

Versatile Reactivity and Theoretical Evaluation of Mono- and Dinuclear Oxidovanadium(V) Compounds of Aroylazines: Electrogeneration of Mixed-Valence V^{IV}V^V Complexes

Subhashree P. Dash,^{†,§} Satabdi Roy,[†] Monalisa Mohanty,[†] M. Fernanda N.N. Carvalho,^{||} Maxim L. Kuznetsov,^{||} João Costa Pessoa,^{||,*} Amit Kumar,^{||,‡} Yogesh P. Patil,[⊥] Aurélien Crochet[£] and Rupam Dinda^{†,*}

[†] Department of Chemistry, National Institute of Technology, Rourkela 769008, Odisha, India

[§] Department of Chemistry, Indira Gandhi Institute of Technology, Sarang, Parjang, Dhenkanal 759146, India

^{||} Centro de Química Estrutural, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1049-001 Lisboa, Portugal

[‡] Centre for Nano and Material Sciences, Jain University, Jain Global Campus, Jakkasandra Post, Bangalore 562112, India

[⊥] Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore 560012, India

[£] Fribourg Center for Nanomaterials, Department of Chemistry, University of Fribourg, CH-1700 Fribourg, Switzerland

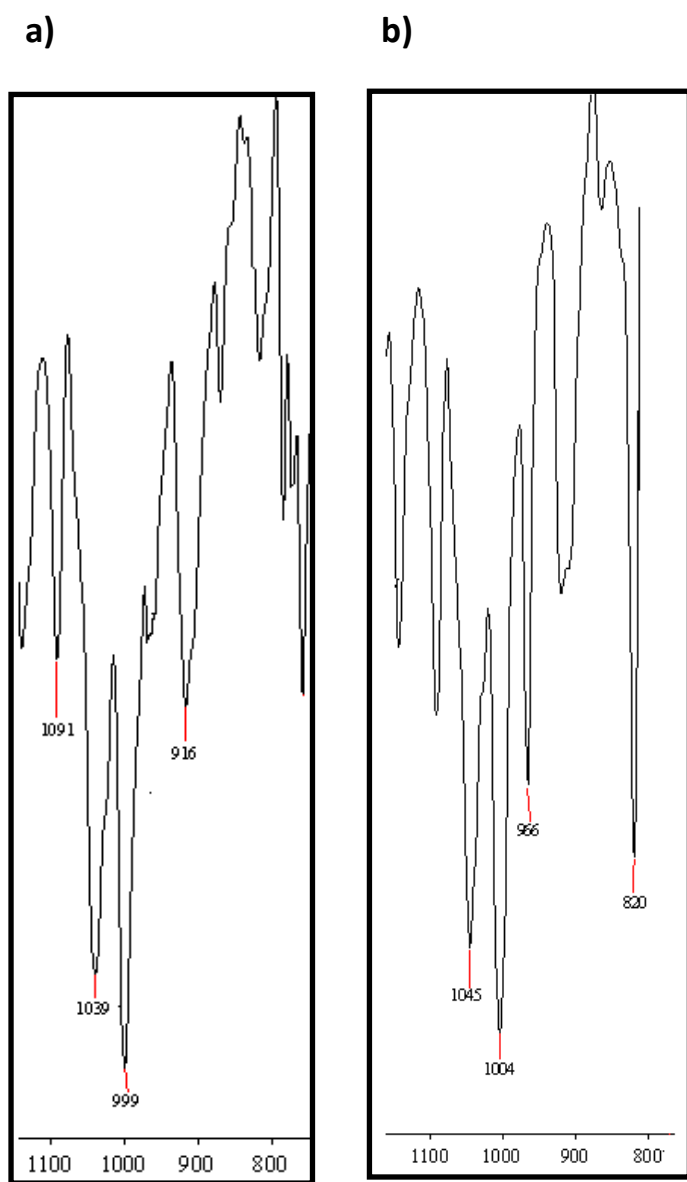


Figure S1. IR spectra of **3**: (a) in KBr pellet; (b) in CHCl₃.

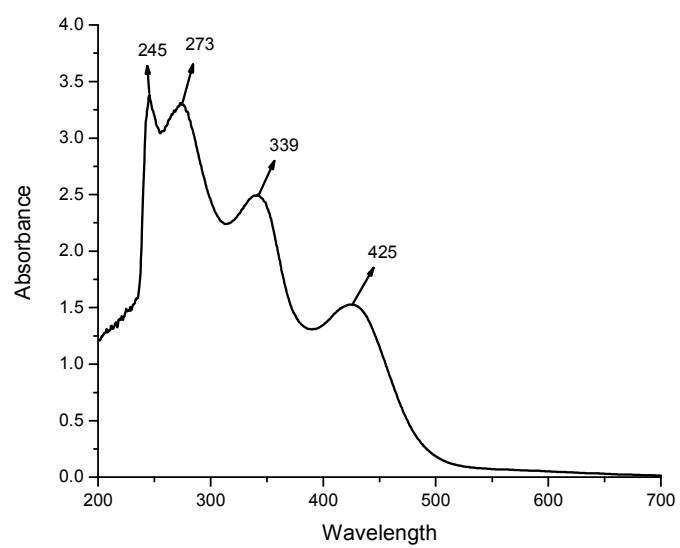
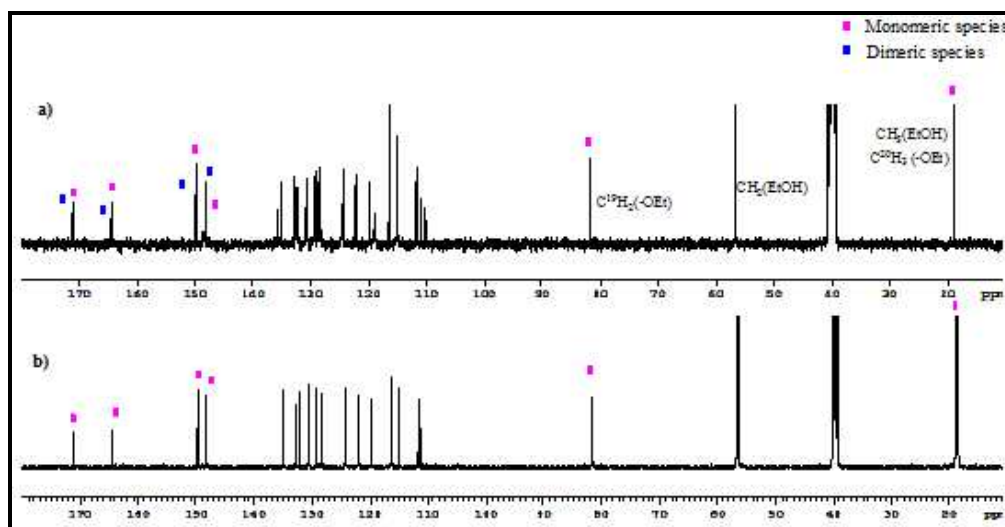


Figure S2. UV-vis spectrum of **2** (1.20×10^{-4} M) in CHCl_3 .

(A)



(B)

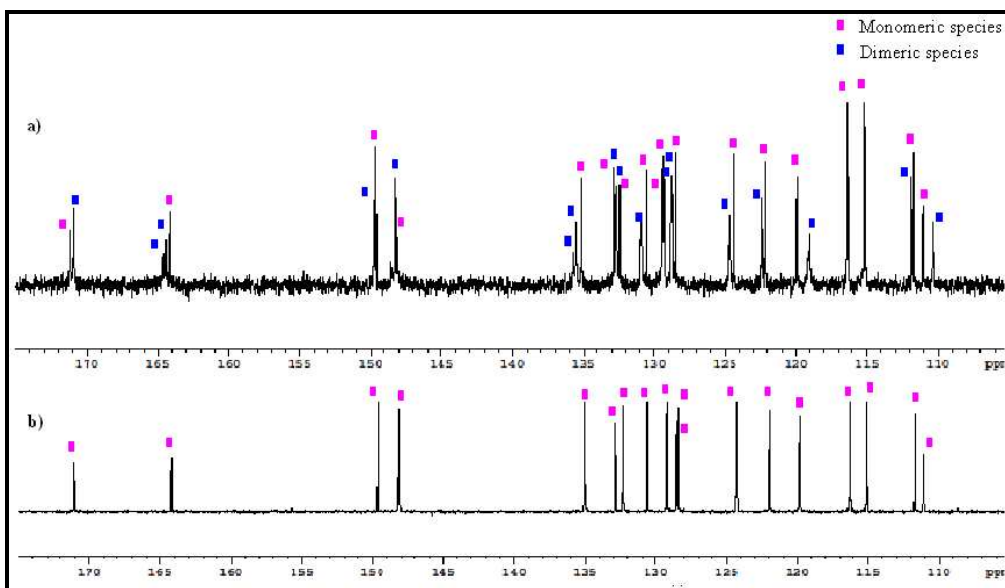


Figure S3. ^{13}C NMR spectra of complex **1** in $\text{DMSO-}d_6$: (A) full range and (B) in the range 110-172 ppm. (a) before addition of ethanol; (b) after addition of ethanol.

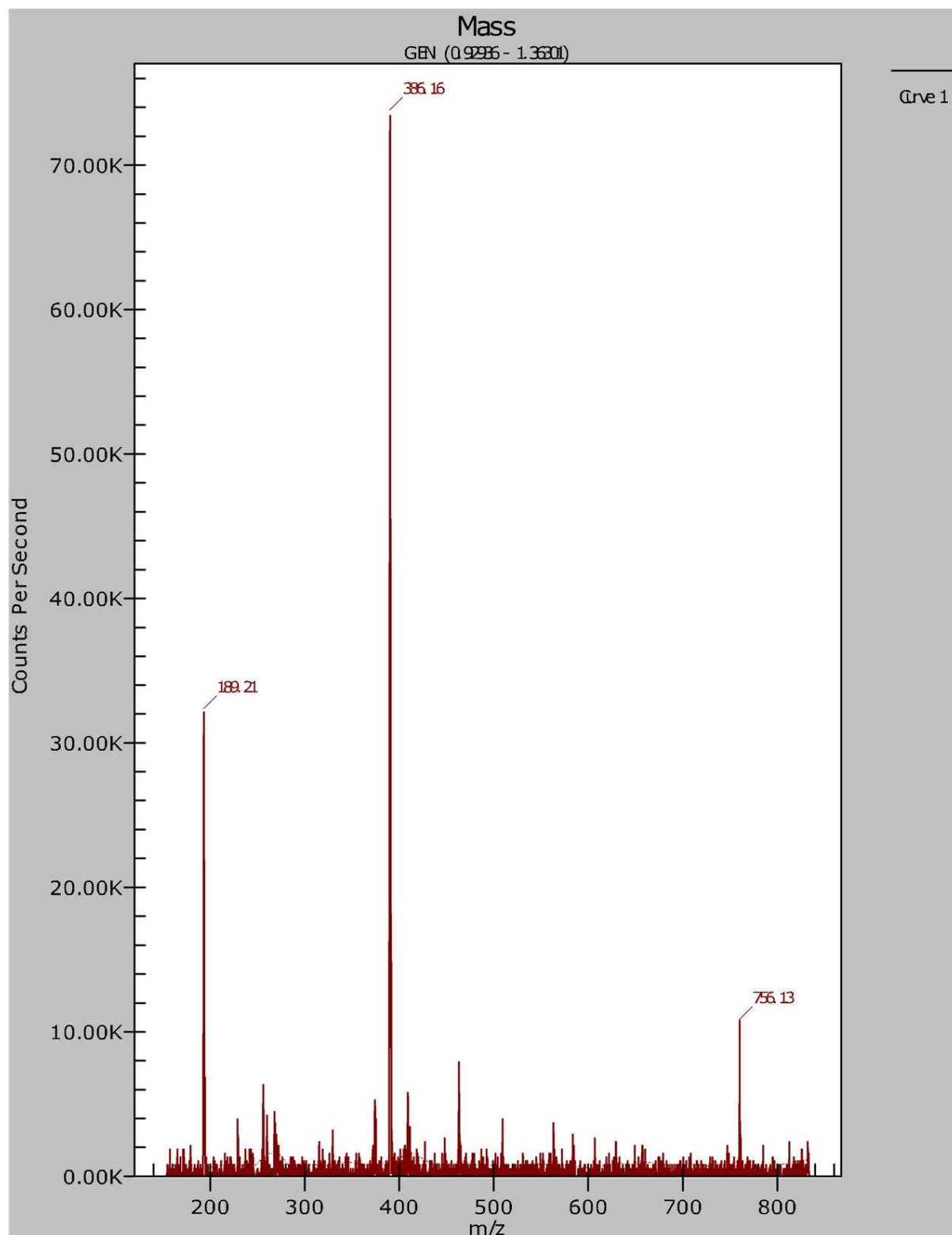


Figure S4. ESI-MS spectrum of complex **1** in DMSO: m/z 386.16 (100%, $[\text{V}^{\text{V}}\text{O}_2(\text{L}^1)]^-$, MW = 386.26); m/z 756.13 (14%, $[\text{V}^{\text{V}}\text{V}^{\text{IV}}\text{O}_3(\text{L}^1)_2]^-$, MW = 756.51).

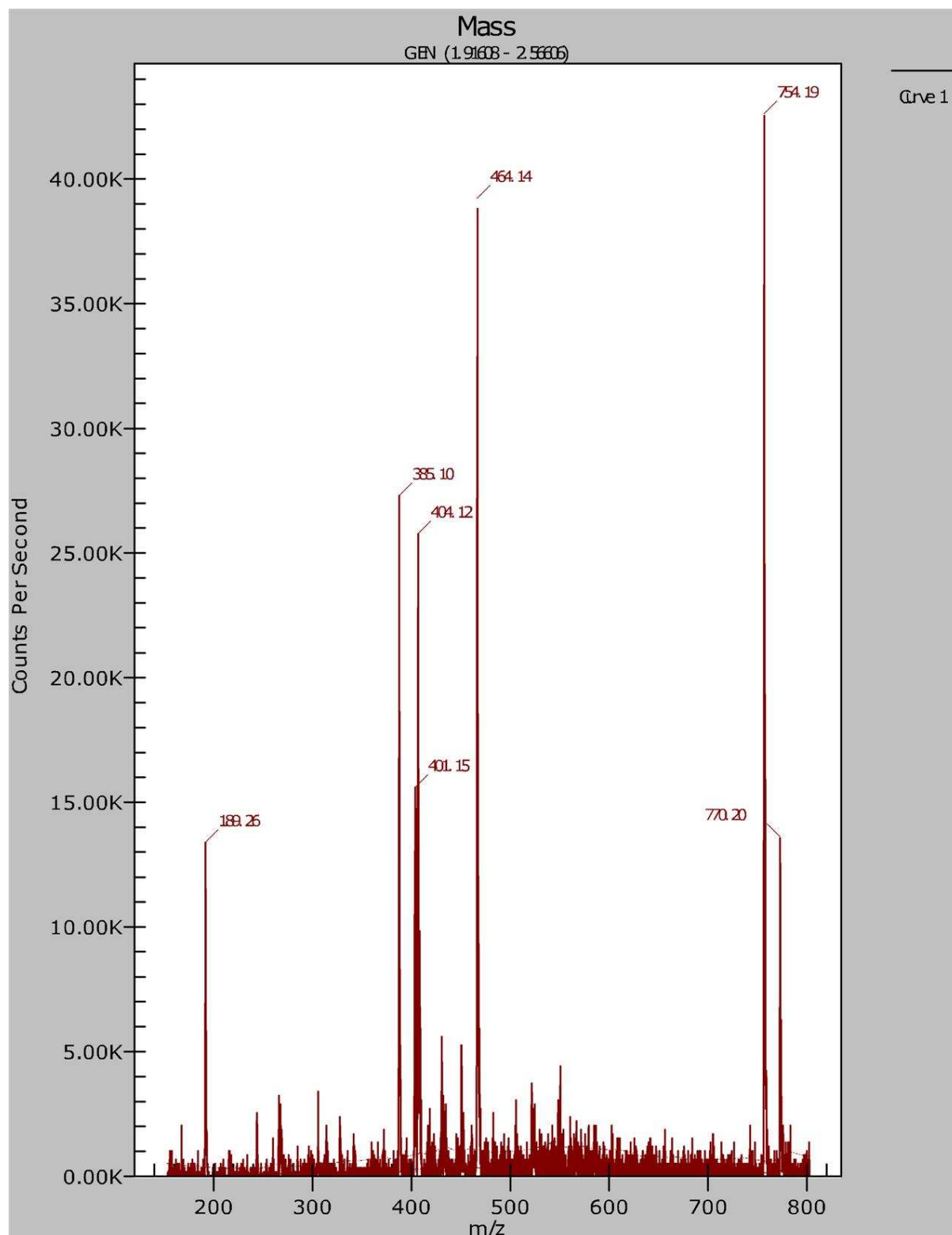


Figure S5. ESI-MS spectrum of complex **3** in DMSO: m/z 385.10 (64%, $[\text{V}^{\text{V}}\text{O}_2(\text{L}^3)]^-$, MW = 385.27); m/z 754.19 (100%, $[\text{V}^{\text{V}}\text{V}^{\text{IV}}\text{O}_3(\text{L}^3)_2]^-$, MW = 754.53).

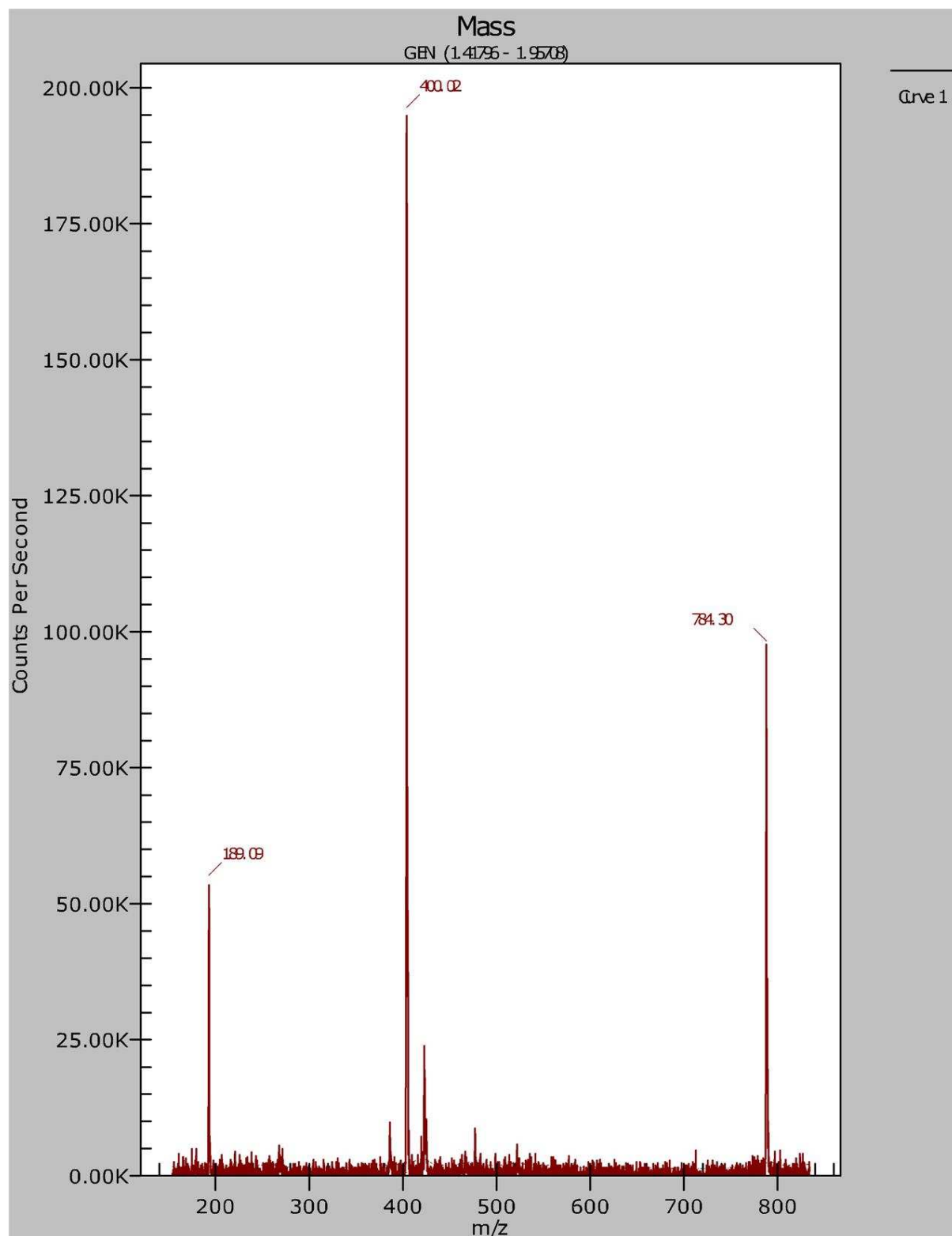


Figure S6. ESI-MS spectrum of complex **4** in DMSO: m/z 400.02 (100%, $[\text{V}^{\text{V}}\text{O}_2(\text{L}^4)]^-$, MW = 400.28); m/z 784.30 (50%, $[\text{V}^{\text{V}}\text{V}^{\text{IV}}\text{O}_3(\text{L}^4)_2]^-$, MW = 784.56).

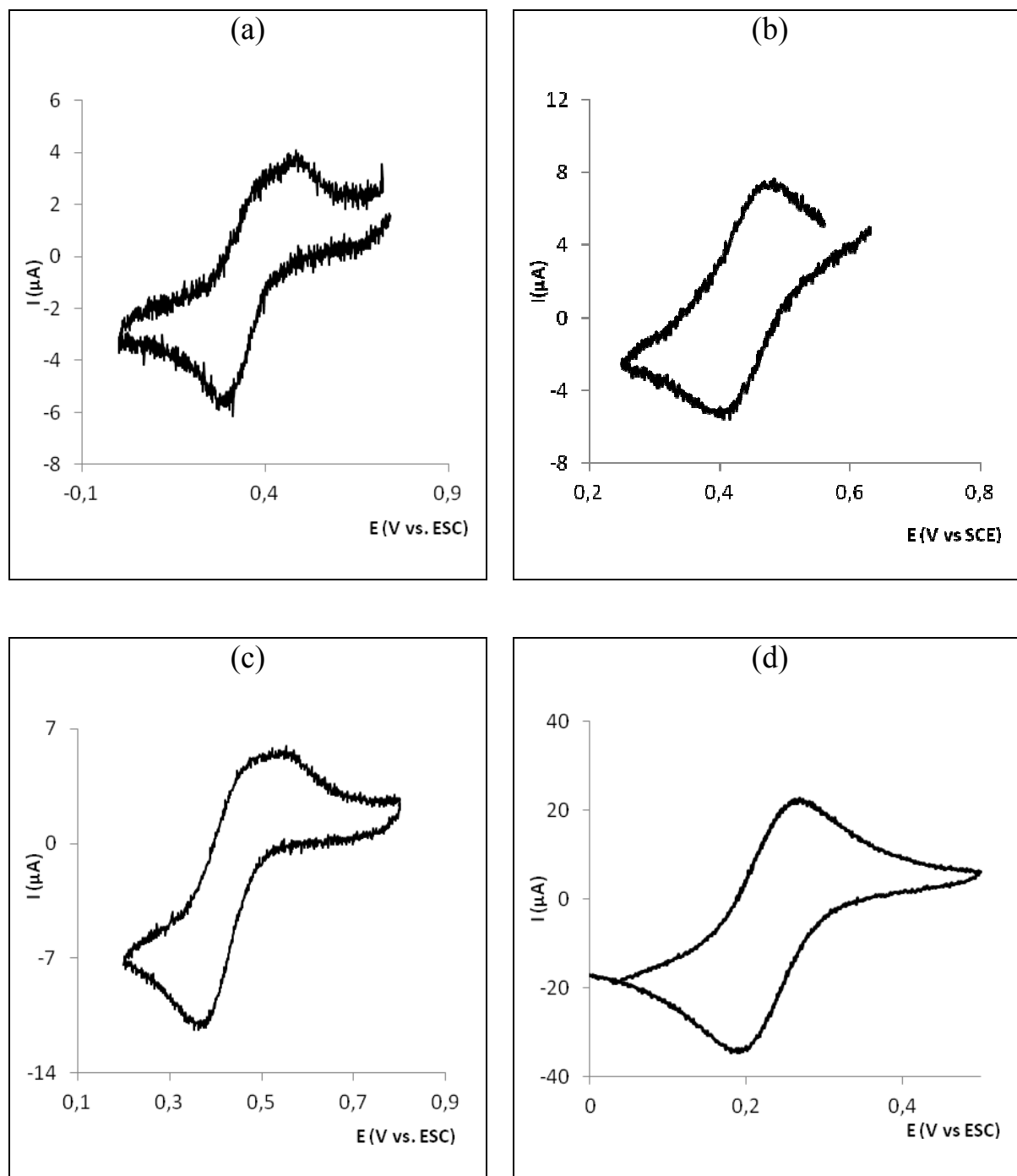


Figure S7. Cyclic voltammograms of: a) $[\text{V}^{\text{VO}}(\text{OEt})(\text{hnal-abhz})]$ (**1**); b) $[\text{V}^{\text{VO}}(\text{OEt})(\text{hnal-hbhz})]$ (**2**); c) $[\text{V}^{\text{VO}}(\text{OEt})(\text{han-bhz})]$ (**3**); d) $[\text{V}^{\text{VO}}(\text{OEt})(\text{han-abhz})]$ (**4**) obtained in $[\text{NBu}_4][\text{BF}_4]$ / acetonitrile (0.10 M) solutions. Values of $E_{1/2}^{\text{red}}$ (vs. SCE) are displayed in Table 4.

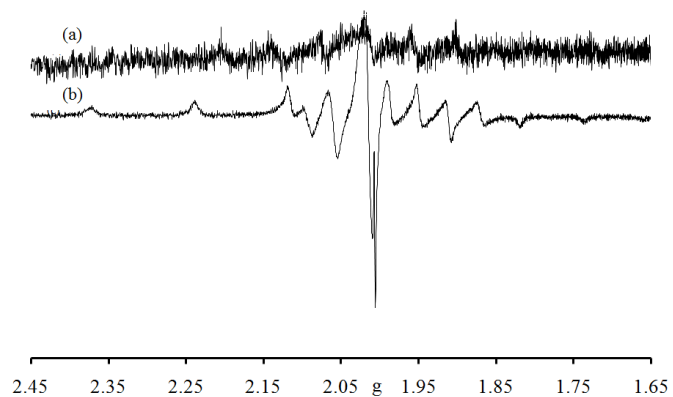


Figure S8. First derivative EPR spectra of **2** in acetonitrile after CPE: a) spectrum at room temperature; b) spectrum of the solution frozen at 77 K. The spin Hamiltonian parameters obtained for the spectrum at 77 K are in Table 4; the A_{iso} value for the spectrum at room temperature is $94.0 \times 10^{-4} \text{ cm}^{-1}$.

Table S1. Cartesian atomic coordinates (in Å) of the calculated equilibrium structures at B3P86 for DMSO taken as solvent for the calculations of the bulky solvent effect (if not stated otherwise)

1

C	1.228491	1.254454	6.086141
C	0.956737	2.444666	5.348828
C	0.672390	3.634665	6.047550
H	0.466772	4.529908	5.465865
C	0.660424	3.689914	7.427002
H	0.443359	4.624231	7.940178
C	0.934402	2.521347	8.150873
H	0.933159	2.540021	9.240471
C	1.208496	1.337671	7.497190
H	1.417638	0.430886	8.064704
C	0.956590	2.497964	3.895215
C	1.460359	0.931378	0.938179
H	1.756445	-0.043546	1.332438
C	1.327787	1.111295	-0.467792
C	0.634565	2.232089	-0.955131
C	0.341035	2.361329	-2.334009
H	-0.218661	3.237250	-2.666058
C	0.762330	1.401540	-3.212122
H	0.541727	1.503963	-4.275130
C	1.495354	0.263074	-2.779564
C	1.937208	-0.706164	-3.708104
H	1.698260	-0.563347	-4.762086
C	2.659811	-1.800630	-3.292678
H	3.000390	-2.542430	-4.013293
C	2.960975	-1.955261	-1.926959
H	3.539407	-2.816910	-1.596040
C	2.541293	-1.025027	-0.998945
H	2.810875	-1.169373	0.045612
C	1.790389	0.105432	-1.393416

C	-1.420230	5.531140	2.163967
H	-1.333651	5.249457	3.225472
H	-2.172457	4.874327	1.700028
C	-1.804525	6.986790	2.014170
H	-1.060880	7.638284	2.487639
H	-2.774358	7.163185	2.495568
H	-1.890575	7.263174	0.956977
N	1.451829	0.047086	5.505293
N	1.276437	1.474473	3.141492
N	1.206285	1.851845	1.827582
O	0.605464	3.634225	3.316920
O	0.187699	3.175179	-0.137062
O	2.303689	4.292872	1.171200
O	-0.161822	5.295086	1.550065
V	0.818766	3.844412	1.450451
H	1.692216	0.009637	4.512448
H	1.832707	-0.697361	6.098469

1 (EtOH solution)

C	1.217994	1.250741	6.089323
C	0.966463	2.446425	5.353501
C	0.700081	3.639732	6.053640
H	0.510226	4.538794	5.472665
C	0.686178	3.692715	7.433324
H	0.483442	4.629441	7.947657
C	0.940796	2.518830	8.155546
H	0.938192	2.535874	9.245018
C	1.197460	1.331625	7.500468
H	1.391357	0.421099	8.067084
C	0.966593	2.501393	3.899398
C	1.461528	0.933331	0.941335
H	1.755040	-0.042204	1.335235
C	1.329068	1.113992	-0.464610
C	0.635146	2.235329	-0.950193

C	0.338863	2.364832	-2.328707
H	-0.221346	3.240700	-2.658962
C	0.758788	1.405387	-3.207999
H	0.536333	1.508172	-4.270395
C	1.493494	0.266978	-2.777226
C	1.935083	-0.701476	-3.706948
H	1.694601	-0.558380	-4.760373
C	2.658924	-1.796003	-3.293324
H	2.998869	-2.536982	-4.014833
C	2.962970	-1.950847	-1.928067
H	3.543063	-2.811715	-1.598558
C	2.544006	-1.021127	-0.999088
H	2.816387	-1.164732	0.044663
C	1.790871	0.108735	-1.391559
C	-1.421228	5.524260	2.154828
H	-1.339381	5.247769	3.217964
H	-2.163610	4.858238	1.688359
C	-1.819877	6.975505	1.996239
H	-1.086311	7.636334	2.472199
H	-2.794893	7.143524	2.469866
H	-1.900747	7.246325	0.937314
N	1.422672	0.040430	5.505309
N	1.279470	1.476330	3.144865
N	1.210100	1.854397	1.831046
O	0.621999	3.639958	3.321914
O	0.188897	3.177566	-0.130939
O	2.310726	4.298433	1.167466
O	-0.156040	5.297994	1.550931
V	0.827943	3.849182	1.454016
H	1.668135	0.005645	4.513973
H	1.796274	-0.708347	6.096232

1•DMSO

V	0.382399	1.103057	-1.029413
O	-1.337078	1.510675	-0.432694
O	2.092967	0.293480	-0.777307
O	-0.005696	0.632752	-2.489151
O	1.130730	2.675135	-1.288406
N	-0.019171	-0.749471	-0.186862
N	1.064411	-1.525765	0.125039
N	2.694262	-3.610494	0.904820
C	-3.675673	1.483294	-0.622442
H	-3.643574	2.565364	-0.761073
C	-4.858459	0.797172	-0.606367
H	-5.799529	1.331872	-0.739266
C	-4.899762	-0.610155	-0.420385
C	-6.133806	-1.300091	-0.413015
H	-7.050005	-0.725880	-0.552131
C	-6.178510	-2.662218	-0.230216
H	-7.132353	-3.187265	-0.221532
C	-4.978020	-3.377970	-0.064110
H	-5.008003	-4.458508	0.070573
C	-3.760003	-2.731724	-0.075381
H	-2.855009	-3.325109	0.038509
C	-3.679156	-1.328640	-0.242364
C	-2.433776	-0.600161	-0.258996
C	-2.450137	0.791266	-0.458080
H	-1.210198	-2.288572	0.394976
C	-1.196260	-1.267782	0.006190
C	2.162556	-0.911605	-0.256519
C	3.477620	-1.534169	-0.145759
C	3.686410	-2.845017	0.376034
C	5.007094	-3.348351	0.382644
H	5.168563	-4.352301	0.775272
C	6.070089	-2.606425	-0.091076
H	7.071362	-3.036117	-0.070215

C	5.868784	-1.314248	-0.594065
H	6.704225	-0.725324	-0.966507
C	4.586315	-0.802221	-0.614152
H	4.406183	0.195216	-1.007664
C	2.067057	3.452235	-0.565670
H	1.576989	3.851958	0.332690
H	2.879523	2.788086	-0.232091
C	2.600535	4.565304	-1.442201
H	3.105516	4.162133	-2.327928
H	3.324313	5.166997	-0.878240
H	1.791126	5.226321	-1.774128
H	2.897666	-4.606271	1.040095
H	1.724680	-3.368214	0.688135
O	0.799054	1.561303	1.223278
S	-0.377071	1.441194	2.214948
C	0.415580	1.376853	3.829409
C	-1.088674	3.090516	2.354962
H	-0.298514	3.814741	2.574261
H	-1.841592	3.085777	3.149550
H	-1.558627	3.316798	1.396680
H	1.102750	2.220844	3.936994
H	0.964148	0.433749	3.888710
H	-0.356827	1.402453	4.604288

1•EtOH

V	0.328350	1.358345	-0.759902
O	-1.346652	1.714772	-0.069956
O	2.028516	0.492626	-0.626197
O	-0.050871	1.140660	-2.278659
O	1.113284	2.931525	-0.730337
N	-0.102095	-0.581731	-0.187557
N	0.965613	-1.420329	-0.004980
N	2.580213	-3.566555	0.641206

C	-3.689908	1.786748	-0.143522
H	-3.625060	2.875958	-0.127841
C	-4.894368	1.140176	-0.169427
H	-5.820387	1.715966	-0.180035
C	-4.978216	-0.277459	-0.186093
C	-6.234257	-0.925281	-0.222356
H	-7.134806	-0.310877	-0.232120
C	-6.319220	-2.297945	-0.246873
H	-7.289530	-2.791086	-0.274564
C	-5.138157	-3.063574	-0.244902
H	-5.200056	-4.150745	-0.274425
C	-3.899935	-2.457965	-0.212456
H	-3.011733	-3.086407	-0.229802
C	-3.778744	-1.049335	-0.171356
C	-2.510266	-0.363067	-0.136293
C	-2.484781	1.042156	-0.135585
H	-1.317306	-2.157225	0.220905
C	-1.287248	-1.093163	-0.024258
C	2.075840	-0.779651	-0.291204
C	3.381894	-1.427997	-0.258309
C	3.579048	-2.775473	0.164342
C	4.895011	-3.289551	0.132457
H	5.048862	-4.319733	0.453615
C	5.962955	-2.525275	-0.292533
H	6.960456	-2.963947	-0.305484
C	5.771589	-1.200238	-0.706250
H	6.610846	-0.595635	-1.043294
C	4.494558	-0.674633	-0.681086
H	4.321886	0.349852	-1.001644
C	2.058890	3.567557	0.108460
H	1.573820	3.817906	1.062148
H	2.866929	2.849120	0.321851
C	2.606355	4.806665	-0.567642

H	3.107134	4.553216	-1.509303
H	3.336204	5.294450	0.090484
H	1.804665	5.523571	-0.780586
H	2.777745	-4.570484	0.709349
H	1.613297	-3.309107	0.430911
O	0.761434	1.433048	1.608958
C	-0.021066	0.785760	2.616809
C	0.344272	1.273140	4.002512
H	0.104390	-0.304860	2.543513
H	-1.063378	1.025131	2.380937
H	1.392114	1.046164	4.237512
H	-0.283061	0.778109	4.754471
H	0.196685	2.356016	4.090123
H	1.720948	1.202427	1.763254

1•MeCN

V	0.286495	1.262390	-0.856731
O	-1.340810	1.681526	-0.101228
O	1.971293	0.411151	-0.642184
O	-0.137912	0.972087	-2.347930
O	1.087786	2.819672	-0.900766
N	-0.149271	-0.627069	-0.144436
N	0.909859	-1.465892	0.072802
N	2.513797	-3.608762	0.754569
C	-3.682808	1.805478	-0.083005
H	-3.593432	2.893047	-0.083859
C	-4.900892	1.185109	-0.056275
H	-5.814140	1.780792	-0.039499
C	-5.015702	-0.230773	-0.058029
C	-6.285468	-0.851162	-0.047957
H	-7.172727	-0.217924	-0.030194
C	-6.400219	-2.221942	-0.062841
H	-7.381324	-2.694011	-0.055201

C	-5.237037	-3.013136	-0.102077
H	-5.323525	-4.098684	-0.128595
C	-3.985362	-2.434094	-0.111552
H	-3.110945	-3.080245	-0.159635
C	-3.834280	-1.029073	-0.077273
C	-2.550557	-0.370790	-0.086485
C	-2.495526	1.033949	-0.110537
H	-1.387213	-2.176046	0.309113
C	-1.342738	-1.120330	0.031753
C	2.022126	-0.845608	-0.246088
C	3.326053	-1.492556	-0.187132
C	3.516361	-2.831308	0.266494
C	4.830827	-3.350439	0.250617
H	4.979734	-4.373878	0.594830
C	5.902926	-2.599377	-0.186208
H	6.898874	-3.041764	-0.185260
C	5.718343	-1.282576	-0.629272
H	6.561544	-0.688216	-0.974505
C	4.443432	-0.752024	-0.621050
H	4.276052	0.265879	-0.964630
C	2.138917	3.459123	-0.203931
H	1.739149	3.863839	0.737034
H	2.893676	2.699030	0.050774
C	2.735437	4.558122	-1.057531
H	3.148906	4.152997	-1.988525
H	3.545409	5.054591	-0.508533
H	1.980527	5.312071	-1.309586
H	2.706508	-4.611117	0.851763
H	1.546556	-3.348377	0.550169
N	0.798263	1.593791	1.789862
C	0.811836	1.787806	2.932504
C	0.828814	2.037059	4.360096
H	1.861074	2.029378	4.727998

H	0.257294	1.260617	4.881127
H	0.380327	3.014339	4.571981

2

V	3.142758	1.855245	8.444006
O	2.617758	0.384239	7.487436
O	2.505662	3.185024	9.655189
O	-0.623982	5.905334	8.698815
O	4.250150	2.568380	7.592681
O	3.942422	1.013445	9.744363
N	1.414173	2.658889	7.551593
N	0.875827	3.749429	8.178153
C	2.077495	0.180488	6.293328
C	2.380874	-1.036525	5.636712
H	3.062527	-1.734383	6.125642
C	1.819427	-1.312797	4.420784
H	2.055573	-2.248967	3.913838
C	0.930334	-0.404319	3.785212
C	0.371444	-0.705916	2.522668
H	0.637514	-1.651152	2.049232
C	-0.486774	0.173190	1.904320
H	-0.914167	-0.065433	0.931719
C	-0.808971	1.388358	2.536508
H	-1.485128	2.088839	2.048031
C	-0.274675	1.709613	3.766597
H	-0.536298	2.665824	4.215765
C	0.604480	0.824700	4.431467
C	1.191878	1.107276	5.719622
C	0.824366	2.269363	6.456019
H	-0.016963	2.880194	6.119732
C	1.529034	3.982335	9.287450
C	1.171830	5.108280	10.142596
C	0.125176	6.003036	9.807793

C	-0.166763	7.065263	10.672284
H	-0.976135	7.743095	10.396650
C	0.553101	7.243407	11.842520
H	0.306213	8.076750	12.499523
C	1.585218	6.363530	12.184237
H	2.148612	6.502542	13.104708
C	1.883057	5.310859	11.337236
H	2.681819	4.615225	11.585545
C	5.279029	1.042256	10.235721
H	5.280396	1.673398	11.137156
H	5.926809	1.512000	9.480870
C	5.743280	-0.359565	10.564430
H	5.093800	-0.822290	11.316284
H	6.762878	-0.319034	10.967426
H	5.752087	-0.990797	9.668444
H	-0.345645	5.106972	8.162894

3

C	7.969474	7.077054	6.755238
C	7.472195	6.855112	5.446081
H	7.858801	6.000909	4.887807
C	6.537848	7.698007	4.917844
H	6.160247	7.533548	3.908260
C	6.003640	8.772828	5.678392
C	4.954315	9.562908	5.158660
H	4.606808	9.361168	4.145250
C	4.363451	10.543241	5.922233
H	3.548951	11.142333	5.518190
C	4.797764	10.741912	7.244896
H	4.300993	11.480986	7.872217
C	5.835593	9.998671	7.768778
H	6.107704	10.144849	8.810381
C	6.499534	9.018017	6.994041

C	7.581558	8.204537	7.499646
C	8.380318	8.581666	8.647614
C	10.481715	7.083562	10.848420
C	11.372216	7.244550	12.003815
C	12.097345	6.147504	12.482755
H	11.994126	5.180615	11.994973
C	12.943855	6.295324	13.576152
H	13.505649	5.437674	13.943527
C	13.072833	7.534869	14.198671
H	13.735516	7.648551	15.055791
C	12.350999	8.630780	13.724591
H	12.448512	9.600696	14.210281
C	11.506472	8.490550	12.631672
H	10.941500	9.343080	12.260679
C	11.275718	3.814535	8.361079
H	11.827561	4.152072	9.252980
H	11.639930	4.395519	7.499264
C	11.462056	2.330605	8.132650
H	11.109585	1.754498	8.996075
H	12.526551	2.111725	7.983001
H	10.914930	1.998762	7.242695
C	8.580722	10.020561	9.016750
H	9.651862	10.202479	9.154246
H	8.096122	10.259145	9.972984
H	8.197666	10.689491	8.245397
N	9.050734	7.665338	9.313759
N	9.847004	8.100835	10.340553
O	8.874231	6.215756	7.207116
O	10.345657	5.883755	10.325417
O	7.664576	5.267538	9.483867
O	9.901337	4.108269	8.563300
V	9.093924	5.624615	8.925210

V	3.927362	2.574968	1.194621
O	4.399329	3.422545	-0.358072
O	4.278083	2.758754	3.036504
O	2.523674	1.899564	0.952707
O	5.138171	1.301954	1.137556
N	3.264308	4.484531	1.681244
N	3.365208	4.835403	3.001304
N	3.190050	6.164268	5.397961
C	3.886289	4.161801	-2.517341
H	4.654743	3.479328	-2.884109
C	3.158002	4.947312	-3.362920
H	3.339628	4.911117	-4.437416
C	2.124043	5.790236	-2.874235
C	1.305770	6.511470	-3.772371
H	1.523174	6.445058	-4.838571
C	0.243006	7.256959	-3.316633
H	-0.388480	7.803772	-4.015052
C	-0.044548	7.276070	-1.939996
H	-0.915296	7.820697	-1.576984
C	0.752666	6.599840	-1.039950
H	0.468372	6.597207	0.008527
C	1.885637	5.867633	-1.468751
C	2.743741	5.132320	-0.568220
C	3.656110	4.217790	-1.119715
C	2.512038	6.765547	1.401572
H	1.593245	6.762243	2.003767
H	2.414732	7.505727	0.606548
H	3.324898	7.060803	2.074409
C	2.811874	5.402920	0.854016
C	3.888835	3.845964	3.679496
C	4.074144	3.892403	5.121052
C	3.702411	5.017121	5.916179

C	3.926387	4.937953	7.309842
H	3.641345	5.793254	7.922392
C	4.484875	3.818707	7.892018
H	4.636397	3.799438	8.971043
C	4.856752	2.716178	7.110665
H	5.299356	1.834024	7.568262
C	4.648978	2.768689	5.746890
H	4.926137	1.923440	5.121568
C	6.486857	1.310031	1.583797
H	7.036207	2.094869	1.040257
H	6.487708	1.576079	2.653075
C	7.116182	-0.047329	1.357680
H	6.575965	-0.825562	1.909180
H	8.155904	-0.035064	1.707318
H	7.114965	-0.307531	0.292859
H	2.758428	6.824049	6.053399
H	2.821237	6.151550	4.444224

4 (B3LYP)

V	3.924207	2.562114	1.203830
O	4.402595	3.421579	-0.353827
O	4.272056	2.757082	3.054809
O	2.515431	1.875425	0.961722
O	5.148137	1.287678	1.134876
N	3.246613	4.487833	1.688281
N	3.345305	4.836246	3.019540
N	3.198317	6.189535	5.427836
C	3.894451	4.165195	-2.520881
H	4.664494	3.482935	-2.883913
C	3.166768	4.949060	-3.372515
H	3.352497	4.910333	-4.446008
C	2.126523	5.793399	-2.888840
C	1.306803	6.512050	-3.793898
H	1.528406	6.444340	-4.858975

C	0.237020	7.255851	-3.343823
H	-0.393710	7.798532	-4.046182
C	-0.056979	7.277565	-1.965020
H	-0.930950	7.820420	-1.607076
C	0.740897	6.605579	-1.058046
H	0.452284	6.607248	-0.011464
C	1.881942	5.873793	-1.479866
C	2.742641	5.140594	-0.570950
C	3.659174	4.223611	-1.120505
C	2.505375	6.784044	1.406469
H	1.583177	6.784644	2.003767
H	2.413529	7.523164	0.610182
H	3.316684	7.079216	2.080935
C	2.803802	5.411696	0.858172
C	3.874649	3.848631	3.699451
C	4.063690	3.896698	5.147423
C	3.702673	5.027382	5.945675
C	3.932719	4.949697	7.341311
H	3.655567	5.808174	7.952930
C	4.487729	3.826109	7.926140
H	4.643479	3.807719	9.004578
C	4.849728	2.718153	7.142992
H	5.288853	1.833843	7.600061
C	4.636506	2.768705	5.776714
H	4.907042	1.919029	5.155590
C	6.517011	1.292146	1.547719
H	7.054187	2.066648	0.977564
H	6.548897	1.569584	2.613280
C	7.134267	-0.077760	1.319496
H	6.605152	-0.846492	1.895851
H	8.184154	-0.066804	1.639934
H	7.101459	-0.350750	0.257694
H	2.755996	6.832099	6.094961

H	2.783655	6.162528	4.493602
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4 (M06)

V	3.843892	2.520179	1.235810
O	4.363374	3.336846	-0.331183
O	4.190907	2.712945	3.088431
O	2.421089	1.892398	0.985058
O	5.021909	1.203408	1.206824
N	3.254154	4.458867	1.703130
N	3.367345	4.824689	3.022171
N	3.217932	6.195552	5.402908
C	3.875960	4.080457	-2.492274
H	4.631053	3.375205	-2.850948
C	3.167211	4.874085	-3.342544
H	3.347337	4.828429	-4.419792
C	2.151287	5.742440	-2.861833
C	1.348709	6.468979	-3.767190
H	1.569284	6.386391	-4.834438
C	0.301748	7.237853	-3.320507
H	-0.321509	7.790152	-4.025322
C	0.015969	7.276741	-1.944942
H	-0.846669	7.841768	-1.587178
C	0.799618	6.596807	-1.039236
H	0.514662	6.610852	0.012072
C	1.916480	5.837987	-1.460253
C	2.757930	5.092750	-0.553357
C	3.646173	4.150179	-1.094755
C	2.566265	6.752546	1.393453
H	1.652626	6.775428	2.007584
H	2.475382	7.490039	0.591797
H	3.390586	7.043441	2.058356
C	2.831249	5.379005	0.864837
C	3.850639	3.823449	3.709744
C	4.048516	3.891402	5.150753

C	3.709174	5.035085	5.926686
C	3.943488	4.976125	7.317076
H	3.678616	5.851164	7.915695
C	4.484119	3.858812	7.915898
H	4.644267	3.856117	8.996004
C	4.828774	2.737471	7.152611
H	5.261800	1.854069	7.621967
C	4.609246	2.770397	5.791383
H	4.868589	1.906891	5.177903
C	6.362099	1.286369	1.662438
H	6.792942	2.259821	1.360040
H	6.343600	1.261945	2.768003
C	7.166842	0.139264	1.105081
H	6.739555	-0.823548	1.416505
H	8.201386	0.193024	1.470175
H	7.187599	0.171215	0.007414
H	2.798031	6.850953	6.073340
H	2.783664	6.169658	4.476200

4 (TPSSH)

V	3.938185	2.573330	1.192964
O	4.411460	3.428592	-0.365667
O	4.287261	2.760037	3.041153
O	2.517286	1.900414	0.946447
O	5.151859	1.289602	1.134793
N	3.266657	4.488115	1.679508
N	3.366341	4.848119	3.007140
N	3.191916	6.180846	5.413678
C	3.896346	4.173569	-2.532169
H	4.668135	3.495013	-2.898652
C	3.164492	4.962082	-3.380813
H	3.349436	4.929298	-4.454710
C	2.122519	5.802077	-2.891079
C	1.300423	6.525060	-3.791769

H	1.520907	6.463641	-4.857609
C	0.228585	7.266042	-3.334602
H	-0.403792	7.812272	-4.032721
C	-0.065499	7.277215	-1.954704
H	-0.941263	7.814504	-1.592821
C	0.735741	6.600065	-1.051022
H	0.448563	6.590911	-0.003006
C	1.878466	5.874900	-1.480459
C	2.740000	5.138758	-0.575772
C	3.660380	4.226053	-1.131903
C	2.495287	6.776693	1.404178
H	1.577045	6.764230	2.007546
H	2.391610	7.515135	0.607393
H	3.310645	7.074587	2.073515
C	2.804765	5.409934	0.849440
C	3.893131	3.853742	3.688532
C	4.078609	3.898251	5.133003
C	3.703000	5.024411	5.933443
C	3.929243	4.944928	7.330862
H	3.641697	5.798704	7.944610
C	4.493504	3.822875	7.913670
H	4.645736	3.802831	8.992515
C	4.868667	2.718573	7.127840
H	5.314093	1.837109	7.584382
C	4.659369	2.771289	5.759647
H	4.938304	1.927365	5.133246
C	6.512345	1.282781	1.587794
H	7.065468	2.061640	1.041529
H	6.508297	1.545229	2.657011
C	7.123083	-0.089916	1.356244
H	6.570086	-0.860115	1.906896
H	8.163326	-0.091306	1.706452
H	7.116831	-0.344755	0.289834

H	2.742070	6.824927	6.077143
H	2.794284	6.156441	4.468666

4 (in EtOH solution)

V	3.923585	2.573632	1.198173
O	4.402946	3.425720	-0.350536
O	4.273581	2.758177	3.040899
O	2.520073	1.899563	0.954109
O	5.134376	1.300368	1.138269
N	3.259852	4.484516	1.685326
N	3.360995	4.835169	3.005372
N	3.203658	6.171564	5.398590
C	3.890796	4.160465	-2.511894
H	4.660588	3.478698	-2.876222
C	3.162925	4.944509	-3.359408
H	3.346353	4.907684	-4.433397
C	2.126705	5.786434	-2.873089
C	1.309825	6.507747	-3.772764
H	1.529328	6.441674	-4.838393
C	0.246151	7.253503	-3.319171
H	-0.383483	7.800593	-4.018800
C	-0.044676	7.272064	-1.943077
H	-0.916202	7.816311	-1.581838
C	0.750499	6.594978	-1.041725
H	0.464357	6.591439	0.006129
C	1.885312	5.863923	-1.468046
C	2.743011	5.130908	-0.565275
C	3.658568	4.217929	-1.114431
C	2.507670	6.765922	1.403819
H	1.589418	6.762411	2.006612
H	2.409208	7.505018	0.608025
H	3.321090	7.062122	2.075513
C	2.808138	5.402467	0.857306

C	3.885043	3.845644	3.683573
C	4.071452	3.892815	5.125529
C	3.707608	5.021016	5.919494
C	3.930097	4.941922	7.313332
H	3.650876	5.799521	7.925070
C	4.482039	3.819652	7.896734
H	4.633344	3.800520	8.975639
C	4.846565	2.713765	7.116613
H	5.283014	1.829196	7.575115
C	4.638595	2.765894	5.752653
H	4.908873	1.917989	5.128106
C	6.486725	1.312644	1.573186
H	7.029101	2.098699	1.024625
H	6.495764	1.579202	2.642197
C	7.118734	-0.043145	1.342406
H	6.585156	-0.822458	1.898596
H	8.161204	-0.027546	1.683305
H	7.108888	-0.303562	0.277799
H	2.772966	6.832797	6.051872
H	2.834208	6.156026	4.445683

4•DMSO

V	0.277653	1.147260	-1.035886
O	-1.262928	1.620137	-0.104649
O	1.959810	0.242210	-1.074593
O	-0.398347	0.780852	-2.418071
O	1.081032	2.679659	-1.382151
N	-0.092455	-0.707964	-0.169421
N	1.020716	-1.445258	0.134999
N	2.667996	-3.520282	0.857835
C	-3.600855	1.742379	-0.148631
H	-3.498377	2.828723	-0.124599
C	-4.824820	1.137312	-0.173825

H	-5.734791	1.737870	-0.163656
C	-4.940414	-0.274854	-0.252971
C	-6.210907	-0.883896	-0.367448
H	-7.094563	-0.245935	-0.339533
C	-6.331289	-2.243161	-0.538842
H	-7.313132	-2.704145	-0.633737
C	-5.168372	-3.029678	-0.632236
H	-5.252999	-4.098840	-0.823076
C	-3.917961	-2.465025	-0.496533
H	-3.044855	-3.099618	-0.617740
C	-3.758573	-1.077359	-0.258292
C	-2.473089	-0.439692	-0.107676
C	-2.416772	0.962599	-0.147399
C	-1.296939	-2.441585	1.010570
H	-1.034764	-3.324298	0.411694
H	-2.279305	-2.595180	1.459961
H	-0.543063	-2.366730	1.802868
C	-1.257318	-1.186196	0.191116
C	2.077145	-0.887504	-0.412948
C	3.399669	-1.497151	-0.325817
C	3.637610	-2.775834	0.260516
C	4.963032	-3.267162	0.254063
H	5.146558	-4.247234	0.694491
C	6.004100	-2.539249	-0.285643
H	7.010910	-2.956001	-0.267801
C	5.774763	-1.277649	-0.850620
H	6.594060	-0.700401	-1.273793
C	4.486087	-0.781259	-0.865797
H	4.284112	0.192379	-1.305736
C	2.202558	3.339060	-0.829900
H	1.918399	3.768586	0.140896
H	2.986482	2.588658	-0.642448
C	2.693192	4.410968	-1.780423

H	2.994880	3.977248	-2.741214
H	3.561533	4.922947	-1.347064
H	1.913134	5.158700	-1.966770
H	2.880496	-4.508947	1.027643
H	1.691110	-3.287037	0.662378
O	1.104218	1.510585	1.120163
S	0.131004	1.364677	2.306933
C	1.218818	1.177745	3.728822
C	-0.465839	3.024929	2.672270
H	0.383851	3.707690	2.766361
H	-1.046349	2.998181	3.599929
H	-1.105980	3.322972	1.840507
H	1.949008	1.991858	3.741633
H	1.728134	0.216532	3.627210
H	0.616400	1.180785	4.642444

4•EtOH

V	0.275153	1.369966	-0.736452
O	-1.250397	1.741152	0.225410
O	1.975287	0.500623	-0.807404
O	-0.350705	1.154851	-2.170852
O	1.078177	2.933545	-0.849655
N	-0.096150	-0.568930	-0.093785
N	1.010217	-1.352081	0.101451
N	2.664129	-3.464749	0.669648
C	-3.584959	1.886762	0.213921
H	-3.472242	2.962673	0.357519
C	-4.813461	1.297846	0.131182
H	-5.718031	1.901438	0.210232
C	-4.942397	-0.096328	-0.104193
C	-6.219279	-0.672646	-0.291231
H	-7.094599	-0.028698	-0.203615
C	-6.355831	-2.006288	-0.597401

H	-7.342509	-2.442264	-0.745332
C	-5.202297	-2.795181	-0.756520
H	-5.298266	-3.839828	-1.050096
C	-3.945193	-2.262160	-0.563152
H	-3.081113	-2.893355	-0.747580
C	-3.768531	-0.906227	-0.192199
C	-2.475714	-0.297880	0.014326
C	-2.408400	1.100654	0.124812
C	-1.300503	-2.421223	0.883811
H	-1.053272	-3.228201	0.180702
H	-2.276980	-2.621495	1.327337
H	-0.534872	-2.446092	1.667711
C	-1.262687	-1.078407	0.218734
C	2.077133	-0.725169	-0.338862
C	3.394289	-1.350528	-0.340555
C	3.630424	-2.678699	0.122424
C	4.951089	-3.176597	0.050038
H	5.134042	-4.192460	0.400264
C	5.987406	-2.414279	-0.449467
H	6.990018	-2.839317	-0.490909
C	5.758122	-1.107686	-0.901803
H	6.573298	-0.504300	-1.295491
C	4.475952	-0.598319	-0.839595
H	4.274427	0.411574	-1.188437
C	2.179445	3.539704	-0.203993
H	1.918054	3.728353	0.846663
H	3.018910	2.825226	-0.217223
C	2.553461	4.825739	-0.909719
H	2.831938	4.636628	-1.953016
H	3.408561	5.291356	-0.403853
H	1.718887	5.536569	-0.894715
H	2.874987	-4.464819	0.754257
H	1.686502	-3.217155	0.497200

O	1.036667	1.477708	1.567195
C	0.371250	0.861045	2.672984
C	0.817916	1.452899	3.993622
H	0.545843	-0.225320	2.652898
H	-0.696393	1.037405	2.509588
H	1.891107	1.291263	4.157460
H	0.276875	0.979247	4.822557
H	0.621640	2.531097	4.026508
H	2.011666	1.276372	1.636006

1-1

V	2.072024	-0.865075	0.511120
O	2.731773	-1.473926	-1.074729
O	2.143235	0.494571	1.798485
H	2.896499	4.143977	6.543451
O	1.815708	-2.166449	1.353503
O	0.545657	-0.251571	-0.139300
N	4.101005	-0.548435	0.880657
N	4.397437	0.308959	1.908365
C	3.814149	-2.106130	-1.502254
C	3.700731	-2.883407	-2.678514
H	2.725344	-2.956862	-3.162666
C	4.805125	-3.514702	-3.180679
H	4.721059	-4.117217	-4.085747
C	5.043429	-1.962501	-0.841059
C	5.126344	-1.096238	0.284021
H	6.104383	-0.833934	0.693465
C	3.288965	0.822095	2.376526
C	3.246402	1.740426	3.502676
C	4.417478	2.268567	4.123363
N	5.678366	2.017274	3.684263
C	4.240905	3.136621	5.225163
H	5.132417	3.535910	5.708659

C	2.985643	3.475417	5.687473
C	1.834444	2.972830	5.065560
H	0.844207	3.242231	5.426356
C	1.980191	2.119947	3.990026
H	1.101196	1.710753	3.497524
V	-1.082417	-0.554344	-0.774268
O	-1.623073	-1.646460	0.580572
C	-2.675181	-2.422291	0.806546
C	-2.485936	-3.578986	1.597743
H	-1.481595	-3.802173	1.962414
C	-3.554695	-4.381139	1.890333
H	-3.411506	-5.275190	2.498099
C	-3.945319	-2.073119	0.324866
C	-4.105776	-0.852077	-0.387353
N	-3.120152	-0.117327	-0.827565
O	-1.208758	1.175862	-1.480834
C	-2.384902	1.687587	-1.813599
N	-3.469867	1.050811	-1.451231
C	-2.405826	2.933800	-2.559057
C	-3.610986	3.541162	-3.024429
N	-4.847939	3.052051	-2.761216
C	-3.497040	4.739638	-3.767085
H	-4.414014	5.207336	-4.125259
C	-2.270725	5.310361	-4.037476
H	-2.229504	6.233982	-4.614455
C	-1.086418	4.713930	-3.581645
H	-0.119059	5.163045	-3.795777
C	-1.170170	3.543039	-2.856894
H	-0.264604	3.060879	-2.495975
O	-0.994116	-1.495677	-2.028612
H	-5.109083	-0.469790	-0.588386
H	-4.947440	2.102621	-2.395112
H	-5.636176	3.435157	-3.292914

C	-6.379827	-2.675705	0.141880
C	-5.073811	-2.922758	0.621224
C	-7.418081	-3.531391	0.443148
C	-4.861263	-4.088321	1.414928
C	-7.206833	-4.675008	1.235225
C	-5.944472	-4.946682	1.710011
H	-6.581410	-1.808574	-0.484317
H	-5.756364	-5.830769	2.319416
H	-8.037488	-5.340676	1.464155
H	-8.414939	-3.317226	0.059744
H	5.838344	1.222077	3.062378
H	6.451788	2.273598	4.306780
C	7.487261	-2.555111	-0.765462
C	6.211653	-2.626401	-1.369138
C	8.565348	-3.226227	-1.303145
C	6.075142	-3.411709	-2.551996
C	8.426183	-3.999123	-2.470664
C	7.197767	-4.086758	-3.083044
H	7.633505	-1.977538	0.145372
H	7.066547	-4.681478	-3.987219
H	9.286483	-4.524043	-2.882868
H	9.536345	-3.155913	-0.814576

4-4

V	1.708976	-0.507170	0.459573
O	2.336709	-1.134072	-1.125560
O	1.579984	1.099769	1.415044
H	1.900041	6.015213	4.908767
O	1.889656	-1.676208	1.493641
O	0.000341	-0.423197	-0.002110
N	3.667941	0.241042	0.554199
N	3.816806	1.423886	1.225064
C	3.449295	-1.819219	-1.380574

C	3.367820	-2.827104	-2.372165
H	2.408832	-2.987615	-2.867668
C	4.475496	-3.560174	-2.688546
H	4.420687	-4.330561	-3.458196
C	4.662042	-1.505864	-0.749815
C	4.746984	-0.267013	-0.000376
C	6.016901	0.525652	0.059393
C	2.661684	1.803365	1.709163
C	2.510998	2.969138	2.563547
C	3.595471	3.836653	2.892093
N	4.851339	3.689381	2.394586
C	3.325569	4.930141	3.746418
H	4.150261	5.596581	3.999011
C	2.062693	5.160833	4.252127
C	0.999167	4.304205	3.936930
H	0.004444	4.480915	4.340320
C	1.235451	3.231341	3.101626
H	0.425040	2.553204	2.844339
V	-1.708719	-0.507738	-0.462300
O	-2.334769	-1.136014	1.122947
C	-3.446813	-1.821806	1.378584
C	-3.363930	-2.830279	2.369439
H	-2.404343	-2.990842	2.863760
C	-4.471056	-3.563852	2.686598
H	-4.415176	-4.334713	3.455697
C	-4.660315	-1.508437	0.749329
C	-4.746439	-0.269170	0.000708
N	-3.668126	0.239683	-0.554547
O	-1.581417	1.099752	-1.416893
C	-2.663597	1.803450	-1.709053
N	-3.818126	1.423049	-1.224290
C	-2.513977	2.970353	-2.562111
C	-3.599189	3.837331	-2.889609

N	-4.854884	3.688523	-2.392096
C	-3.330311	4.931913	-3.742851
H	-4.155589	5.597898	-3.994688
C	-2.067669	5.164229	-4.248418
H	-1.905818	6.019440	-4.904179
C	-1.003381	4.308215	-3.934152
H	-0.008829	4.486204	-4.337393
C	-1.238691	3.234243	-3.099985
H	-0.427685	2.556537	-2.843484
O	-1.889672	-1.676259	-1.496904
C	-6.016718	0.523046	-0.057168
H	-5.118562	2.789154	-1.983104
H	-5.602631	4.228116	-2.840638
H	-6.457417	0.502795	-1.063354
H	-5.787092	1.571689	0.162203
H	-6.750606	0.156473	0.661766
C	-6.991698	-2.312008	0.237467
C	-5.798001	-2.362667	0.997482
C	-8.044915	-3.161597	0.503121
C	-5.699211	-3.376228	1.998499
C	-7.965669	-4.110165	1.538336
C	-6.800555	-4.222409	2.260629
H	-7.073516	-1.632018	-0.605118
H	-6.698165	-4.979305	3.038501
H	-8.808096	-4.769099	1.742466
H	-8.944465	-3.102678	-0.108397
H	5.115800	2.790622	1.984766
H	5.598557	4.229240	2.843676
H	6.456503	0.504910	1.066048
H	5.787086	1.574352	-0.159534
H	6.751709	0.159868	-0.659007
C	6.993190	-2.308935	-0.236054
C	5.800257	-2.359594	-0.997279

C	8.046980	-3.157993	-0.501140
C	5.702818	-3.372659	-1.998935
C	7.969062	-4.106051	-1.536925
C	6.804703	-4.218336	-2.260407
H	7.073954	-1.629367	0.606964
H	6.703348	-4.974850	-3.038786
H	8.811915	-4.764588	-1.740576
H	8.945921	-3.099069	0.111271

4-4 (B3LYP)

V	1.717454	-0.493394	0.463896
O	2.338019	-1.116278	-1.137871
O	1.613846	1.122778	1.426084
H	1.973897	6.021243	4.968375
O	1.890959	-1.675610	1.498896
O	0.000329	-0.389317	-0.001596
N	3.702743	0.239159	0.555576
N	3.862261	1.423193	1.242644
C	3.450463	-1.811987	-1.402628
C	3.351861	-2.821625	-2.396068
H	2.388006	-2.972826	-2.884454
C	4.451756	-3.566840	-2.721891
H	4.383084	-4.335995	-3.491370
C	4.672865	-1.508611	-0.778287
C	4.773602	-0.268943	-0.019201
C	6.055849	0.521497	0.025060
C	2.709943	1.812676	1.730704
C	2.568296	2.976904	2.600476
C	3.656109	3.847199	2.925712
N	4.915969	3.709956	2.410289
C	3.392937	4.939436	3.788309
H	4.219440	5.605328	4.035820
C	2.131617	5.169346	4.307331
C	1.065043	4.310117	3.997982

H	0.073685	4.483499	4.411335
C	1.294699	3.237515	3.155206
H	0.480625	2.561919	2.905650
V	-1.717281	-0.493595	-0.465593
O	-2.336599	-1.116656	1.136674
C	-3.448607	-1.812928	1.402074
C	-3.349248	-2.821955	2.395962
H	-2.385357	-2.972260	2.884528
C	-4.448690	-3.567903	2.722159
H	-4.379438	-4.336567	3.492029
C	-4.671268	-1.510602	0.777782
C	-4.773186	-0.270980	0.018810
N	-3.702941	0.238091	-0.555932
O	-1.614875	1.123262	-1.426882
C	-2.711477	1.812841	-1.730566
N	-3.863343	1.422411	-1.242368
C	-2.570816	2.977850	-2.599442
C	-3.659328	3.847592	-2.923811
N	-4.918977	3.709013	-2.408103
C	-3.397223	4.940576	-3.785706
H	-4.224320	5.606007	-4.032565
C	-2.136214	5.171875	-4.304845
H	-1.979315	6.024342	-4.965330
C	-1.068882	4.313259	-3.996285
H	-0.077751	4.487746	-4.409730
C	-1.297510	3.239909	-3.154244
H	-0.482854	2.564759	-2.905338
O	-1.891257	-1.675475	-1.500562
C	-6.056124	0.518417	-0.025016
H	-5.190405	2.799202	-2.029137
H	-5.663879	4.239027	-2.874674
H	-6.511630	0.489924	-1.024547
H	-5.831040	1.569160	0.188401

H	-6.777295	0.150306	0.705485
C	-7.005866	-2.345011	0.281023
C	-5.802586	-2.380171	1.034769
C	-8.050432	-3.206832	0.556068
C	-5.686561	-3.394054	2.040164
C	-7.954131	-4.154451	1.595442
C	-6.780767	-4.253139	2.311415
H	-7.102818	-1.667361	-0.560895
H	-6.666070	-5.006978	3.090285
H	-8.788391	-4.821595	1.806651
H	-8.955000	-3.158318	-0.048937
H	5.188220	2.800456	2.030946
H	5.660330	4.240139	2.877464
H	6.511502	0.492715	1.024519
H	5.829890	1.572190	-0.187638
H	6.777227	0.154430	-0.705766
C	7.008268	-2.340997	-0.281531
C	5.804843	-2.377295	-1.035051
C	8.053434	-3.202075	-0.556363
C	5.689596	-3.391690	-2.040132
C	7.957777	-4.150213	-1.595377
C	6.784408	-4.249977	-2.311188
H	7.104840	-1.662957	0.560132
H	6.670187	-5.004204	-3.089781
H	8.792526	-4.816750	-1.806451
H	8.958069	-3.152607	0.048457

4-4 (M06)

V	1.715264	-0.525392	0.458223
O	2.346668	-1.167985	-1.130683
O	1.574213	1.088689	1.421696
H	1.890635	6.001858	4.916094
O	1.904485	-1.690103	1.495349
O	0.000476	-0.452563	-0.002859

N	3.663949	0.245617	0.541398
N	3.805246	1.435160	1.211428
C	3.469529	-1.832942	-1.377846
C	3.406188	-2.848435	-2.363709
H	2.446783	-3.022290	-2.859599
C	4.521897	-3.568512	-2.670285
H	4.481776	-4.348280	-3.435326
C	4.676817	-1.499232	-0.749328
C	4.747060	-0.253643	-0.010396
C	6.005503	0.551558	0.043481
C	2.650027	1.798185	1.703311
C	2.500715	2.963566	2.561495
C	3.581634	3.831191	2.887400
N	4.843461	3.700847	2.386438
C	3.311957	4.920591	3.743176
H	4.140061	5.588406	3.992965
C	2.052545	5.147948	4.255124
C	0.991719	4.289921	3.944307
H	-0.003522	4.461236	4.354629
C	1.229062	3.220485	3.107058
H	0.416926	2.539111	2.852355
V	-1.714642	-0.526056	-0.462783
O	-2.343561	-1.171264	1.126047
C	-3.465574	-1.837183	1.374267
C	-3.399901	-2.853692	2.358900
H	-2.439481	-3.027602	2.852806
C	-4.514713	-3.574572	2.666840
H	-4.472789	-4.355111	3.430998
C	-4.674121	-1.503399	0.748264
C	-4.746204	-0.257167	0.010590
N	-3.664265	0.243328	-0.542378
O	-1.576312	1.089539	-1.423657
C	-2.653018	1.798624	-1.703030

N	-3.807412	1.433659	-1.210683
C	-2.505438	2.965920	-2.558901
C	-3.587759	3.832247	-2.883557
N	-4.849544	3.698642	-2.383365
C	-3.319763	4.923693	-3.737241
H	-4.149024	5.590393	-3.986180
C	-2.060566	5.154374	-4.248225
H	-1.899960	6.009818	-4.907521
C	-0.998280	4.297771	-3.938462
H	-0.003134	4.471765	-4.347884
C	-1.233991	3.226324	-3.103326
H	-0.420666	2.546016	-2.849526
O	-1.904169	-1.689624	-1.501158
C	-6.005220	0.547299	-0.040400
H	-5.138671	2.787289	-2.015932
H	-5.582448	4.240267	-2.857597
H	-6.443526	0.544444	-1.050554
H	-5.766171	1.594420	0.188891
H	-6.749633	0.184517	0.673353
C	-7.012236	-2.276030	0.225827
C	-5.822119	-2.345134	0.988048
C	-8.073135	-3.115830	0.479887
C	-5.738621	-3.366264	1.977785
C	-8.007460	-4.074347	1.505639
C	-6.847641	-4.203030	2.229560
H	-7.085125	-1.587717	-0.614890
H	-6.750320	-4.968786	3.003368
H	-8.858659	-4.727803	1.701679
H	-8.971285	-3.043718	-0.136073
H	5.134230	2.790639	2.017462
H	5.575496	4.243199	2.861178
H	6.441908	0.548313	1.054451
H	5.766171	1.598681	-0.185533

H	6.751464	0.189772	-0.669158
C	7.014372	-2.271126	-0.223469
C	5.825637	-2.340188	-0.987849
C	8.076156	-3.110146	-0.476426
C	5.744381	-3.360474	-1.978629
C	8.012724	-4.067807	-1.503130
C	6.854240	-4.196510	-2.229162
H	7.085350	-1.583536	0.618014
H	6.758649	-4.961649	-3.003792
H	8.864593	-4.720673	-1.698230
H	8.973199	-3.038155	0.141157

4-4 (TPSSH)

V	1.721104	-0.486268	0.449592
O	2.344365	-1.104077	-1.150583
O	1.611881	1.116102	1.425429
H	1.969812	5.998649	4.987912
O	1.909874	-1.676481	1.480826
O	0.000571	-0.392643	-0.003098
N	3.694713	0.244601	0.548056
N	3.863771	1.427245	1.234287
C	3.456537	-1.803160	-1.413793
C	3.363520	-2.801313	-2.418831
H	2.403242	-2.946742	-2.916343
C	4.468610	-3.544432	-2.743903
H	4.406317	-4.306052	-3.521670
C	4.675887	-1.505414	-0.775232
C	4.774787	-0.271805	-0.013701
C	6.058101	0.514077	0.053706
C	2.707264	1.811271	1.730158
C	2.564526	2.966494	2.604386
C	3.654884	3.833573	2.936113
N	4.912347	3.694430	2.419504
C	3.391487	4.922603	3.804675

H	4.218506	5.585870	4.058119
C	2.127519	5.150286	4.322358
C	1.058263	4.293310	4.006353
H	0.066734	4.466129	4.419544
C	1.288138	3.224121	3.157281
H	0.475866	2.548312	2.899391
V	-1.720441	-0.486962	-0.454385
O	-2.340712	-1.107600	1.146154
C	-3.451731	-1.808184	1.410162
C	-3.355735	-2.807368	2.413947
H	-2.394633	-2.952427	2.909477
C	-4.459915	-3.551926	2.740173
H	-4.395333	-4.314135	3.516888
C	-4.672308	-1.510826	0.774177
C	-4.773774	-0.276315	0.014375
N	-3.695070	0.242021	-0.548577
O	-1.614603	1.117331	-1.427517
C	-2.711199	1.811780	-1.729306
N	-3.866557	1.425539	-1.232663
C	-2.570608	2.968758	-2.601479
C	-3.662550	3.835371	-2.930113
N	-4.918621	3.694926	-2.411385
C	-3.401197	4.926036	-3.797588
H	-4.229280	5.589217	-4.048549
C	-2.138501	5.155671	-4.317064
H	-1.982522	6.005130	-4.981659
C	-1.067876	4.298968	-4.004129
H	-0.077288	4.473182	-4.418825
C	-1.295729	3.228264	-3.156250
H	-0.482341	2.552620	-2.900968
O	-1.909533	-1.675944	-1.486984
C	-6.057947	0.508474	-0.049206
H	-5.185513	2.787309	-2.015972

H	-5.669548	4.224370	-2.873255
H	-6.496205	0.479058	-1.056466
H	-5.835356	1.559215	0.169800
H	-6.787186	0.134536	0.671715
C	-7.002103	-2.346876	0.269386
C	-5.804525	-2.377577	1.032652
C	-8.050343	-3.207642	0.545413
C	-5.693579	-3.384130	2.047715
C	-7.960812	-4.147195	1.594070
C	-6.789776	-4.241946	2.318815
H	-7.090050	-1.676352	-0.580536
H	-6.679569	-4.990432	3.103685
H	-8.796650	-4.812373	1.805063
H	-8.950663	-3.164456	-0.066286
H	5.180366	2.787597	2.023321
H	5.661769	4.223505	2.883898
H	6.494542	0.483116	1.061733
H	5.834912	1.565034	-0.163608
H	6.788996	0.142253	-0.666600
C	7.005679	-2.339810	-0.267557
C	5.809354	-2.370865	-1.032799
C	8.055278	-3.199136	-0.542901
C	5.701038	-3.376480	-2.049094
C	7.968338	-4.137737	-1.592624
C	6.798539	-4.232974	-2.319236
H	7.091647	-1.670178	0.583243
H	6.690294	-4.980775	-3.105030
H	8.805190	-4.801825	-1.802999
H	8.954625	-3.155585	0.070194

4-4a

C	-1.283473	3.241767	0.324337
C	-4.068091	1.381497	-0.260907
C	-4.544889	0.037970	0.023038

C	-5.947416	-0.304724	0.069189
C	-6.326879	-1.682313	0.069318
C	-5.322542	-2.685119	0.085847
H	-5.628279	-3.731614	0.075333
C	-3.999147	-2.356406	0.153515
H	-3.218806	-3.118530	0.202546
C	-3.604225	-0.995388	0.153186
C	-0.645553	4.548076	0.249849
C	-1.283808	5.693794	-0.313135
N	-2.513379	5.658774	-0.889458
C	-0.572938	6.915914	-0.300765
H	-1.060087	7.794961	-0.722654
C	0.699350	7.007913	0.224485
H	1.211252	7.969950	0.214239
C	1.333116	5.881041	0.766734
H	2.335962	5.953393	1.182095
C	0.655824	4.677169	0.775085
H	1.124299	3.791298	1.197319
C	0.991071	-0.549517	2.460496
H	1.315609	-1.587137	2.290130
C	0.361483	-0.408038	3.825773
H	1.880201	0.091981	2.371445
C	-4.857054	2.327290	-1.115822
H	-4.185661	2.770345	-1.859887
H	-5.264504	3.161355	-0.528141
H	-5.676424	1.818918	-1.626404
O	-0.610940	2.251703	0.879008
O	-2.296791	-0.751428	0.210194
O	0.139076	-0.218025	1.370374
V	-1.422569	0.559361	1.131947
N	-2.490271	3.029192	-0.142651
N	-2.876166	1.749174	0.147858
O	-2.127192	0.613164	2.531378

C	1.235978	-3.212985	-0.353308
C	4.052219	-1.423294	0.294247
C	4.567016	-0.090152	0.028438
C	5.978496	0.216391	-0.001708
C	6.991618	-0.766044	-0.125757
C	6.393040	1.583670	0.009989
C	5.415343	2.612683	-0.010086
H	5.748131	3.650751	0.010383
C	4.084749	2.318647	-0.093856
H	3.324315	3.100539	-0.147235
C	3.655385	0.968239	-0.107950
C	0.572818	-4.508958	-0.323005
C	1.171019	-5.678933	0.232958
N	2.376556	-5.678793	0.860739
C	0.442488	-6.888240	0.159437
H	0.899890	-7.786301	0.574622
C	-0.809087	-6.946855	-0.418393
H	-1.333643	-7.901330	-0.456509
C	-1.405739	-5.795141	-0.950149
H	-2.392897	-5.839230	-1.405130
C	-0.710962	-4.602649	-0.895982
H	-1.149416	-3.698176	-1.310647
C	-0.937150	0.616267	-2.469462
H	-1.390375	1.587115	-2.221607
C	-0.230489	0.689603	-3.802885
H	-1.746393	-0.129211	-2.496705
C	4.806479	-2.396431	1.149487
H	4.115471	-2.828149	1.882165
H	5.199147	-3.235708	0.559142
H	5.632807	-1.913997	1.673958
O	0.592022	-2.200077	-0.900051
O	2.343412	0.759275	-0.184331
O	-0.103003	0.280739	-1.365711

C	7.768795	1.907817	-0.001688
V	1.444596	-0.522632	-1.121613
N	2.439026	-3.033199	0.136485
N	2.856980	-1.757961	-0.132437
O	2.161086	-0.575287	-2.515015
H	-3.116388	4.852477	-0.712979
H	-2.973663	6.556825	-1.070291
C	-6.984233	0.652357	0.195215
C	-7.693538	-2.041915	0.093376
H	-7.949773	-3.101487	0.079648
C	-8.676765	-1.082409	0.150285
C	-8.309926	0.273282	0.224872
H	-6.744789	1.704717	0.311152
H	-9.727492	-1.367312	0.169087
H	-9.080147	1.037017	0.325450
H	3.002428	-4.883678	0.716258
H	2.816166	-6.589640	1.029500
H	8.051841	2.960420	0.020636
C	8.727910	0.924156	-0.058004
C	8.326852	-0.421197	-0.143899
H	6.726013	-1.811084	-0.250083
H	9.785623	1.182337	-0.067714
H	9.077743	-1.204003	-0.244020
H	-0.956044	1.010382	-4.561723
H	0.173908	-0.280815	-4.108255
H	0.587846	1.418514	-3.784700
H	1.099325	-0.709531	4.580635
H	-0.518785	-1.051155	3.934293
H	0.065493	0.626228	4.032058

4-4a (in EtOH solution)

C	-1.290603	-3.229519	-0.330809
C	-4.078108	-1.380602	0.275821

C	-4.563666	-0.039205	-0.002438
C	-5.968301	0.297584	-0.036891
C	-6.354343	1.673208	-0.026086
C	-5.354437	2.680921	-0.044934
H	-5.664507	3.725813	-0.024889
C	-4.030451	2.358352	-0.128789
H	-3.253538	3.123354	-0.182941
C	-3.628904	0.998814	-0.141258
C	-0.652992	-4.537727	-0.273945
C	-1.284537	-5.688288	0.286594
N	-2.503646	-5.655758	0.887228
C	-0.578477	-6.912379	0.245956
H	-1.060669	-7.795122	0.665437
C	0.683847	-7.002488	-0.304169
H	1.191749	-7.966437	-0.316290
C	1.311677	-5.870823	-0.842925
H	2.306279	-5.940809	-1.277704
C	0.638664	-4.664442	-0.822433
H	1.101707	-3.774490	-1.241900
C	0.966525	0.578326	-2.464125
H	1.307599	1.606478	-2.271324
C	0.330675	0.478286	-3.830757
H	1.845591	-0.079209	-2.392768
C	-4.858407	-2.333042	1.132296
H	-4.181672	-2.772938	1.873229
H	-5.262445	-3.168288	0.544172
H	-5.679225	-1.830738	1.646366
O	-0.624612	-2.236287	-0.886569
O	-2.321963	0.762458	-0.217322
O	0.112857	0.236268	-1.379053
V	-1.443683	-0.546996	-1.139244
N	-2.493447	-3.020512	0.148094
N	-2.885875	-1.741471	-0.138643

O	-2.152303	-0.610293	-2.536359
C	1.290851	3.229554	0.331231
C	4.078292	1.380598	-0.275593
C	4.563684	0.039037	0.002169
C	5.968280	-0.297995	0.036392
C	7.001513	0.662910	0.163732
C	6.354121	-1.673674	0.025016
C	5.354070	-2.681253	0.043505
H	5.663985	-3.726181	0.022993
C	4.030144	-2.358516	0.127547
H	3.253111	-3.123414	0.181451
C	3.628791	-0.998923	0.140664
C	0.653279	4.537809	0.274623
C	1.284764	5.688437	-0.285803
N	2.503858	5.655973	-0.886566
C	0.578676	6.912495	-0.245028
H	1.060814	7.795290	-0.664460
C	-0.683612	7.002528	0.305213
H	-1.191533	7.966466	0.317464
C	-1.311366	5.870801	0.843924
H	-2.305924	5.940727	1.278813
C	-0.638326	4.664440	0.823236
H	-1.101306	3.774432	1.242654
C	-0.967082	-0.577314	2.464018
H	-1.308003	-1.605679	2.272095
C	-0.331867	-0.475900	3.830855
H	-1.846136	0.080101	2.391501
C	4.858780	2.333293	-1.131615
H	4.182147	2.773662	-1.872355
H	5.262976	3.168183	-0.543095
H	5.679510	1.831071	-1.645907
O	0.624742	2.236254	0.886722
O	2.321908	-0.762489	0.217082

O	-0.112825	-0.236303	1.379118
C	7.722739	-2.026831	0.039105
V	1.443711	0.546881	1.139136
N	2.493728	3.020602	-0.147580
N	2.886014	1.741422	0.138806
O	2.152323	0.610032	2.536271
H	-3.105134	-4.845906	0.724810
H	-2.966379	-6.553705	1.057346
C	-7.001364	-0.663548	-0.163912
C	-7.723022	2.026137	-0.040392
H	-7.984349	3.084158	-0.017992
C	-8.702226	1.062377	-0.100938
C	-8.329229	-0.291111	-0.186851
H	-6.756508	-1.713679	-0.287906
H	-9.754146	1.342565	-0.113736
H	-9.095870	-1.057823	-0.290344
H	3.105479	4.846293	-0.723758
H	2.966644	6.554001	-1.056165
H	7.983891	-3.084886	0.016258
C	8.702106	-1.063251	0.099946
C	8.329323	0.290253	0.186447
H	6.756853	1.713031	0.288188
H	9.753982	-1.343613	0.112560
H	9.096084	1.056808	0.290207
H	-1.069768	-0.788306	4.580990
H	-0.023769	0.549569	4.061269
H	0.542248	-1.130547	3.918981
H	1.068261	0.791459	-4.580884
H	-0.543479	1.133023	-3.917851
H	0.022493	-0.546943	-4.062100

1-1⁻ (in MeCN solution)

V	-1.635049	0.797138	-0.717019
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O	-2.289288	-1.008234	-0.744070
O	-1.309873	2.286644	0.492961
H	-1.400133	7.546260	3.453426
O	-1.595136	1.329007	-2.219793
O	0.104694	0.129117	-0.248193
N	-3.481411	1.259507	-0.000732
N	-3.582525	2.445544	0.694164
C	-3.497703	-1.448454	-1.013800
C	-3.609890	-2.784056	-1.496688
H	-2.687533	-3.353207	-1.627880
C	-4.828059	-3.327134	-1.784204
H	-4.895502	-4.350345	-2.156117
C	-4.670615	-0.685330	-0.804968
C	-4.589137	0.596623	-0.188113
H	-5.497813	1.067968	0.194877
C	-2.376985	2.934258	0.900992
C	-2.183064	4.207665	1.600025
C	-3.246269	4.971800	2.163771
N	-4.561753	4.630480	2.051081
C	-2.914513	6.171692	2.832177
H	-3.726255	6.753830	3.268988
C	-1.609580	6.613034	2.930744
C	-0.564471	5.869568	2.369839
H	0.465674	6.211923	2.443996
C	-0.865291	4.685826	1.721980
H	-0.069413	4.087147	1.285779
V	1.611916	-0.560431	-0.576947
O	2.542615	1.053220	-0.690978
C	3.786052	1.387764	-0.979637
C	4.001098	2.672323	-1.544308
H	3.130577	3.302691	-1.735103
C	5.268308	3.092623	-1.834986
H	5.428135	4.079051	-2.271945

C	4.874895	0.545875	-0.692851
C	4.645344	-0.690348	-0.023587
N	3.468891	-1.215015	0.179233
O	1.234919	-2.079534	0.521513
C	2.217062	-2.797846	1.023128
N	3.455876	-2.384782	0.897467
C	1.871826	-4.030616	1.724738
C	2.834145	-4.863516	2.367899
N	4.160024	-4.565214	2.436183
C	2.369172	-6.034685	3.008027
H	3.103276	-6.675448	3.496717
C	1.029811	-6.368971	3.024373
H	0.714726	-7.282450	3.528614
C	0.081890	-5.547228	2.400983
H	-0.974456	-5.807458	2.413722
C	0.513273	-4.398733	1.765771
H	-0.204148	-3.747374	1.272139
O	1.653219	-1.130513	-2.056305
H	5.493689	-1.251789	0.374723
H	4.537236	-3.862889	1.794986
H	4.794429	-5.322622	2.713006
C	7.361257	0.177541	-0.804629
C	6.214803	0.978433	-1.012977
C	8.619681	0.639020	-1.129688
C	6.401449	2.269989	-1.588290
C	8.799747	1.919061	-1.685672
C	7.702433	2.717525	-1.911793
H	7.264092	-0.824232	-0.390694
H	7.816100	3.710115	-2.348488
H	9.799425	2.269442	-1.937944
H	9.484250	-0.001015	-0.956967
H	-4.785808	3.666652	1.791351
H	-5.212723	5.089746	2.697809

C	-7.174719	-0.528914	-1.021719
C	-5.961537	-1.248002	-1.134338
C	-8.382184	-1.107582	-1.354753
C	-6.030803	-2.585028	-1.622806
C	-8.443783	-2.432891	-1.822228
C	-7.279747	-3.155306	-1.955058
H	-7.171104	0.505755	-0.684604
H	-7.299917	-4.180942	-2.324730
H	-9.403211	-2.877161	-2.082778
H	-9.297848	-0.525080	-1.258657

4-4⁻ (partially optimized in MeCN solution with frozen V–O_{bridge} bonds and the V–O–V angle)

C	2.745418	5.006058	2.148034
C	1.796812	4.194473	1.457972
C	0.456458	4.620044	1.393071
H	-0.251247	3.984269	0.866180
C	0.029758	5.801394	1.969911
H	-1.013440	6.103175	1.902347
C	0.965032	6.602078	2.637445
H	0.654492	7.540977	3.095669
C	2.287223	6.213122	2.722401
H	3.012147	6.837499	3.245008
C	2.138645	2.927952	0.810462
C	4.594274	0.675722	0.099652
C	5.717074	1.245113	0.915593
C	4.732562	-0.594985	-0.589775
C	3.610821	-1.441901	-0.684377
C	3.773776	-2.806159	-1.057335
H	2.884576	-3.439754	-1.053377
C	4.998447	-3.294301	-1.405537
H	5.114175	-4.342483	-1.683452
C	6.137632	-2.446431	-1.455602
C	7.379426	-2.941003	-1.913176

H	7.449506	-3.996350	-2.178292
C	8.467282	-2.109267	-2.048686
H	9.419195	-2.496578	-2.408738
C	8.325749	-0.742007	-1.751223
H	9.165405	-0.064995	-1.905075
C	7.129572	-0.238361	-1.282904
H	7.047463	0.831222	-1.112997
C	6.005285	-1.076183	-1.077257
N	4.051219	4.655610	2.319391
N	3.368012	2.465634	0.824077
N	3.432249	1.287695	0.117498
O	1.174407	2.251109	0.229211
O	2.383082	-1.058647	-0.381871
O	1.881024	0.949441	-2.273913
O	-0.016868	0.041427	-0.551844
V	1.640596	0.643143	-0.731787
C	-2.631531	-5.001389	2.143056
C	-1.699100	-4.130873	1.505828
C	-0.332080	-4.466892	1.521159
H	0.362159	-3.787382	1.032200
C	0.136294	-5.614261	2.133050
H	1.199343	-5.846270	2.130937
C	-0.781717	-6.469494	2.755329
H	-0.436778	-7.381344	3.242694
C	-2.129903	-6.170607	2.757552
H	-2.841489	-6.839038	3.242588
C	-2.084603	-2.886600	0.840989
C	-4.608175	-0.709756	0.136089
C	-5.709065	-1.307296	0.962490
C	-4.785293	0.555225	-0.555398
C	-3.688137	1.432304	-0.659477
C	-3.889822	2.790217	-1.035814
H	-3.017696	3.447034	-1.040895

C	-5.129545	3.244789	-1.375899
H	-5.274969	4.288625	-1.656166
C	-6.246506	2.367325	-1.413380
C	-7.505556	2.827410	-1.860063
H	-7.606201	3.879730	-2.127316
C	-8.572667	1.966983	-1.981099
H	-9.538269	2.327999	-2.331886
C	-8.391518	0.604716	-1.682306
H	-9.214375	-0.094847	-1.825668
C	-7.177678	0.134517	-1.224981
H	-7.065796	-0.932087	-1.053778
C	-6.074328	1.002208	-1.032320
N	-3.966842	-4.740915	2.225171
N	-3.327168	-2.461351	0.858962
N	-3.429706	-1.289877	0.146425
O	-1.145305	-2.185843	0.247664
O	-2.448071	1.083367	-0.364447
O	-1.906751	-0.915313	-2.254248
V	-1.662184	-0.595216	-0.715984
H	-6.535403	-0.607775	1.097164
H	-5.301669	-1.582151	1.942027
H	-6.094306	-2.234040	0.515854
H	6.528016	0.526173	1.040959
H	5.326271	1.526738	1.900071
H	6.119400	2.163828	0.467450
H	-4.355091	-4.038592	1.589868
H	-4.576203	-5.531193	2.464315
H	4.433917	3.928566	1.709215
H	4.694979	5.401521	2.605889

4-4⁻ (in MeCN solution)

V	1.678410	-0.785429	-1.036926
O	2.439979	0.963323	-0.922517

O	0.937468	-2.119222	0.162252
H	-0.253593	-6.748157	3.848017
O	1.974782	-1.397206	-2.481129
O	-0.057770	0.031785	-1.129114
N	3.279821	-1.331074	0.118303
N	3.048921	-2.352689	1.013810
C	3.718763	1.210039	-1.135246
C	4.032135	2.458770	-1.746513
H	3.200069	3.127626	-1.974722
C	5.320325	2.800708	-2.033071
H	5.544921	3.762439	-2.495736
C	4.760732	0.342211	-0.741576
C	4.463179	-0.763586	0.152721
C	5.430615	-1.185267	1.218012
C	1.790460	-2.732384	0.948340
C	1.298776	-3.845648	1.762878
C	2.102809	-4.546825	2.710007
N	3.426711	-4.291521	2.907113
C	1.496219	-5.588025	3.448087
H	2.107335	-6.121561	4.176360
C	0.173471	-5.936734	3.258764
C	-0.615047	-5.256673	2.322576
H	-1.657211	-5.529566	2.169694
C	-0.046111	-4.226156	1.597670
H	-0.640409	-3.678755	0.869943
V	-1.607208	0.678009	-0.949470
O	-2.487764	-0.950916	-0.807260
C	-3.763402	-1.188955	-1.083724
C	-4.053482	-2.412301	-1.743659
H	-3.219179	-3.077652	-1.973627
C	-5.338641	-2.731235	-2.073811
H	-5.559306	-3.673093	-2.577151
C	-4.795922	-0.322314	-0.689194

C	-4.480930	0.755394	0.232577
N	-3.279598	1.282307	0.224223
O	-0.976392	2.072495	0.188939
C	-1.798395	2.690187	1.010964
N	-3.041931	2.287359	1.125939
C	-1.273357	3.810292	1.784753
C	-2.068714	4.581701	2.683138
N	-3.375866	4.309955	2.951998
C	-1.445941	5.656296	3.357500
H	-2.052237	6.251203	4.040798
C	-0.111412	5.954879	3.168678
H	0.328902	6.792477	3.709531
C	0.672493	5.194203	2.291781
H	1.724621	5.427354	2.141894
C	0.084775	4.142075	1.616143
H	0.673068	3.540821	0.926811
O	-2.066155	1.304051	-2.336244
C	-5.459458	1.195665	1.279555
H	-3.884603	3.706192	2.300320
H	-3.918076	5.051992	3.408762
H	-5.838493	2.207522	1.081156
H	-4.942280	1.241863	2.244898
H	-6.303246	0.508036	1.355121
C	-7.211563	0.315588	-1.011115
C	-6.140211	-0.603892	-1.132826
C	-8.478070	0.004400	-1.460525
C	-6.406581	-1.832128	-1.811318
C	-8.747591	-1.239639	-2.060047
C	-7.717361	-2.132544	-2.245507
H	-7.035536	1.305128	-0.600375
H	-7.890360	-3.085523	-2.746368
H	-9.753984	-1.476895	-2.401612
H	-9.275695	0.739467	-1.358346

H	3.802406	-3.411551	2.543481
H	3.846869	-4.655966	3.769023
H	5.811051	-2.200744	1.044290
H	4.899748	-1.214027	2.177276
H	6.272111	-0.495781	1.295815
C	7.185302	-0.270417	-1.040206
C	6.111754	0.648496	-1.151272
C	8.462069	0.062961	-1.443148
C	6.390074	1.900646	-1.777490
C	8.740719	1.330100	-1.987147
C	7.709103	2.223608	-2.166070
H	7.002898	-1.276479	-0.673650
H	7.888995	3.195649	-2.626403
H	9.754253	1.585463	-2.292541
H	9.260217	-0.672653	-1.348743

I⁻ (in MeCN solution)

C	1.142824	1.152311	6.014826
C	0.888469	2.384710	5.344910
C	0.617218	3.530863	6.112224
H	0.421639	4.458680	5.580323
C	0.600242	3.507266	7.495584
H	0.389317	4.412876	8.060608
C	0.862513	2.298724	8.150907
H	0.860023	2.253537	9.239825
C	1.129140	1.152007	7.427017
H	1.328185	0.211265	7.940642
C	0.892422	2.530606	3.884195
C	1.422237	0.978798	0.910876
H	1.689534	-0.001575	1.312878
C	1.334124	1.151213	-0.501983
C	0.700115	2.297995	-1.039264
C	0.485330	2.376976	-2.448307

H	-0.025638	3.262536	-2.830268
C	0.903797	1.382927	-3.282923
H	0.732415	1.462757	-4.357114
C	1.578127	0.231228	-2.789172
C	2.027250	-0.775620	-3.672143
H	1.835970	-0.652860	-4.738550
C	2.699233	-1.881004	-3.201746
H	3.046309	-2.651263	-3.888619
C	2.939728	-2.003752	-1.821396
H	3.480151	-2.870115	-1.441715
C	2.508443	-1.035405	-0.937784
H	2.735156	-1.160512	0.118911
C	1.805356	0.108491	-1.386556
C	-0.908919	6.069527	2.343818
H	-0.089485	6.798014	2.486109
H	-1.056598	5.565823	3.313430
C	-2.177050	6.813450	1.963089
H	-2.045117	7.348822	1.014579
H	-2.445868	7.545514	2.735767
H	-3.015128	6.114867	1.846221
N	1.341365	-0.026888	5.356723
N	1.214454	1.515102	3.110500
N	1.165375	1.906643	1.790613
O	0.547410	3.689029	3.377801
O	0.252962	3.288015	-0.308460
O	2.242890	4.638012	1.236086
O	-0.567752	5.138940	1.345181
V	0.826430	3.903175	1.447229
H	1.597073	0.031025	4.367300
H	1.762929	-0.788527	5.897429

1' (in MeCN solution)

C	5.605681	0.218358	-0.396781
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C	4.541994	1.164573	-0.304088
C	4.852474	2.512589	-0.042242
H	4.027268	3.216902	0.027015
C	6.151690	2.952331	0.123659
H	6.357940	4.001044	0.326965
C	7.194816	2.023417	0.021996
H	8.228966	2.345237	0.143094
C	6.927078	0.693612	-0.235226
H	7.741479	-0.026851	-0.312233
C	3.132484	0.817209	-0.477661
C	0.816223	-1.647774	-0.797261
H	1.493353	-2.504078	-0.744997
C	-0.593368	-1.863597	-0.787137
C	-1.473245	-0.801056	-0.476103
C	-2.859775	-1.064228	-0.296727
H	-3.505962	-0.224478	-0.035368
C	-3.358661	-2.325098	-0.452430
H	-4.424852	-2.510514	-0.317306
C	-2.518718	-3.419975	-0.796187
C	-3.056497	-4.714754	-0.968999
H	-4.128785	-4.854106	-0.829557
C	-2.248404	-5.774722	-1.311575
H	-2.669217	-6.770042	-1.444869
C	-0.869890	-5.560527	-1.492271
H	-0.225981	-6.393492	-1.771946
C	-0.320362	-4.304773	-1.333204
H	0.746185	-4.178585	-1.507929
C	-1.121239	-3.197252	-0.969268
C	0.236379	4.295418	-0.213072
H	-0.089019	4.641854	-1.203440
H	1.328263	4.219613	-0.204797
C	-0.270682	5.191169	0.890042
H	-1.366999	5.236299	0.889798

H	0.108661	6.208851	0.735956
H	0.068557	4.839566	1.871092
N	5.412634	-1.115813	-0.591436
N	2.750135	-0.429703	-0.656791
N	1.380704	-0.471643	-0.803094
O	2.243192	1.790427	-0.430726
O	-1.068701	0.439655	-0.292663
O	0.266234	1.558380	-2.563874
O	-0.237399	2.937847	-0.023742
V	0.464828	1.309031	-1.004590
H	4.499510	-1.429403	-0.927071
H	6.225369	-1.664531	-0.889795
H	-1.248130	2.931162	0.007738

2-2⁻(in MeCN solution)

V	-1.590592	0.861343	-0.651468
O	-1.987116	-1.012041	-0.748444
O	-1.597824	2.377631	0.594626
H	-3.048339	7.465911	3.578865
O	-1.455789	1.414526	-2.139205
O	0.165412	0.419754	0.011332
N	-3.550191	1.056764	-0.154901
N	-3.875930	2.206678	0.526488
C	-3.087405	-1.619385	-1.130156
C	-2.959916	-2.959435	-1.596405
H	-1.957235	-3.390140	-1.628866
C	-4.054773	-3.674182	-1.985518
H	-3.939077	-4.698535	-2.342117
C	-4.371540	-1.029437	-1.052157
C	-4.532585	0.250667	-0.451065
H	-5.532448	0.591842	-0.170604
C	-2.783003	2.847461	0.877396
C	-2.898114	4.109189	1.614207

C	-4.146392	4.655346	2.002855
O	-5.333902	4.086375	1.734536
C	-4.175281	5.863068	2.712037
H	-5.147902	6.264624	3.001861
C	-3.000065	6.526374	3.028983
C	-1.762812	5.996187	2.652540
H	-0.839181	6.514628	2.902726
C	-1.724503	4.800270	1.955512
H	-0.772201	4.369359	1.654139
V	1.648387	-0.296486	-0.365540
O	2.604394	1.281590	-0.580683
C	3.834996	1.572999	-0.963156
C	4.036458	2.816494	-1.615130
H	3.166239	3.450746	-1.794031
C	5.291426	3.194894	-2.001099
H	5.441047	4.149741	-2.506469
C	4.924469	0.727383	-0.688719
C	4.710328	-0.471913	0.049290
N	3.535193	-0.962725	0.327955
O	1.290128	-1.763452	0.830515
C	2.284382	-2.475240	1.294454
N	3.523568	-2.100385	1.091830
C	1.986949	-3.685940	2.056429
C	3.002670	-4.485659	2.633499
O	4.314723	-4.217479	2.545036
C	2.644739	-5.635617	3.348534
H	3.443650	-6.237510	3.785247
C	1.313605	-5.992158	3.494223
H	1.059999	-6.891458	4.054906
C	0.302072	-5.209205	2.929550
H	-0.743373	-5.488689	3.044430
C	0.645666	-4.069792	2.222575
H	-0.126077	-3.446217	1.776188

O	1.602799	-0.938908	-1.812504
H	5.567521	-1.031820	0.431062
H	4.461101	-3.368462	2.031007
C	7.398152	0.315176	-0.900198
C	6.252027	1.118426	-1.101529
C	8.642709	0.733971	-1.322423
C	6.423552	2.367917	-1.767729
C	8.807083	1.970819	-1.973453
C	7.710165	2.772608	-2.188395
H	7.311884	-0.654745	-0.414250
H	7.812774	3.733367	-2.693622
H	9.795518	2.287244	-2.303096
H	9.507587	0.093369	-1.153674
H	-5.186657	3.226647	1.237526
C	-6.843547	-1.246681	-1.488107
C	-5.532672	-1.777872	-1.483599
C	-7.919488	-1.999572	-1.912135
C	-5.362083	-3.114005	-1.949152
C	-7.744490	-3.321169	-2.360773
C	-6.479463	-3.863772	-2.378439
H	-7.022105	-0.221210	-1.170366
H	-6.315923	-4.883249	-2.728956
H	-8.601401	-3.904175	-2.694695
H	-8.915679	-1.558561	-1.903764

2⁻(in MeCN solution)

C	4.017477	-0.126877	0.039466
C	3.285287	1.032692	-0.327119
C	3.977914	2.228622	-0.565827
H	3.402262	3.109264	-0.843620
C	5.357406	2.297589	-0.454605
H	5.877206	3.234443	-0.645489
C	6.071316	1.150217	-0.095113

H	7.156532	1.189892	-0.004430
C	5.412646	-0.045442	0.148867
H	5.960748	-0.946072	0.430147
C	1.824599	1.002255	-0.447599
C	-0.871346	-1.057237	-0.183737
H	-0.325942	-1.974172	0.053298
C	-2.296118	-1.078322	-0.199065
C	-3.024021	0.137202	-0.196798
C	-4.443499	0.095805	-0.051747
H	-4.975086	1.048732	-0.030075
C	-5.107078	-1.090722	0.055178
H	-6.192384	-1.101736	0.163211
C	-4.418708	-2.335772	0.019316
C	-5.127542	-3.554346	0.105940
H	-6.212242	-3.517005	0.210146
C	-4.468099	-4.761372	0.050746
H	-5.020915	-5.697268	0.114316
C	-3.069298	-4.774983	-0.094804
H	-2.540702	-5.725943	-0.150095
C	-2.353649	-3.597939	-0.179472
H	-1.275508	-3.655758	-0.314030
C	-2.999070	-2.339794	-0.114704
C	-0.300735	4.691659	-0.547700
H	-0.313511	5.045824	-1.594839
H	0.746133	4.443600	-0.308627
C	-0.777285	5.808646	0.364752
H	-1.810536	6.091495	0.127986
H	-0.144109	6.698560	0.253842
H	-0.742799	5.491801	1.414729
O	3.436253	-1.307174	0.286595
N	1.213820	-0.146206	-0.242050
N	-0.143918	0.004564	-0.395044
O	1.168850	2.094916	-0.717380

O	-2.464578	1.317823	-0.276141
O	-0.959010	1.798746	-2.651049
O	-1.126463	3.560425	-0.409327
V	-0.763540	1.852794	-1.056488
H	2.410401	-1.179146	0.135187

2'(in MeCN solution)

C	4.162393	0.609288	-0.147555
C	3.155028	1.600608	-0.043196
C	3.538415	2.926660	0.217546
H	2.757076	3.679005	0.299110
C	4.868145	3.280744	0.367937
H	5.140715	4.314843	0.569194
C	5.853151	2.294527	0.258659
H	6.904367	2.556525	0.374805
C	5.505113	0.977139	0.006320
H	6.263489	0.197297	-0.079620
C	1.732228	1.294339	-0.199471
C	-0.573102	-1.186750	-0.512441
H	0.108809	-2.039728	-0.465784
C	-1.980285	-1.408399	-0.502035
C	-2.864260	-0.348170	-0.192324
C	-4.250175	-0.616189	-0.016014
H	-4.900331	0.221107	0.243267
C	-4.743145	-1.879344	-0.171786
H	-5.808957	-2.068688	-0.038883
C	-3.898863	-2.971994	-0.512671
C	-4.432162	-4.268660	-0.684377
H	-5.504133	-4.411522	-0.546228
C	-3.619790	-5.326128	-1.024805
H	-4.036863	-6.323111	-1.157403
C	-2.241928	-5.107430	-1.203957
H	-1.594699	-5.938482	-1.481642

C	-1.696755	-3.849559	-1.045672
H	-0.630304	-3.720243	-1.219028
C	-2.502161	-2.744870	-0.684036
C	-1.176203	4.757819	0.088072
H	-1.511282	5.101427	-0.899991
H	-0.083710	4.690338	0.089114
C	-1.683315	5.648220	1.195089
H	-2.779948	5.684312	1.201937
H	-1.313478	6.669099	1.038996
H	-1.334646	5.298941	2.173633
O	3.919683	-0.688713	-0.392196
N	1.350715	0.049104	-0.376325
N	-0.016469	-0.006879	-0.516559
O	0.858466	2.270521	-0.145932
O	-2.464425	0.893360	-0.006668
O	-1.137819	2.032699	-2.263418
O	-1.638670	3.396030	0.280205
V	-0.935387	1.776674	-0.708186
H	2.932038	-0.836893	-0.470688
H	-2.649504	3.381974	0.322393

3-3⁻ (in MeCN solution)

V	1.695214	-0.750520	-1.016752
O	2.453892	0.998588	-0.943523
O	0.953559	-2.069610	0.215506
H	0.084762	-6.693912	4.057777
O	1.984414	-1.390124	-2.447662
O	-0.045560	0.056169	-1.113395
N	3.309878	-1.268912	0.138899
N	3.073259	-2.270478	1.054222
C	3.730875	1.246649	-1.164343
C	4.036079	2.485517	-1.799160
H	3.200170	3.146330	-2.036419

C	5.321503	2.826666	-2.098119
H	5.539952	3.780299	-2.580117
C	4.778765	0.391123	-0.758159
C	4.491180	-0.697161	0.159349
C	5.465605	-1.093202	1.227824
C	1.815911	-2.653724	0.999639
C	1.372060	-3.761178	1.849063
C	2.256728	-4.441288	2.720791
O	3.557341	-4.136338	2.843905
C	1.772085	-5.493261	3.508815
H	2.471316	-6.002377	4.174424
C	0.440683	-5.872286	3.436677
C	-0.441661	-5.210647	2.576995
H	-1.486650	-5.509288	2.520567
C	0.028981	-4.166997	1.797808
H	-0.641119	-3.638538	1.122711
V	-1.609247	0.665767	-0.953041
O	-2.461719	-0.976029	-0.828442
C	-3.729337	-1.238410	-1.120928
C	-3.986833	-2.465755	-1.786513
H	-3.136588	-3.113141	-2.009200
C	-5.261844	-2.810775	-2.129311
H	-5.457784	-3.756193	-2.636221
C	-4.784063	-0.394297	-0.735114
C	-4.502862	0.683020	0.197145
N	-3.311744	1.231721	0.203964
O	-1.009912	2.079744	0.200761
C	-1.857504	2.662612	1.008451
N	-3.092958	2.236545	1.108934
C	-1.408490	3.796472	1.810613
C	-2.280908	4.474106	2.697096
O	-3.565802	4.136420	2.882702
C	-1.797315	5.561902	3.435242

H	-2.485565	6.071094	4.112144
C	-0.480298	5.973085	3.304003
H	-0.125391	6.821691	3.888272
C	0.389813	5.310676	2.431851
H	1.423523	5.635303	2.330251
C	-0.078456	4.234153	1.698478
H	0.581720	3.705366	1.013719
O	-2.060535	1.287276	-2.342035
C	-5.501841	1.096726	1.235405
H	-3.793067	3.346694	2.303554
H	-5.892490	2.105306	1.043184
H	-4.999320	1.136755	2.209054
H	-6.336071	0.396027	1.291886
C	-7.208025	0.195633	-1.083685
C	-6.117662	-0.702297	-1.193719
C	-8.462769	-0.140570	-1.548204
C	-6.350880	-1.934494	-1.876807
C	-8.699650	-1.388641	-2.152930
C	-7.649875	-2.260836	-2.326940
H	-7.056626	1.188094	-0.669690
H	-7.797698	-3.216239	-2.831194
H	-9.696929	-1.645496	-2.506841
H	-9.276279	0.578002	-1.454525
H	3.774547	-3.371343	2.227025
H	5.862623	-2.103961	1.062767
H	4.937084	-1.120616	2.188490
H	6.296753	-0.390336	1.296581
C	7.204560	-0.216902	-1.055456
C	6.127134	0.695349	-1.178836
C	8.477430	0.113458	-1.473494
C	6.396280	1.935636	-1.831640
C	8.747614	1.370311	-2.044323
C	7.711404	2.256162	-2.234873

H	7.029079	-1.216143	-0.667667
H	7.884473	3.219427	-2.715765
H	9.758194	1.623281	-2.361260
H	9.279165	-0.616876	-1.369088

3⁻ (in MeCN solution)

C	4.074307	0.961267	-0.722936
C	3.029891	1.895841	-0.748736
C	3.328961	3.250602	-0.929077
H	2.519538	3.976862	-0.947261
C	4.648853	3.664501	-1.079431
H	4.870704	4.721969	-1.217643
C	5.682424	2.731112	-1.052288
H	6.715610	3.056209	-1.169089
C	5.390718	1.378103	-0.875362
H	6.195315	0.644201	-0.853915
C	1.625565	1.473096	-0.575153
C	-0.393741	-1.194149	0.038719
C	0.649450	-2.233946	0.333585
C	-1.806494	-1.468369	0.232915
C	-2.656869	-0.433944	0.689896
C	-3.942129	-0.766011	1.217371
H	-4.537131	0.051180	1.628970
C	-4.405643	-2.046997	1.206159
H	-5.386962	-2.281751	1.619940
C	-3.645612	-3.093724	0.616305
C	-4.181873	-4.395435	0.504262
H	-5.167327	-4.587017	0.929843
C	-3.493133	-5.393033	-0.148241
H	-3.916465	-6.392287	-0.236779
C	-2.251507	-5.094247	-0.737431
H	-1.723506	-5.859617	-1.305168
C	-1.697354	-3.835650	-0.622551

H	-0.762503	-3.630703	-1.136517
C	-2.349514	-2.801378	0.094459
C	-1.214079	4.587392	-0.040705
H	-1.420352	4.805263	-1.105274
H	-0.119488	4.638923	0.085683
C	-1.869723	5.654223	0.819962
H	-2.958675	5.648626	0.685846
H	-1.496355	6.651905	0.554824
H	-1.656871	5.479435	1.882186
H	3.846870	-0.092894	-0.582817
N	1.368025	0.203654	-0.385434
N	0.004338	0.017067	-0.276515
O	0.696449	2.389412	-0.594711
O	-2.320965	0.835589	0.724493
O	-1.767672	1.674727	-2.009139
O	-1.696183	3.310888	0.301882
V	-1.146334	1.725217	-0.525734
H	1.185831	-2.541181	-0.573577
H	0.217528	-3.116703	0.806348
H	1.397763	-1.798380	1.004718

3' (in MeCN solution)

C	5.498918	0.508937	-1.085849
C	4.436521	1.422860	-1.113406
C	4.707782	2.785994	-1.276229
H	3.884569	3.496547	-1.295957
C	6.020184	3.227205	-1.411490
H	6.222060	4.290003	-1.538300
C	7.071970	2.314211	-1.384520
H	8.099216	2.661364	-1.489656
C	6.807345	0.953909	-1.221941
H	7.626698	0.236649	-1.199191
C	3.043136	0.966791	-0.967501

C	1.020264	-1.712496	-0.406842
C	2.051195	-2.753445	-0.085215
C	-0.394464	-1.963693	-0.201430
C	-1.226375	-0.916629	0.253938
C	-2.511939	-1.213509	0.790163
H	-3.092191	-0.382280	1.194419
C	-2.993689	-2.488813	0.796141
H	-3.976414	-2.703371	1.217294
C	-2.252424	-3.554361	0.217387
C	-2.808364	-4.849775	0.128273
H	-3.794135	-5.020942	0.561523
C	-2.137041	-5.865771	-0.513269
H	-2.575131	-6.860029	-0.584496
C	-0.893437	-5.595522	-1.112118
H	-0.379535	-6.378149	-1.669030
C	-0.320302	-4.343587	-1.020750
H	0.616082	-4.160228	-1.540419
C	-0.955970	-3.291098	-0.317254
C	-0.074741	4.218794	-0.578159
H	-0.739286	4.437751	-1.424959
H	0.959757	4.202607	-0.935347
C	-0.261468	5.201248	0.551859
H	-1.293660	5.184570	0.923699
H	-0.048833	6.215497	0.192148
H	0.416761	4.979139	1.383665
H	5.290190	-0.550757	-0.957523
N	2.792563	-0.311016	-0.846502
N	1.429665	-0.511491	-0.749112
O	2.092116	1.870993	-0.949785
O	-0.858448	0.352409	0.273464
O	-0.288055	1.108526	-2.472443
O	-0.338495	2.867669	-0.127595
V	0.300848	1.151339	-0.994616

H	-1.292059	2.790368	0.196814
H	2.583926	-3.085727	-0.985964
H	1.609448	-3.619368	0.408729
H	2.803836	-2.306124	0.573714

4⁻ (in MeCN solution)

C	4.172760	0.980454	-0.668348
C	3.043097	1.847376	-0.728570
C	3.253589	3.217027	-0.970262
H	2.379389	3.861855	-1.008623
C	4.515903	3.749803	-1.160352
H	4.643082	4.814160	-1.347275
C	5.622275	2.894210	-1.108923
H	6.627622	3.287484	-1.258390
C	5.452098	1.544115	-0.869204
H	6.315770	0.880316	-0.826171
C	1.655830	1.400433	-0.547463
C	-0.413242	-1.239927	0.071159
C	0.606785	-2.295695	0.385926
C	-1.833889	-1.490805	0.250484
C	-2.671763	-0.443782	0.699280
C	-3.972231	-0.752625	1.202121
H	-4.557938	0.073939	1.608331
C	-4.461735	-2.023866	1.173707
H	-5.455429	-2.241107	1.566980
C	-3.711603	-3.081616	0.591747
C	-4.271696	-4.371655	0.460927
H	-5.270068	-4.544808	0.863698
C	-3.588737	-5.380692	-0.179521
H	-4.030386	-6.370586	-0.282538
C	-2.327747	-5.105050	-0.738300
H	-1.802068	-5.879135	-1.296329
C	-1.750789	-3.858761	-0.605384

H	-0.800136	-3.672234	-1.096595
C	-2.398575	-2.812856	0.099123
C	-1.151536	4.547537	-0.038775
H	-1.358758	4.779467	-1.100324
H	-0.055293	4.571008	0.081103
C	-1.774352	5.624433	0.834130
H	-2.864061	5.647090	0.708080
H	-1.378040	6.614508	0.573757
H	-1.558562	5.436537	1.893574
N	4.078352	-0.349784	-0.374812
N	1.373755	0.129528	-0.351814
N	0.007158	-0.038346	-0.249982
O	0.717827	2.314192	-0.568578
O	-2.311649	0.819594	0.744535
O	-1.740409	1.621176	-1.998765
O	-1.662983	3.280994	0.296394
V	-1.123355	1.680640	-0.512383
H	3.156671	-0.781441	-0.489978
H	4.887978	-0.930522	-0.615282
H	1.139973	-2.628807	-0.514513
H	0.155693	-3.162330	0.870826
H	1.363675	-1.864006	1.051002

4' (in MeCN solution)

C	5.592008	0.496512	-1.065468
C	4.462064	1.365481	-1.093146
C	4.668605	2.745079	-1.282172
H	3.793695	3.390102	-1.298414
C	5.929358	3.285398	-1.451740
H	6.055890	4.355792	-1.599983
C	7.037708	2.429161	-1.428874
H	8.042468	2.829627	-1.562070
C	6.870808	1.071572	-1.239910

H	7.735928	0.408612	-1.220624
C	3.083796	0.902120	-0.939716
C	1.005365	-1.749761	-0.391357
C	2.018853	-2.806496	-0.067085
C	-0.415475	-1.978153	-0.190855
C	-1.232679	-0.916856	0.256238
C	-2.528406	-1.187986	0.780410
H	-3.096059	-0.345029	1.178227
C	-3.035290	-2.453359	0.782697
H	-4.026299	-2.648356	1.193798
C	-2.308335	-3.532999	0.212936
C	-2.888553	-4.817653	0.120441
H	-3.882161	-4.968129	0.543350
C	-2.229774	-5.848441	-0.510038
H	-2.686226	-6.834188	-0.584178
C	-0.974967	-5.603057	-1.096145
H	-0.470220	-6.396673	-1.645855
C	-0.377996	-4.362900	-1.000110
H	0.567541	-4.199813	-1.509568
C	-1.000500	-3.295530	-0.307086
C	-0.004154	4.200777	-0.552392
H	-0.588290	4.407683	-1.459452
H	1.060025	4.199268	-0.808624
C	-0.313063	5.183349	0.550517
H	-1.375949	5.151885	0.821462
H	-0.081967	6.200255	0.210267
H	0.285082	4.972870	1.444545
N	5.501049	-0.841841	-0.829073
N	2.802012	-0.377471	-0.826787
N	1.436768	-0.556284	-0.733032
O	2.129603	1.810177	-0.908164
O	-0.843272	0.346040	0.276237
O	-0.236932	1.092136	-2.469625

O	-0.290595	2.849300	-0.119603
V	0.337570	1.123954	-0.984355
H	4.589304	-1.287245	-0.953674
H	6.324144	-1.409276	-1.055766
H	-1.257664	2.776916	0.163275
H	2.536101	-3.160017	-0.969263
H	1.565704	-3.658793	0.440501
H	2.787998	-2.365931	0.577996