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TABLE S1: Optimized Geometric Parameters and Total Energies for E and Z Isomers of Propionaldehyde Oxime[a]

E-ac form	ab initio MO[b]		DFT	
Parameters	HF/6-31G*	MP2/6-31G*	BLYP/6-31G	BLYP/6-31G*
C1-C2	1.532	1.531	1.557	1.551
C1-H10	1.086	1.094	1.104	1.104
C1-H11	1.085	1.093	1.103	1.102
C1-H12	1.085	1.093	1.103	1.103
C2-C3	1.500	1.494	1.513	1.510
C2-H8	1.088	1.097	1.108	1.108
C2-H9	1.083	1.094	1.103	1.103
C3-N4	1.251	1.286	1.300	1.290
C3-H7	1.081	1.093	1.100	1.103
N4-O5	1.375	1.417	1.506	1.439
O5-H6	0.946	0.973	0.992	0.981
H10-C1-H11	107.94	108.07	107.97	107.83
H10-C1-H12	107.76	107.96	107.94	107.80
H11-C1-H12	108.13	108.32	108.27	108.21
C1-C2-C3	112.11	111.73	112.52	112.66
H8-C2-H9	107.41	107.41	107.22	107.16
C2-C3-N4	120.79	119.36	119.63	119.86
N4-C3-H7	120.12	120.38	121.10	120.88
C3-N4-O5	111.87	110.05	109.32	110.50
N4-O5-H6	104.26	101.66	101.22	101.04
H10-C1-C2-C3	58.63	58.50	57.78	57.92
H11-C1-C2-C3	-61.60	-61.47	-62.40	-62.20
H12-C1-C2-C3	178.45	178.52	177.65	177.76
C1-C2-C3-N4	119.77	117.09	119.20	118.25
C1-C2-C3-H7	-59.75	-61.65	-60.11	-60.92
H8-C2-C3-N4	-119.30	-121.60	-119.93	-120.82
H9-C2-C3-N4	-2.74	-4.99	-3.44	-4.48
C2-C3-N4-O5	-180.00	-179.11	-179.68	-179.68
C3-N4-O5-H6	-180.00	-180.00	-180.00	-180.00
E	-246.91906	-247.64974	-248.28118	-248.34803

E-sp form	ab initio MO[b]		DFT	
Parameters	HF/6-31G*	MP2/6-31G*	BLYP/6-31G	BLYP/6-31G*
C1-C2	1.526	1.525	1.547	1.541
C1-H10	1.083	1.092	1.102	1.100
C1-H11	1.083	1.092	1.102	1.100
C1-H12	1.085	1.093	1.103	1.102
C2-C3	1.502	1.497	1.515	1.512
C2-H8	1.088	1.098	1.109	1.109
C2-H9	1.088	1.098	1.109	1.109
C3-N4	1.251	1.285	1.300	1.289
C3-H7	1.081	1.093	1.100	1.103
N4-O5	1.376	1.419	1.505	1.439
O5-H6	0.947	0.973	0.992	0.981
H10-C1-H11	107.70	107.59	107.40	107.40
H10-C1-H12	108.36	108.60	108.49	108.43
H11-C1-H12	108.36	108.60	108.49	108.43
C1-C2-C3	114.98	114.37	115.35	115.42
H8-C2-H9	105.54	105.39	105.13	104.80
C2-C3-N4	121.82	120.22	120.59	120.84
N4-C3-H7	119.94	120.07	120.77	120.64
C3-N4-O5	111.79	109.93	109.24	110.50
N4-O5-H6	104.26	101.60	101.18	101.07
H10-C1-C2-C3	59.96	59.73	59.71	59.75
H11-C1-C2-C3	-59.96	-59.73	-59.71	-59.75
H12-C1-C2-C3	180.00	180.00	180.00	180.00
C1-C2-C3-N4	0.00	0.00	0.00	0.00
C1-C2-C3-H7	180.00	180.00	180.00	180.00
H8-C2-C3-N4	123.27	123.18	123.45	123.63
H9-C2-C3-N4	-123.27	-123.18	-123.45	-123.63
C2-C3-N4-O5	180.00	180.00	180.00	180.00
C3-N4-O5-H6	180.00	180.00	180.00	180.00
E	-246.91880	-247.64962	-248.28067	-248.34750

Z-ap form	ab initio MO[b]		DFT	
Parameters	HF/6-31G*	MP2/6-31G*	BLYP/6-31G	BLYP/6-31G*
C1-C2	1.528	1.526	1.547	1.542
C1-H10	1.086	1.094	1.104	1.104
C1-H11	1.086	1.094	1.104	1.104
C1-H12	1.084	1.093	1.102	1.102
C2-C3	1.506	1.500	1.514	1.515
C2-H8	1.086	1.097	1.107	1.107
C2-H9	1.086	1.097	1.107	1.107
C3-N4	1.253	1.289	1.303	1.292
C3-H7	1.077	1.089	1.097	1.098
N4-O5	1.375	1.418	1.510	1.443
O5-H6	0.946	0.973	0.991	0.981
H10-C1-H11	107.83	108.02	107.83	107.70
H10-C1-H12	107.74	107.83	107.74	107.70
H11-C1-H12	107.74	107.83	107.74	107.70
C1-C2-C3	112.45	112.52	113.11	113.22
H8-C2-H9	105.85	105.24	104.80	104.86
C2-C3-N4	126.71	126.21	127.70	127.46
N4-C3-H7	114.10	113.49	112.95	113.05
C3-N4-O5	112.14	109.73	109.34	110.41
N4-O5-H6	104.10	101.42	100.86	100.76
H10-C1-C2-C3	60.17	60.15	60.15	60.09
H11-C1-C2-C3	-60.17	-60.15	-60.15	-60.09
H12-C1-C2-C3	180.00	180.00	180.00	180.00
C1-C2-C3-N4	180.00	180.00	180.00	180.00
C1-C2-C3-H7	0.00	0.00	0.00	0.00
H8-C2-C3-N4	57.32	56.91	56.68	56.70
H9-C2-C3-N4	-57.32	-56.91	-56.68	-56.70
C2-C3-N4-O5	0.00	0.00	0.00	0.00
H7-C3-N4-O5	180.00	180.00	180.00	180.00
C3-N4-O5-H6	180.00	180.00	180.00	180.00
E	-246.91781	-247.64931	-248.28101	-248.34722

[a] The numbering of the atoms is given in Figure 2. Bond lengths are in angstroms and bond angles in degrees. Total energies, E, are in Hartrees. [b] r_e structure.

TABLE S2: Cartesian Coordinates of the Optimized Structures for E and Z Isomers of Propionaldehyde Oxime Calculated by ab initio MO and DFT Methods[a]

E-ac form

HF/6-31G*

	X	Y	Z
C1	-2.232930	-0.470226	-0.196656
C2	-1.187141	0.600445	0.131030
C3	0.168858	0.008336	0.377535
N4	1.145558	0.325317	-0.337004
O5	2.293391	-0.328877	0.045068
H6	2.952593	-0.013675	-0.556531
H7	0.292582	-0.706084	1.179632
H8	-1.495829	1.144776	1.020579
H9	-1.109992	1.317567	-0.677323
H10	-2.320605	-1.195896	0.606578
H11	-1.968956	-1.005021	-1.102903
H12	-3.208544	-0.019199	-0.343001

BLYP/6-31G

	X	Y	Z
C1	-2.281783	-0.480597	-0.218649
C2	-1.222906	0.594990	0.163117
C3	0.150521	0.001865	0.386945
N4	1.144862	0.382252	-0.360589
O5	2.389880	-0.356897	0.052676
H6	3.055537	0.017391	-0.580240
H7	0.288145	-0.754087	1.173674
H8	-1.545878	1.106041	1.091720
H9	-1.154426	1.363243	-0.625524
H10	-2.356881	-1.262339	0.557329
H11	-2.018000	-0.970548	-1.170602
H12	-3.276561	-0.017831	-0.332113

MP2/6-31G*

	X	Y	Z
C1	-2.222874	-0.484943	-0.203717
C2	-1.198770	0.602475	0.133731
C3	0.152609	0.024883	0.404520
N4	1.135910	0.333908	-0.364658
O5	2.311323	-0.337288	0.056003
H6	2.962488	-0.019364	-0.593602
H7	0.298247	-0.669955	1.236248
H8	-1.533762	1.161772	1.016074
H9	-1.107910	1.315797	-0.690925
H10	-2.309935	-1.210903	0.610076
H11	-1.926079	-1.022996	-1.107710
H12	-3.210788	-0.047890	-0.372781

BLYP/6-31G*

	X	Y	Z
C1	-2.265556	-0.476982	-0.210127
C2	-1.207184	0.599463	0.144646
C3	0.159847	0.010278	0.396317
N4	1.151862	0.343888	-0.357996
O5	2.349457	-0.341607	0.051819
H6	2.997136	0.006808	-0.598135
H7	0.292012	-0.713096	1.218019
H8	-1.535382	1.141068	1.053349
H9	-1.126640	1.342773	-0.665852
H10	-2.353353	-1.233279	0.588861
H11	-1.997795	-1.000560	-1.142618
H12	-3.257312	-0.014631	-0.347225

E-sp form

HF/6-31G*

	X	Y	Z
C1	-1.611247	-1.268285	0.000000
C2	-1.427964	0.246728	0.000000
C3	0.000000	0.713009	0.000000
N4	0.956671	-0.092457	0.000000
O5	2.170016	0.555790	0.000000
H6	2.808132	-0.143729	0.000000
H7	0.190681	1.776963	0.000000
H8	-1.920275	0.683968	0.866470
H9	-1.920275	0.683968	-0.866470
H10	-1.156004	-1.716897	0.874836
H11	-1.156004	-1.716897	-0.874836
H12	-2.667813	-1.515207	0.000000

BLYP/6-31G

	X	Y	Z
C1	-1.695097	-1.234370	0.000000
C2	-1.453703	0.293947	0.000000
C3	0.000000	0.721129	0.000000
N4	0.950311	-0.166109	0.000000
O5	2.282108	0.533900	0.000000
H6	2.905181	-0.238183	0.000000
H7	0.233549	1.795486	0.000000
H8	-1.944659	0.756230	0.880877
H9	-1.944659	0.756230	-0.880877
H10	-1.244611	-1.706117	0.887905
H11	-1.244611	-1.706117	-0.887905
H12	-2.776424	-1.450203	0.000000

MP2/6-31G*

	X	Y	Z
C1	-1.631146	-1.219260	0.000000
C2	-1.432815	0.292565	0.000000
C3	0.000000	0.727777	0.000000
N4	0.941723	-0.146900	0.000000
O5	2.203586	0.501275	0.000000
H6	2.813259	-0.257394	0.000000
H7	0.242579	1.793662	0.000000
H8	-1.925695	0.739766	0.873412
H9	-1.925695	0.739766	-0.873412
H10	-1.171965	-1.672088	0.881046
H11	-1.171965	-1.672088	-0.881046
H12	-2.697497	-1.460012	0.000000

BLYP/6-31G*

	X	Y	Z
C1	-1.661099	-1.249531	0.000000
C2	-1.443853	0.276590	0.000000
C3	0.000000	0.726808	0.000000
N4	0.960348	-0.133178	0.000000
O5	2.234838	0.534782	0.000000
H6	2.848770	-0.230998	0.000000
H7	0.214188	1.808318	0.000000
H8	-1.943347	0.732755	0.878436
H9	-1.943347	0.732755	-0.878436
H10	-1.204472	-1.715062	0.887642
H11	-1.204472	-1.715062	-0.887642
H12	-2.738741	-1.481917	0.000000

Z-ap form

HF/6-31G*

	X	Y	Z
C1	-2.238636	-0.443258	0.000000
C2	-0.719522	-0.605277	0.000000
C3	0.000000	0.717838	0.000000
N4	1.240402	0.896010	0.000000
O5	1.934428	-0.291006	0.000000
H6	2.843174	-0.026646	0.000000
H7	-0.575202	1.628796	0.000000
H8	-0.396767	-1.174618	0.866089
H9	-0.396767	-1.174618	-0.866089
H10	-2.577792	0.099085	-0.877653
H11	-2.577792	0.099085	0.877653
H12	-2.728134	-1.410927	0.000000

BLYP/6-31G

	X	Y	Z
C1	-2.293216	-0.381581	0.000000
C2	-0.757064	-0.567154	0.000000
C3	0.000000	0.744155	0.000000
N4	1.291414	0.918714	0.000000
O5	1.977941	-0.426593	0.000000
H6	2.929921	-0.150307	0.000000
H7	-0.559369	1.688316	0.000000
H8	-0.433636	-1.160331	0.877337
H9	-0.433636	-1.160331	-0.877337
H10	-2.629879	0.174860	-0.892339
H11	-2.629879	0.174860	0.892339
H12	-2.805269	-1.357844	0.000000

MP2/6-31G*

	X	Y	Z
C1	-2.246831	-0.396042	0.000000
C2	-0.731636	-0.573960	0.000000
C3	0.000000	0.734142	0.000000
N4	1.279079	0.890909	0.000000
O5	1.916831	-0.376158	0.000000
H6	2.855673	-0.119203	0.000000
H7	-0.552411	1.673049	0.000000
H8	-0.405568	-1.154532	0.871614
H9	-0.405568	-1.154532	-0.871614
H10	-2.578807	0.154433	-0.885135
H11	-2.578807	0.154433	0.885135
H12	-2.751912	-1.365590	0.000000

BLYP/6-31G*

	X	Y	Z
C1	-2.279326	-0.417076	0.000000
C2	-0.746337	-0.586415	0.000000
C3	0.000000	0.731701	0.000000
N4	1.280105	0.910230	0.000000
O5	1.965161	-0.359434	0.000000
H6	2.900466	-0.062931	0.000000
H7	-0.565267	1.673035	0.000000
H8	-0.417971	-1.175792	0.877072
H9	-0.417971	-1.175792	-0.877072
H10	-2.621840	0.136574	-0.891159
H11	-2.621840	0.136574	0.891159
H12	-2.783627	-1.397066	0.000000

[a] The numbering of the atoms is given in Figure 2. Coordinates are in angstroms.