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Catalytically active hybrid complex of fullerene C_{60} and vitamine B_{12}

Valentina S. Romanova, Nadezhda Yu. Shepeta, Zinaida S. Klemenkova and Konstantin A. Kochetkov

General remarks

The IR spectra were measured on aTensor 37 Fourier spectrometer (Bruker) in the region of 4000-400 cm^{-1} for samples in the form of tablets with KBr. UV-Vis spectra were recorded on a spectrophotometer V-780 (Japan) in 1 cm quartz cuvettes in aqueous solutions containing $5 \cdot 10^{-5}$ mol of the test substance at 23°C. The wave length range is 220– 700 nm. Scanning speed 400 nm/min, scanning interval 0.5 nm.

The study of autooxidation of ascorbic acid

UV-Vis spectra were recorded on a V-780 spectrophotometer (Japan) in 1 cm quartz cuvettes in 0.05 M phosphate buffer at pH 6.0 at room temperature. The working wavelength was 262 nm, the number of cycles was 5. The ratio of substrate: complex was 10:1, and the working concentrations of the substrate and complex were $5 \cdot 10^{-5}$ M and $5 \cdot 10^{-6}$ M, respectively.

Syntheses

Compound **1** was synthesized according to the method[1] and the compound **2** to the method from[2]. Complexes **3** and **4** was synthesized by us early [13].

†† Complex $(OH)_2$-Cbi-*e*-$C(O)OCH_2CH_2$-$C_{60}NH(CH_2)_5COOCH_3$ (7)

To a solution 0.0361 g ($3.64 \cdot 10^{-5}$ mol) compound **5** in 5 ml DMF was added 0.0290 g ($3.64 \cdot 10^{-4}$ mol) ethylene chlorohydrin and 0.0091 g ($4.37 \cdot 10^{-5}$ mol) (1,2-fold excess relative to compound **5**) dicyclohexylcarbodiimide. The addition of the ethylene chlorohydrin molecule was carried out with a very large excess of the latter, which greatly impeded the isolation of compound **6**. The mixture was stirred for 2 days at room temperature. Dialysis against water was not possible because, together with the excess ethylene chlorohydrin, the resulting product also passed through the dialysis bag. Therefore, dialysis was performed against chloroform for 2 days. In this case, derivative **6** remained in the dialysis bag, and the excess ethylene chlorohydrin left with the

solvent. Then, 0.0472 g ($5.46 \cdot 10^{-5}$ mol) (1,5-fold excess) of compound **2** in 5 ml of pyridine was added to this solution, and the mixture was stirred at room temperature for 8 hours, then left overnight. The final product **7** was dialyzed against water. In this case, an excess of water-insoluble compound **2** and the urea obtained during the reaction precipitated, and the unreacted chlorine-containing component **6** penetrates through the dialysis bag, staining the water pink. Then the solution was removed from the dialysis bag and the precipitate was filtered off. An aqueous solution of the complex **7** was obtained in almost quantitative yield.

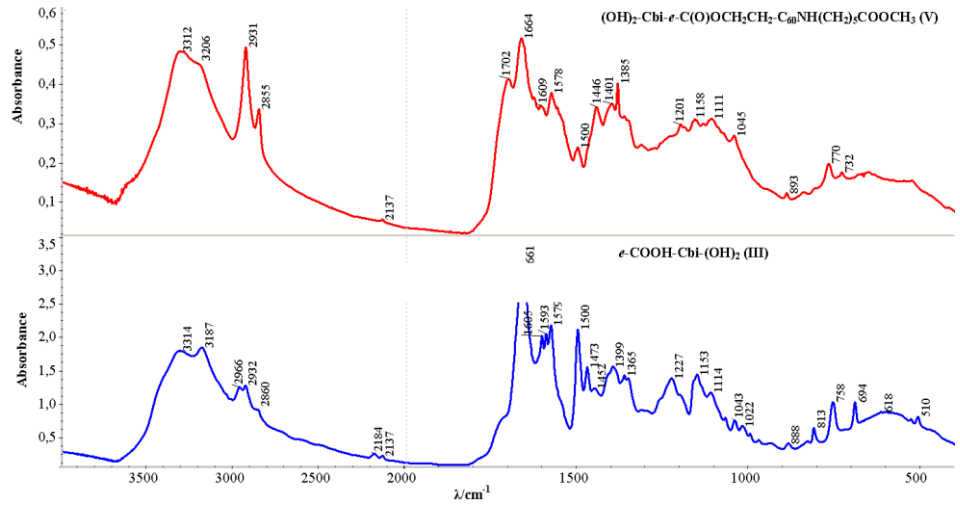


Figure S1. IR spectra of compounds **5** and **7**.

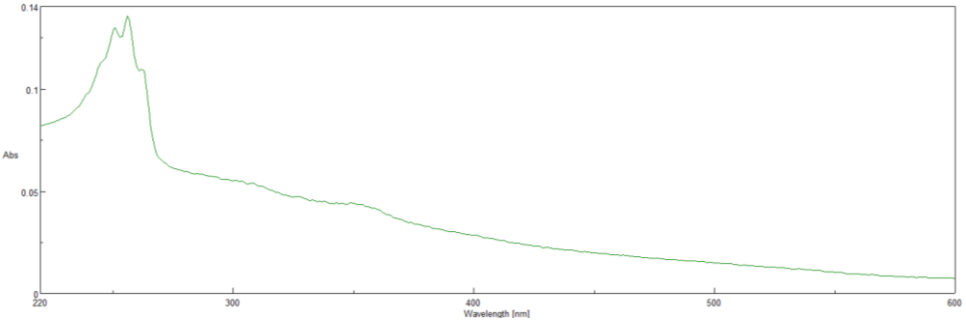
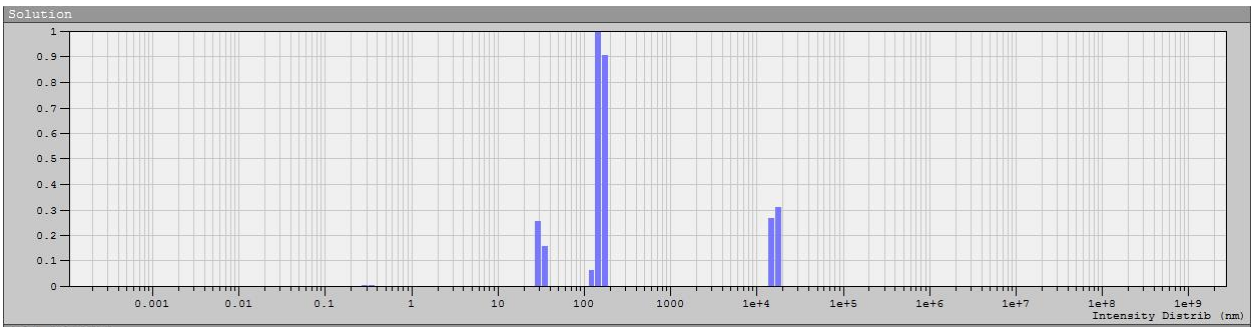


Figure S2. UV- spectra of compound **7**.



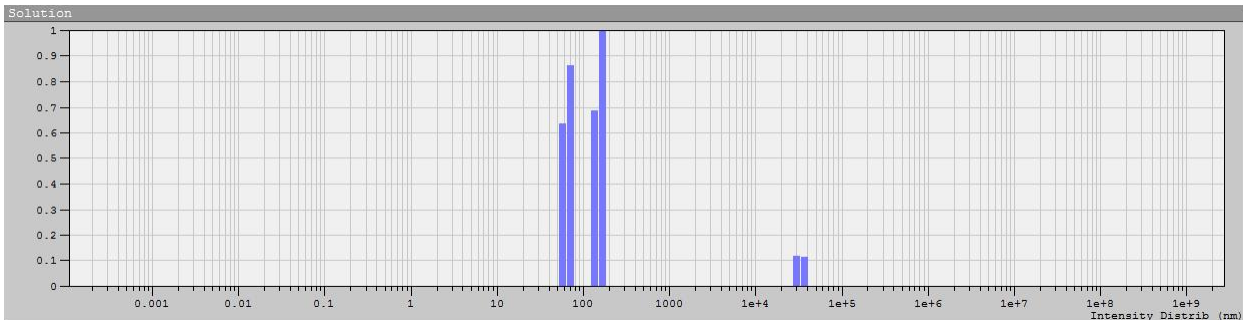
❖ **Distribution analysis**

Fitting range : [50; 240] channels
Number of Intervals : 170
Boundaries : [1.5e-4; 2.0e+9]
Resolution : 0

Peak Num	Area	Mean	Position	STD
1	0.139	31.23	29.09	3.327
2	0.666	156.4	144.3	17.85
3	0.194	1.6e+4	1.8e+4	1731.

χ^2 : 2.2e-4

Figure S3. The light scattering data of compound **3**.



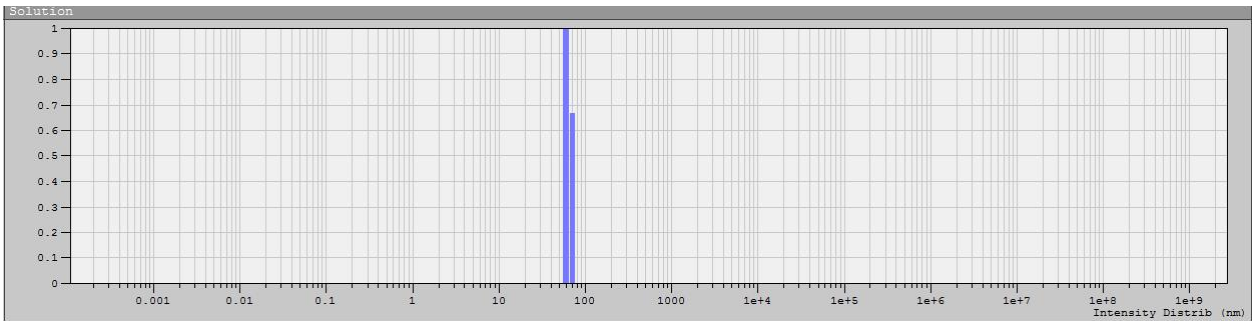
❖ **Distribution analysis**

Fitting range : [50; 200] channels
Number of Intervals : 140
Boundaries : [1.5e-4; 2.0e+9]
Resolution : 0

Peak Num	Area	Mean	Position	STD
1	0.439	64.69	70.50	7.886
2	0.494	154.1	167.3	18.65
3	0.067	3.4e+4	3.0e+4	4171.

χ^2 : 9.2e-5

Figure S4. The light scattering data of compound **4**.



❖ **Distribution analysis**

Fitting range	: [50; 130] channels
Number of Intervals	: 170
Boundaries	: [1.5e-4; 2.0e+9]
Resolution	: 0

Peak Num	Area	Mean	Position	STD
1	1.000	63.89	59.28	6.541

χ^2 : 3.4e-4

Figure S5. The light scattering data of compound **7**.

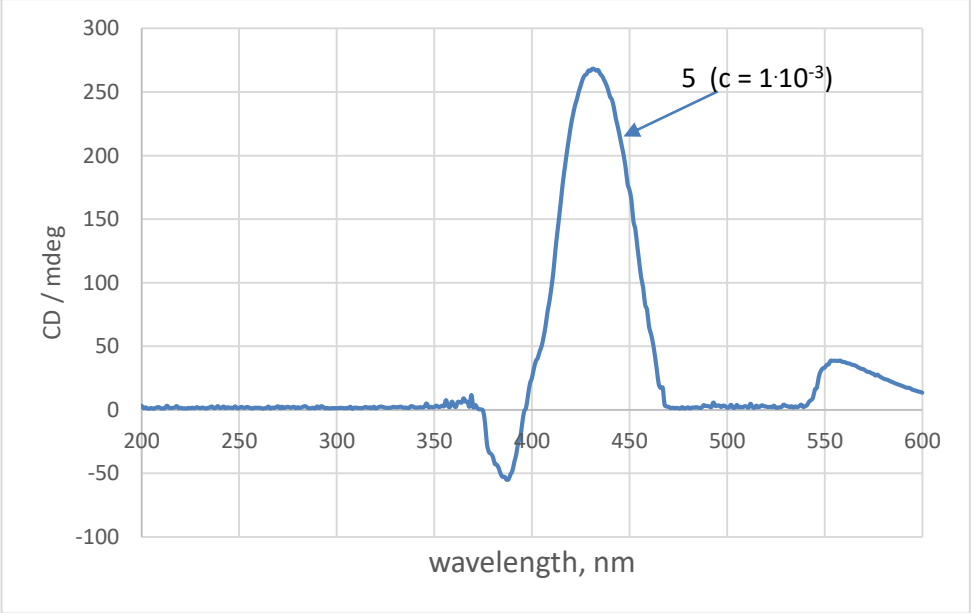


Figure S6. CD spectra of compound **5** ($c=1\cdot10^{-3}$).

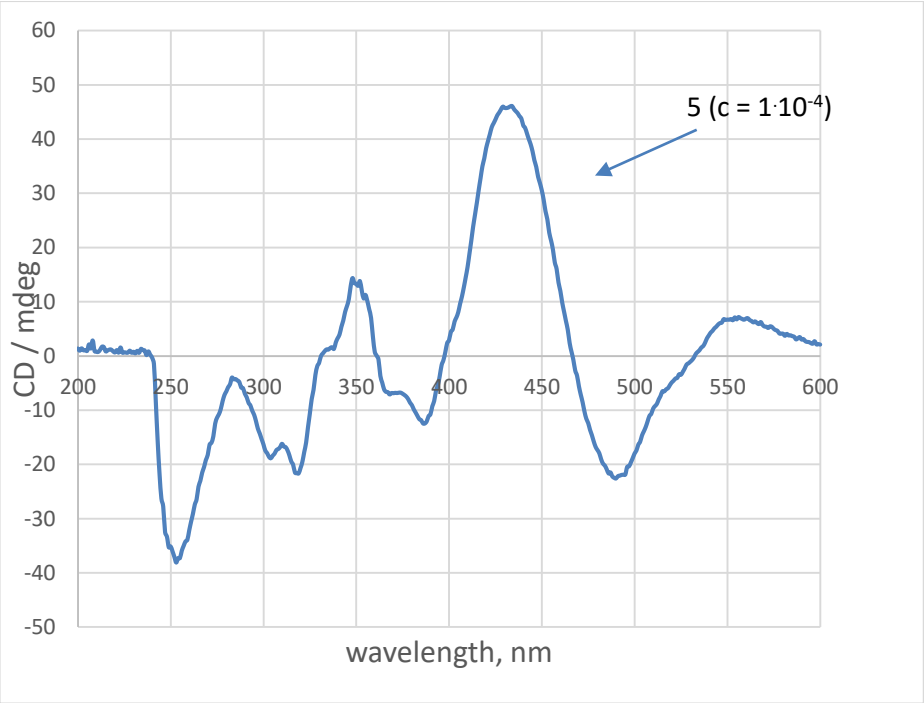


Figure S7. CD spectra of dilute aqueous solutions of compound **5** ($c=1\cdot10^{-4}$)

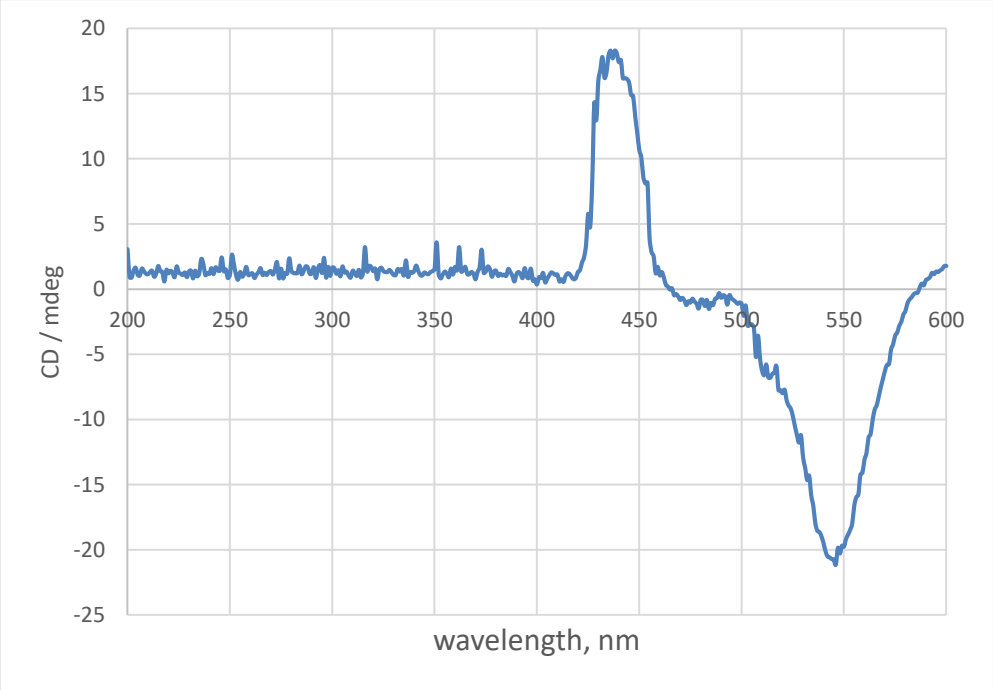


Figure S8. CD spectra of compound **3**.

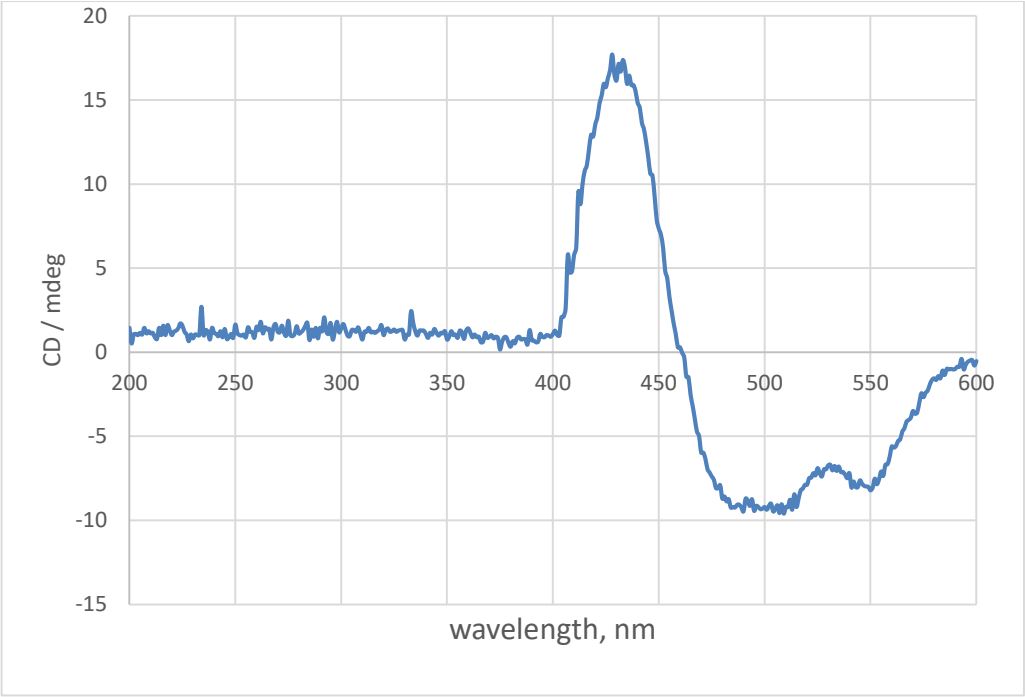


Figure S9. CD spectra of compound **4**.

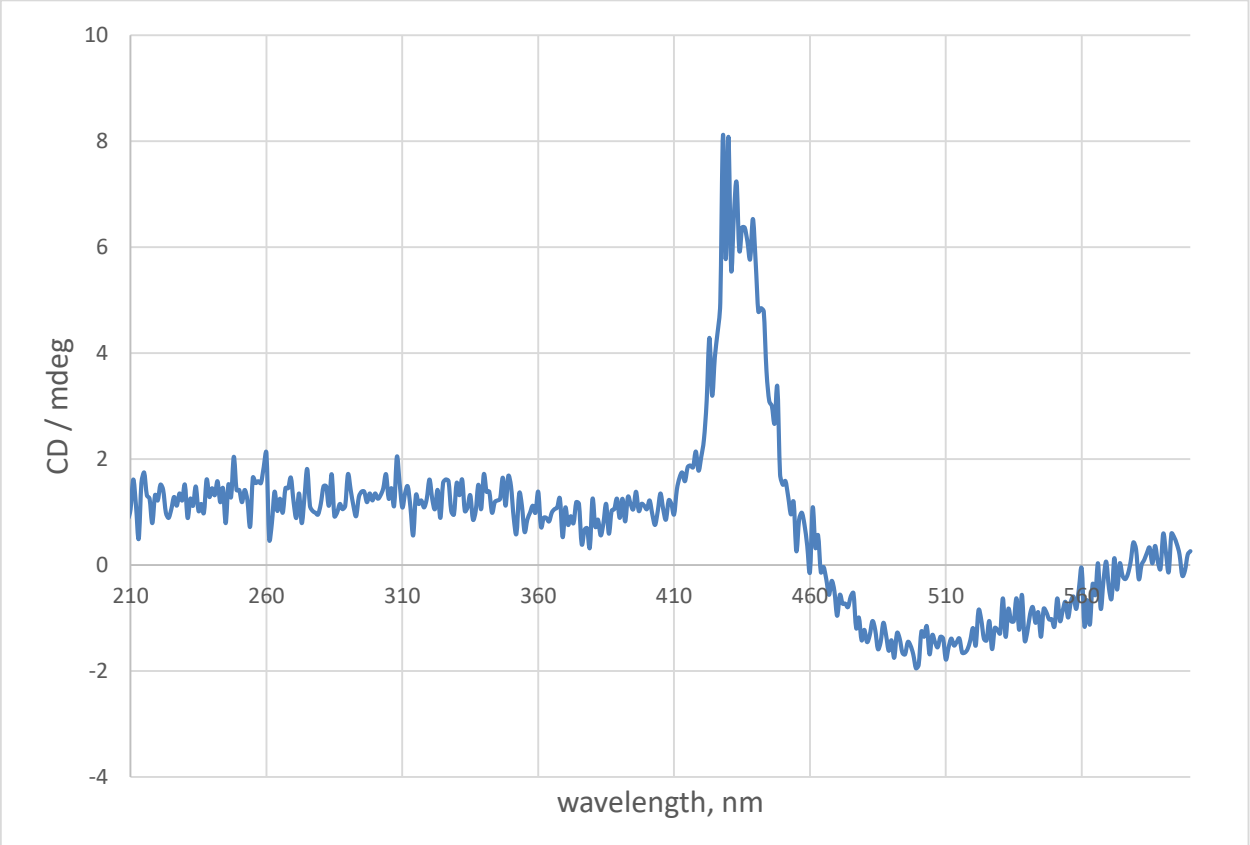


Figure S10. CD spectra of compound **7**.

References

1. H. A. O. Hill, J. M. Pratt and R. J. P. Williams, *Proc. R. Soc.*, 1965, **A288**, 352.
2. Z. S. Klemenkova, V. S. Romanova, V. A. Tsyryapkin, V. E. Muradan, Z. N. Parnes, B. V. Lokshin and M. E. Vol'pin, *Mendeleev Commun*., 1996, **6**, 60.