

Supplementary Information for:

Photoisomerization of Azobenzenes Isolated in Cryogenic Matrices

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Contents

Figure S1. Isomeric forms of 2,2'-dihydroxyazobenzene found at the M06-2X/cc-pVTZ level of theory.....	3
Figure S2. Experimental UV-Vis spectra of azobenzene (AB, blue), 2,2'-dihydroxyazobenzene (DAB, red), and 2,2'-azotoluene (AT, black) in acetonitrile.	4
Figure S3. TD-DFT (M06-2X/cc-pVTZ) simulated UV-visible spectra of the <i>E</i> -AB, <i>Z</i> -AB, <i>E</i> -DOH1, <i>E</i> -DOH2, <i>E</i> -NHOH4, <i>E</i> -AT1, <i>E</i> -AT2, and <i>Z</i> -AT1 isomers.....	5
Table S1. Relative energies of the 2,2'-dihydroxyazobenzene isomeric forms.	6
Table S2. Theoretical wavenumbers and infrared intensities of the 2,2'-dihydroxyazobenzene isomeric forms.	7
Table S3. Experimental wavenumbers of the <i>E</i> -DOH1 azo-enol isomer isolated in argon and xenon matrices.	31
Table S4. TD-DFT (M06-2X/cc-pVTZ and B3LYP/cc-pVTZ) vertical transition wavelengths and oscillator strengths for the lowest twelve excited singlet states and lowest twelve excited triplet states of the <i>E</i> -AB, <i>Z</i> -AB, <i>E</i> -AT1, <i>E</i> -AT2, <i>Z</i> -AT1, <i>E</i> -DOH1, <i>E</i> -DOH2, <i>E</i> -NHOH4, and <i>Z</i> -DOH1 isomers.	34
Table S5. Experimental observed wavenumbers in argon and xenon matrices after irradiation of 2,2'-dihydroxyazobenzene at 323 nm.	43
Table S6. Theoretical wavenumbers and infrared intensities of the 2,2'-azotoluene isomeric forms.....	44
Table S7. Experimental wavenumbers of the <i>E</i> -AT1 isomer isolated in argon and xenon matrices.	51
Table S8. Theoretical wavenumbers and infrared intensities of the <i>E</i> and <i>Z</i> forms of azobenzene.	55

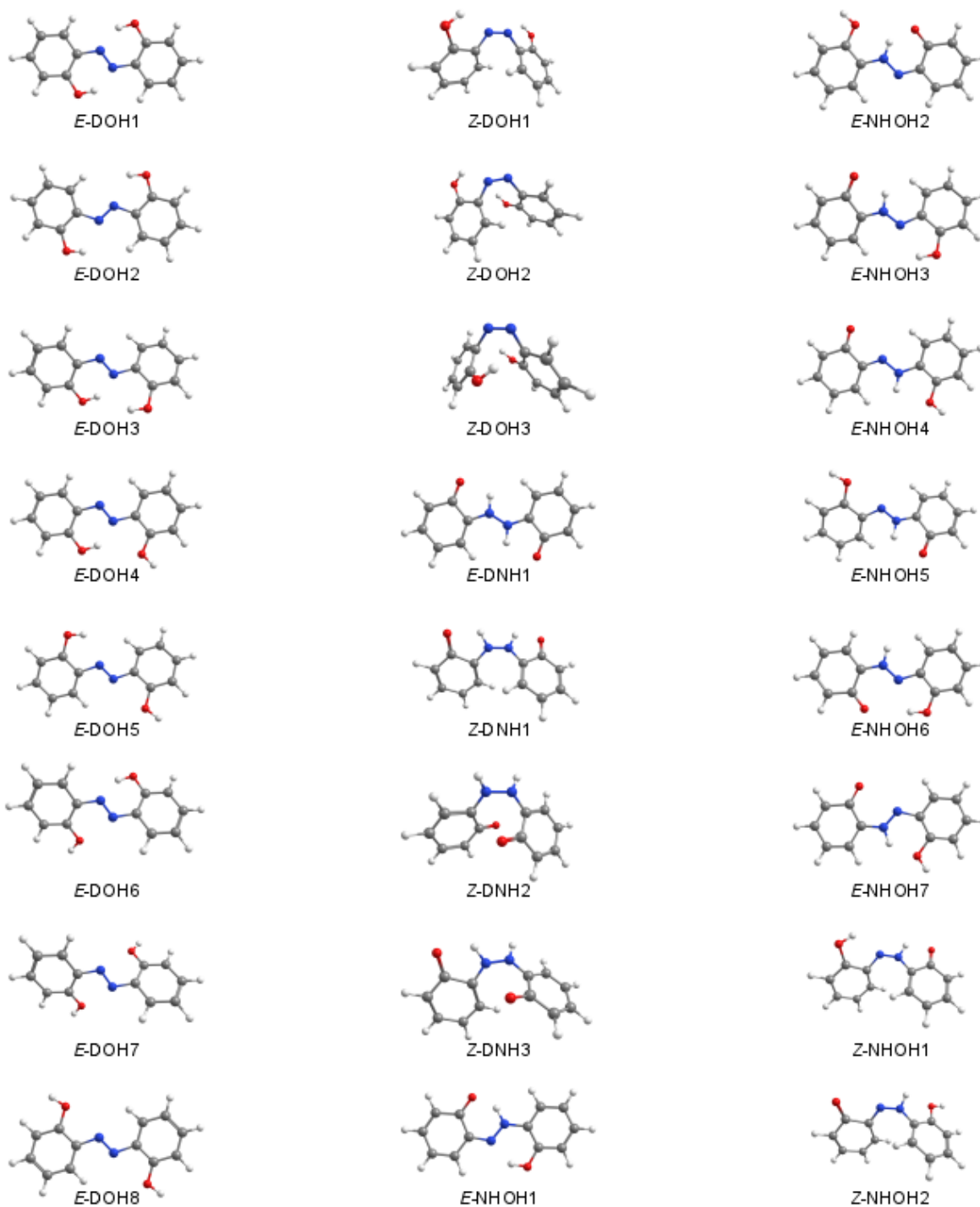


Figure S1. Isomeric forms of 2,2'-dihydroxyazobenzene found at the M06-2X/cc-pVTZ level of theory.

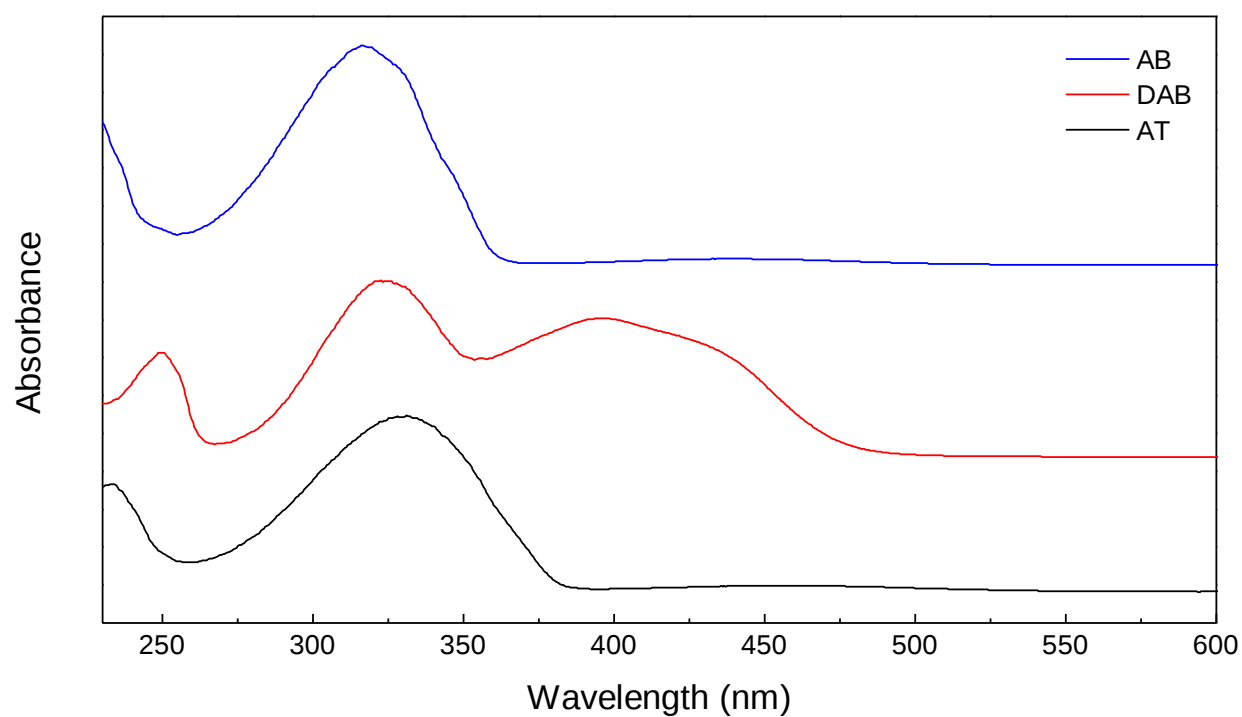


Figure S2. Experimental UV-Vis spectra of azobenzene (AB, blue), 2,2'-dihydroxyazobenzene (DAB, red), and 2,2'-azotoluene (AT, black) in acetonitrile. The spectra were obtained in a Shimadzu UV-2100 spectrometer using quartz cuvettes.

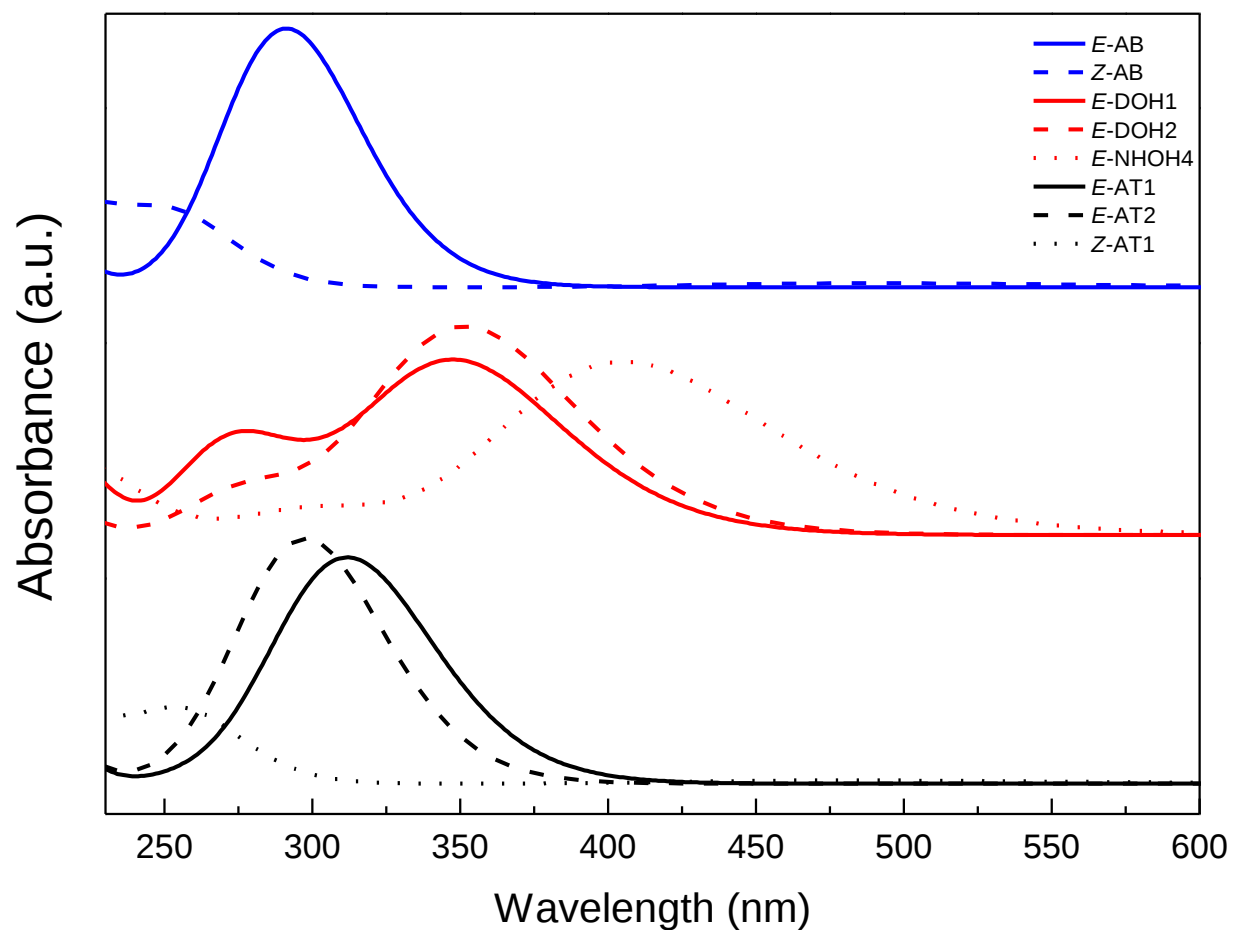


Figure S3. TD-DFT (M06-2X/cc-pVTZ) simulated UV-visible spectra of the *E*-AB, *Z*-AB, *E*-DOH1, *E*-DOH2, *E*-NHOH4, *E*-AT1, *E*-AT2, and *Z*-AT1 isomers. See Table S4 for vertical transition wavelengths (λ /nm) and oscillator strengths (f) for the lowest twelve excited singlet states and lowest twelve excited triplet states.

Table S1. Relative energies (in kJ mol⁻¹) of the 2,2'-dihydroxyazobenzene isomeric forms.^a

DAB	B3LYP		M06-2X	
	ΔE_{ZPVE}	ΔE_{Gibbs}	ΔE_{ZPVE}	ΔE_{Gibbs}
<i>E</i> -DOH1	0.00	0.00	0.00	0.00
<i>E</i> -DOH2	23.97	16.35	16.86	12.23
<i>E</i> -DOH3	22.86	19.91	17.73	14.57
<i>E</i> -DOH4	29.00	25.07	22.64	18.18
<i>E</i> -DOH5	48.58	40.77	40.24	35.07
<i>E</i> -DOH6	45.38	39.79	40.79	36.64
<i>E</i> -DOH7	94.33	86.15	84.37	77.29
<i>E</i> -DOH8	73.23	67.70	62.93	58.72
<i>Z</i> -DOH1	89.93	87.26	76.17	74.55
<i>Z</i> -DOH2	105.60	98.88	84.85	80.41
<i>Z</i> -DOH3	123.02	120.47	96.84	93.46
<i>E</i> -DNH1	153.53	149.31	201.26	197.82
<i>Z</i> -DNH1	177.41	173.69	220.03	217.11
<i>Z</i> -DNH2	194.25	195.96	213.59	215.87
<i>Z</i> -DNH3	198.24	195.20	229.19	226.70
<i>E</i> -NHOH1	23.42	21.40	37.69	34.89
<i>E</i> -NHOH2	41.21	37.30	49.00	44.37
<i>E</i> -NHOH3	77.37	71.08	98.25	93.21
<i>E</i> -NHOH4	95.13	88.61	100.32	93.66
<i>E</i> -NHOH5	100.55	95.15	118.92	114.39
<i>E</i> -NHOH6	110.90	105.49	129.98	124.40
<i>E</i> -NHOH7	129.88	124.68	147.46	142.60
<i>Z</i> -NHOH1	116.87	113.44	129.67	126.69
<i>Z</i> -NHOH2	143.73	137.61	140.60	135.09

^a ΔE_{ZPVE} – Relative energy including zero-point vibrational energy correction. ΔE_{Gibbs} – Relative energy including thermal correction to Gibbs free energy at 298.15 K. The calculations were performed with the cc-pVTZ basis set.

Table S2. Theoretical wavenumbers (ω / cm^{-1} ; unscaled values) and infrared intensities (I / km mol^{-1}) of the 2,2'-dihydroxyazobenzene isomeric forms.

<i>E</i> -DOH1						<i>E</i> -DOH2						<i>E</i> -DOH3					
M06-2X			B3LYP			M06-2X			B3LYP			M06-2X			B3LYP		
ω	I		ω	I		ω	I		ω	I		ω	I		ω	I	
3416	0		3270	0		3756	229		3657	0		3852	86		3762	59	
3406	581		3257	442		3756	0		3656	174		3461	269		3319	208	
3218	0		3202	0		3222	0		3210	16		3230	3		3210	7	
3218	13		3202	34		3222	15		3210	0		3220	6		3203	16	
3212	6		3195	18		3216	4		3200	0		3214	4		3200	11	
3212	0		3195	0		3216	0		3200	22		3212	3		3195	8	
3194	0		3183	0		3207	0		3188	0		3206	5		3189	13	
3194	4		3183	7		3207	5		3188	25		3205	2		3187	3	
3185	0		3174	5		3191	0		3173	0		3192	1		3174	1	
3185	0		3174	0		3191	3		3173	2		3191	1		3174	2	
1700	167		1662	184		1703	0		1653	0		1699	60		1660	102	
1695	0		1655	0		1691	117		1651	123		1693	70		1650	44	
1667	0		1626	0		1672	0		1627	0		1670	48		1624	53	
1652	138		1617	126		1667	104		1623	106		1659	61		1621	49	
1596	0		1534	15		1631	0		1537	0		1605	47		1532	8	
1542	6		1531	0		1541	0		1521	0		1539	74		1527	65	
1531	0		1525	0		1532	212		1512	66		1534	45		1515	79	
1523	195		1503	182		1526	9		1509	147		1520	6		1503	7	
1509	0		1459	0		1518	0		1494	0		1514	76		1467	52	
1422	0		1436	78		1382	0		1387	0		1424	54		1425	65	
1422	89		1415	0		1377	96		1382	86		1368	30		1370	23	
1369	0		1362	0		1358	0		1354	0		1360	5		1355	10	
1364	16		1352	21		1354	23		1344	42		1351	13		1344	8	
1342	0		1323	0		1308	0		1296	143		1325	51		1312	62	

E-DOH1						E-DOH2						E-DOH3				
M06-2X			B3LYP			M06-2X			B3LYP			M06-2X			B3LYP	
ω	I		ω	I		ω	I		ω	I		ω	I		ω	I
1325	141		1316	124		1307	168		1290	0		1296	121		1280	94
1291	94		1276	118		1283	235		1267	267		1292	65		1273	108
1268	0		1264	0		1237	0		1224	0		1255	28		1247	9
1238	75		1239	53		1212	160		1213	171		1216	26		1210	21
1224	0		1219	0		1202	0		1200	0		1198	75		1194	83
1174	0		1179	0		1171	0		1174	139		1174	25		1176	36
1174	54		1177	63		1169	123		1170	0		1173	33		1175	30
1154	0		1149	0		1134	20		1133	7		1143	29		1138	22
1142	20		1137	16		1122	0		1118	0		1129	6		1121	4
1071	12		1055	12		1062	16		1049	0		1068	10		1053	8
1069	0		1053	0		1062	0		1048	16		1068	4		1052	7
1020	1		994	0		1021	0		993	0		1020	0		998	0
1019	0		993	0		1021	0		992	0		1020	0		996	0
984	5		969	0		992	4		973	5		1000	5		979	5
983	0		965	6		990	0		971	0		996	1		976	1
970	0		965	0		946	0		935	0		959	4		954	4
897	2		895	17		898	4		884	10		902	2		886	1
893	0		881	0		895	0		884	2		899	1		885	1
892	17		877	0		882	10		880	0		884	2		884	1
834	0		840	0		855	0		848	0		852	22		842	20
801	12		832	113		807	16		793	14		798	37		814	41
795	0		822	0		795	65		784	55		793	36		785	65
794	75		787	11		784	0		774	0		787	33		779	40
778	158		781	114		775	74		764	72		779	47		775	5
775	0		771	0		760	0		751	0		769	11		765	28
756	42		759	21		659	0		657	0		745	37		750	3

E-DOH1						E-DOH2						E-DOH3				
M06-2X			B3LYP			M06-2X			B3LYP			M06-2X			B3LYP	
ω	I		ω	I		ω	I		ω	I		ω	I		ω	I
742	0		745	0		606	1		640	0		673	2		672	2
684	0		682	0		591	0		635	135		602	2		600	1
603	4		601	6		590	33		605	0		592	23		592	32
592	0		588	53		584	116		588	46		588	1		582	1
588	49		584	0		583	27		574	0		562	1		557	1
567	0		566	0		559	0		556	0		547	10		546	9
567	0		561	0		557	0		550	0		531	18		530	17
511	15		503	12		511	35		507	24		514	6		514	5
494	6		494	6		505	0		501	0		467	7		497	81
462	0		462	0		491	26		491	27		450	82		464	3
458	0		459	0		459	0		461	0		441	1		440	2
422	11		434	10		396	34		386	38		412	15		418	13
352	0		350	0		343	1		336	1		353	0		349	1
340	0		345	0		302	0		301	0		315	6		323	5
283	0		284	0		240	0		239	0		251	1		250	2
235	0		235	0		225	0		223	0		228	2		230	3
221	0		226	0		212	1		209	0		224	3		223	2
217	0		215	0		207	0		199	0		201	0		199	0
139	0		138	0		120	0		122	0		135	1		138	1
91	1		94	1		74	1		74	1		77	1		79	1
64	0		59	1		66	0		61	0		61	0		60	0
42	1		42	1		11	1		4	0		37	0		38	0

E-DOH4						E-DOH5						E-DOH6				
M06-2X			B3LYP			M06-2X			B3LYP			M06-2X			B3LYP	
ω	I		ω	I		ω	I		ω	I		ω	I		ω	I
3885	108		3816	84		3877	101		3810	79		3870	82		3788	57
3336	320		3213	2		3764	117		3656	91		3353	357		3202	13
3219	9		3201	20		3238	2		3212	6		3227	7		3201	22
3218	9		3194	26		3230	5		3208	8		3225	10		3197	254
3212	4		3193	14		3222	4		3199	12		3207	4		3193	5
3209	3		3186	220		3218	8		3191	18		3205	4		3187	29
3197	3		3184	1		3208	7		3186	16		3202	0		3185	4
3192	2		3178	7		3197	5		3177	6		3192	0		3179	1
3187	1		3170	15		3194	1		3170	2		3190	2		3170	9
3175	6		3155	13		3187	6		3152	15		3171	8		3146	16
1698	65		1657	96		1699	13		1653	48		1698	75		1660	101
1687	51		1640	37		1685	83		1641	51		1687	35		1645	21
1681	12		1635	14		1678	9		1633	7		1671	18		1626	26
1657	70		1618	63		1672	65		1626	69		1658	67		1619	70
1609	71		1535	46		1628	3		1540	1		1611	60		1541	10
1548	30		1527	8		1551	41		1527	23		1552	34		1533	14
1530	42		1523	25		1537	67		1516	80		1537	11		1518	36
1520	120		1498	102		1522	7		1503	9		1516	116		1490	86
1507	6		1464	32		1507	79		1482	66		1504	30		1471	31
1409	56		1418	85		1381	42		1385	38		1428	42		1428	58
1364	24		1362	51		1361	35		1364	49		1364	32		1368	37
1360	23		1354	3		1355	16		1350	24		1360	3		1354	4
1348	105		1341	88		1343	91		1332	82		1345	96		1337	76
1325	7		1315	15		1308	12		1292	54		1335	19		1319	16
1308	51		1290	29		1304	106		1288	44		1311	56		1297	40
1292	49		1276	87		1281	145		1263	190		1291	35		1272	80

E-DOH4						E-DOH5						E-DOH6				
M06-2X			B3LYP			M06-2X			B3LYP			M06-2X			B3LYP	
ω	I		ω	I		ω	I		ω	I		ω	I		ω	I
1247	8		1241	2		1230	104		1217	86		1253	31		1245	37
1219	111		1213	85		1208	14		1202	4		1218	38		1205	16
1194	31		1190	25		1194	41		1191	29		1199	29		1195	19
1182	21		1180	39		1176	38		1177	109		1182	10		1184	15
1172	36		1174	51		1169	54		1170	26		1169	29		1173	39
1142	24		1138	16		1133	30		1130	27		1144	16		1141	11
1127	30		1119	37		1119	28		1113	29		1133	54		1126	59
1077	4		1061	3		1080	2		1063	2		1086	5		1070	4
1067	6		1051	7		1065	8		1048	8		1067	6		1051	6
1017	0		998	1		1025	0		1000	0		1018	0		994	0
1016	0		994	0		1018	0		989	0		1014	0		987	0
989	4		973	3		1007	3		983	2		996	3		977	2
987	0		967	1		995	3		965	2		982	2		962	2
961	3		957	2		946	0		935	0		959	2		957	3
895	2		886	15		905	1		885	1		895	1		889	24
883	1		883	1		890	1		881	21		887	23		883	0
882	0		879	36		880	19		862	1		883	1		866	21
850	27		865	1		853	1		847	2		830	3		855	31
816	43		841	27		803	11		789	10		822	53		815	2
796	1		781	2		797	79		783	60		797	9		781	16
790	132		780	83		788	12		771	4		791	120		780	86
781	2		770	5		780	54		765	69		785	32		770	10
775	29		765	48		759	0		747	0		773	3		762	33
753	2		745	1		659	1		657	1		752	4		743	1
674	2		673	2		602	63		633	67		683	0		681	0
599	5		597	6		601	9		599	3		605	3		604	8

E-DOH4						E-DOH5						E-DOH6				
M06-2X			B3LYP			M06-2X			B3LYP			M06-2X			B3LYP	
ω	I		ω	I		ω	I		ω	I		ω	I		ω	I
592	23		592	30		592	24		592	33		593	1		587	0
590	0		583	0		585	0		577	0		586	40		584	45
564	1		558	0		559	1		556	0		570	2		566	2
545	0		543	0		558	1		552	0		566	1		563	0
531	16		530	15		516	18		510	16		514	10		508	8
513	15		510	12		506	19		499	19		496	1		495	1
462	0		462	0		489	19		489	20		469	3		466	4
449	9		449	10		467	4		464	3		449	8		451	9
412	4		422	4		394	10		387	27		407	2		417	75
375	93		372	87		370	90		383	72		382	85		408	3
350	1		346	0		344	5		338	2		358	1		349	0
306	8		312	8		288	1		285	1		307	14		309	13
246	1		245	1		227	0		224	0		289	2		282	0
225	1		228	0		221	0		219	1		223	1		225	1
219	0		223	0		218	3		211	3		219	1		213	1
211	0		209	0		194	1		190	2		191	0		197	1
127	0		131	0		116	1		120	1		132	0		126	0
71	1		78	1		77	1		74	1		79	1		83	1
59	2		60	2		64	2		62	2		58	2		57	2
26	0		28	0		24	0		8	0		26	0		14	0

E-DOH7						E-DOH8						Z-DOH1				
M06-2X			B3LYP			M06-2X			B3LYP			M06-2X			B3LYP	
ω	I		ω	I		ω	I		ω	I		ω	I		ω	I
3874	34		3786	5		3892	0		3810	0		3765	124		3623	65
3874	113		3785	88		3891	187		3810	145		3764	65		3621	81
3214	1		3202	0		3220	18		3210	13		3230	1		3212	2
3214	13		3202	29		3220	0		3210	0		3230	6		3211	3
3205	0		3189	0		3208	0		3190	0		3219	4		3200	1
3205	10		3189	23		3208	10		3190	42		3219	3		3200	20
3192	1		3176	12		3194	0		3174	0		3211	1		3189	15
3192	4		3176	0		3194	8		3174	15		3211	2		3189	6
3161	3		3142	1		3168	0		3150	0		3200	0		3174	1
3161	14		3141	33		3168	18		3149	32		3200	0		3174	2
1691	7		1646	2		1696	0		1643	0		1700	0		1649	14
1688	53		1645	64		1684	74		1639	73		1686	18		1644	31
1675	8		1623	1		1681	0		1635	0		1669	135		1621	81
1662	37		1616	53		1678	50		1632	47		1661	74		1617	82
1628	1		1551	1		1628	0		1541	0		1653	13		1561	76
1550	27		1527	14		1552	61		1529	40		1538	118		1510	123
1542	9		1501	0		1546	0		1522	0		1534	141		1508	0
1505	76		1489	83		1509	114		1491	108		1524	2		1504	128
1502	20		1482	4		1507	0		1474	0		1519	0		1502	5
1363	15		1367	89		1365	0		1365	0		1381	21		1383	17
1363	60		1366	5		1364	66		1364	94		1381	74		1383	80
1339	24		1334	4		1344	0		1338	0		1351	52		1341	28
1335	99		1329	80		1339	202		1330	163		1346	17		1339	24
1322	20		1300	5		1310	0		1291	52		1309	78		1289	140
1304	39		1286	43		1307	66		1288	0		1301	208		1279	277
1277	24		1254	66		1277	110		1253	160		1253	91		1237	47

E-DOH7						E-DOH8						Z-DOH1					
M06-2X			B3LYP			M06-2X			B3LYP			M06-2X			B3LYP		
ω	I		ω	I		ω	I		ω	I		ω	I		ω	I	
1213	10		1196	3		1222	0		1203	0		1243	120		1226	115	
1193	45		1195	34		1195	0		1192	0		1213	35		1204	31	
1193	11		1187	0		1193	72		1191	53		1207	3		1197	3	
1177	8		1180	41		1180	0		1178	107		1178	84		1171	133	
1177	23		1173	4		1177	84		1175	0		1176	1		1161	0	
1134	16		1130	4		1132	112		1125	124		1137	8		1130	11	
1124	80		1119	89		1118	0		1110	0		1122	2		1108	3	
1085	9		1069	9		1079	8		1062	5		1073	7		1052	13	
1083	0		1067	0		1078	0		1062	0		1072	11		1052	7	
1009	1		993	1		1026	1		1007	2		1023	0		996	0	
1009	0		993	0		1025	0		1005	0		1023	0		994	0	
986	3		967	3		995	3		970	3		996	16		973	0	
983	1		965	0		993	0		968	0		992	0		972	15	
945	3		944	1		946	0		935	0		912	8		886	13	
880	18		881	32		888	1		879	36		903	5		883	4	
878	0		866	0		884	0		868	0		885	6		867	3	
875	9		862	0		879	32		865	0		867	6		859	11	
828	10		806	4		852	0		845	0		860	11		852	11	
791	6		773	6		800	8		783	7		800	5		783	4	
775	125		772	114		789	100		776	77		786	144		773	10	
775	22		769	4		785	0		770	0		786	14		771	142	
767	0		762	22		781	51		765	60		764	2		754	1	
754	8		742	2		756	0		744	0		760	15		749	16	
681	0		679	0		658	0		656	0		722	2		720	2	
607	2		607	7		596	13		595	22		639	0		658	12	
594	0		589	0		595	19		592	19		592	0		655	128	

E-DOH7					E-DOH8					Z-DOH1						
M06-2X			B3LYP		M06-2X			B3LYP		M06-2X			B3LYP			
ω	I		ω	I		ω	I		ω	I		ω	I			
584	41		577	54		588	0		578	0		586	17		620	4
571	0		568	0		562	0		557	0		584	139		588	1
563	1		565	1		560	0		554	0		571	22		569	33
518	3		513	4		518	12		514	11		554	8		550	6
494	3		491	3		501	0		495	0		549	7		544	5
471	3		472	0		491	17		489	18		532	7		530	2
444	11		441	9		470	0		469	0		517	8		509	9
394	116		425	148		390	12		385	13		497	5		489	8
393	48		425	12		373	180		382	178		463	5		456	7
380	12		378	9		372	0		381	0		402	2		399	2
361	4		350	2		342	14		336	4		397	15		395	15
293	3		281	1		281	0		275	0		287	1		278	0
271	11		270	3		228	0		224	0		284	1		264	0
215	1		206	2		209	0		206	0		237	4		225	4
192	11		188	5		206	2		199	2		208	0		206	1
164	0		176	0		179	0		167	0		177	0		172	0
112	1		91	1		86	0		92	0		147	2		149	2
55	3		56	4		70	2		72	2		72	0		72	0
47	4		54	3		68	4		62	4		45	0		37	0
22	0		14	1		30	0		18	0		41	0		35	0

Z-DOH2						Z-DOH3						E-DNH1				
M06-2X			B3LYP			M06-2X			B3LYP			M06-2X			B3LYP	
ω	I		ω	I		ω	I		ω	I		ω	I		ω	I
3871	64		3806	51		3859	268		3746	375		3330	232		3319	165
3745	104		3584	99		3854	13		3736	5		3315	0		3303	0
3239	1		3237	2		3226	0		3202	2		3231	0		3202	0
3227	2		3202	7		3226	10		3202	23		3231	4		3202	32
3220	6		3200	15		3206	2		3194	4		3226	0		3197	0
3216	3		3192	9		3206	1		3194	10		3226	14		3197	22
3203	2		3192	10		3199	0		3182	4		3189	0		3170	0
3198	1		3182	4		3199	0		3182	1		3189	16		3170	20
3187	1		3175	3		3191	2		3175	0		3176	19		3162	0
3183	3		3173	0		3191	1		3175	1		3176	0		3161	14
1697	6		1650	33		1693	0		1647	1		1735	0		1684	0
1688	17		1645	11		1687	39		1644	48		1702	387		1651	227
1664	102		1619	76		1670	18		1610	0		1663	0		1616	0
1661	12		1616	15		1647	22		1600	11		1651	0		1600	0
1651	48		1565	100		1645	21		1576	51		1640	269		1596	235
1535	36		1513	35		1530	150		1501	110		1592	0		1557	0
1526	181		1508	9		1530	0		1496	12		1578	290		1549	138
1522	1		1502	180		1506	9		1493	14		1532	0		1509	0
1511	5		1495	9		1504	4		1489	3		1491	1185		1485	1027
1377	53		1386	46		1360	5		1362	21		1448	269		1452	44
1363	34		1365	22		1356	31		1357	2		1446	0		1443	0
1350	25		1348	36		1344	68		1333	3		1426	788		1416	204
1333	47		1318	38		1343	4		1329	66		1394	0		1391	0
1298	160		1285	250		1285	1		1268	37		1336	0		1340	978
1292	32		1267	38		1284	34		1264	2		1326	1987		1308	0
1243	92		1230	71		1217	0		1206	3		1290	0		1274	0

Z-DOH2						Z-DOH3						E-DNH1				
M06-2X			B3LYP			M06-2X			B3LYP			M06-2X			B3LYP	
ω	I		ω	I		ω	I		ω	I		ω	I		ω	I
1229	61		1213	70		1216	96		1200	146		1267	867		1270	97
1208	7		1202	17		1199	62		1190	1		1227	79		1228	33
1194	22		1186	5		1186	1		1185	0		1206	0		1206	0
1173	13		1174	23		1172	20		1174	19		1176	0		1177	0
1167	42		1159	66		1170	5		1157	5		1165	860		1175	308
1130	8		1122	22		1123	5		1113	5		1150	33		1143	6
1120	2		1109	11		1121	0		1112	0		1135	0		1123	0
1072	6		1056	12		1076	14		1060	15		1024	0		1021	0
1070	10		1054	8		1074	1		1057	0		1019	115		1017	17
1018	0		1002	0		1018	0		996	0		1015	1		1002	0
1015	0		988	0		1017	0		995	0		1015	0		1002	0
996	8		976	4		992	7		973	4		973	35		944	16
985	5		963	4		992	2		973	2		967	0		941	0
915	11		893	7		912	10		893	8		947	56		915	0
903	1		883	3		901	0		884	0		917	0		903	58
883	8		866	13		885	15		872	18		892	73		894	36
861	8		855	7		866	1		861	3		871	0		859	0
852	11		843	13		844	17		824	18		868	32		855	41
796	22		782	19		794	24		782	32		857	0		851	0
785	91		774	78		785	78		772	54		827	0		797	0
782	22		766	14		774	7		756	5		786	80		774	29
765	2		758	8		750	12		737	10		778	58		767	43
748	13		736	13		731	1		715	0		762	0		748	0
714	3		713	49		709	7		707	7		749	74		741	78
652	34		703	12		642	3		630	3		744	0		734	0
632	47		630	7		601	3		599	3		626	0		623	0

Z-DOH2					Z-DOH3					E-DNH1				
M06-2X			B3LYP		M06-2X			B3LYP		M06-2X			B3LYP	
ω	I		ω	I	ω	I		ω	I	ω	I		ω	I
594	3		591	2	592	0		588	1	592	8		587	10
583	1		579	4	574	0		566	0	562	418		572	203
552	7		549	10	548	9		546	15	555	0		551	0
550	10		544	5	523	1		520	1	543	0		543	0
534	12		530	19	506	20		494	17	526	1		526	0
513	5		508	5	451	8		453	7	524	0		523	0
481	11		476	11	434	0		437	3	481	14		483	12
441	8		434	11	434	2		425	0	478	16		474	12
424	7		413	12	402	0		400	2	445	0		451	0
394	5		393	5	308	8		315	39	397	56		403	5
314	50		334	83	282	13		296	72	325	0		312	0
301	31		295	1	265	87		284	11	296	1		292	1
265	17		256	2	241	45		262	59	221	0		212	0
235	14		229	2	209	89		245	1	214	0		211	0
195	2		201	2	192	6		191	0	188	0		187	0
178	0		164	1	168	8		173	3	178	7		174	7
138	4		129	2	135	13		143	2	118	0		118	0
65	1		69	1	56	0		66	0	63	3		63	3
48	0		33	0	52	6		52	0	59	1		57	0
31	0		19	1	38	0		38	0	32	4		25	4

Z-DNH1					Z-DNH2					Z-DNH3						
M06-2X			B3LYP		M06-2X			B3LYP		M06-2X			B3LYP			
ω	I		ω	I		ω	I		ω	I		ω	I			
3308	174		3249	114		3587	48		3556	26		3580	146		3563	80
3298	229		3238	173		3580	93		3549	61		3332	173		3260	139
3241	1		3222	2		3218	0		3198	7		3242	4		3223	3
3235	6		3212	10		3218	17		3198	26		3219	3		3202	12
3223	2		3201	0		3208	3		3190	3		3214	8		3198	20
3221	3		3200	26		3208	5		3190	24		3211	5		3194	8
3220	1		3193	11		3181	3		3169	15		3208	4		3192	9
3219	18		3192	3		3181	10		3169	5		3188	8		3166	12
3180	3		3168	5		3168	6		3151	13		3183	9		3166	14
3180	17		3168	22		3168	13		3150	14		3167	11		3146	17
1721	161		1673	102		1694	1		1648	1		1739	210		1682	130
1714	360		1661	200		1692	14		1648	8		1684	110		1641	40
1654	176		1610	37		1644	0		1601	16		1669	67		1621	32
1651	92		1607	205		1624	36		1594	2		1640	241		1602	121
1643	13		1592	4		1601	5		1565	6		1612	41		1573	115
1588	5		1553	80		1597	117		1560	118		1602	102		1566	57
1586	143		1552	27		1563	40		1521	34		1588	101		1547	102
1539	8		1513	15		1523	205		1507	103		1527	86		1509	153
1521	36		1504	32		1499	3		1491	4		1515	375		1500	113
1470	1257		1472	909		1472	1		1468	236		1479	858		1476	525
1456	26		1456	19		1471	276		1439	0		1454	30		1449	16
1423	731		1422	341		1432	128		1414	54		1421	4		1415	7
1412	16		1406	19		1409	41		1403	0		1417	109		1408	39
1354	2104		1363	824		1408	0		1393	8		1375	109		1357	127
1305	2		1279	11		1341	1		1318	2		1308	43		1284	264
1297	81		1276	2		1263	157		1264	116		1290	410		1275	6

Z-DNH1					Z-DNH2					Z-DNH3				
M06-2X			B3LYP		M06-2X			B3LYP		M06-2X			B3LYP	
ω	I		ω	I	ω	I		ω	I	ω	I		ω	I
1289	14		1274	3	1237	0		1232	1	1264	184		1254	32
1223	102		1217	37	1219	222		1216	113	1221	69		1216	33
1216	17		1203	12	1189	0		1185	1	1206	73		1193	18
1173	14		1172	17	1177	3		1176	182	1179	87		1175	13
1164	816		1170	347	1167	274		1156	15	1160	352		1169	252
1154	104		1145	36	1154	203		1150	7	1151	72		1147	15
1128	10		1112	13	1154	13		1150	7	1143	42		1127	17
1033	3		1022	2	1029	1		1026	4	1034	7		1027	1
1024	62		1018	11	1028	28		1024	1	1027	1		1015	8
1023	0		1004	0	1011	0		995	0	1022	0		1003	0
1022	17		1003	1	1011	1		995	0	1017	42		999	1
1007	0		975	0	976	2		953	2	988	0		964	1
990	3		955	3	976	0		953	0	967	4		943	2
914	16		905	14	920	29		924	16	915	24		917	17
889	5		875	10	899	3		899	3	883	7		876	8
882	30		873	23	871	0		860	0	878	2		867	4
881	21		869	18	864	2		854	2	872	16		862	4
875	89		865	18	790	22		779	25	856	80		850	74
864	0		858	3	783	31		771	50	833	53		822	22
836	104		837	78	775	60		767	26	786	11		773	10
802	10		785	6	761	4		750	7	778	53		770	53
785	96		767	58	743	41		736	40	756	24		749	34
757	9		744	9	742	19		730	21	754	39		744	27
753	53		742	67	725	23		722	19	741	27		723	18
751	0		739	0	632	118		627	115	702	45		696	22
700	140		690	70	614	69		606	63	588	4		588	3

Z-DNH1					Z-DNH2					Z-DNH3				
M06-2X			B3LYP		M06-2X			B3LYP		M06-2X			B3LYP	
ω	I		ω	I	ω	I		ω	I	ω	I		ω	I
582	1		584	2	580	21		581	29	576	28		574	58
565	107		565	87	579	41		578	22	561	13		558	4
559	0		553	0	563	42		555	40	554	47		546	96
544	0		543	77	529	102		528	85	541	157		543	11
540	197		537	0	524	46		525	21	525	11		518	7
522	28		522	8	498	41		497	17	509	3		515	1
519	0		497	0	498	0		495	2	480	19		482	5
486	8		486	8	459	3		457	2	453	14		453	17
446	17		447	14	430	1		425	32	436	24		439	17
422	10		424	0	423	58		417	0	426	8		420	4
377	1		352	0	347	12		334	10	359	9		341	5
272	6		275	4	316	1		308	1	292	6		286	6
235	0		229	0	297	21		293	12	267	9		257	2
212	1		206	0	235	3		228	14	242	4		229	5
200	8		197	6	227	54		224	1	211	2		205	2
188	1		175	1	223	0		205	0	198	3		183	4
148	4		146	4	129	1		126	1	139	2		139	2
77	0		76	0	85	0		82	4	78	2		73	2
56	2		52	1	85	5		82	1	66	1		62	1
48	1		42	1	78	7		75	5	37	1		39	1

E-NHOH1						E-NHOH2						E-NHOH3				
M06-2X			B3LYP			M06-2X			B3LYP			M06-2X			B3LYP	
ω	I		ω	I		ω	I		ω	I		ω	I		ω	I
3562	314		3433	240		3888	122		3827	97		3790	86		3685	56
3227	7		3203	15		3222	4		3218	2		3292	36		3245	27
3220	8		3200	18		3215	7		3199	19		3233	5		3204	15
3213	2		3196	7		3213	5		3197	18		3232	4		3203	18
3208	8		3194	11		3209	6		3192	14		3217	5		3197	12
3194	0		3180	3		3200	3		3182	5		3209	6		3195	10
3194	1		3177	1		3189	0		3179	1		3206	0		3187	2
3181	1		3173	0		3178	10		3160	12		3202	5		3180	1
3180	2		3164	10		3178	6		3158	13		3193	1		3169	1
2920	92		2871	78		3130	96		3058	77		3182	10		3164	16
1719	120		1675	76		1721	124		1675	66		1734	258		1676	154
1695	18		1655	41		1689	9		1644	2		1688	46		1646	31
1664	78		1626	122		1685	41		1640	40		1672	3		1627	11
1651	91		1614	95		1659	66		1608	86		1657	124		1611	118
1598	279		1557	288		1599	40		1555	35		1611	219		1561	170
1588	602		1545	133		1571	831		1554	675		1586	299		1560	78
1549	70		1526	52		1554	425		1537	17		1541	157		1518	95
1535	26		1524	25		1521	47		1503	48		1527	35		1512	41
1498	34		1488	47		1496	73		1487	42		1516	1144		1507	652
1451	2		1435	49		1457	5		1426	16		1452	100		1434	140
1419	48		1420	5		1408	28		1395	12		1440	356		1408	157
1411	42		1382	5		1368	113		1366	72		1389	57		1392	35
1361	249		1352	80		1351	307		1346	279		1372	14		1364	3
1351	264		1337	355		1332	29		1318	35		1348	148		1339	144
1337	14		1318	26		1319	148		1306	165		1330	60		1301	95
1303	339		1293	241		1307	197		1286	155		1299	256		1277	228

E-NHOH1						E-NHOH2						E-NHOH3				
M06-2X			B3LYP			M06-2X			B3LYP			M06-2X			B3LYP	
ω	I		ω	I		ω	I		ω	I		ω	I		ω	I
1268	78		1267	8		1239	86		1235	27		1271	169		1263	35
1233	44		1231	33		1201	118		1205	77		1232	181		1227	141
1202	28		1202	2		1185	51		1184	20		1206	7		1203	3
1178	27		1182	20		1181	25		1182	47		1181	26		1182	79
1171	61		1170	86		1170	123		1170	123		1174	282		1175	128
1152	74		1153	29		1153	150		1152	17		1152	5		1144	2
1135	145		1138	18		1117	66		1114	46		1138	3		1128	0
1075	5		1058	4		1076	8		1062	6		1077	11		1058	9
1037	0		1019	4		1030	0		1014	4		1041	38		1009	4
1020	12		1010	0		1014	9		1011	0		1028	0		1009	0
1015	0		989	9		1008	0		988	1		1015	2		996	25
993	23		981	34		996	0		981	0		1010	11		986	9
987	31		971	10		970	3		952	1		992	0		963	1
967	3		951	0		925	52		943	45		980	2		949	0
923	5		929	1		923	2		928	1		931	17		925	5
888	12		892	9		884	0		878	2		895	2		893	9
885	5		877	3		878	0		868	10		890	12		869	9
878	0		868	1		863	16		860	0		879	10		865	3
810	18		799	14		845	16		834	17		853	45		847	29
785	9		777	8		784	8		780	17		797	24		783	11
781	112		770	36		775	100		766	82		787	62		774	26
779	66		769	104		771	80		762	39		782	61		768	79
769	23		767	37		767	38		759	43		767	1		754	2
749	5		748	33		752	4		740	1		756	12		744	18
671	69		733	15		644	4		648	1		644	1		640	0
662	1		663	0		596	9		594	10		598	4		593	5

E-NHOH1						E-NHOH2						E-NHOH3				
M06-2X			B3LYP			M06-2X			B3LYP			M06-2X			B3LYP	
ω	I		ω	I		ω	I		ω	I		ω	I		ω	I
597	2		594	7		585	31		587	30		581	84		591	74
588	60		588	52		578	0		570	0		569	1		581	86
577	0		570	0		540	20		539	9		548	78		559	2
561	9		561	4		536	7		537	5		547	65		548	26
539	1		538	1		531	1		532	3		534	8		528	11
495	4		499	1		488	8		490	7		519	0		519	0
491	13		489	9		469	0		471	0		502	33		497	23
486	11		485	10		455	2		460	2		488	17		487	12
456	0		459	0		426	17		425	16		456	1		455	0
426	2		438	3		396	5		391	4		409	23		400	15
391	2		388	2		338	83		331	67		334	5		329	4
323	1		319	1		316	28		312	37		321	0		313	1
286	6		287	5		240	0		242	0		238	2		235	3
234	0		233	0		233	0		232	0		222	0		220	0
211	0		220	1		207	0		217	1		212	1		201	2
198	1		201	1		193	0		195	0		182	2		186	2
133	1		132	1		127	0		128	0		124	0		121	0
88	1		93	0		68	1		79	1		69	2		70	2
53	1		52	1		50	2		53	2		57	0		58	0
36	2		46	1		33	0		34	0		25	2		15	2

E-NHOH4						E-NHOH5						E-NHOH6				
M06-2X			B3LYP			M06-2X			B3LYP			M06-2X			B3LYP	
ω	I		ω	I		ω	I		ω	I		ω	I		ω	I
3900	115		3827	93		3891	127		3811	102		3663	84		3591	55
3573	64		3511	48		3271	32		3230	21		3399	4		3363	1
3222	4		3217	1		3224	6		3204	15		3229	3		3203	15
3216	3		3197	15		3217	9		3200	16		3228	3		3199	16
3213	7		3195	16		3211	4		3196	13		3211	7		3194	13
3199	3		3186	18		3206	1		3187	5		3205	11		3194	13
3198	9		3182	5		3200	3		3185	5		3197	1		3178	1
3187	6		3160	15		3182	1		3173	1		3184	9		3163	17
3176	4		3156	14		3181	12		3161	17		3180	3		3149	4
3173	9		3152	2		3173	12		3155	20		3142	6		3131	9
1788	208		1708	174		1728	285		1675	173		1731	261		1670	159
1708	12		1664	16		1683	34		1639	23		1691	14		1647	14
1697	34		1655	30		1668	17		1626	17		1681	44		1639	29
1688	21		1642	16		1661	52		1613	66		1655	57		1609	23
1639	64		1593	108		1607	129		1559	102		1638	103		1595	87
1579	760		1557	479		1584	360		1556	152		1565	677		1539	385
1573	668		1539	121		1554	71		1534	45		1535	57		1513	63
1533	98		1509	297		1512	554		1505	570		1525	135		1507	89
1511	62		1493	20		1507	604		1491	84		1504	5		1490	35
1467	225		1457	327		1449	108		1432	142		1471	458		1432	256
1414	53		1411	53		1437	559		1401	321		1440	163		1418	62
1378	28		1366	35		1368	225		1371	142		1415	31		1395	55
1358	24		1348	14		1366	9		1363	5		1392	81		1386	31
1327	125		1313	189		1342	59		1331	67		1355	88		1343	122
1317	103		1286	32		1330	58		1300	88		1314	60		1301	56
1285	358		1263	222		1305	225		1284	135		1305	278		1287	258

E-NHOH4						E-NHOH5						E-NHOH6				
M06-2X			B3LYP			M06-2X			B3LYP			M06-2X			B3LYP	
ω	I		ω	I		ω	I		ω	I		ω	I		ω	I
1253	94		1240	44		1269	56		1254	30		1258	307		1250	121
1218	2		1212	4		1212	46		1203	4		1227	66		1220	48
1192	54		1184	19		1204	20		1203	54		1217	85		1205	53
1180	23		1181	53		1185	23		1188	25		1184	4		1185	3
1177	2		1177	5		1172	130		1175	92		1173	270		1177	153
1143	139		1133	99		1148	37		1140	33		1161	13		1151	9
1120	60		1110	59		1134	83		1123	64		1145	5		1135	1
1080	5		1062	3		1092	5		1072	1		1069	5		1052	6
1040	0		1020	0		1062	49		1015	42		1022	0		1019	4
1018	1		1002	2		1028	0		1009	2		1021	11		1006	0
1001	3		997	1		1011	1		1008	1		1011	0		985	0
982	0		963	0		1010	6		982	0		970	9		945	6
974	3		950	3		996	1		976	1		964	3		939	2
912	45		909	33		969	7		945	6		932	11		931	8
886	4		886	8		933	12		924	4		920	38		885	2
884	0		869	11		889	11		891	11		885	4		866	13
880	13		863	0		883	12		872	8		884	7		862	25
846	44		837	50		875	1		855	8		868	15		857	29
780	3		774	2		853	63		845	45		840	17		828	11
778	83		762	102		795	28		781	7		775	6		765	0
770	83		759	24		784	42		777	44		770	73		761	63
763	52		759	50		776	83		763	82		764	32		747	18
751	0		736	0		766	9		756	6		760	9		747	4
630	1		632	43		756	4		744	4		740	32		731	34
610	50		629	1		645	1		640	0		678	89		693	83
590	9		586	11		598	9		591	13		655	0		652	0

E-NHOH4						E-NHOH5						E-NHOH6				
M06-2X			B3LYP			M06-2X			B3LYP			M06-2X			B3LYP	
ω	I		ω	I		ω	I		ω	I		ω	I		ω	I
578	0		577	30		585	57		585	59		594	5		592	11
576	23		569	0		573	3		564	1		582	74		582	59
545	35		545	26		547	56		547	33		568	1		560	1
526	21		520	14		530	3		524	3		541	10		539	11
492	0		499	0		523	2		521	1		534	0		532	0
479	5		478	3		504	17		500	15		530	20		528	9
475	3		475	3		489	12		488	8		490	16		486	13
408	1		432	2		467	11		465	6		455	2		451	2
401	7		394	6		408	20		399	5		431	1		434	1
329	32		314	1		397	81		389	91		417	28		409	21
303	21		303	7		344	5		330	4		326	1		319	1
295	73		265	107		323	1		315	1		290	3		285	3
223	2		219	2		241	4		233	5		253	4		249	4
219	0		215	2		220	0		217	0		225	4		222	5
213	1		209	1		210	3		210	2		210	1		202	1
173	0		172	0		168	0		168	0		184	1		182	1
85	0		88	0		128	0		125	0		109	0		109	0
71	1		71	2		67	2		67	2		57	0		57	0
45	2		47	1		59	1		57	2		48	1		50	1
34	2		36	2		34	2		26	1		30	1		32	1

E-NHOH7						Z-NHOH1						Z-NHOH2					
M06-2X			B3LYP			M06-2X			B3LYP			M06-2X			B3LYP		
ω	I		ω	I		ω	I		ω	I		ω	I		ω	I	
3886	125		3810	93		3766	89		3661	63		3891	122		3822	100	
3382	84		3370	59		3286	125		3253	107		3595	111		3576	104	
3233	7		3207	7		3246	5		3227	4		3243	2		3219	3	
3219	5		3197	16		3222	2		3212	3		3234	1		3214	1	
3210	1		3196	12		3216	3		3201	10		3225	5		3198	13	
3205	10		3191	15		3216	6		3199	13		3211	4		3194	14	
3200	1		3182	5		3211	1		3191	14		3209	2		3183	3	
3176	13		3159	20		3201	3		3190	4		3199	5		3179	12	
3160	6		3147	15		3189	0		3177	0		3180	10		3158	14	
3157	8		3138	7		3180	10		3165	14		3173	11		3156	16	
1739	244		1683	149		1734	284		1677	180		1800	235		1709	201	
1700	2		1661	7		1685	25		1645	27		1715	13		1664	15	
1681	39		1632	27		1671	72		1625	78		1686	2		1644	1	
1658	10		1616	24		1656	102		1613	91		1680	56		1638	52	
1635	36		1599	14		1607	26		1565	69		1647	8		1596	23	
1578	341		1547	253		1577	286		1547	27		1609	177		1569	40	
1541	21		1517	13		1545	621		1517	311		1562	163		1537	79	
1509	98		1493	37		1531	120		1510	130		1531	278		1505	197	
1498	26		1487	87		1512	299		1497	454		1503	311		1484	234	
1478	1736		1437	926		1487	180		1475	18		1460	189		1448	510	
1448	10		1418	3		1434	167		1423	72		1413	66		1410	80	
1415	35		1388	49		1377	52		1387	42		1372	32		1365	56	
1362	43		1361	50		1351	297		1347	246		1344	28		1333	49	
1327	41		1318	30		1341	73		1329	45		1341	84		1313	62	
1312	131		1299	74		1319	6		1286	1		1321	59		1295	25	
1286	30		1258	25		1302	274		1285	328		1282	219		1268	108	

E-NHOH7						Z-NHOH1						Z-NHOH2					
M06-2X			B3LYP			M06-2X			B3LYP			M06-2X			B3LYP		
ω	I		ω	I		ω	I		ω	I		ω	I		ω	I	
1239	76		1225	13		1251	148		1245	61		1226	21		1217	14	
1221	68		1203	45		1223	50		1219	61		1213	63		1198	32	
1193	32		1186	26		1209	69		1204	33		1197	62		1191	90	
1184	68		1184	10		1172	143		1177	112		1183	14		1183	16	
1179	1		1181	25		1168	79		1171	76		1178	19		1171	27	
1158	9		1149	6		1149	5		1140	2		1143	141		1133	108	
1133	54		1122	56		1124	13		1114	11		1115	20		1104	18	
1082	4		1064	4		1067	8		1054	11		1084	5		1066	4	
1025	0		1018	4		1049	131		1024	84		1035	0		1019	0	
1023	0		1007	0		1029	0		1016	12		1026	4		1001	3	
1021	10		997	0		1022	17		1011	0		1013	0		993	3	
988	21		956	3		1018	3		993	0		999	2		986	0	
973	3		953	17		1007	6		981	0		969	3		946	3	
958	16		935	10		996	8		963	5		907	14		894	10	
935	12		924	20		907	8		892	22		886	19		878	12	
891	10		891	12		895	25		881	2		879	6		867	23	
877	0		864	10		883	12		872	15		872	3		856	2	
873	16		860	5		874	7		867	5		851	17		844	15	
796	10		779	9		858	19		854	14		798	29		785	13	
780	46		767	4		797	13		782	5		782	92		765	111	
778	64		764	90		785	92		768	41		769	52		761	40	
770	36		752	19		777	14		763	39		758	27		746	11	
755	20		744	15		761	26		750	46		742	20		729	13	
740	9		731	13		755	22		746	11		698	55		680	41	
663	1		659	1		709	54		700	39		631	43		626	44	
594	30		593	33		600	13		611	81		591	2		589	2	

E-NHOH7					Z-NHOH1					Z-NHOH2				
M06-2X			B3LYP		M06-2X			B3LYP		M06-2X			B3LYP	
ω	I		ω	I	ω	I		ω	I	ω	I		ω	I
582	24		576	18	585	3		591	4	576	5		569	2
578	0		570	0	568	45		575	4	565	9		565	27
561	26		561	16	562	60		567	68	535	50		531	18
533	0		529	0	548	23		547	12	526	5		524	17
491	15		487	11	536	17		536	1	522	14		512	15
489	1		486	1	534	71		529	25	482	10		481	14
464	1		458	2	521	2		521	2	464	59		472	33
442	3		445	3	490	20		489	16	444	14		454	11
398	19		393	16	455	8		453	9	409	10		404	10
337	5		330	4	413	12		413	9	359	75		351	38
323	85		317	67	400	2		395	2	330	106		343	93
285	16		283	29	290	3		285	2	290	9		284	9
281	3		278	2	247	1		241	2	237	2		227	0
229	7		226	7	218	1		213	2	225	2		216	0
212	0		200	0	211	1		209	1	202	7		192	4
183	1		181	1	192	1		180	1	185	4		179	0
99	0		98	0	140	2		140	2	117	0		113	1
86	1		82	1	76	1		77	0	48	1		56	1
50	2		48	2	52	1		51	1	46	4		41	3
33	1		34	1	45	0		41	0	44	3		37	2

Table S3. Experimental wavenumbers (ω , in cm^{-1}) of the *E*-DOH1 azo-enol isomer isolated in argon and xenon matrices.^a

Ar (15 K)	Xe (30 K)	Calculated			
ω	ω	ω	<i>I</i>	Sym.	Tentative Assignment
3400-2500	3400-2500	3313.5	0.0	A _g	v(OH)s
		3303.4	581.5	B _u	v(OH)as
		3121.8	0.0	A _g	v(CH)
		3121.7	13.3	B _u	v(CH)
		3116.0	5.8	B _u	v(CH)
		3116.0	0.0	A _g	v(CH)
		3098.0	0.0	A _g	v(CH)
		3097.9	4.3	B _u	v(CH)
		3089.5	0.5	B _u	v(CH)
		3089.5	0.0	A _g	v(CH)
1625.7, 1623.6	1622.7, 1622.1	1649.1	166.7	B _u	v(CC)+ δ (CH)+ δ (OH)
		1644.3	0.0	A _g	v(CC)+ δ (CH)+ δ (OH)+v(NN)
		1616.6	0.0	A _g	v(CC)+ δ (CH)+ δ (OH)+v(NN)
1589.7 , 1584.4	1585.0 , 1581.2	1602.5	137.6	B _u	v(CC)+ δ (OH)+ δ (CH)
		1548.4	0.0	A _g	v(NN)+ δ (OH)+v(CC)+ δ (CH)
1518.0	1511.1	1495.4	6.4	B _u	δ (CH)+ δ (OH)+v(CC)
		1485.4	0.0	A _g	δ (CH)+ δ (OH)+v(CC)
1477.2 , 1476.0	1473.3 , 1471.4	1477.8	194.7	B _u	δ (CH)+v(CO)+v(CC)
		1463.8	0.0	A _g	δ (CH)+v(CO)+v(CC)+v(NN)
		1379.6	0.0	A _g	δ (OH)+ δ (CH)
1370.2, 1368.9, 1366.9 , 1364.4	1364.5 , 1362.6	1379.1	89.2	B _u	δ (OH)+ δ (CH)
		1328.3	0.0	A _g	v(CC)+ δ (CH)
1326.7, 1322.8, 1320.6, 1319.8	1323.6, 1322.3, 1318.0 , 1314.6	1322.6	16.1	B _u	v(CC)+v(CO)+ δ (CH)
		1301.4	0.0	A _g	v(CO)+v(CC)
1293.1	1288.0				

Ar (15 K)	Xe (30 K)	Calculated			
ω	ω	ω	I	Sym.	Tentative Assignment
1282.1 , 1280.7	1277.8 , 1277.0	1284.9	140.9	B _u	$\nu(\text{CO})+\nu(\text{CC})$
1249.9, 1247.8, 1245.3, 1244.3, 1240.9, 1239.2	1245.4, 1244.2, 1240.9, 1239.4, 1238.0, 1236.7	1252.0	93.6	B _u	$\nu(\text{CN})+\delta(\text{CH})$
1227.9, 1223.7	1220.8 , 1217.7				
		1229.8	0.0	A _g	$\delta(\text{CH})+\nu(\text{CN})$
1210.2, 1208.0	1205.5 , 1204.3	1200.5	74.9	B _u	$\delta(\text{CH})+\nu(\text{CN})$
1194.3, 1190.4, 1187.5	1185.6, 1183.0				
		1187.0	0.0	A _g	$\nu(\text{CN})+\delta(\text{CH})$
		1139.2	0.0	A _g	$\delta(\text{CH})$
1151.6 , 1149.3, 1147.3	1147.5	1138.9	53.7	B _u	$\delta(\text{CH})$
		1119.0	0.0	A _g	$\delta(\text{CH})+\nu(\text{CC})$
1117.7	1114.5 , 1112.8				
1112.6, 1109.8	1107.9 , 1106.3	1107.3	19.7	B _u	$\delta(\text{CH})+\nu(\text{CC})$
1036.7, 1034.7, 1032.7	1032.1 , 1030.9, 1029.8	1038.4	12.3	B _u	$\delta(\text{CH})+\nu(\text{CC})$
		1036.9	0.0	A _g	$\delta(\text{CH})+\nu(\text{CC})$
974.2	971.0, 969.9	989.0	0.6	A _u	$\gamma(\text{CH})$
		988.7	0.0	B _g	$\gamma(\text{CH})$
943.9, 943.0, 941.6, 940.7	939.8 , 937.8	954.8	5.4	A _u	$\gamma(\text{CH})$
		954.0	0.0	B _g	$\gamma(\text{CH})$
		940.5	0.0	A _g	$\delta(\text{NNC})+\delta(\text{ring})$
899.6	894.3				
889.3	884.7	869.8	1.9	A _u	$\gamma(\text{CH})$
		866.6	0.0	B _g	$\gamma(\text{CH})$
876.5, 876.1 , 874.0, 871.5	875.0 , 874.0, 871.3, 868.9	865.4	17.1	B _u	$\delta(\text{ring})+\nu(\text{CN})$
		809.2	0.0	A _g	$\delta(\text{ring})+\nu(\text{CC})$
774.7	769.2	776.8	12.1	B _u	$\nu(\text{CC})+\delta(\text{ring})+\nu(\text{CN})$
		771.3	0.0	B _g	$\gamma(\text{CH})+\tau(\text{OH})$
770.0, 767.7	765.5 , 762.9	770.3	75.3	A _u	$\gamma(\text{CH})+\gamma(\text{CN})$
762.8, 762.1, 760.8	760.6, 758.5 , 757.3	754.7	157.7	A _u	$\gamma(\text{CH})+\tau(\text{OH})$

Ar (15 K)	Xe (30 K)	Calculated			
ω	ω	ω	I	Sym.	Tentative Assignment
		751.4	0.0	B _g	$\gamma(\text{CH})+\tau(\text{OH})$
752.2 , 744.5	747.5 , 742.9, 741.3	733.0	42.2	A _u	$\tau(\text{OH})+\gamma(\text{CH})$
		720.0	0.0	B _g	$\tau(\text{OH})+\gamma(\text{CH})$
		663.5	0.0	A _g	$\delta(\text{ring})+\delta(\text{NNC})$
592.0, 590.6	590.1	585.2	3.6	B _u	$\delta(\text{ring})+\delta(\text{NCC})$
		574.3	0.0	A _u	$\tau(\text{ring})$
580.2, 579.4, 575.0	577.3 , 574.8, 571.1	570.4	49.2	B _g	$\delta(\text{NNC})+\delta(\text{ring})$
		550.1	0.0	A _g	$\delta(\text{ring})$
		549.7	0.0	B _g	$\tau(\text{ring})$
496.6, 494.5, 493.6 , 493.2	493.6, 492.6, 491.3	495.7	15.3	A _u	$\tau(\text{ring})+\tau(\text{CNNC})$
482.70, 481.4	480.3	479.2	5.8	B _u	$\delta(\text{ring})+\delta(\text{NCC})$
		448.4	0.0	B _g	$\tau(\text{ring})+\tau(\text{CNNC})$
		444.3	0.0	A _g	$\delta(\text{CCO})$
422.8	419.5	409.7	11.1	B _u	$\delta(\text{CCO})$
n.i.	n.i.	341.8	0.5	A _u	$\tau(\text{ring})+\tau(\text{CNNC})$
n.i.	n.i.	330.3	0.0	B _g	$\gamma(\text{NC})+\tau(\text{OH})+\tau(\text{ring})$
n.i.	n.i.	274.9	0.0	A _g	$\delta(\text{NCC})$
n.i.	n.i.	227.8	0.0	B _g	$\gamma(\text{NC})+\tau(\text{ring})+\tau(\text{OH})$
n.i.	n.i.	214.7	0.0	A _g	$\delta(\text{NCC})$
n.i.	n.i.	210.6	0.1	A _u	$\gamma(\text{CO})+\tau(\text{ring})$
n.i.	n.i.	134.9	0.0	B _g	$\tau(\text{NNCC})+\delta(\text{ring})+\gamma(\text{NC})$
n.i.	n.i.	88.4	1.0	B _u	$\delta(\text{NNC})+\delta(\text{NCC})$
n.i.	n.i.	61.8	0.4	A _u	$\tau(\text{CNNC})$
n.i.	n.i.	40.7	1.1	A _u	$\tau(\text{NNCC})$

^a M06-2X/cc-pVTZ wavenumbers and intensities (I , in km mol⁻¹) are also given. Calculated wavenumbers are scaled by 0.97. The strongest components of split bands are given in bold.; ν , stretching; δ , in-plane-bending; γ , out-of-plane bending; τ , torsion; n.o., not observed; n.i., not investigated.

Table S4. TD-DFT (M06-2X/cc-pVTZ and B3LYP/cc-pVTZ) vertical transition wavelengths (λ /nm) and oscillator strengths (f) for the lowest twelve excited singlet states and lowest twelve excited triplet states of the *E*-AB, *Z*-AB, *E*-AT1, *E*-AT2, *Z*-AT1, *E*-DOH1, *E*-DOH2, *E*-NHOH4, and *Z*-DOH1 isomers.

<i>E</i>-AB							
M06-2x/cc-pVTZ				B3LYP/cc-pVTZ			
Mult. ^a	Sym. ^b	λ	f	Mult. ^a	Sym. ^b	λ	f
T	B_g	640.67	0.0000	T	B_g	694.70	0.0000
S	B_g	494.16	0.0000	T	B_u	546.45	0.0000
T	B_u	436.32	0.0000	S	B_g	489.11	0.0000
T	A_g	305.94	0.0000	T	A_g	353.41	0.0000
S	B_u	291.48	0.8095	T	B_u	342.23	0.0000
T	B_u	288.60	0.0000	T	A_g	335.94	0.0000
T	A_g	285.65	0.0000	S	B_u	329.58	0.7728
T	B_u	259.64	0.0000	S	B_u	300.98	0.0492
S	B_u	254.93	0.0278	S	A_g	300.80	0.0000
T	A_g	254.79	0.0000	T	B_u	287.26	0.0000
S	A_g	254.33	0.0000	T	A_g	280.69	0.0000
T	B_u	245.07	0.0000	T	B_u	265.59	0.0000
T	A_g	243.27	0.0000	T	A_g	263.39	0.0000
S	A_g	223.40	0.0000	S	A_g	257.46	0.0000
T	B_u	222.17	0.0000	T	B_g	251.12	0.0000
T	A_g	207.45	0.0000	S	B_g	249.46	0.0000
S	B_u	203.12	0.3406	T	A_u	248.58	0.0000
T	B_g	202.56	0.0000	S	A_u	247.19	0.0000
S	A_g	202.02	0.0000	T	A_g	244.22	0.0000
S	B_g	201.10	0.0000	S	A_u	235.33	0.0003
S	A_u	200.16	0.0000	S	B_u	228.34	0.1534
S	A_u	196.32	0.0004	S	A_g	227.85	0.0000
S	A_g	189.59	0.0000	S	A_g	208.84	0.0000
S	B_g	186.06	0.0000	S	A_u	203.99	0.0008

^a Mult. – Multiplicity: T, triplet; S, singlet; ^b Sym. – Symmetry.

Parameters λ and f were used to construct the simulated spectra shown in Figure S3.

Z-AB							
M06-2x/cc-pVTZ				B3LYP/cc-pVTZ			
Mult. ^a	Sym. ^b	λ	f	Mult. ^a	Sym. ^b	λ	f
T	B	689.08	0.0000	T	B	779.32	0.0000
S	B	490.79	0.0128	S	B	481.94	0.0351
T	B	329.24	0.0000	T	B	387.57	0.0000
T	A	316.67	0.0000	T	A	368.22	0.0000
T	B	269.44	0.0000	T	B	314.91	0.0000
T	A	269.10	0.0000	T	A	310.41	0.0000
T	B	265.14	0.0000	T	B	298.16	0.0000
T	A	260.67	0.0000	S	B	297.92	0.0664
S	B	256.97	0.1658	T	A	297.51	0.0000
T	B	256.11	0.0000	T	B	296.62	0.0000
S	A	254.06	0.0201	S	A	292.53	0.0075
T	A	250.67	0.0000	T	A	285.89	0.0000
T	A	247.08	0.0000	S	B	283.15	0.0530
T	B	244.74	0.0000	S	A	279.23	0.0002
S	B	243.90	0.0449	T	A	275.69	0.0000
S	A	239.86	0.0013	S	B	271.39	0.1075
S	B	222.30	0.1561	T	B	269.68	0.0000
S	A	219.96	0.0677	S	A	259.01	0.0246
S	A	211.65	0.0048	S	A	249.08	0.0487
T	A	209.20	0.0000	T	A	238.06	0.0000
S	B	204.77	0.0088	S	B	235.67	0.0480
S	B	195.29	0.0212	S	B	219.76	0.0169
S	A	193.11	0.0170	S	A	217.65	0.0051
S	A	189.86	0.0059	S	A	208.49	0.0010

^a Mult. – Multiplicity: T, triplet; S, singlet; ^b Sym. – Symmetry.

Parameters λ and f were used to construct the simulated spectra shown in Figure S3.

<i>E</i> -AT1							
M06-2x/cc-pVTZ				B3LYP/cc-pVTZ			
Mult. ^a	Sym. ^b	λ	f	Mult. ^a	Sym. ^b	λ	f
T	B_g	689.40	0.0000	T	B_g	749.43	0.0000
S	B_g	525.13	0.0000	T	B_u	587.41	0.0000
T	B_u	467.16	0.0000	S	B_g	519.60	0.0000
T	A_g	313.79	0.0000	T	A_g	369.16	0.0000
S	B_u	312.38	0.7053	T	B_u	368.17	0.0000
T	B_u	307.34	0.0000	T	A_g	357.75	0.0000
T	A_g	307.22	0.0000	S	B_u	352.77	0.6925
S	A_g	271.10	0.0000	S	A_g	323.97	0.0000
S	B_u	268.83	0.0461	S	B_u	321.56	0.0437
T	B_u	264.22	0.0000	T	B_u	292.41	0.0000
T	A_g	260.23	0.0000	T	A_g	287.25	0.0000
T	B_u	241.26	0.0000	S	A_g	266.62	0.0000
T	A_g	240.68	0.0000	T	A_g	263.28	0.0000
S	A_g	231.10	0.0000	T	B_u	262.60	0.0000
T	B_u	224.43	0.0000	T	A_g	250.40	0.0000
T	A_g	214.42	0.0000	T	A_u	250.13	0.0000
S	A_g	207.84	0.0000	T	B_g	248.53	0.0000
S	B_u	206.12	0.2311	S	A_u	248.07	0.0000
T	A_u	205.53	0.0000	S	B_g	247.03	0.0000
S	A_u	203.39	0.0000	S	A_u	239.10	0.0001
S	B_g	199.27	0.0000	S	A_g	232.03	0.0000
S	A_u	197.57	0.0001	S	B_u	230.06	0.1082
S	A_g	193.77	0.0000	S	A_u	209.95	0.0003
S	B_g	191.43	0.0000	S	B_g	209.18	0.0000

^a Mult. – Multiplicity: T, triplet; S, singlet; ^b Sym. – Symmetry.

Parameters λ and f were used to construct the simulated spectra shown in Figure S3.

<i>E</i> -AT2							
M06-2x/cc-pVTZ				B3LYP/cc-pVTZ			
Mult. ^a	Sym. ^b	λ	f	Mult. ^a	Sym. ^b	λ	f
T	A''	673.75	0.0000	T	A''	731.56	0.0000
S	A''	516.03	0.0000	T	A'	550.95	0.0000
T	A'	443.25	0.0000	S	A''	511.53	0.0000
T	A'	310.39	0.0000	T	A'	361.92	0.0000
T	A'	302.25	0.0000	T	A'	359.01	0.0000
S	A'	298.49	0.7547	T	A'	343.34	0.0000
T	A'	294.67	0.0000	S	A'	336.81	0.7119
S	A'	265.79	0.0367	S	A'	316.12	0.0272
T	A'	263.65	0.0000	S	A'	310.38	0.0515
S	A'	261.85	0.0226	T	A'	291.35	0.0000
T	A'	258.94	0.0000	T	A'	285.03	0.0000
T	A'	242.60	0.0000	T	A'	264.45	0.0000
T	A'	240.48	0.0000	T	A'	261.17	0.0000
S	A'	224.27	0.0033	S	A'	258.02	0.0069
T	A'	222.86	0.0000	T	A''	255.53	0.0000
T	A'	212.71	0.0000	T	A''	253.75	0.0000
T	A''	209.58	0.0000	S	A''	253.72	0.0000
S	A''	206.10	0.0002	S	A''	250.17	0.0000
S	A'	205.54	0.2050	T	A'	249.75	0.0000
S	A'	204.69	0.0475	S	A''	244.58	0.0002
S	A''	203.38	0.0000	S	A'	231.00	0.0774
S	A''	199.57	0.0002	S	A'	228.74	0.0260
S	A'	193.91	0.0179	S	A'	213.32	0.0089
S	A''	188.35	0.0000	S	A''	209.27	0.0000

^a Mult. – Multiplicity: T, triplet; S, singlet; ^b Sym. – Symmetry.

Parameters λ and f were used to construct the simulated spectra shown in Figure S3.

Z-AT1							
M06-2x/cc-pVTZ				B3LYP/cc-pVTZ			
Mult. ^a	Sym. ^b	λ	f	Mult. ^a	Sym. ^b	λ	f
T	B	669.21	0.0000	T	B	768.30	0.0000
S	B	480.66	0.0105	S	B	481.84	0.0364
T	B	326.17	0.0000	T	B	392.17	0.0000
T	A	319.46	0.0000	T	A	375.50	0.0000
T	A	274.49	0.0000	T	B	324.78	0.0000
T	B	268.77	0.0000	T	A	322.04	0.0000
T	A	265.42	0.0000	S	A	307.76	0.0023
T	B	265.36	0.0000	T	A	302.78	0.0000
S	A	261.28	0.0111	T	B	302.66	0.0000
T	A	258.47	0.0000	S	B	300.49	0.0080
S	B	257.34	0.2059	S	B	295.46	0.1798
T	B	256.09	0.0000	T	B	291.71	0.0000
T	B	248.80	0.0000	T	A	291.03	0.0000
S	B	245.61	0.0112	S	A	284.47	0.0023
S	A	244.95	0.0009	T	A	273.65	0.0000
T	A	244.93	0.0000	T	B	272.92	0.0000
S	A	223.88	0.0640	S	B	268.29	0.0501
S	B	219.22	0.1188	S	A	261.03	0.0404
S	A	212.09	0.0003	S	A	245.51	0.0217
T	A	210.92	0.0000	T	A	238.92	0.0000
S	B	209.54	0.0393	S	B	237.93	0.0589
S	B	198.42	0.0848	S	B	222.89	0.0159
S	A	194.40	0.0154	S	A	219.20	0.0096
S	A	192.32	0.0328	S	A	212.19	0.0076

^a Mult. – Multiplicity: T, triplet; S, singlet; ^b Sym. – Symmetry.

Parameters λ and f were used to construct the simulated spectra shown in Figure S3.

<i>E</i> -DOH1							
M06-2x/cc-pVTZ				B3LYP/cc-pVTZ			
Mult. ^a	Sym. ^b	λ	f	Mult. ^a	Sym. ^b	λ	f
T	B_u	523.49	0.0000	T	B_u	649.71	0.0000
T	B_g	522.56	0.0000	T	B_g	536.48	0.0000
S	B_g	428.82	0.0000	T	A_g	451.65	0.0000
T	A_g	367.30	0.0000	S	B_g	422.25	0.0000
S	B_u	348.62	0.5466	T	B_u	414.96	0.0000
T	B_u	338.17	0.0000	S	B_u	406.93	0.3760
S	A_g	304.32	0.0000	S	A_g	373.81	0.0000
T	A_g	299.03	0.0000	T	A_g	339.09	0.0000
T	B_u	279.50	0.0000	S	B_u	324.00	0.4603
S	B_u	275.12	0.3150	T	B_u	306.23	0.0000
T	A_g	273.21	0.0000	T	A_g	300.48	0.0000
T	B_u	239.34	0.0000	T	A_g	273.82	0.0000
T	A_g	234.36	0.0000	T	B_u	265.97	0.0000
S	A_g	227.38	0.0000	S	A_g	258.41	0.0000
T	A_g	226.13	0.0000	T	A_g	253.01	0.0000
T	B_u	221.59	0.0000	T	B_u	249.29	0.0000
S	B_u	216.05	0.2503	S	B_u	241.00	0.0875
S	A_g	210.77	0.0000	S	A_g	237.33	0.0000
T	B_u	206.80	0.0000	T	B_u	235.71	0.0000
S	A_g	199.09	0.0000	S	A_g	220.75	0.0000
S	B_u	192.13	0.3663	S	A_u	218.85	0.0003
S	A_u	187.70	0.0005	S	B_g	217.88	0.0000
S	B_g	185.22	0.0000	S	B_u	217.01	0.0204
S	A_u	182.60	0.0004	S	A_g	213.83	0.0000

^a Mult. – Multiplicity: T, triplet; S, singlet; ^b Sym. – Symmetry.

Parameters λ and f were used to construct the simulated spectra shown in Figure S3.

<i>E</i> -DOH2							
M06-2x/cc-pVTZ				B3LYP/cc-pVTZ			
Mult. ^a	Sym. ^b	λ	f	Mult. ^a	Sym. ^b	λ	f
T	B_g	571.99	0.0000	T	B_u	672.98	0.0000
T	B_u	532.37	0.0000	T	B_g	593.88	0.0000
S	B_g	455.34	0.0000	S	B_g	447.02	0.0000
T	A_g	361.07	0.0000	T	A_g	446.23	0.0000
S	B_u	351.99	0.6535	T	B_u	420.94	0.0000
T	B_u	342.13	0.0000	S	B_u	410.70	0.4957
T	A_g	309.14	0.0000	S	A_g	372.26	0.0000
S	A_g	302.25	0.0000	T	A_g	352.31	0.0000
S	B_u	279.14	0.1552	S	B_u	332.71	0.2899
T	B_u	276.02	0.0000	T	B_u	303.30	0.0000
T	A_g	272.44	0.0000	T	A_g	298.37	0.0000
S	A_g	232.00	0.0000	T	A_g	274.23	0.0000
T	A_g	231.96	0.0000	S	A_g	267.85	0.0000
T	B_u	227.97	0.0000	T	B_u	252.40	0.0000
T	B_u	225.41	0.0000	T	B_u	250.91	0.0000
T	A_g	223.70	0.0000	T	A_g	248.99	0.0000
S	A_g	216.13	0.0000	S	A_g	242.70	0.0000
S	B_u	208.92	0.1122	T	B_u	237.09	0.0000
T	B_u	206.54	0.0000	S	B_u	232.41	0.0433
S	A_g	197.49	0.0000	S	A_u	225.99	0.0001
S	B_u	191.68	0.3290	S	A_g	218.36	0.0000
S	B_g	191.28	0.0000	S	B_g	215.66	0.0000
S	A_u	190.29	0.0001	S	B_u	215.39	0.0519
S	B_g	182.32	0.0000	S	B_g	212.58	0.0000

^a Mult. – Multiplicity: T, triplet; S, singlet; ^b Sym. – Symmetry.

Parameters λ and f were used to construct the simulated spectra shown in Figure S3.

E-NHOH4							
M06-2x/cc-pVTZ				B3LYP/cc-pVTZ			
Mult. ^a	Sym. ^b	λ	f	Mult. ^a	Sym. ^b	λ	f
T	A'	886.07	0.0000	T	A'	1041.88	0.0000
T	A''	461.79	0.0000	T	A''	575.54	0.0000
S	A''	415.01	0.0000	S	A''	500.95	0.0000
T	A'	412.45	0.0000	T	A'	493.66	0.0000
S	A'	405.02	0.5442	S	A'	449.90	0.4989
T	A''	342.79	0.0000	T	A''	369.54	0.0000
T	A'	303.80	0.0000	T	A'	369.51	0.0000
S	A'	302.01	0.0845	S	A'	363.39	0.0174
S	A''	294.29	0.0010	T	A'	340.21	0.0000
T	A'	290.07	0.0000	S	A'	335.03	0.0424
T	A'	283.66	0.0000	T	A'	313.48	0.0000
T	A'	279.02	0.0000	T	A'	312.73	0.0000
S	A'	265.22	0.0060	S	A''	306.70	0.0009
T	A'	261.02	0.0000	T	A'	304.96	0.0000
T	A'	242.51	0.0000	T	A'	272.57	0.0000
S	A'	237.06	0.0851	S	A'	269.57	0.0862
S	A'	220.56	0.1246	S	A'	254.21	0.0798
T	A'	217.82	0.0000	T	A'	251.76	0.0000
T	A''	216.80	0.0000	S	A'	247.46	0.0883
S	A'	215.75	0.0377	T	A''	247.21	0.0000
S	A''	213.00	0.0003	S	A''	243.28	0.0001
S	A''	208.21	0.0002	S	A''	235.65	0.0000
S	A'	202.52	0.0568	S	A'	231.42	0.0148
S	A'	195.07	0.0815	S	A''	227.55	0.0000

^a Mult. – Multiplicity: T, triplet; S, singlet; ^b Sym. – Symmetry.

Parameters λ and f were used to construct the simulated spectra shown in Figure S3.

Z-DOH1							
M06-2x/cc-pVTZ				B3LYP/cc-pVTZ			
Mult. ^a	Sym. ^b	λ	f	Mult. ^a	Sym. ^b	λ	f
T	B	753.43	0.0000	T	B	890.90	0.0000
S	B	526.73	0.0361	S	B	532.78	0.0939
T	B	399.65	0.0000	T	B	479.24	0.0000
T	A	367.26	0.0000	T	A	451.36	0.0000
T	B	336.28	0.0000	T	B	417.71	0.0000
S	B	314.54	0.2647	S	B	383.67	0.1272
T	A	308.34	0.0000	S	A	374.54	0.0001
S	A	305.88	0.0057	T	A	364.80	0.0000
T	B	280.93	0.0000	S	B	323.87	0.1772
S	B	280.16	0.0644	T	B	311.41	0.0000
T	A	272.64	0.0000	T	A	303.10	0.0000
T	A	256.20	0.0000	T	A	289.93	0.0000
T	B	250.73	0.0000	S	A	287.47	0.0200
S	A	250.24	0.0173	T	B	278.46	0.0000
T	B	235.79	0.0000	T	B	261.23	0.0000
S	B	227.44	0.0542	S	B	260.84	0.0236
T	A	226.94	0.0000	T	A	255.62	0.0000
S	A	220.56	0.0663	S	A	249.50	0.0437
T	A	213.45	0.0000	T	B	243.72	0.0000
S	A	207.14	0.0245	S	A	235.60	0.0008
S	B	201.15	0.0403	S	B	223.78	0.0356
S	B	195.47	0.0862	S	B	221.27	0.0118
S	A	191.27	0.0660	S	A	220.09	0.0025
S	B	190.00	0.4127	S	B	218.05	0.0510

^a Mult. – Multiplicity: T, triplet; S, singlet; ^b Sym. – Symmetry.

Table S5. Experimental observed wavenumbers (ω , in cm^{-1}) in argon and xenon matrices after irradiation of 2,2'-dihydroxyazobenzene at 323 nm.^a

Ar (15 K)	Xe (30 K)
ω	ω
3600.7	3605.2
3416.6, 3412.0	3353.1
3332.4	3324.2
1553.7	1550.4
1516.7	1514.5, 1511.0
1506.3	1502.7
1423.8, 1414.0	1421.6
1399.5	n.o.
1379.1	1376.2
1164.8	1153.5
n.o.	1116.6
1104.6	1107.9, 1105.3 , 1103.1
906.8, 906.0	908.0, 906.5, 904.6
819.3	839.1
813.3	831.1
802.7	803.5, 801.8, 800.9
742.3	740.3
733.8	731.7
718.5	721.2
565.3	566.2

^aThe strongest components of split bands are given in bold; n.o., not observed.

Table S6. Theoretical wavenumbers (ω , in cm^{-1} ; unscaled values) and infrared intensities (I , in km mol^{-1}) of the 2,2'-azotoluene isomeric forms.

<i>E</i> -AT1				<i>E</i> -AT2				<i>E</i> -AT3				<i>E</i> -AT4	
M06-2X		B3LYP		M06-2X		B3LYP		M06-2X		B3LYP		M06-2X	
ω	I	ω	I	ω	I	ω	I	ω	I	ω	I	ω	I
3219	15	3212	11	3220	14	3212	6	3222	1	3197	2	3222	0
3219	0	3212	0	3216	11	3199	15	3222	6	3197	33	3222	20
3205	0	3187	0	3214	2	3187	2	3207	0	3186	0	3206	0
3205	19	3187	60	3202	6	3187	49	3207	32	3186	39	3206	9
3192	0	3172	33	3195	4	3175	11	3195	4	3174	17	3193	0
3192	17	3172	0	3194	4	3172	17	3195	14	3174	2	3193	26
3177	0	3162	0	3176	9	3161	6	3184	0	3159	2	3178	0
3177	10	3162	10	3173	11	3160	9	3184	1	3159	16	3178	5
3148	0	3107	0	3147	15	3106	22	3138	7	3103	2	3147	0
3148	27	3107	44	3147	24	3103	30	3137	27	3103	51	3147	18
3137	12	3092	22	3131	4	3093	6	3128	11	3097	16	3133	29
3137	0	3092	0	3122	9	3088	16	3127	2	3096	3	3133	0
3071	0	3040	0	3067	10	3038	22	3060	17	3038	11	3064	0
3071	33	3040	45	3061	18	3037	21	3060	12	3038	36	3064	31
1699	0	1645	0	1697	1	1646	2	1694	1	1647	0	1696	0
1682	14	1638	18	1688	5	1641	9	1689	2	1645	7	1688	3
1665	0	1619	0	1664	1	1619	1	1673	0	1614	0	1672	0
1662	0	1617	2	1657	4	1607	6	1645	5	1604	9	1647	6
1633	0	1543	0	1626	7	1548	4	1627	0	1555	0	1629	0
1540	25	1519	20	1540	10	1519	8	1536	13	1511	8	1536	15
1535	0	1517	0	1526	13	1504	24	1529	5	1497	2	1527	0
1513	27	1502	31	1512	15	1496	7	1508	3	1496	28	1510	0
1510	0	1496	0	1508	11	1488	13	1508	27	1487	5	1510	35
1488	15	1482	13	1491	14	1480	12	1486	11	1476	9	1486	11

E-AT1				E-AT2				E-AT3				E-AT4	
M06-2X		B3LYP		M06-2X		B3LYP		M06-2X		B3LYP		M06-2X	
ω	I	ω	I	ω	I	ω	I	ω	I	ω	I	ω	I
1488	0	1482	0	1484	2	1472	3	1485	3	1476	3	1485	0
1482	15	1473	10	1481	1	1466	6	1480	5	1470	3	1482	8
1476	0	1459	0	1474	12	1462	0	1475	0	1461	0	1475	0
1422	0	1422	0	1419	2	1423	4	1421	0	1423	0	1422	0
1421	4	1422	5	1414	5	1417	3	1420	4	1422	5	1421	4
1345	0	1340	0	1345	0	1342	1	1342	1	1335	1	1341	0
1344	16	1339	14	1335	14	1330	11	1331	9	1325	10	1331	10
1316	0	1313	0	1315	5	1310	6	1316	3	1312	5	1318	5
1309	7	1307	12	1314	5	1310	6	1314	1	1310	1	1315	0
1271	28	1247	31	1270	19	1244	23	1270	4	1243	12	1269	8
1246	0	1216	0	1240	2	1222	6	1242	0	1220	0	1239	0
1230	9	1214	14	1236	0	1214	3	1234	2	1216	6	1233	2
1211	0	1200	0	1208	2	1191	2	1208	0	1188	0	1208	0
1181	0	1183	0	1185	2	1187	4	1186	1	1186	3	1183	0
1179	22	1182	30	1182	6	1181	7	1184	2	1179	0	1183	3
1146	3	1144	4	1150	5	1144	7	1152	0	1144	0	1155	0
1125	0	1118	0	1135	3	1127	3	1143	5	1137	7	1146	6
1081	13	1069	10	1093	5	1075	4	1090	9	1076	9	1092	11
1081	0	1068	0	1084	6	1070	5	1089	1	1073	1	1090	0
1075	5	1068	5	1070	6	1066	6	1066	2	1063	2	1068	6
1074	0	1066	0	1063	0	1061	0	1065	5	1061	5	1067	0
1034	0	1011	2	1035	0	1014	2	1028	0	1013	1	1029	0
1033	0	1010	0	1032	1	1013	0	1028	0	1013	1	1029	0
1018	3	1009	0	1031	0	1007	1	1022	0	1003	0	1023	1
1017	0	1009	0	1013	2	1006	0	1022	1	1003	0	1023	0
1002	2	984	2	1002	1	984	2	1002	3	978	2	996	4

E-AT1				E-AT2				E-AT3				E-AT4	
M06-2X		B3LYP		M06-2X		B3LYP		M06-2X		B3LYP		M06-2X	
ω	I	ω	I	ω	I	ω	I	ω	I	ω	I	ω	I
1000	0	982	0	997	1	979	1	998	1	974	0	994	0
948	0	936	0	953	0	941	0	952	0	941	0	952	0
911	1	895	1	909	1	895	1	912	0	890	1	910	3
910	0	894	0	903	0	893	0	912	1	890	0	909	0
865	0	862	0	865	0	861	0	867	1	865	1	868	1
821	0	814	0	816	1	807	1	816	26	803	31	808	72
813	62	802	52	813	68	802	55	795	26	783	16	797	0
794	0	783	0	795	0	783	0	787	41	776	30	786	0
781	0	765	1	768	0	753	0	771	1	754	0	772	1
756	49	745	48	755	46	746	47	750	25	740	31	755	45
746	0	736	0	743	0	735	0	746	3	736	3	742	0
665	0	663	0	679	1	675	1	687	0	683	0	687	0
597	11	596	15	602	1	601	3	610	0	609	1	611	1
587	2	582	1	590	2	586	15	588	1	583	1	590	5
584	1	579	2	589	14	583	1	574	25	567	31	569	25
552	0	550	0	542	0	537	0	564	0	561	0	563	0
537	0	530	0	532	1	527	1	533	0	534	0	543	0
490	19	489	22	515	16	511	20	488	3	487	3	490	1
479	12	477	10	481	10	481	8	482	5	480	6	480	10
456	0	456	0	454	1	456	0	461	3	458	2	462	0
446	0	444	0	420	1	411	1	408	0	402	0	406	0
352	10	347	10	387	2	368	2	387	1	367	1	389	1
334	0	327	0	368	0	335	0	367	0	347	0	347	2
265	0	257	0	331	1	268	0	294	3	287	2	306	0
228	0	225	0	261	0	239	2	280	9	272	10	289	0
209	0	204	0	246	2	236	0	256	0	230	0	282	1

E-AT1				E-AT2				E-AT3				E-AT4	
M06-2X		B3LYP		M06-2X		B3LYP		M06-2X		B3LYP		M06-2X	
ω	I	ω	I	ω	I	ω	I	ω	I	ω	I	ω	I
202	3	192	4	226	0	210	0	255	1	216	0	262	0
199	0	184	0	194	3	189	4	217	2	208	2	211	0
174	2	118	1	193	1	178	0	193	5	179	4	192	5
169	0	117	0	132	1	118	0	165	1	165	1	185	0
72	1	75	1	84	1	81	1	133	0	112	0	83	1
71	0	71	0	69	0	71	0	61	1	57	1	79	0
68	1	62	1	59	0	57	1	60	2	56	2	57	1
29	0	12	0	13	0	14	0	25	0	18	0	20	0

Z-AT1				Z-AT2				Z-AT3			
M06-2X		B3LYP		M06-2X		B3LYP		M06-2X		B3LYP	
ω	I	ω	I	ω	I	ω	I	ω	I	ω	I
3217	9	3197	10	3212	4	3215	2	3207	2	3195	3
3217	8	3197	6	3210	6	3193	21	3207	12	3195	27
3207	10	3187	14	3203	8	3190	21	3197	5	3185	16
3207	2	3187	26	3201	8	3181	14	3197	1	3185	12
3193	1	3173	1	3190	4	3175	10	3185	2	3172	11
3193	3	3173	14	3187	4	3170	4	3185	1	3172	1
3181	0	3161	1	3177	5	3162	8	3164	2	3160	1
3181	14	3160	18	3174	3	3158	7	3164	5	3160	12
3144	0	3111	0	3148	10	3112	14	3142	6	3108	8
3144	21	3111	34	3146	7	3107	13	3142	6	3108	15
3109	3	3075	7	3119	12	3083	13	3115	0	3092	6
3109	13	3075	17	3116	6	3081	13	3115	17	3092	20
3048	3	3025	6	3055	13	3031	28	3050	17	3038	32

Z-AT1				Z-AT2				Z-AT3			
M06-2X		B3LYP		M06-2X		B3LYP		M06-2X		B3LYP	
ω	I	ω	I	ω	I	ω	I	ω	I	ω	I
3048	24	3025	36	3053	11	3031	8	3050	1	3038	0
1701	7	1645	0	1705	10	1643	2	1705	12	1649	7
1679	11	1633	3	1684	1	1639	2	1678	1	1638	3
1678	4	1620	7	1673	11	1616	6	1676	3	1634	11
1658	1	1612	1	1659	1	1611	10	1646	2	1611	1
1658	2	1598	31	1649	3	1599	23	1642	1	1606	3
1538	10	1515	6	1536	8	1516	8	1530	2	1516	7
1538	20	1513	15	1531	19	1510	13	1528	21	1513	17
1512	2	1503	0	1510	11	1504	13	1506	32	1502	0
1509	21	1502	21	1509	19	1502	18	1504	2	1502	29
1481	6	1479	11	1496	14	1490	13	1495	23	1492	14
1480	1	1479	5	1481	2	1476	5	1494	4	1490	8
1478	3	1470	0	1478	1	1471	1	1471	0	1469	0
1476	7	1468	0	1474	3	1468	1	1469	2	1468	2
1413	5	1419	4	1422	1	1422	1	1411	0	1420	4
1413	3	1419	3	1413	5	1415	5	1410	1	1420	0
1335	1	1330	0	1333	1	1329	1	1327	0	1324	0
1328	1	1325	1	1324	1	1320	1	1319	0	1318	1
1321	0	1315	0	1316	1	1314	2	1307	0	1314	0
1314	0	1306	0	1312	0	1307	1	1304	2	1304	4
1252	0	1223	1	1248	1	1221	2	1237	2	1222	2
1252	0	1220	2	1242	0	1220	1	1233	0	1219	1
1206	1	1189	0	1208	0	1191	0	1203	1	1187	2
1202	0	1188	0	1198	2	1187	0	1185	1	1187	0
1185	0	1184	2	1184	2	1184	2	1171	0	1180	1
1185	0	1179	0	1180	1	1174	5	1171	1	1172	0

Z-AT1				Z-AT2				Z-AT3			
M06-2X		B3LYP		M06-2X		B3LYP		M06-2X		B3LYP	
ω	I	ω	I	ω	I	ω	I	ω	I	ω	I
1138	9	1132	7	1139	3	1131	3	1131	5	1125	6
1131	1	1118	0	1129	6	1118	5	1131	5	1122	10
1087	4	1070	5	1087	4	1071	7	1085	6	1072	5
1084	5	1068	9	1086	4	1070	2	1084	1	1071	2
1066	4	1065	0	1072	4	1066	3	1063	2	1066	7
1065	0	1065	1	1067	3	1064	3	1062	3	1066	1
1020	0	1008	1	1020	0	1010	1	1026	0	1009	1
1020	0	1007	1	1020	0	1006	1	1026	0	1008	0
1005	2	995	0	1013	0	1000	0	1007	1	997	0
1005	2	995	0	1009	1	996	0	1005	1	997	0
980	6	962	8	990	7	967	6	993	4	970	4
978	0	961	0	986	2	965	2	990	0	967	1
917	7	891	9	914	8	893	6	907	9	895	3
896	0	882	1	902	1	884	2	901	1	885	1
882	0	862	1	886	2	861	2	880	7	859	1
837	1	833	1	837	2	831	1	839	2	829	3
832	1	823	0	832	1	823	2	827	10	825	2
803	14	789	16	804	11	790	19	806	11	784	25
771	86	760	83	775	79	764	71	774	79	760	69
764	3	751	6	758	11	747	10	758	13	748	13
747	11	737	10	747	15	737	11	736	4	727	1
744	11	734	10	735	4	722	3	723	1	716	1
702	6	699	5	707	6	699	5	707	2	694	4
643	1	632	1	643	2	634	2	642	2	638	1
596	0	592	0	592	0	589	0	591	1	584	0
568	0	565	1	579	1	576	1	582	0	580	0

Z-AT1				Z-AT2				Z-AT3			
M06-2X		B3LYP		M06-2X		B3LYP		M06-2X		B3LYP	
ω	I	ω	I	ω	I	ω	I	ω	I	ω	I
530	0	526	2	544	0	539	0	561	1	554	1
526	1	519	1	523	2	521	1	525	3	520	2
499	7	504	9	493	9	488	12	484	1	482	0
485	0	478	0	483	3	477	4	469	17	469	15
457	4	458	4	462	1	453	1	443	2	429	2
445	0	445	3	434	4	427	5	428	1	424	2
362	0	368	0	386	2	380	2	397	1	405	2
358	1	354	0	361	0	357	0	357	2	347	2
292	4	292	3	298	2	284	3	293	1	285	2
281	2	266	2	282	2	270	3	271	3	278	6
226	2	225	2	261	3	232	2	263	2	233	1
183	0	180	0	211	0	182	0	260	0	197	0
147	0	152	0	193	0	160	1	259	2	153	0
144	0	137	1	167	0	142	0	205	1	136	0
135	0	126	1	134	2	132	2	178	0	124	0
126	1	124	1	114	0	117	1	131	5	122	3
56	0	58	0	81	1	59	0	88	0	72	1
54	1	42	1	61	0	53	1	60	0	55	0
40	0	38	0	46	0	40	0	30	0	18	0

Table S7. Experimental wavenumbers (ω , in cm^{-1}) of the *E*-AT1 isomer isolated in argon and xenon matrices.^a

Ar (15 K)	Xe (30 K)	Calculated			
ω	ω	ω	I	Sym.	Tentative Assignment
3093.6, 3091.2	3079.8	3122.7	15.0	B _u	$\nu(\text{CH})$
		3122.6	0.0	A _g	$\nu(\text{CH})$
		3108.6	0.0	A _g	$\nu(\text{CH})$
3073.1	3071.3, 3061.2	3108.6	19.1	B _u	$\nu(\text{CH})$
		3096.1	0.0	A _g	$\nu(\text{CH})$
3055.9	3046.4 , 3037.8	3096.0	16.9	B _u	$\nu(\text{CH})$
		3081.6	0.0	A _g	$\nu(\text{CH})$
3042.9 , 3030.4	3024.6	3081.5	10.5	B _u	$\nu(\text{CH})$
		3053.6	0.0	A _g	$\nu(\text{CH}_3)$
2999.5	2973.2	3053.5	27.2	B _u	$\nu(\text{CH}_3)$
2972.1	2956.4	3043.1	12.3	A _u	$\nu(\text{CH}_3)$
		3043.0	0.0	B _g	$\nu(\text{CH}_3)$
		2978.8	0.0	A _g	$\nu(\text{CH}_3)$
2938.4	2932.3	2978.7	33.1	B _u	$\nu(\text{CH}_3)$
		1648.5	0.0	A _g	$\nu(\text{CC})+\nu(\text{NN})+\delta(\text{CH})$
1602.6	1604.6, 1599.9	1631.8	14.3	B _u	$\nu(\text{CC})+\delta(\text{CH})$
		1615.4	0.0	A _g	$\nu(\text{CC})+\delta(\text{CH})+\nu(\text{NN})$
n.o.	1570.5	1612.1	0.2	B _u	$\nu(\text{CC})+\delta(\text{CH})$
		1584.2	0.0	A _g	$\nu(\text{NN})+\nu(\text{CC})+\delta(\text{CH})$
1492.4, 1490.4, 1483.3	1490.2, 1487.9, 1481.6, 1480.1	1493.7	25.2	B _u	$\delta(\text{CH})+\nu(\text{CC})$
		1489.2	0.0	A _g	$\delta(\text{CH})+\nu(\text{CC})$
1464.6	1461.3	1467.2	27.4	B _u	$\delta(\text{CH})+\delta(\text{CH}_3)+\nu(\text{CC})$
		1465.1	0.0	A _g	$\delta(\text{CH})+\delta(\text{CH}_3)+\nu(\text{CC})$
1438.3	1433.5	1443.4	14.8	A _u	$\delta(\text{CH}_3)$
		1443.0	0.0	B _g	$\delta(\text{CH}_3)$
1429.6	1424.8	1437.2	15.4	B _u	$\delta(\text{CH}_3)+\delta(\text{CH})$

Ar (15 K)	Xe (30 K)	Calculated			
ω	ω	ω	I	Sym.	Tentative Assignment
		1431.8	0.0	A _g	$\delta(\text{CH}_3)+\delta(\text{CH})$
		1379.1	0.0	A _g	$\delta(\text{CH}_3)+\nu(\text{C}-\text{CH}_3)$
1380.4	1376.6	1378.8	3.9	B _u	$\delta(\text{CH}_3)+\nu(\text{C}-\text{CH}_3)$
		1304.7	0.0	A _g	$\nu(\text{CC})+\delta(\text{CH})+\delta(\text{CH}_3)$
1304.4	1306.8, 1304.5	1303.4	16.0	B _u	$\nu(\text{CC})+\delta(\text{CH})+\delta(\text{CH}_3)$
		1276.5	0.0	A _g	$\delta(\text{CH})+\nu(\text{CC})+\delta(\text{CH}_3)$
1276.8	1274.8	1269.5	7.1	B _u	$\delta(\text{CH})+\nu(\text{CC})+\delta(\text{CH}_3)$
1222.5	1220.3	1232.5	28.1	B _u	$\nu(\text{CN})+\delta(\text{CH})$
		1208.6	0.0	A _g	$\nu(\text{C}-\text{CH}_3)+\nu(\text{CN})+\nu(\text{CC})+\delta(\text{CH})$
1195.2	1195.5, 1193.1, 1191.6	1192.9	8.5	B _u	$\nu(\text{C}-\text{CH}_3)+\delta(\text{CH})+\delta(\text{ring})$
		1174.7	0.0	A _g	$\nu(\text{CN})+\delta(\text{CH})$
		1145.6	0.0	A _g	$\delta(\text{CH})$
1152.03	1154.4, 1151.7 , 1150.1	1143.3	22.1	B _u	$\delta(\text{CH})$
1117.0	1116.5	1111.8	3.4	B _u	$\delta(\text{CH})$
		1091.4	0.0	A _g	$\delta(\text{CH})+\nu(\text{CN})+\delta(\text{ring})$
1045.6, 1042.4	1045.4, 1041.9	1048.7	13.2	B _u	$\delta(\text{CH})+\nu(\text{CC})$
		1048.4	0.0	A _g	$\delta(\text{CH})+\nu(\text{CC})$
1037.6	1035.9	1043.0	5.0	A _u	$\gamma(\text{CH}_3)$
		1041.9	0.0	B _g	$\gamma(\text{CH}_3)$
		1002.6	0.0	A _u	$\gamma(\text{CH})$
		1002.2	0.0	B _g	$\gamma(\text{CH})$
990.6, 988.4	987.6	987.7	2.8	B _u	$\gamma(\text{CH}_3)$
		986.4	0.0	A _g	$\gamma(\text{CH}_3)$
955.3, 951.3 , 947.8, 945.4, 943.5	955.1, 948.4 , 945.0, 943.7, 942.0	971.8	2.0	A _u	$\gamma(\text{CH})$
		969.6	0.0	B _g	$\gamma(\text{CH})$
		919.5	0.0	A _g	$\delta(\text{NNC})+\delta(\text{ring})$
865.0 , 863.5	863.0 , 861.8	883.3	0.8	A _u	$\gamma(\text{CH})$

Ar (15 K)	Xe (30 K)	Calculated			
ω	ω	ω	I	Sym.	Tentative Assignment
		882.6	0.0	B _g	$\gamma(\text{CH})$
848.8, 847.8	847.2	838.8	0.2	B _u	$\delta(\text{ring})+\nu(\text{CN})$
		796.6	0.0	A _g	$\delta(\text{ring})$
775.9, 773.1	772.4 , 720.6	788.3	61.5	A _u	$\gamma(\text{CH})+\gamma(\text{CN})$
767.2	765.6				
758.8	757.1				
		770.0	0.0	B _g	$\gamma(\text{CH})+\gamma(\text{CN})$
n.o.	n.o.	757.8	0.4	B _u	$\nu(\text{CC})+\delta(\text{ring})+\nu(\text{CN})$
722.9, 721.7, 720.8	721.6, 718.7	733.2	49.0	A _u	$\gamma(\text{CH})+\gamma(\text{CH}_3)+\tau(\text{ring})$
		723.2	0.0	B _g	$\gamma(\text{CH})+\gamma(\text{CH}_3)+\tau(\text{ring})$
		644.9	0.0	A _g	$\delta(\text{ring})+\delta(\text{NCC})$
587.7 , 581.6	587.1 , 582.2	578.7	10.6	B _u	$\delta(\text{ring})+\delta(\text{NCC})$
570.3	577.2	569.7	2.0	A _u	$\tau(\text{ring})$
n.o.	n.o.	566.2	0.7	B _u	$\delta(\text{NCC})+\delta(\text{ring})$
		535.3	0.0	A _g	$\delta(\text{ring})$
		520.6	0.0	B _g	$\tau(\text{ring})$
480.9 , 475.9	480.6 , 476.1	475.0	19.0	B _u	$\delta(\text{ring})+\delta(\text{NCC})$
464.0, 459.0	461.6, 458.7	464.4	12.0	A _u	$\tau(\text{ring})+\tau(\text{CNCC})$
		442.4	0.0	B _g	$\tau(\text{ring})+\tau(\text{CNCC})$
		432.6	0.0	A _g	$\delta(\text{CCCH}_3)$
n.i.	n.i.	341.2	9.9	B _u	$\delta(\text{CCCH}_3)$
n.i.	n.i.	323.6	0.4	A _u	$\tau(\text{ring})+\tau(\text{CNCC})$
n.i.	n.i.	257.5	0.0	B _g	$\gamma(\text{NC})+\tau(\text{ring})$
n.i.	n.i.	221.4	0.0	A _g	$\delta(\text{NCC})$
n.i.	n.i.	202.8	0.0	A _g	$\delta(\text{NCC})$
n.i.	n.i.	196.3	2.8	A _u	$\gamma(\text{C-CH}_3)+\tau(\text{CH}_3)+\tau(\text{CNCC})$
n.i.	n.i.	192.6	0.0	B _g	$\tau(\text{NNCC})+\tau(\text{ring})+\tau(\text{CH}_3)$
n.i.	n.i.	168.9	2.2	A _u	$\tau(\text{CH}_3)$

Ar (15 K)	Xe (30 K)	Calculated			
ω	ω	ω	I	Sym.	Tentative Assignment
n.i.	n.i.	164.1	0.0	B _g	$\tau(\text{CH}_3)$
n.i.	n.i.	69.7	0.7	B _u	$\delta(\text{NNC})+\delta(\text{NCC})$
n.i.	n.i.	69.1	0.0	B _g	$\tau(\text{NNCC})+\tau(\text{ring})$
n.i.	n.i.	65.5	0.8	A _u	$\tau(\text{CNNC})$
n.i.	n.i.	28.2	0.0	A _u	$\tau(\text{NNCC})$

^a M06-2X/cc-pVTZ wavenumbers and intensities (I , in km mol^{-1}) are also given. Calculated wavenumbers are scaled by 0.97. The strongest components of split bands are given in bold.; ν , stretching; δ , in-plane-bending; γ , out-of-plane bending; τ , torsion; n.o., not observed; n.i., not investigated.

Table S8. Theoretical wavenumbers (ω , in cm^{-1} ; unscaled values) and infrared intensities (I , in km mol^{-1}) of the *E* and *Z* forms of azobenzene.

<i>E</i> -AB						<i>Z</i> -AB				
B3LYP			M06-2X			B3LYP			M06-2X	
ω	I		ω	I		ω	I		ω	I
3223	7		3212	9		3210	9		3201	4
3223	0		3212	0		3210	2		3200	2
3209	0		3197	0		3206	2		3194	2
3209	22		3197	32		3205	6		3194	36
3200	0		3187	0		3200	4		3186	7
3200	15		3187	40		3199	6		3186	17
3192	0		3176	0		3191	1		3175	1
3192	7		3176	21		3190	5		3175	11
3183	0		3166	0		3182	0		3167	0
3183	1		3166	3		3182	1		3167	1
1698	0		1645	0		1707	19		1645	11
1682	1		1639	3		1675	9		1635	5
1676	0		1629	0		1671	0		1624	1
1668	4		1623	5		1665	1		1616	6
1635	0		1551	0		1660	6		1600	25
1540	18		1522	12		1531	11		1519	9
1530	0		1509	0		1530	12		1516	7
1504	0		1490	13		1500	3		1488	3
1503	13		1482	0		1493	7		1482	7
1355	0		1352	6		1351	0		1357	0
1354	7		1351	0		1349	0		1355	0
1346	0		1346	0		1332	0		1330	0
1338	4		1337	5		1321	1		1320	2
1272	13		1251	18		1214	1		1204	1

E-AB						Z-AB				
B3LYP			M06-2X			B3LYP			M06-2X	
ω	I		ω	I		ω	I		ω	I
1222	0		1208	0		1208	0		1203	1
1185	12		1184	0		1188	0		1184	0
1183	0		1184	0		1177	0		1184	0
1180	10		1177	31		1175	1		1169	1
1179	0		1160	0		1175	0		1148	0
1113	12		1103	13		1112	1		1105	1
1110	0		1099	0		1111	13		1103	12
1060	12		1044	0		1062	2		1049	2
1060	0		1043	13		1062	4		1049	5
1040	0		1022	2		1029	1		1021	1
1040	0		1021	0		1029	0		1020	0
1027	0		1020	0		1026	1		1008	0
1026	3		1019	0		1026	0		1008	1
1023	0		1004	0		1009	0		990	0
1022	0		1003	0		1009	0		990	0
979	9		965	8		964	25		946	23
973	0		959	0		956	1		940	1
950	0		938	0		891	3		865	4
880	0		866	0		871	1		857	1
879	0		865	0		870	0		856	3
849	0		838	0		809	11		796	14
817	63		806	56		787	48		781	42
794	0		785	0		775	0		764	0
719	87		710	80		721	99		718	83
714	0		705	0		720	22		713	21
686	0		686	0		713	1		708	8

E-AB						Z-AB				
B3LYP			M06-2X			B3LYP			M06-2X	
ω	I		ω	I		ω	I		ω	I
633	0		635	0		640	2		637	0
627	0		629	0		628	0		633	0
569	19		563	14		617	3		615	5
551	4		550	6		554	1		550	0
532	22		529	25		511	4		511	4
495	0		492	0		452	1		455	2
425	0		424	0		449	3		436	3
422	0		420	0		418	0		417	0
315	1		309	1		416	2		414	4
309	0		307	0		298	5		291	5
260	0		253	0		279	0		272	0
231	0		224	0		173	0		172	0
97	0		99	0		153	1		157	3
87	2		86	2		68	0		68	0
69	1		63	1		51	1		47	0
35	0		22	0		46	0		43	1