Supplementary information
Spectroscopic and quantum mechanical study of a scavenger molecule: N,N-diethylhydroxylamine

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6.5-18.5 GHz									
J"	K_a"	K_c"	-	J'	K_a'	K_c	F"-F'	$\nu_{obs.}$ [MHz]	$\nu_{obs.} - \nu_{calc.}$
1	1	1	-	0	0	0	0 - 1	9365.895	-0.005
							2 - 1	9368.363	-0.001
							1 - 1	9370.005	-0.001
1	1	0	-	0	0	0	1 - 1	9626.849	0.002
							2 - 1	9628.706	0.003
							0 - 1	9631.493	0.006
2	1	2	-	1	0	1	1 - 1	12887.987	-0.001
							1 - 0	12888.521	0.000
							3 - 2	12889.306	0.001
							2 - 1	12891.081	0.000
							2 - 2	12891.291	-0.003
2	1	1	-	1	0	1	2 - 1	13667.432	-0.002
							2 - 2	13667.642	-0.005
							3 - 2	13669.406	-0.001
							1 - 1	13670.172	0.000
							1 - 0	13670.708	0.003
2	2	1	-	2	1	1	1 - 1	16762.074	0.001
							3 - 3	16762.929	0.005
							2 - 2	16764.447	-0.008
2	2	0	-	2	1	1	1 - 1	16770.986	-0.000
							3 - 3	16771.787	-0.003
							2 - 2	16773.240	0.003
							3 - 3	17551.894	0.003
							2 - 2	17549.589	-0.001
							1 - 1	17553.168	-0.002
2	2	1	-	2	1	2	2 - 2	17540.810	0.002
							3 - 3	17543.024	-0.001
							1 - 1	17544.254	-0.003
3	1	2	-	2	0	2	3 - 2	17841.106	-0.000
							4 - 3	17843.159	0.002
							2 - 1	17843.938	-0.002
3	1	3	-	2	0	2	2 - 2	16282.778	0.004
							2 - 1	16283.264	0.002
							4 - 3	16283.840	0.001
							3 - 2	16285.674	-0.000
							3 - 3	16285.989	0.002
3	2	1	-	3	1	3	2 - 2	17983.168	0.003
							4 - 4	17982.332	-0.004
							3 - 3	17979.970	0.001
3	2	2	-	3	1	3	2 - 2	17938.865	-0.000
							4 - 4	17938.114	0.000
							3 - 3	17935.964	-0.002
3	2	2	-	3	1	2	2 - 2	16378.185	-0.002
							4 - 4	16378.796	0.000
							3 - 3	16380.526	-0.007
3	2	1	-	3	1	2	4 - 4	16423.022	0.004
							3 - 3	16424.540	0.003
4	0	4	-	3	1	3	4 - 3	10057.201	-0.001
							5 - 4	10058.706	-0.001
							3 - 2	10059.293	0.000
							3 - 2	8498.616	0.002
							5 - 4	8499.388	-0.001
							4 - 3	8501.765	-0.004
4	1	3	-	4	0	4	4 - 4	7122.833	0.004
							5 - 5	7125.179	-0.001

							3 - 3	7125.787	0.002
4	2	2	-	4	1	3	3 - 3	16002.347	-0.003
							5 - 5	16002.722	0.005
							4 - 4	16004.140	-0.001
4	2	3	-	4	1	3	3 - 3	15870.118	0.002
							5 - 5	15870.587	0.001
							4 - 4	15872.415	0.003
4	2	3	-	4	1	4	4 - 4	18465.737	0.001
							5 - 5	18467.879	-0.001
							3 - 3	18468.433	0.002
5	0	5	-	4	1	3	4 - 3	11604.339	0.001
							6 - 5	11604.957	0.001
							5 - 4	11607.534	-0.000
5	0	5	-	4	1	4	4 - 3	14202.652	-0.002
							6 - 5	14202.249	-0.001
							5 - 4	14200.856	-0.003
5	2	3	-	5	1	4	4 - 4	15548.021	-0.006
							6 - 6	15548.277	-0.002
							5 - 5	15549.517	-0.000
6	0	6	-	5	1	5	6 - 5	18369.038	-0.000
							7 - 6	18370.272	0.003
							5 - 4	18370.555	-0.001
6	1	5	-	6	0	6	6 - 6	8907.158	-0.000
							7 - 7	8909.879	-0.002
							5 - 5	8910.345	0.001
59.6-74.4 GHz									
5	5	1	-	4	4	0,1		70360.72	0.006
6	4	3	-	5	3	2		62706.75	-0.021
6	4	2	-	5	3	2		62707.04	0.119
6	4	2	-	5	3	3		62712.24	0.052
7	4	4	-	6	3	3		66477.18	-0.028
7	4	3	-	6	3	3		66477.81	0.054
7	4	4	-	6	3	4		66492.91	-0.065
7	4	3	-	6	3	4		66493.55	0.027
8	4	5	-	7	3	4		70233.71	-0.078
8	4	4	-	7	3	4		70235.50	0.070
8	4	4	-	7	3	5		70274.71	0.001
9	3	7	-	8	2	7	8-7,10-9	63204.46	0.003
							9-8	63203.93	-0.032
9	3	7	-	8	2	6	8-7,10-9	61465.72	0.033
							9-8	61466.76	0.033
9	3	6	-	8	2	6	8-7,10-9	61636.35	-0.003
							9-8	61637.16	-0.043

Table S2: Experimental rotational transition frequencies of *trans*-2-DEHA.

J"	K_a"	K_c"	-	J'	K_a'	K_c	F"-F'	$\nu_{obs.}$ [MHz]	$\nu_{obs.} - \nu_{calc.}$
1	1	0	-	0	0	0	1 - 1	7697.237	0.002
							2 - 1	7699.211	0.003
							0 - 1	7702.170	0.002
1	1	1	-	0	0	0	0 - 1	7105.322	-0.001
							2 - 1	7107.509	-0.001
							1 - 1	7108.966	-0.003
2	0	2	-	1	0	1	1 - 1	8319.233	-0.004
							3 - 2	8320.242	0.002
							1 - 0	8320.519	-0.004
							2 - 1	8320.609	0.004
							2 - 2	8321.119	-0.000
2	1	1	-	1	1	0	1 - 0	8990.727	0.003
							3 - 2	8992.816	0.001
							2 - 1	8993.225	-0.001
2	1	1	-	1	0	1	2 - 1	12489.200	0.006
							2 - 2	12489.713	0.004
							3 - 2	12491.274	0.003
							1 - 1	12491.628	0.002
							1 - 0	12492.915	0.003
2	1	2	-	1	0	1	1 - 1	10715.387	-0.002
							1 - 0	10716.673	-0.002
							3 - 2	10717.073	-0.005
							2 - 1	10718.673	-0.004
							2 - 2	10719.188	-0.004
2	1	2	-	1	1	1	3 - 2	7810.322	0.003
							1 - 0	7811.333	0.000
							2 - 1	7810.976	0.001
3	0	3	-	2	0	2	4 - 3	12286.775	0.000
							2 - 1	12286.775	-0.003
							3 - 2	12287.273	-0.005
3	1	2	-	2	0	2	3 - 2	17603.132	-0.006
							4 - 3	17605.372	-0.003
							2 - 1	17606.337	-0.003
3	1	3	-	2	0	2	2 - 1	14064.386	0.002
							4 - 3	14064.749	0.002
							3 - 2	14066.304	0.004
4	0	4	-	3	0	3	3 - 2	16068.298	-0.002
							5 - 4	16068.318	0.004
							4 - 3	16068.876	0.002

Table S3: Experimental rotational transition frequencies of *trans*-3-DEHA.

J"	K_a"	K_c"	-	J'	K_a'	K_c	F"-F'	$\nu_{obs.}$ [MHz]	$\nu_{obs.} - \nu_{calc.}$
1	1	1	-	0	0	0	0 - 1	7934.709	-0.010
							2 - 1	7936.422	0.002
							1 - 1	7937.548	-0.005
1	1	0	-	0	0	0	1 - 1	8233.627	0.010
							2 - 1	8234.634	0.001
							0 - 1	8236.173	0.015
2	1	2	-	1	0	1	1 - 0	11887.169	-0.003
							1 - 1	11887.468	0.003
							3 - 2	11887.952	-0.000
							2 - 2	11889.039	-0.002
							2 - 1	11889.155	-0.004
2	1	1	-	1	0	1	2 - 2	12780.824	0.009
							2 - 1	12780.936	0.003
							3 - 2	12782.033	0.003
							1 - 0	12782.530	0.001
							1 - 1	12782.821	-0.001
3	0	3	-	2	1	1	2 - 1	8378.271	-0.005
							4 - 3	8378.986	0.000
							3 - 2	8380.295	-0.005
3	0	3	-	2	1	2	3 - 2	9272.079	0.005
							4 - 3	9273.065	0.001
							2 - 1	9273.635	0.002
3	1	3	-	2	0	2	2 - 1	15696.967	-0.001
							4 - 3	15697.378	-0.003
							3 - 2	15698.542	-0.000
3	1	2	-	2	0	2	3 - 2	17483.251	-0.002
							4 - 3	17484.472	-0.006
							2 - 1	17484.894	-0.006
4	0	4	-	3	1	2	3 - 2	12022.345	0.004
							5 - 4	12022.860	0.005
							4 - 3	12024.400	0.001
4	0	4	-	3	1	3	4 - 3	13809.112	0.003
							5 - 4	13809.951	-0.001
							3 - 2	13810.270	-0.004

Table S4: Experimental rotational transition frequencies of ^{15}N-*trans*-1-DEHA.

J"	K_a"	K_c"	-	J'	K_a'	K_c	$\nu_{obs.}$ [MHz]	$\nu_{obs.} - \nu_{calc.}$
1	1	1	-	0	0	0	9362.031	-0.002
1	1	0	-	0	0	0	9621.307	0.004
2	1	2	-	1	0	1	12883.320	0.001
2	1	1	-	1	0	1	13661.126	-0.004
3	1	3	-	2	0	2	16278.360	0.000
3	1	2	-	2	0	2	17833.793	0.001

Table S5: Experimental rotational transition frequencies of $^{13}C_{\alpha}$-*trans*-1-DEHA.

J"	K_a"	K_c"	-	J'	K_a'	K_c	F"-F'	$\nu_{obs.}$ [MHz]	$\nu_{obs.} - \nu_{calc.}$
1	1	1	-	0	0	0	0 - 1	9294.819	0.005
							2 - 1	9297.280	0.002
							1 - 1	9298.916	-0.004
1	1	0	-	0	0	0	1 - 1	9555.059	0.008
							2 - 1	9556.909	0.002
							0 - 1	9559.682	-0.009
2	1	2	-	1	0	1	1 - 0	12794.504	0.003
							3 - 2	12795.288	0.003
							2 - 1	12797.052	-0.009
							1 - 1	12793.969	0.001
							2 - 2	12797.263	-0.011
2	1	1	-	1	0	1	2 - 1	13571.286	0.002
							3 - 2	13573.263	0.006
							1 - 0	13574.553	-0.002
3	1	3	-	2	0	2	4 - 3	16167.256	0.006
3	1	2	-	2	0	2	4 - 3	17722.305	-0.003

Table S6: Experimental rotational transition frequencies of $^{13}C_{\beta}$-*trans*-1-DEHA.

J"	K_a"	K_c"	-	J'	K_a'	K_c	F"-F'	$\nu_{obs.}$ [MHz]	$\nu_{obs.} - \nu_{calc.}$
1	1	1	-	0	0	0	0 - 1	9317.850	-0.005
							2 - 1	9320.322	0.003
							1 - 1	9321.961	-0.000
1	1	0	-	0	0	0	1 - 1	9566.717	-0.001
							2 - 1	9568.577	0.003
							0 - 1	9571.364	0.006
2	1	2	-	1	0	1	1 - 0	12767.660	-0.004
							3 - 2	12768.447	-0.001
							2 - 1	12770.220	-0.004
2	1	1	-	1	0	1	2 - 1	13510.322	-0.003
							3 - 2	13512.298	0.000
							1 - 0	13513.595	-0.001
3	1	3	-	2	0	2	2 - 1	16095.301	-0.001
							4 - 3	16095.882	0.001
							3 - 2	16097.724	0.005
3	1	2	-	2	0	2	4 - 3	17582.723	0.001

Table S7: Theoretical structure of *trans*-1-DEHA calculated at the B3LYP-D3(BJ)/Def2TZVP and MP2/aug-cc-pVTZ levels.

				B3LYP-D3(BJ)/Def2TZVP			MP2/aug-cc-pVTZ		
				d [Å]	α [°]	τ [°]	d [Å]	α [°]	τ [°]
C1									
C2	C1			1.5186			1.5155		
N3	C2	C1		1.4612	112.2		1.4615	111.7	
C4	N3	C2	C1	1.4612	111.9	175.6	1.4615	110.5	177.2
C5	C4	N3	C2	1.5186	112.2	-175.6	1.5155	111.7	-177.2
O6	N3	C2	C1	1.4497	106.3	-68.8	1.4514	105.2	-69.8
H7	O6	N3	C2	0.9632	103.2	120.3	0.9641	102.3	121.7
H8	C2	N3	O6	1.1003	110.4	54.8	1.0984	109.9	53.5
H9	C4	N3	O6	1.0924	106.1	-171.1	1.0913	106.1	-170.1
H10	C2	N3	O6	1.0924	106.1	171.1	1.0913	106.1	170.1
H11	C4	N3	O6	1.1003	110.4	-54.8	1.0984	109.9	-53.5
H12	C1	C2	N3	1.0914	110.3	-176.8	1.0896	110.3	-177.3
H13	C5	C4	N3	1.0914	110.3	176.8	1.0896	110.3	177.3
H14	C1	C2	N3	1.0915	110.6	-56.8	1.0892	110.3	-57.3
H15	C5	C4	N3	1.0896	110.8	-63.6	1.0877	110.6	-63.1
H16	C1	C2	N3	1.0896	110.8	63.6	1.0877	110.6	63.1
H17	C5	C4	N3	1.0915	110.6	56.8	1.0892	110.3	57.3

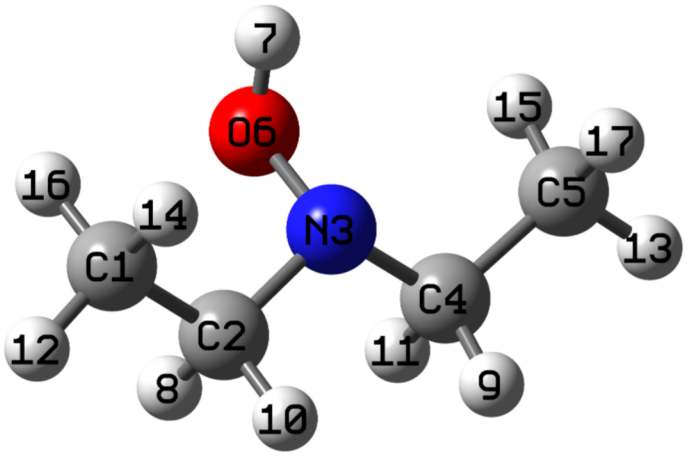


Table S8: Theoretical structure of *trans*-2-DEHA calculated at the B3LYP-D3(BJ)/Def2TZVP and MP2/aug-cc-pVTZ levels.

				B3LYP-D3(BJ)/Def2TZVP			MP2/aug-cc-pVTZ		
				d [Å]	α [°]	τ [°]	d [Å]	α [°]	τ [°]
C1									
C2	C1			1.5225			1.5198		
N3	C2	C1		1.4639	112.1		1.4637	111.6	
C4	N3	C2	C1	1.4606	112.8	73.6	1.4607	111.5	72.8
C5	C4	N3	C2	1.5190	112.2	-175.5	1.5160	111.6	-177.7
O6	N3	C2	C1	1.4501	105.7	-171.0	1.4525	104.6	-174.4
H7	O6	N3	C2	0.9635	103.0	120.4	0.9643	102.0	120.5
H8	C2	N3	O6	1.0896	106.2	-51.5	1.0887	106.2	-54.8
H9	C4	N3	O6	1.0909	106.6	-170.7	1.0898	106.6	-170.4
H10	C2	N3	O6	1.1007	110.9	64.6	1.0986	110.4	61.5
H11	C4	N3	O6	1.1005	110.1	-54.3	1.0988	109.7	-53.6
H12	C1	C2	N3	1.0911	109.6	172.1	1.0894	109.5	170.8
H13	C5	C4	N3	1.0915	110.3	176.9	1.0896	110.2	177.3
H14	C1	C2	N3	1.0903	112.5	-68.5	1.0881	112.4	-69.8
H15	C5	C4	N3	1.0896	110.9	-63.4	1.0875	110.6	-63.0
H16	C1	C2	N3	1.0911	110.5	52.7	1.0891	110.3	51.5
H17	C5	C4	N3	1.0915	110.5	57.0	1.0892	110.3	57.5

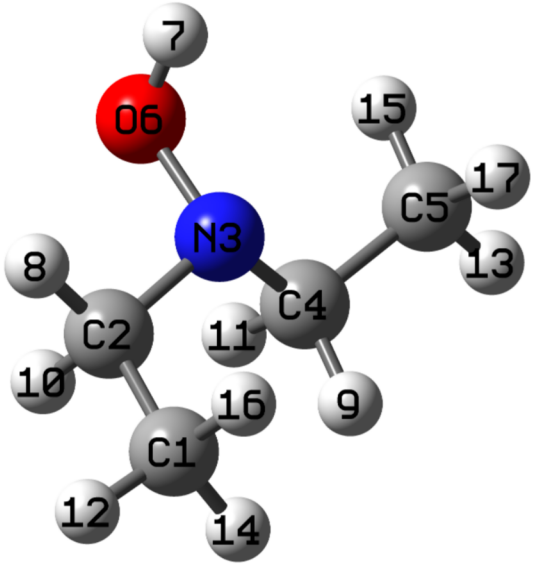


Table S9: Theoretical structure of *trans*-3-DEHA calculated at the B3LYP-D3(BJ)/Def2TZVP and MP2/aug-cc-pVTZ levels.

				B3LYP-D3(BJ)/Def2TZVP			MP2/aug-cc-pVTZ		
				d [Å]	α [°]	τ [°]	d [Å]	α [°]	τ [°]
C1									
C2	C1			1.5280			1.5240		
N3	C2	C1		1.4640	116.8		1.4650	116.2	
C4	N3	C2	C1	1.4600	114.0	-58.4	1.4610	112.6	-56.0
C5	C4	N3	C2	1.5190	111.6	-169.9	1.5160	111.0	-170.9
O6	N3	C2	C1	1.4490	107.0	59.5	1.4510	106.1	59.1
H7	O6	N3	C2	0.9630	102.9	117.7	0.9640	101.8	118.8
H8	C2	N3	O6	1.0930	105.9	-177.0	1.0920	105.7	-177.6
H9	C4	N3	O6	1.0930	106.1	-168.0	1.0920	106.1	-166.3
H10	C2	N3	O6	1.0910	106.5	-63.5	1.0900	106.3	-63.7
H11	C4	N3	O6	1.0980	111.3	-51.2	1.0960	110.8	-49.1
H12	C1	C2	N3	1.0920	109.7	-174.8	1.0900	109.5	-173.4
H13	C5	C4	N3	1.0920	110.5	177.3	1.0900	110.5	178.2
H14	C1	C2	N3	1.0900	110.6	-55.5	1.0880	110.5	-54.1
H15	C5	C4	N3	1.0900	110.6	-63.2	1.0880	110.3	-62.3
H16	C1	C2	N3	1.0910	112.1	65.7	1.0890	112.0	67.2
H17	C5	C4	N3	1.0910	110.6	57.1	1.0890	110.4	57.9

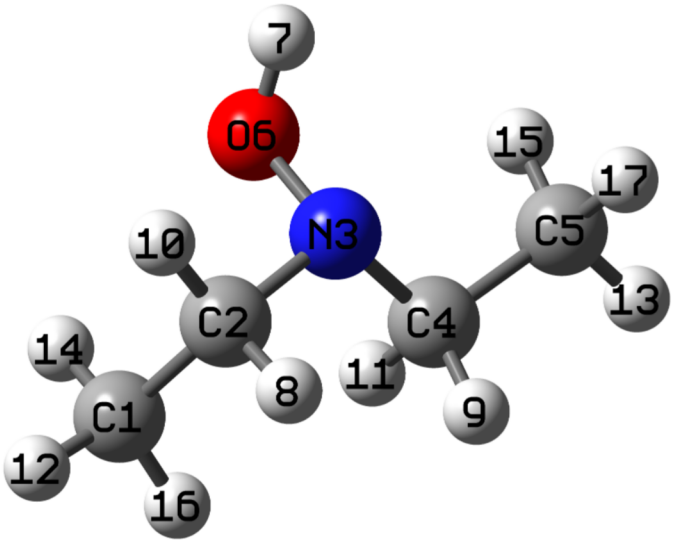


Table S10: Theoretical structures of the S_0, D_0 and D_1 states of *trans*-1-DEHA calculated at B3LYP-D3(BJ)/Def2TZVP level.

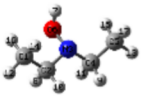
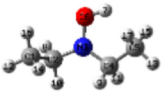
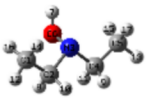
				S_0			D_0			D_1		
				d [Å]	α [°]	τ [°]	d [Å]	α [°]	τ [°]	d [Å]	α [°]	τ [°]
C1				-	-	-	-	-	-	-	-	-
C2	C1			1.5186	-	-	1.5314	-	-	1.5087	-	-
N3	C2	C1		1.4612	112.2	-	1.4565	111.5	-	1.5849	105.9	-
C4	N3	C2	C1	1.4612	111.9	175.6	1.4661	124.4	98.4	1.5848	100.6	174.0
C5	C4	N3	C2	1.5186	112.2	-175.6	1.5163	114.1	-165.2	1.5087	105.9	-174.1
O6	N3	C2	C1	1.4497	106.3	-68.8	1.3242	114.0	-79.2	1.3581	105.2	-76.9
H7	O6	N3	C2	0.9632	103.2	120.3	0.9775	108.7	175.9	0.9784	106.7	127.2
H8	C2	N3	O6	1.1003	110.4	54.8	1.0904	106.8	42.7	1.0892	109.2	46.1
H9	C4	N3	O6	1.0924	106.1	-171.1	1.0928	105.5	135.4	1.0855	103.6	-164.3
H10	C2	N3	O6	1.0924	106.1	171.1	1.0893	106.0	159.1	1.0855	103.6	164.2
H11	C4	N3	O6	1.1003	110.4	-54.8	1.0959	106.2	-111.1	1.0892	109.2	-46.1
H12	C1	C2	N3	1.0914	110.3	-176.8	1.0894	108.1	-179.4	1.1024	104.4	-170.3
H13	C5	C4	N3	1.0914	110.3	176.8	1.0893	108.1	178.4	1.1024	104.4	170.3
H14	C1	C2	N3	1.0915	110.6	-56.8	1.0897	111.4	-60.6	1.0887	112.8	-54.3
H15	C5	C4	N3	1.0896	110.8	-63.6	1.0934	112.6	-64.8	1.0876	112.6	-71.6
H16	C1	C2	N3	1.0896	110.8	63.6	1.0886	110.9	61.7	1.0876	112.6	71.6
H17	C5	C4	N3	1.0915	110.6	56.8	1.0914	112.2	60.4	1.0887	112.8	54.3
												

Table S11: Theoretical structures of the S_0, D_0 and D_1 states of hydroxylamine calculated at B3LYP-D3(BJ)/Def2TZVP level.

				S_0			D_0			D_1		
				d [Å]	α [°]	τ [°]	d [Å]	α [°]	τ [°]	d [Å]	α [°]	τ [°]
N1				-	-	-	-	-	-	-	-	-
O2	N1			1.4429	-	-	1.2946	-	-	1.3967	-	-
H3	O2	N1		0.9634	102.6	-	0.9832	111.2	-	0.9964	105.5	-
H4	N1	O2	H3	1.0170	104.1	124.5	1.0214	121.8	0.0	1.0428	102.0	128.3
H5	N1	O2	H3	1.0170	104.1	-124.5	1.0203	114.3	180.0	1.0428	102.0	-128.3
												

Table S12: Theoretical vibrational wavenumbers ($\tilde{\nu}_k$) and main Huang-Rhys factors (S_k) for the D_1 state of *trans*-1-DEHA calculated at the B3LYP-D3(BJ)/Def2TZVP level.

$\tilde{\nu}_k$ [cm^{-1}]	S_k
100	0.017 16
219	0.535 99
245	0.202 75
311	0.297 17
312	0.002 13
453	0.284 80
637	1.495 23
803	0.155 22
914	0.575 99
984	0.002 90
1043	0.909 23
1131	0.019 94
1227	0.000 49
1308	0.030 97
1349	0.003 19
1392	0.125 81
1501	0.006 41
2943	0.032 37
3097	0.000 64
3149	0.007 11
3177	0.000 58
3613	0.056 36

Table S13: Theoretical vibrational wavenumbers ($\tilde{\nu}_k$) and main Huang-Rhys factors (S_k) for the D_1 state of hydroxylamine calculated at the B3LYP-D3(BJ)/Def2TZVP level.

$\tilde{\nu}_k$ [cm^{-1}]	S_k
977	0.330 84
1119	0.109 08
1303	0.001 79
1557	0.000 21
3187	0.035 36
3443	0.062 16

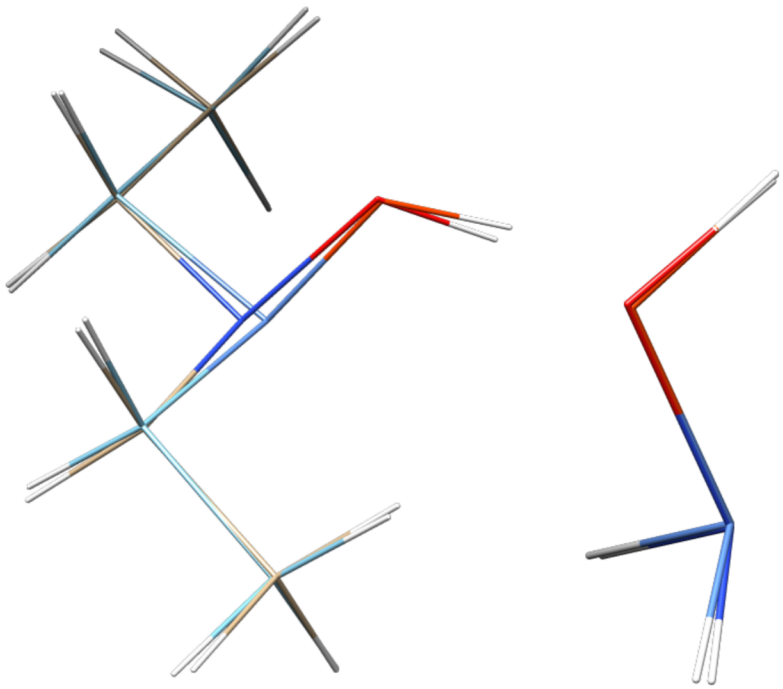


Figure S1: Superposition of the neutral (S_0, darker colors) and cation-excited (D_1, lighter colors) geometries for the *trans*-1-DEHA and HA.

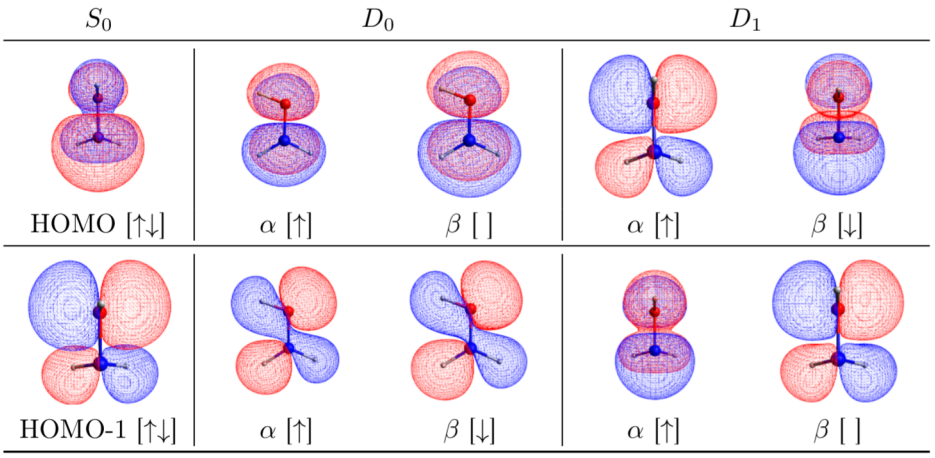


Figure S2: Structure and frontier's orbitals of the S_0, D_0 and D_1 states of hydroxylamine.

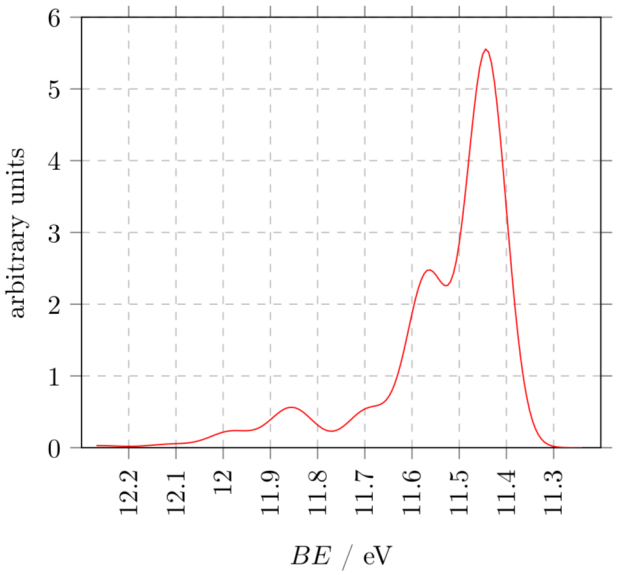


Figure S3: Simulated hydroxylamine $S_0 \rightarrow D_1$ ionization transition.