Electronic Supplementary Information (ESI)

Creation of spin-switching in graphene oxide-based hybrid film materials with anionic Fe(III) 5Cl-salicyaldehyde-thiosemicarbazone complex

Nataliya G. Spitsyna*[a], Anatoly S. Lobach,[a] Maxim A. Blagov,[a] Nadezhda N. Dremova,[a] Alexei I. Dmitriev,[a] Mikhail V. Zhidkov,[a] Sergei V. Simonov[b]

[a]*Federal Research Center of Problems of Chemical Physics and Medicinal Chemistry, Russian Academy of Sciences, Chernogolovka, Moscow region 142432, Russia.*
E-mail: spitsina@icp.ac.ru
[b]*Institute of Solid State Physics RAS, Chernogolovka, MD 142432, Russia*

Author Contributions

N.G.S., A.S.L. conceived the idea and designed experiments, synthesized samples and wrote the paper. N.N.D performed SEM, EDX investigation. S.V.S performed PXRD analysis. K.V.Z., A.N.V performed *dc* magnetic measurements. M.A.B measured and contributed to analyses of ^{57}Fe Mössbauer spectral data, performed the DFT calculations. All authors discussed the results and contributed to the final manuscript.

Contents

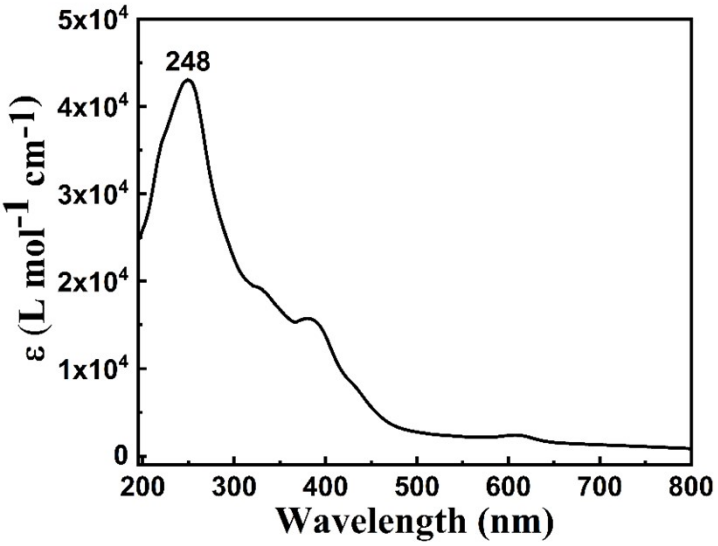

Figure S1. UV-vis spectrum of salt $[Et_4N][^{57}Fe^{III}(5Cl\text{-}thsa)_2]$ (**1**) in acetonitrile solution.

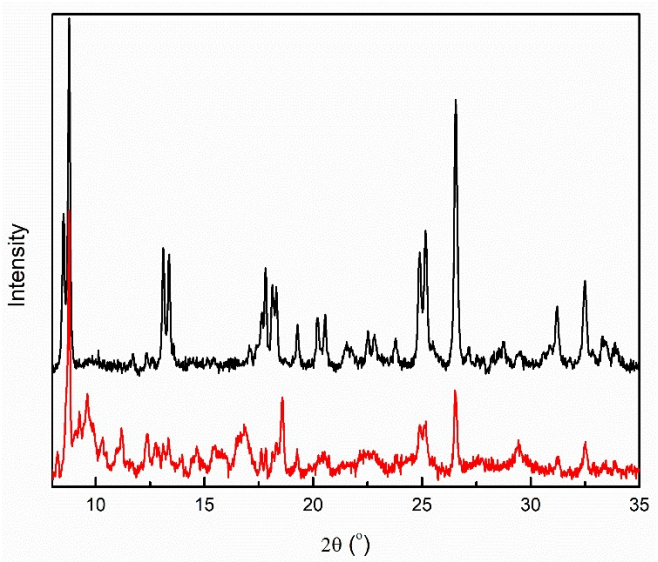

Figure S2. Normalized powder X-ray diffraction patterns in the 8° to 35° region for initial (**1,** black line) and recrystallized (**1´**, red line) from acetonitrile $[Et_4N][^{57}Fe(5Cl\text{-}thsa)_2]$ salt.

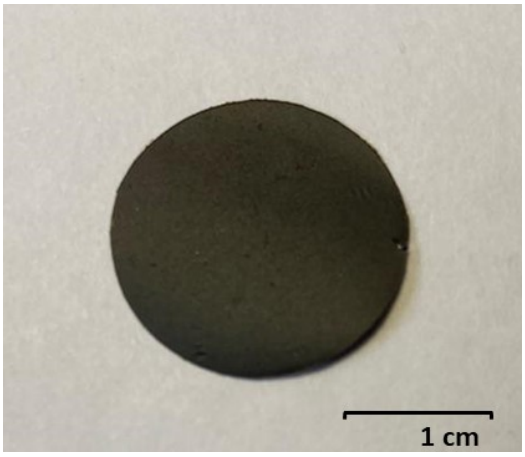

Figure S3. Photo of the film GO-**1** hybrid material: the thickness ~45 μm and 2 cm in diameter.

Table S1. Table of experimental ATR FT-IR vibrational modes of compound $[Et_4N][^{57}Fe^{III}(5Cl\text{-}thsa)_2]$, films GO and hybrid GO-**1**.

$[Et_4N][^{57}Fe^{III}(5Cl\text{-}thsa)_2]$ (**1**), ν, cm^{-1}	Film GO, ν, cm^{-1}	Film GO-**1**, ν, cm^{-1}	Assignment of the most significant of vibration modes
3533(w)		3533(sh)*	ν(N-H)
3458(s)		3457(w)*	ν(N-H)
3406(s)		3408(w)*	ν(N-H)
	~3292(s)	~3330 (s)	ν(C-OH)
3270(s)		~3270(w)*	ν(N-H), $\nu(C_{arom}\text{-}H)$
2979(m)		~2979(sh)*	$\nu_{asym}\text{-}CH_3$ (Et_4N^+)
	2962(sh)	2962(sh)*	ν(C-H) $\text{-}CH_2$
	2929(sh)	2929(sh)*	ν(C–H) –CH
	1724(s)	1732(m)	ν(C=O)
1635(m)		1635(w)*	$\nu(C_{arom}\text{-}C_{arom})$
1604(w)	1614(s)	1607(s)	δ(-OH),
	1577(s)	1571(sh)	ν(>C=C<)
1588(m)		1591(sh)	$\nu(C{=}N_{im})$ (azomethine group)
1437(w)		1419w	$\nu(C_{arom}\text{-}O)$
1359(m)	1363(s)	1352w	δ(OH) in C-OH
1313 (sh)		1318w	C-H, C-OH; GO
1295(s)		1294m*	ν(N-H)
	1225(w)	1225(w)	ν(C-O-C)epoxy
1184(s)		1188(m)	δ(N-H)
1122(sh)		1128(sh)	$\nu(C_{arom}\text{-}Cl)$
1093(m)		1084(sh)	$\nu(C_{arom}\text{-}Cl)$
	1045(s)	~1050(s)	ν(C-O)alkoxy
1031(m)		1036(sh)	ν_{sym}(C-N),ν_{asym}(C-N) (Et_4N^+)
970(w)		977(sh)	$\delta(C_{arom}\text{–}H)$, δ(C–H)
930(m)		934(sh)	$\delta(C_{arom}\text{–}H)$, δ(C–H)
818(s)		821(m)	δ(N–H), ν(C–S)
661(s)		660(w)*	ν_{sym}(C-N) (Et_4N^+), $\delta(C_{arom}\text{–}H)$, $\nu(C_{arom}\text{–}C_{arom})$, δ(N–H), δ(Fe–O),
535(m)		533(w)*	ν(Fe-S), ν(Fe-N)
456(m)		456(w)*	ν(Fe-O)

(w): weak, (m): middle, (s): strong, (sh): shoulder, *- bands are coincided.

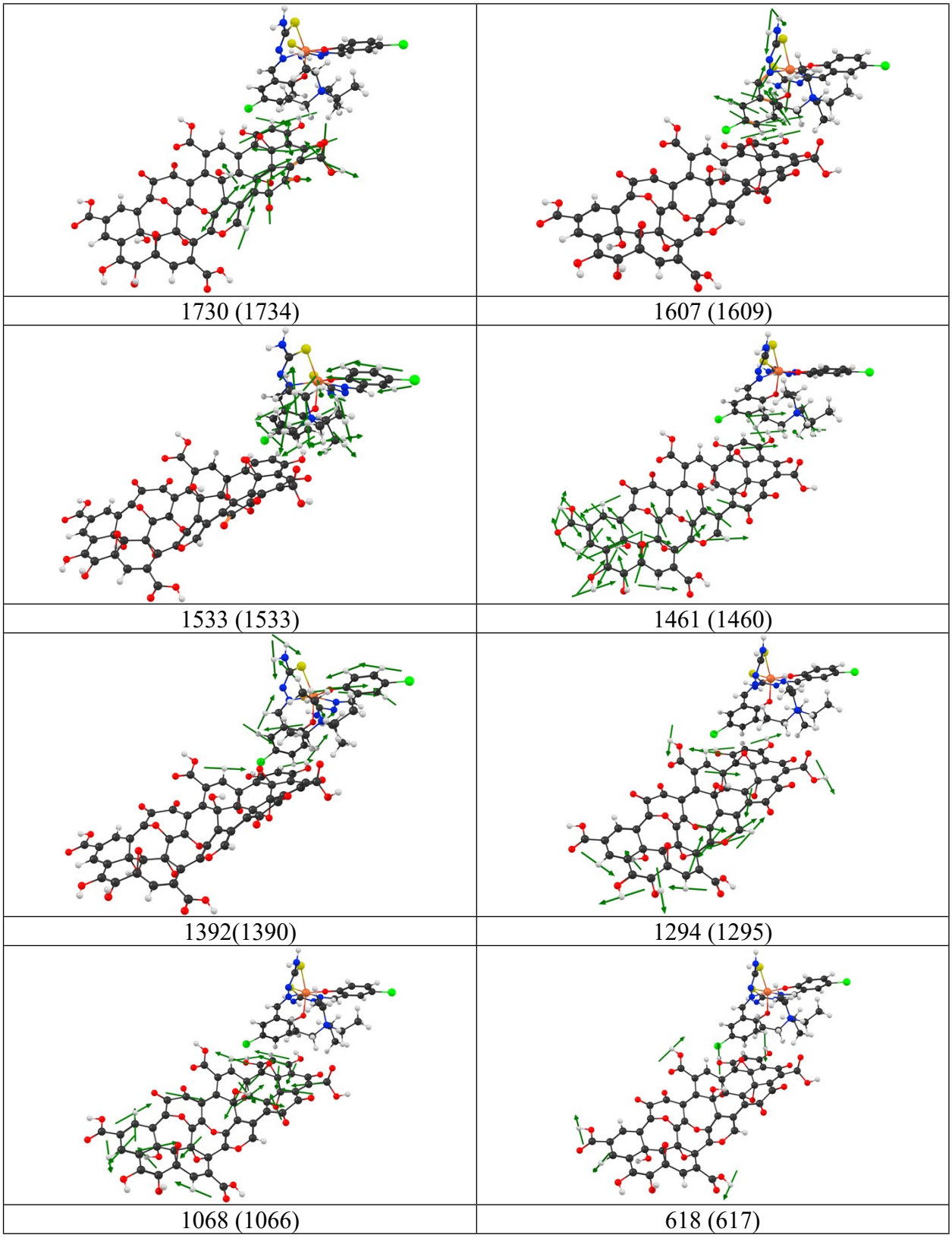

Figure S4. Selected experimental and calculated (in brackets) IR vibrational modes of the GO-**1** system in HS state (wB97XD/6-31G(d,p)).

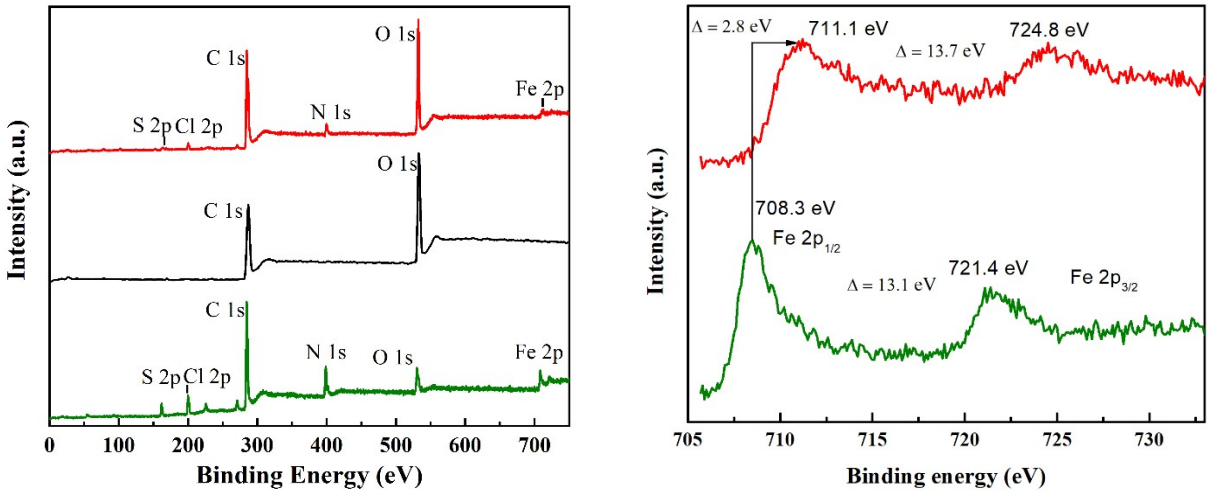

Figure S5. *Left:* XPS full spectra of salt **1** (green line), GO (black line) and GO-**1** (red line) films. *Right:* High-resolution XPS spectra of Fe2p for bulk salt **1** (708.2 eV, green line) and GO-**1** film (712.7 eV, red line).

Figure S5/right demonstrates the existence of Fe $2p_{3/2}$ (for salt **1** – 721.4 eV; GO-**1** – 724.8 eV) and Fe $2p_{1/2}$ (for salt **1** – 708.3 eV; GO-**1** – 711.1 eV) peaks. This shift and broadening of these peaks in spectra of GO-**1** compared to salt **1** are due to electronic interactions between the spin-crossover complexes and GO nanosheets.

Method: XPS analyses were carried out using monochromated Al (Kα = 1486.6 eV) X -ray source of Kratos Ultra DLD spectrometer. The analysis area was 300 x 700 μm^2. A scan was performed at a pass energies were 80 and 40 eV for the survey and high-resolution spectra, respectively. The spectra were calibrated to the C 1s signal (284.7 eV).

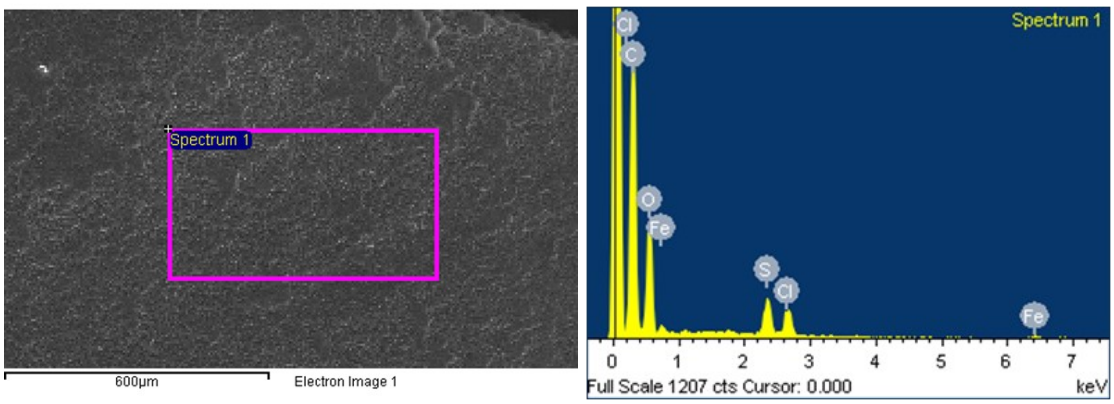

Figure S6. EDX elemental analysis of GO-**1** hybrid film.

Fe:S:Cl=1:2:2.

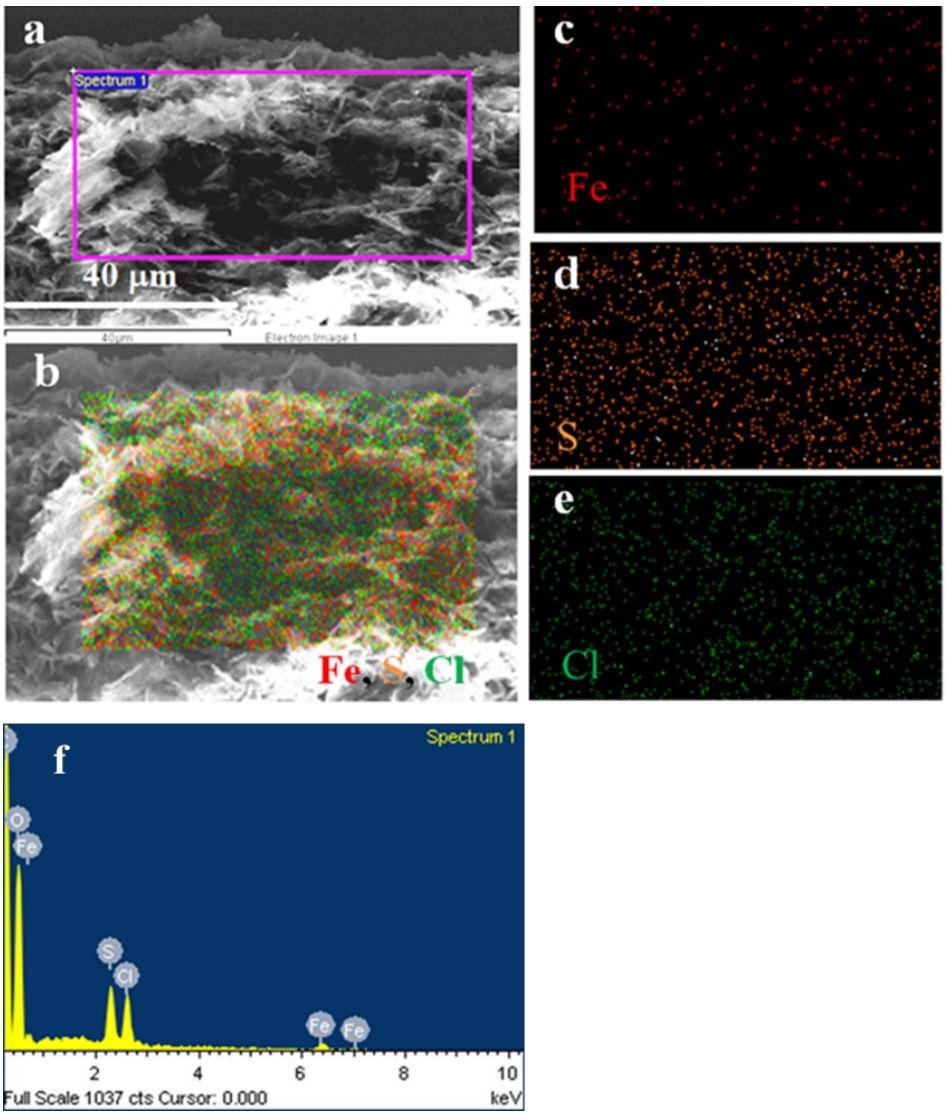

Figure S7. Cross-section SEM image of (a) GO-**1** hybrid film, (b) corresponding EDX combined map of Fe, S, Cl and maps of (c) Fe, (d) S and (e) Cl elements, (f) EDX spectrum.

The distribution of Fe, S and Cl elements in the (b) image proves the uniform distribution of **1** in the volume of the GO-**1** film. Fe:S:Cl=1:2:2.

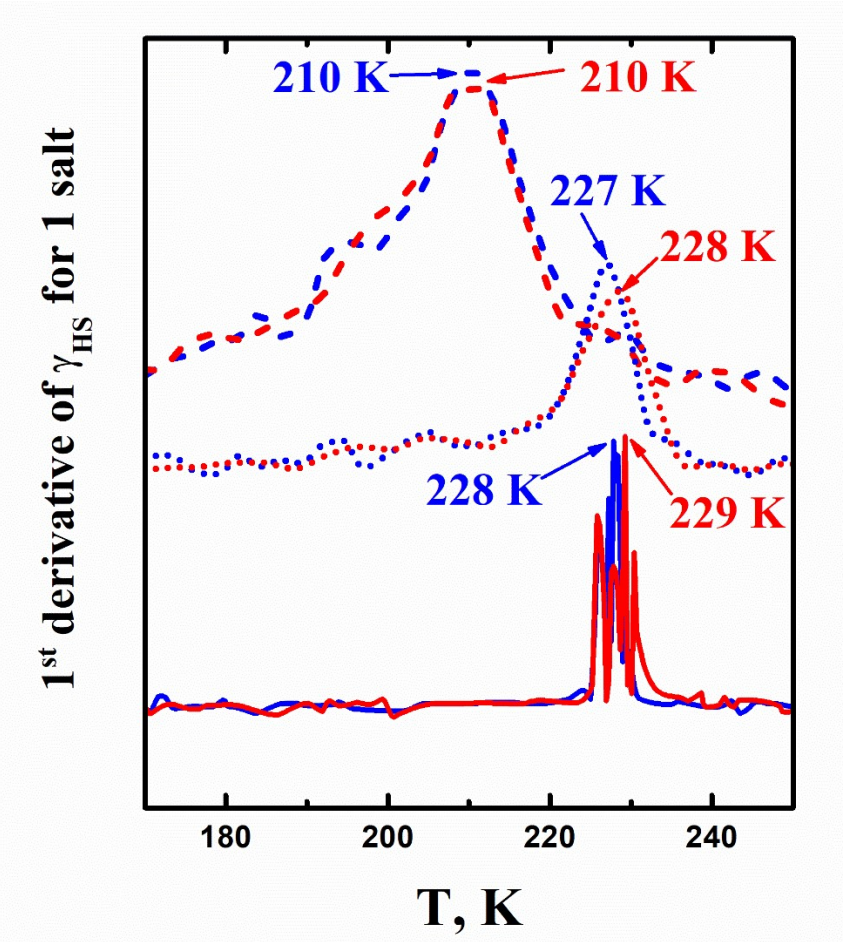

Figure S8. The first order differentiation of γ_{HS} *versus* T in temperature range 80–300 K plots for $[Et_4N][^{57}Fe(5Cl\text{-}thsa)_2]$ salt (dash line; dotes line- from CH_3CN) and GO-**1** hybrid film (solid line) on cooling (blue) and heating (red) mode.

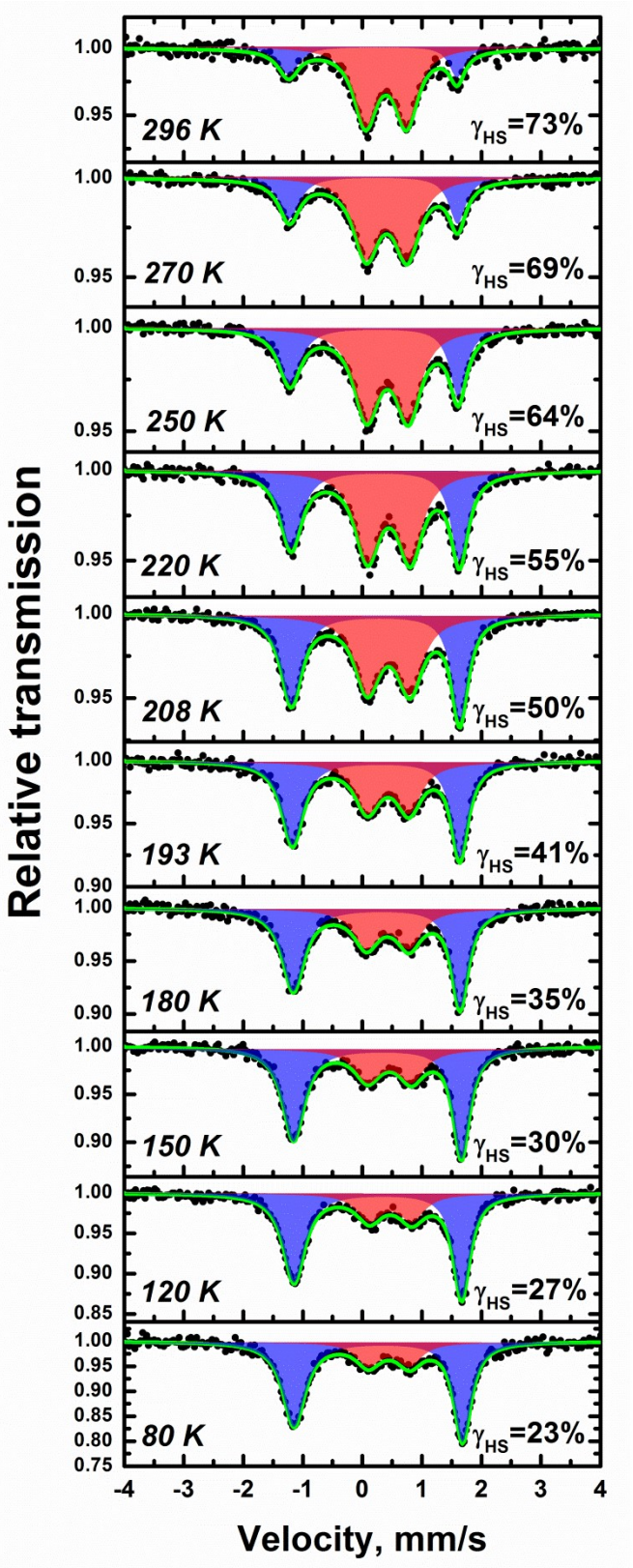

Figure S9. Mössbauer spectra for the salt **1** in the temperature range 296-80 K in cooling mode. Fit line colored in green. A doublet highlighted in red corresponds to Fe(III) ions in the HS state (S=5/2), whereas the doublet highlighted in blue corresponds to Fe(III) ions in the LS state (S=1/2).

Table S2. Mössbauer parameters for spectra of $[Et_4N][^{57}Fe(5Cl\text{-}thsa)_2]$ salt in the temperature range 296-80 K in cooling mode.

T., K	ΔE_Q, mm/s		δ, mm/s		Γ, mm/s			γ_{HS}, %
	HS	LS	HS	LS	HS	LS		
						—	+	
296	0.689(6)	2.83(1)	0.397(4)	0.176(7)	0.464(9)	0.42(4)	0.31(2)	73
270	0.686(4)	2.823(6)	0.409(2)	0.187(3)	0.518(6)	0.42(1)	0.34(1)	69
250	0.702(5)	2.83(1)	0.423(4)	0.197(7)	0.515(7)	0.44(4)	0.35(2)	64
220	0.720(4)	2.830(4)	0.446(3)	0.218(2)	0.500(7)	0.44(1)	0.353(8)	55
208	0.715(4)	2.828(3)	0.443(3)	0.223(1)	0.517(7)	0.429(7)	0.333(5)	50
193	0.697(8)	2.809(9)	0.435(5)	0.232(2)	0.52(1)	0.433(9)	0.344(7)	41
180	0.72(1)	2.800(4)	0.427(6)	0.241(2)	0.53(2)	0.453(9)	0.34(1)	35
150	0.73(1)	2.820(3)	0.458(7)	0.254(2)	0.54(2)	0.447(8)	0.336(6)	30
120	0.71(1)	2.815(3)	0.476(7)	0.261(1)	0.53(2)	0.443(7)	0.340(5)	27
80	0.69(1)	2.830(3)	0.448(7)	0.269(1)	0.50(2)	0.457(7)	0.351(5)	23

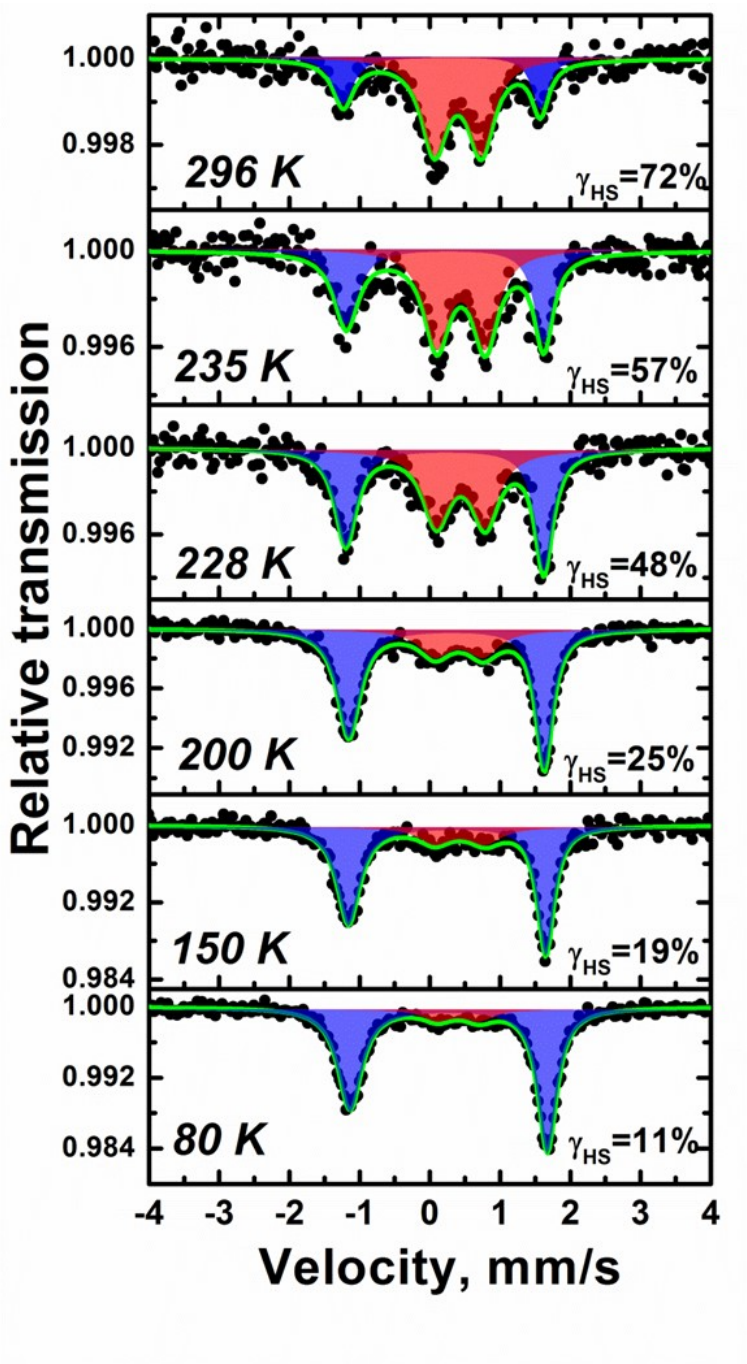

Figure S10. Mössbauer spectra for the salt **1´** recrystallized from acetonitrile at the temperature range 296–80 K in cooling mode. Fit line colored in green. A doublet highlighted in red corresponds to Fe(III) ions in the HS state (S=5/2), whereas the doublet highlighted in blue corresponds to Fe(III) ions in the LS state (S=1/2).

Table S3. Mössbauer parameters for spectra of salt **1** from acetonitrile solution at the temperature range 296–80 K in cooling mode.

T, K	ΔE_Q, mm/s		δ, mm/s		Γ, mm/s			γ_{HS},%
	HS	LS	HS	LS	HS	LS		
						–	+	
296	0.67(1)	2.81(1)	0.399(7)	0.169(9)	0.45(2)	0.36(4)	0.29(4)	72
235	0.69(1)	2.81(1)	0.445(7)	0.216(7)	0.44(2)	0.42(3)	0.33(2)	57
228	0.70(1)	2.821(9)	0.442(9)	0.213(5)	0.47(2)	0.37(2)	0.31(2)	48
200	0.68(2)	2.786(3)	0.42(1)	0.238(2)	0.56(3)	0.400(8)	0.297(6)	25
150	0.72(4)	2.810(4)	0.43(2)	0.247(2)	0.57(6)	0.40(1)	0.292(8)	19
80	0.60(3)	2.810(3)	0.41(2)	0.268(1)	0.52(6)	0.419(7)	0.334(4)	11

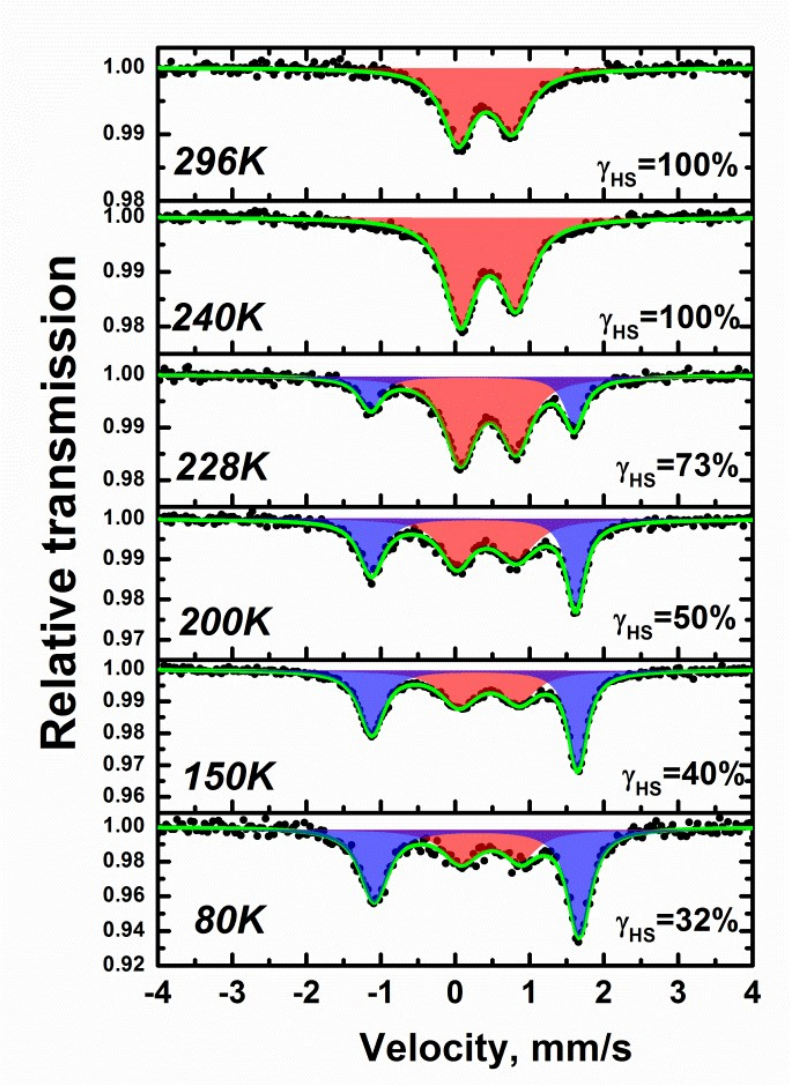

Figure S11. Mössbauer spectra for the GO-**1** hybrid film in the temperature range 296-80 K in cooling mode. Fit line colored in green. A doublet highlighted in red corresponds to Fe(III) ions

in the HS state (S=5/2), whereas the doublet highlighted in blue corresponds to Fe(III) ions in the LS state (S=1/2).

Table S4. Mössbauer parameters for spectra of GO-**1** hybrid film in the temperature range temperature range 296-80 K in cooling mode.

T., K	ΔE_Q, mm/s		δ, mm/s		Γ, mm/s		γ_{HS},%
	HS	LS	HS	LS	HS	LS	
296	0.732(6)	—	0.404(4)	—	0.50(2) 0.55(2)	—	100
240	0.752(3)	—	0.446(2)	—	0.51(1)	—	100
228	0.751(4)	2.735(7)	0.446(2)	0.232(4)	0.50(1) 0.49(1)	0.37(2) 0.33(1)	73
200	0.81(1)	2.747(4)	0.422(6)	0.248(2)	0.51(2) 0.63(3)	0.39(1) 0.30(1)	50
150	0.82(1)	2.768(2)	0.459(5)	0.264(1)	0.59(2) 0.57(2)	0.40(1) 0.30(1)	40
80	0.81(2)	2.757(6)	0.480(9)	0.291(3)	0.59(5) 0.54(6)	0.45(2) 0.37(1)	32

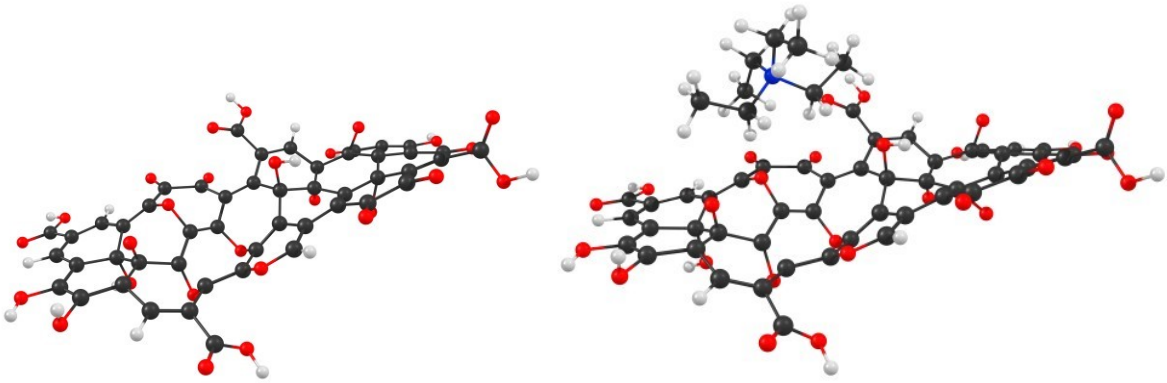

Figure S12. Optimized geometries of isolated GO (left) and $[Et_4N]^+$-GO (right) system with (C/O=1.82). Calculations were performed at the M062X/6-31G(d,p) theory level.

Table S5. Electronic energy (Eel), zero-point vibration energy (E_{ZPV}) for $[Et_4N]$+, GO and $[Et_4N]^+$ on the GO surface (C/O=1.82). Interaction energy of $[Et_4N]^+$ with the GO surface is E(ads). Calculations were performed with 6-31G(d,p) basis set.

Functional	$[Et_4N]^+$···GO system		GO		$[Et_4N]^+$ cation		E(ads), kJ/mol
	E_{el}, a.u.	E_{ZPV}, a.u.	E_{el}, a.u.	E_{ZPV}, a.u.	E_{el}, a.u.	E_{ZPV}, a.u.	
M06-2X	-4277.378423	0.881768	-3906.088594	0.598170	-371.251737	0.280674	**-92**
wB97XD	-4277.645072	0.881276	-3906.245394	0.597557	-371.3556706	0.281173	**-109**
B97D	-4276.150537	0.841155	-3904.896192	0.565876	-371.2083175	0.273976	**-117**

Table S6. Electronic energy (E_{el}), zero-point vibration energy (E_{ZPV}), total energy (E_0) and relative energy E_0(wB97XD) of the optimized (wB97XD/6-31G(d,p)) GO-**1** hybrid system.

State	E_{el}, a.u.	E_{ZPV}, a.u.	E_0(wB97XD), kJ/mol
HS1	-8353.809758	1.161034	-17.7
LS1	-8353.804501	1.162514	0
LS2	-8353.801163	1.164184	13.2

Table S7. Electronic energy (E_{el}) and relative electronic energy E_0(B3LYP*) of the single point calculation by B3LYP* functional of the optimized GO-**1** hybrid system in wB97XD functional.

State	E_{el}, a.u.	E_{el}(B3LYP*), kJ/mol
HS	-8351.72	14.7
LS1	-8351.73	0
LS2	-8351.71	41.28

Table S8. Electronic energy (E_{el}), zero-point vibration energy (E_{ZPV}), total energy (E_0) and total energy difference between the HS and LS states (ΔE_0(HS-LS)) of the optimized **1** isolated molecule.

Функционал	E_{el}, a.u.		E_{ZPV}, a.u.		ΔE_0(HS-LS), kJ/mol
	HS	LS	HS	LS	
B3LYP*	-4446.5197925	-4446.5249792	0.547761	0.550093	**16**
wB97XD	-4447.515352	-4447.5133741	0.560890	0.562801	**-3**

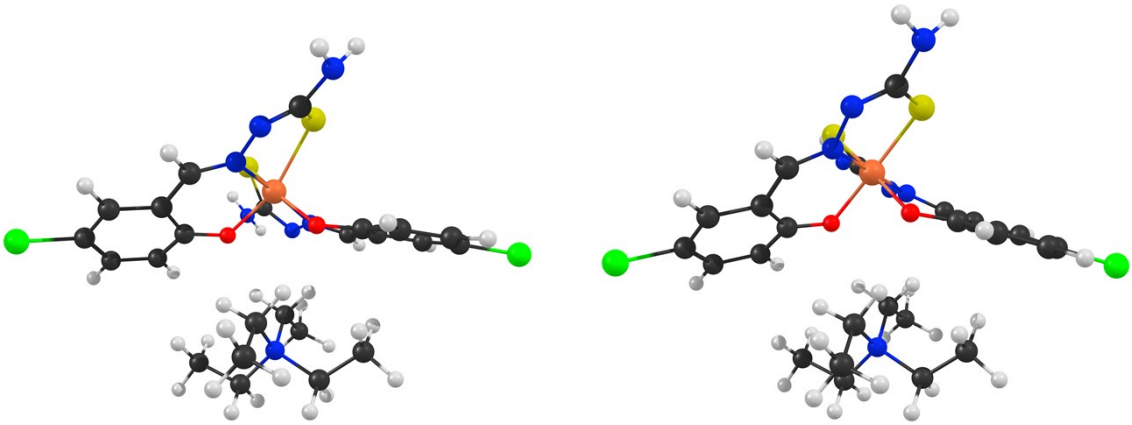

Figure S13. Optimized structures of isolated $[Et_4N][Fe(5Cl\text{-}thsa)_2]$ complex in HS (left) and LS (right) state. Calculations were performed at the wB97XD /6-31G(d,p) theory level.

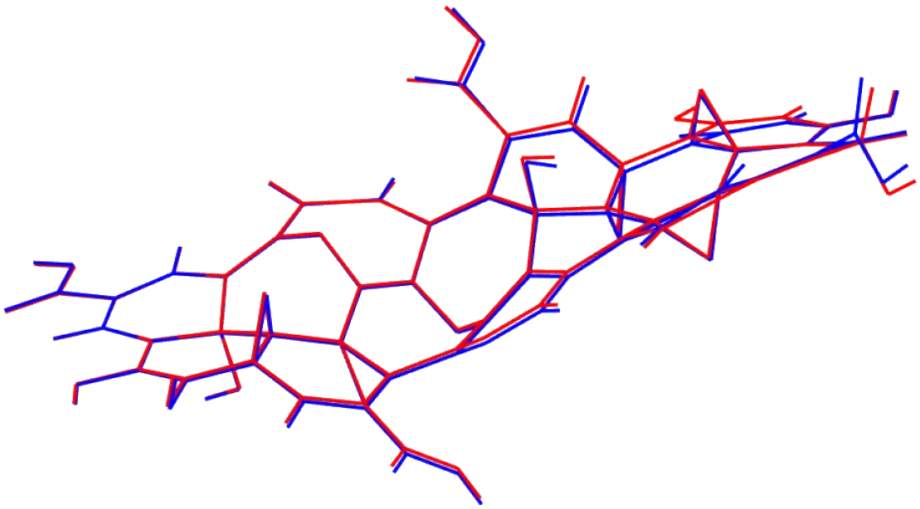

Figure S14. The overlay of GO from optimized structures of GO-**1** hybrid system in HS (red) and LS (blue) state. Calculations were performed at the wB97XD /6-31G(d,p) theory level.

Table S9. Table of parameters of Fe(III)-ligand bond lengths and the angle α value between the phenoxy planes of the 5Cl-thsa^{2-} ligand for optimized HS and LS states of the GO-**1** hybrid system and **1** isolated complex.

Optimized structure	Spin state	Functional	Structural parameter			
			Fe–S, Å	Fe–N, Å	Fe–O, Å	α, °
1	HS	B3LYP*	2.45291 2.48532	2.18936 2.23419	1.97259 1.98258	112.7
	LS		2.28226 2.29059	1.94822 1.95184	1.93688 1.94254	126.5
	HS	wB97XD	2.41658 2.46727	2.16470 2.16528	1.93835 1.96562	142.3
	LS		2.26437 2.27919	1.95431 1.95557	1.91865 1.92768	131.2
GO-**1**	HS1		2.39133 2.51982	2.16898 2.19331	1.89934 2.00681	151.0
	LS1		2.26494 2.28483	1.94904 1.95330	1.91211 1.93925	129.1
	LS2		2.27035 2.27231	1.95003 1.95004	1.90987 1.94792	129.8

Table S10. Optimized coordinates (B97D/6-31G(d,p)) of $[Et_4N]^+$ cation in the singlet state. Units are in Å.

C	0.000017000000	1.232408000000	0.918271000000
H	0.885101000000	1.124829000000	1.554600000000
H	-0.885042000000	1.124823000000	1.554631000000
N	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	2.579751000000	0.202161000000
H	0.000078000000	3.359859000000	0.975390000000
H	-0.895354000000	2.728085000000	-0.414646000000
H	0.895269000000	2.728041000000	-0.414781000000
C	1.232408000000	-0.000017000000	-0.918271000000
H	1.124829000000	-0.885101000000	-1.554600000000
H	1.124823000000	0.885042000000	-1.554631000000
C	-2.579751000000	0.000000000000	-0.202161000000
H	-2.728041000000	0.895269000000	0.414781000000
H	-2.728085000000	-0.895354000000	0.414646000000
H	-3.359859000000	0.000078000000	-0.975390000000
C	-0.000017000000	-1.232408000000	0.918271000000
H	0.885042000000	-1.124823000000	1.554631000000
H	-0.885101000000	-1.124829000000	1.554600000000
C	-1.232408000000	0.000017000000	-0.918271000000
H	-1.124829000000	0.885101000000	-1.554600000000
H	-1.124823000000	-0.885042000000	-1.554631000000
C	2.579751000000	0.000000000000	-0.202161000000
H	2.728085000000	0.895354000000	0.414646000000
H	3.359859000000	-0.000078000000	-0.975390000000
H	2.728041000000	-0.895269000000	0.414781000000
C	0.000000000000	-2.579751000000	0.202161000000
H	0.895354000000	-2.728085000000	-0.414646000000
H	-0.895269000000	-2.728041000000	-0.414781000000
H	-0.000078000000	-3.359859000000	0.975390000000

Table S11. Optimized coordinates (wB97XD/6-31G(d,p)) of $[Et_4N]^+$ cation in the singlet state. Units are in Å.

C	-1.216145000000	0.000135000000	0.910024000000
H	-1.114338000000	0.877308000000	1.550204000000
H	-1.114336000000	-0.876807000000	1.550523000000
N	0.000000000000	0.000000000000	0.000000000000
C	-2.564584000000	0.000000000000	0.213657000000
H	-3.331537000000	0.000376000000	0.991319000000
H	-2.728870000000	-0.890306000000	-0.396620000000
H	-2.728708000000	0.889851000000	-0.397328000000
C	0.000135000000	1.216145000000	-0.910024000000
H	0.877308000000	1.114338000000	-1.550204000000
H	-0.876807000000	1.114336000000	-1.550523000000
C	0.000000000000	-2.564584000000	-0.213657000000
H	-0.889851000000	-2.728708000000	0.397328000000
H	0.890306000000	-2.728870000000	0.396620000000
H	-0.000376000000	-3.331537000000	-0.991319000000
C	1.216145000000	-0.000135000000	0.910024000000
H	1.114336000000	0.876807000000	1.550523000000
H	1.114338000000	-0.877308000000	1.550204000000
C	-0.000135000000	-1.216145000000	-0.910024000000
H	-0.877308000000	-1.114338000000	-1.550204000000
H	0.876807000000	-1.114336000000	-1.550523000000
C	0.000000000000	2.564584000000	-0.213657000000
H	-0.890306000000	2.728870000000	0.396620000000
H	0.000376000000	3.331537000000	-0.991319000000
H	0.889851000000	2.728708000000	0.397328000000
C	2.564584000000	0.000000000000	0.213657000000
H	2.728870000000	0.890306000000	-0.396620000000
H	2.728708000000	-0.889851000000	-0.397328000000
H	3.331537000000	-0.000376000000	0.991319000000

Table S12. Optimized coordinates (M062-2X/6-31G(d,p)) of $[Et_4N]^+$ cation in the singlet state. Units are in Å.

C	0.000024000000	1.215417000000	0.909482000000
H	0.878372000000	1.111415000000	1.548905000000
H	-0.878278000000	1.111421000000	1.548971000000
N	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	2.559875000000	0.205662000000
H	0.000202000000	3.331782000000	0.978536000000
H	-0.890535000000	2.718823000000	-0.405945000000
H	0.890331000000	2.718695000000	-0.406279000000
C	1.215417000000	-0.000024000000	-0.909482000000
H	1.111415000000	-0.878372000000	-1.548905000000
H	1.111421000000	0.878278000000	-1.548971000000
C	-2.559875000000	0.000000000000	-0.205662000000
H	-2.718695000000	0.890331000000	0.406279000000
H	-2.718823000000	-0.890535000000	0.405945000000
H	-3.331782000000	0.000202000000	-0.978536000000
C	-0.000024000000	-1.215417000000	0.909482000000
H	0.878278000000	-1.111421000000	1.548971000000
H	-0.878372000000	-1.111415000000	1.548905000000
C	-1.215417000000	0.000024000000	-0.909482000000
H	-1.111415000000	0.878372000000	-1.548905000000
H	-1.111421000000	-0.878278000000	-1.548971000000
C	2.559875000000	0.000000000000	-0.205662000000
H	2.718823000000	0.890535000000	0.405945000000
H	3.331782000000	-0.000202000000	-0.978536000000
H	2.718695000000	-0.890331000000	0.406279000000
C	0.000000000000	-2.559875000000	0.205662000000
H	0.890535000000	-2.718823000000	-0.405945000000
H	-0.890331000000	-2.718695000000	-0.406279000000
H	-0.000202000000	-3.331782000000	0.978536000000

Table S13. Optimized coordinates (B97D/6-31G(d,p)) of GO in the singlet state. Units are in Å.

C	-6.281777000000	-2.472003000000	-0.188991000000
C	-5.261023000000	-1.466590000000	-0.283689000000
C	-3.949174000000	-1.805874000000	-0.547503000000
C	-3.261040000000	-3.106317000000	-0.282395000000
C	-1.699413000000	-3.129827000000	0.221123000000
C	-7.616426000000	-2.114698000000	-0.232087000000
C	2.609930000000	-3.083225000000	-0.253178000000
C	3.378048000000	-2.009826000000	0.423956000000
C	4.882298000000	-2.132305000000	0.343903000000
C	5.528902000000	-3.248448000000	1.093788000000
C	6.865980000000	-3.230109000000	1.366895000000
C	1.272274000000	-3.000266000000	-0.474172000000
C	2.778046000000	-0.653721000000	0.434258000000
C	1.341199000000	-0.512294000000	-0.107367000000
C	0.833011000000	0.842797000000	0.434765000000
C	1.593084000000	1.995693000000	0.018719000000
C	2.971031000000	1.824260000000	-0.319980000000
C	3.650266000000	0.607639000000	0.243342000000
C	-0.338117000000	1.060935000000	1.140068000000
C	0.841259000000	3.187703000000	-0.086234000000
C	-1.079053000000	2.241742000000	0.928852000000
C	3.717124000000	2.880401000000	-0.965532000000
C	0.509234000000	-1.835992000000	0.020806000000
C	-0.832591000000	-1.888108000000	0.295355000000
C	-1.526292000000	-0.704559000000	0.792026000000
C	-2.611477000000	-0.164974000000	0.210835000000
C	-3.346137000000	1.048176000000	0.611446000000
C	-2.570637000000	2.326225000000	0.987260000000
C	-3.243978000000	3.645333000000	0.721030000000
C	-5.687166000000	-0.012461000000	0.119467000000
C	-7.115995000000	0.292027000000	-0.345901000000
C	-7.528857000000	1.658073000000	-0.580856000000
C	-6.638962000000	2.701841000000	-0.620870000000
C	-5.189532000000	2.513497000000	-0.413559000000
C	-4.677896000000	1.149199000000	-0.147973000000
C	-4.435409000000	3.697220000000	0.084499000000
C	-8.019307000000	-0.739265000000	-0.400426000000
C	7.997139000000	0.233268000000	0.108597000000
C	7.280302000000	1.353686000000	-0.617557000000
C	7.703725000000	-2.093268000000	1.045936000000
C	7.182102000000	-0.934251000000	0.482376000000
C	5.748607000000	-0.936229000000	0.091355000000
C	5.111014000000	0.433254000000	0.070245000000
C	5.923576000000	1.478706000000	-0.625864000000
C	5.235988000000	2.663427000000	-1.232908000000
O	1.364048000000	-0.360620000000	-1.542315000000
O	9.020774000000	-2.173079000000	1.341853000000
O	-8.854271000000	1.855995000000	-0.824684000000
O	-3.075207000000	-0.795013000000	-0.934951000000
H	2.031222000000	0.321301000000	-1.758779000000
C	8.214820000000	2.314994000000	-1.313475000000
O	8.694560000000	2.069122000000	-2.402912000000
O	8.502246000000	3.394310000000	-0.552490000000
H	9.114247000000	3.943493000000	-1.079216000000
H	9.218341000000	-3.054156000000	1.698007000000
C	-8.708690000000	-3.137459000000	-0.216947000000
O	-9.898222000000	-2.873377000000	-0.319374000000
O	-8.243631000000	-4.411072000000	-0.064145000000
H	-9.031899000000	-4.984610000000	-0.073736000000
C	0.631232000000	-3.969032000000	-1.427639000000

O	-0.336591000000	-3.713839000000	-2.125956000000
O	1.289945000000	-5.159720000000	-1.483282000000
H	0.829254000000	-5.679893000000	-2.167920000000
C	-2.723876000000	4.931216000000	1.299702000000
O	-3.073087000000	6.042701000000	0.939972000000
O	-1.846811000000	4.710747000000	2.319251000000
H	-1.582051000000	5.590730000000	2.647226000000
O	4.566579000000	0.843532000000	1.360352000000
O	-4.513735000000	1.665258000000	-1.462826000000
O	-0.908379000000	0.003419000000	1.822100000000
O	4.676555000000	-4.230437000000	1.477543000000
H	5.137708000000	-4.863025000000	2.053157000000
O	-5.684371000000	-0.030565000000	1.574178000000
H	-6.390241000000	-0.640199000000	1.847716000000
O	5.377732000000	-1.862557000000	-0.988535000000
H	-8.976136000000	2.803717000000	-1.013401000000
H	-4.921035000000	4.669700000000	0.006708000000
H	7.319365000000	-4.079328000000	1.886224000000
H	3.178262000000	-3.911176000000	-0.668219000000
H	-5.986724000000	-3.517480000000	-0.206835000000
H	-9.070317000000	-0.540552000000	-0.595621000000
H	1.209401000000	4.108741000000	-0.522186000000
O	5.842547000000	3.471830000000	-1.926256000000
O	3.221452000000	3.956108000000	-1.347677000000
O	-0.458195000000	3.240520000000	0.268209000000
O	-3.811547000000	-4.194346000000	-0.331155000000
O	-7.154912000000	3.967201000000	-0.867450000000
H	-6.604378000000	4.412965000000	-1.531457000000
O	9.205056000000	0.356745000000	0.337328000000
O	2.866066000000	-1.404854000000	1.649356000000
O	-1.309618000000	-4.208720000000	0.624736000000
O	-3.236384000000	1.493024000000	1.964792000000

Table S14. Optimized coordinates (wB97XD/6-31G(d,p)) of GO in the singlet state. Units are in Å.

C	6.193337000000	-2.476242000000	0.054075000000
C	5.179818000000	-1.450541000000	0.218816000000
C	3.906745000000	-1.772390000000	0.537242000000
C	3.204834000000	-3.079597000000	0.316084000000
C	1.686862000000	-3.097775000000	-0.216244000000
C	7.499945000000	-2.137218000000	0.135113000000
C	-2.551295000000	-3.062840000000	0.325069000000
C	-3.326940000000	-2.012270000000	-0.377248000000
C	-4.821756000000	-2.137861000000	-0.298018000000
C	-5.455307000000	-3.274056000000	-1.015219000000
C	-6.772469000000	-3.274521000000	-1.301792000000
C	-1.233793000000	-2.955302000000	0.538810000000
C	-2.743824000000	-0.662713000000	-0.406897000000
C	-1.323230000000	-0.495345000000	0.128751000000
C	-0.824605000000	0.855386000000	-0.418950000000
C	-1.582587000000	1.985220000000	-0.001682000000
C	-2.952519000000	1.792516000000	0.329158000000
C	-3.614583000000	0.586084000000	-0.249609000000
C	0.338516000000	1.081685000000	-1.120501000000
C	-0.835483000000	3.163763000000	0.128251000000
C	1.063157000000	2.245581000000	-0.876698000000
C	-3.701902000000	2.859399000000	0.913038000000
C	-0.484808000000	-1.798276000000	0.007627000000
C	0.827618000000	-1.858324000000	-0.297674000000
C	1.516381000000	-0.670838000000	-0.796615000000
C	2.577948000000	-0.141163000000	-0.207342000000
C	3.311575000000	1.075042000000	-0.595592000000
C	2.554230000000	2.337684000000	-0.946118000000
C	3.225690000000	3.641704000000	-0.649359000000
C	5.618520000000	-0.009617000000	-0.152617000000
C	7.034531000000	0.255563000000	0.335436000000
C	7.461633000000	1.622677000000	0.598229000000
C	6.603251000000	2.657024000000	0.657823000000
C	5.150278000000	2.484017000000	0.458113000000
C	4.635828000000	1.146191000000	0.144998000000
C	4.403270000000	3.681757000000	-0.018620000000
C	7.911709000000	-0.765199000000	0.383924000000
C	-7.927292000000	0.189349000000	-0.146625000000
C	-7.224749000000	1.335942000000	0.540454000000
C	-7.615866000000	-2.130607000000	-1.015158000000
C	-7.106112000000	-0.975713000000	-0.485355000000
C	-5.685212000000	-0.953805000000	-0.084863000000
C	-5.063198000000	0.409506000000	-0.098748000000
C	-5.888530000000	1.460272000000	0.557484000000
C	-5.217053000000	2.662557000000	1.138134000000
O	-1.353940000000	-0.330707000000	1.537814000000
O	-8.913284000000	-2.223648000000	-1.316471000000
O	8.779389000000	1.791056000000	0.821142000000
O	3.044731000000	-0.772014000000	0.915746000000
H	-2.005881000000	0.357422000000	1.746622000000
C	-8.170355000000	2.319733000000	1.175151000000
O	-8.666904000000	2.137455000000	2.255627000000
O	-8.438600000000	3.350886000000	0.372150000000
H	-9.053408000000	3.921567000000	0.854269000000
H	-9.115952000000	-3.101829000000	-1.651921000000
C	8.579069000000	-3.160228000000	0.064545000000
O	9.753685000000	-2.911670000000	0.210524000000
O	8.119324000000	-4.396178000000	-0.184611000000
H	8.889977000000	-4.979350000000	-0.199049000000

C	-0.570026000000	-3.883243000000	1.502913000000
O	0.461885000000	-3.643910000000	2.086437000000
O	-1.271975000000	-5.005713000000	1.708382000000
H	-0.785807000000	-5.509097000000	2.375600000000
C	2.703350000000	4.927128000000	-1.202762000000
O	3.074354000000	6.021016000000	-0.854148000000
O	1.798826000000	4.727841000000	-2.174591000000
H	1.530670000000	5.600345000000	-2.494755000000
O	-4.504124000000	0.789973000000	-1.362058000000
O	4.487356000000	1.643484000000	1.453681000000
O	0.904992000000	0.043028000000	-1.801999000000
O	-4.590958000000	-4.244145000000	-1.350073000000
H	-5.013357000000	-4.900877000000	-1.913599000000
O	5.613462000000	0.019443000000	-1.583489000000
H	6.360268000000	-0.500620000000	-1.899348000000
O	-5.321397000000	-1.830379000000	1.000687000000
H	8.921406000000	2.736526000000	0.964652000000
H	4.889368000000	4.645813000000	0.091258000000
H	-7.215965000000	-4.132090000000	-1.803303000000
H	-3.104450000000	-3.884195000000	0.762913000000
H	5.886463000000	-3.512801000000	-0.017350000000
H	8.954598000000	-0.584894000000	0.615922000000
H	-1.202187000000	4.067571000000	0.590166000000
O	-5.838282000000	3.489024000000	1.766216000000
O	-3.220214000000	3.935551000000	1.268586000000
O	0.451319000000	3.211012000000	-0.213467000000
O	3.740926000000	-4.153056000000	0.419539000000
O	7.116382000000	3.916520000000	0.904236000000
H	6.796445000000	4.230687000000	1.757776000000
O	-9.120804000000	0.293166000000	-0.369568000000
O	-2.821671000000	-1.435842000000	-1.586327000000
O	1.307802000000	-4.162106000000	-0.629868000000
O	3.195246000000	1.528070000000	-1.923280000000

Table S15. Optimized coordinates (M062-2X/6-31G(d,p)) of GO in the singlet state. Units are in Å.

C	6.207404000000	-2.475105000000	0.013989000000
C	5.198499000000	-1.450317000000	0.219426000000
C	3.931719000000	-1.772086000000	0.560632000000
C	3.224057000000	-3.078907000000	0.342434000000
C	1.692074000000	-3.099276000000	-0.150895000000
C	7.515136000000	-2.129551000000	0.060540000000
C	-2.552827000000	-3.072756000000	0.327363000000
C	-3.327774000000	-2.021260000000	-0.377035000000
C	-4.820721000000	-2.146458000000	-0.290442000000
C	-5.455058000000	-3.291830000000	-0.989720000000
C	-6.779258000000	-3.314044000000	-1.240675000000
C	-1.235363000000	-2.961575000000	0.543401000000
C	-2.744815000000	-0.666713000000	-0.401784000000
C	-1.327875000000	-0.498984000000	0.139123000000
C	-0.824564000000	0.854911000000	-0.398309000000
C	-1.590738000000	1.987362000000	0.011219000000
C	-2.966729000000	1.801781000000	0.307148000000
C	-3.620007000000	0.581270000000	-0.255725000000
C	0.345084000000	1.081064000000	-1.087064000000
C	-0.836869000000	3.165320000000	0.158721000000
C	1.069926000000	2.247161000000	-0.837588000000
C	-3.726800000000	2.887911000000	0.846504000000
C	-0.484294000000	-1.801167000000	0.022149000000
C	0.836170000000	-1.857571000000	-0.253666000000
C	1.531025000000	-0.672959000000	-0.752426000000
C	2.594820000000	-0.143164000000	-0.165980000000
C	3.324353000000	1.074074000000	-0.560203000000
C	2.559408000000	2.340286000000	-0.902133000000
C	3.229735000000	3.642108000000	-0.593222000000
C	5.630122000000	-0.007642000000	-0.151764000000
C	7.055120000000	0.257522000000	0.310236000000
C	7.486011000000	1.621970000000	0.579672000000
C	6.629317000000	2.656231000000	0.660725000000
C	5.171639000000	2.484008000000	0.482174000000
C	4.653941000000	1.144150000000	0.166043000000
C	4.416164000000	3.684670000000	0.020322000000
C	7.937046000000	-0.761185000000	0.319095000000
C	-7.949532000000	0.161055000000	-0.128950000000
C	-7.244173000000	1.338499000000	0.499661000000
C	-7.627722000000	-2.173723000000	-0.948956000000
C	-7.118243000000	-1.003136000000	-0.458526000000
C	-5.692847000000	-0.961603000000	-0.076199000000
C	-5.075256000000	0.402860000000	-0.112671000000
C	-5.909617000000	1.470560000000	0.504995000000
C	-5.250588000000	2.711969000000	1.022355000000
O	-1.373170000000	-0.345217000000	1.549589000000
O	-8.933255000000	-2.284243000000	-1.216479000000
O	8.810106000000	1.784049000000	0.783445000000
O	3.072016000000	-0.772793000000	0.957149000000
H	-2.028369000000	0.339148000000	1.765675000000
C	-8.193418000000	2.354411000000	1.080766000000
O	-8.678827000000	2.245147000000	2.172731000000
O	-8.472726000000	3.325566000000	0.208586000000
H	-9.092301000000	3.927193000000	0.650204000000
H	-9.137880000000	-3.172362000000	-1.530968000000
C	8.593348000000	-3.151672000000	-0.050484000000
O	9.768467000000	-2.902842000000	0.065750000000
O	8.125032000000	-4.385275000000	-0.298680000000
H	8.893701000000	-4.973714000000	-0.340097000000

C	-0.577961000000	-3.885259000000	1.519767000000
O	0.427531000000	-3.627183000000	2.134474000000
O	-1.264736000000	-5.023209000000	1.693825000000
H	-0.791547000000	-5.526468000000	2.373957000000
C	2.690870000000	4.931879000000	-1.126192000000
O	3.063954000000	6.021208000000	-0.775036000000
O	1.771069000000	4.734013000000	-2.084547000000
H	1.493740000000	5.607768000000	-2.401493000000
O	-4.501756000000	0.761825000000	-1.371341000000
O	4.526872000000	1.637700000000	1.474476000000
O	0.923448000000	0.041843000000	-1.762066000000
O	-4.577687000000	-4.244775000000	-1.347088000000
H	-4.997964000000	-4.907449000000	-1.910120000000
O	5.599117000000	0.029137000000	-1.581165000000
H	6.323482000000	-0.518111000000	-1.913281000000
O	-5.311122000000	-1.824838000000	1.004905000000
H	8.965085000000	2.729612000000	0.926458000000
H	4.898762000000	4.651719000000	0.128953000000
H	-7.224158000000	-4.179341000000	-1.727155000000
H	-3.106616000000	-3.896646000000	0.763082000000
H	5.904749000000	-3.513493000000	-0.060032000000
H	8.986344000000	-0.583820000000	0.526361000000
H	-1.198052000000	4.071287000000	0.620312000000
O	-5.890261000000	3.580228000000	1.565264000000
O	-3.247385000000	3.964392000000	1.195202000000
O	0.452092000000	3.208282000000	-0.173928000000
O	3.762541000000	-4.150373000000	0.424604000000
O	7.142348000000	3.915772000000	0.904529000000
H	6.824091000000	4.234623000000	1.760483000000
O	-9.148208000000	0.241690000000	-0.318025000000
O	-2.821310000000	-1.440372000000	-1.577658000000
O	1.294603000000	-4.174700000000	-0.508192000000
O	3.199663000000	1.534907000000	-1.880253000000

Table S16. Optimized coordinates (B97D/6-31G(d,p)) of $[Et_4N]^+$-GO system in the singlet state. Units are in Å.

C	6.042363000000	-2.308611000000	-0.739707000000
C	5.003966000000	-1.330926000000	-0.586137000000
C	3.694505000000	-1.711473000000	-0.373084000000
C	3.015897000000	-2.986127000000	-0.725915000000
C	1.429773000000	-2.993068000000	-1.146554000000
C	7.369200000000	-1.931815000000	-0.641357000000
C	-2.863058000000	-2.990824000000	-0.523945000000
C	-3.666884000000	-1.870928000000	-1.070703000000
C	-5.161820000000	-2.002625000000	-0.889728000000
C	-5.869994000000	-3.049417000000	-1.682767000000
C	-7.223545000000	-3.008799000000	-1.846415000000
C	-1.516507000000	-2.917458000000	-0.351347000000
C	-3.062451000000	-0.517417000000	-1.009080000000
C	-1.595392000000	-0.408314000000	-0.546349000000
C	-1.114045000000	0.979329000000	-1.025391000000
C	-1.847397000000	2.096493000000	-0.483025000000
C	-3.187517000000	1.880570000000	-0.037962000000
C	-3.917970000000	0.718938000000	-0.651925000000
C	0.019866000000	1.246906000000	-1.774345000000
C	-1.107535000000	3.294561000000	-0.366876000000
C	0.765460000000	2.417557000000	-1.527159000000
C	-3.857803000000	2.847909000000	0.802827000000
C	-0.772278000000	-1.719804000000	-0.788639000000
C	0.557789000000	-1.750797000000	-1.127227000000
C	1.223052000000	-0.530319000000	-1.576774000000
C	2.320324000000	-0.022002000000	-0.991548000000
C	3.045782000000	1.217876000000	-1.312649000000
C	2.255815000000	2.509190000000	-1.608639000000
C	2.919971000000	3.815648000000	-1.269543000000
C	5.407064000000	0.159774000000	-0.873660000000
C	6.823877000000	0.451997000000	-0.366463000000
C	7.216155000000	1.804150000000	-0.042032000000
C	6.308346000000	2.833406000000	0.055643000000
C	4.867668000000	2.638529000000	-0.191038000000
C	4.375340000000	1.286522000000	-0.540703000000
C	4.104614000000	3.841663000000	-0.620925000000
C	7.744384000000	-0.567554000000	-0.369005000000
C	-8.232344000000	0.309409000000	-0.159346000000
C	-7.449385000000	1.356627000000	0.612448000000
C	-8.028336000000	-1.910110000000	-1.349599000000
C	-7.456534000000	-0.809489000000	-0.718506000000
C	-5.997027000000	-0.839552000000	-0.454497000000
C	-5.357399000000	0.525456000000	-0.363138000000
C	-6.097563000000	1.494813000000	0.503332000000
C	-5.354262000000	2.606682000000	1.173093000000
O	-1.557660000000	-0.338640000000	0.905286000000
O	-9.361814000000	-1.960097000000	-1.540131000000
O	8.532898000000	1.999908000000	0.224270000000
O	2.806111000000	-0.738968000000	0.095688000000
H	-2.213388000000	0.341905000000	1.171079000000
C	-8.312048000000	2.213986000000	1.508139000000
O	-8.651545000000	1.826519000000	2.609131000000
O	-8.695505000000	3.361057000000	0.914745000000
H	-9.263181000000	3.832474000000	1.554955000000
H	-9.604165000000	-2.795728000000	-1.971141000000
C	8.485505000000	-2.934374000000	-0.704381000000
O	9.661586000000	-2.649582000000	-0.542912000000
O	8.045634000000	-4.194644000000	-0.968881000000
H	8.838650000000	-4.762135000000	-0.995999000000

C	-0.846365000000	-3.960411000000	0.490701000000
O	0.085190000000	-3.731423000000	1.256581000000
O	-1.424521000000	-5.176214000000	0.380112000000
H	-0.953963000000	-5.768710000000	0.996360000000
C	2.389183000000	5.131548000000	-1.777717000000
O	2.731419000000	6.217534000000	-1.345768000000
O	1.519836000000	4.957185000000	-2.807877000000
H	1.251832000000	5.847831000000	-3.104855000000
O	-4.918137000000	1.046300000000	-1.657091000000
O	4.181797000000	1.708467000000	0.808721000000
O	0.569917000000	0.233856000000	-2.537660000000
O	-5.049325000000	-3.989743000000	-2.212874000000
H	-5.549306000000	-4.572951000000	-2.808435000000
O	5.412146000000	0.246188000000	-2.321432000000
H	6.153904000000	-0.294086000000	-2.642713000000
O	-5.530846000000	-1.858761000000	0.503358000000
H	8.663424000000	2.938742000000	0.447845000000
H	4.578034000000	4.814382000000	-0.489396000000
H	-7.722069000000	-3.806927000000	-2.402974000000
H	-3.408577000000	-3.858695000000	-0.161998000000
H	5.767354000000	-3.357458000000	-0.809143000000
H	8.789846000000	-0.366065000000	-0.147698000000
H	-1.459038000000	4.194915000000	0.122252000000
C	1.450940000000	-0.295547000000	5.304795000000
H	2.393491000000	-0.216820000000	5.857831000000
H	0.853921000000	-1.089965000000	5.765926000000
N	1.826856000000	-0.812792000000	3.913438000000
C	0.693836000000	1.029821000000	5.317696000000
H	0.469534000000	1.273954000000	6.364804000000
H	-0.259516000000	0.967354000000	4.778352000000
H	1.287892000000	1.855225000000	4.905243000000
C	2.769376000000	0.167149000000	3.203926000000
H	2.901239000000	-0.223757000000	2.194515000000
H	2.212527000000	1.105702000000	3.117960000000
C	-0.547597000000	-1.787020000000	3.620534000000
H	-0.953508000000	-1.347653000000	4.541408000000
H	-0.247113000000	-2.825405000000	3.802836000000
H	-1.343162000000	-1.806779000000	2.867484000000
C	2.506243000000	-2.173965000000	4.116217000000
H	3.307847000000	-1.996545000000	4.842394000000
H	1.752209000000	-2.809184000000	4.593231000000
C	0.580060000000	-0.956347000000	3.020684000000
H	0.247112000000	0.064124000000	2.808408000000
H	0.923899000000	-1.395517000000	2.081336000000
C	4.117105000000	0.387714000000	3.882531000000
H	4.027108000000	0.852185000000	4.873620000000
H	4.683207000000	1.065846000000	3.231471000000
H	4.694212000000	-0.541833000000	3.972200000000
C	3.048559000000	-2.826742000000	2.848058000000
H	3.813097000000	-2.211692000000	2.358101000000
H	2.253819000000	-3.067534000000	2.134567000000
H	3.522785000000	-3.772063000000	3.145588000000
O	-5.882661000000	3.336833000000	2.002078000000
O	-3.301792000000	3.853555000000	1.278138000000
O	0.169210000000	3.378684000000	-0.788634000000
O	3.578951000000	-4.068730000000	-0.777998000000
O	6.813608000000	4.080633000000	0.370246000000
H	6.210435000000	4.548522000000	0.968863000000
O	-9.453607000000	0.449906000000	-0.263935000000
O	-3.221717000000	-1.169874000000	-2.269146000000
O	1.012160000000	-4.064778000000	-1.540076000000
O	2.920896000000	1.739771000000	-2.634850000000

Table S17. Optimized coordinates (wB97XD/6-31G(d,p)) of $[Et_4N]^+$-GO system in the singlet state. Units are in Å.

C	5.966400000000	-2.322947000000	-0.881063000000
C	4.936218000000	-1.326669000000	-0.645776000000
C	3.670395000000	-1.689327000000	-0.347437000000
C	2.973028000000	-2.979743000000	-0.630631000000
C	1.417741000000	-2.986300000000	-1.049288000000
C	7.264007000000	-1.967985000000	-0.755739000000
C	-2.803892000000	-2.993291000000	-0.403108000000
C	-3.611804000000	-1.898773000000	-0.992465000000
C	-5.098308000000	-2.032231000000	-0.822548000000
C	-5.784536000000	-3.112213000000	-1.576677000000
C	-7.118244000000	-3.094325000000	-1.764263000000
C	-1.479725000000	-2.893511000000	-0.221314000000
C	-3.026494000000	-0.550289000000	-0.957496000000
C	-1.579803000000	-0.410146000000	-0.489379000000
C	-1.106466000000	0.967540000000	-0.987743000000
C	-1.840904000000	2.068820000000	-0.462793000000
C	-3.176295000000	1.842640000000	-0.038541000000
C	-3.884690000000	0.680510000000	-0.655223000000
C	0.022251000000	1.231608000000	-1.730232000000
C	-1.092845000000	3.247470000000	-0.320811000000
C	0.754634000000	2.386306000000	-1.466096000000
C	-3.873932000000	2.851049000000	0.702093000000
C	-0.746578000000	-1.704938000000	-0.700236000000
C	0.556204000000	-1.745271000000	-1.059336000000
C	1.216377000000	-0.528479000000	-1.529799000000
C	2.295978000000	-0.022054000000	-0.953953000000
C	3.016935000000	1.216274000000	-1.289601000000
C	2.243331000000	2.487592000000	-1.569535000000
C	2.905848000000	3.781923000000	-1.216191000000
C	5.349876000000	0.145123000000	-0.919405000000
C	6.758657000000	0.400727000000	-0.407711000000
C	7.168462000000	1.759409000000	-0.078561000000
C	6.293939000000	2.777431000000	0.037588000000
C	4.844966000000	2.591655000000	-0.175111000000
C	4.347383000000	1.265743000000	-0.556313000000
C	4.082316000000	3.804073000000	-0.584541000000
C	7.650621000000	-0.608420000000	-0.413215000000
C	-8.174817000000	0.254724000000	-0.231481000000
C	-7.416441000000	1.344940000000	0.492008000000
C	-7.936075000000	-1.980913000000	-1.319147000000
C	-7.384172000000	-0.871804000000	-0.733663000000
C	-5.937836000000	-0.873325000000	-0.446888000000
C	-5.317761000000	0.490368000000	-0.403314000000
C	-6.083719000000	1.480536000000	0.402804000000
C	-5.366905000000	2.627924000000	1.032675000000
O	-1.558386000000	-0.305264000000	0.933807000000
O	-9.249894000000	-2.049279000000	-1.523336000000
O	8.482615000000	1.931319000000	0.136400000000
O	2.798993000000	-0.723088000000	0.114948000000
H	-2.208270000000	0.379430000000	1.176150000000
C	-8.303750000000	2.249422000000	1.305521000000
O	-8.676571000000	1.951027000000	2.409264000000
O	-8.660931000000	3.342147000000	0.634606000000
H	-9.241389000000	3.853715000000	1.216263000000
H	-9.491840000000	-2.889908000000	-1.923717000000
C	8.368362000000	-2.965805000000	-0.879181000000
O	9.529085000000	-2.698541000000	-0.680583000000
O	7.935092000000	-4.182129000000	-1.233131000000
H	8.711712000000	-4.756081000000	-1.288696000000

C	-0.797247000000	-3.892180000000	0.648904000000
O	0.168716000000	-3.642682000000	1.344691000000
O	-1.395827000000	-5.079295000000	0.648606000000
H	-0.912284000000	-5.648948000000	1.262976000000
C	2.363496000000	5.090355000000	-1.701923000000
O	2.725985000000	6.163688000000	-1.291478000000
O	1.458210000000	4.924965000000	-2.676049000000
H	1.181172000000	5.805196000000	-2.968457000000
O	-4.850446000000	0.962522000000	-1.674685000000
O	4.188018000000	1.685890000000	0.783886000000
O	0.566619000000	0.224488000000	-2.475964000000
O	-4.943193000000	-4.048855000000	-2.043258000000
H	-5.399472000000	-4.664068000000	-2.627594000000
O	5.337086000000	0.259382000000	-2.342224000000
H	6.132023000000	-0.153659000000	-2.697348000000
O	-5.484187000000	-1.830314000000	0.535843000000
H	8.632016000000	2.873885000000	0.293422000000
H	4.559142000000	4.766287000000	-0.428406000000
H	-7.600717000000	-3.910449000000	-2.297190000000
H	-3.337302000000	-3.854595000000	-0.019665000000
H	5.678437000000	-3.356161000000	-1.034272000000
H	8.690393000000	-0.427054000000	-0.167041000000
H	-1.437137000000	4.127946000000	0.200568000000
C	1.458712000000	-0.141587000000	5.262681000000
H	2.389174000000	-0.076648000000	5.828567000000
H	0.839091000000	-0.897588000000	5.746757000000
N	1.826476000000	-0.702453000000	3.905172000000
C	0.749905000000	1.200844000000	5.249177000000
H	0.527104000000	1.466660000000	6.284927000000
H	-0.199795000000	1.172433000000	4.711348000000
H	1.368195000000	2.000861000000	4.837132000000
C	2.774512000000	0.227559000000	3.172823000000
H	2.909567000000	-0.193495000000	2.179021000000
H	2.238242000000	1.167324000000	3.038715000000
C	-0.549531000000	-1.642029000000	3.625313000000
H	-0.973712000000	-1.171680000000	4.515426000000
H	-0.278962000000	-2.675200000000	3.849050000000
H	-1.328088000000	-1.673221000000	2.861598000000
C	2.475522000000	-2.050278000000	4.157050000000
H	3.274063000000	-1.870910000000	4.878716000000
H	1.720741000000	-2.659668000000	4.655307000000
C	0.596962000000	-0.855280000000	3.021250000000
H	0.278008000000	0.154261000000	2.762057000000
H	0.929689000000	-1.330802000000	2.098692000000
C	4.114803000000	0.470526000000	3.840334000000
H	4.031956000000	0.984985000000	4.800600000000
H	4.683287000000	1.110257000000	3.162330000000
H	4.693104000000	-0.445981000000	3.977355000000
C	3.008659000000	-2.767399000000	2.930311000000
H	3.798209000000	-2.206726000000	2.424860000000
H	2.218581000000	-3.020107000000	2.221219000000
H	3.448077000000	-3.708594000000	3.268960000000
O	-5.922661000000	3.391542000000	1.787324000000
O	-3.350380000000	3.882669000000	1.119191000000
O	0.170525000000	3.317409000000	-0.730764000000
O	3.520505000000	-4.052545000000	-0.617684000000
O	6.793964000000	4.034214000000	0.305975000000
H	6.497118000000	4.333653000000	1.172642000000
O	-9.381063000000	0.370372000000	-0.343369000000
O	-3.163766000000	-1.239508000000	-2.179883000000
O	0.996952000000	-4.057064000000	-1.399458000000
O	2.873961000000	1.729225000000	-2.590841000000

Table S18. Optimized coordinates (M06-2X/6-31G(d,p)) of $[Et_4N]^+$-GO system in the singlet state. Units are in Å.

C	6.003055000000	-2.313545000000	-0.985218000000
C	4.980093000000	-1.328232000000	-0.674184000000
C	3.727071000000	-1.697012000000	-0.333010000000
C	3.020556000000	-2.985025000000	-0.616013000000
C	1.435925000000	-2.999305000000	-0.915176000000
C	7.302905000000	-1.947251000000	-0.909855000000
C	-2.792129000000	-3.000945000000	-0.334705000000
C	-3.595302000000	-1.920052000000	-0.957972000000
C	-5.081474000000	-2.055458000000	-0.800884000000
C	-5.750707000000	-3.164459000000	-1.525676000000
C	-7.085594000000	-3.178322000000	-1.703902000000
C	-1.470147000000	-2.889411000000	-0.140385000000
C	-3.014405000000	-0.564253000000	-0.932363000000
C	-1.576395000000	-0.411754000000	-0.445392000000
C	-1.098497000000	0.963682000000	-0.944518000000
C	-1.851131000000	2.072934000000	-0.450867000000
C	-3.201859000000	1.860346000000	-0.084564000000
C	-3.885373000000	0.669100000000	-0.676837000000
C	0.043418000000	1.220213000000	-1.666118000000
C	-1.094915000000	3.250791000000	-0.291311000000
C	0.774489000000	2.378710000000	-1.399207000000
C	-3.931235000000	2.903296000000	0.580019000000
C	-0.733065000000	-1.707248000000	-0.629801000000
C	0.579305000000	-1.753001000000	-0.961313000000
C	1.247162000000	-0.544047000000	-1.444367000000
C	2.333366000000	-0.036298000000	-0.880818000000
C	3.044865000000	1.205826000000	-1.227918000000
C	2.262102000000	2.480211000000	-1.492616000000
C	2.923437000000	3.769363000000	-1.117078000000
C	5.381229000000	0.148468000000	-0.931402000000
C	6.804453000000	0.403311000000	-0.461657000000
C	7.215277000000	1.755122000000	-0.107975000000
C	6.338880000000	2.764602000000	0.059500000000
C	4.883324000000	2.575443000000	-0.118371000000
C	4.385720000000	1.252698000000	-0.519489000000
C	4.106122000000	3.791763000000	-0.496615000000
C	7.703491000000	-0.597499000000	-0.539243000000
C	-8.197755000000	0.210693000000	-0.298010000000
C	-7.456934000000	1.353838000000	0.357108000000
C	-7.919196000000	-2.062325000000	-1.291557000000
C	-7.383876000000	-0.921873000000	-0.756720000000
C	-5.939243000000	-0.891321000000	-0.462103000000
C	-5.330126000000	0.477951000000	-0.457183000000
C	-6.125955000000	1.500684000000	0.277482000000
C	-5.442241000000	2.708425000000	0.835159000000
O	-1.579464000000	-0.300503000000	0.979588000000
O	-9.234851000000	-2.158884000000	-1.485104000000
O	8.536956000000	1.926345000000	0.072825000000
O	2.864021000000	-0.741111000000	0.177454000000
H	-2.243502000000	0.372602000000	1.217612000000
C	-8.368258000000	2.309828000000	1.084915000000
O	-8.745276000000	2.109908000000	2.206026000000
O	-8.735065000000	3.329214000000	0.310377000000
H	-9.333045000000	3.885999000000	0.834029000000
H	-9.467752000000	-3.019097000000	-1.854063000000
C	8.405854000000	-2.934818000000	-1.114976000000
O	9.570822000000	-2.663905000000	-0.969341000000
O	7.959529000000	-4.144779000000	-1.477073000000
H	8.734584000000	-4.716757000000	-1.589170000000

C	-0.798115000000	-3.856961000000	0.775185000000
O	0.123256000000	-3.564007000000	1.510525000000
O	-1.363238000000	-5.059928000000	0.764160000000
H	-0.896469000000	-5.612601000000	1.410262000000
C	2.364931000000	5.083958000000	-1.573522000000
O	2.720568000000	6.149445000000	-1.145008000000
O	1.456939000000	4.926101000000	-2.547147000000
H	1.171680000000	5.809530000000	-2.830950000000
O	-4.826029000000	0.905844000000	-1.724903000000
O	4.257398000000	1.646523000000	0.829210000000
O	0.600109000000	0.206343000000	-2.396723000000
O	-4.886541000000	-4.090686000000	-1.977173000000
H	-5.327909000000	-4.725529000000	-2.556760000000
O	5.325140000000	0.292059000000	-2.349920000000
H	6.092285000000	-0.149115000000	-2.739865000000
O	-5.481748000000	-1.812062000000	0.543220000000
H	8.695333000000	2.867787000000	0.240726000000
H	4.575859000000	4.756804000000	-0.329697000000
H	-7.556628000000	-4.016085000000	-2.212787000000
H	-3.328097000000	-3.857274000000	0.060669000000
H	5.720148000000	-3.346030000000	-1.155904000000
H	8.752930000000	-0.419186000000	-0.331853000000
H	-1.439719000000	4.138866000000	0.216454000000
C	1.415786000000	-0.258665000000	5.343565000000
H	2.359002000000	-0.233794000000	5.892089000000
H	0.808867000000	-1.057352000000	5.773764000000
N	1.756506000000	-0.704545000000	3.938393000000
C	0.703081000000	1.078236000000	5.440279000000
H	0.475217000000	1.258214000000	6.492965000000
H	-0.243025000000	1.090832000000	4.895497000000
H	1.323280000000	1.908634000000	5.097032000000
C	2.677079000000	0.291439000000	3.260048000000
H	2.816247000000	-0.066950000000	2.240561000000
H	2.117914000000	1.226475000000	3.197511000000
C	-0.634912000000	-1.601703000000	3.685341000000
H	-1.054286000000	-1.130221000000	4.577188000000
H	-0.356670000000	-2.632862000000	3.908798000000
H	-1.416003000000	-1.642952000000	2.923902000000
C	2.424171000000	-2.061333000000	4.063845000000
H	3.198519000000	-1.947864000000	4.825178000000
H	1.663631000000	-2.732168000000	4.465693000000
C	0.504497000000	-0.806164000000	3.076495000000
H	0.194759000000	0.219427000000	2.869997000000
H	0.812967000000	-1.250512000000	2.127966000000
C	4.013498000000	0.509562000000	3.945016000000
H	3.919510000000	0.986974000000	4.923092000000
H	4.590952000000	1.172742000000	3.297643000000
H	4.587500000000	-0.413639000000	4.053797000000
C	3.006281000000	-2.621173000000	2.779030000000
H	3.823336000000	-2.008932000000	2.389870000000
H	2.240645000000	-2.757803000000	2.012246000000
H	3.413265000000	-3.609227000000	3.006147000000
O	-6.040628000000	3.536318000000	1.477069000000
O	-3.421742000000	3.944957000000	0.980995000000
O	0.176542000000	3.310761000000	-0.676405000000
O	3.574587000000	-4.049973000000	-0.677106000000
O	6.835710000000	4.019533000000	0.341788000000
H	6.557231000000	4.302712000000	1.223355000000
O	-9.405509000000	0.292224000000	-0.396906000000
O	-3.130856000000	-1.275861000000	-2.141282000000
O	0.987054000000	-4.089095000000	-1.146564000000
O	2.888115000000	1.729453000000	-2.519373000000

Table S19. Optimized coordinates (B3LYP*/6-31G(d,p)) of $[Et_4N][Fe(5Cl\text{-}thsa)_2]$ complex in the sextet (HS) state. Units are in Å.

Fe	-0.190627000000	-1.234875000000	0.366008000000
S	1.077340000000	-3.331475000000	0.250783000000
O	-1.529681000000	0.192171000000	0.048074000000
N	-1.462422000000	-2.451773000000	-0.935909000000
N	-1.063005000000	-3.670588000000	-1.429880000000
N	0.528667000000	-5.298882000000	-1.469603000000
C	-2.807884000000	0.158039000000	-0.246813000000
C	-3.656213000000	1.235301000000	0.112219000000
C	-4.995418000000	1.277759000000	-0.254945000000
C	-5.537761000000	0.223890000000	-1.000086000000
C	-4.756016000000	-0.868380000000	-1.340217000000
C	-3.398278000000	-0.934084000000	-0.959926000000
C	-2.669939000000	-2.125153000000	-1.313224000000
C	0.078824000000	-4.111321000000	-0.953193000000
H	-3.235269000000	2.030140000000	0.720391000000
H	-5.624555000000	2.114381000000	0.038222000000
H	-5.191572000000	-1.694757000000	-1.896977000000
H	-3.188744000000	-2.855801000000	-1.939990000000
H	1.219973000000	-5.800636000000	-0.931200000000
H	-0.160362000000	-5.850406000000	-1.966387000000
S	-1.332544000000	-1.632447000000	2.537359000000
O	0.994718000000	-0.243756000000	-0.860272000000
N	1.367462000000	-0.648385000000	1.855976000000
N	1.138525000000	-0.625296000000	3.209074000000
N	-0.322422000000	-0.981674000000	4.918220000000
C	2.304999000000	-0.292202000000	-0.962496000000
C	2.923356000000	-0.183225000000	-2.232003000000
C	4.305270000000	-0.153388000000	-2.370630000000
C	5.116149000000	-0.222622000000	-1.228589000000
C	4.552417000000	-0.336343000000	0.032003000000
C	3.149425000000	-0.382199000000	0.191135000000
C	2.621836000000	-0.470469000000	1.531895000000
C	-0.060432000000	-1.048307000000	3.569866000000
H	2.277705000000	-0.141977000000	-3.106143000000
H	4.761563000000	-0.081248000000	-3.354469000000
H	5.191536000000	-0.400829000000	0.909744000000
H	3.333579000000	-0.383831000000	2.358908000000
H	-1.076124000000	-1.565433000000	5.253831000000
H	0.497562000000	-0.923866000000	5.511110000000
Cl	6.873127000000	-0.165291000000	-1.403616000000
Cl	-7.233717000000	0.283173000000	-1.489890000000
C	0.559720000000	2.543062000000	1.120022000000
H	1.193909000000	1.754941000000	0.716579000000
H	-0.438641000000	2.103497000000	1.182264000000
N	0.483925000000	3.610068000000	0.016949000000
C	1.059645000000	3.006935000000	2.478538000000
H	1.093962000000	2.112140000000	3.112754000000
H	0.394672000000	3.730499000000	2.963200000000
H	2.073319000000	3.422353000000	2.449881000000
C	1.861970000000	4.201493000000	-0.278556000000

H	1.696607000000	4.976352000000	-1.032830000000
H	2.169146000000	4.706214000000	0.641688000000
C	-1.824710000000	4.468801000000	0.811423000000
H	-1.895900000000	3.794010000000	1.669407000000
H	-2.392348000000	4.040082000000	-0.018807000000
H	-2.310914000000	5.410034000000	1.092575000000
C	-0.095033000000	2.892104000000	-1.211968000000
H	0.541412000000	2.019670000000	-1.381924000000
H	-1.053918000000	2.479485000000	-0.892327000000
C	-0.385370000000	4.789177000000	0.439856000000
H	0.131570000000	5.252169000000	1.285142000000
H	-0.352596000000	5.501021000000	-0.389684000000
C	2.937181000000	3.228531000000	-0.735803000000
H	3.180844000000	2.473592000000	0.015955000000
H	3.846293000000	3.812039000000	-0.921966000000
H	2.684668000000	2.708819000000	-1.663826000000
C	-0.239782000000	3.744437000000	-2.463969000000
H	0.717039000000	4.107708000000	-2.854131000000
H	-0.914780000000	4.597713000000	-2.333935000000
H	-0.679169000000	3.104805000000	-3.237397000000

Table S20. Optimized coordinates (B3LYP*/6-31G(d,p)) of $[Et_4N][Fe(5Cl\text{-}thsa)_2]$ complex in the doublet (LS) state. Units are in Å.

Fe	-0.121648000000	-1.638866000000	0.192796000000
S	1.148770000000	-3.443881000000	-0.387429000000
O	-1.213592000000	-0.103299000000	0.665174000000
N	-1.187277000000	-2.067911000000	-1.385184000000
N	-0.767601000000	-3.024374000000	-2.286022000000
N	0.787597000000	-4.631335000000	-2.763179000000
C	-2.445925000000	0.088794000000	0.253161000000
C	-3.293037000000	0.947296000000	1.001747000000
C	-4.572963000000	1.289409000000	0.578717000000
C	-5.059577000000	0.763714000000	-0.623655000000
C	-4.290097000000	-0.121686000000	-1.362451000000
C	-2.996220000000	-0.492135000000	-0.937959000000
C	-2.298521000000	-1.478788000000	-1.724818000000
C	0.299175000000	-3.683300000000	-1.901794000000
H	-2.913606000000	1.316123000000	1.951804000000
H	-5.199073000000	1.944745000000	1.179154000000
H	-4.690569000000	-0.554145000000	-2.276544000000
H	-2.755792000000	-1.807825000000	-2.660071000000
H	1.394174000000	-5.337285000000	-2.370631000000
H	0.144766000000	-4.938246000000	-3.482882000000
S	-1.399423000000	-2.870907000000	1.640605000000
O	0.945728000000	-0.525205000000	-0.978519000000
N	0.991921000000	-1.249795000000	1.743329000000
N	0.569343000000	-1.564551000000	3.016445000000
N	-1.011911000000	-2.626141000000	4.280107000000
C	2.222104000000	-0.283771000000	-0.800161000000
C	3.018435000000	0.065735000000	-1.922631000000
C	4.358357000000	0.410152000000	-1.801379000000
C	4.952813000000	0.423813000000	-0.531641000000
C	4.222390000000	0.067685000000	0.591730000000
C	2.863709000000	-0.307107000000	0.484865000000
C	2.177486000000	-0.704540000000	1.692094000000
C	-0.524857000000	-2.294723000000	3.041893000000
H	2.540808000000	0.036144000000	-2.899287000000
H	4.947905000000	0.662082000000	-2.679260000000
H	4.702148000000	0.054376000000	1.568101000000
H	2.699423000000	-0.587309000000	2.644717000000
H	-1.656760000000	-3.402753000000	4.322018000000
H	-0.351516000000	-2.548348000000	5.043865000000
Cl	6.651785000000	0.887216000000	-0.365979000000
Cl	-6.674606000000	1.212652000000	-1.185517000000
C	0.593256000000	2.568203000000	1.262180000000
H	1.351495000000	1.883020000000	0.879183000000
H	-0.308150000000	1.962443000000	1.390892000000
N	0.305267000000	3.545219000000	0.113364000000
C	1.054151000000	3.200844000000	2.567028000000
H	1.238268000000	2.378997000000	3.267860000000
H	0.302573000000	3.852643000000	3.024686000000
H	1.992590000000	3.758329000000	2.470829000000
C	1.575449000000	4.280038000000	-0.315826000000
H	1.258881000000	4.992520000000	-1.083024000000
H	1.888838000000	4.861434000000	0.555899000000
C	-2.001994000000	4.181123000000	1.115322000000
H	-1.879099000000	3.632840000000	2.053349000000
H	-2.587834000000	3.559310000000	0.434017000000
H	-2.590029000000	5.080398000000	1.333416000000
C	-0.269674000000	2.691026000000	-1.028545000000
H	0.406151000000	1.840290000000	-1.152038000000

H	-1.201345000000	2.274210000000	-0.642556000000
C	-0.675181000000	4.639166000000	0.531580000000
H	-0.136380000000	5.259327000000	1.253688000000
H	-0.837885000000	5.249769000000	-0.360863000000
C	2.718792000000	3.417822000000	-0.822526000000
H	3.115679000000	2.734877000000	-0.066644000000
H	3.533522000000	4.091871000000	-1.111689000000
H	2.453767000000	2.825333000000	-1.700923000000
C	-0.501546000000	3.417334000000	-2.345432000000
H	0.421744000000	3.783657000000	-2.806224000000
H	-1.212756000000	4.246985000000	-2.267493000000
H	-0.938277000000	2.687183000000	-3.035673000000

Table S21. Optimized coordinates (wB97XD/6-31G(d,p)) of $[Et_4N][Fe(5Cl\text{-}thsa)_2]$ complex in the sextet (HS) state. Units are in Å.

Fe	-0.027784000000	-1.369048000000	0.426599000000
S	1.134764000000	-3.429029000000	-0.068215000000
O	-1.446910000000	-0.051589000000	0.513606000000
N	-1.046244000000	-2.026755000000	-1.366747000000
N	-0.359091000000	-2.798903000000	-2.272710000000
N	1.440899000000	-4.137154000000	-2.614423000000
C	-2.703038000000	-0.102076000000	0.151230000000
C	-3.668039000000	0.644658000000	0.857941000000
C	-4.988127000000	0.699965000000	0.446896000000
C	-5.382667000000	0.000695000000	-0.694166000000
C	-4.471470000000	-0.766602000000	-1.394366000000
C	-3.133986000000	-0.843903000000	-0.979829000000
C	-2.230766000000	-1.684821000000	-1.742740000000
C	0.671927000000	-3.414047000000	-1.753266000000
H	-3.345300000000	1.160236000000	1.756291000000
H	-5.716439000000	1.274977000000	1.008461000000
H	-4.793109000000	-1.323607000000	-2.269016000000
H	-2.582411000000	-2.076517000000	-2.699279000000
H	2.071932000000	-4.814114000000	-2.221448000000
H	1.035653000000	-4.337734000000	-3.515421000000
S	-0.922994000000	-2.364897000000	2.498864000000
O	1.167437000000	-0.330567000000	-0.738159000000
N	1.162204000000	-0.439881000000	1.978699000000
N	0.598336000000	-0.211629000000	3.213699000000
N	-1.066136000000	-0.792076000000	4.644233000000
C	2.468794000000	-0.225294000000	-0.644998000000
C	3.255618000000	-0.187400000000	-1.815169000000
C	4.618398000000	0.032328000000	-1.761116000000
C	5.240663000000	0.225714000000	-0.524436000000
C	4.507934000000	0.173872000000	0.643778000000
C	3.124410000000	-0.064388000000	0.605326000000
C	2.389927000000	-0.064312000000	1.855453000000
C	-0.402253000000	-1.020944000000	3.474636000000
H	2.752770000000	-0.345616000000	-2.763172000000
H	5.209022000000	0.054244000000	-2.670687000000
H	5.001609000000	0.311812000000	1.600972000000
H	2.894193000000	0.307418000000	2.750288000000
H	-1.650710000000	-1.533980000000	4.990689000000
H	-0.582753000000	-0.227358000000	5.325759000000
Cl	6.965921000000	0.532119000000	-0.462020000000
Cl	-7.048969000000	0.088260000000	-1.232438000000
C	0.284083000000	2.427334000000	0.867108000000
H	1.007247000000	1.690550000000	0.530567000000
H	-0.617517000000	1.852123000000	1.080567000000
N	-0.018749000000	3.275539000000	-0.356025000000
C	0.784221000000	3.161662000000	2.092621000000
H	0.895573000000	2.396756000000	2.868340000000
H	0.077249000000	3.906953000000	2.468313000000
H	1.757650000000	3.637405000000	1.944245000000
C	1.217658000000	4.009347000000	-0.823808000000
H	0.901902000000	4.631826000000	-1.663594000000
H	1.495506000000	4.682379000000	-0.010617000000
C	-2.351457000000	3.838684000000	0.547854000000
H	-2.204220000000	3.374247000000	1.524371000000
H	-2.876477000000	3.127202000000	-0.091708000000
H	-3.004565000000	4.703876000000	0.686172000000
C	-0.523352000000	2.305438000000	-1.415624000000

H	0.200551000000	1.488038000000	-1.455001000000
H	-1.431926000000	1.866546000000	-1.008041000000
C	-1.049773000000	4.336517000000	-0.050576000000
H	-0.568056000000	5.042520000000	0.628742000000
H	-1.232966000000	4.863906000000	-0.988369000000
C	2.395365000000	3.136752000000	-1.213853000000
H	2.798477000000	2.568247000000	-0.373836000000
H	3.188330000000	3.793901000000	-1.578848000000
H	2.154360000000	2.431838000000	-2.010935000000
C	-0.770262000000	2.904422000000	-2.786570000000
H	0.140218000000	3.281603000000	-3.258792000000
H	-1.525324000000	3.694982000000	-2.786818000000
H	-1.150214000000	2.098626000000	-3.418956000000

Table S22. Optimized coordinates (wB97XD/6-31G(d,p)) of $[Et_4N][Fe(5Cl\text{-}thsa)_2]$ complex in the doublet (LS) state. Units are in Å.

Fe	-0.044873000000	-1.562008000000	0.229226000000
S	1.320303000000	-3.286984000000	-0.307554000000
O	-1.236987000000	-0.123134000000	0.664816000000
N	-1.039656000000	-2.048406000000	-1.382628000000
N	-0.508081000000	-2.938665000000	-2.291366000000
N	1.177911000000	-4.402331000000	-2.720375000000
C	-2.462209000000	-0.010702000000	0.234903000000
C	-3.369872000000	0.780641000000	0.975374000000
C	-4.648842000000	1.053724000000	0.525676000000
C	-5.075121000000	0.522213000000	-0.691562000000
C	-4.240155000000	-0.304118000000	-1.418347000000
C	-2.944529000000	-0.598517000000	-0.967339000000
C	-2.158377000000	-1.527703000000	-1.752444000000
C	0.576727000000	-3.525089000000	-1.867521000000
H	-3.030063000000	1.159090000000	1.933654000000
H	-5.321677000000	1.666420000000	1.116483000000
H	-4.592767000000	-0.744429000000	-2.346042000000
H	-2.554205000000	-1.853046000000	-2.714126000000
H	1.839973000000	-5.051250000000	-2.330706000000
H	0.617609000000	-4.722448000000	-3.494491000000
S	-1.240489000000	-2.818643000000	1.707760000000
O	0.971013000000	-0.402825000000	-0.928457000000
N	1.011362000000	-1.042165000000	1.789176000000
N	0.518519000000	-1.235552000000	3.059744000000
N	-1.081769000000	-2.261345000000	4.305209000000
C	2.247734000000	-0.185748000000	-0.762610000000
C	3.044334000000	0.106402000000	-1.892875000000
C	4.372274000000	0.467263000000	-1.777305000000
C	4.957726000000	0.546951000000	-0.510852000000
C	4.227676000000	0.227436000000	0.616552000000
C	2.881138000000	-0.159399000000	0.512625000000
C	2.176376000000	-0.490163000000	1.736590000000
C	-0.522270000000	-2.029736000000	3.084665000000
H	2.569764000000	0.035381000000	-2.865758000000
H	4.962161000000	0.689737000000	-2.660049000000
H	4.698893000000	0.265644000000	1.594116000000
H	2.662136000000	-0.276020000000	2.689035000000
H	-1.715755000000	-3.037948000000	4.386000000000
H	-0.510008000000	-2.045412000000	5.106436000000
Cl	6.632934000000	1.045277000000	-0.357723000000
Cl	-6.685599000000	0.884917000000	-1.284779000000
C	0.426697000000	2.373313000000	1.169823000000
H	1.125995000000	1.669321000000	0.725513000000
H	-0.476041000000	1.789550000000	1.354377000000
N	0.093564000000	3.364583000000	0.068691000000
C	0.998721000000	2.961769000000	2.442688000000
H	1.149908000000	2.123531000000	3.127918000000
H	0.322740000000	3.665145000000	2.936449000000
H	1.968832000000	3.444128000000	2.295196000000
C	1.328327000000	4.110026000000	-0.387951000000
H	0.986509000000	4.830316000000	-1.133951000000
H	1.672596000000	4.680007000000	0.476915000000
C	-2.153850000000	3.938452000000	1.181527000000
H	-1.973579000000	3.366680000000	2.093733000000
H	-2.759249000000	3.327983000000	0.510617000000
H	-2.741403000000	4.819313000000	1.453079000000
C	-0.514269000000	2.533769000000	-1.054261000000

H	0.141475000000	1.670586000000	-1.198355000000
H	-1.442987000000	2.130402000000	-0.653361000000
C	-0.867953000000	4.428852000000	0.547622000000
H	-0.308605000000	5.042611000000	1.256331000000
H	-1.084768000000	5.055687000000	-0.319325000000
C	2.450696000000	3.257059000000	-0.938917000000
H	2.880318000000	2.585542000000	-0.193294000000
H	3.245508000000	3.928589000000	-1.272574000000
H	2.143231000000	2.655165000000	-1.794560000000
C	-0.767686000000	3.271004000000	-2.354545000000
H	0.149054000000	3.617697000000	-2.837376000000
H	-1.456242000000	4.113678000000	-2.249058000000
H	-1.239334000000	2.555942000000	-3.032611000000

Table S23. Optimized coordinates (wB97XD/6-31G(d,p)) of GO-**1** (HS1) hybrid system in the sextet (HS) state. Units are in Å.

C	10.093498000000	-3.532072000000	0.694752000000
C	9.392038000000	-2.261367000000	0.702081000000
C	8.052347000000	-2.204587000000	0.866288000000
C	7.044721000000	-3.283588000000	0.600977000000
C	5.654724000000	-2.923941000000	-0.123432000000
C	11.425028000000	-3.556177000000	0.929068000000
C	1.555790000000	-1.701799000000	-0.105065000000
C	1.179879000000	-0.526567000000	-0.927338000000
C	-0.290082000000	-0.226728000000	-1.026312000000
C	-1.165648000000	-1.219108000000	-1.707186000000
C	-2.396710000000	-0.876917000000	-2.140444000000
C	2.821902000000	-1.945122000000	0.257108000000
C	2.122397000000	0.604697000000	-0.941580000000
C	3.465496000000	0.413199000000	-0.238083000000
C	4.378735000000	1.543304000000	-0.753122000000
C	3.925019000000	2.859406000000	-0.460374000000
C	2.524083000000	3.060856000000	-0.290278000000
C	1.633893000000	2.054496000000	-0.938823000000
C	5.629809000000	1.400951000000	-1.311280000000
C	4.945343000000	3.798249000000	-0.277685000000
C	6.615522000000	2.337474000000	-1.009231000000
C	2.033075000000	4.307634000000	0.200297000000
C	3.916974000000	-1.072727000000	-0.214270000000
C	5.187148000000	-1.505388000000	-0.351473000000
C	6.229036000000	-0.582462000000	-0.794583000000
C	7.321589000000	-0.324452000000	-0.091103000000
C	8.402944000000	0.620097000000	-0.417199000000
C	8.071703000000	2.017773000000	-0.895603000000
C	9.040145000000	3.106052000000	-0.555205000000
C	10.251895000000	-1.019917000000	0.346160000000
C	11.621087000000	-1.119266000000	1.001703000000
C	12.377063000000	0.094366000000	1.279007000000
C	11.837144000000	1.324280000000	1.200582000000
C	10.426635000000	1.540292000000	0.821716000000
C	9.601054000000	0.375438000000	0.483873000000
C	10.103056000000	2.863534000000	0.217980000000
C	12.169486000000	-2.334683000000	1.190111000000
C	-2.559357000000	2.875643000000	-1.473392000000
C	-1.681400000000	3.806516000000	-0.674316000000
C	-2.888257000000	0.473514000000	-2.065629000000
C	-2.098004000000	1.506911000000	-1.611414000000
C	-0.786958000000	1.165890000000	-1.024726000000
C	0.192666000000	2.296129000000	-1.000735000000
C	-0.381797000000	3.557970000000	-0.458211000000
C	0.505057000000	4.510434000000	0.276308000000
O	3.321130000000	0.667565000000	1.150834000000
O	-4.143564000000	0.690472000000	-2.447551000000
O	13.655329000000	-0.087111000000	1.662168000000
O	7.463090000000	-0.985352000000	1.100177000000
H	2.865780000000	1.518715000000	1.253896000000
C	-2.421286000000	5.002119000000	-0.146568000000
O	-3.197042000000	4.919702000000	0.777309000000
O	-2.191429000000	6.108266000000	-0.844885000000
H	-2.697064000000	6.819748000000	-0.427338000000
H	-4.594551000000	-0.150586000000	-2.627803000000
C	12.180771000000	-4.835546000000	1.022531000000
O	13.352472000000	-4.905041000000	1.313660000000
O	11.431175000000	-5.913027000000	0.744171000000
H	12.006774000000	-6.683224000000	0.843189000000

C	3.092844000000	-2.961276000000	1.318640000000
O	4.076099000000	-2.970829000000	2.022696000000
O	2.094709000000	-3.842849000000	1.458337000000
H	2.346956000000	-4.425075000000	2.188045000000
C	8.959076000000	4.446531000000	-1.208723000000
O	9.583023000000	5.416825000000	-0.855853000000
O	8.139444000000	4.440996000000	-2.272412000000
H	8.164676000000	5.329845000000	-2.653346000000
O	0.994436000000	2.437746000000	-2.174079000000
O	9.445564000000	0.976441000000	1.747400000000
O	5.957423000000	0.208751000000	-1.888487000000
O	-0.618429000000	-2.428971000000	-1.832566000000
H	-1.196316000000	-3.031595000000	-2.329235000000
O	10.416407000000	-1.080434000000	-1.073926000000
H	11.021065000000	-1.802112000000	-1.278010000000
O	-0.813017000000	0.351107000000	0.172177000000
H	14.036423000000	0.791638000000	1.793976000000
H	10.824704000000	3.661820000000	0.358962000000
H	-3.040604000000	-1.626168000000	-2.584469000000
H	0.755385000000	-2.317572000000	0.284486000000
H	9.522428000000	-4.449196000000	0.613744000000
H	13.187294000000	-2.431351000000	1.548880000000
H	4.793755000000	4.795517000000	0.106293000000
O	0.043011000000	5.429981000000	0.913300000000
O	2.741332000000	5.233957000000	0.597421000000
O	6.225904000000	3.473339000000	-0.457762000000
O	7.244897000000	-4.452332000000	0.810197000000
O	12.646057000000	2.410938000000	1.475504000000
H	12.336197000000	2.844373000000	2.279142000000
O	-3.618540000000	3.321499000000	-1.900212000000
O	1.948352000000	-0.195956000000	-2.089625000000
O	5.044572000000	-3.868765000000	-0.549729000000
O	8.567747000000	1.004961000000	-1.760785000000
Fe	-8.348320000000	-2.027138000000	0.573700000000
S	-8.677076000000	-4.212905000000	-0.338871000000
O	-8.944044000000	-0.366509000000	1.277193000000
N	-9.839936000000	-1.649072000000	-0.989230000000
N	-9.872429000000	-2.482454000000	-2.083408000000
N	-9.269188000000	-4.507288000000	-2.918352000000
C	-9.922284000000	0.471744000000	1.066878000000
C	-10.203208000000	1.471059000000	2.023510000000
C	-11.156107000000	2.447704000000	1.795880000000
C	-11.872320000000	2.444543000000	0.598640000000
C	-11.660770000000	1.451453000000	-0.338586000000
C	-10.704239000000	0.449668000000	-0.117284000000
C	-10.566219000000	-0.592043000000	-1.114911000000
C	-9.327978000000	-3.647144000000	-1.862148000000
H	-9.669884000000	1.435258000000	2.967432000000
H	-11.356675000000	3.206669000000	2.544303000000
H	-12.243867000000	1.439061000000	-1.254299000000
H	-11.136109000000	-0.487966000000	-2.040021000000
H	-9.108189000000	-5.479414000000	-2.717171000000
H	-9.862622000000	-4.285556000000	-3.702833000000
S	-8.868884000000	-2.960909000000	2.855493000000
O	-7.118178000000	-1.372376000000	-0.870364000000
N	-6.420554000000	-2.304016000000	1.528444000000
N	-6.286557000000	-2.097351000000	2.883804000000
N	-7.384655000000	-2.024955000000	4.870690000000
C	-6.167401000000	-2.109247000000	-1.359761000000
C	-5.970917000000	-2.192363000000	-2.760280000000
C	-4.988211000000	-3.006066000000	-3.305812000000
C	-4.137027000000	-3.714948000000	-2.458515000000

C	-4.262794000000	-3.623666000000	-1.083215000000
C	-5.271808000000	-2.838951000000	-0.521913000000
C	-5.368514000000	-2.730166000000	0.921768000000
C	-7.408391000000	-2.317289000000	3.533046000000
H	-6.677585000000	-1.669777000000	-3.396623000000
H	-4.878354000000	-3.091809000000	-4.381518000000
H	-3.582235000000	-4.168625000000	-0.435970000000
H	-4.497830000000	-2.989299000000	1.527559000000
H	-8.119787000000	-2.429024000000	5.427817000000
H	-6.466905000000	-1.998667000000	5.290245000000
Cl	-2.812591000000	-4.656500000000	-3.143698000000
Cl	-13.064106000000	3.693537000000	0.298173000000
C	-6.547414000000	1.316769000000	2.521968000000
H	-6.526770000000	0.268709000000	2.229764000000
H	-7.597031000000	1.578793000000	2.627687000000
N	-6.030849000000	2.112582000000	1.343972000000
C	-5.807150000000	1.511594000000	3.830198000000
H	-6.244991000000	0.806205000000	4.541186000000
H	-5.917886000000	2.518771000000	4.240514000000
H	-4.743117000000	1.276443000000	3.753514000000
C	-4.576748000000	1.793538000000	1.067930000000
H	-4.340221000000	2.309557000000	0.140396000000
H	-3.997915000000	2.277249000000	1.856267000000
C	-7.492664000000	4.143857000000	1.869744000000
H	-7.937401000000	3.733060000000	2.779003000000
H	-8.185014000000	3.969446000000	1.043771000000
H	-7.402510000000	5.224053000000	2.006504000000
C	-6.905154000000	1.727462000000	0.160167000000
H	-6.760577000000	0.659044000000	-0.002028000000
H	-7.929767000000	1.853844000000	0.504695000000
C	-6.100610000000	3.598822000000	1.603604000000
H	-5.441130000000	3.797187000000	2.449311000000
H	-5.640403000000	4.080881000000	0.740349000000
C	-4.247202000000	0.318129000000	0.973240000000
H	-4.462821000000	-0.226682000000	1.895247000000
H	-3.176748000000	0.229593000000	0.772774000000
H	-4.782038000000	-0.163565000000	0.153116000000
C	-6.683622000000	2.503786000000	-1.122394000000
H	-5.673788000000	2.420032000000	-1.525273000000
H	-6.938825000000	3.562484000000	-1.028031000000
H	-7.367172000000	2.070307000000	-1.857542000000

Table S24. Optimized coordinates (wB97XD/6-31G(d,p)) of GO-**1** (LS1) hybrid system in the doublet (LS) state. Units are in Å.

C	10.244676000000	-3.545108000000	0.762300000000
C	9.520988000000	-2.286992000000	0.774038000000
C	8.173982000000	-2.257211000000	0.872204000000
C	7.201306000000	-3.344185000000	0.523794000000
C	5.842552000000	-2.984773000000	-0.257397000000
C	11.564096000000	-3.554444000000	1.057706000000
C	1.728081000000	-1.828888000000	-0.399717000000
C	1.370727000000	-0.641990000000	-1.213578000000
C	-0.097616000000	-0.361123000000	-1.376685000000
C	-0.936505000000	-1.361271000000	-2.093848000000
C	-2.138320000000	-1.024892000000	-2.604387000000
C	2.980334000000	-2.061059000000	0.013955000000
C	2.293765000000	0.504309000000	-1.158553000000
C	3.603817000000	0.318164000000	-0.392955000000
C	4.520933000000	1.477744000000	-0.830185000000
C	4.028073000000	2.776917000000	-0.525015000000
C	2.616259000000	2.948578000000	-0.424494000000
C	1.782708000000	1.946262000000	-1.149541000000
C	5.802177000000	1.372010000000	-1.324642000000
C	5.020012000000	3.726410000000	-0.261082000000
C	6.753332000000	2.315407000000	-0.943179000000
C	2.076046000000	4.171094000000	0.075673000000
C	4.080905000000	-1.159627000000	-0.383991000000
C	5.363435000000	-1.567733000000	-0.470583000000
C	6.410278000000	-0.615999000000	-0.833790000000
C	7.460167000000	-0.361197000000	-0.067073000000
C	8.539006000000	0.611187000000	-0.308697000000
C	8.207275000000	2.017266000000	-0.761697000000
C	9.136401000000	3.110532000000	-0.337722000000
C	10.374926000000	-1.021439000000	0.496940000000
C	11.713263000000	-1.118352000000	1.213768000000
C	12.433009000000	0.098113000000	1.565237000000
C	11.875084000000	1.320809000000	1.500141000000
C	10.481258000000	1.525432000000	1.058395000000
C	9.694190000000	0.358558000000	0.644853000000
C	10.163105000000	2.861683000000	0.481032000000
C	12.274059000000	-2.329926000000	1.390465000000
C	-2.373893000000	2.725665000000	-1.931944000000
C	-1.568312000000	3.643798000000	-1.042794000000
C	-2.649838000000	0.322081000000	-2.545092000000
C	-1.896805000000	1.353805000000	-2.036824000000
C	-0.612780000000	1.023714000000	-1.387877000000
C	0.344919000000	2.168644000000	-1.291166000000
C	-0.281617000000	3.406899000000	-0.750111000000
C	0.542434000000	4.347061000000	0.067788000000
O	3.383849000000	0.534196000000	0.992891000000
O	-3.883823000000	0.535713000000	-2.994700000000
O	13.694043000000	-0.074581000000	2.005125000000
O	7.551786000000	-1.055179000000	1.110271000000
H	2.912552000000	1.377274000000	1.092376000000
C	-2.361517000000	4.812649000000	-0.537905000000
O	-3.197562000000	4.691766000000	0.328848000000
O	-2.106931000000	5.941061000000	-1.185538000000
H	-2.666009000000	6.628637000000	-0.796374000000
H	-4.360576000000	-0.303061000000	-3.101629000000
C	12.337964000000	-4.823526000000	1.144232000000
O	13.498625000000	-4.882231000000	1.478539000000
O	11.618235000000	-5.904462000000	0.806743000000
H	12.203136000000	-6.667751000000	0.904816000000

C	3.219469000000	-3.098182000000	1.062898000000
O	4.168529000000	-3.108487000000	1.812413000000
O	2.231981000000	-3.999903000000	1.134502000000
H	2.462453000000	-4.597033000000	1.859368000000
C	9.064247000000	4.469740000000	-0.952718000000
O	9.645350000000	5.440208000000	-0.533437000000
O	8.308687000000	4.481782000000	-2.062670000000
H	8.336524000000	5.382591000000	-2.414247000000
O	1.210009000000	2.349906000000	-2.411663000000
O	9.465519000000	0.916448000000	1.916634000000
O	6.180765000000	0.202653000000	-1.917075000000
O	-0.397245000000	-2.580852000000	-2.167618000000
H	-1.022706000000	-3.196287000000	-2.580581000000
O	10.606898000000	-1.036172000000	-0.914879000000
H	11.236837000000	-1.738138000000	-1.111095000000
O	-0.681297000000	0.198902000000	-0.195760000000
H	14.052562000000	0.805488000000	2.183465000000
H	10.860584000000	3.667755000000	0.684974000000
H	-2.745679000000	-1.778658000000	-3.088893000000
H	0.921305000000	-2.466128000000	-0.062035000000
H	9.695441000000	-4.469005000000	0.625947000000
H	13.275091000000	-2.421539000000	1.794756000000
H	4.831581000000	4.709315000000	0.143064000000
O	0.026322000000	5.235908000000	0.707115000000
O	2.744023000000	5.095206000000	0.541505000000
O	6.314006000000	3.427674000000	-0.381086000000
O	7.411747000000	-4.515495000000	0.707052000000
O	12.649708000000	2.411130000000	1.848793000000
H	12.294067000000	2.812720000000	2.650032000000
O	-3.373108000000	3.178429000000	-2.468540000000
O	2.188806000000	-0.273393000000	-2.330388000000
O	5.267594000000	-3.925981000000	-0.737374000000
O	8.765256000000	1.039697000000	-1.629599000000
Fe	-8.978896000000	-1.766889000000	0.402939000000
S	-9.332462000000	-3.765400000000	-0.602498000000
O	-8.742233000000	-0.079825000000	1.271247000000
N	-10.406444000000	-1.108759000000	-0.756523000000
N	-10.888713000000	-1.884785000000	-1.793443000000
N	-10.829547000000	-3.925078000000	-2.801043000000
C	-9.587184000000	0.912106000000	1.252036000000
C	-9.478278000000	1.917328000000	2.242097000000
C	-10.260647000000	3.056665000000	2.231062000000
C	-11.212719000000	3.225726000000	1.225927000000
C	-11.392774000000	2.243317000000	0.272968000000
C	-10.608830000000	1.079508000000	0.277209000000
C	-10.908197000000	0.076504000000	-0.719904000000
C	-10.426869000000	-3.100390000000	-1.790347000000
H	-8.767172000000	1.759066000000	3.045161000000
H	-10.148453000000	3.809896000000	3.003847000000
H	-12.157294000000	2.364805000000	-0.488247000000
H	-11.641896000000	0.318303000000	-1.487943000000
H	-10.727526000000	-4.915198000000	-2.655578000000
H	-11.641855000000	-3.621520000000	-3.315250000000
S	-10.242719000000	-2.328818000000	2.221570000000
O	-7.766706000000	-1.227669000000	-1.011461000000
N	-7.494176000000	-2.462254000000	1.456902000000
N	-7.595399000000	-2.553828000000	2.825016000000
N	-9.034929000000	-2.550659000000	4.582966000000
C	-6.740528000000	-1.937937000000	-1.355177000000
C	-6.268448000000	-1.874293000000	-2.692994000000
C	-5.208177000000	-2.650718000000	-3.132240000000
C	-4.538729000000	-3.474452000000	-2.223229000000

C	-4.928767000000	-3.526790000000	-0.899576000000
C	-6.027221000000	-2.783418000000	-0.451551000000
C	-6.372744000000	-2.860052000000	0.956311000000
C	-8.840586000000	-2.480725000000	3.238171000000
H	-6.829106000000	-1.255985000000	-3.386294000000
H	-4.920650000000	-2.645948000000	-4.180018000000
H	-4.394277000000	-4.164916000000	-0.202417000000
H	-5.645322000000	-3.283547000000	1.650205000000
H	-9.972138000000	-2.707071000000	4.912779000000
H	-8.279864000000	-2.934428000000	5.128857000000
Cl	-3.195787000000	-4.477488000000	-2.779471000000
Cl	-12.199395000000	4.675077000000	1.194423000000
C	-5.903470000000	0.425139000000	2.530947000000
H	-6.028015000000	-0.479290000000	1.941807000000
H	-6.917752000000	0.747276000000	2.754350000000
N	-5.312971000000	1.459696000000	1.596596000000
C	-5.115166000000	0.135928000000	3.791312000000
H	-5.631446000000	-0.688810000000	4.288862000000
H	-5.081909000000	0.982873000000	4.481577000000
H	-4.092590000000	-0.193602000000	3.588569000000
C	-3.957993000000	1.025363000000	1.085653000000
H	-3.630221000000	1.805269000000	0.396769000000
H	-3.279959000000	1.051970000000	1.940509000000
C	-6.298765000000	3.410520000000	2.949474000000
H	-6.708989000000	2.790095000000	3.749859000000
H	-7.096699000000	3.638451000000	2.240995000000
H	-5.974666000000	4.353630000000	3.396099000000
C	-6.313853000000	1.603498000000	0.456888000000
H	-6.588977000000	0.594082000000	0.146671000000
H	-7.208773000000	2.024535000000	0.911376000000
C	-5.082453000000	2.782847000000	2.294907000000
H	-4.312711000000	2.593732000000	3.046019000000
H	-4.643133000000	3.452807000000	1.554974000000
C	-3.923098000000	-0.336772000000	0.431094000000
H	-4.189217000000	-1.137456000000	1.122646000000
H	-2.897615000000	-0.508186000000	0.103320000000
H	-4.580418000000	-0.400851000000	-0.437983000000
C	-5.852809000000	2.430317000000	-0.723886000000
H	-5.115039000000	1.917666000000	-1.340968000000
H	-5.451273000000	3.409730000000	-0.452772000000
H	-6.729806000000	2.597080000000	-1.353858000000

Table S25. Optimized coordinates (wB97XD/6-31G(d,p)) of GO-**1** (LS2) hybrid system in the doublet (LS) state. Units are in Å.

C	7.964270000000	3.116835000000	2.360468000000
C	7.314996000000	2.216502000000	1.425121000000
C	5.987571000000	1.974825000000	1.494763000000
C	5.085049000000	2.128475000000	2.680635000000
C	3.934439000000	1.039957000000	2.973026000000
C	9.165151000000	3.649441000000	2.041383000000
C	0.115509000000	-0.843107000000	2.735432000000
C	0.029880000000	-2.236888000000	2.233281000000
C	-1.353470000000	-2.823011000000	2.244269000000
C	-2.003583000000	-3.069320000000	3.554811000000
C	-3.105787000000	-3.834855000000	3.650646000000
C	1.166191000000	-0.050729000000	2.490855000000
C	0.923730000000	-2.604626000000	1.126694000000
C	1.977436000000	-1.585256000000	0.696659000000
C	3.030052000000	-2.381855000000	-0.095893000000
C	2.538728000000	-3.009875000000	-1.272633000000
C	1.144682000000	-3.313534000000	-1.333532000000
C	0.451119000000	-3.499059000000	-0.022789000000
C	4.386620000000	-2.411102000000	0.140113000000
C	3.482266000000	-3.156165000000	-2.293196000000
C	5.260480000000	-2.465898000000	-0.943081000000
C	0.552229000000	-3.702650000000	-2.571088000000
C	2.366087000000	-0.590062000000	1.823209000000
C	3.605415000000	-0.094881000000	2.032623000000
C	4.754409000000	-0.701815000000	1.365969000000
C	5.600051000000	-0.030128000000	0.598247000000
C	6.753845000000	-0.559995000000	-0.149292000000
C	6.610573000000	-1.825605000000	-0.968662000000
C	7.459582000000	-1.949408000000	-2.194001000000
C	8.265243000000	1.443076000000	0.473864000000
C	9.377727000000	2.353567000000	-0.021858000000
C	10.043685000000	2.056526000000	-1.282767000000
C	9.575867000000	1.148130000000	-2.158945000000
C	8.343591000000	0.375061000000	-1.904557000000
C	7.630027000000	0.580274000000	-0.639413000000
C	8.239930000000	-0.941188000000	-2.594409000000
C	9.822630000000	3.338143000000	0.782284000000
C	-3.558972000000	-5.177466000000	0.098716000000
C	-2.847822000000	-4.890555000000	-1.206029000000
C	-3.654019000000	-4.532355000000	2.504945000000
C	-3.014607000000	-4.533468000000	1.288982000000
C	-1.863634000000	-3.630810000000	1.112365000000
C	-0.928612000000	-3.996378000000	0.001410000000
C	-1.620756000000	-4.350864000000	-1.267859000000
C	-0.938950000000	-4.096306000000	-2.570142000000
O	1.396195000000	-0.700977000000	-0.258591000000
O	-4.779034000000	-5.217665000000	2.678426000000
O	11.149295000000	2.778800000000	-1.543314000000
O	5.376661000000	1.312974000000	0.454606000000
H	1.040912000000	-1.264972000000	-0.970044000000
C	-3.674884000000	-5.226322000000	-2.415554000000
O	-4.538204000000	-4.489774000000	-2.823019000000
O	-3.391074000000	-6.424057000000	-2.918415000000
H	-3.980688000000	-6.558593000000	-3.674165000000
H	-5.235246000000	-4.905066000000	3.473482000000
C	9.835662000000	4.648818000000	2.919410000000
O	10.868275000000	5.208705000000	2.633155000000
O	9.179594000000	4.863280000000	4.069521000000

H	9.684336000000	5.527789000000	4.557488000000
C	1.018414000000	1.424365000000	2.679561000000
O	1.619112000000	2.249821000000	2.031156000000
O	0.081811000000	1.740079000000	3.580053000000
H	0.011197000000	2.704838000000	3.580943000000
C	7.608766000000	-3.255555000000	-2.903131000000
O	8.124460000000	-3.389102000000	-3.985147000000
O	7.139274000000	-4.281434000000	-2.174564000000
H	7.301138000000	-5.088136000000	-2.683463000000
O	0.157717000000	-4.846372000000	0.381079000000
O	7.121075000000	1.172630000000	-1.810682000000
O	4.840360000000	-2.077233000000	1.381687000000
O	-1.378000000000	-2.475760000000	4.583116000000
H	-1.791082000000	-2.720382000000	5.418370000000
O	8.838903000000	0.415088000000	1.287488000000
H	9.470965000000	0.821601000000	1.890261000000
O	-2.168922000000	-2.222826000000	1.237943000000
H	11.498395000000	2.467396000000	-2.389395000000
H	8.904987000000	-1.113836000000	-3.434546000000
H	-3.596664000000	-3.964121000000	4.609869000000
H	-0.770044000000	-0.429406000000	3.201437000000
H	7.427117000000	3.436242000000	3.245343000000
H	10.689017000000	3.927148000000	0.505338000000
H	3.249796000000	-3.467372000000	-3.300179000000
O	-1.535733000000	-4.175104000000	-3.621737000000
O	1.134881000000	-3.706826000000	-3.656488000000
O	4.752634000000	-2.793064000000	-2.118305000000
O	5.210895000000	2.991686000000	3.510499000000
O	10.291295000000	0.932108000000	-3.321121000000
H	9.773927000000	1.232784000000	-4.077190000000
O	-4.541524000000	-5.898178000000	0.064391000000
O	1.118006000000	-3.146862000000	2.415036000000
O	3.394351000000	1.155668000000	4.041705000000
O	7.312747000000	-1.782189000000	0.266040000000
Fe	-6.512479000000	2.610899000000	0.054810000000
S	-8.564861000000	1.812501000000	0.606858000000
O	-4.796489000000	3.280274000000	-0.450094000000
N	-7.110905000000	2.420541000000	-1.791337000000
N	-8.245053000000	1.699363000000	-2.092020000000
N	-10.122866000000	0.729012000000	-1.255847000000
C	-4.503844000000	3.825912000000	-1.589887000000
C	-3.304984000000	4.575127000000	-1.688685000000
C	-2.837831000000	5.062113000000	-2.894937000000
C	-3.571078000000	4.828723000000	-4.060326000000
C	-4.774291000000	4.150879000000	-4.000529000000
C	-5.264467000000	3.652952000000	-2.783587000000
C	-6.495013000000	2.890718000000	-2.822042000000
C	-8.952182000000	1.389344000000	-1.038376000000
H	-2.756653000000	4.753111000000	-0.768955000000
H	-1.909138000000	5.621214000000	-2.941772000000
H	-5.346299000000	3.990705000000	-4.909799000000
H	-6.949145000000	2.694426000000	-3.793142000000
H	-10.531758000000	0.232153000000	-0.483422000000
H	-10.257059000000	0.349508000000	-2.179420000000
S	-7.172137000000	4.774601000000	0.270775000000
O	-5.850074000000	0.782588000000	-0.058776000000
N	-5.899038000000	2.787642000000	1.897395000000
N	-5.720925000000	4.034760000000	2.454104000000
N	-6.131886000000	6.259175000000	2.221749000000
C	-5.919549000000	-0.027145000000	0.964768000000
C	-6.145845000000	-1.407516000000	0.752142000000
C	-6.228623000000	-2.314403000000	1.792447000000

C	-6.078721000000	-1.855343000000	3.100983000000
C	-5.835113000000	-0.522543000000	3.362379000000
C	-5.761522000000	0.403582000000	2.313456000000
C	-5.598817000000	1.801380000000	2.669100000000
C	-6.269466000000	4.987756000000	1.748478000000
H	-6.294906000000	-1.741820000000	-0.268379000000
H	-6.421259000000	-3.362906000000	1.590324000000
H	-5.741556000000	-0.175663000000	4.387141000000
H	-5.263092000000	2.048434000000	3.676380000000
H	-6.749567000000	6.960505000000	1.849912000000
H	-5.867506000000	6.344765000000	3.190498000000
Cl	-6.309877000000	-2.967011000000	4.462223000000
Cl	-2.963414000000	5.407430000000	-5.602199000000
C	-2.551994000000	1.218111000000	-0.666770000000
H	-3.580753000000	0.947924000000	-0.418549000000
H	-2.564531000000	2.287031000000	-0.865913000000
N	-2.238129000000	0.549840000000	-1.996850000000
C	-1.596433000000	0.892296000000	0.459434000000
H	-2.012859000000	1.344426000000	1.363550000000
H	-0.594812000000	1.303923000000	0.309335000000
H	-1.515427000000	-0.179954000000	0.637825000000
C	-2.375596000000	-0.954796000000	-1.901876000000
H	-2.158637000000	-1.343235000000	-2.898566000000
H	-1.577645000000	-1.292839000000	-1.234416000000
C	-0.487520000000	2.293013000000	-2.688543000000
H	-0.701398000000	2.926421000000	-1.825604000000
H	-1.012814000000	2.703320000000	-3.553029000000
H	0.585028000000	2.356073000000	-2.887345000000
C	-3.237376000000	1.122575000000	-2.982149000000
H	-4.214448000000	1.040557000000	-2.504996000000
H	-3.013669000000	2.185161000000	-3.048182000000
C	-0.820585000000	0.833851000000	-2.431393000000
H	-0.182034000000	0.443292000000	-1.639026000000
H	-0.645006000000	0.235805000000	-3.328213000000
C	-3.723997000000	-1.431324000000	-1.400220000000
H	-3.781428000000	-1.392989000000	-0.313039000000
H	-3.878366000000	-2.461915000000	-1.723380000000
H	-4.557297000000	-0.848938000000	-1.796621000000
C	-3.247136000000	0.491842000000	-4.360161000000
H	-3.614996000000	-0.536451000000	-4.355113000000
H	-2.270342000000	0.520828000000	-4.850458000000
H	-3.931548000000	1.084524000000	-4.971963000000