SUPPORTING INFORMATION

Determination of the Absolute Configuration of a Chiral Oxadiazol-3-one Calcium Channel Blocker, resolved using Chiral Chromatography, via Concerted Density Functional Theory Calculations of its Vibrational Circular Dichroism, Electronic Circular Dichroism and Optical Rotation.

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CONTENTS

S2 **Table S1**: Key dihedral angles of the B3LYP/6-31G* conformations of (*S*)-**2**.

S3 **Table S2**: Calculated and experimental frequencies, dipole strengths and rotational strengths for conformations **a**-**c** of **2**.

S6 **Table S3**: Calculated B3LYP/aug-cc-pVDZ//B3LYP/6-31G* excitation energies, oscillator strengths and rotational strengths for *S*-**2**.

S8 **Table S4**. Calculated B3PW91/aug-cc-pVDZ//B3LYP/6-31G* excitation energies, oscillator strengths and rotational strengths for S-**2**.

S10 **Figure S1**: B3LYP/TZ2P IR and VCD spectra of conformations **a**-**c** of (*S*)-**2**.

S11 **Figure S2**: B3PW91/TZ2P IR and VCD spectra of conformations **a**-**c** of (*S*)-**2**.

S12 **Figure S3**: Comparison of calculated and experimental vibrational frequencies.

S13 B3PW91/TZ2P optimized geometries of **2a**-**2c**.

Table S1: Key dihedral angles[a] of the B3LYP/6-31G* conformations of (*S*)-**2**.

Conformer	N4C9C8S7	C9C8O10C11	C8O10C11C12	C9C8C13C14	O2C3N4C5
a	46.4	170.2	170.1	-87.7	-173.5
b	44.9	-58.3	-173.5	151.7	-175.8
c	34.3	59.3	-177.7	130.0	-176.5
d	-38.2	51.7	160.4	167.2	176.6
e	-38.7	60.9	-160.1	165.7	176.1
f	-40.7	52.0	163.5	-117.1	174.6
g	-45.3	-78.2	176.8	-175.2	173.1
h	-45.0	-175.8	179.5	-124.3	173.9
i	46.2	154.9	66.9	-91.4	-173.4
j	44.8	-40.0	-68.8	152.6	-175.9
k	-46.2	-104.0	82.2	-162.1	172.9
l	-38.3	78.9	-69.3	-12.0	178.4
m	-44.2	-53.2	-61.9	179.0	175.7

[a] Dihedral angles are in degrees.

Table S2: Calculated and experimental frequencies, dipole strengths and rotational strengths for conformations **a-c** of **2**[a].

	B3LYP/TZ2P									B3PW91/TZ2P									Experiment[b]					
	2a			**2b**			**2c**			**2a**			**2b**			**2c**			IR			VCD		
Mode	ν	*D*	*R*	ν	*D*	*R*	ν	*D*	*R*	ν	*D*	*R*	ν	*D*	*R*	ν	*D*	*R*	ν	*D*	γ	ν	*R*	γ
83	1842	1660.9	71.3	1844	1672.9	67.8	1841	1632.0	52.7	1865	1660.3	75.5	1866	1670.6	71.6	1864	1630.5	55.5						
82	1675	68.1	11.6	1678	44.5	-2.0	1681	34.2	1.6	1688	72.8	11.6	1690	47.0	-3.2	1693	35.5	1.3	1630	31.1	5.7	1629	7.7	4.6
81	1629	46.3	-11.1	1628	70.6	0.3	1630	60.4	-2.8	1644	66.3	0.1	1641	73.5	0.6	1643	61.8	-3.2						
																			1590	103.3	5.7	1592	11.1	6.1
80										1642	72.1	13.2												
80	1627	100.3	24.1	1617	83.7	-53.0	1613	21.8	-43.1				1633	85.1	-48.7	1628	28.8	-48.0	1579	15.5	3.7	1580	-2.7	2.0
79	1608	8.9	17.6	1606	31.0	34.5	1605	76.7	34.0	1622	9.2	16.7	1619	22.6	30.4	1620	64.0	39.4	1572	9.3	3.6	1571	20.9	3.8
78	1529	7.2	-6.0	1528	8.3	6.9	1525	174.1	1.9	1523	168.7	-5.7	1523	177.4	5.7	1524	182.3	3.7	1489	99.6	3.6			
77	1524	161.4	5.0	1525	169.9	-2.9	1522	9.9	1.4	1520	7.0	6.4	1519	7.8	-1.6	1512	8.9	0.7	1483	14.4	2.9			
76	1505	8.8	-4.5	1504	7.5	2.6	1505	15.4	0.8	1497	9.0	-4.7	1496	6.9	2.9	1497	14.9	0.5	1456	6.1	2.8			
75	1491	24.0	-12.1	1490	24.1	-12.5	1489	24.2	-2.2	1481	5.4	1.1	1481	13.7	-7.0	1481	24.1	-0.8						
																			1444	13.2	3.6			
74	1489	19.3	1.4	1489	19.8	2.6	1489	32.0	-1.5	1481	25.0	-9.4	1480	20.5	-1.7	1479	23.4	-3.1						
73	1471	37.0	-21.9	1473	36.2	-20.9	1474	31.8	-15.7	1460	38.2	-22.5	1461	37.4	-21.1	1463	33.2	-16.0				1434	-8.3	2.6
																			1425	271.7	8.0			
72	1432	88.2	80.7	1431	7.8	14.0	1432	72.9	81.0	1454	268.1	87.9										1424	43.5	4.4
72													1443	255.6	36.1							1419	18.3	4.6
																			1415	27.3	4.1			
72																1437	266.4	198.0				1408	19.3	5.9
71	1428	38.5	-15.8	1429	26.0	5.7	1432	34.5	-37.1	1429	50.0	-37.7	1430	22.2	-32.0	1430	94.3	-125.4	1396	70.9	3.4	1396	-67.0	3.4
70	1426	110.5	-80.7	1427	94.6	2.4	1428	7.6	2.5	1418	59.1	69.7	1422	71.4	-8.7	1424	27.6	-16.5						
																			1389	34.5	3.0	1390	63.6	3.6
69	1421	135.9	114.1	1415	222.9	-21.4	1409	2.6	4.7	1416	13.2	-9.7	1417	6.2	6.1	1419	3.2	-2.3						
68	1401	13.8	18.2	1407	1.8	-2.0	1407	272.1	-2.0	1390	7.6	15.0	1395	0.6	-4.6	1396	1.1	-2.0	1362	2.2	3.6	1364	9.1	4.3
67	1351	212.9	68.2	1343	192.9	63.4	1343	136.0	81.3	1365	217.0	52.8							1337	150.8	3.6	1337	63.2	3.7

67													1358	207.0	64.1	1357	178.1	61.6	1331	44.0	4.4	1330	21.6	4.7
66	1338	2.5	-7.1	1340	11.1	-11.6	1338	65.8	-48.9	1337	9.3	-12.2	1339	7.9	3.2	1344	47.7	-29.2	1303	1.2	1.9	1301	-1.5	1.0
65	1311	7.9	-7.7	1313	4.0	1.0	1317	17.2	-3.7	1327	1.7	4.4	1328	1.1	-3.6	1327	3.9	-1.0						
64	1299	5.6	-21.1	1311	1.3	9.5	1313	10.0	10.3				1307	0.6	5.5	1307	11.3	15.7						
64										1294	6.3	-22.1							1275	5.2	2.9	1274	-22.1	4.5
63	1258	131.2	21.4	1256	128.4	33.8	1257	131.6	44.5	1261	127.2	22.7	1259	123.5	36.9	1261	122.8	50.5	1242	107.3	4.0	1242	20.4	3.3
62	1226	121.5	-30.2	1224	108.4	-27.0	1224	91.1	-42.2	1242	149.5	-44.5							1223	69.1	4.3	1222	-34.9	6.4
62													1238	175.3	-48.9	1238	151.6	-77.0	1216	23.6	3.2			
61	1213	54.7	-1.9	1213	102.7	-20.2	1212	98.9	-24.3	1206	35.5	-0.4	1207	51.1	-11.2	1206	60.2	-14.4	1184	18.8	2.7	1183	-3.1	2.8
60	1181	13.5	6.0	1178	14.7	-0.2	1180	13.2	-20.5	1182	37.4	9.8	1179	23.2	25.5	1180	36.6	41.9	1164	13.3	3.3	1164	16.0	4.0
59	1169	36.2	11.8	1167	24.0	14.6	1167	33.1	16.7	1176	26.7	26.6	1173	15.9	0.1	1174	29.1	-28.1	1158	15.5	3.5	1158	15.1	4.2
58	1143	42.1	-4.3	1146	4.5	1.1	1146	22.0	4.2	1148	261.4	27.3	1145	17.9	9.6	1146	326.1	60.6						
																			1121	134.0	4.1	1120	32.4	4.4
57																1145	54.9	-3.4						
57	1141	135.0	32.2	1135	39.7	9.7	1141	87.5	3.9	1138	21.4	7.6	1135	34.9	11.3									
																			1114	54.5	4.3	1113	11.4	4.8
56																1129	434.8	50.2						
56	1110	185.6	6.3	1105	223.8	8.8	1111	585.6	120.3	1119	208.7	-18.0	1113	255.4	-30.7				1095	124.8	5.2	1091	-16.0	3.2
55	1092	179.1	-1.8	1091	105.9	5.7	1094	526.8	79.7	1102	219.0	0.5	1100	119.7	0.8	1104	340.7	110.7	1075	157.0	4.2			
54	1076	592.9	250.4	1070	16.6	34.0	1091	40.3	13.9	1096	432.9	160.5				1101	39.5	-11.8	1065	223.2	4.0	1064	155.6	4.3
54													1081	529.8	432.4				1059	97.3	4.4	1057	74.7	3.4
53	1070	83.4	-81.0	1062	147.1	228.5	1070	27.5	-0.3	1072	112.7	-128.9	1071	259.8	-286.6	1072	91.9	-98.0	1048	153.0	4.2	1047	-174.3	3.5
52	1061	104.8	-139.4	1055	660.8	-173.1	1063	90.8	-102.5	1059	16.2	12.8	1060	17.5	-14.3	1059	7.6	-1.7	1041	79.9	5.0	1042	-45.3	4.6
51	1034	212.3	-15.5	1034	255.4	29.3	1034	264.2	-5.4	1039	41.3	-18.6	1038	27.1	19.7	1041	80.9	13.7						
																			1012	156.6	2.4	1013	-29.2	3.8
50	1025	29.4	11.8	1022	50.6	-24.5	1026	23.9	-1.6	1031	182.8	-15.4	1031	176.4	-59.2	1032	171.6	-42.0						
49	1011	58.4	11.9	1008	64.7	2.6	1007	45.0	22.9	1017	34.4	32.7	1015	49.2	21.7	1013	36.6	39.4	999	35.5	2.8	999	44.2	4.0
48	1002	1.2	0.4	1002	2.6	-1.1	997	2.9	-0.3	999	1.9	0.1	999	3.4	-1.1	995	4.4	-0.8						
47	986	16.5	-3.0	987	17.3	-5.1	982	8.9	-3.3	984	28.0	-7.2	985	36.6	-14.2	980	25.4	-16.1						
46	944	131.6	3.7	950	97.5	-36.9	946	62.6	-20.6	963	182.4	-32.2	968	84.4	-39.4	966	79.4	-40.2						
45	909	247.0	-68.8	912	166.8	37.7	906	324.3	-99.9	923	125.2	-35.5	923	139.6	38.1	920	254.0	-58.6						

44																898	5.7	5.7
44	871	118.1	20.5	873	82.3	-31.8	889	2.5	0.8	881	164.5	28.9	887	136.1	-43.0			
43	868	239.2	17.4	868	129.9	-35.8	868	0.3	2.2	879	202.9	27.4	878	30.7	-10.5	876	12.8	3.6
42	848	11.2	-6.4	847	7.5	-3.2	841	6.5	-2.3	847	10.9	0.8	846	18.6	-6.8	840	30.4	-2.5
41	827	182.8	-3.1	824	116.5	-46.6	835	6.3	2.3	833	182.5	2.2	834	51.5	-9.3	834	126.8	-15.8
40	823	10.6	5.6	823	15.7	17.7	824	216.8	-24.8	822	62.6	53.4	825	215.6	44.9	826	36.4	3.2
39	812	88.2	85.6	819	134.3	56.2	803	258.6	122.2	817	13.2	3.7	817	5.4	3.4	812	245.1	100.5
38	787	60.8	-62.1	789	81.2	-57.5	790	61.7	-52.6	787	43.7	-67.0	788	60.9	-54.0	789	68.7	-50.6

[a] Frequencies ν in cm^{-1}; dipole strengths *D* in 10^{-40} esu^2 cm^2; rotational strengths *R* in 10^{-44} esu^2 cm^2. Experimental rotational strengths are for (+)-**2**; calculated rotational strengths are for (*S*)-**2**.

[b] From Lorentzian fitting to the IR and the VCD spectra.

Table S3: Calculated B3LYP/aug-cc-pVDZ//B3LYP/6-31G* excitation energies, oscillator strengths and rotational strengths for (*S*)-**2**.

		Excitation Energy					
	#	eV	ν^a	λ^b	f^c	$R_{velocity}{}^d$	$R_{length}{}^d$
	1	4.21	33980	294.3	0.0732	81.55	81.35
	2	4.55	36724	272.3	0.0182	7.14	7.36
	3	4.69	37789	264.6	0.0185	11.04	12.08
	4	4.92	39709	251.8	0.0197	-3.57	-3.55
	5	5.05	40708	245.7	0.0390	4.57	4.60
	6	5.17	41674	240.0	0.0636	-0.65	0.45
2a	7	5.30	42728	234.0	0.1953	17.34	17.43
	8	5.32	42909	233.1	0.0584	2.92	3.10
	9	5.37	43333	230.8	0.0144	9.51	9.61
	10	5.45	43966	227.5	0.0059	2.95	2.90
	11	5.51	44448	225.0	0.0067	1.17	1.20
	12	5.64	45452	220.0	0.0182	-3.44	-3.92
	13	5.69	45928	217.7	0.0290	6.73	7.27
	14	5.72	46096	216.9	0.0046	-1.99	-1.96
	15	5.77	46546	214.8	0.0081	16.73	16.19
	1	4.15	33492	298.6	0.0595	67.57	67.69
	2	4.58	36919	270.9	0.0309	-16.31	-15.91
	3	4.71	38010	263.1	0.0337	4.43	5.30
	4	4.89	39403	253.8	0.1338	-31.68	-32.09
	5	4.97	40096	249.4	0.0026	2.67	2.68
	6	5.11	41213	242.6	0.0745	36.69	37.18
2b	7	5.24	42237	236.8	0.0061	-9.82	-9.35
	8	5.32	42941	232.9	0.2140	-18.07	-18.28
	9	5.39	43469	230.1	0.0017	0.06	0.01
	10	5.41	43611	229.3	0.0104	-4.47	-4.14
	11	5.51	44427	225.1	0.0177	-11.99	-12.38
	12	5.56	44881	222.8	0.0213	13.04	13.13
	13	5.59	45124	221.6	0.0146	-24.06	-23.56
	14	5.66	45662	219.0	0.0089	-12.02	-12.23
	15	5.77	46572	214.7	0.0069	-12.09	-12.18

	1	4.24	34183	292.5	0.0537	100.27	100.29
	2	4.47	36069	277.3	0.0314	-35.58	-35.57
	3	4.79	38673	258.6	0.0097	10.86	11.16
	4	4.87	39256	254.7	0.0619	-30.94	-30.95
	5	5.01	40407	247.5	0.0775	-18.71	-17.98
	6	5.05	40722	245.6	0.0001	1.01	0.77
2c	7	5.07	40932	244.3	0.0266	21.07	21.05
	8	5.19	41876	238.8	0.2864	-31.47	-31.97
	9	5.32	42878	233.2	0.0089	13.37	13.30
	10	5.39	43491	229.9	0.0364	-19.22	-19.15
	11	5.45	43995	227.3	0.0070	9.09	9.14
	12	5.52	44482	224.8	0.0051	-0.40	-0.36
	13	5.64	45463	220.0	0.0023	-1.10	-1.00
	14	5.67	45714	218.8	0.0149	-5.38	-5.35
	15	5.68	45819	218.3	0.0121	11.24	10.82

[a] ν in cm^{-1}. [b] λ in nm. [c] Oscillator Strengths. [d] R values in 10^{-40} esu^2cm^2.

Table S4. Calculated B3PW91/aug-cc-pVDZ//B3LYP/6-31G* excitation energies, oscillator strengths and rotational strengths for (*S*)-**2**.

	#	Excitation Energy eV	ν^a	λ^b	f^c	$R_{velocity}{}^d$	$R_{length}{}^d$
	1	4.23	34122	293.1	0.0713	78.63	78.47
	2	4.56	36750	272.1	0.0188	7.57	7.76
	3	4.70	37920	263.7	0.0201	13.14	14.24
	4	4.96	40026	249.8	0.0161	-3.17	-3.17
	5	5.10	41098	243.3	0.0460	4.68	4.64
	6	5.26	42411	235.8	0.1391	9.61	11.30
2a	7	5.36	43253	231.2	0.2021	12.91	12.95
	8	5.47	44109	226.7	0.0082	1.39	1.71
	9	5.47	44142	226.5	0.0008	-0.46	-0.44
	10	5.54	44681	223.8	0.0077	-2.60	-2.69
	11	5.56	44869	222.9	0.0012	2.25	2.35
	12	5.68	45840	218.2	0.0142	-2.11	-2.40
	13	5.74	46290	216.0	0.0302	39.30	39.32
	14	5.79	46681	214.2	0.0009	1.71	1.56
	15	5.84	47110	212.3	0.0323	-17.24	-17.13
	1	4.17	33630	297.4	0.0569	64.26	63.94
	2	4.59	37059	269.8	0.0346	-14.17	-13.92
	3	4.72	38078	262.6	0.0367	2.69	3.43
	4	4.94	39815	251.2	0.1373	-31.21	-31.57
	5	5.00	40363	247.8	0.0027	2.57	2.52
	6	5.14	41483	241.1	0.0783	35.76	36.39
2b	7	5.37	43335	230.8	0.2181	-28.41	-28.52
	8	5.46	44072	226.9	0.0134	-1.65	-0.70
	9	5.49	44299	225.7	0.0005	0.23	0.22
	10	5.51	44415	225.2	0.0102	-10.76	-10.42
	11	5.52	44561	224.4	0.0179	-1.02	-1.31
	12	5.60	45161	221.4	0.0100	1.14	1.29
	13	5.65	45554	219.5	0.0152	-8.86	-8.95
	14	5.73	46247	216.2	0.0177	-25.19	-25.53
	15	5.87	47319	211.3	0.0047	-8.00	-8.83

	1	4.25	34291	291.6	0.0492	95.04	95.07
	2	4.48	36149	276.6	0.0367	-33.17	-32.87
	3	4.81	38791	257.8	0.0186	9.81	10.18
	4	4.91	39609	252.5	0.0515	-28.66	-28.73
	5	5.07	40875	244.7	0.1164	9.38	9.65
	6	5.08	40977	244.0	0.0003	0.75	0.52
2c	7	5.23	42198	237.0	0.2496	-80.24	-80.86
	8	5.27	42488	235.4	0.0524	39.73	40.77
	9	5.42	43704	228.8	0.0055	6.94	6.81
	10	5.51	44433	225.1	0.0104	7.64	7.74
	11	5.51	44466	224.9	0.0260	-8.04	-8.21
	12	5.62	45319	220.7	0.0035	1.47	1.44
	13	5.68	45806	218.3	0.0075	-16.86	-16.46
	14	5.74	46328	215.9	0.0177	18.71	18.33
	15	5.84	47094	212.3	0.0155	4.69	4.68

[a] ν in cm^{-1}. [b] λ in nm. [c] Oscillator Strengths. [d] R values in 10^{-40} esu^2cm^2.

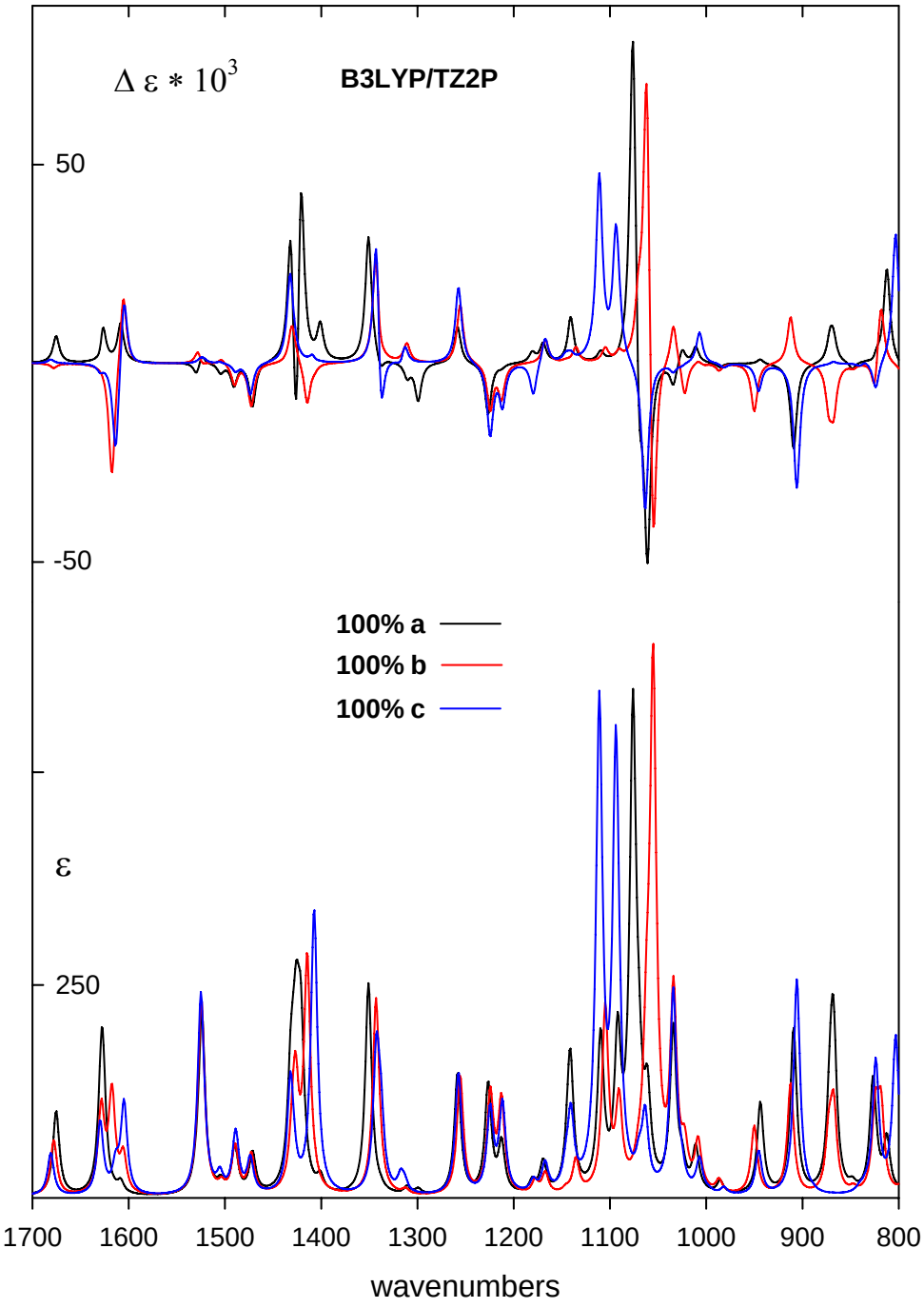

Figure S1: B3LYP/TZ2P IR and VCD spectra of conformations **a**-**c** of (*S*)-**2**. Lorentzian bandwidths γ = 4.0 cm^{-1}.

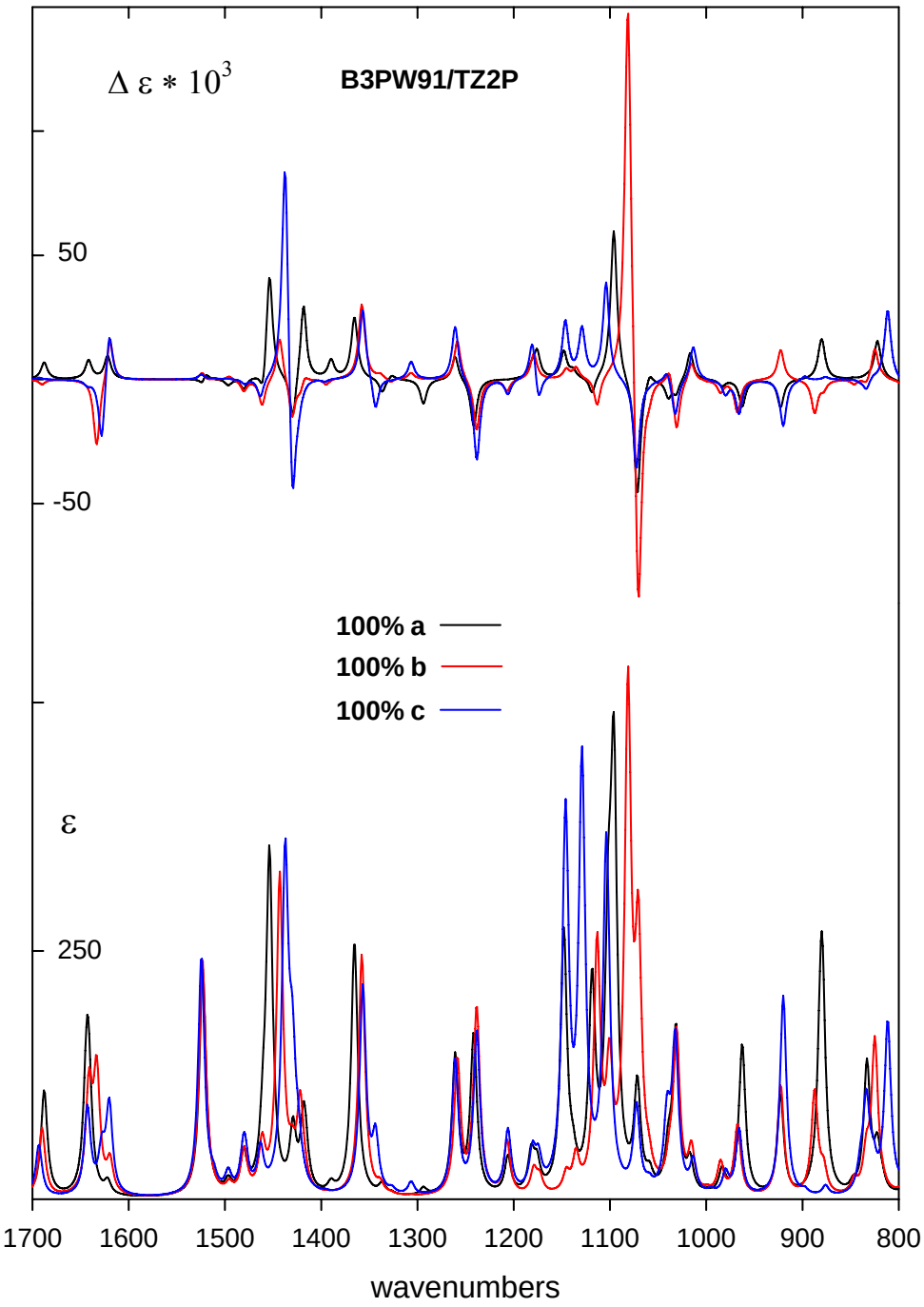

Figure S2: B3PW91/TZ2P IR and VCD spectra of conformations **a**-**c** of (*S*)-**2**. Lorentzian bandwidths $\gamma = 4.0\ cm^{-1}$.

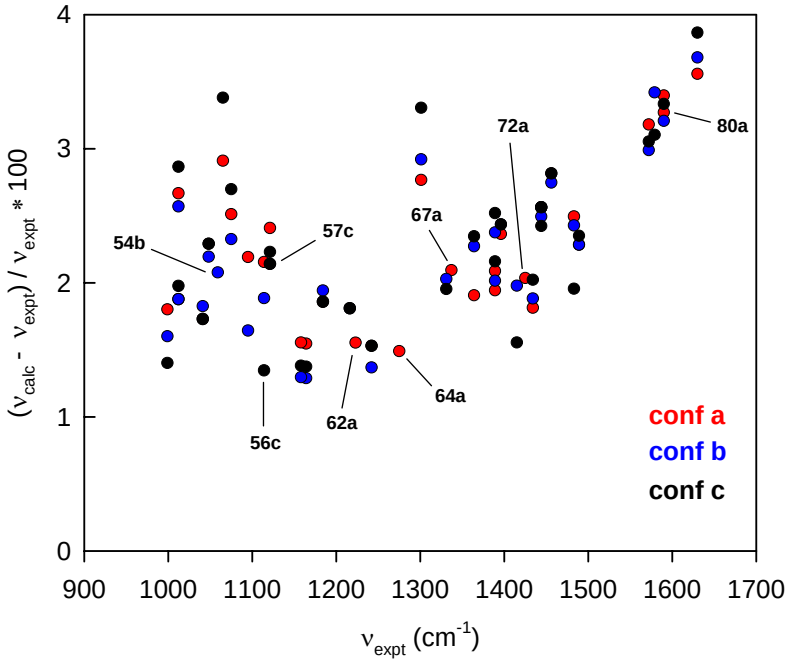

Figure S3: Comparison of calculated and experimental vibrational frequencies of (*S*)-**2**.

Oxadiazol-3-one **2** conformer **a** (*S*)-configuration
B3PW91/TZ2P optimized geometry [E=-3848.20162950 hartrees]
Cartesian coordinates (Angstroms)

O	-2.17307500	-2.60771800	-1.12879000
S	-1.48904600	0.90241200	1.84078600
N	-2.98434300	-0.85363500	-0.10575500
C	-0.88259700	0.51854400	0.11515200
C	-3.21368400	0.82505400	1.53375400
C	-3.79909500	0.01410600	0.64699400
C	-1.62850800	-0.71836000	-0.28944700
O	-1.27708000	1.48497600	-0.81714400
H	-3.81323700	1.51534400	2.10932300
C	-5.26619700	0.00215300	0.37395600
N	-1.10539600	-1.72334300	-0.89454900
C	-3.33714200	-2.09154000	-0.64502200
H	-5.69632500	-0.98102200	0.55874300
H	-5.46958500	0.24929100	-0.66985400
H	-5.75745600	0.73640200	1.00880300
O	-4.39996500	-2.63759200	-0.69287900
C	0.62037500	0.28286000	0.14542700
C	3.35516900	-0.18617900	0.07765000
C	1.28381100	-0.19413600	1.27096000
C	1.34851000	0.50484800	-1.02045800
C	2.71441200	0.27511100	-1.06063300
C	2.65123000	-0.42741800	1.24467700
H	0.73685700	-0.40023400	2.18163600
H	0.83918800	0.85028500	-1.90936800
H	3.27129300	0.44745900	-1.97084100
H	3.15844100	-0.79616500	2.12495800
Br	5.23162200	-0.49853900	0.03371400
C	-0.88393400	2.83933300	-0.56465100
C	-1.26729800	3.65787300	-1.77386700
H	0.19259200	2.88675400	-0.38051700
H	-1.39408900	3.19612200	0.33288700
H	-0.74531800	3.31225300	-2.66621400
H	-1.00580300	4.70367400	-1.60787000
H	-2.33977500	3.59814900	-1.95857800

Oxadiazol-3-one **2** conformer **b** (*S*)-configuration
B3PW91/TZ2P optimized geometry [E=-3848.20012117 hartrees]
Cartesian coordinates (Angstroms)

O	-2.54846300	-2.03138600	-1.67512000
S	-1.18416100	0.41145000	2.07158700
N	-3.04217000	-0.66731000	-0.03635700
C	-0.82289000	0.48166400	0.26238700
C	-2.93343600	0.47651800	2.02459100
C	-3.68747000	-0.02788200	1.04419300
C	-1.71257800	-0.54890800	-0.37332900
O	-1.19842900	1.76574300	-0.17411000
H	-3.39960000	0.99224700	2.85168900
C	-5.17548900	0.08612600	1.00018900
N	-1.38020800	-1.32318900	-1.34591300

C	-3.58197000	-1.64271900	-0.87668200
H	-5.65250300	-0.89251500	0.98559700
H	-5.50339600	0.61463300	0.10305300
H	-5.51586500	0.63920400	1.87299600
O	-4.68955800	-2.08937100	-0.93040500
C	0.66734500	0.21318800	0.14094500
C	3.41293800	-0.18083400	0.06942700
C	1.53683900	1.29842100	0.08659900
C	1.19729500	-1.07402300	0.18185900
C	2.56800300	-1.27621000	0.14262200
C	2.91011800	1.10874400	0.04505700
H	1.13584500	2.30246600	0.08626900
H	0.54345700	-1.93223100	0.23802000
H	2.97127100	-2.27851600	0.16779500
H	3.57840600	1.95692100	-0.00082500
Br	5.29541400	-0.45313500	0.00805900
C	-1.17841200	1.98504100	-1.59474100
C	-1.43817500	3.45352600	-1.82910200
H	-1.94861900	1.37480700	-2.07429900
H	-0.21202200	1.68226600	-2.00626900
H	-2.39732700	3.74972200	-1.40477000
H	-1.45804400	3.65766600	-2.90032000
H	-0.65897700	4.06755700	-1.37750400

Oxadiazol-3-one **2** conformer **c** (*S*)-configuration
B3PW91/TZ2P optimized geometry [E=-3848.19859162 hartrees]
Cartesian coordinates (Angstroms)

O	-2.14742300	-2.14058800	-1.73535700
S	-1.23485700	0.78528400	1.90800800
N	-2.83802500	-0.89017100	-0.07804700
C	-0.78948200	0.65243300	0.09758400
C	-2.93821000	0.38461100	1.90724200
C	-3.57375700	-0.37098600	1.00740900
C	-1.57253300	-0.50881400	-0.47174500
O	-1.01588100	1.82956700	-0.61148700
H	-3.49252500	0.80391900	2.73531400
C	-5.03786700	-0.66241700	1.07009400
N	-1.12903300	-1.22075000	-1.44699500
C	-3.20494200	-1.96022700	-0.89930800
H	-5.23214700	-1.72919500	1.16844300
H	-5.55050700	-0.33011000	0.16591400
H	-5.46439000	-0.14116900	1.92472000
O	-4.20544100	-2.61525300	-0.91151400
C	0.70918200	0.38144600	0.06744600
C	3.43874200	-0.10313600	0.04671800
C	1.57807700	1.28358100	-0.53247300
C	1.22813300	-0.76796100	0.65850300
C	2.58923900	-1.01805500	0.64996700
C	2.94631900	1.04547300	-0.54474400
H	1.18735100	2.17555600	-0.99740200
H	0.56696700	-1.48101600	1.13332900
H	2.98350800	-1.91470300	1.10648200
H	3.61720000	1.75101100	-1.01413400
Br	5.31287600	-0.43631500	0.03441000
C	-2.34023900	2.35352100	-0.69137000

C	-2.28853800	3.59527200	-1.54904600
H	-2.69639300	2.58794800	0.31454000
H	-3.01223300	1.61111100	-1.13285000
H	-1.62626800	4.34117200	-1.10989300
H	-3.28609500	4.02865100	-1.63024600
H	-1.93279600	3.36148200	-2.55219500