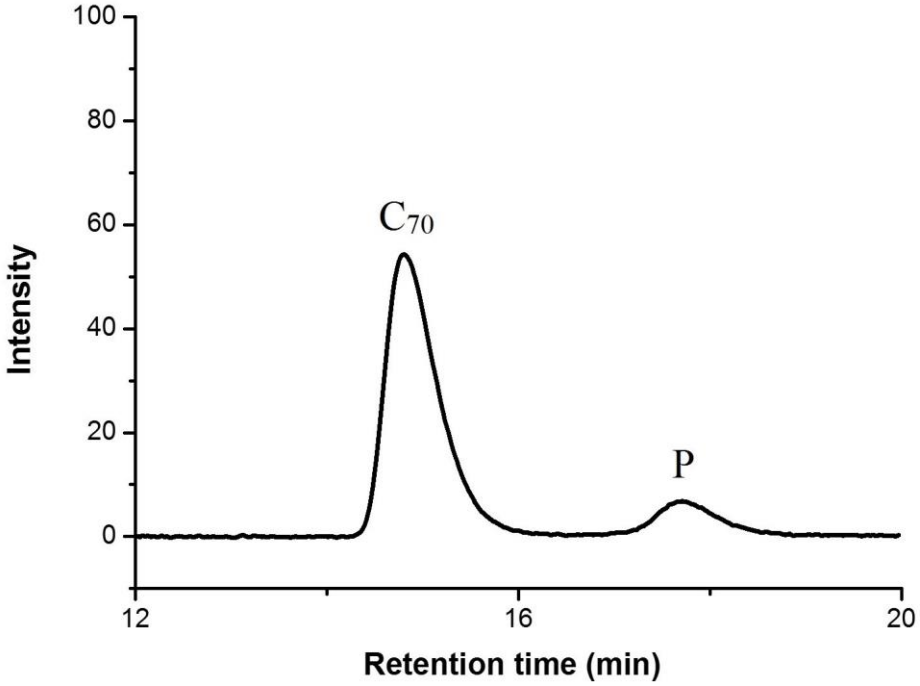

Figure S18. HPLC profile of C_{70} treated with plasma jet (Ar: 200 mL/min, O_2: 400 mL/min, 3.5 kV, 0 ^{o}C, 30 min) on a Buckyprep column (4.6 × 250 mm) with toluene as the eluent (1 mL/min)

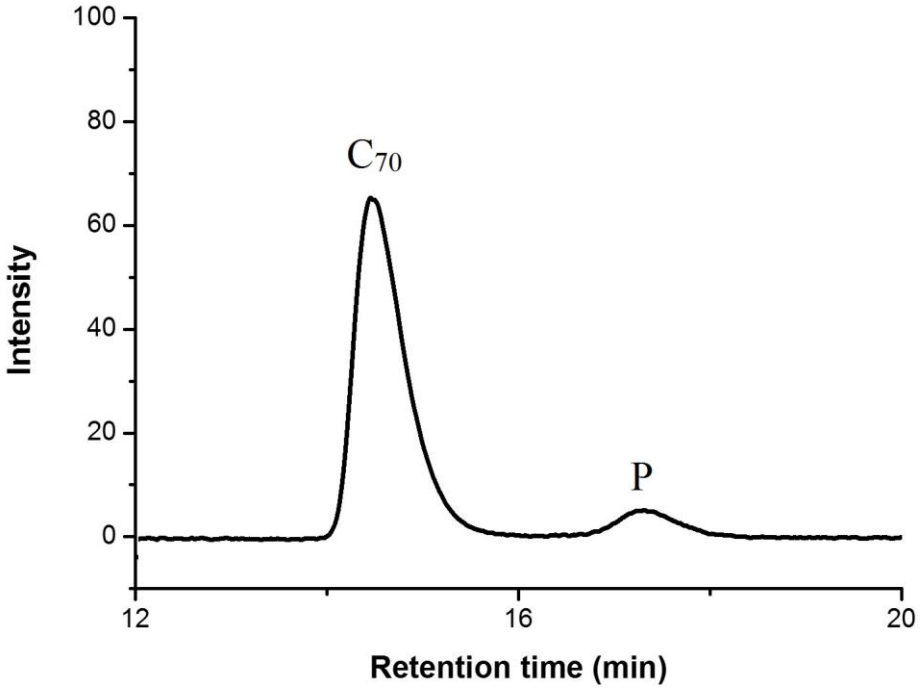

Figure S19. HPLC profile of C_{70} treated with plasma jet (Ar: 200 mL/min, O_2: 400 mL/min, 3.5 kV, –10 ^{o}C, 15 min) on a Buckyprep column (4.6 × 250 mm) with toluene as the eluent (1 mL/min)

The xyz coordinates for the structure of $C_{60}O_2$ (*cis*-1)

Charge = 0 Multiplicity = 1

C	2.58423	-0.99588	-2.30013
C	1.82872	0.01545	-3.02217
C	1.83007	1.34066	-2.57934
C	2.60067	1.7169	-1.40341
C	3.33269	0.74146	-0.71865
C	3.32216	-0.63958	-1.17228
C	1.80606	-2.21966	-2.304
C	0.57238	-1.96244	-3.03201
C	0.59279	-0.57984	-3.47575
C	-0.58283	0.17831	-3.47251
C	0.63169	2.13689	-2.62453
C	1.89752	2.75523	-0.69128
C	1.89752	2.75523	0.69128
C	2.60067	1.7169	1.40341
C	3.33269	0.74146	0.71865
C	3.32216	-0.63958	1.17228
C	3.31454	-1.49469	0.00000
C	2.56312	-2.67262	0.00000
C	1.79317	-3.04086	-1.17453
C	-0.62272	-2.53724	-2.59901

C	-0.63617	-3.39134	-1.42485
C	0.54688	-3.63811	-0.72613
C	0.54688	-3.63811	0.72613
C	1.79317	-3.04086	1.17453
C	1.80606	-2.21966	2.304
C	2.58423	-0.99588	2.30013
C	1.82872	0.01545	3.02217
C	1.83007	1.34066	2.57934
C	0.68406	3.11367	-1.49803
C	-1.8129	1.81068	2.29476
C	-1.82292	2.63503	1.18002
C	-2.54441	2.23031	0.00000
C	-3.31273	1.05802	0.00000
C	-3.32883	0.21604	1.17129
C	-1.82856	-0.42488	3.02101
C	-0.58283	0.17831	3.47251
C	-0.56443	1.55942	3.03324
C	0.63169	2.13689	2.62453
C	0.68406	3.11367	1.49803
C	-0.62051	3.4005	0.75671
C	-1.82292	2.63503	-1.18002
C	-1.8129	1.81068	-2.29476

C	-2.57968	0.58269	-2.29745
C	-3.32883	0.21604	-1.17129
C	-3.3498	-1.16606	-0.72878
C	-3.3498	-1.16606	0.72878
C	-2.62247	-2.1311	1.42264
C	-1.84949	-1.75306	2.59584
C	0.59279	-0.57984	3.47575
C	0.57238	-1.96244	3.03201
C	-0.62272	-2.53724	2.59901
C	-0.63617	-3.39134	1.42485
C	-1.87142	-3.13835	0.6979
C	-1.87142	-3.13835	-0.6979
C	-2.62247	-2.1311	-1.42264
C	-1.84949	-1.75306	-2.59584
C	-1.82856	-0.42488	-3.02101
C	-0.62051	3.4005	-0.75671
C	-0.56443	1.55942	-3.03324
C	-2.57968	0.58269	2.29745
O	0.04453	4.39121	1.51955
O	0.04453	4.39121	-1.51955

The xyz coordinates for the structure of $C_{60}O_2$ (*cis*-2)

Charge = 0 Multiplicity = 1

C	1.33859	2.6236	1.86904
C	2.02815	1.42346	2.37812
C	2.92215	0.71537	1.58223
C	3.3054	1.19881	0.22627
C	2.58949	2.44843	-0.30349
C	1.56823	3.08321	0.58117
C	-0.0086	2.60775	2.40138
C	-0.154	1.42605	3.23522
C	1.10556	0.7013	3.21479
C	1.10556	-0.7013	3.21479
C	2.92215	-0.71537	1.58223
C	3.37173	0.00000	-0.6514
C	2.81304	0.00000	-1.90145
C	2.11129	1.18885	-2.42171
C	1.97226	2.33862	-1.65417
C	0.70345	3.01701	-1.60872
C	0.45692	3.47261	-0.24767
C	-0.84604	3.47917	0.2593
C	-1.08303	3.03652	1.61442
C	-1.35991	0.72801	3.25441
C	-2.47472	1.17581	2.43848

C	-2.33946	2.30818	1.63382
C	-2.87886	2.30573	0.28355
C	-1.95295	3.03115	-0.56787
C	-1.71718	2.59855	-1.8727
C	-0.36618	2.59277	-2.4028
C	-0.21007	1.42283	-3.23508
C	1.00326	0.72743	-3.22954
C	3.3054	-1.19881	0.22627
C	-0.36618	-2.59277	-2.4028
C	0.70345	-3.01701	-1.60872
C	0.45692	-3.47261	-0.24766
C	-0.84604	-3.47917	0.25931
C	-1.95295	-3.03115	-0.56786
C	-2.40189	-1.42271	-2.38518
C	-1.47051	-0.69725	-3.2292
C	-0.21007	-1.42283	-3.23508
C	1.00326	-0.72743	-3.22954
C	2.11129	-1.18885	-2.42171
C	1.97226	-2.33863	-1.65417
C	1.56823	-3.08321	0.58117
C	1.33859	-2.6236	1.86904
C	-0.0086	-2.60774	2.40138

C	-1.08303	-3.03652	1.61442
C	-2.33946	-2.30818	1.63383
C	-2.87886	-2.30573	0.28355
C	-3.53511	-1.17516	-0.2058
C	-3.29379	-0.72546	-1.56706
C	-1.47051	0.69725	-3.2292
C	-2.40189	1.42271	-2.38518
C	-3.29379	0.72545	-1.56706
C	-3.53511	1.17516	-0.2058
C	-3.68135	0.00000	0.63468
C	-3.15998	0.00000	1.93083
C	-2.47472	-1.1758	2.43848
C	-1.35991	-0.72801	3.25441
C	-0.154	-1.42605	3.23522
C	2.58949	-2.44843	-0.30349
C	2.02815	-1.42346	2.37812
C	-1.71718	-2.59856	-1.8727
O	3.98689	2.42271	-0.03568
O	3.98689	-2.42271	-0.03568

The xyz coordinates for the structure of $C_{60}O_2$ (*cis*-3)

Charge = 0 Multiplicity = 1

C	-0.56087	-3.39237	0.76438
C	-1.01835	-2.69034	1.97853
C	-2.14318	-1.8794	1.95659
C	-2.99765	-1.75443	0.74373
C	-2.51925	-2.49575	-0.52711
C	-1.24793	-3.26715	-0.43442
C	0.88779	-3.37931	0.76926
C	1.3356	-2.6911	1.96912
C	0.16187	-2.26855	2.7105
C	0.17424	-1.04685	3.38927
C	-2.11573	-0.59221	2.60863
C	-3.35332	-0.31275	0.61204
C	-3.35361	0.31208	-0.61184
C	-2.84861	-0.37119	-1.80658
C	-2.43696	-1.69583	-1.77586
C	-1.23974	-2.09042	-2.47455
C	-0.51438	-3.05017	-1.65716
C	0.88275	-3.05247	-1.66721
C	1.59955	-3.22226	-0.42483
C	2.47097	-1.88058	1.93035
C	3.20329	-1.71324	0.68488
C	2.77698	-2.37118	-0.46844

C	2.78207	-1.67526	-1.74529
C	1.61062	-2.09832	-2.4888
C	0.91299	-1.18115	-3.27511
C	-0.53921	-1.18136	-3.26914
C	-0.98913	0.18979	-3.337
C	-2.11587	0.59162	-2.60839
C	-2.84872	0.3701	1.80699
C	-0.56198	3.39234	-0.76434
C	-1.24895	3.26671	0.43457
C	-0.51528	3.05008	1.65701
C	0.8818	3.05292	1.66697
C	1.59847	3.22265	0.42483
C	1.3346	2.69151	-1.96909
C	0.16093	2.26868	-2.71047
C	-1.0191	2.69005	-1.97885
C	-2.14362	1.87827	-1.95666
C	-2.99814	1.75381	-0.74422
C	-2.52004	2.49526	0.52777
C	-1.2402	2.08996	2.47437
C	-0.53958	1.18092	3.26905
C	0.91282	1.18136	3.27501
C	1.61004	2.09861	2.48888

C	2.78157	1.67599	1.74511
C	2.77632	2.37208	0.46832
C	3.20275	1.71421	-0.68495
C	2.47008	1.88126	-1.93032
C	0.17368	1.0467	-3.38923
C	1.35509	0.20065	-3.34964
C	2.48073	0.60838	-2.63151
C	3.20863	-0.34664	-1.81591
C	3.65312	0.33633	-0.61212
C	3.65331	-0.33527	0.61211
C	3.2087	0.34754	1.81587
C	2.48106	-0.60769	2.63135
C	1.3552	-0.20035	3.34962
C	-2.43692	1.69505	1.77608
C	-0.98908	-0.18987	3.33697
C	0.88655	3.37972	-0.76938
O	-3.72308	-2.82396	0.15288
O	-3.72346	2.82307	-0.15268

The xyz coordinates for the structure of $C_{60}O_2$ (*e*)

Charge = 0 Multiplicity = 1

C	0.23554	2.56308	2.29968

C	1.62877	2.08008	2.30205
C	2.44629	2.25752	1.19523
C	1.98653	3.02426	0.
C	0.53305	3.5269	0.
C	-0.30287	3.21243	1.19361
C	-0.56091	1.59884	3.01505
C	0.30668	0.52309	3.46542
C	1.65593	0.82135	3.0215
C	2.48958	-0.21997	2.59743
C	3.26481	1.16973	0.7287
C	2.44629	2.25752	-1.19523
C	1.62877	2.08008	-2.30205
C	0.23554	2.56308	-2.29968
C	-0.30287	3.21243	-1.19361
C	-1.62701	2.88564	-0.73789
C	-1.62701	2.88564	0.73789
C	-2.42044	1.99448	1.45199
C	-1.86046	1.31041	2.57943
C	-0.15539	-0.79128	3.4744
C	-1.50632	-1.09108	3.02605
C	-2.34303	-0.06396	2.58527
C	-3.21356	-0.25694	1.45309

C	-3.35897	1.05937	0.76818
C	-3.35897	1.05937	-0.76818
C	-2.42044	1.99448	-1.45199
C	-1.86046	1.31041	-2.57943
C	-0.56091	1.59884	-3.01505
C	3.26481	1.16973	-0.7287
C	0.70958	-1.87152	-3.03193
C	2.00762	-1.5911	-2.60193
C	2.53997	-2.2589	-1.4264
C	1.75297	-3.17713	-0.72778
C	0.40446	-3.46584	-1.17608
C	-1.47832	-2.342	-2.30745
C	-1.50632	-1.09108	-3.02605
C	-0.15539	-0.79128	-3.4744
C	0.30668	0.52309	-3.46542
C	1.65593	0.82135	-3.0215
C	2.48958	-0.21997	-2.59743
C	3.35042	-1.29975	-0.69703
C	3.35042	-1.29975	0.69703
C	2.53997	-2.2589	1.4264
C	1.75297	-3.17713	0.72778
C	0.40446	-3.46584	1.17608

C	-0.43264	-3.6413	0.00000
C	-1.74569	-3.1706	0.00000
C	-2.28569	-2.51058	-1.1766
C	-2.34303	-0.06396	-2.58527
C	-3.21356	-0.25694	-1.45309
C	-3.16398	-1.44492	-0.73838
C	-3.16398	-1.44492	0.73838
C	-2.28569	-2.51058	1.1766
C	-1.47832	-2.342	2.30745
C	-0.10778	-2.82786	2.30685
C	0.70958	-1.87152	3.03193
C	2.00762	-1.5911	2.60193
C	3.31303	-0.04207	-1.42438
C	3.31303	-0.04207	1.42438
C	-0.10778	-2.82786	-2.30685
O	1.65154	4.4063	0.00000
O	-4.48888	1.45759	0.00000

The xyz coordinates for the structure of $C_{60}O_2$ (*trans*-4)

Charge = 0 Multiplicity = 1

C	-0.60389	0.45963	3.49148
C	-1.82954	-0.22599	3.04025

C	-1.79483	-1.54945	2.62506
C	-0.54413	-2.36149	2.69689
C	0.73271	-1.64372	3.16726
C	0.61658	-0.19833	3.51215
C	-0.67445	1.83271	3.03062
C	-1.91987	2.00553	2.30241
C	-2.62864	0.73824	2.3092
C	-3.35324	0.34526	1.17737
C	-2.49541	-1.938	1.42802
C	-0.46259	-3.12964	1.42159
C	0.73296	-3.26908	0.72257
C	1.95365	-2.57876	1.17768
C	1.94667	-1.77903	2.31045
C	2.60758	-0.49627	2.28672
C	1.79712	0.46569	3.01588
C	1.74505	1.79656	2.59202
C	0.47924	2.49425	2.59804
C	-1.96368	2.82744	1.17535
C	-0.76068	3.51143	0.7251
C	0.43606	3.35062	1.42487
C	1.68318	3.18254	0.69842
C	2.4949	2.2197	1.42236

C	3.27527	1.29716	0.72517
C	3.33578	-0.08673	1.16777
C	3.37383	-0.937	0.
C	2.68686	-2.15874	0.
C	-1.67668	-2.89646	0.69975
C	0.73271	-1.64372	-3.16726
C	-0.54413	-2.36149	-2.69689
C	-1.79483	-1.54945	-2.62506
C	-1.82954	-0.22599	-3.04025
C	-0.60389	0.45963	-3.49148
C	1.79712	0.46569	-3.01588
C	2.60758	-0.49627	-2.28672
C	1.94667	-1.77903	-2.31045
C	1.95365	-2.57876	-1.17768
C	0.73296	-3.26908	-0.72257
C	-0.46259	-3.12964	-1.42159
C	-2.49541	-1.938	-1.42802
C	-3.28469	-1.02446	-0.7271
C	-3.35324	0.34526	-1.17737
C	-2.62864	0.73824	-2.3092
C	-1.91987	2.00553	-2.30241
C	-0.67445	1.83271	-3.03062

C	0.47924	2.49425	-2.59804
C	1.74505	1.79656	-2.59202
C	3.33578	-0.08673	-1.16777
C	3.27527	1.29716	-0.72517
C	2.4949	2.2197	-1.42236
C	1.68318	3.18254	-0.69842
C	0.43606	3.35062	-1.42487
C	-0.76068	3.51143	-0.7251
C	-1.96368	2.82744	-1.17535
C	-2.70981	2.41313	0.
C	-3.39439	1.19814	0.
C	-1.67668	-2.89646	-0.69975
C	-3.28469	-1.02446	0.7271
C	0.61658	-0.19833	-3.51215
O	0.13299	-2.70532	3.89898
O	0.13299	-2.70532	-3.89898

The xyz coordinates for the structure of $C_{60}O_2$ (*trans*-3)

Charge = 0 Multiplicity = 1

C	-2.99771	0.10821	-1.90986
C	-2.30446	-1.084	-2.42832
C	-2.16659	-2.22594	-1.65386

C	-2.78488	-2.32997	-0.29923
C	-3.50639	-1.08216	0.24429
C	-3.5292	0.12636	-0.6282
C	-2.30419	1.27662	-2.41816
C	-1.19668	0.82774	-3.24082
C	-1.19334	-0.62641	-3.24047
C	0.02257	-1.31646	-3.23153
C	-0.89616	-2.90571	-1.60615
C	-1.76396	-2.96230	0.58417
C	-1.53133	-2.507	1.87236
C	-2.22213	-1.31427	2.39429
C	-3.12552	-0.61292	1.60799
C	-3.07779	0.826	1.57651
C	-3.325	1.27719	0.21477
C	-2.67751	2.41575	-0.27038
C	-2.15651	2.41576	-1.61781
C	0.00726	1.53075	-3.24237
C	0.15907	2.7135	-2.40836
C	-0.90163	3.14667	-1.61158
C	-0.65095	3.59988	-0.25262
C	-1.75084	3.14666	0.57859
C	-1.50997	2.71321	1.88213

C	-2.18973	1.53208	2.3929
C	-1.2695	0.80569	3.23335
C	-1.28	-0.59305	3.22773
C	-0.65345	-3.34834	-0.24976
C	2.30473	-1.08576	2.42759
C	2.16685	-2.22694	1.65198
C	2.78566	-2.32939	0.29774
C	3.50654	-1.08127	-0.24599
C	3.52934	0.12627	0.62821
C	2.30385	1.27476	2.41923
C	1.19647	0.82496	3.24156
C	1.19345	-0.62918	3.24006
C	-0.0223	-1.31957	3.23042
C	-0.17887	-2.48847	2.39587
C	0.8968	-2.90717	1.60344
C	1.76523	-2.96133	-0.58685
C	1.53197	-2.50466	-1.87444
C	2.22241	-1.31145	-2.39577
C	3.12544	-0.61038	-1.60879
C	3.07754	0.82842	-1.57572
C	3.32473	1.27808	-0.21346
C	2.67692	2.41605	0.27263

C	2.15585	2.41463	1.62003
C	-0.00766	1.52763	3.24377
C	-0.1598	2.71109	2.41083
C	0.90083	3.14529	1.61452
C	0.6501	3.59974	0.25598
C	1.75009	3.14757	-0.57565
C	1.50923	2.71543	-1.87963
C	2.18929	1.53496	-2.39152
C	1.26929	0.80911	-3.23266
C	1.28007	-0.58963	-3.2284
C	0.65457	-3.34845	0.24655
C	0.1795	-2.48605	-2.398
C	2.99757	0.10697	1.90974
O	-4.18202	-2.30104	-0.03732
O	4.18263	-2.30004	0.03516

The xyz coordinates for the structure of $C_{60}O_2$ (*trans*-2)

Charge = 0 Multiplicity = 1

C	3.20434	1.48765	0.60677
C	2.95582	0.74832	1.85889
C	2.96514	-0.63975	1.88406
C	3.31699	-1.4413	0.67577

C	3.5807	-0.66731	-0.63091
C	3.45755	0.81795	-0.58114
C	2.34219	2.65317	0.60761
C	1.57053	2.64923	1.83765
C	1.94936	1.47481	2.60564
C	0.97805	0.78459	3.34035
C	1.93049	-1.34864	2.59218
C	2.34394	-2.56844	0.61699
C	1.76567	-2.96985	-0.57716
C	2.01921	-2.22972	-1.82919
C	2.84339	-1.11342	-1.84759
C	2.43436	0.06724	-2.56781
C	2.8066	1.24241	-1.79554
C	1.98621	2.37413	-1.81099
C	1.74893	3.09589	-0.58003
C	0.24669	3.08968	1.83544
C	-0.36893	3.54357	0.59793
C	0.36927	3.5457	-0.58496
C	-0.24638	3.09652	-1.82403
C	0.75935	2.37516	-2.58562
C	0.40075	1.2509	-3.32781
C	1.25752	0.07578	-3.32231

C	0.41521	-1.09667	-3.32949
C	0.78582	-2.22261	-2.58904
C	1.54736	-2.5208	1.818
C	-2.3445	-2.56581	-0.62613
C	-1.7662	-2.97148	0.5662
C	-2.01966	-2.23646	1.82124
C	-2.84353	-1.12004	1.84369
C	-3.58123	-0.66968	0.62885
C	-2.96474	-0.63236	-1.88647
C	-1.93066	-1.33879	-2.59707
C	-1.54751	-2.51373	-1.82729
C	-0.21891	-2.94381	-1.82632
C	0.38088	-3.40051	-0.59437
C	-0.3812	-3.40267	0.58192
C	-0.78619	-2.23218	2.58088
C	-0.41535	-1.10898	3.32534
C	-1.25737	0.06347	3.32234
C	-2.43428	0.05791	2.56791
C	-2.80646	1.23588	1.79989
C	-3.45735	0.81595	0.5843
C	-3.20395	1.49009	-0.60119
C	-2.95562	0.75572	-1.85631

C	-0.96743	-0.64851	-3.33642
C	-0.97789	0.79696	-3.33731
C	-1.94921	1.48463	-2.60011
C	-1.57023	2.6563	-1.82777
C	-2.34217	2.65585	-0.59792
C	-1.7487	3.09398	0.59144
C	-1.9859	2.36747	1.81949
C	-0.75903	2.36554	2.59425
C	-0.4005	1.2386	3.33235
C	0.21845	-2.95059	1.81531
C	0.96741	-0.66109	3.33396
C	-3.31689	-1.43803	-0.68118
O	4.58476	-1.42443	0.03271
O	-4.58494	-1.42392	-0.03808

The xyz coordinates for the structure of $C_{60}O_2$ (*trans*-1)

Charge = 0 Multiplicity = 1

C	2.60921	0.7399	2.29778
C	2.60921	-0.7399	2.29778
C	3.0535	-1.45244	1.19572
C	3.62739	-0.76961	0.00000
C	3.62739	0.76961	0.00000

C	3.0535	1.45244	1.19572
C	1.42881	1.17894	3.01273
C	0.69717	0.00000	3.45308
C	1.42881	-1.17894	3.01273
C	0.72666	-2.30857	2.59567
C	2.29913	-2.58814	0.73009
C	3.0535	-1.45244	-1.19572
C	2.60921	-0.7399	-2.29778
C	2.60921	0.7399	-2.29778
C	3.0535	1.45244	-1.19572
C	2.29913	2.58814	-0.73009
C	2.29913	2.58814	0.73009
C	1.17188	3.03578	1.42266
C	0.72666	2.30857	2.59567
C	-0.69717	0.00000	3.45308
C	-1.42881	1.17894	3.01273
C	-0.72666	2.30857	2.59567
C	-1.17188	3.03578	1.42266
C	0.00000	3.48744	0.6942
C	0.00000	3.48744	-0.6942
C	1.17188	3.03578	-1.42266
C	0.72666	2.30857	-2.59567

C	1.42881	1.17894	-3.01273
C	2.29913	-2.58814	-0.73009
C	-1.42881	-1.17894	-3.01273
C	-0.72666	-2.30857	-2.59567
C	-1.17188	-3.03578	-1.42266
C	-2.29913	-2.58814	-0.73009
C	-3.0535	-1.45244	-1.19572
C	-2.60921	0.7399	-2.29778
C	-1.42881	1.17894	-3.01273
C	-0.69717	0.00000	-3.45308
C	0.69717	0.00000	-3.45308
C	1.42881	-1.17894	-3.01273
C	0.72666	-2.30857	-2.59567
C	0.00000	-3.48744	-0.6942
C	0.0000	-3.48744	0.6942
C	-1.17188	-3.03578	1.42266
C	-2.29913	-2.58814	0.73009
C	-3.0535	-1.45244	1.19572
C	-3.62739	-0.76961	0.00000
C	-3.62739	0.76961	0.00000
C	-3.0535	1.45244	-1.19572
C	-0.72666	2.30857	-2.59567

C	-1.17188	3.03578	-1.42266
C	-2.29913	2.58814	-0.73009
C	-2.29913	2.58814	0.73009
C	-3.0535	1.45244	1.19572
C	-2.60921	0.7399	2.29778
C	-2.60921	-0.7399	2.29778
C	-1.42881	-1.17894	3.01273
C	-0.72666	-2.30857	2.59567
C	1.17188	-3.03578	-1.42266
C	1.17188	-3.03578	1.42266
C	-2.60921	-0.7399	-2.29778
O	4.82305	0.00000	0.00000
O	-4.82305	0.00000	0.00000

Reference

1 Only two peaks for the 2 sp^3-carbons and four peaks for the half-intensity sp^3-carbons of the C_{60} skeleton were given in the literature: Balch AL, Costa DA, Noll BC, Olmstead MM. 1995 Oxidation of buckminsterfullerene with *m*-chloroperoxybenzoic acid, Characterization of a C_s isomer of the diepoxide $C_{60}O_2$. *J. Am. Chem. Soc.* **117**, 8926–8931. (doi:10.1021/ja00140a005)