

# Mononuclear oxidovanadium(IV) complexes with BIAN-ligands: synthesis and catalytic activity in the oxidation of hydrocarbons and alcohols with peroxides

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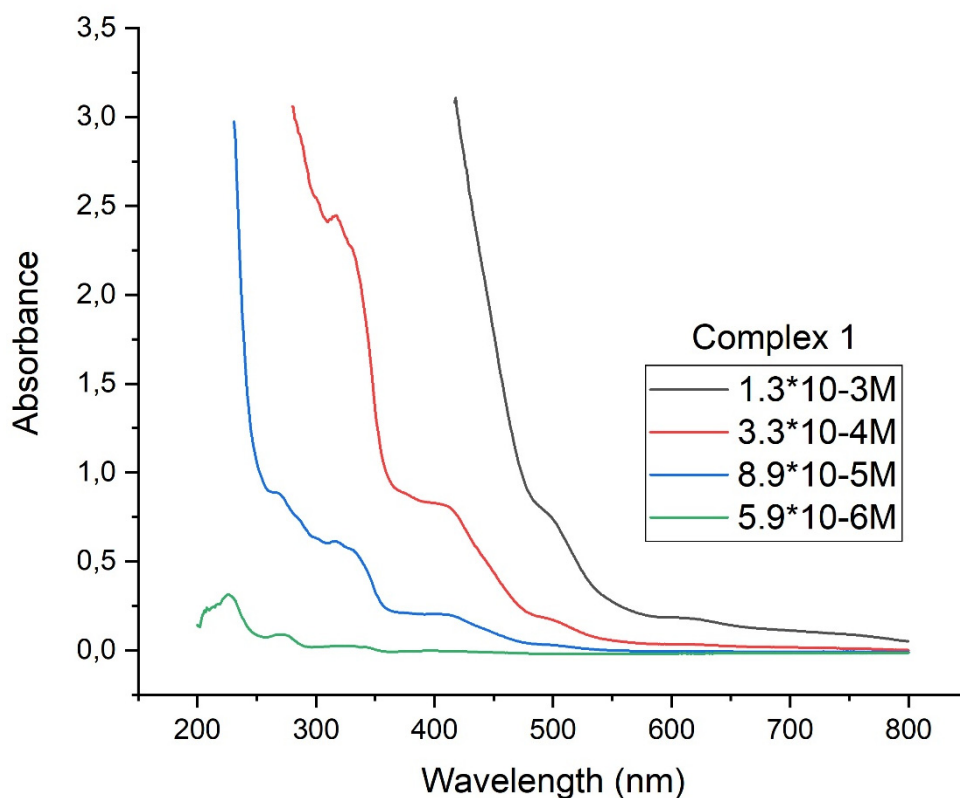
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**Figure S1.** UV-spectrum of **1** in the CH<sub>3</sub>CN

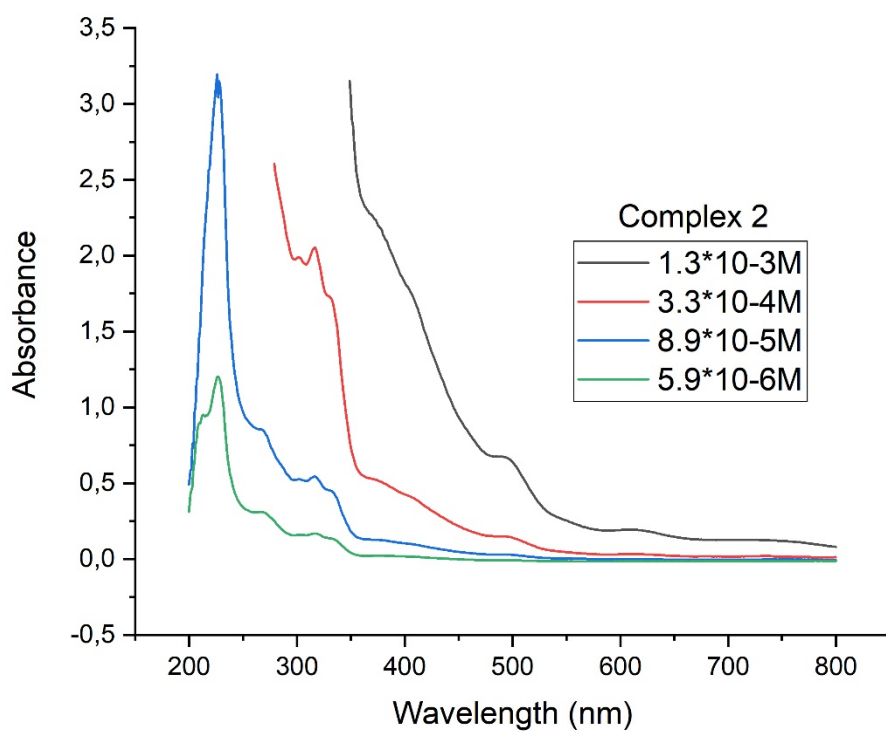
**Figure S2.** UV-spectrum of **2** in the CH<sub>3</sub>CN

**Table S1.** Optimized coordinates for complex **1**

**Table S2.** Optimized coordinates for complex **2**



**Figure S1.** UV-spectrum of **1** in the CH<sub>3</sub>CN



**Figure S2.** UV-spectrum of **2** in the  $\text{CH}_3\text{CN}$

**Table S1**

Optimized coordinates for complex **1**

C	1.49949717	0.28498388	1.68212075
C	0.82814364	-0.58158546	2.53533486
C	1.39600563	-1.85453682	2.79517774
C	2.59598527	-2.26494038	2.22693550
C	5.16449755	-0.68482962	-0.06613558
C	4.56939671	0.58023297	-0.30097895
C	3.34234788	0.85775728	0.28803980
C	2.73127624	-0.13550496	1.10547353
C	3.31286052	-1.39763677	1.35562916
C	4.56571111	-1.65332815	0.73111182
H	-0.11365154	-0.30577092	3.00665989
H	0.86948762	-2.53102625	3.46904662
H	2.99805037	-3.25318665	2.45588518

H	6.12939839	-0.89900037	-0.52660030
H	5.07956253	1.30701338	-0.93085073
C	1.31859948	1.67845110	1.25951302
H	5.06091633	-2.61315327	0.88785401
C	2.47997391	2.03917528	0.38767544
N	0.39700200	2.58232560	1.47031306
N	2.52719007	3.24574878	-0.11952918
C	3.36485338	3.49307018	-1.24979672
C	3.14239641	2.75925117	-2.42771807
C	3.91949993	3.00151724	-3.56041509
C	4.93882247	3.96662797	-3.54812429
C	5.14463989	4.69330499	-2.36009178
C	4.36230899	4.47951454	-1.22596453
H	2.35495487	2.00372070	-2.45513635
H	3.72638240	2.43013844	-4.47078915
H	-3.08291425	2.63994048	4.49855209
H	5.93082692	5.45044179	-2.32444508
H	4.52549156	5.05918329	-0.31897775
C	-0.88396120	2.16880375	1.94542026
C	-1.62756847	1.25187964	1.18344024
C	-2.88765100	0.84099037	1.61834881
C	-3.43473392	1.32190484	2.81840940
C	-2.67942453	2.24773957	3.56257090
C	-1.42715086	2.68456460	3.13224204
H	-1.21786695	0.86872209	0.24746904
H	-3.45518767	0.13223647	1.01176924
H	-0.85899300	3.40722990	3.71549818
C	5.77996419	4.22862203	-4.77234435

H	5.65325832	5.26361666	-5.12334673
H	6.84931812	4.09100356	-4.55417174
H	5.50776507	3.55472882	-5.59445150
C	-4.79323502	0.86942710	3.29277269
H	-5.22564214	0.12503458	2.61262169
H	-4.73261478	0.42341174	4.29667613
H	-5.49116223	1.71739662	3.35925127
V	1.22777828	4.56611678	1.02730309
Cl	-0.73695225	5.62874640	1.71604579
Cl	1.95711343	6.48817315	-0.08852802
O	-0.07297528	4.27987587	-0.93738115
H	0.28286596	3.77310930	-1.69321537
H	-0.97033546	3.92367180	-0.78653601
O	2.14721256	4.58646759	2.34394862
O	-0.07297528	4.27987587	-0.93738115
H	0.28286596	3.77310930	-1.69321537
H	-0.97033546	3.92367180	-0.78653601
O	2.14721256	4.58646759	2.34394862

**Table S2**

Optimized coordinates for complex **2**

C	1.33367067	0.20249808	1.58707061
C	0.66296821	-0.65339698	2.45204617
C	1.22499187	-1.92723175	2.71743735
C	2.42107283	-2.34592104	2.14797466
C	4.98403324	-0.80747110	-0.17868367
C	4.39374949	0.45715243	-0.42624750
C	3.17060530	0.74775374	0.16473201

C	2.56232464	-0.22702458	1.00721721
C	3.13958115	-1.48877267	1.26826561
C	4.38441756	-1.76093710	0.63509676
H	-0.27704217	-0.37041820	2.92157391
H	0.69555779	-2.59848529	3.39396413
H	2.81787215	-3.33569520	2.37914830
H	5.94218416	-1.03497054	-0.64639531
H	4.90365642	1.17465520	-1.06692792
C	1.13195914	1.57279176	1.11002881
H	4.87201070	-2.72366198	0.79718079
C	2.27611281	1.90558947	0.19109568
N	0.26040957	2.50561669	1.36083579
N	2.29269204	3.09034835	-0.34410533
C	3.35999451	3.50236464	-1.21221065
C	3.50412067	2.96707796	-2.51186470
C	4.55859859	3.46724870	-3.29535118
C	5.43191983	4.44782955	-2.82286876
C	5.25655085	4.97558688	-1.53870094
C	4.21031694	4.51472711	-0.74200116
H	3.00479654	0.90352578	-2.93594949
H	4.68520472	3.07432112	-4.30649778
H	-2.38071204	2.90539803	5.12220143
H	5.92309631	5.75218189	-1.16173394
H	4.03981647	4.92732843	0.25238557
C	-0.89965373	2.20636759	2.15308320
C	-1.89055275	1.38658452	1.59177260
C	-3.06175632	1.12007321	2.30102380
C	-3.23637018	1.66964301	3.57497593

C	-2.24090505	2.48130334	4.12587221
C	-1.05635745	2.77700062	3.43309703
H	-1.73993663	0.97231923	0.59405220
H	-3.83274007	0.48986068	1.85616350
H	0.92803010	3.06178910	4.24610003
H	6.23884077	4.81030193	-3.46149176
H	-0.31030589	3.47131056	-2.13374264
H	-1.38676496	3.07262939	-1.11925212
O	1.38281226	5.26808061	1.30401988
H	-4.14843023	1.46894224	4.13933490
O	-0.47531574	2.83443214	-1.40084697
Cl	0.82559926	5.57085008	-1.76885612
Cl	-1.62861936	4.97496106	0.51736001
V	0.62288256	4.33929064	0.23556063
C	2.58696130	1.91228577	-3.08070455
H	1.59511532	1.92363791	-2.61454586
H	2.46378770	2.06073152	-4.16116962
C	0.01281979	3.64002571	4.04747534
H	0.29552470	4.46207972	3.37413049
H	-0.33296977	4.06534528	4.99732663