Table S1. Some additinal charge data to Table 1 and two lowest eigenvalues of Hessian matrix for simplified model complexes.

Optimized geometry atdef2-TZVP/BP86 level										
			NPA			MPA				
Entry	r(W---N)	θ (C1-R1-R2-N)	δ N	δ W	Δ(δ W–δ N)	δ N	δ W	Δ(δ W–δ N)	Two lowest frequencies	
1	2.376	38.9	-0.800	1.242	2.042	-0.459	0.905	1.364	3.59	23.66
2	2.437	38.2	-0.601	1.253	1.854	-0.335	0.904	1.215	25.69	31.47
3	2.462	39.1	-0.609	1.249	1.858	-0.306	0.880	1.193	16.27	23.26
4	2.47	37.9	-0.619	1.254	1.873	-0.317	0.887	1.204	17.5	20.42
5	2.597	37.2	-0.407	1.265	1.672	-0.232	0.922	1.154	20.43	27.03
6	2.677	35.8	-0.411	1.275	1.687	-0.205	0.884	1.089	31.13	34.99
7	3.063	34.7	-0.416	1.307	1.722	-0.184	0.877	1.061	23.75	24.17
8	2.376	-	-0.424	1.22877	1.653	-0.155	0.861	1.016	10.23	40.15
9	2.406	-	-0.442	1.22667	1.669	-0.210	0.860	1.069	19.32	36.51

Table S2. Cartesian coordinates of simplified model complexes

Entry 1 from table 1

C	-3.68358	7.46033	7.38563
C	-2.64657	6.59311	7.74839
C	-2.87272	5.44903	8.51957
C	-4.19043	5.16107	8.93235
C	-5.26272	6.01867	8.58731
C	-4.98147	7.14924	7.81982
C	-1.71430	4.58657	8.95071
N	-1.98560	3.13732	8.75695
H	-1.18786	2.58066	9.07876
O	-4.48713	4.07194	9.67439
W	-3.87721	2.24988	9.88782
Cl	-2.60966	0.26463	9.70431
C	-6.65929	5.69204	9.03772
C	-3.42203	8.68840	6.55195
H	-2.12466	2.92432	7.76292
Cl	-2.59265	2.86340	11.79242
Cl	-4.60372	1.88765	7.64061
N	-5.24927	1.56967	10.73493
C	-6.29722	0.93137	11.43630
H	-5.80803	7.81069	7.54649
H	-1.62557	6.81579	7.42672
H	-0.80979	4.89313	8.40268
H	-1.51678	4.71991	10.02517
H	-7.36401	6.46880	8.71533
H	-6.99113	4.72722	8.62703
H	-6.71272	5.60275	10.13266
H	-2.35633	8.78814	6.30835
H	-3.98258	8.65522	5.60518
H	-3.73481	9.60307	7.07832
H	-6.08083	-0.14289	11.55988
H	-6.41827	1.38316	12.43505
H	-7.24785	1.03874	10.88794

Entry 2 from table 1

C	-5.02284	7.16185	7.84147
C	-3.72966	7.44934	7.38085
C	-2.69529	6.57455	7.73957
C	-2.92715	5.44273	8.52403
C	-4.24159	5.17680	8.95762
C	-5.30833	6.04308	8.62779
C	-3.46735	8.64855	6.50622
C	-1.79168	4.56512	8.98003
N	-2.01013	3.11933	8.68208
W	-3.99351	2.23833	9.79123
N	-5.31625	1.59085	10.73075
C	-6.30138	0.98948	11.54617
O	-4.52386	4.09544	9.72019
C	-6.69999	5.74483	9.11191
Cl	-2.85336	0.20610	9.40009
Cl	-2.56376	2.63929	11.66480
Cl	-4.93156	2.03706	7.61873
H	-1.31593	2.59510	9.22664
C	-1.79042	2.81154	7.24931
H	-5.84335	7.83484	7.57844
H	-1.67460	6.78462	7.40846
H	-0.85321	4.90663	8.51129
H	-1.67258	4.64136	10.07060
H	-7.39691	6.53481	8.80496
H	-7.06036	4.78638	8.71050
H	-6.72883	5.65843	10.20805
H	-2.41624	8.96262	6.55866

H	-3.69147	8.42526	5.45056
H	-4.09512	9.50261	6.79631
H	-6.32991	-0.09966	11.37643
H	-6.07122	1.17217	12.60951
H	-7.29692	1.40932	11.32692
H	-1.92279	1.73625	7.08965
H	-2.52907	3.34875	6.64493
H	-0.77616	3.11247	6.93860

Entry 3 from table 1

C	-4.99192	7.24731	8.05032
C	-3.71209	7.43255	7.50333
C	-2.72807	6.48265	7.80006
C	-2.98602	5.37741	8.61772
C	-4.28362	5.21934	9.14656
C	-5.30453	6.16122	8.86700
C	-3.41620	8.61542	6.61752
C	-1.88014	4.41169	8.95453
N	-2.29858	2.98604	8.82463
H	-2.87887	2.91580	7.97801
O	-4.60325	4.18117	9.94260
W	-4.09833	2.37128	10.38837
N	-5.46617	1.95729	11.39097
C	-6.53447	1.49685	12.19284
C	-6.67960	5.96957	9.44336
C	-1.12825	2.08461	8.58331
C	-0.10637	2.06261	9.71142
Cl	-3.06840	0.25650	10.52928
Cl	-2.65118	3.18612	12.07950
Cl	-5.03326	1.69791	8.28355
H	-5.77689	7.97560	7.82936
H	-1.72341	6.60630	7.38705
H	-1.02445	4.60875	8.28587
H	-1.53579	4.56248	9.98838
H	-0.64079	2.40302	7.64345
H	-1.53793	1.07873	8.42542
H	-7.34275	6.79332	9.15078
H	-7.12469	5.02406	9.10041
H	-6.64590	5.92044	10.54171
H	-2.36126	8.63584	6.31478
H	-4.02846	8.59211	5.70278
H	-3.63972	9.56387	7.12905
H	-6.34833	0.46024	12.52101
H	-6.64662	2.13514	13.08498
H	-7.47878	1.52246	11.62401
H	0.69254	1.35402	9.45163
H	0.36215	3.04396	9.86879
H	-0.55951	1.73890	10.65568

Entry 4 from table 1

C	-5.17653	6.04834	8.75703
C	-4.93236	7.14008	7.92441
C	-3.65603	7.42479	7.41371
C	-2.60466	6.56800	7.75989
C	-2.79240	5.46147	8.59441
C	-4.08798	5.20471	9.08936
C	-3.42825	8.62386	6.52959
C	-1.62100	4.59571	8.98019
N	-1.92583	3.13908	8.85651
C	-0.70301	2.28363	8.62380
C	-0.12717	2.48919	7.21783
O	-4.34337	4.15937	9.89947
W	-3.68302	2.42733	10.43941
Cl	-4.50633	1.55131	8.36499
C	-6.54836	5.74958	9.29433
H	-2.50233	3.02086	8.01236
N	-5.02578	1.93879	11.44213
C	-6.05679	1.41893	12.25630
Cl	-2.46049	0.43237	10.72943
Cl	-2.35161	3.45572	12.11242
C	0.34631	2.48089	9.71445
H	-5.76983	7.79152	7.66065
H	-1.60237	6.76733	7.37135
H	-0.76698	4.86704	8.34090
H	-1.32875	4.78369	10.02368
H	-1.07783	1.25283	8.69209
H	-7.27026	6.50567	8.96097
H	-6.89838	4.76151	8.96133
H	-6.54716	5.72774	10.39409
H	-2.43303	8.59797	6.06686
H	-4.17685	8.67794	5.72564
H	-3.50426	9.56094	7.10364
H	-5.83267	0.37641	12.53905
H	-6.15544	2.01993	13.17564
H	-7.01978	1.44067	11.71971
H	1.14945	1.74378	9.57819
H	0.80498	3.47967	9.66920
H	-0.08315	2.33800	10.71336
H	0.68964	1.77386	7.04690
H	-0.88873	2.31398	6.44356
H	0.28862	3.49758	7.07461

Entry 5 from table 1

C	-5.25801	5.98749	8.55837
C	-5.03407	7.14154	7.79365
C	-3.71929	7.42263	7.39774
C	-2.65030	6.59461	7.74834
C	-2.91351	5.44322	8.51583
C	-4.22502	5.12644	8.93661
C	-6.16879	8.06582	7.43287
C	-1.23760	6.96212	7.38192
N	-0.48476	5.91317	6.62340
C	-1.17064	5.64361	5.33572
O	-1.91564	4.61218	8.88331
W	-0.30865	3.82682	8.16051
N	-0.12742	2.49079	9.26081
C	0.14907	1.40865	10.12563
C	-4.47784	3.88897	9.75185
C	0.85058	6.48012	6.30377
Cl	1.50626	3.27992	6.76795
Cl	1.04860	5.31766	9.42811
Cl	-1.72912	2.75188	6.58026

H	-6.27733	5.74530	8.87075
H	-3.51732	8.31733	6.80265
H	-1.25485	7.88893	6.77867
H	-0.65087	7.16744	8.28972
H	0.73120	7.40788	5.71579
H	1.42405	5.75259	5.72114
H	1.39324	6.69985	7.22899
H	-2.18861	5.28527	5.51427
H	-0.61853	4.87138	4.78897
H	-1.20738	6.56713	4.72918
H	-5.53828	3.81055	10.02262
H	-4.19147	2.98435	9.19572
H	-3.88031	3.89408	10.67540
H	-6.34386	8.80779	8.22880
H	-5.95661	8.62192	6.50964
H	-7.10791	7.51326	7.29210
H	0.87557	0.72143	9.66083
H	0.57476	1.78389	11.07168
H	-0.77360	0.85018	10.35410

Entry 6 from table 1

C	-4.97149	7.29186	8.19002
C	-3.68988	7.50282	7.67096
C	-2.68983	6.52376	7.71285
C	-3.00294	5.28426	8.30792
C	-4.29596	5.02911	8.83004
C	-5.25212	6.04057	8.76037
C	-1.31821	6.89494	7.19380
N	-0.48942	5.83262	6.56335
C	0.85177	6.43129	6.19822
O	-2.11107	4.27819	8.39250
W	-0.24754	3.82426	8.31741
Cl	2.07542	3.89648	7.93983
C	-4.60482	3.69112	9.44284
C	-6.01541	8.37800	8.15490
C	-1.06348	5.42593	5.22872
Cl	0.05584	5.55657	9.93508
Cl	-0.46650	2.46957	6.38367
N	-0.23388	2.47719	9.41559
C	-0.13765	1.32891	10.23236
H	-6.25002	5.84656	9.16225
H	-3.45599	8.46572	7.20843
H	-1.43534	7.73057	6.47543
H	-0.74055	7.27896	8.04520
H	0.68397	7.09962	5.33153
H	1.46704	5.59324	5.84596
C	1.61253	7.21409	7.26156
C	-2.47901	4.86460	5.15941
H	-0.36182	4.68895	4.81715
H	-1.01542	6.32022	4.57685
H	-5.64416	3.65499	9.79275
H	-4.45038	2.87450	8.72242
H	-3.94254	3.48511	10.29660
H	-5.76967	9.14844	7.41204
H	-7.00893	7.97360	7.91450
H	-6.09814	8.87779	9.13351
H	0.88369	1.23056	10.63630
H	-0.84965	1.38411	11.07211
H	-0.36633	0.42888	9.63630
H	2.59554	7.46927	6.83927
H	1.12029	8.15999	7.52514
H	1.78027	6.63746	8.17637
H	-2.64988	4.54460	4.12061
H	-2.61679	3.98706	5.79916
H	-3.24425	5.61052	5.40418

Entry 7 from table 1

C	-4.24823	4.97248	8.86111
C	-5.21980	5.96783	8.78362
C	-4.96556	7.20356	8.16962
C	-3.69752	7.41304	7.61763
C	-2.67930	6.45100	7.65940
C	-2.97110	5.22810	8.30136
C	-6.02489	8.27388	8.11870
C	-1.32222	6.86039	7.11304
N	-0.47037	5.88878	6.37893
C	0.89207	6.53997	6.12185
C	0.88729	7.66993	5.06891
O	-2.06965	4.23316	8.39057
W	-0.26995	3.62434	8.43133
Cl	-0.61691	2.16949	6.59724
C	-4.52521	3.64910	9.51954
C	-1.08262	5.52553	5.03684
C	-0.13010	4.68471	4.17378
C	-2.44211	4.82003	5.11898
N	-0.30341	2.38073	9.63607
C	-0.30137	1.38798	10.64318
Cl	2.01173	3.66557	7.93708
Cl	0.08858	5.41056	9.97963
C	1.59264	7.08022	7.37180
H	-6.20588	5.77340	9.21333
H	-3.48707	8.36554	7.12373
H	-1.49752	7.75634	6.48649
H	-0.73211	7.19057	7.97916
H	1.51067	5.71524	5.74587
H	-1.26723	6.48228	4.50884
H	-5.55721	3.60883	9.88995
H	-4.37248	2.81372	8.82067
H	-3.84533	3.47907	10.36757
H	-5.75788	9.07027	7.41179
H	-6.99901	7.86135	7.81837
H	-6.16360	8.74003	9.10729
H	0.51709	0.66955	10.47452
H	-0.15350	1.86358	11.62753
H	-1.25946	0.84359	10.65744
H	2.63977	7.28495	7.10653
H	1.15906	8.02960	7.71926
H	1.59404	6.37298	8.20416
H	-2.76179	4.58813	4.09274
H	-2.38277	3.87489	5.67098
H	-3.22139	5.44616	5.56510
H	1.91495	8.04573	4.96639

H	0.55684	7.35466	4.07223
H	0.26687	8.52174	5.38332
H	-0.66552	4.36908	3.26776
H	0.76202	5.23175	3.84679
H	0.18939	3.77979	4.70429

Entry 8 from table 1

C	3.35423	6.13234	1.45065
C	3.58307	7.00316	2.53546
C	2.74019	6.92289	3.67103
C	1.68325	5.97904	3.70676
C	1.50866	5.13823	2.60858
C	2.32966	5.19027	1.46575
C	4.66016	7.96052	2.41034
N	5.07118	8.81033	3.29235
W	4.14602	9.01887	5.47094
Cl	5.91759	10.49352	5.96029
O	2.88987	7.71835	4.72827
C	0.79111	5.90645	4.91384
C	2.09932	4.25262	0.30880
C	6.17016	9.68746	2.88630
N	3.38103	9.16223	7.03601
C	2.81057	9.36899	8.31075
Cl	5.61132	7.20625	5.91144
Cl	2.97818	10.78021	4.39622
H	0.69472	4.40856	2.64090
H	5.16931	7.94487	1.43318
H	4.00771	6.20738	0.57759
H	1.37121	5.67719	5.81968
H	0.02264	5.13391	4.78589
H	0.29322	6.86993	5.09648
H	2.77832	4.47184	-0.52523
H	1.06744	4.32563	-0.06613
H	2.26055	3.20516	0.60684
H	1.87799	9.95144	8.22231
H	3.51174	9.92581	8.95552
H	2.57832	8.40528	8.79389
H	5.85952	10.73372	3.00229
H	7.03086	9.52486	3.54728
H	6.46186	9.50112	1.84115

Entry 9 from table 1

W	3.40042	6.10690	1.47881
Cl	2.72465	6.97105	3.58555
Cl	4.55693	5.69720	-0.55361
Cl	2.04622	7.70163	0.43356
N	2.26024	4.79240	1.34451
N	5.04756	7.84701	1.69997
O	4.78468	5.11402	2.44532
C	7.62555	4.39402	4.55558
H	8.04125	3.53884	5.09591
C	6.45363	4.20462	3.82607
C	4.87046	9.32106	-0.25974
H	5.01693	8.45280	-0.90131
C	8.29379	5.63267	4.62705
C	6.09920	7.73490	2.45500
H	6.74668	8.61839	2.55687
C	6.55840	6.57059	3.17290
C	4.85210	9.15121	1.13049
C	4.65086	10.25401	1.97102
H	4.59468	10.10051	3.04946
C	5.90696	5.31206	3.12851
C	7.74524	6.70109	3.92611
H	8.23924	7.67578	3.94983
C	5.75996	2.87292	3.76632
C	4.47639	11.52548	1.42024
H	4.30584	12.37806	2.07908
C	4.51097	11.70205	0.03569
H	4.37571	12.69547	-0.39362
C	4.70979	10.59736	-0.79831
H	4.73599	10.72742	-1.88107
C	9.55608	5.77998	5.43669
C	1.28443	3.78799	1.16538
H	4.73531	2.94415	4.15961
H	6.30673	2.12111	4.34902
H	5.67308	2.51818	2.72899
H	9.96752	6.79420	5.35511
H	10.33024	5.07289	5.10243
H	9.37204	5.57593	6.50264
H	1.64379	3.02990	0.44938
H	0.35227	4.22834	0.77246
H	1.06181	3.28874	2.12305