Electronic Supplementary Material (ESI) for CrystEngComm

SUPPORTING INFORMATION TO

On Two Alizarin Polymorphs

by

Michał K. Cyrański,[a] *Michał H. Jamróz,*[b] *Anna Rygula,*[c]
Jan Cz. Dobrowolski,[b,d] *Łukasz Dobrzycki*[*,a,] *and Malgorzata Baranska**[c,e]

[a] FACULTY OF CHEMISTRY,UNIVERSITY OF WARSAW,PASTEURA 1, 02-093 WARSAW, POLAND
[b] SPECTROSCOPY AND MOLECULAR MODELING GROUP, INDUSTRIAL CHEMISTRY RESEARCH INSTITUTE, 8 RYDYGIERA STREET, 01-793 WARSAW, POLAND
[c] FACULTY OF CHEMISTRY, JAGIELLONIAN UNIVERSITY,INGARDENA 3, 30-060 CRACOW, POLAND
[d] LABORATORY FOR THEORETICAL METHODS AND CALCULATIONS,NATIONAL MEDICINES INSTITUTE, 30/34 CHEŁMSKA STREET, 00-725 WARSAW, POLAND
[e] JAGIELLONIAN CENTER FOR EXPERIMENTAL THERAPEUTICS (JCET), JAGIELLONIAN UNIVERSITY, 14 BOBRZYNSKIEGO STR., 30-348 KRAKOW, POLAND

Juxtaposition of the theoretical and experimental PXRD patterns

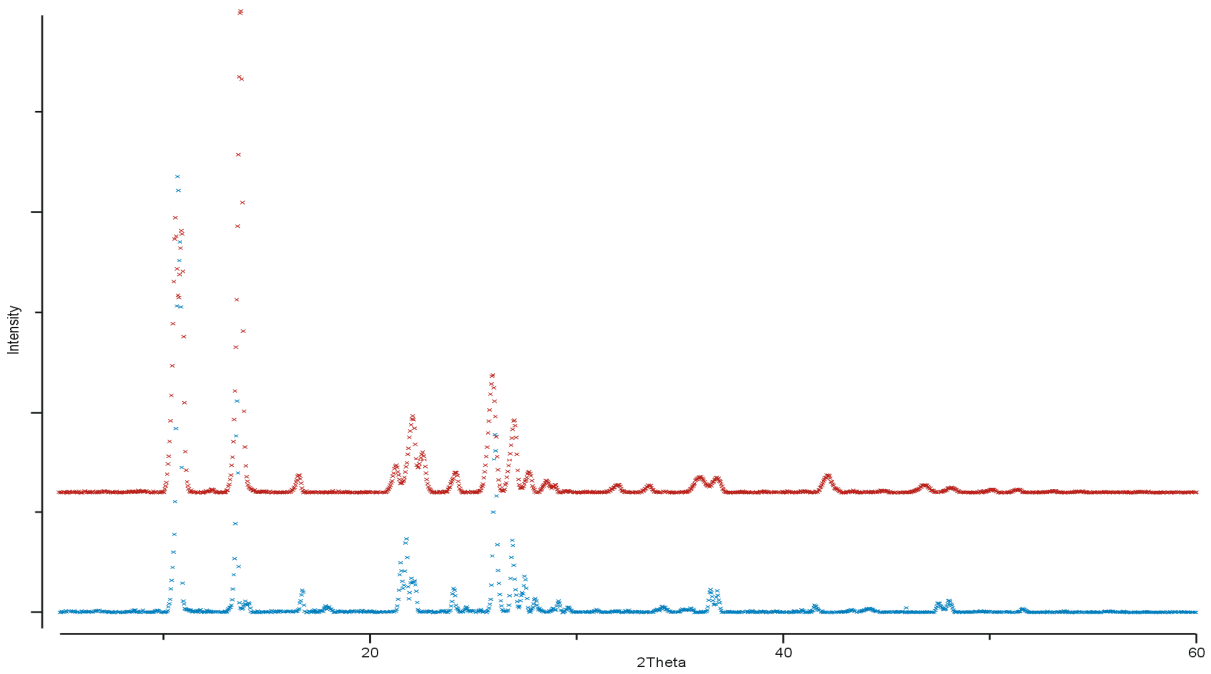

Figure 1SI. Comparison of PXRD patterns of polymorph I (dashed blue line) and of polymorph II (dashed red line).

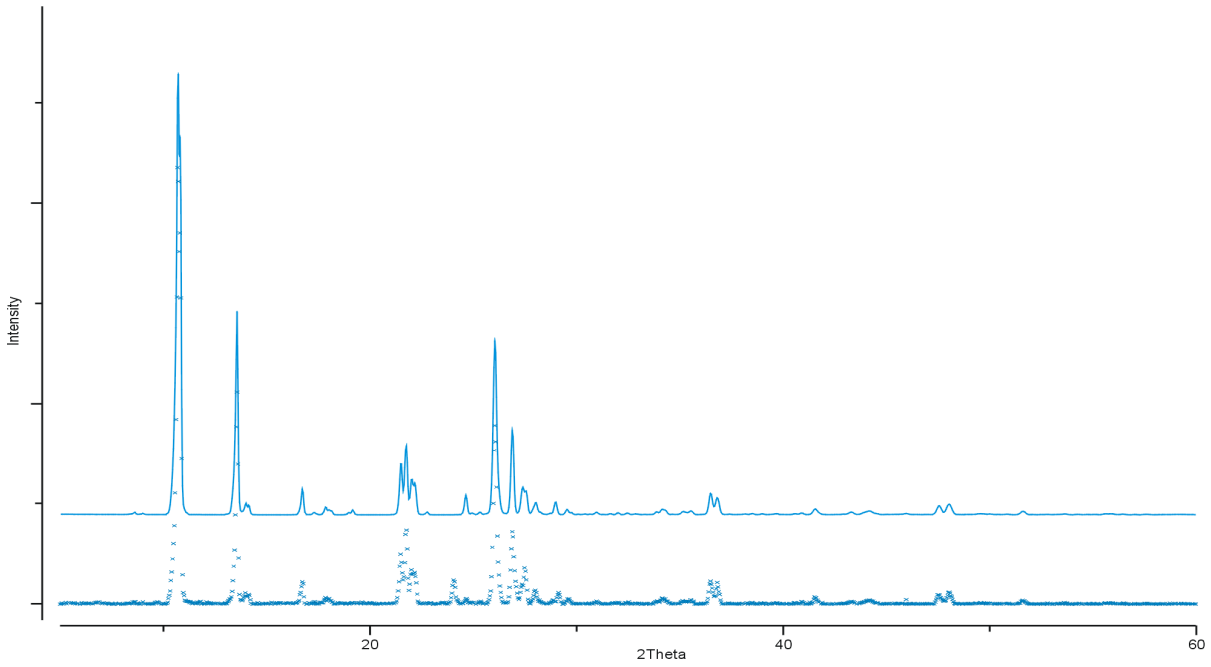

Figure 2SI. PXRD pattern (dashed line) and theoretically calculated pattern (solid line) of polymorph I. Note that the unit cell parameters slightly differ in 295K. They are a=20.188Å, b=3.639Å, c=21.149Å, β=104.54°.

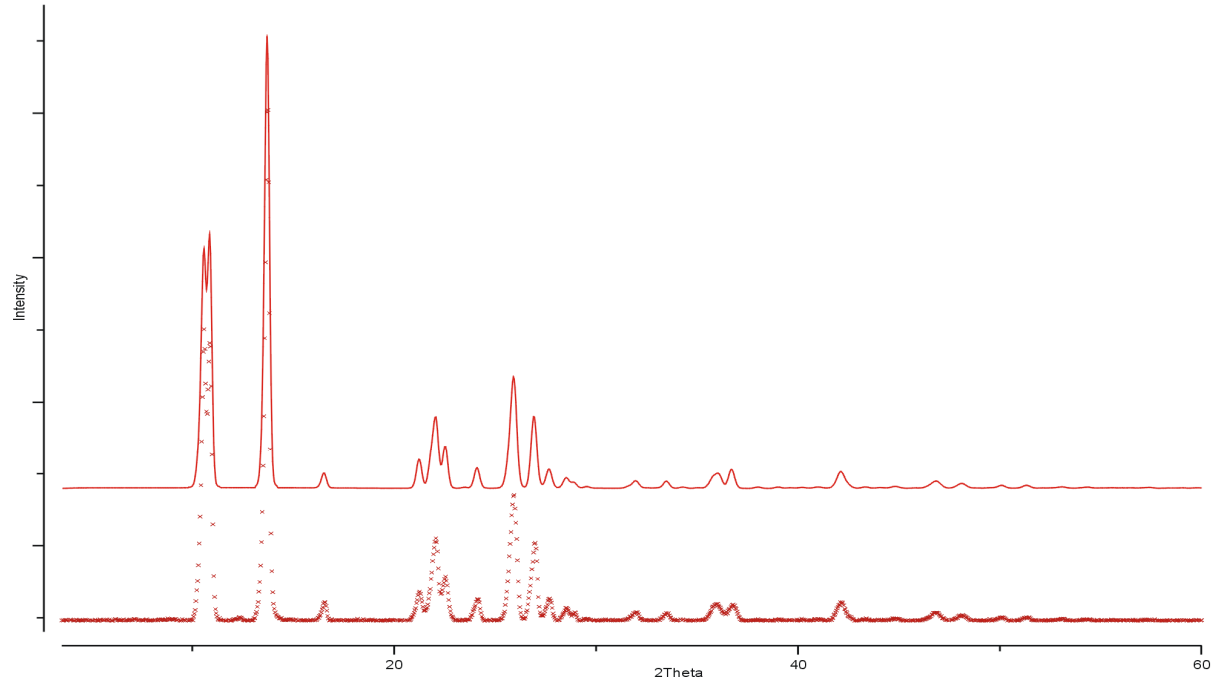

Fig. 3SI. PXRD pattern (dashed line) and theoretically calculated pattern (solid line) of polymorph II. Note that the unit cell parameters slightly differ in 295K. They are a=8.265Å, b=3.783Å, c=17.014Å, β=100.43°

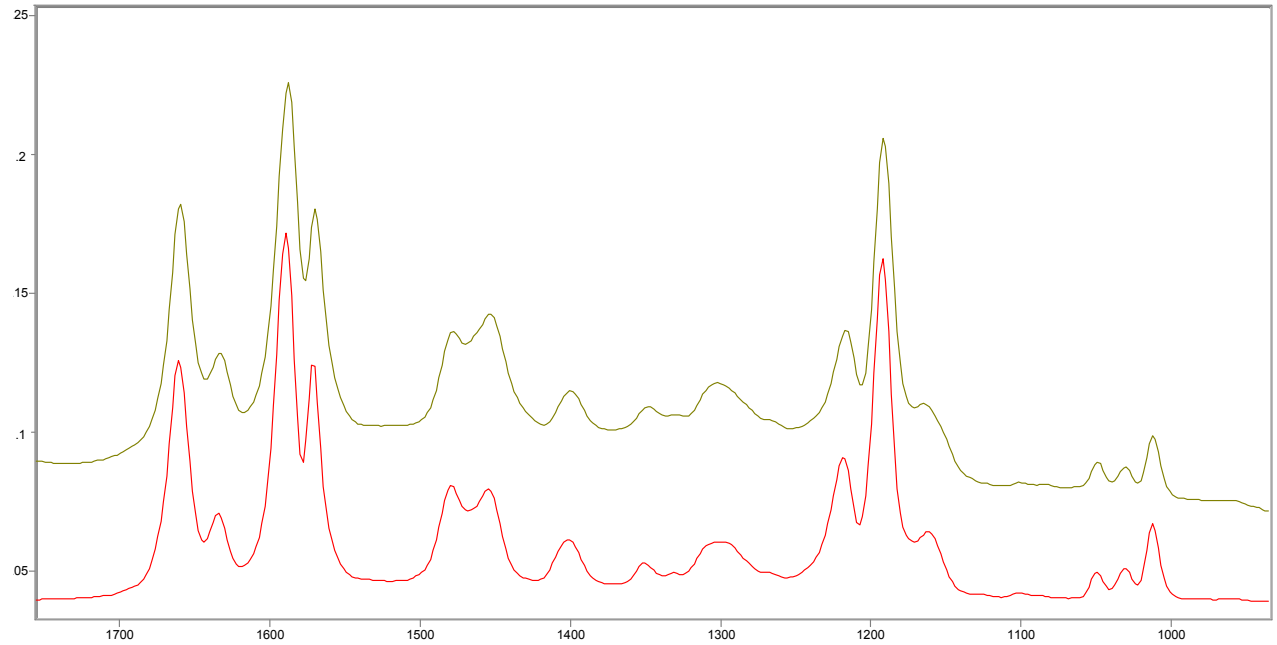

Fig. 4SI. The Raman spectra of the alizarin form I (olive) and form II (red) crystals in the range 1700-1000 cm^{-1}.

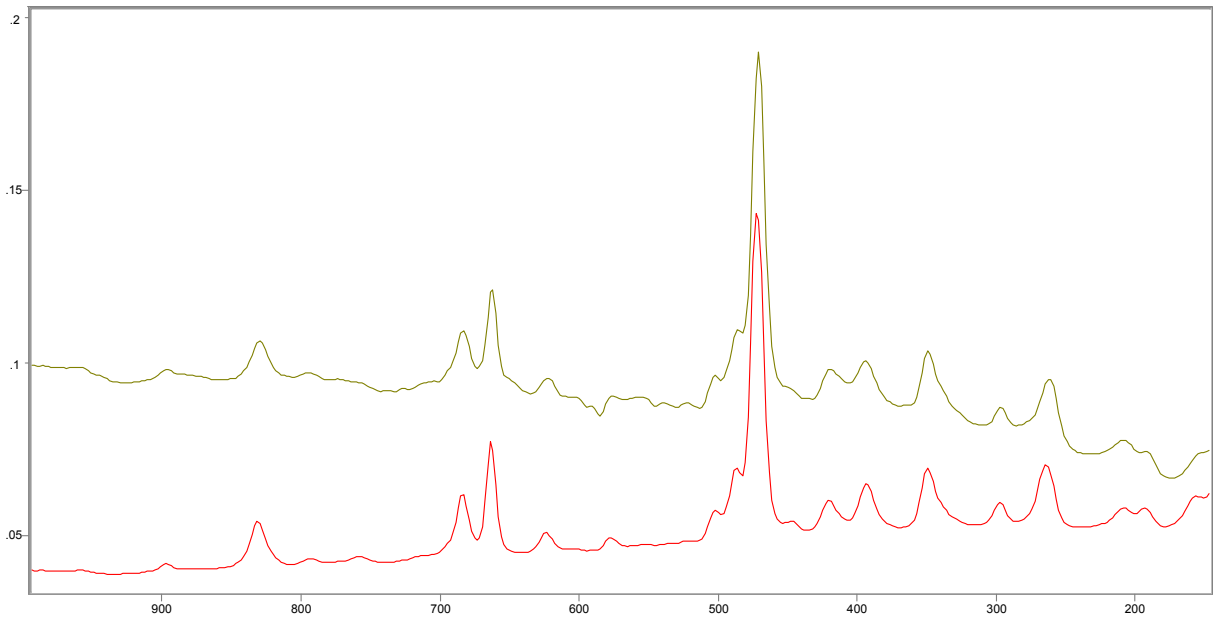

Figure 5SI. The Raman spectra of the alizarin form I (olive) and form II (red) crystals in the range 1000-200 cm^{-1}.

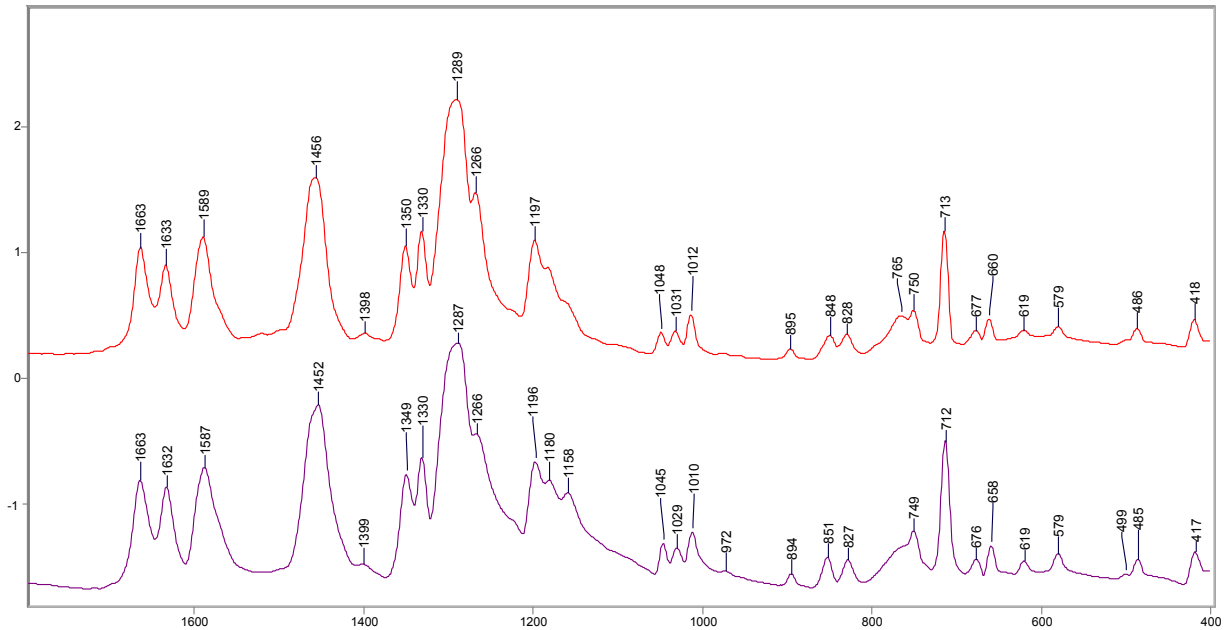

Figure 6SI. The IR spectra of the alizarin form I (red) and form II (dark blue) crystals in the range 1700-400 cm^{-1}.

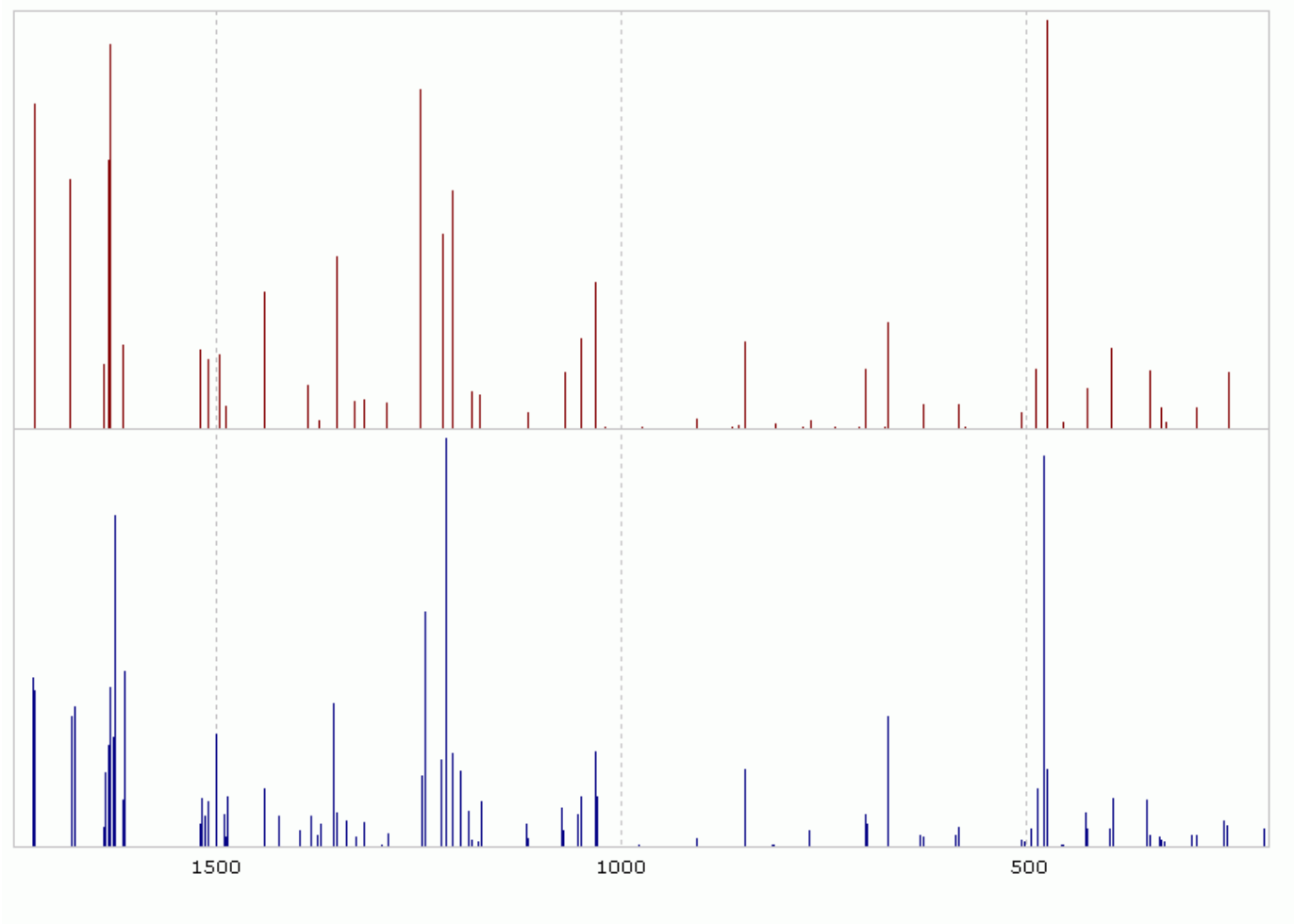

Fig. 7SI. Comparison of the Raman theoretical B3LYP/6-31++G** spectra of alizarin monomer (top) and dimer (bottom)

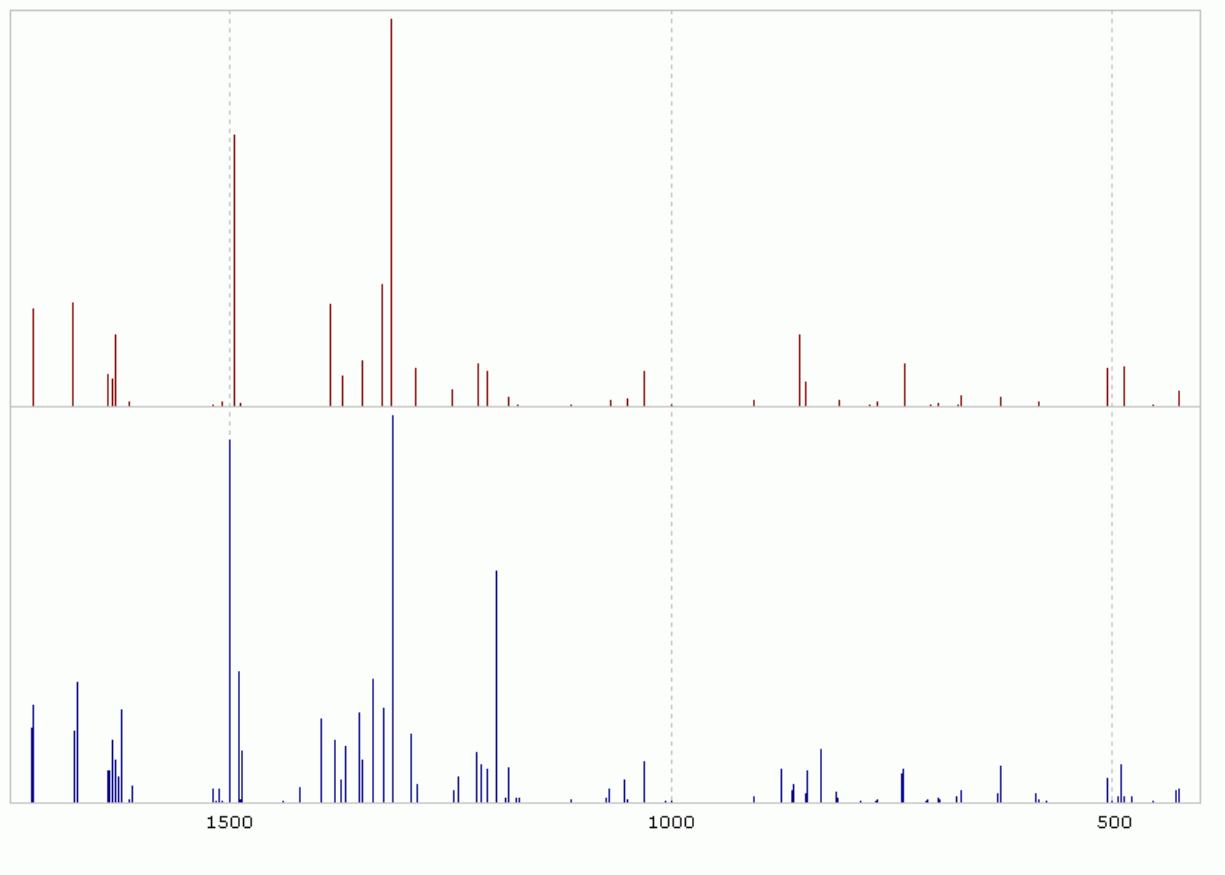

Fig. 8SI. Comparison of the IR theoretical B3LYP/6-31++G** spectra of alizarin monomer (top) and dimer (bottom)

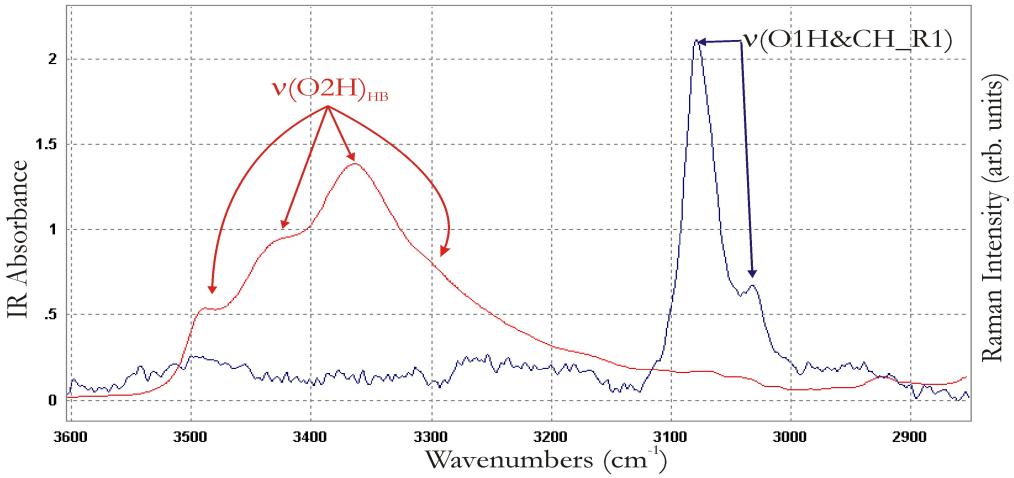

Fig. 9SI. The ν(OH) and ν(CH) region of the experimental IR (red) and Raman (blue) spectra.

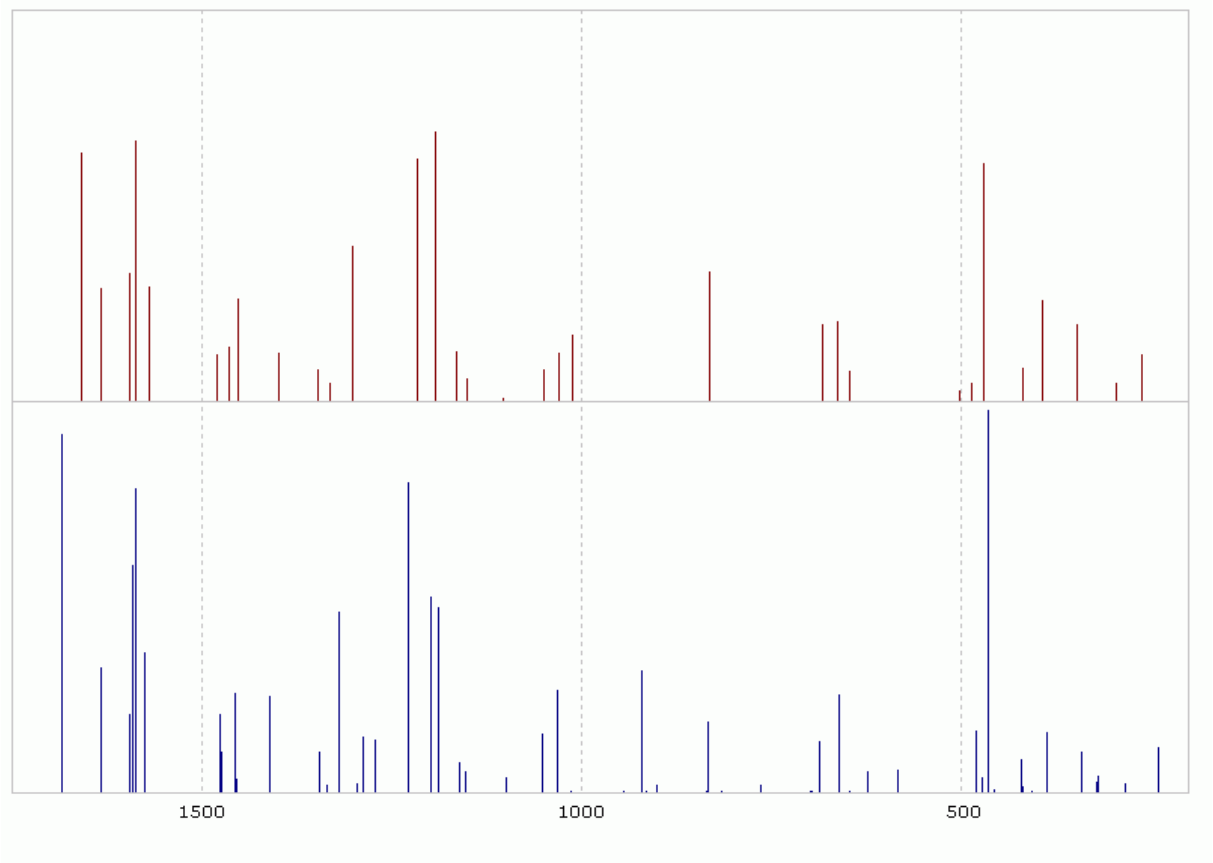

Figure 10SI. Comparison of the Raman experimental digitized (top) and theoretical (bottom) spectra of alizarin.

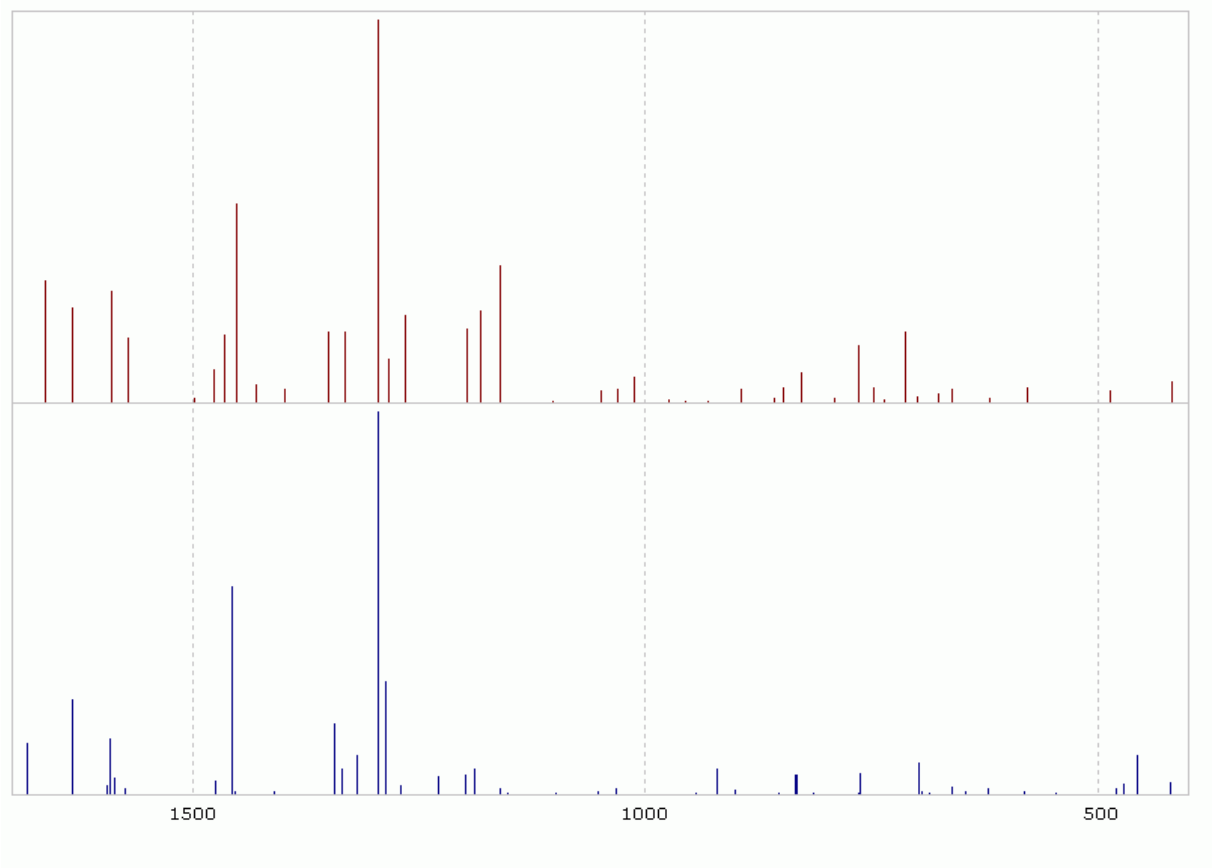

Figure 11SI. Comparison of the IR experimental digitized (top) and theoretical (bottom) spectra of alizarin.

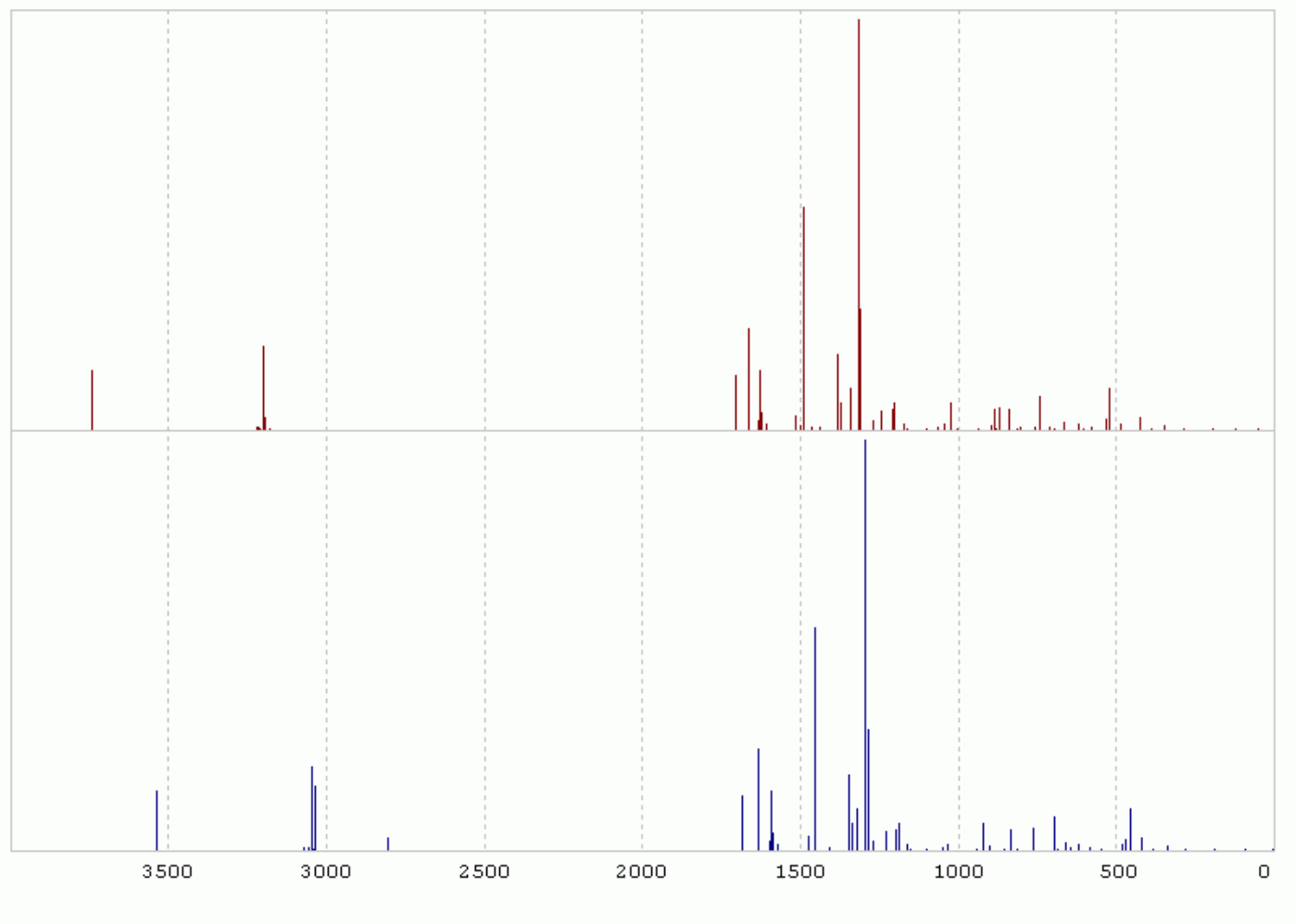

Fig. 12SI. Comparison of the IR theoretical harmonic (top, red) and anharmonic (bottom, blue) B3LYP/aug –cc-pVDZ spectra of the alizarin molecule. Observe that in the anharmonic spectrum different bands are shifted by different factors.

Table 1SI. The B3LYP/aug-cc-pVDZ calculated fundamental frequencies of the alizarin molecule

ν_{har} (cm^{-1})	ν_{anh} (cm^{-1})	I_{IR} (km/mol)	A_R (A^4/amu)	$A_{R(ANHAR)}$ (%)	Symm.	PED (%)
3740	3537	119.4	143.2	7.7	A'	ν(O2-H)100
3218	3071	5.3	33.7	2.8	A'	85 ν^s(CH_R1); 14 ν^s(CH_R2)
3214	3057	4.6	284.1	24.2	A'	83 ν^s(CH_R2); 14 ν^s(CH_R1)
3212	3071	2.4	82.4	6.9	A'	99 $\nu^a{}_1$(CH_R2)
3200	3044	166.2	137.7	11.9	A'	96 $\nu^a{}_1$(O1-H&CH_R1)
3198	3037	127.5	392.6	34.1	A'	96 $\nu^a{}_2$(O1-H&CH_R1)
3195	2803	25.9	154.2	16.8	A'	97 $\nu^a{}_2$(CH_R2)
3181	3040	3.2	82.8	7.2	A'	98 $\nu^a{}_3$(CH_R2)
1707	1683	109.0	276.3	93.7	A'	80 ν(C=04)
1666	1633	201.7	91.4	32.8	A'	67 ν(C=03)
1631	1595	17.4	54.1	20.3	A'	60 ν_1(CC)
1627	1591	117.3	158.3	59.5	A'	50 ν_2(CC); 17 β(O1-H)
1623	1586	35.5	210.6	79.7	A'	62 ν_3(CC)
1606	1574	11.0	95.1	36.5	A'	67 ν_4(CC)
1513	1475	26.7	47.7	20.5	A'	54 ν_5(CC); 12 β_4(CH)
1500	1474	7.6	24.8	10.7	A'	41 β_1(CH_R2); 20 ν_{11}(CC)
1491	1456	443.4	58.5	25.8	A'	54 ν_6(CC); 19 β(O1-H)
1464	1453	5.4	7.6	3.4	A'	39 ν_7(CC); 22 β_2(CH); 12 β_6(CH)
1438	1410	4.2	54.1	25.2	A'	42 ν_8(CC); 38 β(O2-H)
1383	1344	151.9	20.9	10.5	A'	24 β(O1-H); 13 ν_6(CC); 13 ν_9(CC); 11 ν_{12}(CC); 10 β_8(CCC)
1370	1335	54.4	3.7	1.9	A'	68 ν_9(CC)
1341	1319	81.9	91.1	47.4	A'	44 ν(C-O1); 10 β_2(CH)
1318	1295	816.8	4.0	2.1	A'	56 ν(C-O2); 10 ν_{10}(CC)
1310	1287	241.5	26.7	14.5	A'	39 ν_{70}(CC); 17 β_4(CH); 12 β(O2-H)
1271	1271	18.6	24.9	13.8	A'	46 β_2(CH); 39 ν_{10}(CC); 16 ν_7(CC)
1245	1228	36.6	138.8	81.1	A'	14 ν_8(CC); 19 β(O2-H)
1209	1198	42.1	83.9	51.0	A'	46 β_3(CH)
1202	1188	54.8	78.8	48.6	A'	34 β_4(CH); 11 ν_1(CC)
1172	1160	11.2	11.9	7.6	A'	81 β_5(CH_R2); 14 ν_{13}(CC)
1162	1152	3.2	8.0	5.2	A'	48 β_6(CH)
1103	1099	1.1	5.8	4.0	A'	55 β_1(CCC)
1064	1052	4.8	20.4	15.2	A'	56 ν_{11}(CC); 21 β_1(CH_R2)
1042	1032	11.0	35.0	26.8	A'	45 ν_{12}(CC); 13 β_1(CCC)
1029	1014	0.0	0.1	0.1	A"	87 τ_1(CH_R2)
1026	921	52.5	35.4	32.0	A'	53 ν_{13}(CC)
1001	944	1.1	0.1	0.1	A"	86 τ_2(CH)
997	915	0.4	0.2	0.2	A"	87 τ_3(CH_R1)
935	853	1.1	0.0	0.0	A"	69 τ_4(CH_R2); 18 τ(C=O3)
897	900	8.4	1.9	1.8	A'	63 β_2(CCC)
885	834	41.1	0.2	0.2	A"	36 τ(C=O3); 25 τ(O1-H); 12 τ_4(CH_R2)
879	815	2.2	0.2	0.2	A"	64 τ_5(CH_R1&O1-H); 11 τ(C=O3&C=O4)
868	763	44.8	0.6	0.7	A"	56 τ(O1-H); 16 τ(C=O3)
841	833	39.8	17.8	18.5	A'	59 ν_{14}(CC)
816	764	2.4	1.0	1.2	A"	36 τ(C=O3&C=O4); 34 τ_6(CH_R2)

806	695	4.9	0.1	0.1	A"	75 τ_1(CCCC)
757	763	6.4	1.6	1.9	A'	68 β_3(CCC)
741	697	65.7	0.3	0.4	A"	57 τ_6(CH_R2); 30 τ(C=O3&C=O4)
713	647	6.3	0.1	0.1	A"	79 τ_2(CCCC)
694	686	3.0	9.9	13.4	A'	79 β_4(CCC)
668	661	15.3	18.0	25.6	A'	71 β_5(CCC)
620	622	11.5	3.5	5.4	A'	61 β_6(CCC)
605	547	0.7	0.0	0.0	A"	83 τ_3(CCCC)
577	582	5.7	3.5	5.9	A'	56 β_7(CCC)
532	472	22.8	1.8	3.9	A"	51 τ_4(CCCC); 36 τ(O2-H)
522	456	84.3	0.3	0.7	A"	59 τ(O2-H); 29 τ_4(CCCC)
484	480	12.2	7.5	15.9	A'	63 β_1(CCO)
472	464	0.3	45.2	100.0	A'	68 ν(quinone)
470	418	0.2	0.5	1.3	A"	80 τ_5(CCCC)
437	406	0.2	0.1	0.3	A"	83 τ_6(CCCC)
425	420	24.2	3.5	8.7	A'	62 β_8(CCC)
389	386	3.7	5.7	15.7	A'	60 β_9(CCC); 11 ν_{10}(CC)
346	340	7.3	3.3	10.5	A'	81 β_2(CCO)
342	320	0.5	1.2	4.1	A"	91 τ_7(CCCC)
328	321	0.2	0.8	2.7	A'	79 ν(accordion)
286	283	1.4	0.6	2.4	A'	81 β_{10}(CCC)
271	239	0.0	2.5	11.9	A"	88 τ_8(CCCC)
196	190	0.6	0.3	1.8	A'	74 β_{11}(CCC)
188	166	0.1	0.6	4.2	A"	83 τ_9(CCCC)
147	131	0.2	0.3	2.7	A"	87 τ_{10}(CCCC)
125	92	1.2	1.2	16.0	A"	82 τ_{11}(CCCC)
95	62	0.4	0.3	6.2	A"	86 τ_{12}(CCCC)
49	6	2.9	0.1	83.1	A"	90 τ(Butterfly)

Table 2SI. The parameters of experimental FT-IR and FT-Raman spectra of alizarin in polycrystalline powder

IR				Raman				Calculations		
Freq	I_{INT}(%)	I_{max}(%)	FWHM	Freq	I_{INT}(%)	I_{max}(%)	FWHM	Freq anh	I_{INT}(%)	$I^{REL,anh}$ (%)
3491	8.80	7.20	31.8					3537	14.62	7.7
3436	31.31	13.60	70.3							
3366	61.82	21.40	73.8							
3307	44.65	10.40	116.9							
								3071	0.65	2.8
				3077	61.70	30.86	30.3	3071	0.29	6.9
								3057	0.56	24.2
3060	4.69	2.00	75.6							
				3035	14.49	7.41	33.0	3044	20.35	11.9
								3040	0.39	7.2
								3037	15.61	34.1
								2803	3.17	16.8
1663	31.84	45.40	19.4	1658	64.83	62.96	14.3	1683	13.34	93.7
1633	24.83	34.20	16.9	1632	29.45	22.22	16.5	1633	24.69	32.8
				1595	33.38	24.69	19.0	1595	2.13	20.3
1590	29.09	46.20	19.4	1587	68.28	82.72	12.9	1591	14.36	59.5
								1586	4.35	79.7
1571 sh	17.03	16.60	24.3	1569	29.92	49.38	8.7	1574	1.35	36.5
1498???	1.00									
1477	8.65	18.40	14.5	1478	22.10	14.81	15.00	1475	3.27	20.5
								1474	0.93	10.7
1465 sh	17.58	37.00	14.6	1463	14.16	13.58	13.2			
1452	52.06	67.40	21.2	1451	26.80	23.46	17.7	1456	54.29	25.8
								1453	0.66	3.4
1429	4.64	8.00	17.7							
1398	3.51	4.60	19.2	1399	12.50	12.35	17.5	1410	0.51	25.2
1350	18.50	39.20	14.5	1347	8.18	8.64	15.8	1344	18.60	10.5
1332	18.30	46.20	12.1	1331	4.65	6.17	13.3	1335	6.66	1.9
								1319	10.03	47.4
1295	100.00	100.00	30.7	1302	40.49	19.75	34.9	1295	100.00	2.1
1283 sh	11.28	30.00	11.5					1287	29.57	14.5

1266	22.72	41.00	14.8					1271	2.28	13.8	
				1216	63.50	40.74	21.2	1228	4.48	81.1	
1198	19.27	39.60	15.0					1198	5.15	51.0	
				1191	70.35	93.83	12.7	1188	6.71	48.6	
1182	23.78	36.60	20.0								
1160	35.72	34.00	31.7	1164	12.77	13.58	16.5	1160	1.37	7.6	
				1150	5.92	7.41	11.2	1152	0.39	5.2	
1102	0.42	1.20	10.8	1102	0.80	1.23	5.5	1099	0.13	4.0	
1048	3.21	10.20	9.7	1048	8.18	12.35	9.5	1052	0.59	15.2	
1031	3.59	9.80	11.3	1030	12.57	13.58	12.9	1032	1.35	26.8	
1012	6.61	19.20	10.5	1012	17.15	23.46	10.0	1014	0.00	0.1	
974	0.78	1.60	15.5								
955	0.22	0.80	9.2								
931	0.28	0.80	10.2					921	6.43	32.0	
895	3.52	6.60	13.6					900	1.03	1.8	
858	0.86	3.40	7.9					853	0.13	0.0	
848	3.91	11.60	10.3					834	5.03	0.2	
828	7.69	12.80	15.9	830	33.84	16.05	25.8	833	4.87	18.5	
792	1.23	2.60	15.1								
765	14.90	17.60	26.0					763	5.48	0.7	
748	4.00	12.00	10.2					763	0.78	1.9	
736	0.47	1.60	6.8								
713	18.36	56.40	10.0					697	8.04	0.4	
700	1.62	3.80	9.6					695	0.60	0.1	
677	2.07	6.00	9.9	682	20.08	18.52	13.3	686	0.37	13.4	
660	3.45	12.40	8.5	662	20.94	35.80	7.3	661	1.87	25.6	
				646	7.65	7.41	14.7	647	0.77	0.1	
620	0.87	2.60	10.0					622	1.41	5.4	
579	3.69	6.80	13.2					582	0.70	5.9	
				501	2.79	7.41	6.2				
486	3.07	9.00	10.3	486	4.52	9.88	8.1	480	1.49	15.9	
				470	62.37	100.00	8.5	464	0.04	100.0	
419	5.27	15.40	10.5	419	8.38	8.64	12.0	420	2.96	8.7	
				392	26.26	13.58	24.6	386	0.45	15.7	
				347	19.88	16.05	15.2	340	0.89	10.5	
				296	4.39	4.94	10.5	283	0.17	2.4	
				261	11.97	16.05	13.0				
				193	100.00	58.02	30.1	190	0.07	1.8	
				182	26.40	48.15	9.7				
				169	38.76	48.15	13.6	166	0.01	4.2	

Table 3SI. Definitions of the local coordinates for PED analysis of alizarin calculated at the B3LYP/aug-cc-pVDZ level.

coor.	coef.	inter mode type	Atom				fragment	Geom. value	Freq 1	Freq 2	Freq 3	Notati
			No1	No2	No3	No4			PED %			
s 1	1.00	STRE	16	20			OH	0.970410	f3740 100			ν(O2-H
s 2	1.00	STRE	3	21			CH	1.089395	f3218 85	f3214 14		ν^{s}(CH_
	3.00		4	22			CH	1.087996				
s 3	1.00	STRE	5	23			CH	1.088567	f3214 83	f3218 14		ν^{s}(CH_
	1.00		6	24			CH	1.090330				
	1.00		7	25			CH	1.090156				
	2.00		8	26			CH	1.088349				
s 4	-3.00	STRE	5	23			CH	1.088567	f3212 99			$\nu^{a}{}_{1}$(CH_
	-1.00		6	24			CH	1.090330				
	1.00		8	26			CH	1.088349				
s 5	-2.00	STRE	3	21			CH	1.089395	f3200 96			$\nu^{a}{}_{1}$(O1-H&CH_R
	1.00		4	22			CH	1.087996				
	2.00		15	19			OH	0.996409				
s 6	2.00	STRE	3	21			CH	1.089395	f3198 96			$\nu^{a}{}_{2}$(O1-H&CH_R
	-1.00		4	22			CH	1.087996				
	2.00		15	19			OH	0.996409				
s 7	-1.00	STRE	5	23			CH	1.088567	f3195 97			$\nu^{a}{}_{2}$(CH_
	2.00		6	24			CH	1.090330				
	3.00		7	25			CH	1.090156				
	-1.00		8	26			CH	1.088349				
s 8	-1.00	STRE	6	24			CH	1.090330	f3181 98			$\nu^{a}{}_{3}$(CH_
	1.00		7	25			CH	1.090156				
s 9	1.00	STRE	18	10			OC	1.227412	f1707 80			ν(C=04
s 10	1.00	STRE	17	9			OC	1.246636	f1666 67			ν(C=03
s 11	3.00	STRE	2	3			CC	1.392095	f1631 60	f1202 11		ν_{1}(CC)
	-2.00		4	14			CC	1.394778				
	2.00		5	6			CC	1.394906				
	-1.00		16	2			OC	1.355710				
	-1.00		17	9			OC	1.246636				
	-1.00		18	10			OC	1.227412				
s 12	1.00	STRE	1	2			CC	1.414741	f1627 50			ν_{2}(CC)
	-1.00		1	13			CC	1.406723				
	1.00		2	3			CC	1.392095				

	-1.00		3	4			CC	1.399714				
	1.00		4	14			CC	1.394778				
	1.00		18	10			OC	1.227412				
s 13	-3.00	STRE	2	3			CC	1.392095	f162362			ν_3(CC)
	3.00		4	14			CC	1.394778				
	-4.00		5	11			CC	1.401102				
	-5.00		7	8			CC	1.393725				
	3.00		17	9			OC	1.246636				
s 14	1.00	STRE	4	14			CC	1.394778	f160667			ν_4(CC)
	1.00		5	6			CC	1.394906				
	-1.00		6	7			CC	1.401921				
	-1.00		11	12			CC	1.411714				
	1.00		17	9			OC	1.246636				
	1.00		18	10			OC	1.227412				
s 15	-2.00	STRE	2	3			CC	1.392095	f151354			ν_5(CC)
	-5.00		3	4			CC	1.399714				
	-1.00		9	13			CC	1.467399				
	8.00		13	14			CC	1.421718				
	-5.00		17	9			OC	1.246636				
s 16	1.00	BEND	23	5	11		HCC	118.40	f150041	f106421		β_1(CH_
	1.00		24	6	5		HCC	119.84				
	1.00		25	7	8		HCC	119.93				
	1.00		26	8	12		HCC	118.77				
s 17	-10.00	STRE	1	13			CC	1.406723	f149154	f138313		ν_6(CC)
	8.00		3	4			CC	1.399714				
	-2.00		9	12			CC	1.483478				
	4.00		9	13			CC	1.467399				
	7.00		15	1			OC	1.348683				
	5.00		16	2			OC	1.355710				
s 18	-1.00	STRE	5	6			CC	1.394906	f146439	f127116		ν_7(CC)
	-1.00		5	11			CC	1.401102				
	1.00		7	8			CC	1.393725				
	1.00		8	12			CC	1.403283				
	-1.00		9	12			CC	1.483478				
s 19	-1.00	STRE	1	2			CC	1.414741	f124514	f143842		ν_8(CC)
	1.00		2	3			CC	1.392095				
	2.00		4	14			CC	1.394778				
	-1.00		10	14			CC	1.483912				
	-1.00		13	14			CC	1.421718				
s 20	1.00	BEND	20	16	2		HOC	108.19	f143838	f124519	f131012	β(O2-H
s 21	1.00	BEND	19	15	1		HOC	105.97	f138324	f149119	f162717	β(O1-H
s 22	1.00	STRE	5	6			CC	1.394906	f137068	f138313		ν_9(CC)
	-1.00		5	11			CC	1.401102				
	-1.00		6	7			CC	1.401921				

	1.00		7	8			CC	1.393725				
	-1.00		8	12			CC	1.403283				
	1.00		11	12			CC	1.411714				
s 23	1.00	STRE	15	1			OC	1.348683	f134144			ν(C-O1
s 24	1.00	STRE	16	2			OC	1.355710	f131856			ν(C-O2
s 25	-1.00	STRE	10	11			CC	1.498389	f131039	f38911	f131810	ν_{10}(CC)
	1.00		10	14			CC	1.483912				
s 26	-2.00	BEND	19	15	1		HOC	105.97	f127146	f146422	f134110	β_2(CH)
	-3.00		22	4	14		HCC	118.62				
	3.00		25	7	8		HCC	119.93				
	6.00		26	8	12		HCC	118.77				
s 27	-1.00	BEND	20	16	2		HOC	108.19	f120946			β_3(CH)
	-1.00		21	3	2		HCC	118.68				
	1.00		22	4	3		HCC	120.59				
	-1.00		24	6	5		HCC	119.84				
	-1.00		26	8	12		HCC	118.77				
s 28	2.00	BEND	20	16	2		HOC	108.19	f120234	f131017	f151312	β_4(CH)
	2.00		21	3	2		HCC	118.68				
	2.00		22	4	3		HCC	120.59				
	1.00		25	7	6		HCC	120.03				
s 29	1.00	BEND	23	5	6		HCC	121.35	f117281			β_5(CH_
	-1.00		23	5	11		HCC	118.40				
	2.00		24	6	5		HCC	119.84				
	-2.00		24	6	7		HCC	119.93				
	-2.00		25	7	6		HCC	120.03				
	2.00		25	7	8		HCC	119.93				
	1.00		26	8	7		HCC	121.19				
	-1.00		26	8	12		HCC	118.77				
s 30	-1.00	BEND	21	3	4		HCC	121.11	f116248	f146412		β_6(CH)
	1.00		22	4	14		HCC	118.62				
	-1.00		24	6	5		HCC	119.84				
	-1.00		26	8	12		HCC	118.77				
s 31	-1.00	BEND	6	5	11		CCC	120.25	f110355	f104213		β_1(CCC
	1.00		7	8	12		CCC	120.04				
s 32	1.00	STRE	1	2			CC	1.414741	f106456	f150020		ν_{11}(CC)
	-2.00		4	14			CC	1.394778				
	-3.00		5	6			CC	1.394906				
	2.00		5	11			CC	1.401102				
	-5.00		6	7			CC	1.401921				
	-3.00		7	8			CC	1.393725				
	1.00		8	12			CC	1.403283				
	-2.00		9	13			CC	1.467399				
	2.00		11	12			CC	1.411714				
	-1.00		13	14			CC	1.421718				

	2.00		16	2			OC	1.355710				
s 33	1.00	STRE	3	4			CC	1.399714	f104245	f138311		ν_{12}(CC)
	1.00		5	6			CC	1.394906				
	1.00		6	7			CC	1.401921				
	1.00		7	8			CC	1.393725				
	-1.00		9	13			CC	1.467399				
	1.00		16	2			OC	1.355710				
s 34	1.00	TORS	23	5	11	10	HCCC	0.00	f102987			τ_1(CH_
	1.00		24	6	7	25	HCCH	0.00				
s 35	1.00	STRE	4	14			CC	1.394778	f102653	f120214		ν_{13}(CC)
	-1.00		5	6			CC	1.394906				
	-1.00		5	11			CC	1.401102				
	-1.00		6	7			CC	1.401921				
	-1.00		7	8			CC	1.393725				
	-1.00		8	12			CC	1.403283				
	1.00		10	14			CC	1.483912				
	-1.00		11	12			CC	1.411714				
	-1.00		15	1			OC	1.348683				
s 36	-1.00	TORS	21	3	4	22	HCCH	0.00	f100186			τ_2(CH)
	1.00		23	5	6	24	HCCH	0.00				
	1.00		25	7	6	5	HCCC	-180.00				
	1.00		26	8	12	9	HCCC	0.00				
	1.00		26	8	12	11	HCCC	-180.00				
s 37	1.00	TORS	21	3	4	22	HCCH	0.00	f99787			τ_3(CH_
	-1.00		22	4	3	2	HCCC	-180.00				
	-1.00		22	4	14	10	HCCC	0.00				
s 38	1.00	TORS	23	5	11	10	HCCC	0.00	f93569	f88612		τ_4(CH_
	1.00		24	6	5	11	HCCC	-180.00				
	1.00		25	7	8	12	HCCC	-180.00				
	1.00		26	8	12	9	HCCC	0.00				
s 39	1.00	BEND	3	4	14		CCC	120.79	f89763			β_2(CCC
	-1.00		4	14	13		CCC	119.63				
	1.00		5	6	7		CCC	120.23				
	-1.00		5	11	10		CCC	119.14				
	1.00		11	10	14		CCC	117.48				
	1.00		11	10	18		CCO	120.65				
s 40	1.00	OUT	17	12	13	9	OCCC	0.00	f88636	f93518	f86816	τ(C=O3
s 41	-1.00	TORS	19	15	1	2	HOCC	-180.00	f87964			τ_5(CH_ H)
	-1.00		19	15	1	13	HOCC	0.00				
	1.00		21	3	2	16	HCCO	0.00				
	1.00		22	4	3	2	HCCC	-180.00				
s 42	1.00	TORS	19	15	1	2	HOCC	-180.00	f86856	f88625		τ(O1-H
s 43	1.00	STRE	1	2			CC	1.414741	f84159			ν_{14}(CC)

	1.00		1	13			CC	1.406723				
	1.00		2	3			CC	1.392095				
	1.00		3	4			CC	1.399714				
	-1.00		7	8			CC	1.393725				
	-1.00		8	12			CC	1.403283				
	-1.00		9	12			CC	1.483478				
	-1.00		11	12			CC	1.411714				
	1.00		15	1			OC	1.348683				
	1.00		16	2			OC	1.355710				
s 44	-1.00	OUT	17	12	13	9	OCCC	0.00	f81636	f74130	f87911	τ(C=O3
	1.00		18	11	14	10	OCCC	0.00				
s 45	1.00	OUT	9	8	11	12	CCCC	0.00	f80775			τ_1(CCC
	1.00	TORS	1	2	3	4	CCCC	0.00				
	1.00		2	3	4	14	CCCC	0.00				
	1.00		5	6	7	8	CCCC	0.00				
	1.00		6	7	8	12	CCCC	0.00				
	1.00		7	6	5	11	CCCC	0.00				
	-1.00	OUT	15	2	13	1	OCCC	0.00				
	-1.00		16	1	3	2	OCCC	0.00				
s 46	-1.00	BEND	2	3	4		CCC	120.21	f75768			β_3(CCC
	1.00		6	7	8		CCC	120.04				
	-1.00		11	10	14		CCC	117.48				
	1.00		11	10	18		CCO	120.65				
	1.00		12	9	13		CCC	118.42				
	-1.00		12	9	17		CCO	120.74				
s 47	1.00	TORS	23	5	11	12	HCCC	-180.00	f74157	f81634		τ_6(CH_
	1.00		24	6	5	11	HCCC	-180.00				
	1.00		25	7	6	5	HCCC	-180.00				
	1.00		26	8	7	6	HCCC	-180.00				
s 48	1.00	TORS	6	7	8	12	CCCC	0.00	f71379			τ_2(CCC
	1.00		7	6	5	11	CCCC	0.00				
	1.00	OUT	15	2	13	1	OCCC	0.00				
	1.00		16	1	3	2	OCCC	0.00				
	1.00		17	12	13	9	OCCC	0.00				
s 49	-1.00	BEND	3	4	14		CCC	120.79	f69479			β_4(CCC
	1.00		4	14	10		CCC	119.83				
	-1.00		5	6	7		CCC	120.23				
	1.00		13	9	17		CCO	120.84				
	-1.00		14	10	18		CCO	121.88				
s 50	1.00	BEND	5	6	7		CCC	120.23	f66871			β_5(CCC
	1.00		6	7	8		CCC	120.04				
s 51	-1.00	BEND	2	1	13		CCC	120.13	f62061			β_6(CCC
	1.00		3	2	16		CCO	120.46				
	-1.00		3	4	14		CCC	120.79				
	-1.00		9	12	11		CCC	120.52				
	-1.00		9	13	14		CCC	121.64				

s 52	1.00	TORS	3	4	14	13	CCCC	0.00	f60583			τ3(CCC
	-1.00		5	6	7	8	CCCC	0.00				
	-1.00		6	5	11	10	CCCC	-180.00				
	1.00		14	13	1	15	CCCO	-180.00				
	-1.00		14	13	9	17	CCCO	-180.00				
	-1.00	OUT	16	1	3	2	OCCC	0.00				
s 53	1.00	BEND	2	1	13		CCC	120.13	f57756			β7(CCC
	1.00		2	3	4		CCC	120.21				
	1.00		3	4	14		CCC	120.79				
	-1.00		6	5	11		CCC	120.25				
	1.00		8	12	11		CCC	119.98				
	-1.00		9	12	11		CCC	120.52				
	1.00		11	10	18		CCO	120.65				
	1.00		12	9	13		CCC	118.42				
s 54	-1.00	TORS	1	2	3	4	CCCC	0.00	f53251	f52229		τ4(CCC
	1.00		2	3	4	14	CCCC	0.00				
	-1.00		5	6	7	8	CCCC	0.00				
	-1.00		9	13	1	15	CCCO	0.00				
	-1.00		13	1	2	16	CCCO	-180.00				
s 55	1.00	TORS	20	16	2	1	HOCC	0.00	f52259	f53236		τ(O2-H
s 56	1.00	BEND	3	2	16		CCO	120.46	f48463			β1(CCO
	1.00		5	11	12		CCC	119.45				
	1.00		11	10	14		CCC	117.48				
	-1.00		13	1	15		CCO	123.53				
s 57	-1.00	STRE	1	4			CC	2.801175	f47268			ν(quin
	-1.00		5	8			CC	2.801882				
	4.00		9	10			CC	2.945785				
s 58	1.00	TORS	5	6	7	8	CCCC	0.00	f47080			τ5(CCC
	1.00		5	11	12	8	CCCC	0.00				
	-1.00		6	7	8	12	CCCC	0.00				
	1.00		11	12	9	17	CCCO	-180.00				
	1.00		12	11	10	18	CCCO	-180.00				
	-1.00		13	1	2	16	CCCO	-180.00				
s 59	-1.00	TORS	6	7	8	12	CCCC	0.00	f43783			τ6(CCC
	1.00		7	6	5	11	CCCC	0.00				
s 60	1.00	BEND	1	13	9		CCC	118.99	f42562	f138310		β8(CCC O1H... breaki
	1.00		2	1	13		CCC	120.13				
	-1.00		8	12	9		CCC	119.50				
	1.00		8	12	11		CCC	119.98				
	-1.00		11	10	18		CCO	120.65				
	-2.00		12	9	17		CCO	120.74				
	2.00		13	9	17		CCO	120.84				
s 61	-1.00	BEND	2	1	15		CCO	116.35	f38960			β9(CCC

	-2.00		4	14	13		CCC	119.63				
	2.00		5	11	12		CCC	119.45				
	-2.00		8	12	9		CCC	119.50				
	-2.00		8	12	11		CCC	119.98				
	3.00		10	14	13		CCC	120.55				
	-2.00		12	9	13		CCC	118.42				
	3.00		13	1	15		CCO	123.53				
	3.00		14	10	18		CCO	121.88				
s 62	1.00	BEND	1	2	16		CCO	119.67	f34681			β_2(CCO
	1.00		2	1	15		CCO	116.35				
	1.00		14	10	18		CCO	121.88				
s 63	1.00	OUT	10	4	13	14	CCCC	0.00	f34291			τ_7(CCC
	2.00	TORS	1	2	3	4	CCCC	0.00				
	-2.00		2	3	4	14	CCCC	0.00				
	4.00		4	3	2	16	CCCO	-180.00				
	-1.00		5	11	10	18	CCCO	0.00				
	-2.00		9	13	1	15	CCCO	0.00				
	1.00		12	9	13	14	CCCC	0.00				
	-1.00		12	11	10	18	CCCO	-180.00				
	-3.00		14	13	1	15	CCCO	-180.00				
	-2.00	OUT	16	1	3	2	OCCC	0.00				
s 64	1.00	STRE	2	13			CC	2.445020	f32879			ν(accc
	1.00		3	14			CC	2.429681				
	1.00		6	11			CC	2.424505				
	1.00		7	12			CC	2.422830				
	2.00		11	14			CC	2.549280				
	2.00		12	13			CC	2.534937				
s 65	3.00	BEND	1	2	16		CCO	119.67	f28681			β_{10}(CCC
	-1.00		2	1	13		CCC	120.13				
	-1.00		4	14	10		CCC	119.83				
	3.00		5	11	10		CCC	119.14				
	-2.00		8	12	9		CCC	119.50				
	-2.00		9	13	14		CCC	121.64				
	1.00		11	10	18		CCO	120.65				
	-1.00		12	9	17		CCO	120.74				
s 66	-1.00	TORS	1	2	3	4	CCCC	0.00	f27188			τ_8(CCC
	-4.00		4	14	13	9	CCCC	-180.00				
	-2.00		6	5	11	10	CCCC	-180.00				
	2.00		7	8	12	9	CCCC	-180.00				
	-2.00		14	13	1	15	CCCO	-180.00				
s 67	-1.00	BEND	1	13	9		CCC	118.99	f19674			β_{11}(CCC
	-1.00		8	12	9		CCC	119.50				
	1.00		12	9	13		CCC	118.42				
s 68	1.00	TORS	6	5	11	10	CCCC	-180.00	f18883			τ_9(CCC
	-1.00		7	8	12	9	CCCC	-180.00				
	-1.00		11	12	9	17	CCCO	-180.00				
	1.00		12	11	10	18	CCCO	-180.00				

s 69	1.00	TORS	1	13	9	17	CCCO	0.00	f147 87			τ_{10}(CCC
	1.00		2	1	13	9	CCCC	-180.00				
	1.00		5	11	12	8	CCCC	0.00				
	1.00		9	13	1	15	CCCO	0.00				
	-1.00		11	12	9	13	CCCC	0.00				
	-1.00		13	1	2	16	CCCO	-180.00				
s 70	1.00	TORS	3	2	1	13	CCCC	0.00	f125 82			τ_{11}(CCC (^{f}(^{g}
	1.00		3	4	14	10	CCCC	-180.00				
	1.00		5	11	12	8	CCCC	0.00				
	-1.00		6	5	11	10	CCCC	-180.00				
	-1.00		7	6	5	11	CCCC	0.00				
	-1.00		12	11	10	18	CCCO	-180.00				
	1.00		13	1	2	16	CCCO	-180.00				
s 71	1.00	TORS	1	2	3	4	CCCC	0.00	f95 86			τ_{12}(CCC
	1.00		1	13	14	10	CCCC	-180.00				
	-1.00		2	1	13	9	CCCC	-180.00				
	-1.00		3	4	14	10	CCCC	-180.00				
	-1.00		9	13	1	15	CCCO	0.00				
	-1.00		11	12	9	13	CCCC	0.00				
s 72	1.00	TORS	1	13	9	12	CCCC	-180.00	f49 90			τ(Butt
	-1.00		2	1	13	9	CCCC	-180.00				
	1.00		5	11	10	14	CCCC	-180.00				
	-1.00		8	12	9	17	CCCO	0.00				
	1.00		12	9	13	14	CCCC	0.00				