

Table S1

Optimized geometric parameters^a (Å and degree), relative energy, and rotational constants for *anti* and *syn* forms of 2-cyclohexen-1-one oxime

	<i>anti</i> form		<i>syn</i> form	
	MP2/6-31G(d, p)	HF/6-31G(d, p)	MP2/6-31G(d, p)	HF/6-31G(d, p)
r(C1-C2)	1.504	1.510	1.504	1.508
r(C2-C3)	1.528	1.531	1.528	1.530
r(C1-C4)	1.459	1.473	1.460	1.475
r(C1=N)	1.299	1.260	1.297	1.259
r(C3-C6)	1.527	1.529	1.528	1.530
r(C4=C7)	1.347	1.324	1.349	1.325
r(N-O)	1.414	1.375	1.478	1.377
r(C2-H9)	1.095	1.089	1.095	1.089
r(C2-H10)	1.089	1.081	1.090	1.083
r(C3-H11)	1.091	1.086	1.091	1.086
r(C3-H12)	1.093	1.087	1.093	1.087
r(C4-H13)	1.083	1.075	1.080	1.072
r(C6-H14)	1.096	1.090	1.096	1.090
r(C6-H15)	1.092	1.086	1.093	1.087
r(C7-H16)	1.084	1.077	1.085	1.078
r(O-H17)	0.966	0.942	0.966	0.942
∠C3-C2-C1	110.54	111.12	109.46	110.40
∠C4-C1-C2	118.84	117.78	117.50	116.80
∠C2-C1-N	125.46	125.86	116.54	117.48
∠C6-C3-C2	111.32	111.91	110.26	110.80
∠C7-C4-C1	121.62	122.13	120.67	121.02
∠O-N-C1	110.84	113.09	111.22	113.26
∠H9-C2-C1	108.53	107.77	109.15	108.43
∠H10-C2-C1	109.43	109.85	109.36	109.33
∠H11-C3-C2	110.03	109.67	110.59	110.23
∠H12-C3-C2	108.85	109.00	108.95	109.16
∠H13-C4-C1	116.93	116.35	118.31	117.88
∠H14-C6-C3	109.88	110.35	109.83	110.24
∠H15-C6-C3	110.23	110.10	110.42	110.35
∠H16-C7-C4	119.35	119.25	119.02	118.88
∠H17-O-N	101.10	103.97	100.96	103.88
∠C4-C1-C2-C3	-28.89	-30.41	-40.38	-39.58
∠N-C1-C2-C3	153.44	151.93	140.43	141.48
∠C6-C3-C2-C1	54.47	53.30	59.27	57.14
∠C7-C4-C1-C2	0.35	2.64	9.82	10.26
∠O-N-C1-C2	-0.15	-0.64	179.54	178.97
∠H7-C2-C1-C4	91.84	90.14	78.88	80.08
∠H10-C2-C1-C4	-152.06	-153.77	-163.56	-162.95
∠H11-C3-C2-C1	177.47	176.10	181.73	179.44
∠H12-C3-C2-C1	-65.32	-67.14	-60.53	-63.22
∠H13-C4-C1-C2	181.87	184.16	190.18	190.67
∠H14-C6-C3-C2	69.65	73.04	73.25	75.60
∠H15-C6-C3-C2	-173.75	-170.21	-170.28	-167.69
∠H16-C7-C4-C1	182.76	182.56	182.27	181.78
∠H17-O-N-C1	-178.11	-178.80	-178.94	-179.59
A/MHz	4424.43	4447.04	4362.08	4386.45
B/MHz	1509.03	1519.57	1511.75	1526.14
C/MHz	1169.18	1175.24	1178.56	1186.39
$\Delta I^b / \text{u}\text{\AA}^2$	-16.878	-16.204	-21.346	-20.384
$\Delta E^c / \text{kJmol}^{-1}$	0.00	0.00	1.51	1.84

^a See Fig. 1 for the numbering of the atoms.

^b $\Delta I = I_c - I_a - I_b$

^c Relative energy