Supplementary Information

Assembly of Imidazolyl-substituted Nitronyl Nitroxides into Ferromagnetically Coupled Chains

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Contents:

NMR spectra of IBX-OTs and 4,5-Dichloro-1*H*-imidazole-2-carbaldehyde

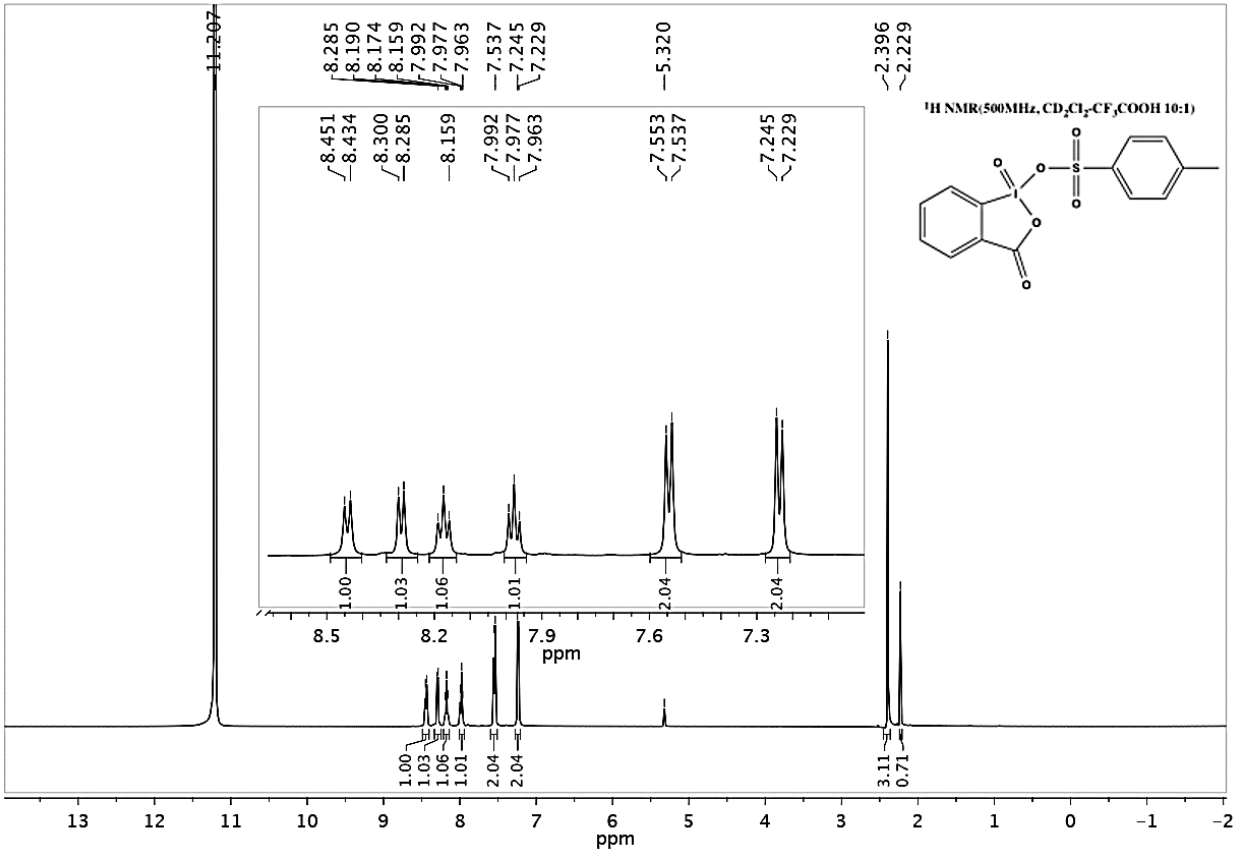

Figure S1. [1]H NMR spectrum of IBX-OTs.

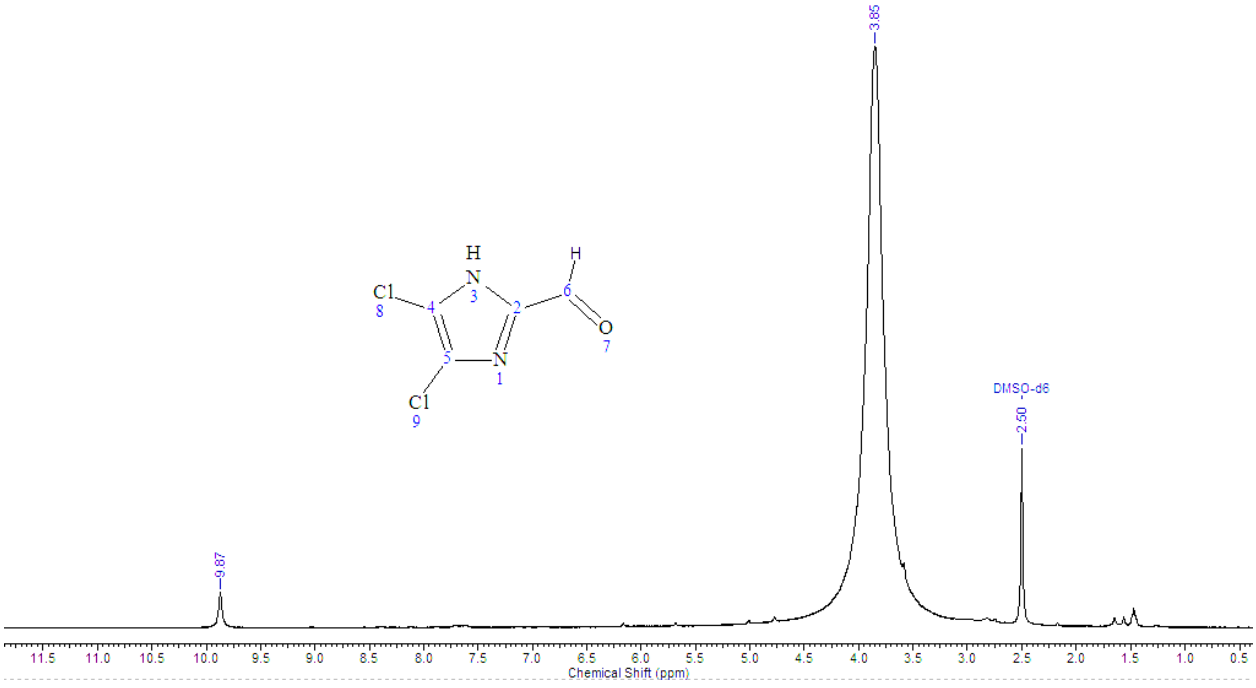

Figure S2. [1]H NMR spectrum of 4,5-dichloro-1*H*-imidazole-2-carbaldehyde.

EPR spectra of 1a,b

EPR spectra were acquired in a diluted and oxygen-free toluene solution at 295 K at the concentrations of 10^{-4} M by means of the commercial Bruker X-Band (9 GHz) spectrometer Elexys E540. For determining the isotropic g-factors (g_{iso}), we simultaneously recorded X-band CW EPR spectra of two samples placed in separate sample tubes (Finland trityl as a reference and the radical being analyzed, and thus obtained the target g_{iso} value relative to the known g_{iso} of Finland trityl). The simulations of the solution EPR lines were carried out in the software package Easy Spin which is available at http://www.easypin.org.

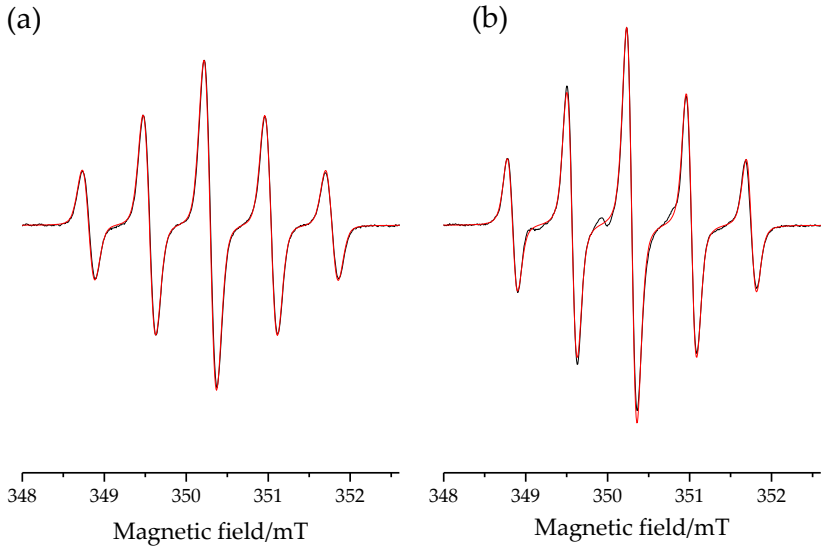

Figure S3. EPR spectra of (a) **1a**; (b) **1b** in diluted (C ≈ 10^{-4}M) and oxygen-free toluene solutions (black curves) at 295K. The red curves represent the computer simulations with the following parameters: **1a**: $A_{N1} = A_{N3} = 0.76$ mT, $g_{iso} = 2.0057$; **1b**: $A_{N1} = A_{N3} = 0.75$ mT, $g_{iso} = 2.0057$.

IR and UV/Vis spectra of 1a,b

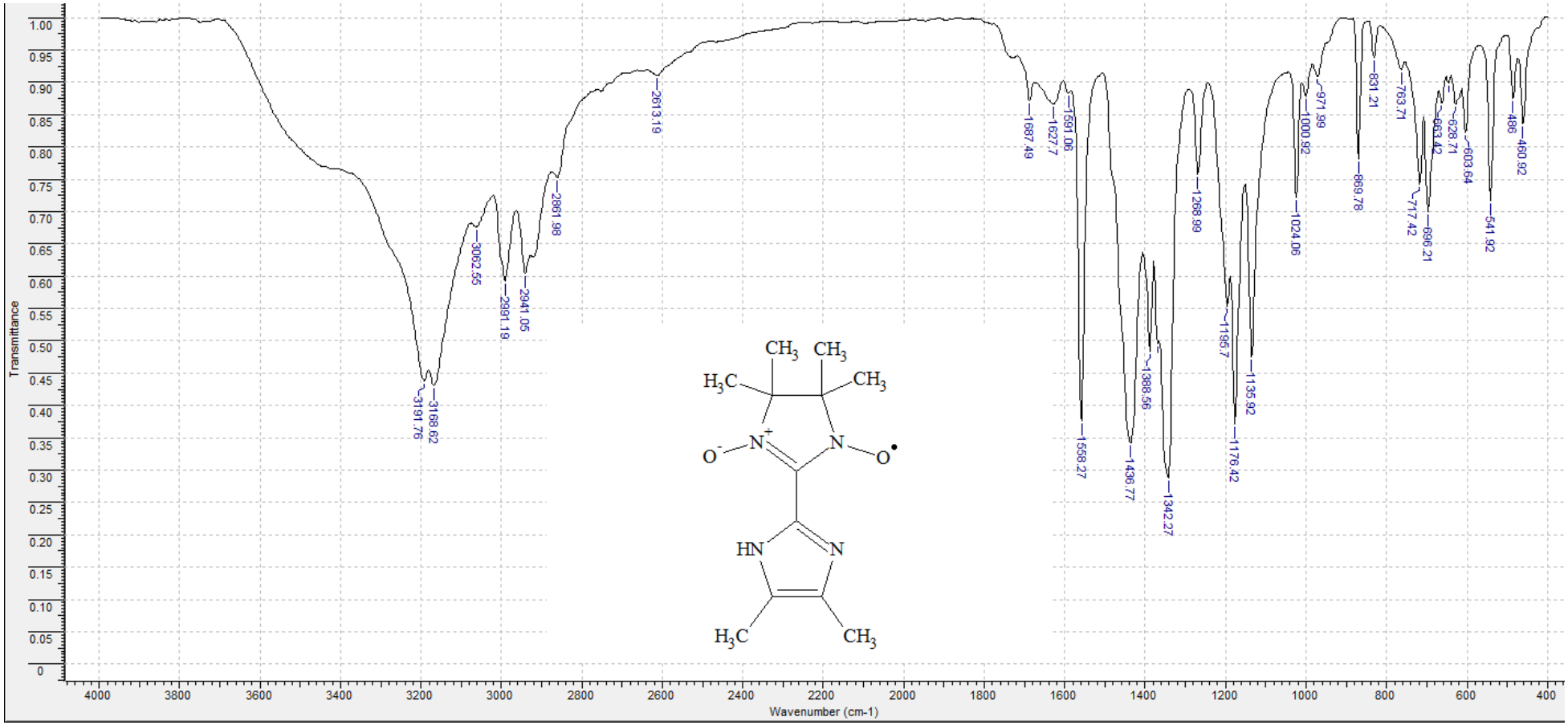

Figure S4. IR spectrum of **1a** (KBr).

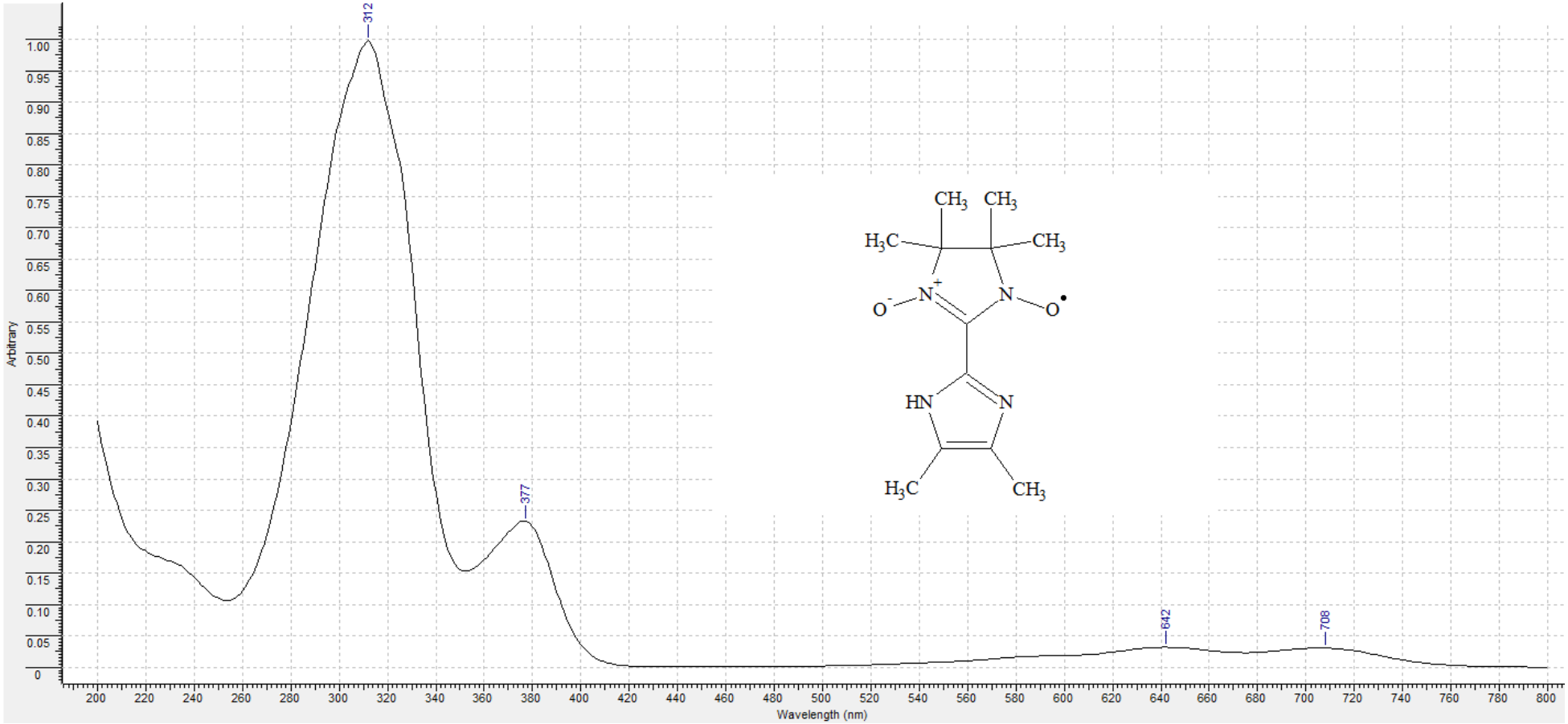

Figure S5. UV/Vis spectrum of **1a** (EtOH; C = 0.630 mg/25 ml; L = 1 cm).

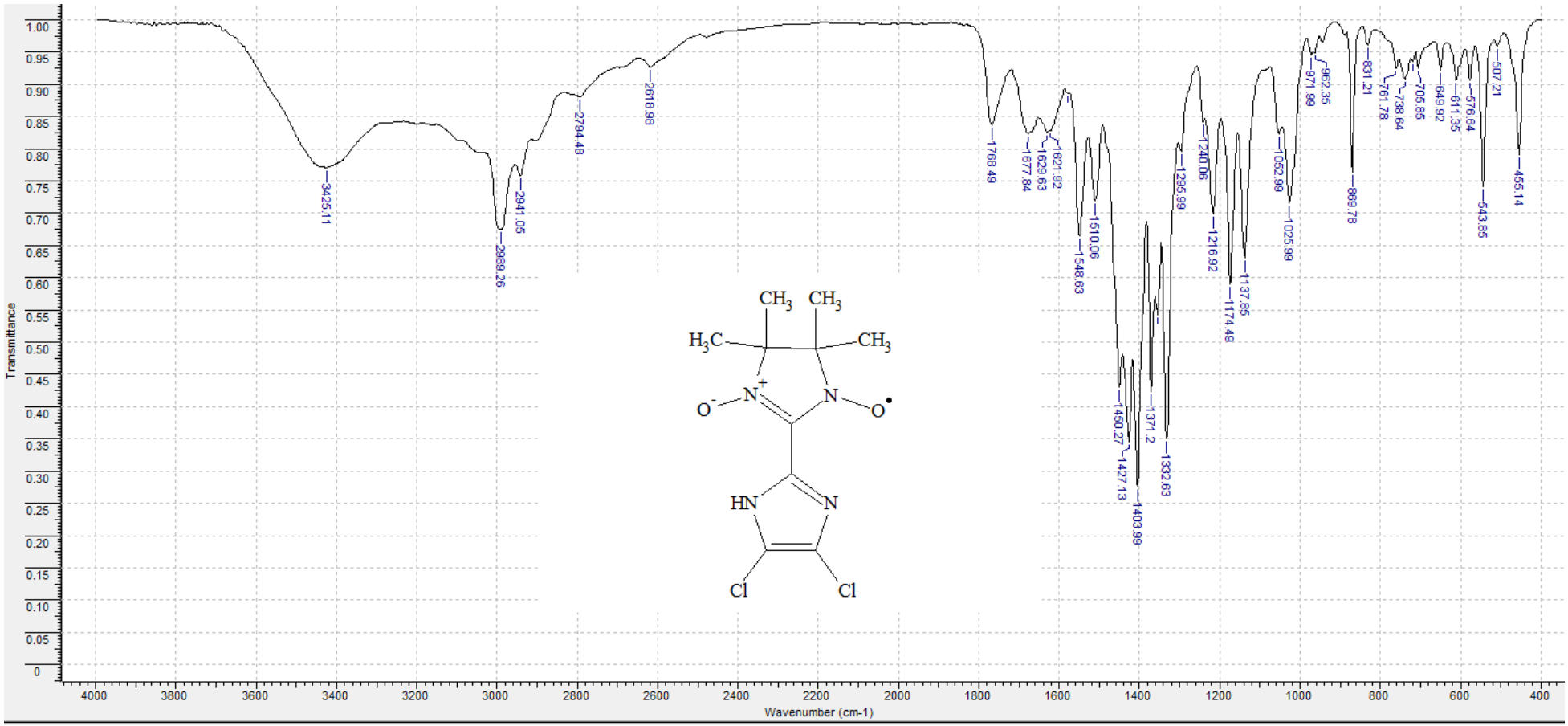

Figure S6. IR spectrum of **1b** (KBr).

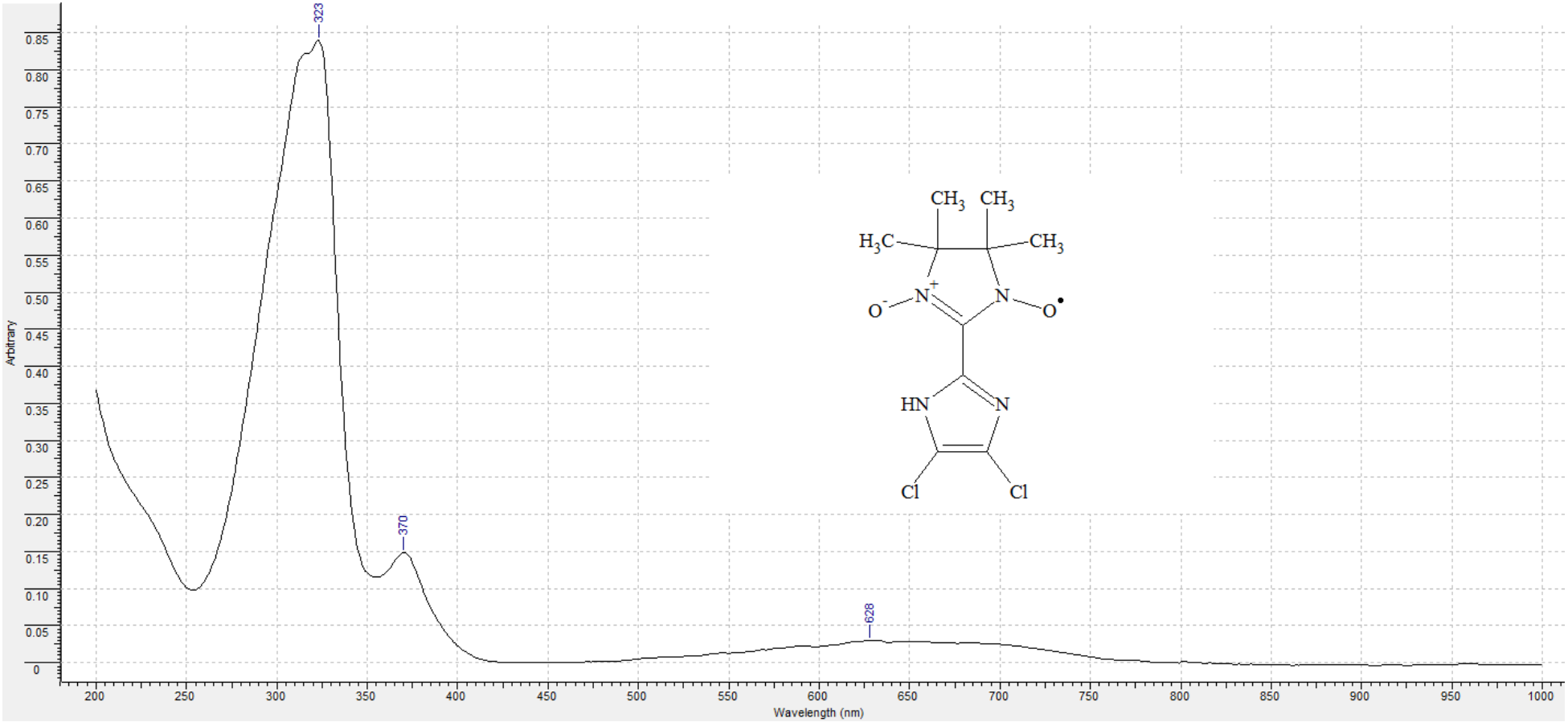

Figure S7. UV/Vis spectrum of **1b** (EtOH; C = 0.733 mg/25 ml; L = 1 cm).

PXRD analysis of 1a

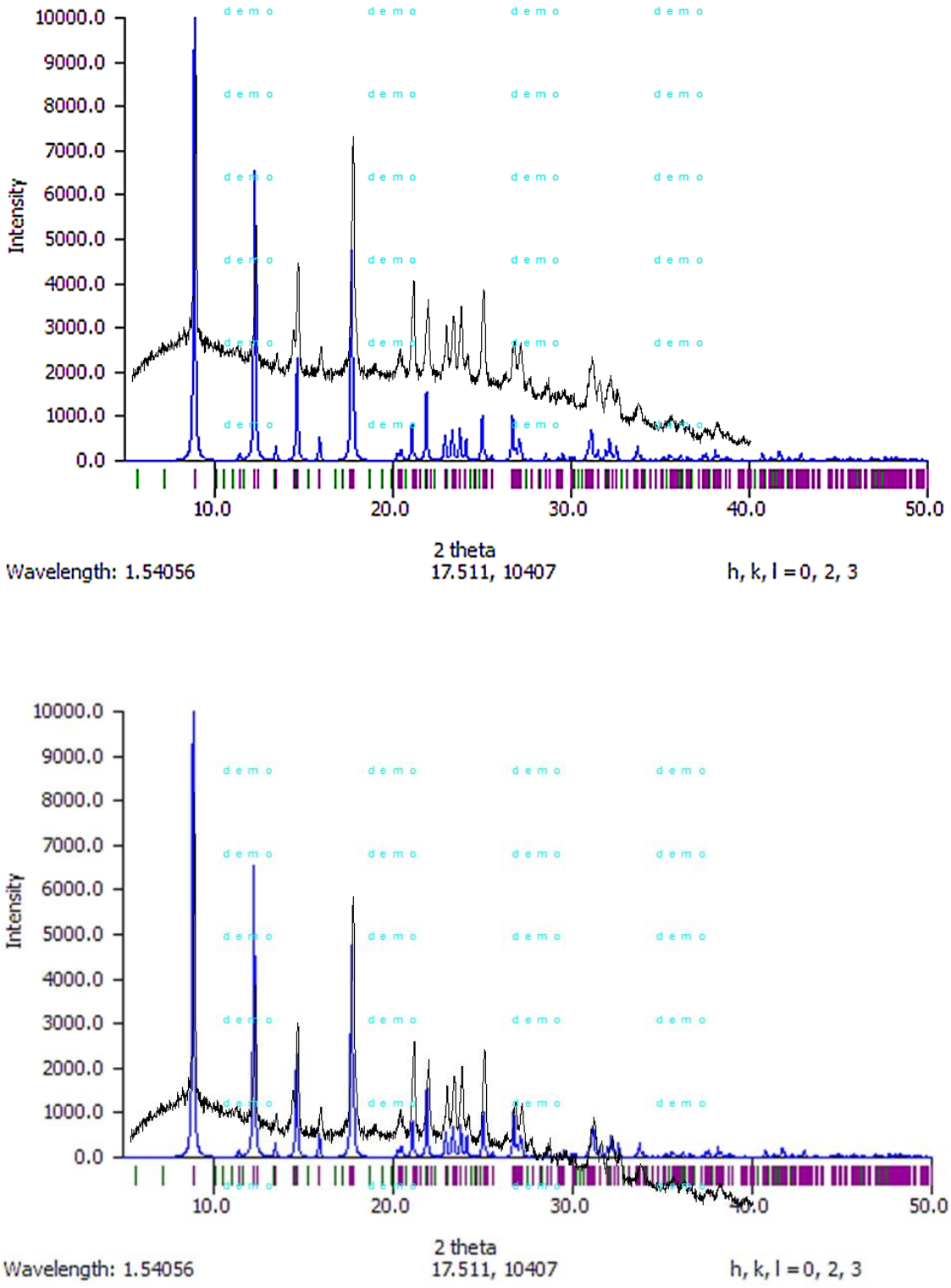

Figure S8. Calculated and experimental X-ray powder diffractograms for **1a**.

Picture of crystals of 1b

Figure S9. Well-shaped crystals of **1b**.

Results of quantum chemical calculations for exchange interaction in the crystals of 1a-c

Table S1. Selected interatomic distances (Å) and angles (°) and parameters of exchange interaction (J_1) calculated at the BS-DFT level (with B3LYP[a] and BHandHLYP[b] functionals and def2-TZVP basis set) for the closest radicals in the FM chains or AFM pairs for crystals of radicals **1a-c**.

Properties	Compound		
	1a	**1b**	**1c**
R(O_1…O_2),[c] Å	3.292	3.125	3.484
R(C1…O2), Å	3.146	3.049	3.701
∠N_1–O_1–O_2–N_2,[d] °	–118.4	–121.6	180.0
[a] *J*, K (*J*, cm^{-1})	21.1 (14.6)	23.8 (16.5)	–52.8 (–36.7)
[b] *J*, K (*J*, cm^{-1})	26.8 (18.6)	29.7 (20.6)	–38.9 (–27.0)

[a] Parameters of the exchange interaction calculated at the BS-B3LYP level.

[b] Parameters of the exchange interaction calculated at the BS-BHandHLYP level.

[c] Shortest distance between nitroxide oxygen atoms of neighboring radicals.

[d] N_1O_1 – nitroxide group of first radical and N_2O_2 – nitroxide group of the 2nd radical of the pair.

Geometry of the pair **1a…1a** in the FM chain (X, Y, Z in Å).

O	1.606880	1.342883	7.405515
O	4.450622	3.506650	4.474397
N	3.806435	3.203902	5.539248
N	1.413781	0.621886	4.518071
N	3.265620	1.202024	3.452824
H	4.021135	1.581773	3.295399
N	2.459469	2.169951	6.919543
C	3.245418	5.386686	6.399823
H	3.751777	5.813750	5.705407
H	3.219182	5.956001	7.172455
H	2.350764	5.224644	6.090532
C	3.908319	4.051225	6.768868
C	2.928922	2.194227	5.665902
C	2.532843	1.315206	4.585766
C	1.442116	0.025358	3.278326
C	0.334074	-0.863713	2.814390
H	0.327953	-0.893709	1.854158
H	-0.505484	-0.519527	3.128644
H	0.467004	-1.748764	3.162392
C	3.081004	0.071899	1.241135
H	3.102868	0.878247	0.720620
H	2.494188	-0.562820	0.823850
H	3.965164	-0.298419	1.296323
C	2.586889	0.377430	2.609122

C	3.087126	3.207922	7.789251
C	5.374923	4.222700	7.108334
H	5.783333	3.358368	7.204218
H	5.458879	4.709756	7.930794
H	5.812193	4.705117	6.404191
C	3.945924	2.422911	8.795539
H	3.402835	1.764226	9.233072
H	4.306235	3.027479	9.449457
H	4.665671	1.988426	8.331800
C	1.960719	3.936651	8.498556
H	1.457858	4.448446	7.859328
H	2.328025	4.525757	9.161606
H	1.383522	3.298066	8.923384
O	-2.765820	1.342883	2.520385
O	0.077922	3.506650	5.451503
N	-0.566265	3.203902	4.386652
N	-2.958919	0.621886	5.407829
N	-1.107080	1.202024	6.473076
H	-0.351565	1.581773	6.630501
N	-1.913231	2.169951	3.006357
C	-1.127282	5.386686	3.526077
H	-0.620923	5.813750	4.220493
H	-1.153518	5.956001	2.753445
H	-2.021936	5.224644	3.835368
C	-0.464381	4.051225	3.157032
C	-1.443778	2.194227	4.259998
C	-1.839857	1.315206	5.340134
C	-2.930584	0.025358	6.647574
C	-4.038626	-0.863713	7.111510
H	-4.044747	-0.893709	8.071742
H	-4.878184	-0.519527	6.797256
H	-3.905696	-1.748764	6.763508
C	-1.291696	0.071899	8.684765
H	-1.269832	0.878247	9.205280
H	-1.878512	-0.562820	9.102050
H	-0.407536	-0.298419	8.629577
C	-1.785811	0.377430	7.316778
C	-1.285574	3.207922	2.136649
C	1.002223	4.222700	2.817566
H	1.410633	3.358368	2.721682
H	1.086179	4.709756	1.995106
H	1.439493	4.705117	3.521709
C	-0.426776	2.422911	1.130361
H	-0.969865	1.764226	0.692828
H	-0.066465	3.027479	0.476443
H	0.292971	1.988426	1.594100
C	-2.411981	3.936651	1.427344
H	-2.914842	4.448446	2.066572
H	-2.044675	4.525757	0.764294
H	-2.989178	3.298066	1.002516

Geometry of the pair **1b…1b** in the FM chain

Cl	4.173327	8.874097	7.033791
Cl	1.290050	7.938143	8.765601
O	2.783264	6.493706	2.435834
O	-0.223219	4.515586	5.333849
N	0.449926	4.769132	4.276151
N	2.890514	7.314173	5.264248
N	1.048084	6.749261	6.368282
H	0.289487	6.383475	6.545608
N	1.873821	5.720701	2.906813
C	1.048084	2.569469	3.485908
H	1.942705	2.745714	3.785035
H	1.072499	1.972709	2.733202
H	0.545841	2.165960	4.197557
C	0.383658	3.877393	3.074559
C	1.362858	5.748065	4.148680
C	1.762211	6.621561	5.221237
C	2.886155	7.893927	6.482654
C	1.763083	7.567719	7.181595
C	1.195443	4.706054	2.034456
C	2.274918	3.945418	1.290353
H	2.767569	4.551453	0.733155
H	1.869461	3.266719	0.744885
H	2.870459	3.534179	1.921844
C	0.341804	5.505342	1.052224
H	-0.337445	5.983059	1.534738
H	-0.071500	4.907036	0.426207
H	0.897237	6.129930	0.578704
C	-1.082962	3.654768	2.729292
H	-1.517193	3.203333	3.456581
H	-1.147486	3.116756	1.937484
H	-1.509345	4.500435	2.578751
Cl	8.533077	8.874097	2.741609
Cl	5.649800	7.938143	1.009799
O	7.143014	6.493706	7.339566
O	4.136531	4.515586	4.441551
N	4.809676	4.769132	5.499249
N	7.250264	7.314173	4.511152
N	5.407834	6.749261	3.407118
H	4.649237	6.383475	3.229792
N	6.233571	5.720701	6.868587
C	5.407834	2.569469	6.289492
H	6.302455	2.745714	5.990365
H	5.432249	1.972709	7.042198
H	4.905591	2.165960	5.577843
C	4.743408	3.877393	6.700841
C	5.722608	5.748065	5.626720
C	6.121961	6.621561	4.554163
C	7.245905	7.893927	3.292746
C	6.122833	7.567719	2.593805
C	5.555193	4.706054	7.740944

C	6.634668	3.945418	8.485047
H	7.127319	4.551453	9.042245
H	6.229211	3.266719	9.030515
H	7.230209	3.534179	7.853556
C	4.701554	5.505342	8.723176
H	4.022305	5.983059	8.240662
H	4.288250	4.907036	9.349193
H	5.256987	6.129930	9.196696
C	3.276788	3.654768	7.046108
H	2.842557	3.203333	6.318819
H	3.212264	3.116756	7.837916
H	2.850405	4.500435	7.196649

Geometry of the AFM pair **1c…1c**

O	3.379826	0.242259	0.615166
O	6.128462	1.488331	4.108188
N	4.107161	0.187091	1.671668
N	5.433946	0.757958	3.310500
N	5.755257	3.391620	1.642696
N	3.564073	3.235711	1.520049
C	4.757498	1.210094	2.246273
C	4.176324	-1.064978	2.493498
C	5.444164	-0.747164	3.380032
C	4.333084	-2.284667	1.614690
C	2.899165	-1.116548	3.281529
C	6.731828	-1.186108	2.746518
C	5.378680	-1.180111	4.829584
C	4.681673	2.600082	1.816526
C	5.312449	4.586123	1.181080
C	3.954559	4.469791	1.121205
H	6.736940	3.272770	1.792093
H	4.386159	-3.102949	2.151342
H	5.149227	-2.201075	1.077458
H	3.561714	-2.342593	1.013720
H	2.953246	-1.933152	3.820499
H	2.133258	-1.152407	2.672254
H	2.814600	-0.325970	3.855265
H	6.727069	-2.164377	2.785726
H	7.487864	-0.825958	3.256034
H	6.799169	-0.879926	1.817105
H	5.375923	-2.159100	4.870530
H	4.562971	-0.830275	5.244265
H	6.156593	-0.832674	5.313797
H	5.959074	5.307982	1.040857
H	3.343136	5.186613	0.850899
O	6.603174	-0.242259	-0.615166
O	3.854538	-1.488331	-4.108188
N	5.875839	-0.187091	-1.671668
N	4.549054	-0.757958	-3.310500
N	4.227743	-3.391620	-1.642696
N	6.418927	-3.235711	-1.520049

C	5.225502	-1.210094	-2.246273
C	5.806676	1.064978	-2.493498
C	4.538836	0.747164	-3.380032
C	5.649916	2.284667	-1.614690
C	7.083835	1.116548	-3.281529
C	3.251172	1.186108	-2.746518
C	4.604320	1.180111	-4.829584
C	5.301327	-2.600082	-1.816526
C	4.670551	-4.586123	-1.181080
C	6.028441	-4.469791	-1.121205
H	3.246060	-3.272770	-1.792093
H	5.596841	3.102949	-2.151342
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H	6.421286	2.342593	-1.013720
H	7.029754	1.933152	-3.820499
H	7.849742	1.152407	-2.672254
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H	3.255931	2.164377	-2.785726
H	2.495136	0.825958	-3.256034
H	3.183831	0.879926	-1.817105
H	4.607077	2.159100	-4.870530
H	5.420029	0.830275	-5.244265
H	3.826407	0.832674	-5.313797
H	4.023926	-5.307982	-1.040857
H	6.639864	-5.186613	-0.850899

Table S2. Selected interatomic distances (Å) and angles (°) and parameters of exchange interaction (J_2) calculated at the BS-DFT level (with B3LYP[a] and BHandHLYP[b] functional and def2-TZVP basis set) for the closest radicals of the neighboring FM chains or between radical from neighboring AFM pairs for crystals of radicals **1a-c**.

Properties	Compound		
	1a	**1b**	**1c**
R(O_1…O_2),[c] Å	6.513	6.687	4.301
∠N_1–O_1–O_2–N_2,[d]	112.3	107.0	180.0
[a] J, K (J, cm^{-1})	–0.33 (–0.23)	–0.29 (–0.20)	–1.28 (–0.89)
[b] J, K (J, cm^{-1})	–0.45 (–0.31)	–0.39 (–0.27)	-

[a] Parameters of the exchange interaction calculated at the BS-B3LYP level.

[b] Parameters of the exchange interaction calculated at the BS-BHandHLYP level.

[c] Shortest distance between nitroxide oxygen atoms of neighboring radicals.

[d] N_1O_1 – nitroxide group of first radical and N_2O_2 – nitroxide group of the 2nd radical of the pair.

Cartesian coordinates of the **1a…1a** pair of radicals of the neighboring FM chains

O	1.606880	1.342883	7.405515
O	4.450622	3.506650	4.474397
N	3.806435	3.203902	5.539248
N	1.413781	0.621886	4.518071
N	3.265620	1.202024	3.452824
H	4.021135	1.581773	3.295399
N	2.459469	2.169951	6.919543
C	3.245418	5.386686	6.399823
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C	2.928922	2.194227	5.665902
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C	1.442116	0.025358	3.278326
C	0.334074	-0.863713	2.814390
H	0.327953	-0.893709	1.854158
H	-0.505484	-0.519527	3.128644
H	0.467004	-1.748764	3.162392
C	3.081004	0.071899	1.241135
H	3.102868	0.878247	0.720620
H	2.494188	-0.562820	0.823850
H	3.965164	-0.298419	1.296323
C	2.586889	0.377430	2.609122
C	3.087126	3.207922	7.789251
C	5.374923	4.222700	7.108334
H	5.783333	3.358368	7.204218
H	5.458879	4.709756	7.930794
H	5.812193	4.705117	6.404191
C	3.945924	2.422911	8.795539

H	3.402835	1.764226	9.233072
H	4.306235	3.027479	9.449457
H	4.665671	1.988426	8.331800
C	1.960719	3.936651	8.498556
H	1.457858	4.448446	7.859328
H	2.328025	4.525757	9.161606
H	1.383522	3.298066	8.923384
O	2.765820	-6.388167	7.405515
O	-0.077922	-4.224400	4.474397
N	0.566265	-4.527148	5.539248
N	2.958919	-7.109164	4.518071
N	1.107080	-6.529026	3.452824
H	0.351565	-6.149277	3.295399
N	1.913231	-5.561099	6.919543
C	1.127282	-2.344364	6.399823
H	0.620923	-1.917300	5.705407
H	1.153518	-1.775049	7.172455
H	2.021936	-2.506406	6.090532
C	0.464381	-3.679825	6.768868
C	1.443778	-5.536823	5.665902
C	1.839857	-6.415844	4.585766
C	2.930584	-7.705692	3.278326
C	4.038626	-8.594763	2.814390
H	4.044747	-8.624759	1.854158
H	4.878184	-8.250577	3.128644
H	3.905696	-9.479814	3.162392
C	1.291696	-7.659151	1.241135
H	1.269832	-6.852803	0.720620
H	1.878512	-8.293870	0.823850
H	0.407536	-8.029469	1.296323
C	1.785811	-7.353620	2.609122
C	1.285574	-4.523128	7.789251
C	-1.002223	-3.508350	7.108334
H	-1.410633	-4.372682	7.204218
H	-1.086179	-3.021294	7.930794
H	-1.439493	-3.025933	6.404191
C	0.426776	-5.308139	8.795539
H	0.969865	-5.966824	9.233072
H	0.066465	-4.703571	9.449457
H	-0.292971	-5.742624	8.331800
C	2.411981	-3.794399	8.498556
H	2.914842	-3.282604	7.859328
H	2.044675	-3.205293	9.161606
H	2.989178	-4.432984	8.923384

Cartesian coordinates of the **1b…1b** pair of radicals of neighboring chains

Cl	4.173327	8.874097	7.033791
Cl	1.290050	7.938143	8.765601
O	2.783264	6.493706	2.435834
O	-0.223219	4.515586	5.333849
N	0.449926	4.769132	4.276151

N	2.890514	7.314173	5.264248
N	1.048084	6.749261	6.368282
H	0.289487	6.383475	6.545608
N	1.873821	5.720701	2.906813
C	1.048084	2.569469	3.485908
H	1.942705	2.745714	3.785035
H	1.072499	1.972709	2.733202
H	0.545841	2.165960	4.197557
C	0.383658	3.877393	3.074559
C	1.362858	5.748065	4.148680
C	1.762211	6.621561	5.221237
C	2.886155	7.893927	6.482654
C	1.763083	7.567719	7.181595
C	1.195443	4.706054	2.034456
C	2.274918	3.945418	1.290353
H	2.767569	4.551453	0.733155
H	1.869461	3.266719	0.744885
H	2.870459	3.534179	1.921844
C	0.341804	5.505342	1.052224
H	-0.337445	5.983059	1.534738
H	-0.071500	4.907036	0.426207
H	0.897237	6.129930	0.578704
C	-1.082962	3.654768	2.729292
H	-1.517193	3.203333	3.456581
H	-1.147486	3.116756	1.937484
H	-1.509345	4.500435	2.578751
Cl	0.186423	1.144047	7.033791
Cl	3.069700	0.208093	8.765601
O	1.576486	-1.236344	2.435834
O	4.582969	-3.214464	5.333849
N	3.909824	-2.960918	4.276151
N	1.469236	-0.415877	5.264248
N	3.311666	-0.980789	6.368282
H	4.070263	-1.346575	6.545608
N	2.485929	-2.009349	2.906813
C	3.311666	-5.160581	3.485908
H	2.417045	-4.984336	3.785035
H	3.287251	-5.757341	2.733202
H	3.813909	-5.564090	4.197557
C	3.976092	-3.852657	3.074559
C	2.996892	-1.981985	4.148680
C	2.597539	-1.108489	5.221237
C	1.473596	0.163877	6.482654
C	2.596667	-0.162331	7.181595
C	3.164307	-3.023996	2.034456
C	2.084832	-3.784632	1.290353
H	1.592181	-3.178597	0.733155
H	2.490289	-4.463331	0.744885
H	1.489291	-4.195871	1.921844
C	4.017946	-2.224708	1.052224
H	4.697195	-1.746991	1.534738

H	4.431250	-2.823014	0.426207
H	3.462513	-1.600120	0.578704
C	5.442712	-4.075282	2.729292
H	5.876943	-4.526717	3.456581
H	5.507236	-4.613294	1.937484
H	5.869095	-3.229615	2.578751

Cartesian coordinates of the **1c…1c** pair

O	3.379826	0.242259	0.615166
O	6.128462	1.488331	4.108188
N	4.107161	0.187091	1.671668
N	5.433946	0.757958	3.310500
N	5.755257	3.391620	1.642696
N	3.564073	3.235711	1.520049
C	4.757498	1.210094	2.246273
C	4.176324	-1.064978	2.493498
C	5.444164	-0.747164	3.380032
C	4.333084	-2.284667	1.614690
C	2.899165	-1.116548	3.281529
C	6.731828	-1.186108	2.746518
C	5.378680	-1.180111	4.829584
C	4.681673	2.600082	1.816526
C	5.312449	4.586123	1.181080
C	3.954559	4.469791	1.121205
H	6.736940	3.272770	1.792093
H	4.386159	-3.102949	2.151342
H	5.149227	-2.201075	1.077458
H	3.561714	-2.342593	1.013720
H	2.953246	-1.933152	3.820499
H	2.133258	-1.152407	2.672254
H	2.814600	-0.325970	3.855265
H	6.727069	-2.164377	2.785726
H	7.487864	-0.825958	3.256034
H	6.799169	-0.879926	1.817105
H	5.375923	-2.159100	4.870530
H	4.562971	-0.830275	5.244265
H	6.156593	-0.832674	5.313797
H	5.959074	5.307982	1.040857
H	3.343136	5.186613	0.850899
O	11.627290	-0.242259	9.042070
O	8.878653	-1.488331	5.549048
N	10.899954	-0.187091	7.985568
N	9.573169	-0.757958	6.346735
N	9.251859	-3.391620	8.014540
N	11.443042	-3.235711	8.137187
C	10.249618	-1.210094	7.410963
C	10.830792	1.064978	7.163737
C	9.562952	0.747164	6.277203
C	10.674032	2.284667	8.042546
C	12.107951	1.116548	6.375707
C	8.275288	1.186108	6.910718

C	9.628436	1.180111	4.827652
C	10.325443	-2.600082	7.840710
C	9.694666	-4.586123	8.476156
C	11.052557	-4.469791	8.536031
H	8.270175	-3.272770	7.865142
H	10.620957	3.102949	7.505893
H	9.857889	2.201075	8.579778
H	11.445401	2.342593	8.643516
H	12.053870	1.933152	5.836737
H	12.873858	1.152407	6.984982
H	12.192516	0.325970	5.801971
H	8.280047	2.164377	6.871509
H	7.519251	0.825958	6.401202
H	8.207946	0.879926	7.840130
H	9.631193	2.159100	4.786705
H	10.444144	0.830275	4.412970
H	8.850523	0.832674	4.343438
H	9.048042	-5.307982	8.616379
H	11.663980	-5.186613	8.806337

Table S3. Selected interatomic distances (Å) and angles (°) and parameters of the exchange interaction (J_3) calculated at the BS-DFT level (with B3LYP[a] and BHandHLYP[b] functional and def2-TZVP basis set) for the next closest radicals of neighboring FM chains or of neighboring AFM pairs for crystals **1a-c**.

Properties	Compound		
	1a	**1b**	**1c**
R(O_1…O_2),[c] Å	6.484	6.607	5.834
∠N_1–O_1–O_2–N_2,[d] °	–35.08	33.824	69.4
[a] *J*, K (*J*, cm^{-1})	0.09 (0.06)	0.01 (0.01)	–0.09 (–0.06)
[b] *J*, K (*J*, cm^{-1})	0.09 (0.06)	0.01 (0.01)	-

[a] Parameters of the exchange interaction calculated at the BS-B3LYP level.

[b] Parameters of the exchange interaction calculated at the BS-BHandHLYP level.

[c] Shortest distance between nitroxide oxygen atoms of neighboring radicals.

[d] N_1O_1 – nitroxide group of first radical and N_2O_2 – nitroxide group of the 2nd radical of the pair.

Cartesian coordinates of the **1a…1a** pair of radicals from neighboring FM chains

O	1.606880	1.342883	7.405515
O	4.450622	3.506650	4.474397
N	3.806435	3.203902	5.539248
N	1.413781	0.621886	4.518071
N	3.265620	1.202024	3.452824
H	4.021135	1.581773	3.295399
N	2.459469	2.169951	6.919543
C	3.245418	5.386686	6.399823
H	3.751777	5.813750	5.705407
H	3.219182	5.956001	7.172455
H	2.350764	5.224644	6.090532
C	3.908319	4.051225	6.768868
C	2.928922	2.194227	5.665902
C	2.532843	1.315206	4.585766
C	1.442116	0.025358	3.278326
C	0.334074	-0.863713	2.814390
H	0.327953	-0.893709	1.854158
H	-0.505484	-0.519527	3.128644
H	0.467004	-1.748764	3.162392
C	3.081004	0.071899	1.241135
H	3.102868	0.878247	0.720620
H	2.494188	-0.562820	0.823850
H	3.965164	-0.298419	1.296323
C	2.586889	0.377430	2.609122
C	3.087126	3.207922	7.789251
C	5.374923	4.222700	7.108334
H	5.783333	3.358368	7.204218
H	5.458879	4.709756	7.930794
H	5.812193	4.705117	6.404191

C	3.945924	2.422911	8.795539
H	3.402835	1.764226	9.233072
H	4.306235	3.027479	9.449457
H	4.665671	1.988426	8.331800
C	1.960719	3.936651	8.498556
H	1.457858	4.448446	7.859328
H	2.328025	4.525757	9.161606
H	1.383522	3.298066	8.923384
O	7.138520	-6.388167	2.520385
O	4.294778	-4.224400	5.451503
N	4.938965	-4.527148	4.386652
N	7.331619	-7.109164	5.407829
N	5.479780	-6.529026	6.473076
H	4.724265	-6.149277	6.630501
N	6.285931	-5.561099	3.006357
C	5.499982	-2.344364	3.526077
H	4.993623	-1.917300	4.220493
H	5.526218	-1.775049	2.753445
H	6.394636	-2.506406	3.835368
C	4.837081	-3.679825	3.157032
C	5.816478	-5.536823	4.259998
C	6.212557	-6.415844	5.340134
C	7.303284	-7.705692	6.647574
C	8.411326	-8.594763	7.111510
H	8.417447	-8.624759	8.071742
H	9.250884	-8.250577	6.797256
H	8.278396	-9.479814	6.763508
C	5.664396	-7.659151	8.684765
H	5.642532	-6.852803	9.205280
H	6.251212	-8.293870	9.102050
H	4.780236	-8.029469	8.629577
C	6.158511	-7.353620	7.316778
C	5.658274	-4.523128	2.136649
C	3.370477	-3.508350	2.817566
H	2.962067	-4.372682	2.721682
H	3.286521	-3.021294	1.995106
H	2.933207	-3.025933	3.521709
C	4.799476	-5.308139	1.130361
H	5.342565	-5.966824	0.692828
H	4.439165	-4.703571	0.476443
H	4.079729	-5.742624	1.594100
C	6.784681	-3.794399	1.427344
H	7.287542	-3.282604	2.066572
H	6.417375	-3.205293	0.764294
H	7.361878	-4.432984	1.002516

Cartesian coordinates of the **1b…1b** pair of radicals from neighboring FM chains

Cl	4.173327	8.874097	7.033791
Cl	1.290050	7.938143	8.765601
O	2.783264	6.493706	2.435834
O	-0.223219	4.515586	5.333849

N	0.449926	4.769132	4.276151
N	2.890514	7.314173	5.264248
N	1.048084	6.749261	6.368282
H	0.289487	6.383475	6.545608
N	1.873821	5.720701	2.906813
C	1.048084	2.569469	3.485908
H	1.942705	2.745714	3.785035
H	1.072499	1.972709	2.733202
H	0.545841	2.165960	4.197557
C	0.383658	3.877393	3.074559
C	1.362858	5.748065	4.148680
C	1.762211	6.621561	5.221237
C	2.886155	7.893927	6.482654
C	1.763083	7.567719	7.181595
C	1.195443	4.706054	2.034456
C	2.274918	3.945418	1.290353
H	2.767569	4.551453	0.733155
H	1.869461	3.266719	0.744885
H	2.870459	3.534179	1.921844
C	0.341804	5.505342	1.052224
H	-0.337445	5.983059	1.534738
H	-0.071500	4.907036	0.426207
H	0.897237	6.129930	0.578704
C	-1.082962	3.654768	2.729292
H	-1.517193	3.203333	3.456581
H	-1.147486	3.116756	1.937484
H	-1.509345	4.500435	2.578751
Cl	-4.173327	1.144047	2.741609
Cl	-1.290050	0.208093	1.009799
O	-2.783264	-1.236344	7.339566
O	0.223219	-3.214464	4.441551
N	-0.449926	-2.960918	5.499249
N	-2.890514	-0.415877	4.511152
N	-1.048084	-0.980789	3.407118
H	-0.289487	-1.346575	3.229792
N	-1.873821	-2.009349	6.868587
C	-1.048084	-5.160581	6.289492
H	-1.942705	-4.984336	5.990365
H	-1.072499	-5.757341	7.042198
H	-0.545841	-5.564090	5.577843
C	-0.383658	-3.852657	6.700841
C	-1.362858	-1.981985	5.626720
C	-1.762211	-1.108489	4.554163
C	-2.886154	0.163877	3.292746
C	-1.763083	-0.162331	2.593805
C	-1.195443	-3.023996	7.740944
C	-2.274918	-3.784632	8.485047
H	-2.767569	-3.178597	9.042245
H	-1.869461	-4.463331	9.030515
H	-2.870459	-4.195871	7.853556
C	-0.341804	-2.224708	8.723176

H	0.337445	-1.746991	8.240662
H	0.071500	-2.823014	9.349193
H	-0.897237	-1.600120	9.196696
C	1.082962	-4.075282	7.046108
H	1.517193	-4.526717	6.318819
H	1.147486	-4.613294	7.837916
H	1.509345	-3.229615	7.196649

Cartesian coordinates of the **1c…1c** pair of radicals from neighboring AFM pairs

O	3.379826	0.242259	0.615166
O	6.128462	1.488331	4.108188
N	4.107161	0.187091	1.671668
N	5.433946	0.757958	3.310500
N	5.755257	3.391620	1.642696
N	3.564073	3.235711	1.520049
C	4.757498	1.210094	2.246273
C	4.176324	-1.064978	2.493498
C	5.444164	-0.747164	3.380032
C	4.333084	-2.284667	1.614690
C	2.899165	-1.116548	3.281529
C	6.731828	-1.186108	2.746518
C	5.378680	-1.180111	4.829584
C	4.681673	2.600082	1.816526
C	5.312449	4.586123	1.181080
C	3.954559	4.469791	1.121205
H	6.736940	3.272770	1.792093
H	4.386159	-3.102949	2.151342
H	5.149227	-2.201075	1.077458
H	3.561714	-2.342593	1.013720
H	2.953246	-1.933152	3.820499
H	2.133258	-1.152407	2.672254
H	2.814600	-0.325970	3.855265
H	6.727069	-2.164377	2.785726
H	7.487864	-0.825958	3.256034
H	6.799169	-0.879926	1.817105
H	5.375923	-2.159100	4.870530
H	4.562971	-0.830275	5.244265
H	6.156593	-0.832674	5.313797
H	5.959074	5.307982	1.040857
H	3.343136	5.186613	0.850899
O	8.371326	5.754241	0.615166
O	11.119962	4.508169	4.108188
N	9.098661	5.809409	1.671668
N	10.425446	5.238542	3.310500
N	10.746757	2.604880	1.642696
N	8.555573	2.760789	1.520049
C	9.748998	4.786406	2.246273
C	9.167824	7.061478	2.493498
C	10.435664	6.743664	3.380032
C	9.324584	8.281166	1.614690
C	7.890665	7.113048	3.281529

C	11.723328	7.182608	2.746518
C	10.370180	7.176611	4.829584
C	9.673173	3.396418	1.816526
C	10.303949	1.410377	1.181080
C	8.946059	1.526709	1.121205
H	11.728440	2.723730	1.792093
H	9.377659	9.099449	2.151342
H	10.140727	8.197575	1.077458
H	8.553214	8.339093	1.013720
H	7.944746	7.929652	3.820499
H	7.124758	7.148907	2.672254
H	7.806100	6.322470	3.855265
H	11.718569	8.160877	2.785726
H	12.479364	6.822458	3.256034
H	11.790669	6.876426	1.817105
H	10.367423	8.155600	4.870530
H	9.554471	6.826775	5.244265
H	11.148093	6.829174	5.313797
H	10.950574	0.688518	1.040857
H	8.334636	0.809887	0.850899