Supporting information for:

Tautomers and UV-Induced Photoisomerization of a Strongly Intramolecularly H-bonded Aromatic Azo-Dye: 1-(Cyclopropyl)diazo-2-Naphthol

Luís Duarte,[*,†] Barbara Michela Giuliano,[†,‡] Igor Reva,[†] and Rui Fausto[†]

Department of Chemistry, University of Coimbra, P-3004-535 Coimbra (Portugal)

E-mail: lduarte@qui.uc.pt

[*]To whom correspondence should be addressed

[†]University of Coimbra

[‡]Current address: Centro de Astrobiología, INTA-CSIC, Carretera de Ajalvir, km 4, Torrejón de Ardoz, 28850 Madrid (Spain)

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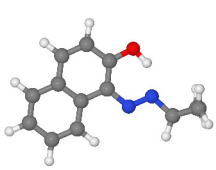
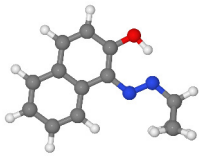
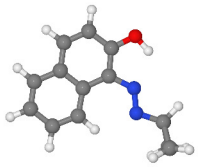


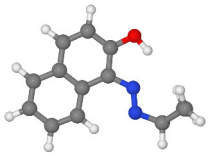
E1
(0.00)
(0.00)
(1.19 D)



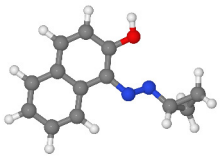
E2
(6.98)
(6.80)
(1.33 D)



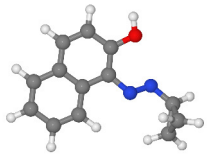
E3
(18.00)
(17.54)
(1.20 D)



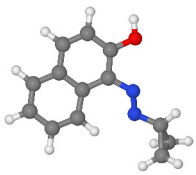
E4
(29.47)
(28.61)
(0.78 D)



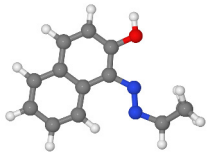
E5
(49.80)
(47.02)
(1.42 D)



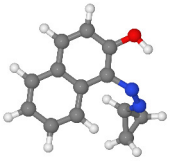
E6
(61.17)
(56.41)
(1.29 D)



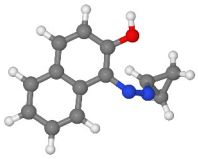
E7
(53.80)
(49.58)
(1.26 D)



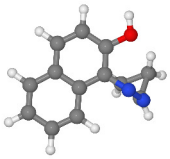
E8
(61.16)
(55.62)
(1.99 D)



E9
(67.84)
(67.01)
(2.93 D)

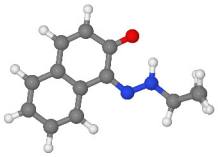


E10
(78.13)
(75.99)
(3.78 D)

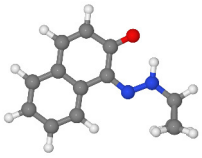


E11
(116.50)
(113.19)
(3.69 D)

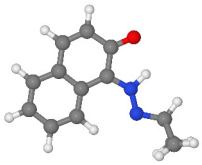
Figure S2: Structures of the calculated (B3LYP/6-311+G(2df,2p) keto-hydrazone forms of CPDNO. The relative energies, in kJ mol^{-1}, with zero point correction (top) and thermal correction to Gibbs Free Energy at 298 K (middle), and the dipole moments (bottom) are given below each structure.



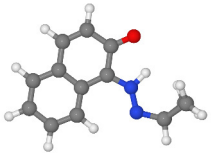
K1
(8.36)
(4.79)
(2.16 D)



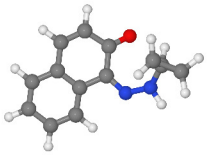
K2
(9.50)
(7.48)
(2.20 D)



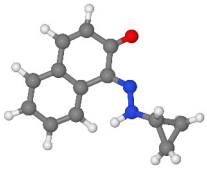
K3
(52.75)
(51.50)
(2.97 D)



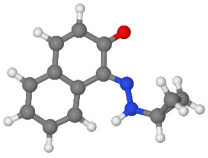
K4
(66.32)
(62.16)
(2.39 D)



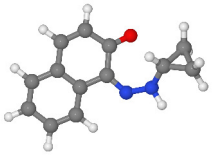
K5
(68.05)
(66.30)
(2.64 D)



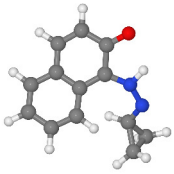
K6
(73.45)
(70.31)
(5.46 D)



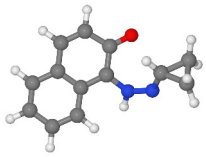
K7
(74.48)
(71.84)
(5.39 D)



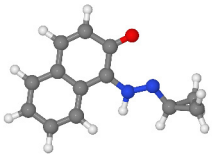
K8
(76.82)
(75.22)
(2.34 D)



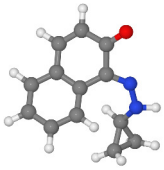
K9
(99.08)
(98.90)
(4.73 D)



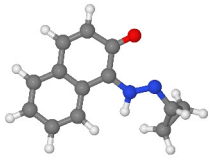
K10
(105.46)
(104.74)
(2.94 D)



K11
(105.61)
(102.46)
5.15 D)



K12
(107.41)
(106.08)
(5.97 D)



K13
(120.60)
(116.46)
(5.38 D)

Figure S3: Relaxed potential energy surface for the proton shift between the E3 and K3 minima in CPDNO calculated at the B3LYP/6-311+G(2df,2p) level of theory. The lowest energy vibrational levels are designated by horizontal lines. The change in the reaction coordinate (OH vs. NH distance) is designated by the vertical dashed line. The energy of E1 form was chosen as the relative zero.

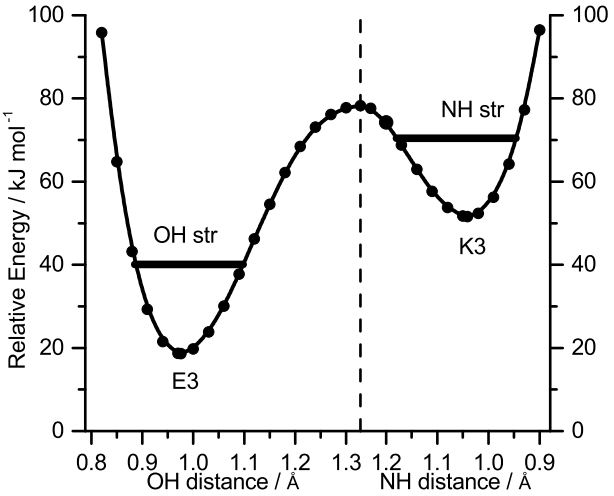


Figure S4: Relaxed potential energy surface for the proton shift between the E4 and K4 minima in CPDNO calculated at the B3LYP/6-311+G(2df,2p) level of theory. The lowest energy vibrational levels are designated by horizontal lines. The change in the reaction coordinate (OH vs. NH distance) is designated by the vertical dashed line. The energy of E1 form was chosen as the relative zero.

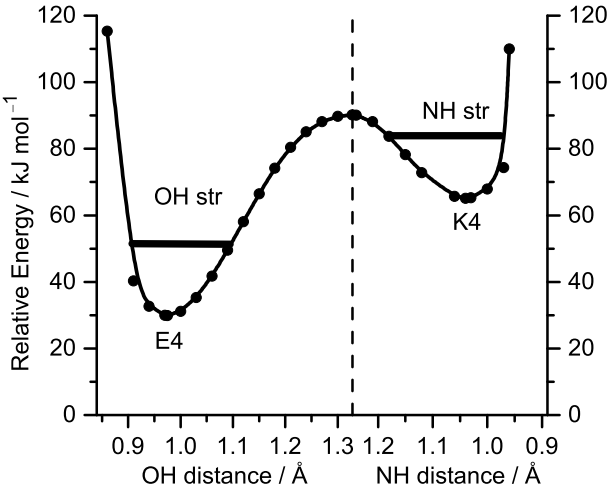


Figure S5: Experimental infrared spectrum of CPDNO in a KBr pellet compared with the calculated infrared spectra of CPDNO most stable isomeric forms. The calculated frequencies were scaled by a factor of 0.975. The calculated infrared spectra were simulated by fitting to a Lorentzian function (FWHM = 10 cm^{-1}).

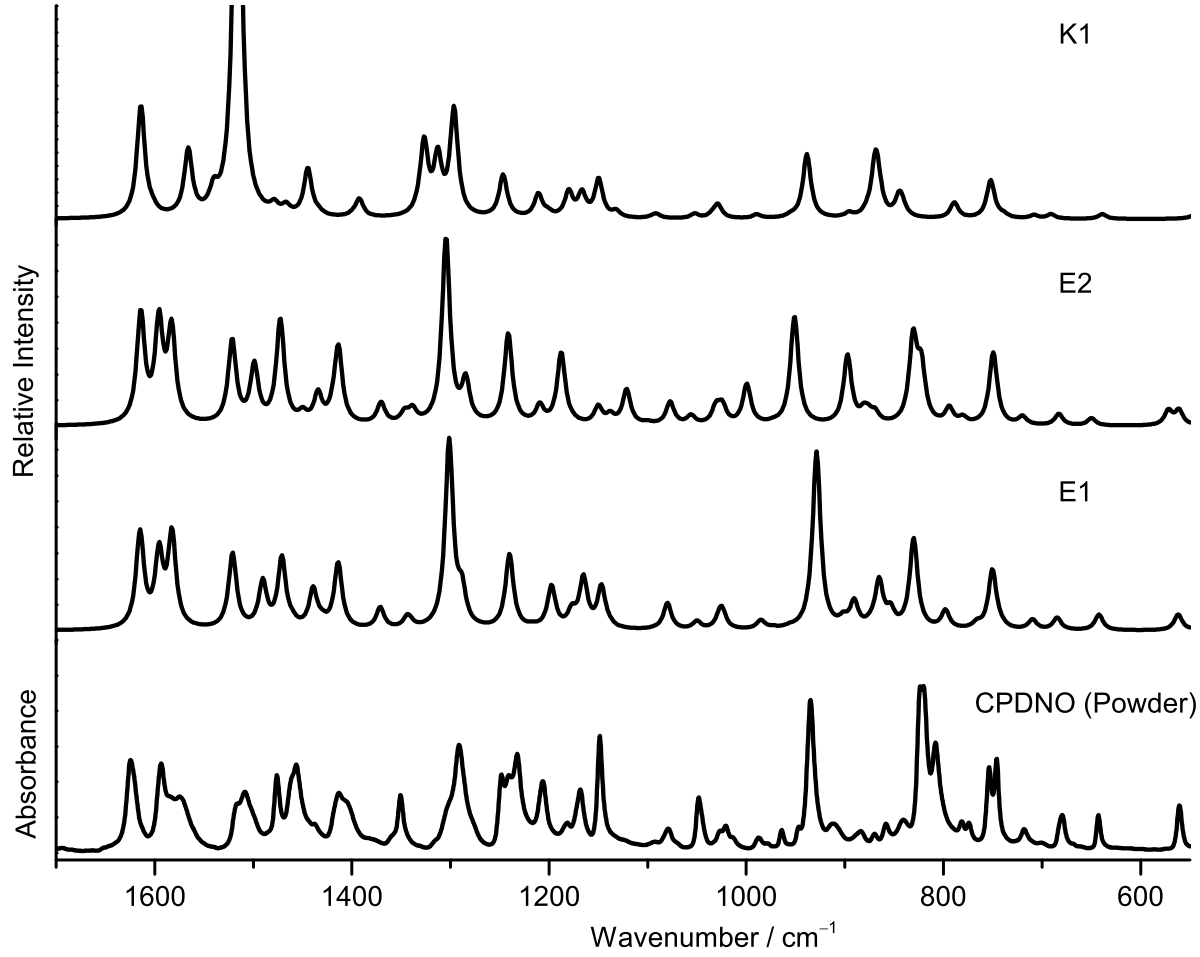


Figure S6: Experimental Raman spectrum of CPDNO in the solid state (powder) compared with the calculated Raman spectra of CPDNO most stable isomeric forms. The Raman spectrum of the sample was recorded with a DXR SmartRaman Spectrometer in the 3300-50 cm^{-1} range with excitation provided by a Nicolet DXR 780 nm laser (14 mW). The Raman activities were calculated at the B3LYP/6-311+G(2df,2p) level of theory and converted to relative Raman intensities using relations derived from the intensity theory of Raman scattering (see aditional references given at the end). The calculated Raman spectra were simulated by fitting to a Lorentzian function (FWHM = 10 cm^{-1}) and the calculated frequencies were scaled by a factor of 0.975.

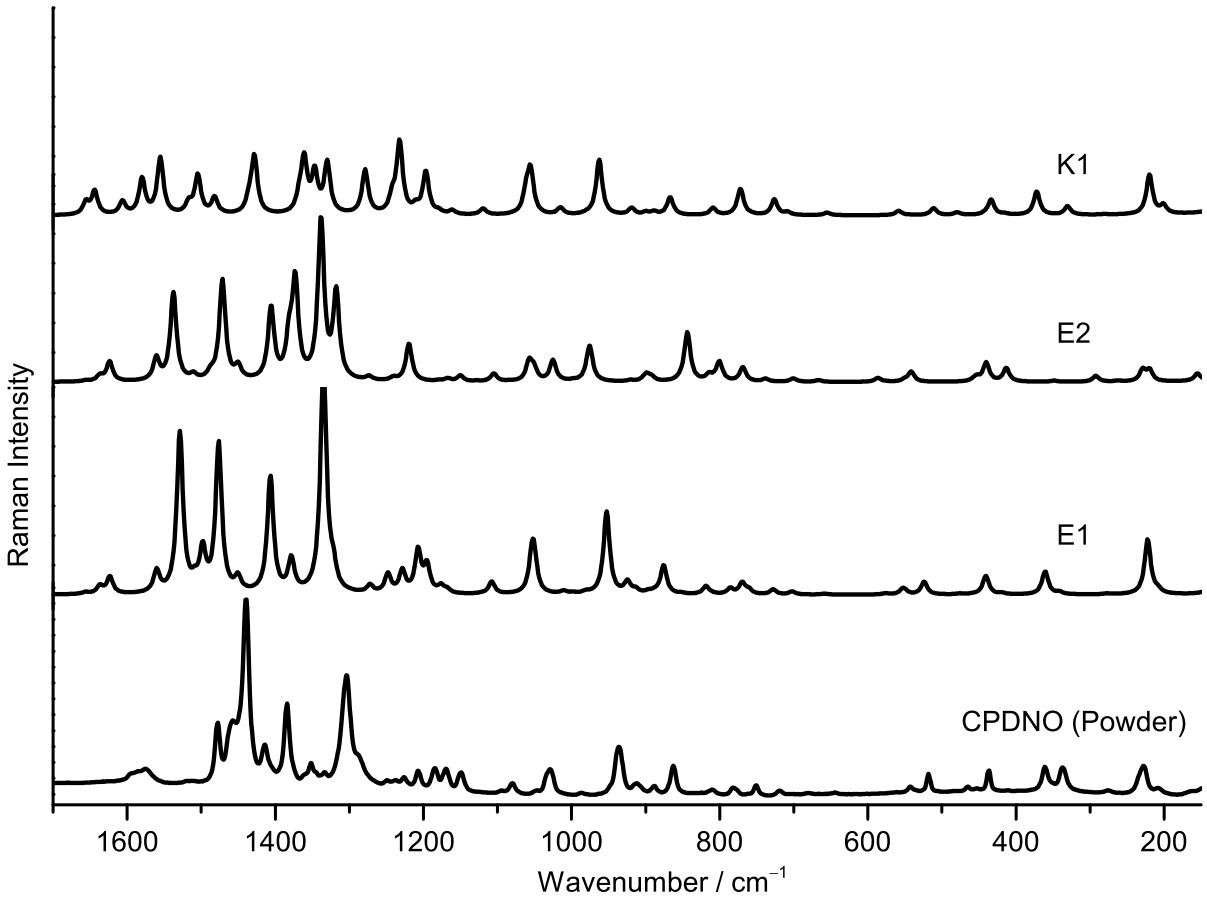


Figure S7: Experimental UV-visible spectrum of CPDNO in acetonitrile. The spectrum was obtained in a Shimadzu UV-2100 spectrometer using quartz cuvettes.

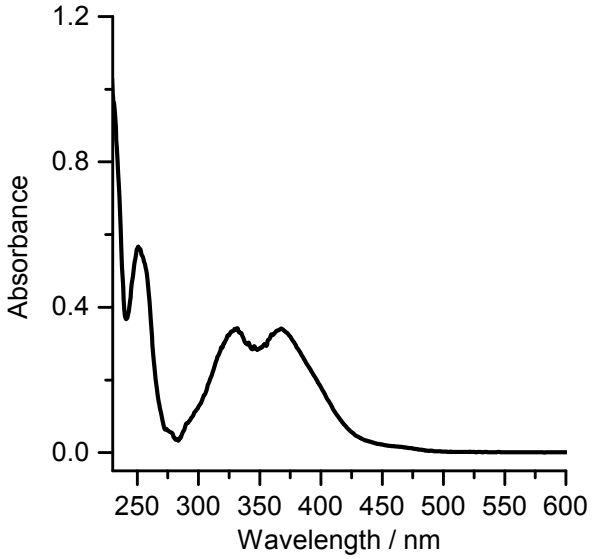


Table S1: **Cartesian coordinates of the optimized geometries of all considered isomeric forms. All calculations were carried out at the B3LYP/6-311+G(2df,2p) level of theory.**

Atom	E1			E2			E3			E4		
	x	y	z	x	y	z	x	y	z	x	y	z
C	-2.758860	-2.286090	0.000000	2.157790	-2.519680	0.000000	1.395760	-2.763600	0.000000	-2.264530	-2.439050	0.000000
C	-3.892860	-1.451430	0.000000	3.426980	-1.910830	0.000000	2.780690	-2.531350	0.000000	-3.503210	-1.777780	0.000000
C	-3.731150	-0.088870	0.000000	3.521250	-0.541730	0.000000	3.244260	-1.239170	0.000000	-3.531010	-0.405250	0.000000
C	-2.440880	0.488900	0.000000	2.361280	0.266020	0.000000	2.352840	-0.144000	0.000000	-2.336960	0.348480	0.000000
C	-1.293130	-0.355090	0.000000	1.076420	-0.349300	0.000000	0.940280	-0.375610	0.000000	-1.071730	-0.321050	0.000000
C	-1.490820	-1.755210	0.000000	1.010840	-1.761550	0.000000	0.496640	-1.720020	0.000000	-1.079310	-1.736730	0.000000
C	0.014660	0.242750	0.000000	-0.097040	0.482230	0.000000	0.069690	0.770120	0.000000	0.118740	0.488840	0.000000
C	0.138080	1.640370	0.000000	0.042020	1.879710	0.000000	0.622420	2.057460	0.000000	0.002790	1.884970	0.000000
C	-1.014900	2.457550	0.000000	1.327950	2.466910	0.000000	2.016150	2.263410	0.000000	-1.252420	2.523900	0.000000
C	-2.258990	1.896880	0.000000	2.445080	1.683710	0.000000	2.851470	1.185840	0.000000	-2.386950	1.767790	0.000000
N	1.098050	-0.633760	0.000000	-1.325780	-0.169990	0.000000	-1.327780	0.828820	0.000000	1.460090	0.094660	0.000000
N	2.253960	-0.137210	0.000000	-2.364540	0.538420	0.000000	-2.019350	-0.212960	0.000000	1.772060	-1.114710	0.000000
O	1.326470	2.253160	0.000000	-1.010860	2.700020	0.000000	-0.163770	3.148990	0.000000	1.095320	2.671460	0.000000
C	3.306110	-1.095020	0.000000	-3.610020	-0.172490	0.000000	-3.419510	0.036230	0.000000	3.182720	-1.382380	0.000000
C	4.567810	-0.722900	0.747460	-3.766830	-1.479710	-0.746640	-4.276600	-0.964590	-0.746590	4.163280	-0.501200	-0.746110
C	4.567810	-0.722900	-0.747460	-3.766830	-1.479710	0.746640	-4.276600	-0.964590	0.746590	4.163280	-0.501200	0.746110
H	-2.887150	-3.360840	0.000000	2.083600	-3.599520	0.000000	1.024460	-3.780420	0.000000	-2.236400	-3.521130	0.000000
H	-4.884020	-1.884800	0.000000	4.320200	-2.520990	0.000000	3.472850	-3.362690	0.000000	-4.424200	-2.345260	0.000000
H	-4.593220	0.566780	0.000000	4.490250	-0.057950	0.000000	4.308500	-1.037780	0.000000	-4.475530	0.124850	0.000000
H	-0.626820	-2.401790	0.000000	0.042390	-2.237580	0.000000	-0.560050	-1.919020	0.000000	-0.140740	-2.261600	0.000000
H	-0.872870	3.529480	0.000000	1.388640	3.546500	0.000000	2.388080	3.278180	0.000000	-1.281950	3.604250	0.000000
H	-3.135650	2.532890	0.000000	3.425100	2.144810	0.000000	3.924220	1.333980	0.000000	-3.356910	2.249370	0.000000
H	2.014390	1.535700	0.000000	-1.821340	2.118480	0.000000	-1.079900	2.813430	0.000000	1.856450	2.062650	0.000000
H	2.981410	-2.128280	0.000000	-4.445300	0.511110	0.000000	-3.716410	1.079450	0.000000	3.369870	-2.445480	0.000000
H	5.075920	-1.518560	1.273200	-4.695270	-1.641930	-1.275520	-5.136190	-0.573160	-1.271630	4.970170	-0.989820	-1.273570
H	5.075920	-1.518560	-1.273200	-4.695270	-1.641930	1.275520	-5.136190	-0.573160	1.271630	4.970170	-0.989820	1.273570
H	4.568210	0.231270	1.254470	-2.875800	-1.837220	-1.243180	-3.753370	-1.761670	-1.254260	3.730400	0.352030	-1.249510
H	4.568210	0.231270	-1.254470	-2.875800	-1.837220	1.243180	-3.753370	-1.761670	1.254260	3.730400	0.352030	1.249510

Atom	E5			E6			E7			E8		
	x	y	z	x	y	z	x	y	z	x	y	z
C	2.573380	-2.381140	-0.051340	2.056460	-2.574100	0.034710	1.241090	-2.766200	-0.046100	-2.222200	-2.451710	0.000000
C	3.754390	-1.629460	0.117570	3.350130	-2.014780	0.000800	2.638740	-2.604010	-0.024430	-3.472440	-1.810140	0.000000
C	3.684910	-0.262490	0.188720	3.498990	-0.652590	-0.024160	3.165530	-1.339690	0.006490	-3.519220	-0.440060	0.000000
C	2.441620	0.407850	0.096420	2.371180	0.202620	-0.014750	2.328050	-0.199230	0.023080	-2.333980	0.330600	0.000000
C	1.244630	-0.351010	-0.065120	1.061030	-0.359880	0.029420	0.904460	-0.356860	0.024450	-1.055110	-0.314860	0.000000
C	1.350980	-1.762690	-0.136490	0.942580	-1.772110	0.052750	0.398200	-1.681140	-0.018210	-1.048310	-1.733290	0.000000
C	-0.019510	0.317990	-0.136500	-0.085290	0.499880	0.062410	0.078280	0.821670	0.020910	0.134230	0.504090	0.000000
C	-0.058310	1.706550	-0.083520	0.098610	1.878620	0.011180	0.685550	2.075490	-0.001960	-0.005550	1.894290	0.000000
C	1.139070	2.443550	0.056100	1.403660	2.416770	-0.054180	2.088850	2.207740	0.015380	-1.276510	2.506140	0.000000
C	2.350260	1.818120	0.151540	2.505910	1.609690	-0.057910	2.886810	1.100280	0.029610	-2.407200	1.744210	0.000000
N	-1.143680	-0.503230	-0.381540	-1.342490	-0.140960	0.030410	-1.329870	0.875780	-0.043960	1.479600	0.099350	0.000000
N	-2.221560	-0.147390	0.131870	-2.287850	0.442060	0.592040	-1.984050	-0.074810	0.428710	1.761810	-1.115480	0.000000
O	-1.241820	2.367110	-0.209780	-0.971280	2.716440	-0.020600	-0.099900	3.184910	-0.007850	1.107860	2.672110	0.000000
C	-3.314620	-0.993830	-0.199410	-3.557340	-0.220460	0.485790	-3.392060	0.092820	0.287790	3.172840	-1.391930	0.000000
C	-4.367160	-1.155400	0.877860	-3.945780	-0.986940	-0.761590	-4.202860	-1.172880	0.109990	4.148970	-0.504900	-0.745710
C	-4.660220	-0.308160	-0.314850	-3.666440	-1.732440	0.498660	-4.237580	-0.453640	1.418350	4.148970	-0.504900	0.745710
H	2.632030	-3.460110	-0.113420	1.940500	-3.650120	0.048090	0.819610	-3.762530	-0.082130	-2.177030	-3.533260	0.000000
H	4.709450	-2.132750	0.188330	4.218190	-2.660340	-0.007570	3.287520	-3.469580	-0.038170	-4.384710	-2.391630	0.000000
H	4.583990	0.327890	0.316110	4.486130	-0.207840	-0.052810	4.238330	-1.190610	0.011420	-4.470290	0.078250	0.000000
H	0.451230	-2.344670	-0.265460	-0.043240	-2.209390	0.079070	-0.666340	-1.833260	-0.012980	-0.103610	-2.245490	0.000000
H	1.079020	3.525870	0.093580	1.516240	3.494790	-0.093930	2.523560	3.200860	0.020310	-1.339900	3.588370	0.000000
H	3.254320	2.402300	0.267240	3.496400	2.044720	-0.098360	3.964050	1.207070	0.041600	-3.381000	2.217440	0.000000
H	-1.065990	3.307040	-0.318860	-0.666100	3.608230	-0.216180	0.456570	3.967860	-0.061490	0.845540	3.597910	0.000000
H	-3.092170	-1.831090	-0.851610	-4.327920	0.340480	0.992190	-3.710130	0.997540	-0.217250	3.359780	-2.455290	0.000000
H	-4.831850	-2.127590	0.958950	-4.966070	-0.892460	-1.105710	-5.059620	-1.113440	-0.545980	4.956550	-0.989680	-1.276130
H	-5.331140	-0.683710	-1.074180	-4.488060	-2.164710	1.052030	-5.118740	0.112490	1.684230	4.956550	-0.989680	1.276130
H	-4.171860	-0.657740	1.816410	-3.189400	-1.018500	-1.533450	-3.650790	-2.099980	0.057610	3.705290	0.350230	-1.236160
H	-4.661610	0.764100	-0.186270	-2.726910	-2.261950	0.565060	-3.703340	-0.890450	2.249450	3.705290	0.350230	1.236160

Atom	E9			E10			E11			K1		
	x	y	z	x	y	z	x	y	z	x	y	z
C	3.358010	1.871090	-0.597980	2.721147	2.103629	0.210281	-2.611167	1.930670	-0.310506	2.799740	2.295070	0.000000
C	4.017000	2.458570	0.500730	3.706996	1.268394	-0.355476	-3.542780	1.057554	0.289400	3.918880	1.454120	0.000000
C	3.768960	1.997040	1.768010	3.423562	-0.048677	-0.610195	-3.184624	-0.235038	0.572246	3.737410	0.086550	0.000000
C	2.867580	0.930230	1.995240	2.148490	-0.588792	-0.316355	-1.886242	-0.714736	0.274116	2.446880	-0.470330	0.000000
C	2.227730	0.309120	0.876700	1.146896	0.261037	0.242565	-0.938855	0.174970	-0.319965	1.314730	0.380110	0.000000
C	2.487440	0.824910	-0.417510	1.471365	1.616262	0.499662	-1.341398	1.503546	-0.606637	1.521800	1.769270	0.000000
C	1.324590	-0.766130	1.124580	-0.147480	-0.268579	0.517841	0.372286	-0.300833	-0.604972	-0.014690	-0.218670	0.000000
C	0.998800	-1.114300	2.425800	-0.404282	-1.604831	0.280279	0.698308	-1.616257	-0.350667	-0.175870	-1.671600	0.000000
C	1.645240	-0.507740	3.520290	0.596361	-2.442943	-0.256360	-0.241668	-2.487882	0.234975	1.032230	-2.469600	0.000000
C	2.566650	0.479280	3.304640	1.837551	-1.949182	-0.552222	-1.501807	-2.049688	0.542821	2.256000	-1.895860	0.000000
N	0.524140	-1.408900	0.124900	-1.065707	0.555263	1.249251	1.256064	0.505568	-1.401210	-1.053180	0.614570	0.000000
N	0.986610	-2.073820	-0.820910	-2.168125	0.912529	0.807156	2.087911	1.313519	-0.983440	-2.256030	0.148260	0.000000
O	0.067120	-2.064200	2.690500	-1.644843	-2.093431	0.584203	1.966322	-2.034993	-0.659641	-1.309500	-2.210310	0.000000
C	2.383340	-2.322330	-0.967270	-2.596257	0.595879	-0.517117	2.408972	1.592121	0.400444	-3.361180	1.049670	0.000000
C	2.868740	-2.408190	-2.402960	-3.503436	1.642040	-1.137380	3.258204	0.612237	1.183386	-4.611780	0.680020	0.753030
C	2.693600	-3.659070	-1.618870	-4.084613	0.357683	-0.658153	1.898173	0.990806	1.691686	-4.611780	0.680020	-0.753030
H	3.534860	2.253580	-1.594780	2.954567	3.139483	0.419120	-2.902498	2.946875	-0.541496	2.934510	3.369000	0.000000
H	4.704240	3.278740	0.342350	4.685937	1.668996	-0.582757	-4.539260	1.409863	0.520212	4.915930	1.873480	0.000000
H	4.253520	2.454170	2.622040	4.175879	-0.698568	-1.040040	-3.895310	-0.913915	1.027348	4.592570	-0.578210	0.000000
H	1.980670	0.400280	-1.271900	0.721602	2.259573	0.937622	-0.639146	2.179794	-1.072927	0.664130	2.425490	0.000000
H	1.388430	-0.839050	4.516960	0.364315	-3.486861	-0.436402	0.049466	-3.511334	0.443650	0.903280	-3.543460	0.000000
H	3.065200	0.946810	4.144120	2.595593	-2.600257	-0.968025	-2.217286	-2.725422	0.992832	3.142160	-2.520640	0.000000
H	-0.383280	-2.283770	1.860820	-1.656102	-3.047731	0.467029	2.031720	-2.987351	-0.543193	-3.032780	2.078260	0.000000
H	3.065170	-1.950090	-0.215560	-1.922087	0.050274	-1.164062	2.742612	2.619025	0.458281	-4.622120	-0.278180	1.254010
H	3.865980	-2.038670	-2.592830	-3.391378	1.805387	-2.199639	4.143349	0.996713	1.669657	-4.622120	-0.278180	-1.254010
H	2.138990	-2.184760	-3.167440	-3.679851	2.529950	-0.548169	1.833873	1.679162	2.524042	-5.131710	1.468090	1.278980
H	1.844710	-4.286650	-1.846740	-4.656055	0.370179	0.258172	3.362970	-0.371867	0.749036	-5.131710	1.468090	-1.278980
H	3.568040	-4.175490	-1.250040	-4.385649	-0.387634	-1.380012	1.125368	0.243204	1.671207	-2.345900	-0.885410	0.000000

Atom	K2			K3			K4			K5		
	x	y	z	x	y	z	x	y	z	x	y	z
C	2.215730	-2.519260	0.000000	1.574610	2.736720	0.000000	-2.414600	-2.349930	0.000000	3.132933	1.882621	-0.062901
C	3.467820	-1.894140	0.000000	2.935210	2.426850	0.000000	-3.604540	-1.621240	0.000000	3.977207	0.852941	0.358812
C	3.535830	-0.515940	0.000000	3.328220	1.100220	0.000000	-3.553650	-0.238380	0.000000	3.463638	-0.420156	0.516679
C	2.367380	0.264570	0.000000	2.384840	0.065660	0.000000	-2.329020	0.440310	0.000000	2.112853	-0.690851	0.251520
C	1.100270	-0.367320	0.000000	0.995280	0.379970	0.000000	-1.113390	-0.302320	0.000000	1.255666	0.351383	-0.168335
C	1.053770	-1.770860	0.000000	0.615930	1.736160	0.000000	-1.186180	-1.708600	0.000000	1.793149	1.638067	-0.310536
C	-0.099860	0.461760	0.000000	0.078940	-0.724220	0.000000	0.107730	0.450740	0.000000	-0.174997	0.064770	-0.396815
C	0.005330	1.921660	0.000000	0.509310	-2.124340	0.000000	0.146950	1.914660	0.000000	-0.611614	-1.360134	-0.452026
C	1.338940	2.487500	0.000000	1.941380	-2.347860	0.000000	-1.136720	2.585880	0.000000	0.319021	-2.347265	0.087069
C	2.438020	1.701770	0.000000	2.807400	-1.311360	0.000000	-2.288870	1.880290	0.000000	1.587033	-2.027350	0.404493
N	-1.271540	-0.166970	0.000000	-1.269960	-0.654480	0.000000	1.364010	-0.045170	0.000000	-0.914686	1.112487	-0.657932
N	-2.372730	0.504140	0.000000	-2.050610	0.353960	0.000000	1.772570	-1.253210	0.000000	-2.226097	1.152265	-0.683309
O	-1.010410	2.655790	0.000000	-0.324850	-3.048940	0.000000	1.235850	2.521220	0.000000	-1.648841	-1.712414	-1.014674
C	-3.639030	-0.166060	0.000000	-3.427600	0.015630	0.000000	3.187710	-1.436220	0.000000	-3.172297	0.289437	-0.028369
C	-3.832860	-1.454560	0.752480	-4.362880	0.943380	-0.747670	4.156250	-0.538510	0.748550	-4.246375	0.953986	0.776277
C	-3.832860	-1.454560	-0.752480	-4.362880	0.943380	0.747670	4.156250	-0.538510	-0.748550	-3.140370	0.197423	1.473486
H	2.154270	-3.599860	0.000000	1.258510	3.771830	0.000000	-2.446070	-3.431730	0.000000	3.525703	2.882548	-0.194143
H	4.372900	-2.486380	0.000000	3.675590	3.215330	0.000000	-4.558090	-2.131780	0.000000	5.021578	1.049960	0.560095
H	4.496890	-0.016420	0.000000	4.380740	0.844470	0.000000	-4.469420	0.340010	0.000000	4.103671	-1.230027	0.844636
H	0.092280	-2.262470	0.000000	-0.430300	1.991550	0.000000	-0.275450	-2.283630	0.000000	1.142960	2.442145	-0.621151
H	1.406380	3.566960	0.000000	2.276810	-3.375700	0.000000	-1.125870	3.666980	0.000000	-0.049953	-3.361997	0.152607
H	3.422820	2.155390	0.000000	3.874510	-1.502910	0.000000	-3.238770	2.402830	0.000000	2.265284	-2.794568	0.761112
H	-4.444140	0.553330	0.000000	-3.667620	-1.045180	0.000000	3.415540	-2.491070	0.000000	-3.402312	-0.616964	-0.567733
H	-2.957110	-1.852940	1.244640	-3.901660	1.778120	-1.254620	3.743250	0.324060	1.256110	-5.236507	0.523124	0.740243
H	-2.957110	-1.852940	-1.244640	-3.901660	1.778120	1.254620	3.743250	0.324060	-1.256110	-4.232584	2.033144	0.859568
H	-4.765570	-1.596040	1.279800	-5.190180	0.487200	-1.272550	4.968510	-1.016730	1.277070	-2.397548	0.781418	1.997844
H	-4.765570	-1.596040	-1.279800	-5.190180	0.487200	1.272550	4.968510	-1.016730	-1.277070	-3.361314	-0.761543	1.919365
H	-2.284770	1.534010	0.000000	-1.644340	-1.625640	0.000000	2.015520	0.765620	0.000000	-2.556441	2.079806	-0.899092

Atom	K6			K7			K8			K9		
	x	y	z	x	y	z	x	y	z	x	y	z
C	1.679100	2.668520	-0.456180	-2.274796	-2.406116	-0.378528	3.275670	1.851420	-0.103730	-0.603091	-2.788569	0.564597
C	2.961730	2.358980	-0.019580	-3.416197	-1.816609	0.152407	4.136040	0.782840	0.158040	-1.892766	-2.937907	0.049493
C	3.267100	1.046850	0.310690	-3.393440	-0.467911	0.474359	3.611570	-0.488080	0.297570	-2.587917	-1.814274	-0.355317
C	2.302040	0.039280	0.238590	-2.237812	0.298500	0.303297	2.233340	-0.717470	0.171800	-2.012623	-0.537654	-0.288787
C	0.971070	0.360310	-0.133930	-1.045167	-0.312220	-0.166262	1.360520	0.363650	-0.087260	-0.665013	-0.390628	0.151808
C	0.698900	1.683670	-0.511790	-1.108599	-1.665673	-0.535245	1.910980	1.646490	-0.213540	-0.002349	-1.543644	0.619739
C	-0.025120	-0.722300	-0.149770	0.159355	0.518735	-0.286872	-0.092470	0.116090	-0.175370	-0.134548	0.945616	0.206074
C	0.453590	-2.148130	-0.199890	0.021994	2.013727	-0.293520	-0.571760	-1.294570	-0.244290	-0.990239	2.129180	0.082612
C	1.830940	-2.366560	0.264820	-1.238315	2.535480	0.251197	0.391830	-2.329250	0.121440	-2.348281	1.886271	-0.368083
C	2.671460	-1.342820	0.482700	-2.270017	1.727857	0.544825	1.695640	-2.051400	0.305670	-2.801251	0.631749	-0.576581
N	-1.314820	-0.631630	-0.009130	1.405573	0.131613	-0.288451	-0.829540	1.189610	-0.307980	1.138506	1.341268	0.517050
N	-1.960070	0.507800	0.175290	1.801582	-1.109693	-0.160964	-2.135240	1.277660	-0.218940	2.331459	0.903366	0.378907
O	-0.250630	-3.075840	-0.557760	0.905160	2.763975	-0.677252	-1.687690	-1.585680	-0.670420	-0.545667	3.268171	0.309670
C	-3.305160	0.415380	0.674850	3.192197	-1.362108	0.133054	-3.049060	0.435090	0.513100	2.557733	-0.245094	-0.406304
C	-4.389850	0.025670	-0.280490	3.922747	-0.598734	1.210754	-4.199760	-0.242780	-0.163920	3.620940	-1.218436	0.086869
C	-4.286970	1.448960	0.201780	4.239435	-0.368204	-0.246860	-4.443970	0.966770	0.698660	3.942423	-0.294818	-1.034514
H	1.438130	3.677200	-0.764470	-2.290543	-3.444077	-0.683507	3.675760	2.850520	-0.218210	-0.067509	-3.652045	0.937324
H	3.721100	3.126880	0.038620	-4.319586	-2.395346	0.288762	5.200930	0.948150	0.251370	-2.352125	-3.915460	-0.002429
H	4.273680	0.784620	0.612130	-4.288073	0.014681	0.848049	4.263920	-1.328020	0.502710	-3.607703	-1.903997	-0.709058
H	-0.265920	1.946420	-0.918870	-0.268505	-2.140356	-1.019648	1.250630	2.479700	-0.401680	0.979349	-1.461837	1.058163
H	2.136510	-3.397170	0.384650	-1.294517	3.608204	0.377728	0.007470	-3.339060	0.174310	-2.969060	2.755937	-0.534020
H	3.689930	-1.532970	0.802330	-3.193451	2.143198	0.932631	2.391560	-2.850360	0.536520	-3.815226	0.474860	-0.926414
H	-3.391030	0.064590	1.697880	3.417966	-2.412681	0.013446	-2.576070	-0.076770	1.340290	1.103440	2.316926	0.846476
H	-5.188330	-0.596010	0.097020	4.629486	-1.134573	1.828914	-4.483860	-1.218860	0.199880	1.737851	-0.647441	-0.982504
H	-4.089830	-0.187380	-1.295680	3.364402	0.178541	1.713396	-4.264590	-0.124510	-1.235080	3.453556	-2.265035	-0.123486
H	-3.929990	2.188570	-0.501450	3.890939	0.557897	-0.679361	-4.695060	1.895780	0.200960	4.046137	-1.004579	1.056348
H	-5.014150	1.816270	0.911390	5.168569	-0.749429	-0.646059	-4.906740	0.846530	1.667960	4.584826	0.549186	-0.832536
H	-1.434890	1.330680	0.454180	1.146938	-1.812730	0.166499	-2.423900	2.241830	-0.288350	3.994861	-0.689838	-2.038994

Atom	K10			K11			K12			K13		
	x	y	z	x	y	z	x	y	z	x	y	z
C	3.049470	2.007340	-0.000824	-2.600556	-2.394026	0.079883	0.214263	2.675928	-0.847159	2.208300	-2.499004	-0.464880
C	4.008228	1.012321	0.208367	-3.770889	-1.648069	-0.077852	-0.870004	3.224808	-0.169116	3.437231	-1.934356	-0.117847
C	3.604663	-0.306517	0.301172	-3.686230	-0.270268	-0.140509	-1.794680	2.382252	0.430230	3.500308	-0.583146	0.165298
C	2.257592	-0.667891	0.160231	-2.451466	0.390048	-0.074084	-1.638918	0.994093	0.383011	2.354603	0.223648	0.134185
C	1.280866	0.336879	-0.081674	-1.252798	-0.363580	0.049834	-0.486802	0.437043	-0.223685	1.094926	-0.350266	-0.183283
C	1.711279	1.680149	-0.123767	-1.371202	-1.765323	0.156574	0.402465	1.300114	-0.871265	1.065281	-1.721107	-0.510193
C	-0.093652	-0.059668	-0.234046	0.003267	0.350576	0.086301	-0.357353	-1.029719	-0.279582	-0.070614	0.510577	-0.180880
C	-0.517986	-1.450781	-0.191646	0.080603	1.811531	0.103475	-1.624130	-1.847880	-0.157429	0.021209	1.958537	0.032666
C	0.542208	-2.404079	0.125705	-1.208588	2.492399	-0.021580	-2.707143	-1.197966	0.598767	1.364011	2.447310	0.351448
C	1.832223	-2.036311	0.271122	-2.376786	1.827339	-0.111180	-2.691956	0.118462	0.863689	2.437976	1.636992	0.403069
N	-0.962502	0.904788	-0.711020	1.142855	-0.387161	-0.012264	0.692523	-1.780355	-0.405903	-1.284450	-0.085552	-0.270912
N	-2.213170	1.116970	-0.576449	2.353279	-0.022697	0.155300	1.966575	-1.406302	-0.292926	-2.437568	0.442117	-0.424168
O	-1.665222	-1.825461	-0.477881	1.139044	2.439559	0.171029	-1.741810	-2.980798	-0.586246	-0.948580	2.714838	-0.002359
C	-2.920089	0.429190	0.414270	3.305365	-1.015934	-0.160836	2.470654	-0.365459	0.579061	-3.520286	-0.495558	-0.349884
C	-4.347020	0.036889	0.069848	4.603279	-0.981610	0.620362	3.413357	0.696550	0.077505	-4.330925	-0.611841	0.909009
C	-4.125358	1.203093	0.959482	4.594913	-0.540538	-0.806219	3.925090	-0.428887	0.937293	-3.499474	-1.784410	0.443767
H	3.349499	3.046205	-0.042936	-2.652725	-3.471519	0.164700	0.913876	3.320129	-1.363464	2.147537	-3.548454	-0.721263
H	5.051768	1.274520	0.316098	-4.731187	-2.142279	-0.130395	-1.007930	4.297103	-0.134485	4.330266	-2.543354	-0.089788
H	4.333626	-1.085988	0.486513	-4.585566	0.325275	-0.238829	-2.669591	2.795057	0.917093	4.449192	-0.123924	0.413772
H	0.992369	2.485139	-0.210907	-0.503505	-2.386966	0.342331	1.233985	0.890326	-1.421874	0.150726	-2.196634	-0.843422
H	0.234823	-3.439035	0.193086	-1.164288	3.572975	-0.040066	-3.538271	-1.831272	0.878328	1.439391	3.509011	0.543594
H	2.589732	-2.784718	0.474532	-3.307856	2.374972	-0.203811	-3.522922	0.578950	1.386440	3.414155	2.043602	0.642016
H	-0.533602	1.593475	-1.324823	2.922772	-1.990278	-0.468505	2.543289	-2.234234	-0.293544	-4.096597	-0.494723	-1.268573
H	-2.380654	-0.218406	1.086112	5.047989	-1.934127	0.871692	1.769180	-0.086598	1.354282	-5.406374	-0.658513	0.816888
H	-4.679620	-0.901765	0.486706	4.673014	-0.221857	1.384605	3.337282	1.687037	0.503127	-3.970898	-0.067187	1.770390
H	-4.650642	0.220785	-0.949420	4.653768	0.518137	-1.010120	3.670836	0.670401	-0.972160	-2.637983	-2.034992	1.049342
H	-4.280533	2.193772	0.558940	5.031220	-1.184045	-1.557088	4.524273	-1.190547	0.454086	-3.995689	-2.646099	0.020343
H	-4.300935	1.098723	2.020917	0.981774	-1.361777	-0.289764	4.206049	-0.227498	1.960989	-1.259606	-1.106234	-0.174102

Table S2: Theoretical Frequencies (ν / cm^{-1}) and IR Intensities (I / km mol^{-1}) of all considered isomeric forms. All calculations were carried out at the B3LYP/6-311+G(2df,2p) level of theory. The calculated frequencies are not scaled.

E1		E2		E3		E4		E5	
ν	I	ν	I	ν	I	ν	I	ν	I
3226.9	4.8	3225.5	10.0	3588.6	98.7	3603.7	93.4	3817.6	70.7
3213.2	0.1	3213.2	0.6	3253.8	5.9	3251.9	6.2	3230.2	5.8
3212.9	4.7	3212.2	5.2	3228.4	6.5	3222.9	12.5	3217.0	0.1
3193.4	9.4	3193.6	8.3	3215.0	0.1	3209.0	0.4	3210.8	3.7
3186.1	24.1	3186.7	8.8	3198.9	6.8	3199.2	6.1	3185.2	24.4
3168.9	12.0	3186.3	28.3	3186.2	23.0	3186.3	23.7	3174.5	16.3
3165.6	3.9	3169.0	15.4	3168.6	20.7	3184.1	15.2	3168.5	10.6
3159.0	1.1	3165.1	1.3	3166.3	0.4	3169.1	20.3	3158.4	1.3
3157.1	163.7	3159.3	0.7	3158.5	0.9	3166.7	0.4	3143.5	11.1
3145.2	92.5	3131.7	9.5	3139.1	17.4	3158.5	1.0	3140.1	19.4
3135.7	5.2	3131.7	13.7	3135.9	13.5	3129.7	14.8	3136.8	13.4
3135.2	12.6	3089.1	216.7	3121.8	24.7	3129.1	11.2	3127.0	14.7
1656.5	57.5	1655.8	65.8	1653.2	77.4	1653.1	72.9	1658.6	32.9
1636.7	43.3	1636.8	59.6	1635.4	61.5	1635.3	50.9	1640.9	13.5
1623.3	55.9	1623.7	55.4	1616.2	31.3	1617.2	19.8	1614.8	15.8
1560.2	45.4	1560.6	50.3	1565.2	23.6	1568.2	33.7	1568.3	2.1
1528.8	27.5	1537.6	34.6	1549.2	67.4	1551.7	71.9	1543.6	41.4
1508.9	42.1	1510.5	63.0	1497.8	38.2	1496.6	32.5	1503.0	4.5
1498.0	2.7	1487.2	5.4	1495.9	11.7	1483.9	9.5	1494.3	1.8
1476.4	22.9	1471.3	17.3	1478.7	11.3	1477.9	7.7	1466.6	19.5
1467.1	3.3	1454.9	4.9	1464.0	3.3	1456.2	4.7	1461.9	3.2
1450.4	39.6	1450.1	44.9	1425.4	54.7	1424.9	43.4	1418.3	4.0
1406.6	12.6	1405.7	12.7	1403.7	21.8	1402.7	15.3	1396.2	5.7
1378.5	6.2	1381.2	6.1	1379.9	0.8	1372.5	4.6	1377.2	16.3
1375.1	1.8	1373.0	7.8	1368.8	3.2	1370.6	1.3	1372.1	30.5
1334.9	114.0	1338.2	112.7	1311.3	37.7	1313.6	35.4	1303.9	23.8
1321.7	19.8	1317.7	24.6	1301.5	25.0	1302.7	27.0	1276.4	104.3
1272.1	45.1	1273.4	54.7	1255.3	157.5	1251.0	173.6	1244.8	1.6
1248.0	1.1	1240.6	10.3	1236.1	28.9	1236.4	29.9	1231.0	27.1
1228.4	25.5	1219.6	3.9	1218.8	18.9	1213.1	15.8	1220.5	4.5
1207.2	9.2	1218.1	39.6	1199.8	0.6	1205.2	0.7	1200.8	0.7
1199.7	0.5	1206.2	0.8	1197.3	39.4	1202.5	14.5	1196.9	13.8
1195.1	29.9	1179.8	10.4	1183.2	4.9	1182.0	15.4	1192.3	11.9
1176.4	24.9	1167.3	5.1	1178.7	73.3	1167.6	3.5	1174.8	9.6
1167.8	1.4	1150.3	21.1	1167.3	5.7	1147.6	38.0	1167.8	8.2
1122.5	0.3	1128.0	1.1	1119.5	0.2	1129.7	0.8	1122.8	0.2
1107.8	16.0	1105.0	13.9	1095.8	11.0	1088.9	12.3	1091.1	40.6
1077.1	4.8	1083.2	5.2	1075.8	4.0	1075.5	4.4	1076.3	3.5
1053.5	6.3	1057.3	9.8	1061.5	7.1	1065.1	0.8	1052.5	6.0
1050.7	9.0	1050.8	10.5	1047.1	4.8	1048.2	15.5	1047.5	3.5
1014.6	0.2	1025.2	24.2	1022.2	0.4	1023.6	0.6	1013.0	0.3
1010.5	5.1	1012.8	0.1	1016.0	11.6	1022.9	19.7	991.5	30.9
998.2	0.9	998.1	0.8	999.0	0.7	998.5	0.8	987.2	3.2
980.3	0.8	979.4	0.8	981.9	0.8	982.0	0.8	964.2	0.1
952.6	107.8	975.5	65.4	949.7	114.7	960.7	75.9	938.1	140.8
924.6	4.7	920.4	41.7	910.4	0.3	904.3	0.8	923.0	1.0
913.5	15.4	903.5	6.3	905.0	1.0	900.3	0.2	903.0	4.8
896.4	2.0	898.7	4.7	900.4	0.5	894.2	5.6	887.6	0.9
887.5	28.3	891.7	5.8	870.4	2.0	849.7	46.0	872.6	5.7
875.7	9.4	852.2	50.4	850.3	44.0	828.2	18.7	825.3	54.7
851.6	54.8	843.6	31.9	818.0	7.2	815.2	1.6	821.5	13.2
818.6	10.9	814.6	9.5	811.6	3.0	809.7	6.7	803.6	1.6
810.3	0.0	806.9	0.0	780.1	3.1	791.0	9.8	783.6	2.7
785.7	3.1	800.4	3.7	770.3	30.9	770.3	31.9	764.7	24.9
769.7	36.3	768.9	36.0	753.3	7.8	762.2	4.1	756.2	3.0
760.8	1.5	768.3	8.1	726.0	51.4	735.0	7.1	724.6	4.5
727.9	6.0	738.3	4.9	722.3	5.6	715.7	26.8	687.8	18.6
702.3	7.4	700.6	7.0	697.5	32.8	692.6	47.5	654.4	8.8
658.8	9.4	666.6	4.4	630.4	2.7	655.3	5.7	584.8	8.4
576.4	9.6	586.5	8.8	595.7	19.8	583.8	5.3	559.3	2.7
552.7	2.3	575.6	8.8	584.5	4.7	578.3	12.2	541.5	1.8
550.1	0.0	550.3	0.0	548.3	1.4	547.4	1.6	525.3	4.1
524.0	2.7	541.4	5.4	532.5	4.2	542.9	5.2	466.3	2.7
475.9	16.1	458.0	4.2	460.0	20.4	491.0	25.6	452.2	0.9
459.1	3.8	453.1	23.6	458.2	2.8	455.6	3.8	434.9	2.1
440.7	2.7	440.1	4.1	439.6	0.9	439.2	1.2	418.0	3.4
419.1	0.3	413.5	0.2	419.8	2.0	413.4	0.8	360.9	26.0
363.9	0.1	413.1	2.7	356.5	2.3	350.4	7.7	349.5	39.4
360.4	3.3	348.6	0.2	346.9	7.4	336.1	1.7	338.1	34.7
341.2	9.4	292.2	5.6	274.7	0.7	314.9	1.5	301.7	0.5
277.1	0.0	262.4	0.0	271.4	1.1	256.2	1.5	267.2	0.6
222.2	2.3	228.9	0.6	263.4	1.3	199.3	0.1	224.6	4.5
208.4	2.9	219.6	2.8	197.6	0.6	191.9	0.0	166.9	3.2
139.1	0.3	155.0	0.6	141.1	0.3	155.2	0.9	137.1	0.7
125.3	0.1	120.1	0.3	106.6	1.0	118.7	0.6	117.9	2.2
96.8	1.1	97.2	0.8	85.9	1.1	100.1	1.3	75.5	1.3
71.4	0.4	78.2	0.7	72.2	0.6	62.8	0.1	67.9	0.7
49.1	0.5	38.6	0.2	39.8	0.0	34.9	0.5	32.7	0.7

E6		E7		E8		E9		E10	
ν	*I*	ν	*I*	ν	*I*	ν	*I*	ν	*I*
3814.8	72.6	3826.4	89.4	3822.8	82.1	3706.5	75.4	3837.6	90.3
3225.0	10.6	3249.2	3.8	3257.8	10.1	3232.7	4.0	3231.1	5.5
3215.6	4.7	3227.5	7.5	3224.0	10.2	3219.6	0.1	3218.1	0.1
3211.5	0.6	3213.8	0.3	3210.8	0.8	3198.9	6.6	3198.0	5.5
3186.7	6.3	3185.8	23.0	3185.6	24.1	3194.8	7.1	3184.9	21.5
3185.7	32.5	3175.2	16.4	3181.1	18.1	3186.0	20.1	3176.9	13.7
3174.6	16.3	3168.0	12.2	3174.4	16.2	3170.6	14.0	3169.7	9.4
3168.8	10.0	3158.2	1.3	3167.3	12.7	3168.8	1.7	3158.8	1.7
3159.1	1.1	3149.0	11.7	3157.6	1.2	3167.3	3.4	3153.8	6.9
3143.5	11.7	3140.4	25.4	3149.0	10.1	3159.5	1.7	3146.2	10.5
3132.3	15.7	3135.4	14.5	3128.0	16.3	3140.0	8.3	3139.1	11.0
3127.8	15.1	3132.7	9.1	3127.0	17.1	3139.0	8.3	3137.4	11.2
1658.4	31.9	1657.0	47.6	1656.4	57.3	1654.4	33.9	1658.4	26.8
1641.5	19.3	1642.9	17.1	1642.0	9.9	1635.0	68.9	1641.1	13.5
1617.1	11.0	1612.7	16.6	1612.9	22.7	1615.0	9.2	1616.5	16.5
1573.5	2.7	1569.5	7.1	1570.9	22.3	1580.4	22.5	1596.8	18.1
1543.7	48.8	1541.7	53.8	1541.0	55.0	1552.3	33.4	1544.1	33.0
1502.4	6.6	1505.1	9.2	1504.4	9.4	1499.1	37.7	1504.1	4.7
1480.7	2.3	1495.6	2.9	1479.2	5.6	1493.9	3.0	1494.0	1.0
1468.1	22.7	1464.4	28.4	1463.6	29.3	1473.7	1.9	1465.5	14.1
1453.9	3.9	1463.5	2.7	1450.1	4.5	1463.6	3.6	1462.6	2.7
1417.1	4.7	1420.2	3.8	1424.1	3.2	1414.4	65.7	1415.6	6.0
1395.5	6.5	1383.6	17.6	1380.4	65.5	1385.2	16.8	1392.5	3.9
1375.9	36.9	1375.2	46.8	1372.6	28.9	1379.0	5.3	1371.8	34.6
1371.2	8.0	1372.6	28.4	1367.3	1.3	1370.6	4.0	1366.9	11.8
1305.4	18.6	1304.2	17.9	1309.2	6.3	1316.0	6.7	1298.4	34.6
1278.6	130.1	1274.9	122.5	1276.8	104.3	1292.7	9.8	1273.3	110.1
1244.3	2.4	1243.8	8.0	1243.8	1.1	1237.0	14.3	1238.4	3.9
1235.6	30.8	1229.8	60.3	1231.3	50.3	1235.0	206.9	1222.8	25.5
1216.3	9.8	1219.2	9.8	1214.3	19.7	1218.4	7.0	1217.6	30.3
1206.1	1.2	1199.4	0.5	1208.1	0.7	1203.9	0.6	1201.3	0.2
1195.1	16.3	1196.4	12.2	1196.9	17.3	1182.1	10.5	1184.7	2.7
1176.4	7.4	1189.2	7.1	1181.5	3.9	1173.0	8.1	1174.2	2.9
1171.9	6.9	1179.8	14.3	1174.7	26.6	1168.0	2.2	1170.5	7.1
1154.3	9.2	1171.6	11.4	1151.3	22.4	1166.0	32.6	1165.3	11.9
1129.7	1.0	1125.6	0.3	1127.5	1.0	1119.1	1.1	1115.4	0.3
1086.8	47.3	1087.5	17.7	1083.1	9.3	1084.8	4.2	1079.8	2.9
1081.0	5.9	1075.5	4.0	1082.9	4.4	1061.9	0.2	1059.4	26.8
1050.5	6.9	1057.5	1.7	1067.2	20.4	1057.1	2.4	1055.9	1.1
1046.8	8.9	1050.5	3.8	1051.6	19.3	1050.4	2.6	1045.4	5.1
1011.7	0.4	1013.6	0.3	1026.9	0.6	1008.6	0.0	1011.5	0.1
1001.2	35.6	1005.2	72.8	1019.3	70.8	996.6	14.1	986.3	2.7
987.1	1.6	988.0	1.6	992.5	1.6	989.8	1.0	977.5	52.8
964.8	0.3	966.0	0.1	968.8	0.0	974.8	1.1	960.3	0.1
952.1	90.0	946.7	105.8	953.2	77.2	924.3	72.1	925.1	94.1
903.1	6.2	913.3	3.3	903.5	0.3	909.8	13.2	909.8	10.2
895.7	5.1	900.5	2.0	896.0	0.1	888.9	26.5	893.8	24.9
886.0	0.6	887.1	3.4	891.7	12.0	886.2	26.7	882.3	15.9
838.8	28.6	869.6	4.4	829.5	14.7	855.5	14.7	857.9	8.2
822.7	47.5	827.8	50.5	828.5	58.2	841.7	45.1	826.0	6.1
816.3	10.5	821.7	14.9	815.1	10.8	824.5	3.2	823.5	51.3
803.4	3.5	799.1	1.5	801.5	0.7	808.0	1.8	813.1	6.2
794.1	2.5	778.6	2.6	791.5	13.7	782.8	0.6	779.6	0.2
766.0	10.7	764.2	27.0	767.4	25.0	764.8	25.9	762.9	18.6
764.0	21.2	749.9	8.0	762.1	2.8	747.8	15.2	745.5	15.0
735.5	4.8	721.5	4.6	735.6	6.6	736.4	4.8	734.8	11.9
684.6	13.9	691.0	10.2	690.3	10.1	687.6	7.8	686.3	8.2
664.9	4.8	626.2	7.7	654.2	5.9	660.8	6.5	659.1	2.6
582.2	10.0	596.5	15.2	584.2	7.3	627.7	9.3	625.9	1.1
578.5	12.7	574.5	5.8	576.2	10.3	572.8	1.6	556.3	2.3
544.4	0.5	543.4	2.0	546.4	2.4	565.4	67.5	539.9	2.8
541.8	2.6	532.5	0.3	544.9	0.9	534.7	14.3	530.0	1.9
459.6	5.1	461.4	2.0	487.8	17.9	529.5	18.3	518.1	6.1
442.2	5.2	451.4	4.0	455.9	3.3	518.0	5.9	463.8	1.6
439.6	2.5	437.8	3.3	437.8	3.0	461.5	1.7	438.4	2.8
420.5	0.6	418.1	2.0	409.4	0.6	441.4	1.4	427.3	4.4
383.3	9.0	367.3	39.7	366.8	66.7	429.9	2.3	356.0	5.0
363.1	71.9	356.1	38.7	341.5	0.6	355.1	3.7	334.3	2.5
318.9	11.0	332.4	16.8	325.7	14.0	311.7	10.6	310.0	40.9
289.4	5.9	282.9	1.9	319.9	6.5	309.1	2.8	304.8	42.4
244.5	3.8	265.0	3.1	232.8	3.0	265.8	1.2	267.4	2.7
207.7	2.3	236.8	3.3	197.1	0.1	237.5	3.2	227.1	8.6
156.2	2.6	175.8	5.0	157.9	3.0	167.1	0.9	159.8	0.5
140.6	3.5	139.6	1.2	126.9	0.0	163.9	1.5	150.3	1.0
115.6	2.0	112.4	1.8	112.0	1.6	112.7	0.2	125.0	0.6
89.9	0.6	76.2	1.7	100.6	1.8	90.0	1.1	83.0	0.5
54.8	1.5	61.5	1.1	51.4	0.4	66.9	0.4	68.1	0.7
16.2	0.5	19.2	1.7	12.6	0.4	42.4	1.5	31.7	1.4

E11		K1		K2		K3		K4	
ν	*I*	ν	*I*	ν	*I*	ν	*I*	ν	*I*
3836.1	148.2	3221.8	8.5	3227.3	10.5	3238.3	1.9	3236.9	2.3
3255.4	0.7	3207.1	0.6	3214.2	0.7	3230.6	1.7	3215.8	8.6
3219.8	2.2	3204.5	5.7	3204.4	6.1	3217.0	2.6	3200.5	0.3
3197.5	5.2	3190.2	2.7	3190.0	9.3	3194.5	9.3	3194.9	6.7
3185.1	17.2	3189.6	11.5	3187.0	19.1	3188.0	17.3	3188.2	40.0
3178.6	10.8	3186.8	22.9	3186.7	9.7	3169.8	6.9	3187.4	15.6
3170.5	8.5	3168.5	12.6	3168.8	10.2	3160.6	6.2	3170.6	22.8
3162.5	11.6	3159.7	5.7	3160.0	7.0	3151.9	8.1	3160.8	6.1
3159.3	0.8	3151.0	5.9	3156.5	106.9	3149.9	80.2	3156.3	50.7
3148.4	9.6	3132.3	6.3	3150.8	6.9	3137.9	11.2	3152.4	2.2
3139.8	13.0	3130.1	11.2	3135.0	8.1	3135.9	11.3	3123.7	6.8
3133.7	12.4	3098.2	93.6	3133.2	12.5	3087.5	24.3	3122.4	1.8
1658.4	19.2	1655.6	131.3	1655.4	133.9	1670.2	377.7	1668.8	338.4
1654.1	34.1	1643.9	6.2	1643.3	9.3	1646.0	10.0	1645.1	10.4
1642.1	16.7	1606.3	76.6	1607.1	89.6	1620.6	47.5	1619.7	38.0
1607.8	4.5	1579.8	22.7	1580.5	24.2	1583.2	19.3	1583.9	17.1
1545.2	38.7	1555.3	592.3	1552.5	485.9	1566.3	167.8	1564.0	84.6
1505.9	8.0	1516.8	10.6	1516.6	14.0	1512.6	75.9	1514.9	5.5
1497.3	0.6	1504.6	9.9	1495.4	4.1	1498.3	268.0	1503.0	115.6
1470.9	5.7	1481.9	56.1	1482.3	47.4	1494.7	56.3	1497.4	264.0
1464.5	13.3	1470.4	3.3	1457.4	4.8	1463.4	16.4	1479.6	3.9
1416.6	11.0	1435.5	2.1	1434.6	1.6	1458.8	239.5	1458.3	200.3
1389.3	4.0	1428.3	21.1	1431.6	5.9	1432.6	16.2	1430.9	26.1
1384.2	1.6	1367.5	1.7	1411.8	48.1	1424.8	65.0	1425.4	19.8
1365.7	50.2	1361.0	86.2	1352.2	8.2	1369.3	22.6	1372.9	29.8
1298.3	30.1	1346.7	65.4	1344.0	23.8	1348.1	2.9	1348.3	0.4
1275.2	138.5	1329.8	125.1	1314.5	274.6	1324.8	34.2	1324.1	47.9
1238.0	3.2	1278.7	49.9	1277.4	44.9	1281.3	111.9	1279.0	176.4
1223.6	53.8	1242.1	27.0	1245.3	16.8	1240.1	65.0	1240.4	71.2
1216.0	34.8	1232.1	4.8	1236.5	67.4	1226.1	23.6	1227.5	4.3
1203.4	2.1	1210.5	29.5	1222.9	15.6	1209.8	12.5	1209.6	9.3
1184.5	0.4	1197.5	0.5	1201.4	0.6	1200.0	5.5	1203.8	2.9
1174.7	5.7	1196.7	26.8	1183.6	10.0	1198.8	16.9	1186.5	13.1
1168.2	16.9	1179.2	45.0	1160.3	7.6	1184.9	4.6	1160.3	17.4
1150.3	9.5	1161.1	7.2	1138.3	27.7	1159.6	23.9	1147.6	22.3
1132.5	6.8	1124.0	1.3	1119.1	0.9	1115.8	0.7	1130.4	2.7
1086.9	8.1	1119.4	5.0	1103.2	0.5	1109.3	1.3	1112.4	5.8
1055.2	28.2	1079.4	5.2	1081.0	4.3	1073.6	0.0	1074.0	4.4
1053.2	9.7	1061.4	3.2	1061.5	7.3	1071.7	7.7	1072.3	14.1
1045.6	10.2	1055.3	16.4	1054.9	26.2	1054.1	6.4	1049.5	15.6
1009.8	2.9	1015.7	0.1	1030.1	4.1	1050.8	28.6	1035.9	90.9
985.0	4.3	1015.1	4.1	1015.7	0.1	1033.2	38.3	1034.6	20.2
975.4	53.1	1011.6	0.3	1010.6	0.1	1015.6	1.7	1016.1	0.2
958.2	0.8	979.5	2.4	981.8	59.7	1012.2	0.7	1013.8	0.3
942.0	34.7	962.7	75.8	978.7	2.3	977.9	2.4	979.4	3.1
896.7	36.5	918.9	4.9	922.1	7.1	956.6	146.2	966.7	62.7
887.1	0.5	899.8	3.8	897.5	0.0	909.8	2.1	903.8	1.4
861.3	1.1	891.4	64.8	881.6	28.3	902.1	1.1	894.3	1.4
844.7	21.3	888.1	20.2	878.1	83.0	896.8	1.1	890.5	7.8
834.6	9.0	867.1	19.7	856.3	1.1	870.0	10.9	859.1	49.0
815.8	43.8	863.7	12.9	814.7	4.3	859.1	54.8	829.8	13.1
793.8	3.4	810.4	3.8	811.3	17.2	809.7	0.9	810.5	0.4
770.8	24.9	809.0	14.8	798.6	0.5	803.5	11.6	799.3	6.6
761.5	20.9	772.9	2.4	786.8	0.3	780.5	6.9	786.0	10.9
738.2	5.3	771.4	42.8	770.6	40.4	771.7	41.4	772.7	40.8
718.8	8.1	758.0	3.7	760.9	13.9	753.8	14.2	755.5	9.0
683.8	6.4	726.2	3.9	736.1	4.4	726.3	1.2	735.7	2.2
660.3	3.8	708.6	5.3	705.2	5.6	699.3	0.7	698.9	0.3
628.9	3.9	655.3	5.8	661.4	4.4	622.1	9.4	644.0	2.6
569.4	6.1	558.6	1.0	587.4	3.2	605.0	14.8	598.2	10.7
550.4	1.6	557.2	5.0	557.1	3.6	572.3	2.9	571.8	1.8
537.0	1.8	541.8	16.8	537.1	19.0	544.6	5.9	543.6	2.5
511.8	4.0	511.4	5.4	536.2	6.3	527.2	12.1	535.3	8.5
452.0	4.1	479.6	0.6	472.0	12.2	474.4	0.3	479.3	34.8
438.7	2.1	441.3	0.2	443.3	2.0	440.5	1.3	443.0	3.8
430.7	1.3	433.5	6.3	432.7	6.3	437.9	10.3	440.4	8.5
362.9	3.4	414.8	2.0	431.6	0.5	412.1	9.2	411.2	2.6
318.5	20.1	373.8	3.5	416.2	1.6	364.4	12.0	354.5	3.0
307.1	80.2	371.9	3.6	369.4	3.0	352.1	3.0	353.6	4.5
306.3	0.8	330.3	14.1	287.9	1.3	264.1	7.2	329.4	3.9
270.6	8.6	280.9	0.8	282.5	0.7	263.3	0.7	263.5	8.8
233.6	9.4	219.8	2.3	218.5	2.9	257.4	7.6	213.8	0.6
161.3	3.7	200.9	4.8	205.7	4.1	202.8	2.6	185.5	0.0
146.8	1.7	128.4	0.1	137.0	0.4	142.4	1.6	151.0	2.6
119.8	0.9	111.8	0.0	109.9	0.0	98.6	0.8	105.5	0.1
69.6	0.5	92.6	0.9	92.7	0.5	84.3	2.6	95.8	2.3
41.5	1.0	52.6	1.4	62.3	1.4	68.8	2.4	65.2	1.8
32.2	1.1	17.6	0.1	27.1	0.2	45.9	0.4	10.9	1.9

K5		K6		K7		K8		K9	
ν	*I*	ν	*I*	ν	*I*	ν	*I*	ν	*I*
3586.8	73.7	3463.8	3.0	3467.4	5.9	3569.5	62.0	3293.5	112.1
3223.7	8.0	3230.4	10.5	3229.9	6.0	3232.6	11.1	3234.5	2.6
3206.5	5.1	3211.7	4.9	3213.4	5.3	3206.6	4.5	3220.3	0.3
3204.9	4.2	3200.7	5.8	3199.5	5.9	3198.5	7.8	3217.9	3.8
3188.0	7.6	3191.1	7.4	3190.7	7.7	3187.3	8.0	3193.6	8.5
3187.0	21.8	3189.2	16.9	3189.0	17.2	3186.9	30.0	3189.9	18.6
3179.8	4.0	3173.0	6.3	3172.5	7.0	3169.1	15.0	3177.9	4.3
3169.4	12.7	3163.1	6.9	3165.5	13.9	3159.8	5.4	3169.7	9.9
3160.2	5.1	3150.0	8.1	3162.7	7.9	3155.2	4.0	3161.4	8.0
3149.2	7.6	3145.2	6.4	3149.6	8.1	3148.5	8.8	3152.7	6.0
3137.5	3.7	3133.4	10.7	3137.7	11.8	3146.8	11.5	3140.0	7.4
3125.0	13.6	3112.4	30.1	3129.3	10.8	3116.4	18.7	3137.6	8.2
1674.5	323.9	1719.5	295.8	1710.4	305.2	1681.6	318.8	1662.2	328.2
1654.3	7.2	1659.9	9.7	1659.4	8.3	1654.7	15.5	1644.8	7.2
1631.4	38.7	1629.7	4.7	1629.0	7.1	1632.2	27.3	1618.2	58.4
1586.3	7.4	1593.3	3.7	1592.4	2.9	1592.2	50.1	1582.3	50.7
1580.4	77.7	1563.2	234.1	1559.7	315.8	1585.7	23.0	1555.2	80.4
1511.9	10.1	1519.5	15.1	1521.0	121.4	1511.8	12.5	1519.9	75.9
1504.6	3.0	1502.0	60.3	1503.0	1.4	1503.0	7.4	1504.0	176.1
1486.4	26.6	1487.7	12.5	1484.8	8.5	1488.0	69.2	1490.8	151.4
1471.1	31.3	1480.7	5.2	1477.5	16.0	1471.2	273.4	1480.1	9.2
1467.0	247.6	1467.5	3.1	1458.0	5.1	1468.4	38.2	1464.7	3.5
1430.3	21.4	1425.5	8.7	1426.4	12.2	1430.2	21.0	1429.1	43.5
1365.6	42.7	1388.9	150.9	1416.1	4.2	1385.2	60.6	1400.6	90.2
1351.4	40.3	1338.2	0.4	1339.5	3.8	1351.1	17.4	1384.6	81.3
1323.3	25.0	1323.7	9.6	1325.3	20.8	1321.9	13.3	1347.9	3.4
1310.9	2.2	1288.6	25.1	1308.5	48.3	1310.0	1.0	1317.0	23.7
1260.7	16.2	1256.4	82.7	1259.1	65.9	1260.5	17.7	1284.1	28.7
1239.3	14.7	1243.4	24.3	1240.2	15.0	1237.7	14.4	1237.7	56.4
1230.6	16.8	1232.3	14.9	1229.9	6.5	1225.2	2.5	1215.0	2.1
1200.9	61.8	1196.8	16.4	1202.5	97.2	1210.4	58.9	1204.8	0.3
1191.5	3.8	1193.6	1.3	1200.0	21.8	1192.9	1.4	1193.6	57.0
1183.5	5.8	1190.2	0.8	1190.6	9.3	1185.2	2.9	1187.4	0.9
1171.7	0.2	1171.2	90.2	1154.6	15.1	1182.7	12.1	1168.5	6.1
1155.4	5.3	1153.2	26.3	1139.9	9.9	1155.4	6.6	1158.6	39.3
1122.3	4.9	1132.5	0.8	1119.4	11.0	1120.5	2.8	1119.1	0.3
1105.8	28.0	1115.2	43.8	1099.5	12.5	1106.7	22.6	1099.6	10.2
1079.0	3.7	1080.4	1.5	1089.7	7.2	1075.7	7.7	1082.9	5.5
1062.6	2.3	1077.2	20.2	1079.1	5.9	1062.7	4.1	1071.0	4.6
1053.4	16.3	1058.3	10.1	1053.7	13.7	1057.8	5.0	1052.3	7.4
1022.7	17.7	1045.6	3.1	1043.5	19.4	1017.7	1.6	1033.3	15.4
1016.8	0.4	1021.1	0.6	1020.8	0.5	1013.4	0.2	1013.8	0.1
1013.3	0.6	1012.4	1.1	1010.4	0.6	1008.6	10.5	1005.7	0.7
988.6	2.6	986.2	4.4	984.4	0.4	980.4	2.2	995.8	38.7
981.1	2.3	980.2	4.7	976.1	5.0	976.5	7.0	972.7	4.4
943.5	5.0	955.6	6.4	929.2	16.7	931.7	27.4	933.3	241.9
901.8	0.7	909.3	4.8	907.2	3.6	901.5	0.5	901.6	11.7
866.3	36.5	882.4	14.3	884.4	16.2	873.1	39.4	892.2	17.0
860.9	10.4	862.0	39.2	862.4	40.2	860.6	28.3	882.8	16.2
851.6	20.3	851.5	7.2	823.8	15.2	852.2	6.2	858.0	39.3
834.0	1.2	830.8	5.2	817.8	7.2	827.2	11.0	851.6	27.9
814.6	10.5	818.3	9.7	809.0	3.3	813.4	6.0	811.0	8.5
777.5	3.3	779.4	16.1	781.0	9.6	772.1	42.0	797.7	1.3
772.6	37.9	772.7	14.9	771.0	20.8	762.5	14.9	781.4	7.1
754.1	3.8	753.2	8.3	755.0	8.8	752.8	2.6	766.1	41.3
722.9	23.8	722.8	1.2	730.2	1.5	716.8	17.8	749.6	17.9
700.7	19.0	701.0	4.6	701.0	4.5	694.4	14.5	725.2	13.4
687.1	2.9	648.8	106.6	643.0	104.1	686.3	10.1	697.9	0.5
644.8	35.6	627.7	10.6	639.8	3.6	649.0	73.9	674.1	31.7
560.4	11.0	587.3	1.8	589.8	5.1	555.2	0.9	593.4	7.6
555.8	1.6	559.5	45.0	556.6	31.1	552.1	5.5	584.6	42.2
539.0	14.6	524.1	18.1	535.5	5.5	535.9	20.0	553.1	1.6
509.2	18.4	513.1	41.5	509.6	65.7	513.4	72.9	539.7	7.7
468.4	41.3	468.4	4.9	484.4	26.9	467.9	21.8	492.8	11.3
452.8	0.9	446.8	1.7	439.8	4.6	452.5	31.4	466.7	6.5
432.1	4.1	436.5	2.9	434.6	5.5	429.9	3.2	442.5	10.8
414.3	5.0	417.5	1.6	421.4	14.3	402.6	1.9	416.2	3.3
355.1	2.0	353.4	3.0	359.1	3.4	352.4	10.5	364.0	14.5
335.8	14.0	329.1	13.2	328.0	0.6	342.1	19.2	327.5	4.4
291.3	3.9	289.9	4.0	317.4	7.4	292.4	1.1	296.2	2.5
281.3	3.4	238.7	3.7	235.7	1.0	278.3	1.9	276.1	2.0
212.1	4.5	219.5	8.6	198.9	4.5	208.4	4.4	218.3	5.1
189.4	8.7	179.9	2.5	187.5	2.0	171.5	7.5	181.6	0.9
169.3	0.5	145.4	0.4	151.1	1.3	164.9	1.6	177.3	0.3
116.0	0.7	92.2	0.9	90.1	1.7	116.5	1.3	106.2	1.8
85.4	1.9	85.8	2.4	87.8	2.0	78.7	0.8	85.9	0.5
45.0	0.8	49.2	1.9	57.3	2.0	49.6	2.5	63.5	0.4
39.9	0.5	36.5	0.2	35.4	0.6	48.2	3.5	58.5	0.6

K10		K11		K12		K13	
ν	*I*	ν	*I*	ν	*I*	ν	*I*
3460.0	21.4	3324.0	0.4	3564.0	52.1	3334.9	9.4
3240.8	2.6	3233.9	2.4	3220.0	3.4	3222.9	9.5
3222.8	1.0	3220.6	0.5	3218.6	7.7	3200.0	3.7
3204.4	6.4	3191.7	17.9	3202.0	1.3	3192.1	16.3
3191.1	19.5	3190.1	9.7	3189.8	7.2	3191.1	8.7
3188.4	9.1	3174.6	13.8	3188.3	18.6	3175.5	13.4
3175.1	14.8	3162.1	7.5	3171.1	9.8	3163.0	6.7
3161.8	6.0	3149.9	8.5	3161.6	5.5	3150.5	8.6
3154.8	8.5	3143.7	12.2	3153.8	2.3	3146.1	11.3
3150.6	7.3	3138.6	11.9	3148.7	8.8	3136.3	11.7
3150.0	5.6	3136.7	10.1	3130.2	5.3	3125.1	9.0
3137.2	9.7	3043.8	36.0	3122.2	12.3	3123.9	9.3
1655.4	163.8	1671.6	247.3	1726.6	306.0	1674.4	286.4
1641.3	10.1	1649.1	0.3	1656.2	12.2	1651.4	0.6
1613.9	114.2	1631.7	26.5	1631.2	10.0	1631.3	33.9
1583.0	36.4	1602.9	78.0	1613.9	162.4	1599.7	27.3
1563.5	39.3	1573.1	90.4	1589.9	26.8	1571.1	90.9
1523.1	2.9	1517.7	52.7	1513.7	46.2	1519.5	31.1
1498.3	80.2	1494.4	3.6	1503.8	3.0	1502.1	3.4
1480.4	50.2	1483.7	4.5	1493.8	155.0	1485.0	6.0
1478.3	124.1	1463.0	4.0	1482.0	8.8	1469.3	14.3
1464.7	3.6	1441.4	514.6	1467.1	4.4	1433.2	403.5
1428.0	11.7	1427.5	77.3	1422.3	9.6	1427.5	208.5
1396.1	6.3	1409.5	51.2	1385.9	55.2	1397.1	11.0
1360.4	13.1	1371.9	21.1	1336.8	1.9	1367.1	81.1
1356.8	44.0	1361.1	63.8	1318.8	1.3	1351.4	131.0
1336.2	95.1	1341.8	42.6	1280.3	20.2	1339.1	83.4
1279.3	54.2	1276.7	23.6	1248.7	32.9	1277.2	14.0
1238.2	29.1	1235.6	43.0	1232.7	43.3	1236.9	47.3
1218.3	6.4	1227.7	21.0	1223.5	1.2	1224.8	0.3
1209.3	41.9	1206.5	5.6	1200.9	10.2	1207.8	9.4
1200.4	0.6	1202.0	0.4	1195.2	13.4	1194.2	6.2
1188.7	9.0	1197.3	4.7	1187.2	0.4	1193.6	5.9
1178.6	12.8	1191.9	5.3	1170.5	30.5	1161.9	10.1
1161.3	6.6	1161.5	8.0	1147.5	17.3	1151.0	9.8
1100.7	5.0	1110.2	4.8	1125.2	2.0	1127.3	7.7
1098.1	1.0	1102.4	0.1	1092.5	52.0	1111.5	2.5
1069.6	2.2	1074.2	5.7	1083.9	2.7	1081.9	4.2
1068.7	3.9	1072.6	5.2	1066.8	1.5	1073.5	3.6
1047.7	9.4	1057.2	13.8	1060.5	8.7	1047.5	14.0
1011.7	0.8	1018.8	20.5	1019.3	0.7	1028.8	0.8
1005.9	6.8	1013.8	0.1	1016.3	4.5	1015.5	0.1
998.9	0.0	996.8	0.1	1010.2	2.5	999.0	0.1
966.1	2.9	963.4	3.0	982.2	1.6	972.2	3.2
936.3	128.3	951.7	148.2	978.5	4.2	965.2	8.2
914.2	231.1	934.6	70.7	935.1	35.1	957.2	59.4
891.5	53.4	895.3	3.4	904.5	3.4	925.3	19.2
880.9	2.8	879.1	22.0	879.7	27.7	877.8	11.0
857.9	16.2	874.7	7.9	858.8	29.9	867.0	3.7
851.7	17.5	864.3	25.5	851.2	9.6	854.8	33.3
837.3	123.7	852.7	33.1	822.4	6.0	830.3	10.1
798.3	13.3	800.0	7.1	817.4	6.8	811.3	12.1
788.0	2.4	792.4	4.2	775.6	16.7	793.5	0.1
776.8	19.8	784.1	1.4	772.3	12.3	780.4	3.2
765.1	39.5	760.7	24.9	753.1	15.4	760.2	44.1
755.8	18.9	756.1	27.9	714.0	28.9	754.8	6.3
726.4	16.4	721.6	0.8	701.0	2.0	724.9	1.7
692.0	23.4	695.5	0.5	690.9	24.3	697.2	0.4
680.0	3.1	656.5	8.1	609.6	115.1	658.5	8.3
588.7	15.3	559.6	0.5	598.6	32.1	570.5	2.1
560.3	3.1	549.1	0.9	564.3	8.2	549.6	0.1
552.0	3.0	532.4	5.4	534.1	9.3	541.0	7.8
535.3	0.8	507.9	7.5	524.4	37.3	520.3	4.7
497.3	17.3	474.9	7.2	477.4	9.2	458.4	10.0
464.0	17.9	437.4	3.2	436.0	4.1	443.6	4.3
435.1	5.3	430.2	5.6	425.4	23.6	430.0	6.8
407.8	1.0	398.4	2.3	405.7	0.7	404.0	3.3
352.0	3.4	360.2	2.6	358.5	9.3	370.8	1.0
348.1	10.6	326.8	6.4	323.3	10.7	330.0	11.3
305.2	4.8	297.1	6.4	290.9	1.6	303.0	2.4
277.6	0.2	261.4	6.5	269.1	5.2	262.1	1.6
213.6	7.7	217.5	2.8	203.6	2.0	217.4	7.0
173.8	1.2	173.5	0.3	175.4	1.6	166.3	2.6
164.3	0.1	127.9	2.1	162.0	0.6	127.5	2.4
133.5	1.2	98.0	0.8	91.8	1.4	95.2	1.8
77.9	2.1	72.4	1.6	82.3	1.3	72.1	3.2
54.2	0.8	48.5	3.2	63.2	1.2	40.8	2.9
52.8	1.3	43.9	1.5	52.5	0.9	32.9	1.2

Table S3: Experimental Observed Wavenumbers (ν) and Tentative Assignments for the E1 Azo-enol Isomer Isolated in Argon and Xenon Matrices.[a]

Ar (15 K)	Xe (30 K)	calculated		Sym.	appr. description
ν	ν	ν	*I*		
3095.0	3099.4	3147.8	4.8	A´	$\nu_{as}(CH_2)cp$
n.o.	3087.4	3134.5	0.1	A´´	$\nu_{as}(CH_2)cp$
3084.8	3078.0	3134.1	4.7	A´	ν(CH)ar
3068.9	3063.3	3115.1	9.4	A´	ν(CH)ar
3057.4	3051.2	3108.0	24.1	A´	ν(CH)ar
n.o.	3040.6	3091.2	12.0	A´	ν(CH)ar
n.o.	n.o.	3088.1	3.9	A´	ν(CH)ar + ν(OH)
n.o.	n.o.	3081.6	1.1	A´	ν(CH)ar
2850 - 2570	2850 - 2570	3079.7	163.7	A´	ν(OH)
3022.0	3020.2	3068.1	92.5	A´	ν(CH)cp + ν(OH)
n.o.	3014.4	3058.8	5.2	A´	$\nu_s(CH_2)cp$ + ν(CH)cp
n.o.	3004.9	3058.3	12.6	A´´	$\nu_s(CH_2)cp$ + ν(CH)cp
1630.0	1627.0	1615.9	57.5	A´	ν(CC)ar + δ(OH)
1599.9	1598.6	1596.6	43.3	A´	ν(CC)ar + δ(OH)
1572.8	1571.0	1583.5	55.9	A´	δ(OH) + ν(CC)ar + ν(NN)
1520.0, 1511.4	**1518.1**, 1508.8, 1505.9	1522.0	45.4	A´	δ(OH) + ν(CC)ar
1481.9, **1480.1**	**1478.9**, 1476.9	1491.3	27.5	A´	ν(N=N) + ν(CC)ar + δ(OH)
1467.6, **1463.0**	1464.9, 1461.0	1471.9	42.1	A´	δ(OH) + ν(CC)ar
1449.2	1445.7	1461.3	2.7	A´	$sci(CH_2)cp$ + δ(CH)cp + ν(CC)cp
1439.3	1437.0	1440.2	22.9	A´	δ(CH)ar + ν(NN) + ν(CC)ar
1428.3	1424.6	1431.2	3.3	A´´	$sci(CH_2)cp$
1415.1	1413.4	1414.8	39.6	A´	δ(CH)ar + δ(OH) + ν(CC)ar
1386.1	1386.4	1372.1	12.6	A´	ν(CC)ar + ν(CO) + δ(CH)cp
1351.1	1347.7	1344.7	6.2	A´	ν(CC) ar + δ(CH)cp + ν(CO)
1345.0	1342.4	1341.4	1.8	A´	δ(CH)cp + ν(CC)cp + ν(NCcp)
1304.0	1302.6, **1300.8**	1302.2	114.0	A´	ν(CarN) + δ(OH) + ν(CC)ar
1292.5	1289.2	1289.3	19.8	A´	ν(CO) + δ(CH)ar + ν(CC)ar
1248.5, 1240.3	**1246.1**, 1237.9, 1236.4	1240.9	45.1	A´	δ(CH)ar + ν(CO) + ν(CC)ar + δ(OH)
1235.4	1233.1	1217.4	1.1	A´	δ(CH)ar + ν(NCcp) + ν(CC)ar
1208.3	1206.6	1198.3	25.5	A´	ν(NCcp) + δ(CH)ar + ν(CC)ar
1188.4	1186.7	1177.6	9.2	A´	δ(CH)cp + ν(CC)cp + ν(NCcp)
1180.9	1180.6	1170.3	0.5	A´´	$r(CH_2)cp$
1170.0	**1172.2**, 1168.7	1165.8	29.9	A´	δ(CH)ar + ν(CarN)
1149.5, **1148.3**	1147.4	1147.6	24.9	A´	δ(CH)ar
1143.4	1140.5	1139.2	1.4	A´	δ(CH)ar
1091.7	1089.5	1094.9	0.3	A´´	$tw(CH_2)cp$ + γ(CH)
1080.7	1078.9	1080.7	16.0	A´	δ(CH)ar + ν(CarN)
1047.0	1046.1, **1044.0**	1050.7	4.8	A´´	$w(CH_2)cp$ + γ(CH)cp
1028.5	1028.0	1027.7	6.3	A´	$w(CH_2)cp$ + δ(CH)ar
1025.2	**1021.9**, 1020.8	1024.9	9.0	A´	δ(CH)ar + $wag(CH_2)cp$
n.o.	n.o.	989.7	0.2	A´´	γ(CH)ar
991.2	990.2	985.8	5.1	A´	δ(ar) + γ(CH) cp
978.5	976.1, **974.6**	973.8	0.9	A´´	γ(CH)ar
n.o.	n.o.	956.3	0.8	A´´	γ(CH)ar
937.8	**938.0**, 936.6	929.3	107.8	A´	δ(cp) + ν(NCcp)
910.3	**915.0**, 909.4	902.0	4.7	A´	δ(NNC) + δ(cp)
889.2	888.4	891.1	15.4	A´´	τ(OH) + γ(NCcp)
866.5	865.0	874.5	2.0	A´´	τ(OH) + γ(CH)ar

862.14, 860.01	**862.4**, 858.7	865.8	28.3	A´´	τ(OH)
n.o.	847.7	854.2	9.4	A´	δ(ar) + δ(cp)
824.3, 822.9, 818.7, 816.8, 811.1	822.5, 820.8, **819.6**, 817.3, 815.0, 813.3, 811.5	830.7	54.8	A´´	γ(CH)ar
n.o.	800.3	798.5	10.9	A´´	ν(CC)cp
n.o.	n.o.	790.5	0.01	A´´	γ(CH)ar
773.7	777.6	766.4	3.1	A´	r(CH_2)cp
750.4	**749.2**, 747.8	750.8	36.3	A´´	γ(CH)ar
		742.1	1.5	A´	δ(ar) + r(CH_2)cp
719.4	720.6, **718.1**	710.1	6.0	A´	δ(ar)
681.2	678.8	685.1	7.4	A´´	τ(ar)
644.2	**644.7**, 643.3	642.7	9.4	A´	δ(ar) + δ(CNN)
561.5	560.1, **559.3**	562.3	9.6	A´´	τ(ar)
540.0	542.4, **539.7**	539.1	2.3	A´	δ(ar)
n.o.	n.o.	536.6	0.02	A´´	τ(ar)
516.4	**517.2**, 515.5	511.1	2.7	A´	δ(ar) + δ(NNC)
464.7	465.4, 466.4, **464.2**	464.2	16.1	A´	δ(NNC)
450.2	453.1, **450.2**	447.9	3.8	A´´	γ(NNC)
433.9	435.4 , **433.3**	429.9	2.7	A´	δ(ar)
n.o.	n.o.	408.8	0.3	A´´	τ(ar) + γ(NCcp)
n.i	n.i	354.9	0.1	A´´	τ(ar) + γ(NCcp)
n.i	n.i	351.5	3.3	A´	δ(NNC) + δ(CCO) + δ(ar)
n.i	n.i	332.8	9.4	A´	δ(NNC) + δ(CCO) + δ(ar)
n.i	n.i	270.3	≈ 0.0	A´´	τ(ar) + γ(NC)
n.i	n.i	216.7	2.3	A´	δ(NCC)ar +δ(NCCcp)
n.i	n.i	203.3	2.9	A´´	τ(ar) + γ(NC)
n.i	n.i	135.7	0.3	A´´	τ(ar) + γ(CcpN)
n.i	n.i	122.2	0.1	A´´	τ(ar) + γ(CO)
n.i	n.i	94.4	1.1	A´	δ(NNCcp)
n.i	n.i	69.7	0.4	A´´	τ(ar) + γ(NCcp)
n.i	n.i	47.9	0.5	A´´	τ(NCcp)

[a] B3LYP/6-311+G(2df,2p) calculated wavenumbers (ν) in cm^{-1} and intensities (*I*) in km mol^{-1} are also given. The theoretical wavenumbers are scaled by a factor of 0.976. The strongest components of split bands are given in bold. ν, bond stretching; δ, in-plane-bending; γ, out-of-plane bending; w, wagging; sci, scissoring; r, rocking; τ, torsion; ar, aromatic ring; cp, cyclopropane ring; n.o., not observed; n.i., not investigated.

Table S4: Experimental Observed Wavenumbers (ν) and Tentative Assignments for the E2 Azo-enol Isomer Isolated in Argon and Xenon Matrices.[a]

Ar (15 K)	Xe (30 K)	calculated		Sym.	appr. description
ν	ν	ν	*I*		
1630 [c]	1627.8 [b]	1615.2	65.8	A´	ν(CC)ar + δ(OH)
1600 [c]	1599.8 [b]	1596.7	59.6	A´	ν(CC)ar + δ(OH)
1579.5	1579.4 [b]	1583.9	55.4	A´	δ(OH) + ν(ar)
1520 [c]	1518.5 [b]	1522.4	50.3	A´	ν(CC)ar + δ(OH)
1485.0	1484.5 [b]	1499.9	34.6	A´	ν(NN) + δ(CH)cp + δ(OH) + ν(CC)ar
1467.6	1465.0 [b]	1473.5	63.0	A´	δ(OH) + ν(CC)ar
1430.3	1427.5 [b]	1435.3	17.3	A´	sci(CH_2)cp + δ(CH)ar + ν(NN)
1304 [c]	1303.6 [b]	1305.4	112.7	A´	ν(CarN) + δ(OH) + ν(CC)ar + δ(CH)ar
1249 [c]	1247.1 [b]	1242.2	54.7	A´	δ(CH)ar + ν(CO) + ν(CC)ar + δ(OH)
1215.2	1213.7 [b]	1210.2	10.3	A´	δ(CH)ar
1188 [c]	1186.7 [b]	1188.3	39.6	A´	δ(CH)ar + ν(CC)cp + ν(NCcp) + ν(NCar)
1149 [c]	1151.0 [b]	1150.8	10.4	A´	δ(CH)ar
1128 [c]	1126.3	1122.1	21.1	A´	δ(CH)ar + ν(NCcp)
1053.4	1051.5 [b]	1056.7	5.2	A´´	w(CH_2)cp
1037.7	1035.2 [b]	1031.4	9.8	A´	w(CH_2)cp
n.o.	1028.6	1025.0	10.5	A´	δ(CH)ar
1005.7	1003.2	1000.1	24.2	A´	δ(cp) + ν(NCcp) + ν(CC)cp
959.4	957.5	951.6	65.4	A´	δ(cp) + ν(NCcp)
837.7	836.9	831.3	50.4	A´´	γ(CH)ar
833.5	835.4	823.0	31.9	A´	δ(cp)
725.5	724.6	720.2	4.9	A´	δ(ar)
651.5	650.8	650.2	4.4	A´	δ(ar)
577.2	575.3	572.1	8.8	A´	δ(ar) + δ(NNC)
530.2	530.8	528.1	5.4	A´	δ(ar)
445.2	443.7	442.0	23.6	A´	δ(ar)

[a] B3LYP/6-311+G(2df,2p) calculated wavenumbers (ν) in cm^{-1} and intensities (*I*) in km mol^{-1} are also given. The theoretical wavenumbers are scaled by a factor of 0.976. The strongest components of split bands are given in bold. ν, bond stretching; δ, in-plane-bending; γ, out-of-plane bending; w, wagging; sci, scissoring; ar, aromatic ring; cp, cyclopropane ring; n.o., not observed.

[b] Bands assigned based on annealing experiments.

[c] Estimated values for E2 bands masked by E1 absorptions.

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