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Supplementary Information

Synthesis, Molecular Structure of Diethyl Phenylenebis(Methylene)Dicarbamates and FTIR Spectroscopy Molecular Recognition Study with Benzenediols

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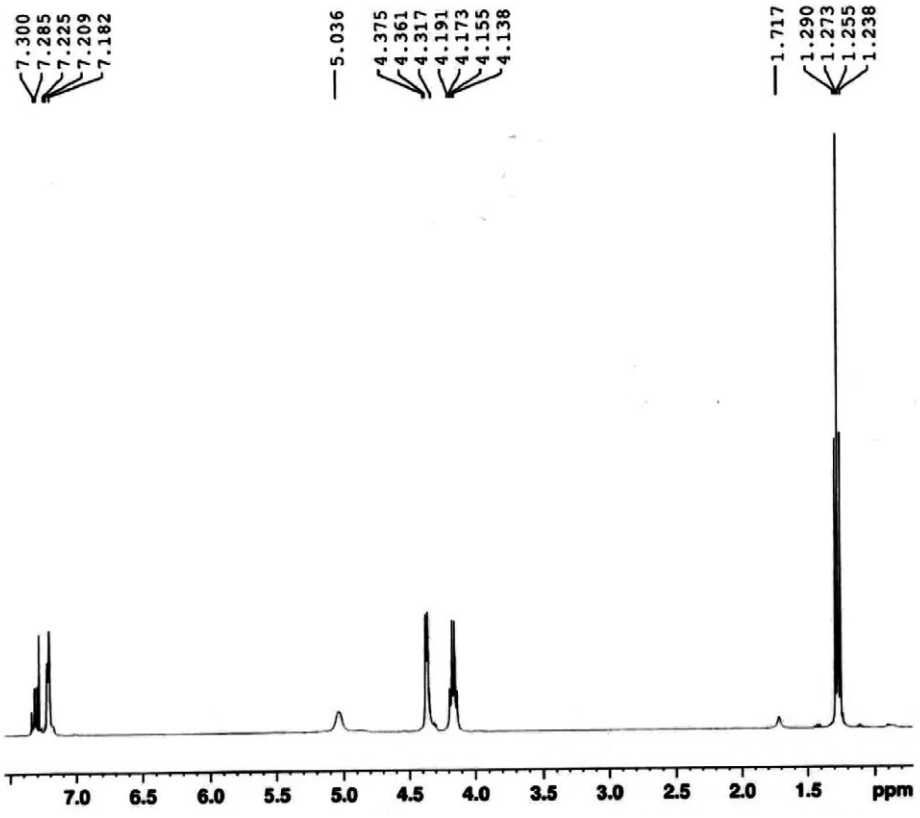

Figure S1. ^{1}H NMR (400 MHz, $CDCl_3$) spectra of **1a**.

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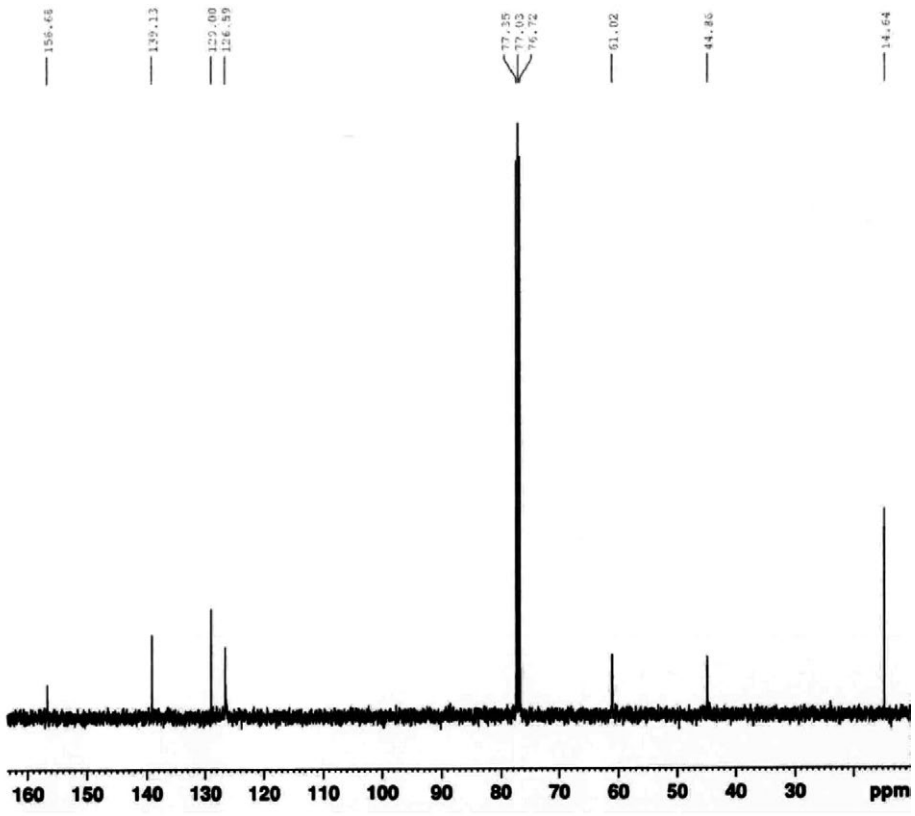

Figure S2. ^{13}C NMR (100 MHz, $CDCl_3$) spectra of **1a**.

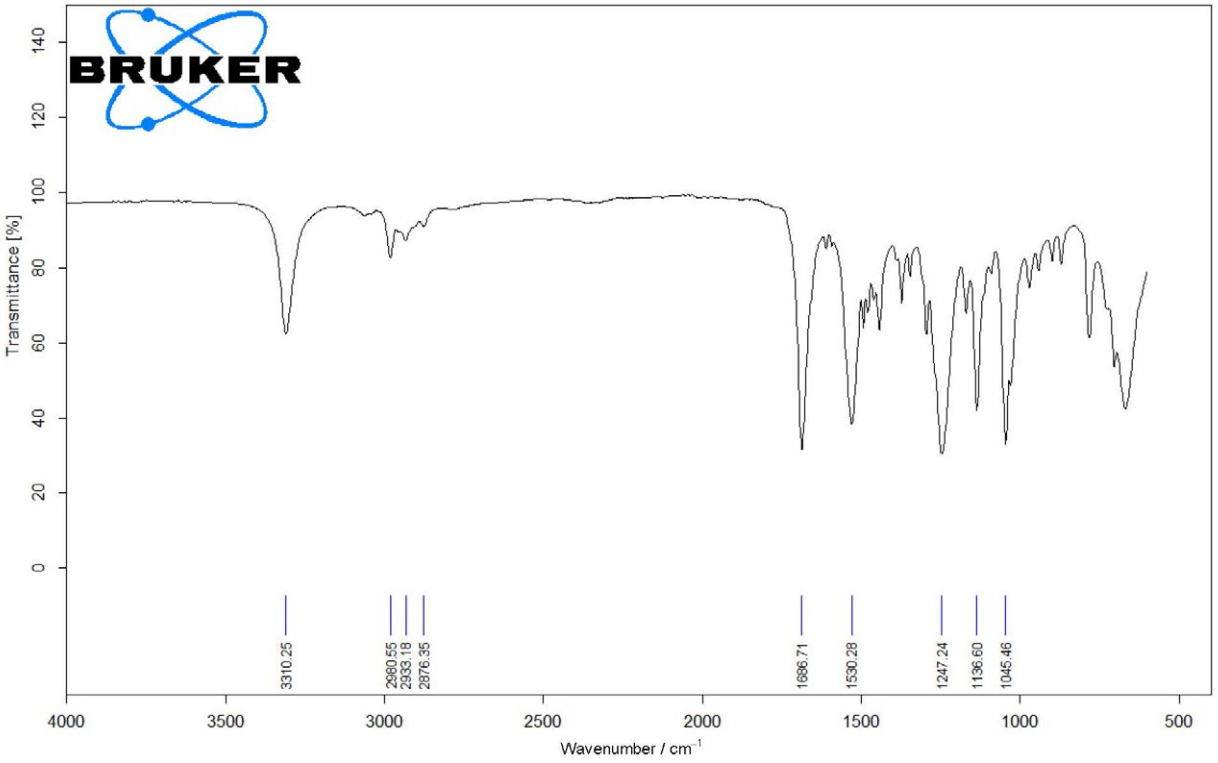

Figure S3. FT-IR spectra (neat, ATR) of **1a**.

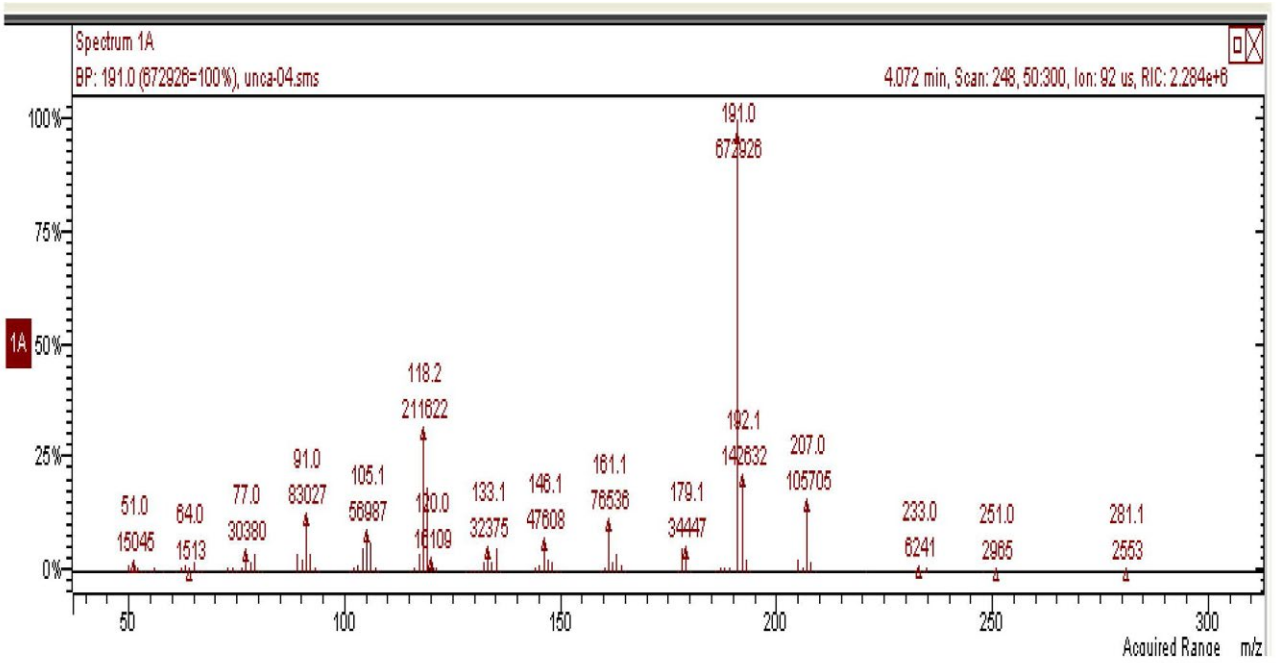

Figure S4. E.I. mass spectra of **1a**.

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Centro Conjunto de Investigación en Química Sustentable
Muestra: UNCA-01 Realizó: Alejandra Núñez
Teóricos: 9.99%N 59.99%C 7.19%H No.reg. 1096

Text report

No.	Name	Weight [mg]	N [%]	C [%]	H [%]
47	UNCA-01	1.6230	9.91	60.06	7.28

Figure S5. Elemental analysis data for **1a**.

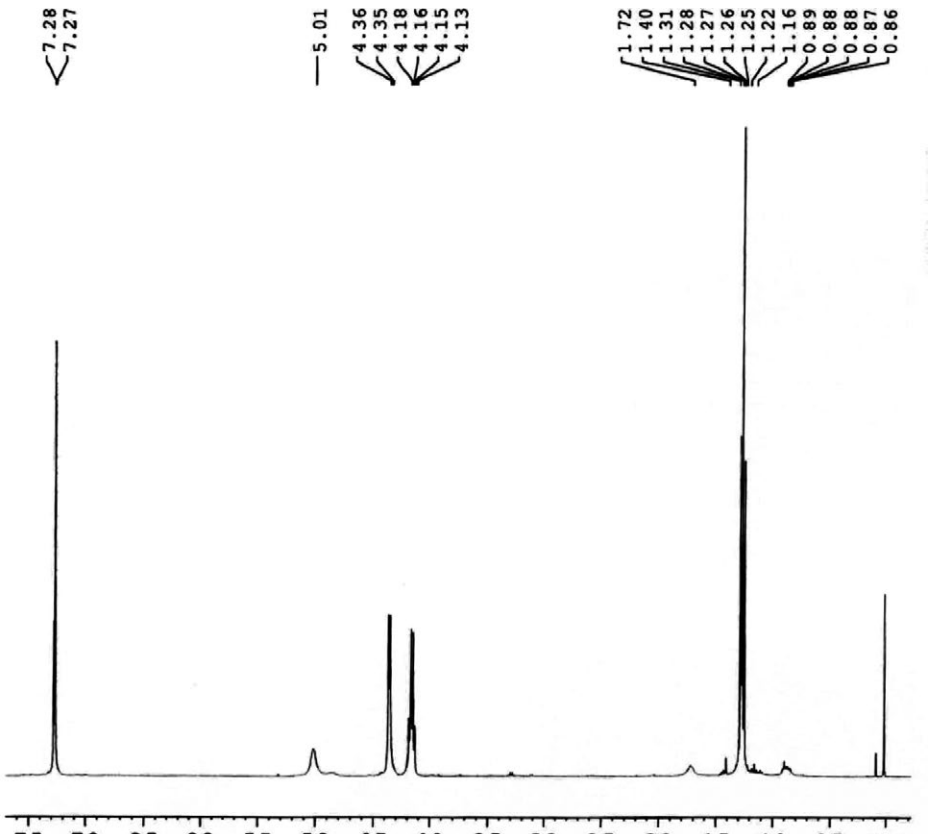

Figure S6. ^{1}H NMR (400 MHz, $CDCl_3$) spectra of **2a**.

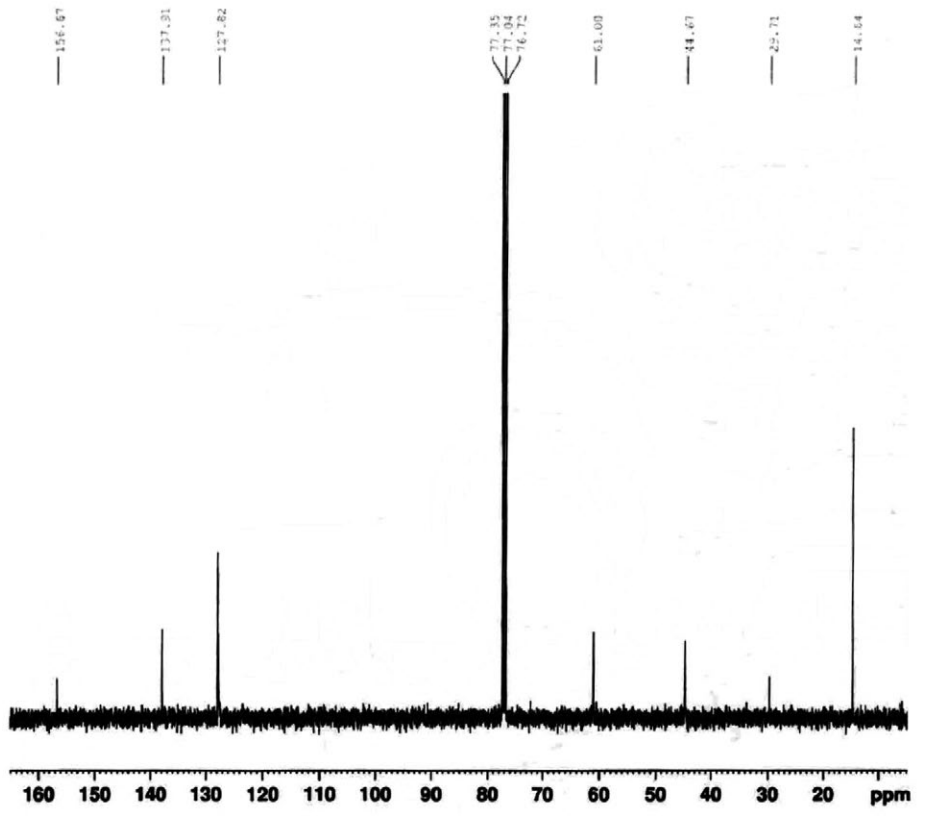

Figure S7. ^{13}C NMR (100 MHz, $CDCl_3$) spectra of **2a**.

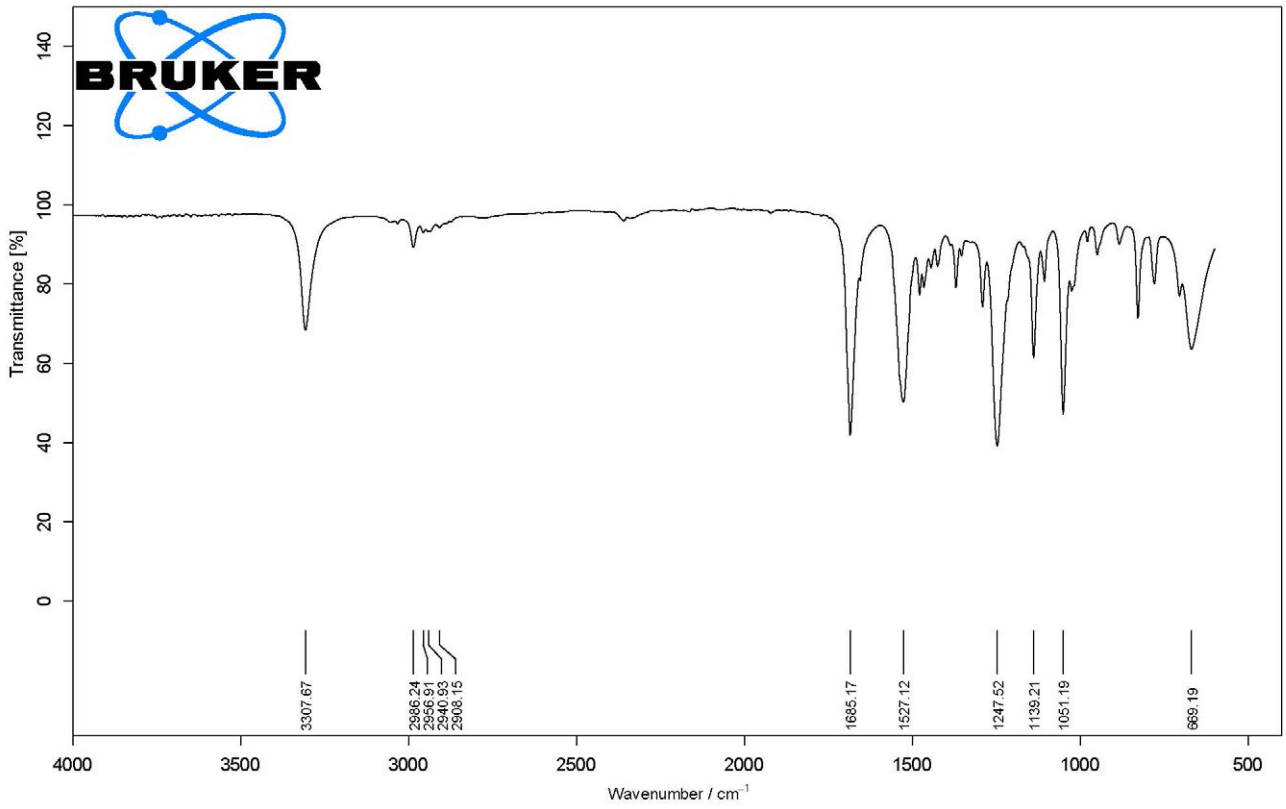

Figure S8. FT-IR spectra (neat, ATR) of **2a**.

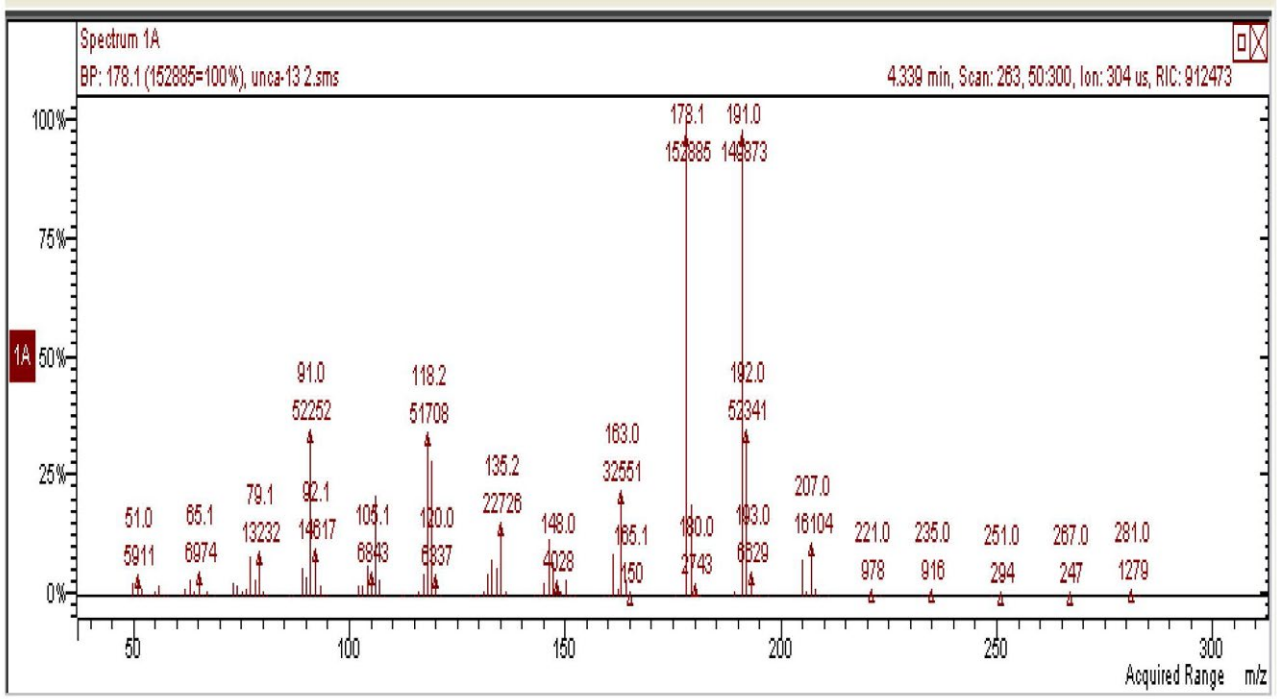

Figure S9. E.I. mass spectra of **2a**.

Document: 30-01-2014 (VarioMICRO) from: 30/01/2014 17:53:33

Centro Conjunto de Investigación en Química Sustentable
Muestra: UNCA-02 Realizó: Alejandra Núñez
Teóricos: 9.99%N 59.99%C 7.19%H No.reg. 1097

Text report

No.	Name	Weight [mg]	N [%]	C [%]	H [%]
48	UNCA-02	1.7880	10.00	59.91	7.25

Figure S10. Elemental analysis data for **2a**.

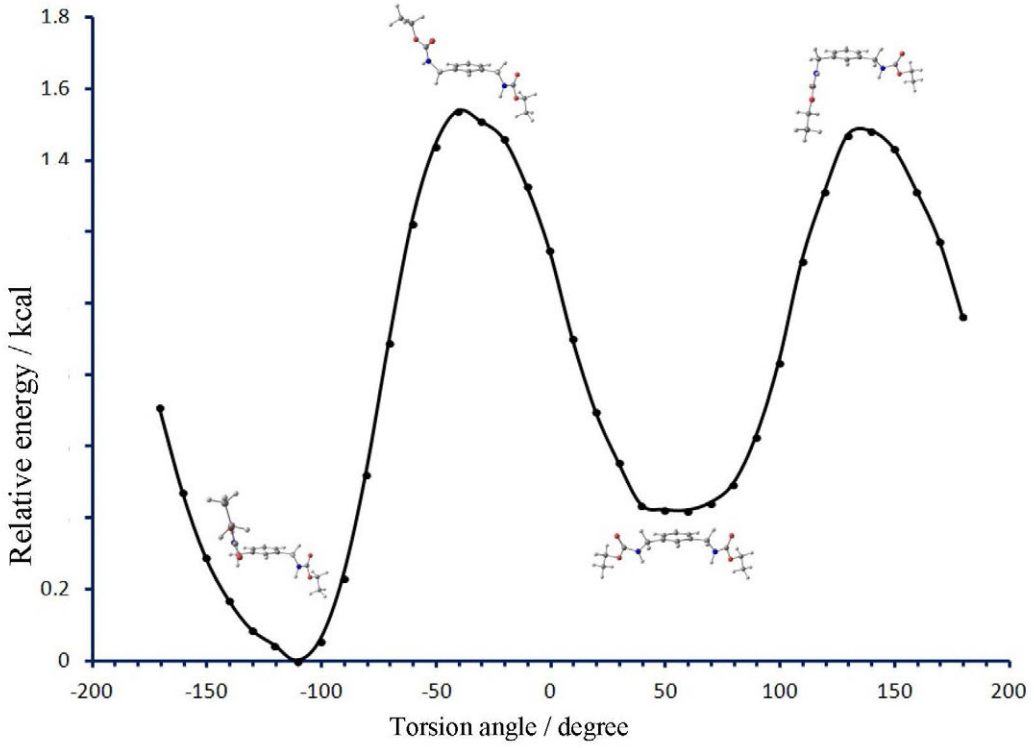

Figure S11. Potential energy as function of the C(2)-C(1)-C(7)-N(7) torsion angle in **1a.**

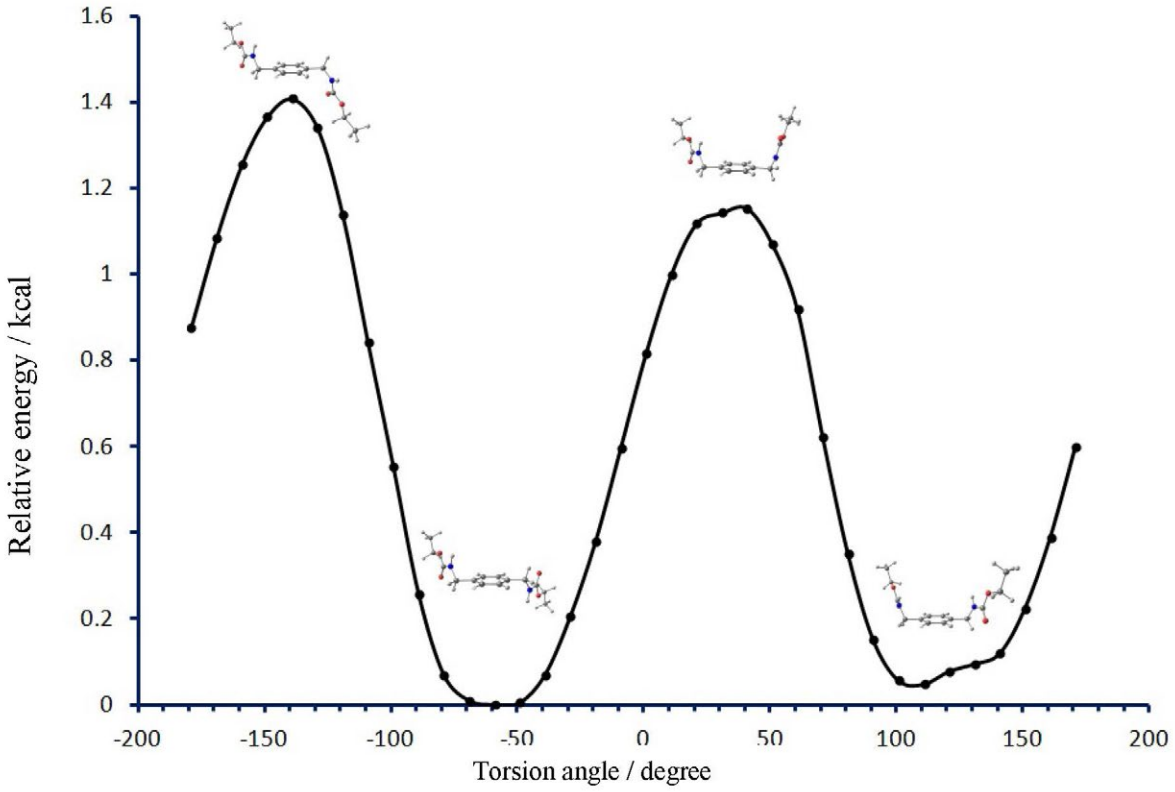

Figure S12. Potential energy as function of the C(2)-C(1)-C(7)-N(7) torsion angle in **2a.**

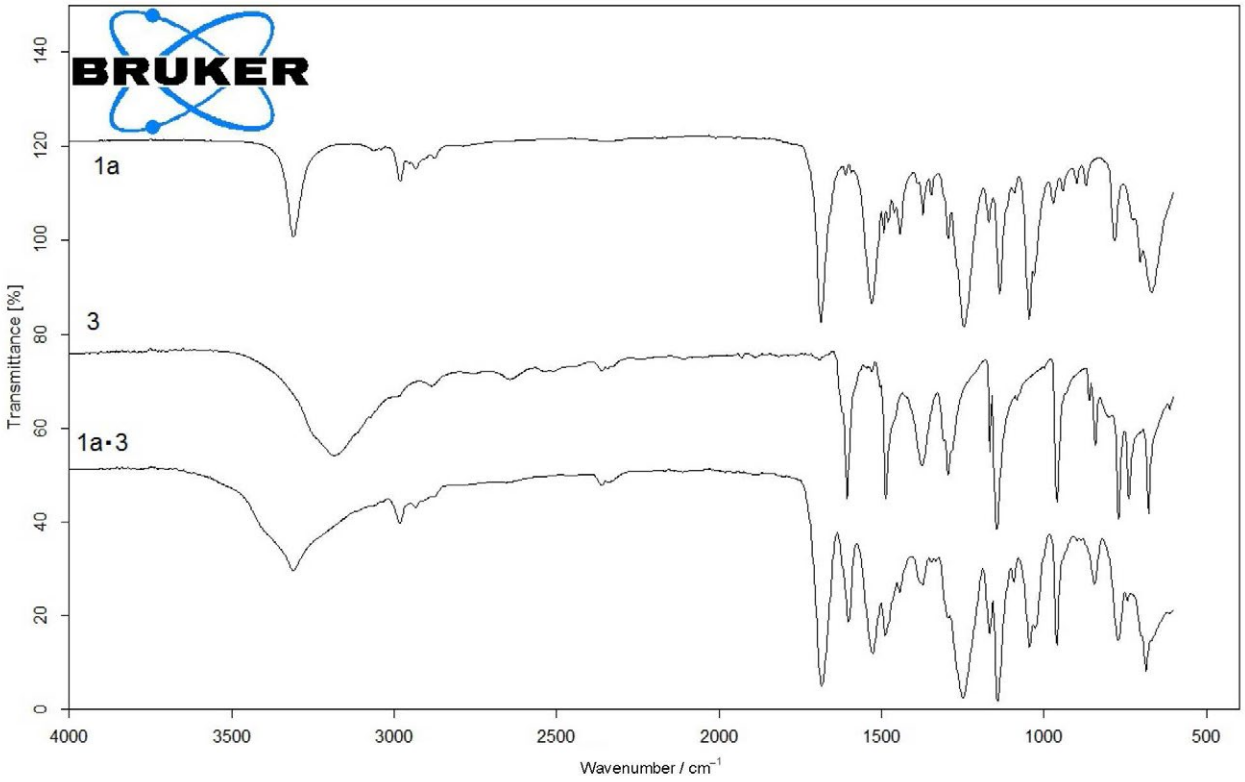

Figure S13. FT-IR spectra of **1a**, **3** and **1a·3** complex.

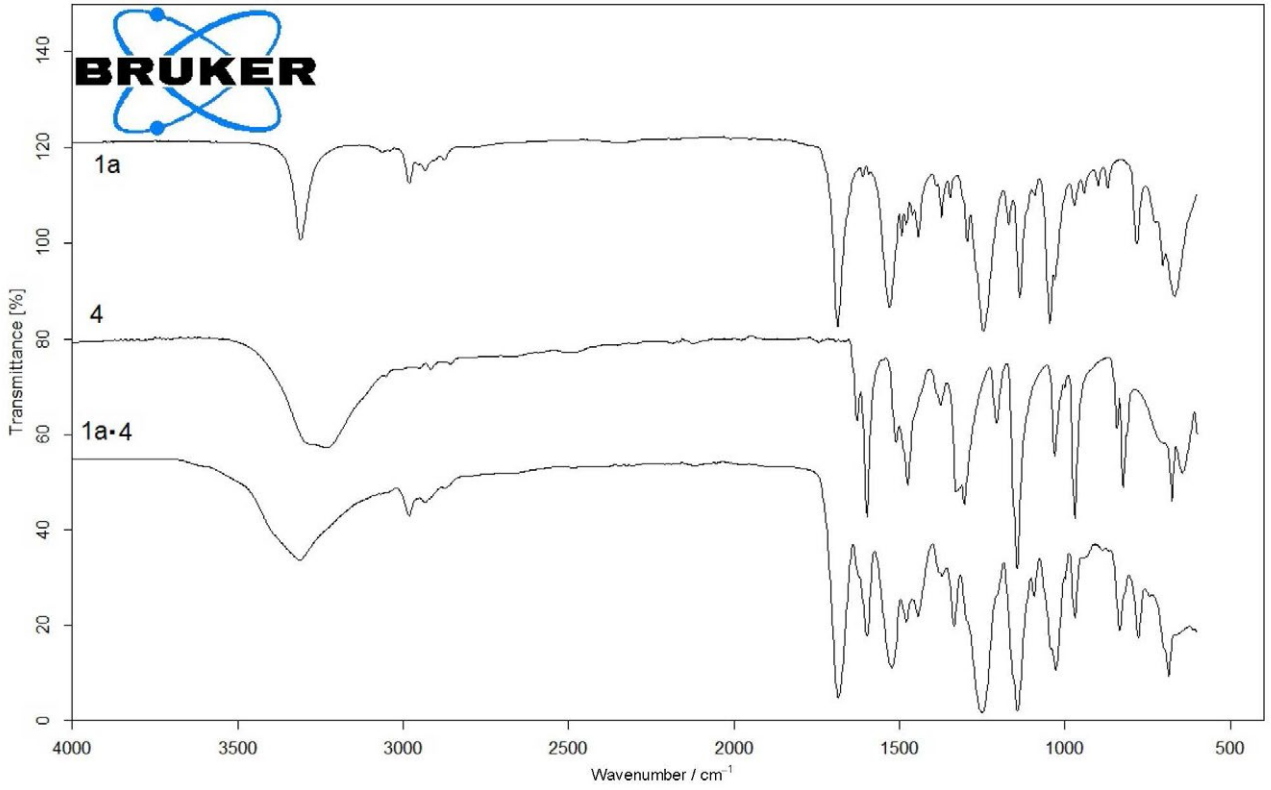

Figure S14. FT-IR spectra of **1a**, **4** and **1a·4** complex.

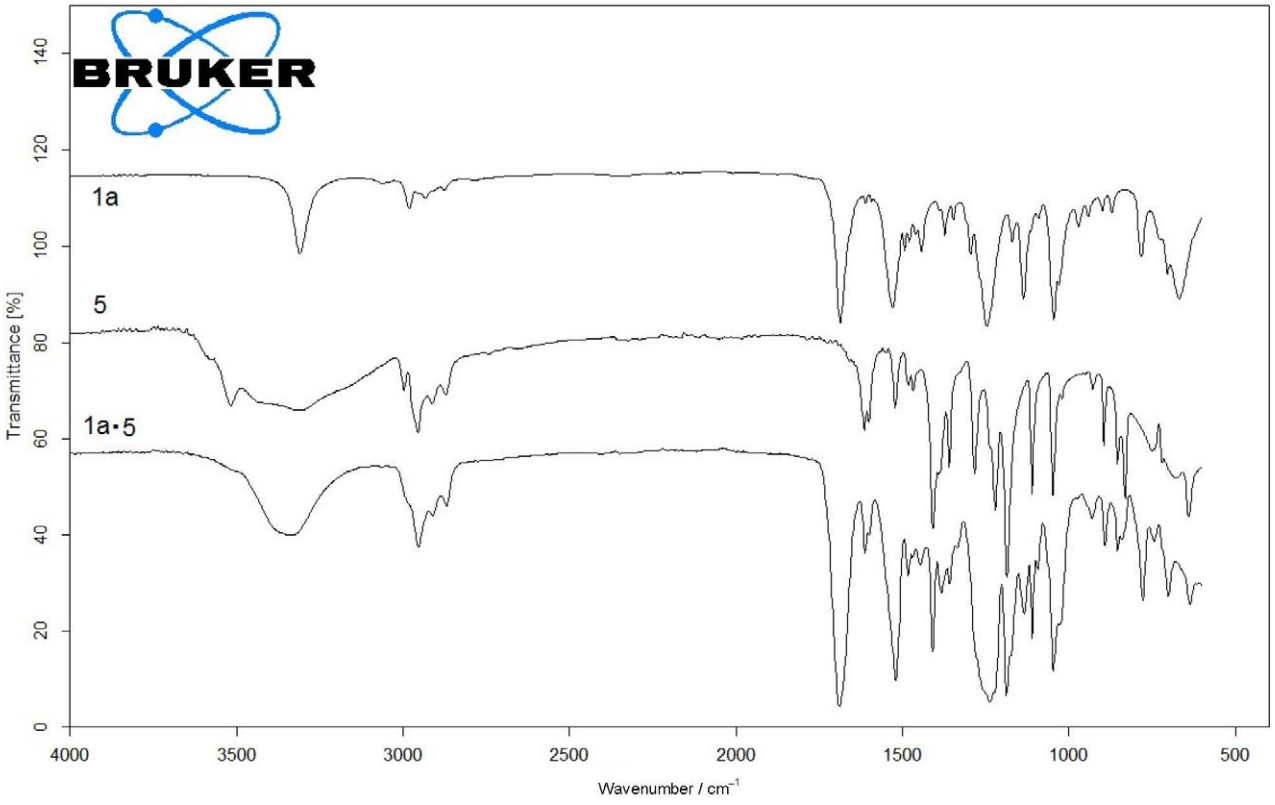

Figure S15. FT-IR spectra of **1a**, **5** and **1a·5** complex.

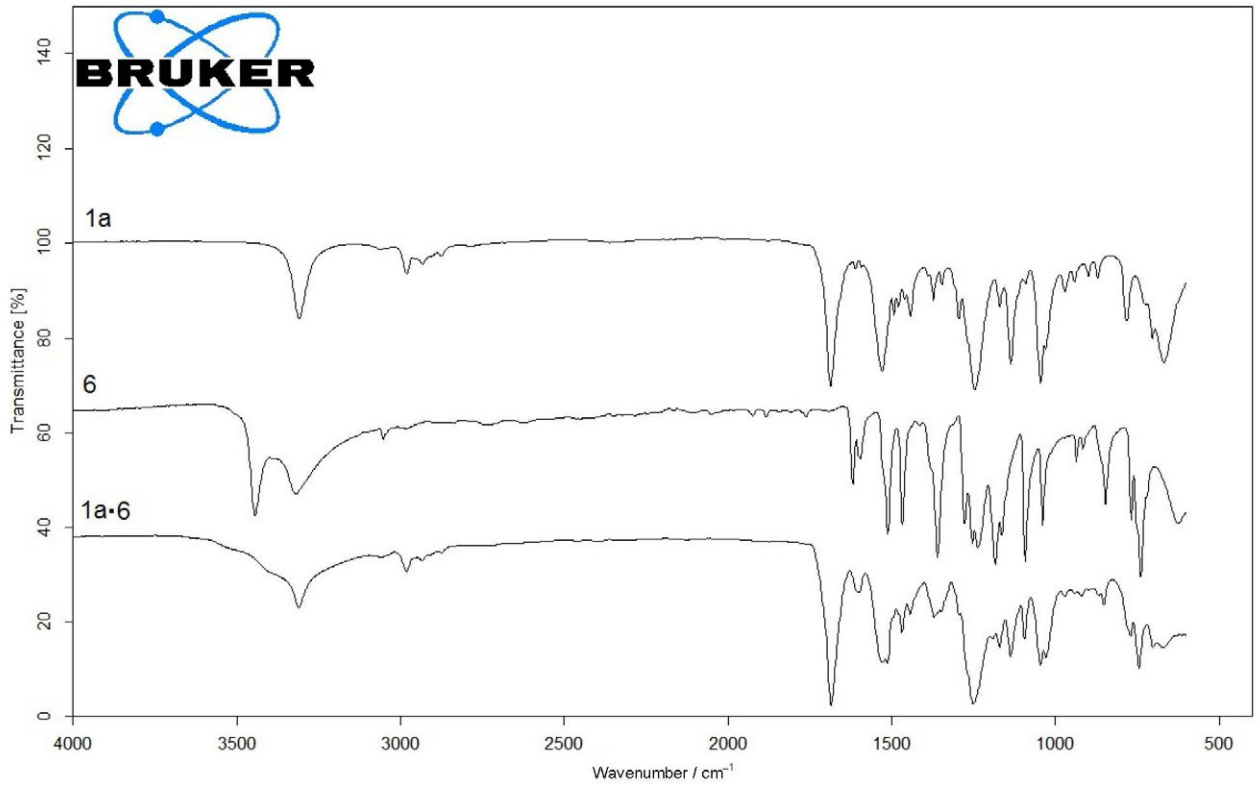

Figure S16. FT-IR spectra of **1a**, **6** and **1a·6** complex.

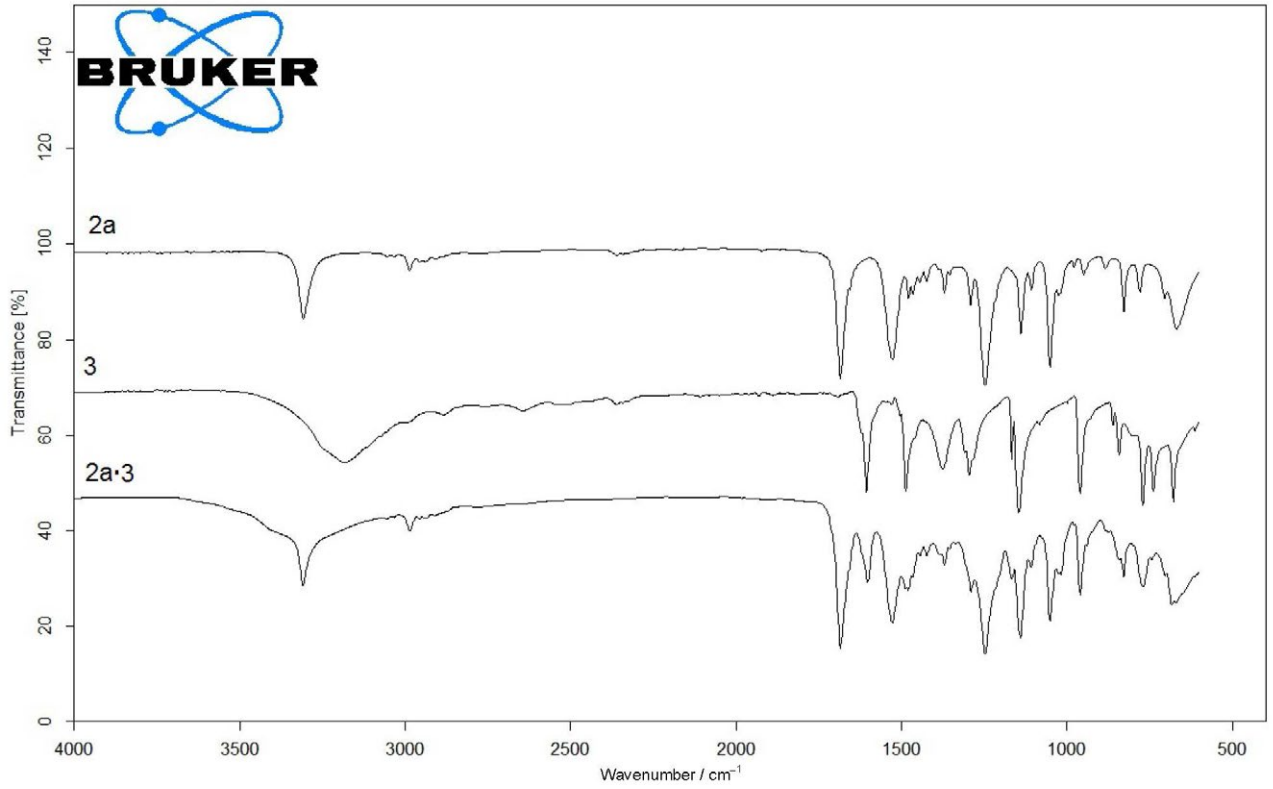

Figure S17. FT-IR spectra of **2a**, **3** and **2a·3** complex.

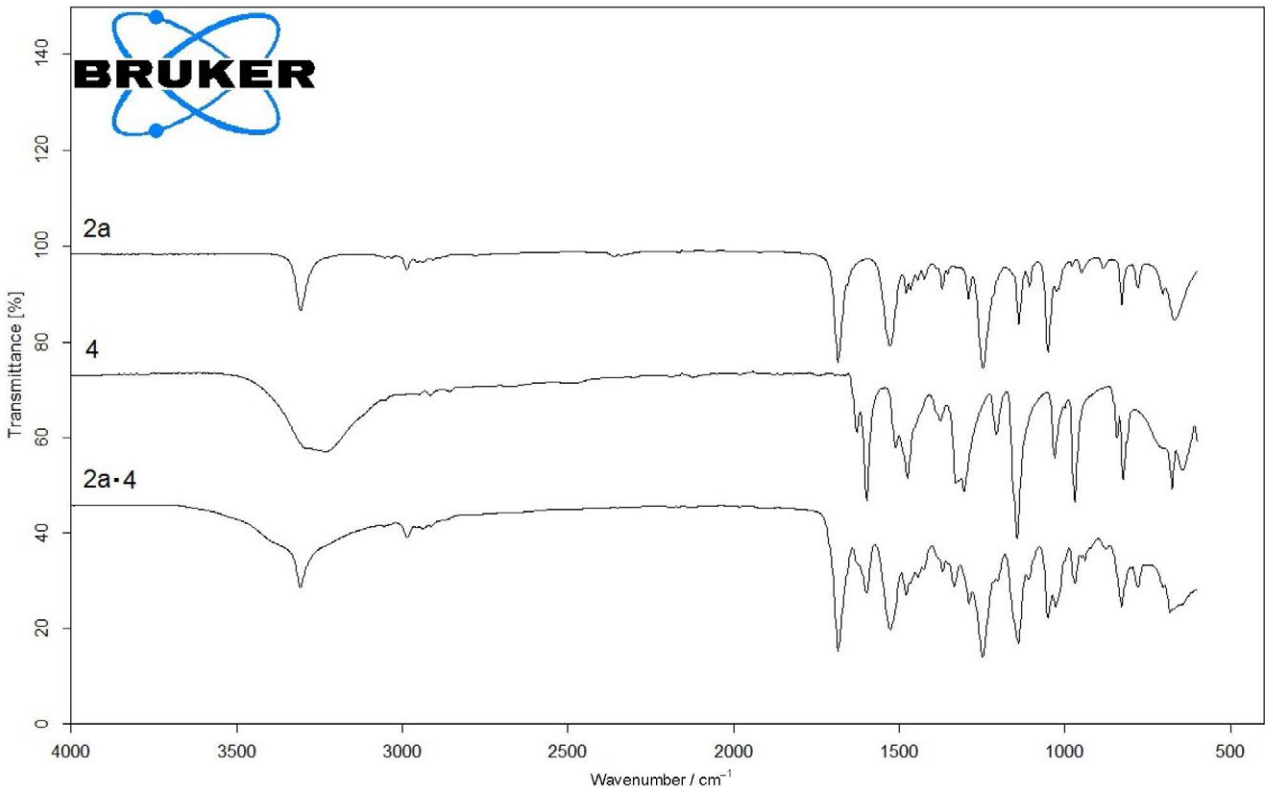

Figure S18. FT-IR spectra of **2a**, **4** and **2a·4** complex.

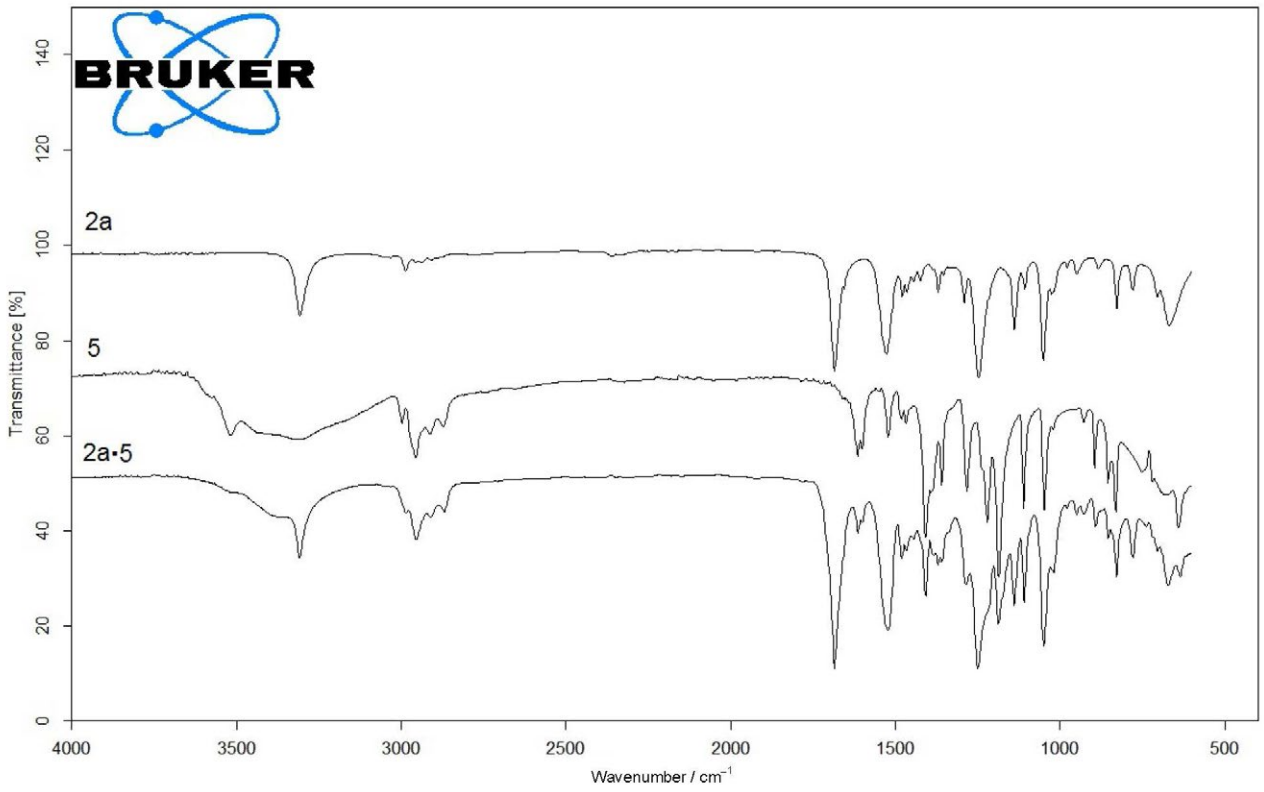

Figure S19. FT-IR spectra of **2a**, **5** and **2a·5** complex.

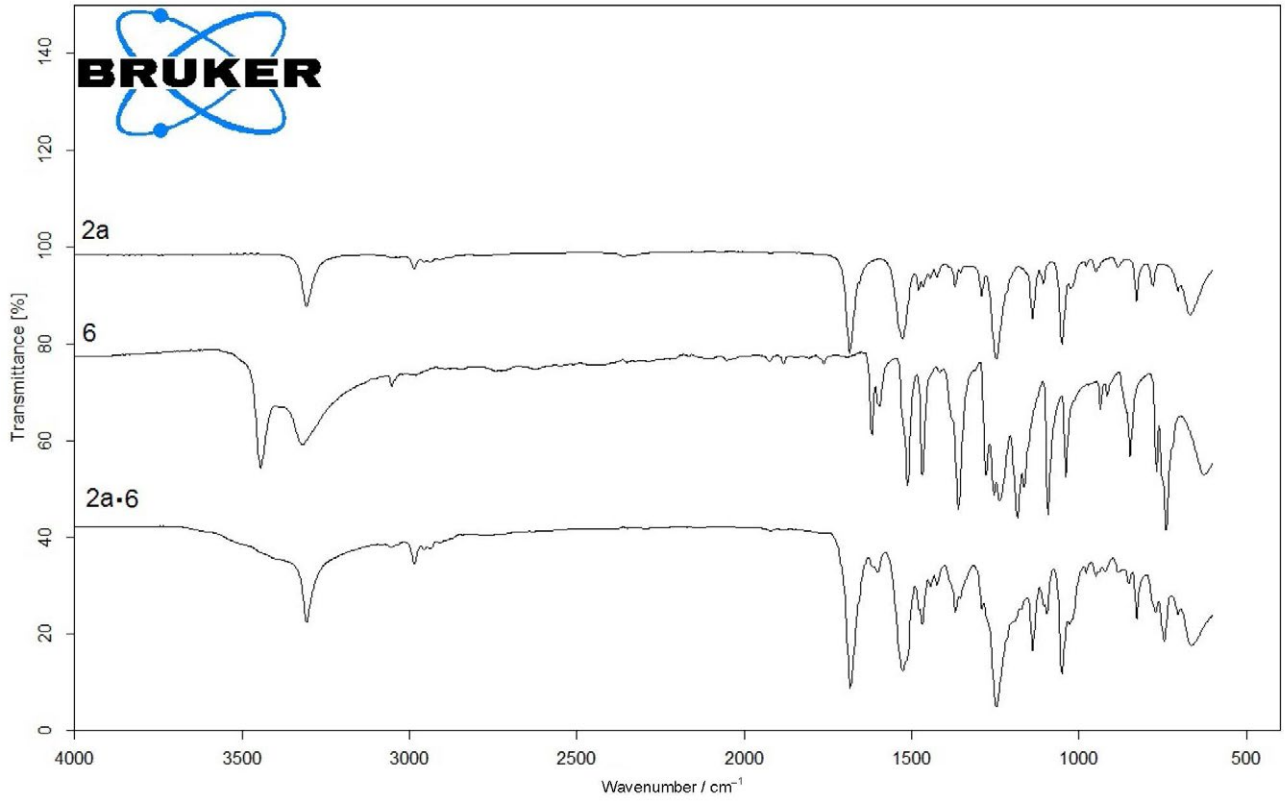

Figure S20. FT-IR spectra of **2a**, **6** and **2a·6** complex.