Core-hole excitation spectra of the oxides and reactions involving water of fullerene C_{60} and azafullerene $C_{59}N$

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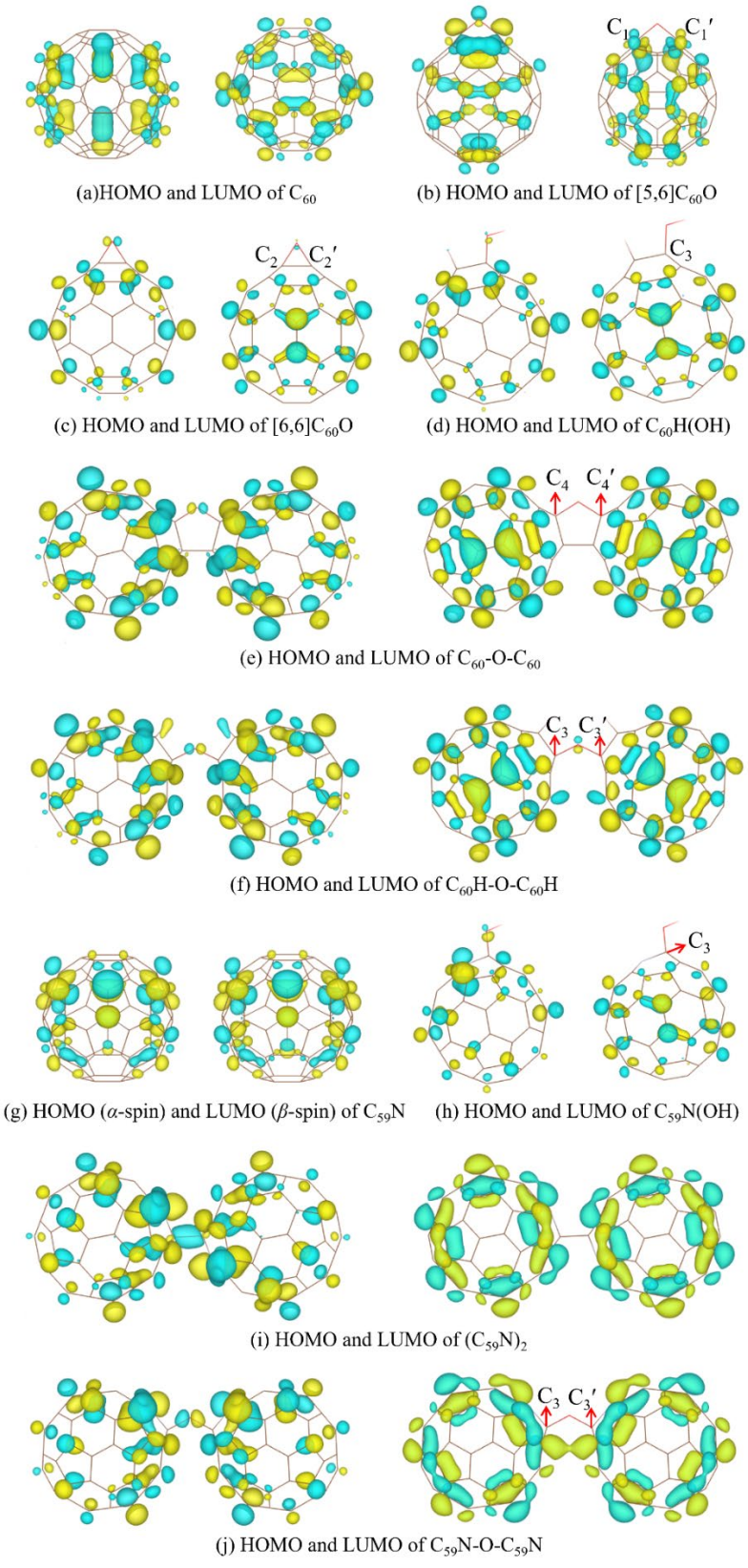

(a)HOMO and LUMO of C_{60} (b) HOMO and LUMO of $[5,6]C_{60}O$

(c) HOMO and LUMO of $[6,6]C_{60}O$ (d) HOMO and LUMO of $C_{60}H(OH)$

(e) HOMO and LUMO of C_{60}-O-C_{60}

(f) HOMO and LUMO of $C_{60}H$-O-$C_{60}H$

(g) HOMO (α-spin) and LUMO (β-spin) of $C_{59}N$ (h) HOMO and LUMO of $C_{59}N(OH)$

(i) HOMO and LUMO of $(C_{59}N)_2$

(j) HOMO and LUMO of $C_{59}N$-O-$C_{59}N$

Figure S1. The HOMOs and LUMOs of the fullerene C_{60}, aza[60]fullerene, their oxides, and reactions involving H_2O calculated at B3LYP/6-311+G* level. The carbon atoms C_1 and C_1', C_2 and C_2', C_3 and C_3', C_4 and C_4', which were connected to the oxygen atom, were symmetrically equivalent.

B. Supplementary Tables

Table S1. MO transitions and the corresponding energies for peak or shoulder A in the nitrogen *K*-edge NEXAFS of the $C_{59}N$, $C_{59}N(OH)$, $(C_{59}N)_2$, and $C_{59}N$-O-$C_{59}N$ molecules.

Molecule	MO transition of peak (shoulder) A	Energy of peak (shoulder) A (eV)
$C_{59}N$	$1s \rightarrow$ LUMO (β spin)	399.96
$C_{59}N(OH)$	$1s \rightarrow$ LUMO	399.97
$(C_{59}N)_2$	$1s \rightarrow$ LUMO	399.94
$C_{59}N$-O-$C_{59}N$	$1s \rightarrow$ LUMO	399.95

Table S2. MO transitions and the corresponding energies for peak A in the oxygen *K*-edge XES of the open [5,6] and closed [6,6] isomers of $C_{60}O$, $C_{59}N(OH)$, and $C_{59}N$-O-$C_{59}N$ molecules.

Molecule	MO transition of peak A	Energy of peak A (eV)
[5,6]$C_{60}O$	HOMO → 1s	515.88
[6,6]$C_{60}O$	HOMO → 1s	515.82
$C_{59}N(OH)$	HOMO → 1s	515.33
$C_{59}N$-O-$C_{59}N$	HOMO → 1s	515.74

Table S3. Assignments of the nitrogen *K*-edge XPS shake-up satellites of the $C_{59}N$, $C_{59}N(OH)$, $(C_{59}N)_2$, and $C_{59}N$-O-$C_{59}N$ molecules.

Molecule	A	B
$C_{59}N$	HOMO→ LUMO+ 2(α)	HOMO− 5 → LUMO+ 2(α)
$C_{59}N(OH)$	HOMO→ LUMO+ 2	HOMO→ LUMO+ 6
		HOMO−5→ LUMO+ 2
		HOMO−4→ LUMO+ 4
$(C_{59}N)_2$	HOMO→ LUMO+ 9	HOMO− 6 → LUMO+ 8
	HOMO −5→ LUMO+ 2	HOMO− 18 → LUMO+ 2
$C_{59}N$-O-$C_{59}N$	HOMO→ LUMO+ 6	HOMO−6→ LUMO+ 8
	HOMO−9→ LUMO	HOMO−9→ LUMO+ 2
		HOMO−12→ LUMO+ 6

Table S4. Assignments of the oxygen *K*-edge XPS shake-up satellites of the open [5,6] and closed [6,6] isomers of $C_{60}O$, $C_{60}H(OH)$, C_{60}-O-C_{60}, $C_{60}H$-O-C_60H, $C_{59}N(OH)$, and $C_{59}N$-O-$C_{59}N$ molecules.

Molecule	**A**	**B**	**C**
[5,6]$C_{60}O$	HOMO − 3 → LUMO + 1 HOMO − 4 → LUMO	—	HOMO − 9 → LUMO + 1 HOMO − 8 → LUMO + 1
[6,6]$C_{60}O$	HOMO − 4 → LUMO	HOMO − 4 → LUMO + 3	HOMO − 8 → LUMO + 2
$C_{60}H(OH)$	HOMO → LUMO	HOMO − 4→ LUMO	HOMO − 5 → LUMO
C_{60}-O-C_{60}	HOMO − 2→ LUMO + 3 HOMO → LUMO+ 5 HOMO − 8 → LUMO	HOMO − 12 → LUMO	HOMO − 12 → LUMO + 3 HOMO − 10 → LUMO + 5
$C_{60}H$-O-$C_{60}H$	HOMO − 4 → LUMO	HOMO −5 → LUMO + 4 HOMO → LUMO + 5	HOMO − 12 → LUMO
$C_{59}N(OH)$	HOMO → LUMO	—	HOMO − 5 → LUMO
$C_{59}N$-O-$C_{59}N$	HOMO −2→ LUMO + 1 HOMO − 2→ LUMO + 3 HOMO → LUMO + 5	—	HOMO − 11 → LUMO + 3 HOMO − 10 → LUMO + 5

Table S5. The lowest frequencies of all optimized structures.

Molecule	**lowest (1) (cm^{-1})**	**lowest (2) (cm^{-1})**	**lowest (3) (cm^{-1})**	**lowest (4) (cm^{-1})**	**lowest (5) (cm^{-1})**
C_{60}	264.6337	264.6340	264.6345	264.6350	264.6355
[5,6]$C_{60}O$	240.0953	241.8540	264.1200	266.9012	268.6820
[6,6]$C_{60}O$	257.8139	258.6538	258.8951	266.2602	267.5548
$C_{60}H(OH)$	191.7129	242.1027	252.0298	255.4117	262.1784
C_{60}-O-C_{60}	14.6776	15.8952	36.8433	94.9132	112.9805
$C_{60}H$-O-$C_{60}H$	3.0406	12.6583	25.2719	64.5702	84.2552
$C_{59}N$	257.8487	261.8285	262.6928	265.9646	268.9307
$C_{59}N(OH)$	181.7198	229.4904	251.5736	259.2045	260.5026
$(C_{59}N)_2$	3.9451	17.9744	19.1445	75.9561	98.5405
$C_{59}N$-O-$C_{59}N$	4.4088	8.8023	20.9036	66.7224	77.9017

Table S6. The energies of the fullerene C_{60}, aza[60]fullerene $C_{59}N$, their oxides, and hydrates molecules at different spin multiplicities. ΔE are the energy differences between the spin triplet (quartet) state and the spin singlet (doublet) state.

Molecule	singlet (a.u.)	doublet (a.u.)	triplet (a.u.)	quartet (a.u.)	ΔE (eV)
C_{60}	-2286.1731	—	-2286.1127	—	1.6436
[5,6]$C_{60}O$	-2361.3595	—	-2361.2957	—	1.7338
[6,6]$C_{60}O$	-2361.3561	—	-2361.2929	—	1.5783
$C_{60}H(OH)$	-2362.5966	—	-2362.5353	—	1.6505
C_{60}-O-C_{60}	-4647.5566	—	-4647.4891	—	1.8387
$C_{60}H$-O-$C_{60}H$	-4648.7582	—	-4648.6925	—	1.7867
$C_{59}N$	—	-2302.7913	—	-2302.7265	1.7635
$C_{59}N(OH)$	-2378.6354	—	-2378.5782	—	1.5558
$(C_{59}N)_2$	-4605.6333	—	-4605.5779	—	1.5088
$C_{59}N$-O-$C_{59}N$	-4680.8402	—	-4680.7847	—	1.5120

C. Molecules Coordinate

Table S7. Molecules Coordinate of the open [5,6] and closed [6,6] isomers of $C_{60}O$, $C_{60}H(OH)$, C_{60}-O-C_{60}, $C_{60}H$-O-C_60H, $C_{59}N(OH)$, and $C_{59}N$-O-$C_{59}N$ molecules.

Molecule	Atom	x	y	z
[5,6]$C_{60}O$	C	0.338440	1.690738	3.081764
	C	1.506536	2.104967	2.331710
	C	1.386131	2.991251	1.249923
	C	0.102088	3.625611	1.075475
	C	-1.048578	3.028019	1.556771
	C	-0.922801	2.095162	2.640554
	C	0.537081	0.319455	3.512067
	C	1.845100	-0.107699	3.048197
	C	2.431872	0.999020	2.311965
	C	3.182547	0.769431	1.167156
	C	2.126932	2.718732	0.000000
	C	-1.048578	3.028019	-1.556771
	C	-2.189512	2.595151	-0.704174
	C	-2.189512	2.595151	0.704174
	C	-2.799361	1.463057	1.406102
	C	-2.023789	1.165148	2.596567
	C	-1.843772	-0.144344	3.037250
	C	-0.533118	-0.578374	3.497333
	C	2.040450	-1.414972	2.607661
	C	0.931778	-2.353674	2.605529
	C	-0.331496	-1.940865	3.038674
	C	-1.519231	-2.351950	2.307090
	C	-2.453044	-1.239311	2.306551
	C	-3.219089	-0.966885	1.174309
	C	-3.399264	0.405225	0.720641
	C	-3.399264	0.405225	-0.720641
	C	-2.799361	1.463057	-1.406102
	C	1.386131	2.991251	-1.249923
	C	-0.533118	-0.578374	-3.497333
	C	0.537081	0.319455	-3.512067
	C	1.845100	-0.107699	-3.048197
	C	2.040450	-1.414972	-2.607661
	C	0.931778	-2.353674	-2.605529

	C	-1.519231	-2.351950	-2.307090
	C	-2.453044	-1.239311	-2.306551
	C	-1.843772	-0.144344	-3.037250
	C	-2.023789	1.165148	-2.596567
	C	-0.922801	2.095162	-2.640554
	C	0.338440	1.690738	-3.081764
	C	2.431872	0.999020	-2.311965
	C	3.182547	0.769431	-1.167156
	C	3.410801	-0.596500	-0.723443
	C	2.846282	-1.665012	-1.423795
	C	2.243994	-2.769534	-0.697436
	C	1.056855	-3.191213	-1.425782
	C	-0.084218	-3.587897	-0.726873
	C	-1.397828	-3.159205	-1.175562
	C	-3.219089	-0.966885	-1.174309
	C	-3.101086	-1.813420	0.000000
	C	-2.208662	-2.888070	0.000000
	C	-1.397828	-3.159205	1.175562
	C	-0.084218	-3.587897	0.726873
	C	1.056855	-3.191213	1.425782
	C	2.243994	-2.769534	0.697436
	C	2.846282	-1.665012	1.423795
	C	3.410801	-0.596500	0.723443
	C	1.506536	2.104967	-2.331710
	C	3.016505	1.624736	0.000000
	C	-0.331496	-1.940865	-3.038674
	C	0.102088	3.625611	-1.075475
	O	-0.017544	4.491316	0.000000
[6,6]$C_{60}O$	C	-2.299383	0.737840	2.501362
	C	-2.299383	-0.737840	2.501362
	C	-1.195160	-1.452753	2.941543
	C	0.000000	-0.768956	3.516743
	C	0.000000	0.768956	3.516743
	C	-1.195160	1.452753	2.941543
	C	-3.017554	1.176500	1.321292
	C	-3.462188	0.000000	0.593610
	C	-3.017554	-1.176500	1.321292
	C	-2.594543	-2.308018	0.615257
	C	-0.727853	-2.585895	2.183636
	C	2.299383	-0.737840	2.501362
	C	2.299383	0.737840	2.501362
	C	1.195160	1.452753	2.941543
	C	0.727853	2.585895	2.183636
	C	-0.727853	2.585895	2.183636
	C	-1.423774	3.030322	1.056329
	C	-2.594543	2.308018	0.615257
	C	-3.471101	0.000000	-0.801034
	C	-3.027197	1.176309	-1.532041
	C	-2.599344	2.308184	-0.837733
	C	-1.425312	3.036188	-1.291663
	C	-0.696999	3.483982	-0.118061
	C	0.696999	3.483982	-0.118061
	C	1.423774	3.030322	1.056329
	C	2.594543	2.308018	0.615257
	C	3.017554	1.176500	1.321292
	C	0.727853	-2.585895	2.183636
	C	3.027197	-1.176309	-1.532041

	C	2.599344	-2.308184	-0.837733
	C	1.425312	-3.036188	-1.291663
	C	0.727030	-2.602801	-2.420184
	C	1.175662	-1.425226	-3.142456
	C	2.304006	0.727479	-2.707408
	C	3.027197	1.176309	-1.532041
	C	3.471101	0.000000	-0.801034
	C	3.462188	0.000000	0.593610
	C	3.017554	-1.176500	1.321292
	C	2.594543	-2.308018	0.615257
	C	0.696999	-3.483982	-0.118061
	C	-0.696999	-3.483982	-0.118061
	C	-1.425312	-3.036188	-1.291663
	C	-0.727030	-2.602801	-2.420184
	C	-1.175662	-1.425226	-3.142456
	C	0.000000	-0.697560	-3.590530
	C	0.000000	0.697560	-3.590530
	C	1.175662	1.425226	-3.142456
	C	2.599344	2.308184	-0.837733
	C	1.425312	3.036188	-1.291663
	C	0.727030	2.602801	-2.420184
	C	-0.727030	2.602801	-2.420184
	C	-1.175662	1.425226	-3.142456
	C	-2.304006	0.727479	-2.707408
	C	-2.304006	-0.727479	-2.707408
	C	-3.027197	-1.176309	-1.532041
	C	-2.599344	-2.308184	-0.837733
	C	1.423774	-3.030322	1.056329
	C	-1.423774	-3.030322	1.056329
	C	2.304006	-0.727479	-2.707408
	C	1.195160	-1.452753	2.941543
	O	0.000000	0.000000	4.712202
$C_{60}H(OH)$	C	1.959187	-2.868579	1.175359
	C	2.984529	-1.943128	0.726945
	C	3.204631	-0.753716	1.424780
	C	2.406040	-0.441584	2.599072
	C	1.418756	-1.332246	3.026237
	C	1.193073	-2.568597	2.303818
	C	1.326125	-3.442389	0.000000
	C	1.959187	-2.868579	-1.175359
	C	2.984529	-1.943128	-0.726945
	C	3.204631	-0.753716	-1.424780
	C	3.430167	0.482498	0.696766
	C	2.140496	0.985202	2.593355
	C	0.894269	1.468369	3.006578
	C	-0.128878	0.539904	3.452197
	C	0.127274	-0.830874	3.469488
	C	-0.895731	-1.765427	3.027818
	C	-0.238126	-2.835661	2.303833
	C	-0.844123	-3.392180	1.175445
	C	-0.046150	-3.697659	0.000000
	C	1.193073	-2.568597	-2.303818
	C	-0.238126	-2.835661	-2.303833
	C	-0.844123	-3.392180	-1.175445
	C	-2.134382	-2.899270	-0.727081
	C	-2.134382	-2.899270	0.727081
	C	-2.768956	-1.869844	1.424956

	C	-2.137243	-1.290598	2.599617
	C	-2.407342	0.135760	2.595620
	C	-1.419042	1.037132	3.007086
	C	2.767678	1.554062	1.424490
	C	0.857445	3.105318	-1.181648
	C	0.249499	2.541764	-2.281616
	C	-1.206363	2.272558	-2.286821
	C	-2.954376	1.627762	-0.725941
	C	-2.954376	1.627762	0.725941
	C	-1.966939	2.569648	1.177533
	C	-1.206363	2.272558	2.286821
	C	0.249499	2.541764	2.281616
	C	0.857445	3.105318	1.181648
	C	2.115444	2.576628	-0.727616
	C	2.767678	1.554062	-1.424490
	C	2.140496	0.985202	-2.593355
	C	0.894269	1.468369	-3.006578
	C	-0.128878	0.539904	-3.452197
	C	-1.419042	1.037132	-3.007086
	C	-2.407342	0.135760	-2.595620
	C	-3.195513	0.439254	-1.426216
	C	-3.195513	0.439254	1.426216
	C	-3.425601	-0.797615	0.697184
	C	-3.425601	-0.797615	-0.697184
	C	-2.768956	-1.869844	-1.424956
	C	-2.137243	-1.290598	-2.599617
	C	-0.895731	-1.765427	-3.027818
	C	0.127274	-0.830874	-3.469488
	C	1.418756	-1.332246	-3.026237
	C	2.406040	-0.441584	-2.599072
	C	2.115444	2.576628	0.727616
	C	3.430167	0.482498	-0.696766
	C	-1.966939	2.569648	-1.177533
	C	0.087731	3.726303	0.000000
	C	-1.461373	3.404780	0.000000
	O	0.138785	5.159327	0.000000
	H	1.070339	5.422345	0.000000
	H	-1.929081	4.398361	0.000000
C_{60}-O-C_{60}	C	-3.027339	5.783460	-1.516255
	C	-3.470201	5.360137	-0.197051
	C	-3.452647	4.007161	0.141202
	C	-3.003777	3.019341	-0.824276
	C	-2.594053	3.426578	-2.098015
	C	-2.599787	4.835119	-2.448054
	C	-2.303993	7.030374	-1.364233
	C	-2.304003	7.382959	0.048395
	C	-3.027535	6.353574	0.768413
	C	-2.599603	5.954122	2.036732
	C	-3.009084	3.589064	1.458438
	C	-2.280394	1.987099	-0.115956
	C	-0.725416	1.841425	-1.974434
	C	-1.424434	2.821969	-2.687411
	C	-0.696801	3.850445	-3.413021
	C	-1.425083	5.098418	-3.263426
	C	-0.727140	6.298469	-3.114667
	C	-1.175442	7.283892	-2.146938
	C	-1.175429	7.974346	0.620116

C	0.000000	8.231743	-0.194411
C	0.000000	7.893824	-1.548735
C	1.175442	7.283892	-2.146938
C	0.727140	6.298469	-3.114667
C	1.425083	5.098418	-3.263426
C	0.696801	3.850445	-3.413021
C	1.424434	2.821969	-2.687411
C	0.725416	1.841425	-1.974434
C	-2.283599	2.345241	1.318651
C	2.283599	2.345241	1.318651
C	1.180306	2.091820	2.099338
C	0.726826	3.089638	3.027405
C	1.424583	4.290123	3.195816
C	3.452647	4.007161	0.141202
C	3.003777	3.019341	-0.824276
C	2.280394	1.987099	-0.115956
C	1.175660	1.392817	-0.684952
C	-0.726826	3.089638	3.027405
C	-1.424583	4.290123	3.195816
C	-0.696936	5.539323	3.352192
C	0.696936	5.539323	3.352192
C	1.424770	6.569776	2.632702
C	2.599603	5.954122	2.036732
C	3.027535	6.353574	0.768413
C	3.470201	5.360137	-0.197051
C	2.594053	3.426578	-2.098015
C	2.599787	4.835119	-2.448054
C	3.027339	5.783460	-1.516255
C	2.303993	7.030374	-1.364233
C	2.304003	7.382959	0.048395
C	1.175429	7.974346	0.620116
C	0.727166	7.559653	1.937687
C	-0.727166	7.559653	1.937687
C	-1.424770	6.569776	2.632702
C	-1.180306	2.091820	2.099338
C	-2.594832	4.546805	2.389990
C	3.009084	3.589064	1.458438
C	2.594832	4.546805	2.389990
C	0.000000	0.808081	0.116535
C	0.000000	-0.808081	0.116535
C	1.175660	-1.392817	-0.684952
C	-1.175660	-1.392817	-0.684952
C	2.280394	-1.987099	-0.115956
C	0.725416	-1.841425	-1.974434
C	1.180306	-2.091820	2.099338
C	-1.180306	-2.091820	2.099338
C	-0.725416	-1.841425	-1.974434
C	-2.280394	-1.987099	-0.115956
C	2.283599	-2.345241	1.318651
C	3.003777	-3.019341	-0.824276
C	1.424434	-2.821969	-2.687411
C	0.726826	-3.089638	3.027405
C	-0.726826	-3.089638	3.027405
C	-2.283599	-2.345241	1.318651
C	-1.424434	-2.821969	-2.687411
C	-3.003777	-3.019341	-0.824276
C	3.009084	-3.589064	1.458438

	C	3.452647	-4.007161	0.141202
	C	2.594053	-3.426578	-2.098015
	C	0.696801	-3.850445	-3.413021
	C	1.424583	-4.290123	3.195816
	C	-1.424583	-4.290123	3.195816
	C	-3.009084	-3.589064	1.458438
	C	-2.594053	-3.426578	-2.098015
	C	-0.696801	-3.850445	-3.413021
	C	-3.452647	-4.007161	0.141202
	C	2.594832	-4.546805	2.389990
	C	3.470201	-5.360137	-0.197051
	C	2.599787	-4.835119	-2.448054
	C	1.425083	-5.098418	-3.263426
	C	0.696936	-5.539323	3.352192
	C	-2.594832	-4.546805	2.389990
	C	-0.696936	-5.539323	3.352192
	C	-2.599787	-4.835119	-2.448054
	C	-1.425083	-5.098418	-3.263426
	C	-3.470201	-5.360137	-0.197051
	C	2.599603	-5.954122	2.036732
	C	3.027535	-6.353574	0.768413
	C	3.027339	-5.783460	-1.516255
	C	0.727140	-6.298469	-3.114667
	C	1.424770	-6.569776	2.632702
	C	-2.599603	-5.954122	2.036732
	C	-1.424770	-6.569776	2.632702
	C	-3.027339	-5.783460	-1.516255
	C	-0.727140	-6.298469	-3.114667
	C	-3.027535	-6.353574	0.768413
	C	2.304003	-7.382959	0.048395
	C	2.303993	-7.030374	-1.364233
	C	1.175442	-7.283892	-2.146938
	C	0.727166	-7.559653	1.937687
	C	-0.727166	-7.559653	1.937687
	C	-2.303993	-7.030374	-1.364233
	C	-1.175442	-7.283892	-2.146938
	C	-2.304003	-7.382959	0.048395
	C	1.175429	-7.974346	0.620116
	C	0.000000	-7.893824	-1.548735
	C	-1.175429	-7.974346	0.620116
	C	0.000000	-8.231743	-0.194411
	C	0.000000	1.210811	1.657056
	C	0.000000	-1.210811	1.657056
	C	-1.175660	1.392817	-0.684952
	O	0.000000	0.000000	2.419174
$C_{60}H$-O-$C_{60}H$	C	1.175557	-6.638021	-2.910960
	C	0.727085	-5.382844	-3.487466
	C	1.424959	-4.203501	-3.219000
	C	2.599094	-4.232198	-2.361661
	C	3.026350	-5.440206	-1.806892
	C	2.304251	-6.665347	-2.088695
	C	0.000000	-7.415091	-2.556139
	C	-1.175557	-6.638021	-2.910960
	C	-0.727085	-5.382844	-3.487466
	C	-1.424959	-4.203501	-3.219000
	C	0.696628	-2.979543	-2.936838
	C	2.591060	-3.027450	-1.552432

C	3.002086	-3.073574	-0.216978
C	3.450222	-4.330414	0.354431
C	3.469273	-5.489004	-0.422458
C	3.028063	-6.751929	0.147724
C	2.303968	-7.475652	-0.879397
C	1.175483	-8.226181	-0.542667
C	0.000000	-8.191546	-1.396288
C	-2.304251	-6.665347	-2.088695
C	-2.303968	-7.475652	-0.879397
C	-1.175483	-8.226181	-0.542667
C	-0.727103	-8.283050	0.837309
C	0.727103	-8.283050	0.837309
C	1.425377	-7.588975	1.827096
C	2.599983	-6.806704	1.475620
C	2.595971	-5.602968	2.287024
C	3.007310	-4.383928	1.735844
C	1.421635	-2.258829	-1.903088
C	-1.184188	-1.566357	0.464068
C	-2.277855	-2.338468	0.799920
C	-2.287350	-3.163703	2.028575
C	-0.725653	-4.451476	3.377742
C	0.725653	-4.451476	3.377742
C	1.176494	-3.197289	2.840374
C	2.287350	-3.163703	2.028575
C	2.277855	-2.338468	0.799920
C	1.184188	-1.566357	0.464068
C	-0.725797	-1.579184	-0.900071
C	-1.421635	-2.258829	-1.903088
C	-2.591060	-3.027450	-1.552432
C	-3.002086	-3.073574	-0.216978
C	-3.450222	-4.330414	0.354431
C	-3.007310	-4.383928	1.735844
C	-2.595971	-5.602968	2.287024
C	-1.426534	-5.637591	3.131397
C	1.426534	-5.637591	3.131397
C	0.697434	-6.864577	2.854463
C	-0.697434	-6.864577	2.854463
C	-1.425377	-7.588975	1.827096
C	-2.599983	-6.806704	1.475620
C	-3.028063	-6.751929	0.147724
C	-3.469273	-5.489004	-0.422458
C	-3.026350	-5.440206	-1.806892
C	-2.599094	-4.232198	-2.361661
C	-0.696628	-2.979543	-2.936838
C	-1.176494	-3.197289	2.840374
C	1.184188	1.566357	0.464068
C	-1.184188	1.566357	0.464068
C	2.277855	2.338468	0.799920
C	0.725797	1.579184	-0.900071
C	1.176494	3.197289	2.840374
C	-1.176494	3.197289	2.840374
C	-2.277855	2.338468	0.799920
C	2.287350	3.163703	2.028575
C	3.002086	3.073574	-0.216978
C	1.421635	2.258829	-1.903088
C	0.725653	4.451476	3.377742
C	-0.725653	4.451476	3.377742

	C	-2.287350	3.163703	2.028575
	C	-1.421635	2.258829	-1.903088
	C	-3.002086	3.073574	-0.216978
	C	3.007310	4.383928	1.735844
	C	3.450222	4.330414	0.354431
	C	2.591060	3.027450	-1.552432
	C	0.696628	2.979543	-2.936838
	C	1.426534	5.637591	3.131397
	C	-1.426534	5.637591	3.131397
	C	-3.007310	4.383928	1.735844
	C	-2.591060	3.027450	-1.552432
	C	-0.696628	2.979543	-2.936838
	C	-3.450222	4.330414	0.354431
	C	2.595971	5.602968	2.287024
	C	3.469273	5.489004	-0.422458
	C	2.599094	4.232198	-2.361661
	C	1.424959	4.203501	-3.219000
	C	0.697434	6.864577	2.854463
	C	-2.595971	5.602968	2.287024
	C	-0.697434	6.864577	2.854463
	C	-2.599094	4.232198	-2.361661
	C	-1.424959	4.203501	-3.219000
	C	-3.469273	5.489004	-0.422458
	C	2.599983	6.806704	1.475620
	C	3.028063	6.751929	0.147724
	C	3.026350	5.440206	-1.806892
	C	0.727085	5.382844	-3.487466
	C	1.425377	7.588975	1.827096
	C	-2.599983	6.806704	1.475620
	C	-1.425377	7.588975	1.827096
	C	-3.026350	5.440206	-1.806892
	C	-0.727085	5.382844	-3.487466
	C	-3.028063	6.751929	0.147724
	C	2.303968	7.475652	-0.879397
	C	2.304251	6.665347	-2.088695
	C	1.175557	6.638021	-2.910960
	C	0.727103	8.283050	0.837309
	C	-0.727103	8.283050	0.837309
	C	-2.304251	6.665347	-2.088695
	C	-1.175557	6.638021	-2.910960
	C	-2.303968	7.475652	-0.879397
	C	1.175483	8.226181	-0.542667
	C	0.000000	7.415091	-2.556139
	C	-1.175483	8.226181	-0.542667
	C	0.000000	8.191546	-1.396288
	C	-0.725797	1.579184	-0.900071
	C	0.725797	-1.579184	-0.900071
	C	0.000000	1.296911	1.416511
	C	0.000000	-1.296911	1.416511
	C	0.000000	-2.235194	2.706054
	C	0.000000	2.235194	2.706054
	O	0.000000	0.000000	2.061802
	H	0.000000	-1.518373	3.536137
	H	0.000000	1.518373	3.536137
$C_{59}N(OH)$	C	1.950493	-2.861800	1.175510
	C	2.978653	-1.939400	0.726807
	C	3.202400	-0.750728	1.424539

C	2.406560	-0.437732	2.600656
C	1.414477	-1.323550	3.026408
C	1.185865	-2.560365	2.304715
C	1.317582	-3.435377	0.000000
C	1.950493	-2.861800	-1.175510
C	2.978653	-1.939400	-0.726807
C	3.202400	-0.750728	-1.424539
C	3.429934	0.484919	0.696365
C	2.145009	0.989485	2.597471
C	0.904003	1.473858	3.021294
C	-0.125606	0.554696	3.466098
C	0.124168	-0.818265	3.472870
C	-0.901067	-1.750409	3.032705
C	-0.245787	-2.820940	2.304117
C	-0.852662	-3.374851	1.175685
C	-0.056045	-3.682622	0.000000
C	1.185865	-2.560365	-2.304715
C	-0.245787	-2.820940	-2.304117
C	-0.852662	-3.374851	-1.175685
C	-2.140902	-2.875147	-0.727487
C	-2.140902	-2.875147	0.727487
C	-2.772748	-1.846639	1.427216
C	-2.138533	-1.268606	2.603002
C	-2.408712	0.158218	2.605925
C	-1.416597	1.061986	3.017091
C	2.768458	1.558582	1.425441
C	0.859717	3.107802	-1.186114
C	0.261071	2.545525	-2.291563
C	-1.182228	2.295654	-2.302393
C	-2.937743	1.636386	-0.717066
C	-2.937743	1.636386	0.717066
C	-1.894269	2.530191	1.136309
C	-1.182228	2.295654	2.302393
C	0.261071	2.545525	2.291563
C	0.859717	3.107802	1.186114
C	2.115132	2.578600	-0.726386
C	2.768458	1.558582	-1.425441
C	2.145009	0.989485	-2.597471
C	0.904003	1.473858	-3.021294
C	-0.125606	0.554696	-3.466098
C	-1.416597	1.061986	-3.017091
C	-2.408712	0.158218	-2.605925
C	-3.188909	0.459328	-1.432649
C	-3.188909	0.459328	1.432649
C	-3.427159	-0.772774	0.698452
C	-3.427159	-0.772774	-0.698452
C	-2.772748	-1.846639	-1.427216
C	-2.138533	-1.268606	-2.603002
C	-0.901067	-1.750409	-3.032705
C	0.124168	-0.818265	-3.472870
C	1.414477	-1.323550	-3.026408
C	2.406560	-0.437732	-2.600656
C	2.115132	2.578600	0.726386
C	3.429934	0.484919	-0.696365
C	-1.894269	2.530191	-1.136309
C	0.052879	3.679838	0.000000
N	-1.331155	3.146329	0.000000

	O	-0.090428	5.090277	0.000000
	H	0.798822	5.474122	0.000000
$C_{59}N$-O-$C_{59}N$	C	-1.175591	6.880127	-2.732438
	C	-0.726916	5.680890	-3.417827
	C	-1.424775	4.482457	-3.255395
	C	-2.600919	4.436087	-2.401443
	C	-3.026792	5.589250	-1.739096
	C	-2.305003	6.835122	-1.911807
	C	0.000000	7.623617	-2.312345
	C	1.175591	6.880127	-2.732438
	C	0.726916	5.680890	-3.417827
	C	1.424775	4.482457	-3.255395
	C	-0.696311	3.238491	-3.081105
	C	-2.596447	3.164490	-1.702660
	C	-3.018696	3.094745	-0.372476
	C	-3.465685	4.291057	0.314281
	C	-3.472988	5.515681	-0.355341
	C	-3.032928	6.723288	0.323991
	C	-2.304349	7.533240	-0.635194
	C	-1.175717	8.249838	-0.233680
	C	0.000000	8.290994	-1.086529
	C	2.305003	6.835122	-1.911807
	C	2.304349	7.533240	-0.635194
	C	1.175717	8.249838	-0.233680
	C	0.727497	8.181241	1.146390
	C	-0.727497	8.181241	1.146390
	C	-1.427483	7.404438	2.070026
	C	-2.603555	6.656131	1.650279
	C	-2.606556	5.386835	2.355787
	C	-3.018782	4.216456	1.699465
	C	-1.423704	2.428957	-2.114333
	C	1.188120	1.547211	0.183752
	C	2.290101	2.277972	0.575590
	C	2.304365	2.970736	1.865295
	C	0.716944	4.151714	3.322140
	C	-0.716944	4.151714	3.322140
	C	-1.136552	2.976583	2.610939
	C	-2.304365	2.970736	1.865295
	C	-2.290101	2.277972	0.575590
	C	-1.188120	1.547211	0.183752
	C	0.725105	1.667664	-1.173170
	C	1.423704	2.428957	-2.114333
	C	2.596447	3.164490	-1.702660
	C	3.018696	3.094745	-0.372476
	C	3.465685	4.291057	0.314281
	C	3.018782	4.216456	1.699465
	C	2.606556	5.386835	2.355787
	C	1.432952	5.347523	3.191140
	C	-1.432952	5.347523	3.191140
	C	-0.698582	6.591621	3.029281
	C	0.698582	6.591621	3.029281
	C	1.427483	7.404438	2.070026
	C	2.603555	6.656131	1.650279
	C	3.032928	6.723288	0.323991
	C	3.472988	5.515681	-0.355341
	C	3.026792	5.589250	-1.739096
	C	2.600919	4.436087	-2.401443

C	0.696311	3.238491	-3.081105
C	1.136552	2.976583	2.610939
C	-1.188120	-1.547211	0.183752
C	1.188120	-1.547211	0.183752
C	-2.290101	-2.277972	0.575590
C	-0.725105	-1.667664	-1.173170
C	-1.136552	-2.976583	2.610939
C	1.136552	-2.976583	2.610939
C	2.290101	-2.277972	0.575590
C	-2.304365	-2.970736	1.865295
C	-3.018696	-3.094745	-0.372476
C	-1.423704	-2.428957	-2.114333
C	-0.716944	-4.151714	3.322140
C	0.716944	-4.151714	3.322140
C	2.304365	-2.970736	1.865295
C	1.423704	-2.428957	-2.114333
C	3.018696	-3.094745	-0.372476
C	-3.018782	-4.216456	1.699465
C	-3.465685	-4.291057	0.314281
C	-2.596447	-3.164490	-1.702660
C	-0.696311	-3.238491	-3.081105
C	-1.432952	-5.347523	3.191140
C	1.432952	-5.347523	3.191140
C	3.018782	-4.216456	1.699465
C	2.596447	-3.164490	-1.702660
C	0.696311	-3.238491	-3.081105
C	3.465685	-4.291057	0.314281
C	-2.606556	-5.386835	2.355787
C	-3.472988	-5.515681	-0.355341
C	-2.600919	-4.436087	-2.401443
C	-1.424775	-4.482457	-3.255395
C	-0.698582	-6.591621	3.029281
C	2.606556	-5.386835	2.355787
C	0.698582	-6.591621	3.029281
C	2.600919	-4.436087	-2.401443
C	1.424775	-4.482457	-3.255395
C	3.472988	-5.515681	-0.355341
C	-2.603555	-6.656131	1.650279
C	-3.032928	-6.723288	0.323991
C	-3.026792	-5.589250	-1.739096
C	-0.726916	-5.680890	-3.417827
C	-1.427483	-7.404438	2.070026
C	2.603555	-6.656131	1.650279
C	1.427483	-7.404438	2.070026
C	3.026792	-5.589250	-1.739096
C	0.726916	-5.680890	-3.417827
C	3.032928	-6.723288	0.323991
C	-2.304349	-7.533240	-0.635194
C	-2.305003	-6.835122	-1.911807
C	-1.175591	-6.880127	-2.732438
C	-0.727497	-8.181241	1.146390
C	0.727497	-8.181241	1.146390
C	2.305003	-6.835122	-1.911807
C	1.175591	-6.880127	-2.732438
C	2.304349	-7.533240	-0.635194
C	-1.175717	-8.249838	-0.233680
C	0.000000	-7.623617	-2.312345

C	1.175717	-8.249838	-0.233680
C	0.000000	-8.290994	-1.086529
C	0.725105	-1.667664	-1.173170
C	-0.725105	1.667664	-1.173170
C	0.000000	-1.262251	1.129499
C	0.000000	1.262251	1.129499
N	0.000000	2.221743	2.262717
N	0.000000	-2.221743	2.262717
O	0.000000	0.000000	1.807137