

Supplementary Material

4. Vibration analysis and vibrational spectra

4.1. PED based vibrational assignment



Fig. S1. The atomic number of DBDS-2 in VEDA4

Table. S1. Internal coordinates and related atoms in DBDS-2

Stretching	Related atoms	Bending	Related atoms
ν_1	C(1)-H(7)	δ_{30}	C(21)-C(23)-C(27)
ν_2	C(2)-H(8)	δ_{31}	C(3)-C(12)-S(15)
ν_3	C(4)-H(9)	δ_{32}	H(7)-C(1)-C(2)
ν_4	C(5)-H(10)	δ_{33}	H(8)-C(2)-C(1)
ν_5	C(6)-H(11)	δ_{34}	H(9)-C(4)-C(5)
ν_6	C(12)-H(13)	δ_{35}	H(10)-C(5)-C(6)
ν_7	C(12)-H(14)	δ_{36}	H(11)-C(6)-C(1)
ν_8	C(17)-H(18)	δ_{37}	H(13)-C(12)-S(15)
ν_9	C(17)-H(19)	δ_{38}	H(14)-C(12)-H(13)
ν_{10}	C(21)-H(24)	δ_{39}	H(18)-C(17)-S(16)
ν_{11}	C(22)-H(26)	δ_{40}	H(19)-C(17)-H(18)
ν_{12}	C(23)-H(28)	δ_{41}	H(24)-C(21)-C(23)
ν_{13}	C(25)-H(29)	δ_{42}	H(26)-C(22)-C(25)
ν_{14}	C(27)-H(30)	δ_{43}	H(28)-C(23)-C(27)
ν_{15}	C(2)-C(1)	δ_{44}	H(29)-C(25)-C(27)
ν_{16}	C(21)-C(23)	δ_{45}	H(30)-C(27)-C(25)
ν_{17}	C(1)-C(6)	δ_{46}	C(2)-C(1)-C(6)
ν_{18}	C(6)-C(5)	δ_{47}	C(1)-C(6)-C(5)
ν_{19}	C(22)-C(25)	δ_{48}	C(6)-C(5)-C(4)
ν_{20}	C(4)-C(3)	δ_{49}	C(22)-C(25)-C(27)
ν_{21}	C(5)-C(4)	δ_{50}	C(4)-C(3)-C(12)

v22	C(23)-C(27)	δ51	C(5)-C(4)-C(3)
v23	C(27)-C(25)	δ52	C(23)-C(27)-C(25)
v24	C(20)-C(22)	δ53	C(20)-C(22)-C(25)
v25	C(3)-C(12)	δ54	C(17)-C(20)-C(22)
v26	C(17)-C(20)	δ55	C(12)-S(15)-S(16)
v27	S(15)-C(12)	δ56	S(16)-C(17)-C(20)
v28	S(16)-C(17)	δ57	S(15)-S(16)-C(17)
v29	S(15)-S(16)		
Torsion		Related atoms	
	τ58	H(7)-C(1)-C(2)-C(3)	
	τ59	H(8)-C(2)-C(1)-C(6)	
	τ60	H(9)-C(4)-C(5)-C(6)	
	τ61	H(10)-C(5)-C(6)-C(1)	
	τ62	H(11)-C(6)-C(1)-C(2)	
	τ63	H(13)-C(12)-S(15)-S(16)	
	τ64	H(14)-C(12)-S(15)-S(16)	
	τ65	H(18)-C(17)-S(16)-S(15)	
	τ66	H(19)-C(17)-S(16)-S(15)	
	τ67	H(24)-C(21)-C(23)-C(27)	
	τ68	H(26)-C(22)-C(25)-C(27)	
	τ69	H(28)-C(23)-C(27)-C(25)	
	τ70	H(29)-C(25)-C(27)-C(23)	
	τ71	H(30)-C(27)-C(25)-C(22)	
	τ72	C(2)-C(1)-C(6)-C(5)	
	τ73	C(21)-C(23)-C(27)-C(25)	
	τ74	C(1)-C(6)-C(5)-C(4)	
	τ75	C(6)-C(5)-C(4)-C(3)	
	τ76	C(4)-C(3)-C(12)-S(15)	
	τ77	C(5)-C(4)-C(3)-C(12)	
	τ78	C(23)-C(27)-C(25)-C(22)	
	τ79	C(20)-C(22)-C(25)-C(27)	
	τ80	C(3)-C(12)-S(15)-S(16)	
	τ81	C(12)-S(15)-S(16)-C(17)	
	τ82	S(16)-C(17)-C(20)-C(21)	
	τ83	S(15)-S(16)-C(17)-C(20)	
	γ84	C(17)-C(21)-C(22)-C(20)	

Table. S2. Assignment of normal mode of DBDS-2.

Mode	Frequency	Vibration assignment (>10%)
#1	3077.9556	% 20v(1)+% 17v(3)+% 22v(4)+% 35v(5)
#2	3076.77952	% 18v(11)+% 21v(12)+% 23v(13)+% 31v(14)
#3	3070.44604	% 25v(1)+% 50v(3)
#4	3069.69412	% 48v(11)+% 26v(12)
#5	3062.7244	% 24v(1)+% 19v(2)+% 17v(3)+% 11v(4)+% 28v(5)

#6	3061.84716	%22v(10)+%18v(11)+%18v(12)+%13v(13)+%28v(14)
#7	3052.77592	%30v(2)+%12v(3)+%44v(4)+%13v(5)
#8	3052.44816	%38v(10)+%10v(11)+%36v(13)
#9	3047.48356	%27v(1)+%42v(2)+%12v(4)+%15v(5)
#10	3046.74128	%29v(10)+%28v(12)+%18v(13)+%23v(14)
#11	3041.44892	%78v(8)+%21v(9)
#12	3007.36188	%23v(6)+%76v(7)
#13	2971.53964	%21v(8)+%79v(9)
#14	2947.3818	%76v(6)+%23v(7)
#15	1589.85772	%29v(16)
#16	1588.58524	%29v(15)+%11v(18)
#17	1570.115	%28v(23)+%21v(24)+%10δ(30)
#18	1569.27632	%27v(18)+%23v(20)
#19	1474.89108	%14δ(41)+%14δ(42)+%16δ(43)+%15δ(44)
#20	1474.5344	%18δ(32)+%14δ(33)+%14δ(34)+%15δ(35)
#21	1437.16012	%28δ(40)+%10δ(45)
#22	1434.42236	%15δ(36)
#23	1431.04836	%39δ(40)+%11τ(66)
#24	1417.31136	%56δ(38)+%12τ(63)+%16τ(64)
#25	1311.91724	%24δ(41)+%26δ(42)+%10δ(43)+%10δ(45)
#26	1311.46416	%10δ(32)+%24δ(33)+%25δ(34)
#27	1295.7124	%18v(15)+%17v(17)+%23v(20)+%16v(21)
#28	1294.88336	%17v(16)+%17v(19)+%18v(22)+%23v(24)
#29	1226.55504	%10v(26)+%25δ(40)+%20τ(65)+%28τ(66)
#30	1220.2312	%10v(25)+%29δ(38)+%14τ(63)+%20τ(64)
#31	1189.11328	%32v(25)
#32	1187.12744	%33v(26)
#33	1161.48504	%17δ(32)+%21δ(33)+%20δ(34)+%18δ(35)
#34	1160.897	%21δ(41)+%21δ(42)+%16δ(43)+%17δ(44)
#35	1141.12536	%16δ(36)+%11δ(43)+%10δ(44)+%22δ(45)
#36	1140.894	%10δ(32)+%11δ(35)+%22δ(36)+%17δ(45)
#37	1122.0478	%46δ(37)+%12τ(63)+%17τ(64)
#38	1111.84868	%39δ(39)+%10τ(65)+%27τ(66)
#39	1060.81452	%13v(15)+%15v(21)+%12δ(36)+%12δ(37)
#40	1057.86468	%12v(16)+%13v(19)+%17δ(39)+%11δ(45)
#41	1015.41976	%22v(22)+%20v(23)+%13δ(30)+%11δ(43)+%11δ(44)
#42	1014.61	%24v(17)+%21v(18)+%11δ(35)+%15δ(46)
#43	985.91172	%20δ(46)+%15δ(47)+%10δ(48)
#44	985.48756	%20δ(30)+%10δ(49)+%15δ(52)
#45	967.7596	%14τ(58)+%17τ(61)+%23τ(62)+%12τ(72)
#46	966.70884	%16τ(69)+%14τ(70)+%25τ(71)
#47	947.3228	%23τ(58)+%19τ(59)+%14τ(60)+%22τ(61)
#48	944.54648	%18τ(67)+%20τ(68)+%27τ(69)+%26τ(70)
#49	899.52768	%24τ(67)+%25τ(68)+%30τ(71)

#50	894.70768	%24 τ (59)+%27 τ (60)+%28 τ (62)
#51	878.13652	%28 δ (39)+%38 τ (65)
#52	863.33912	%20 δ (37)+%30 τ (63)+%11 τ (64)
#53	826.7264	%14 τ (70)+%13 τ (69)+%12 τ (60)+%12 τ (59)+%15 τ (67)+%13 τ (68)
#54	824.20072	%13 τ (58)+%14 τ (59)+%15 τ (60)+%12 τ (61)+%12 τ (67)+%11 τ (68)
#55	797.48828	%21 ν (26)+%33 δ (52)
#56	795.41568	%21 ν (25)+%35 δ (47)+%11 δ (48)
#57	759.52596	%10 ν (28)+%10 τ (69)+%11 τ (70)+%11 τ (71)+%17 τ (79)+%14 γ (84)
#58	750.715	%18 τ (58)+%15 τ (61)+%14 τ (62)+%22 τ (75)
#59	687.36092	%12 τ (67)+%11 τ (68)+%18 τ (71)+%14 τ (73)+%11 τ (78)+%27 τ (79)
#60	685.7414	%13 τ (59)+%13 τ (60)+%19 τ (62)+%13 τ (72)+%12 τ (74)+%25 τ (75)
#61	665.2082	%44 ν (28)+%20 τ (79)
#62	631.59352	%57 ν (27)
#63	615.42724	%23 δ (30)+%34 δ (49)+%20 δ (53)
#64	614.07764	%23 δ (46)+%32 δ (48)+%19 δ (51)
#65	555.37968	%12 δ (31)+%15 δ (51)
#66	551.78396	%15 δ (53)
#67	472.63956	%13 ν (28)+%25 ν (29)+%16 γ (84)
#68	466.66276	%13 ν (27)+%10 τ (72)+%25 τ (74)
#69	457.28304	%69 ν (29)

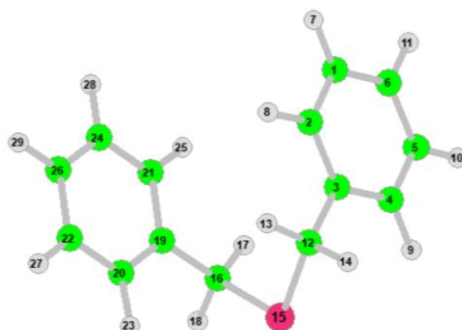


Fig. S2. The atomic number of DBS in VEDA4

Table. S3. Internal coordinates and related atoms in DBS

Stretching	Related atoms	Bending	Related atoms
ν 1	C(1)-H(7)	δ 29	δ 29
ν 2	C(2)-H(8)	δ 30	δ 30
ν 3	C(4)-H(9)	δ 31	δ 31
ν 4	C(5)-H(10)	δ 32	δ 32
ν 5	C(6)-H(11)	δ 33	δ 33
ν 6	C(12)-H(13)	δ 34	δ 34
ν 7	C(12)-H(14)	δ 35	δ 35
ν 8	C(16)-H(17)	δ 36	δ 36
ν 9	C(16)-H(18)	δ 37	δ 37

v10	C(20)-H(23)	δ38	δ38
v11	C(21)-H(25)	δ39	δ39
v12	C(22)-H(27)	δ40	δ40
v13	C(24)-H(28)	δ41	δ41
v14	C(26)-H(29)	δ42	δ42
v15	C(1)-C(6)	δ43	δ43
v16	C(2)-C(1)	δ44	δ44
v17	C(4)-C(5)	δ45	δ45
v18	C(20)-C(22)	δ46	δ46
v19	C(26)-C(24)	δ47	δ47
v20	C(3)-C(2)	δ48	δ48
v21	C(6)-C(5)	δ49	δ49
v22	C(21)-C(19)	δ50	δ50
v23	C(22)-C(26)	δ51	δ51
v24	C(24)-C(21)	δ52	δ52
v25	C(12)-C(3)	δ53	δ53
v26	C(19)-C(16)	δ54	δ54
v27	S(15)-C(12)	δ55	δ55
v28	S(15)-C(16)		

Torsion	Related atoms
τ56	H(7)-C(1)-C(2)-C(3)
τ57	H(8)-C(2)-C(1)-C(6)
τ58	H(9)-C(4)-C(5)-C(6)
τ59	H(10)-C(5)-C(6)-C(1)
τ60	H(11)-C(6)-C(1)-C(2)
τ61	H(13)-C(12)-S(15)-C(16)
τ62	H(14)-C(12)-S(15)-C(16)
τ63	H(17)-C(16)-S(15)-C(12)
τ64	H(18)-C(16)-S(15)-C(12)
τ65	H(23)-C(20)-C(22)-C(26)
τ66	H(25)-C(21)-C(24)-C(26)
τ67	H(27)-C(22)-C(26)-C(24)
τ68	H(28)-C(24)-C(26)-C(22)
τ69	H(29)-C(26)-C(24)-C(21)
τ70	C(2)-C(1)-C(6)-C(5)
τ71	C(4)-C(5)-C(6)-C(1)
τ72	C(20)-C(22)-C(26)-C(24)
τ73	C(26)-C(24)-C(21)-C(19)
τ74	C(3)-C(2)-C(1)-C(6)
τ75	C(21)-C(19)-C(16)-S(15)
τ76	C(22)-C(26)-C(24)-C(21)
τ77	C(24)-C(21)-C(19)-C(16)
τ78	C(19)-C(16)-S(15)-C(12)
τ79	S(15)-C(12)-C(3)-C(4)

τ_{80}

C(16)-S(15)-C(12)-C(3)

 γ_{81}

C(12)-C(4)-C(2)-C(3)

Table. S4. Assignment of normal mode of DBS.

Mode	Frequency	Vibration assignment (>10%)
#1	3075.748	% 10 ν (1)+% 10 ν (4)+% 16 ν (5)+% 13 ν (12)+% 12 ν (13)+% 21 ν (14)
#2	3075.555	% 12 ν (1)+% 14 ν (4)+% 21 ν (5)+% 11 ν (12)+% 17 ν (14)
#3	3067.515	% 13 ν (12)+% 13 ν (2)+% 12 ν (13)+% 11 ν (3)+% 13 ν (10)+% 18 ν (11)
#4	3066.908	% 14 ν (1)+% 13 ν (2)+% 16 ν (3)+% 13 ν (4)+% 11 ν (10)+% 11 ν (11)
#5	3061.664	% 13 ν (2)+% 13 ν (3)+% 14 ν (5)+% 20 ν (10)+% 19 ν (11)+% 21 ν (14)
#6	3061.163	% 20 ν (2)+% 18 ν (3)+% 21 ν (5)+% 12 ν (10)+% 13 ν (11)+% 14 ν (14)
#7	3053.171	% 15 ν (13)+% 12 ν (3)+% 13 ν (4)+% 14 ν (10)+% 12 ν (1)+% 14 ν (12)
#8	3052.573	% 13 ν (12)+% 13 ν (2)+% 13 ν (3)+% 16 ν (4)+% 12 ν (10)+% 12 ν (1)
#9	3046.51	% 12 ν (1)+% 10 ν (4)+% 11 ν (5)+% 15 ν (12)+% 17 ν (13)+% 17 ν (14)
#10	3046.307	% 18 ν (1)+% 14 ν (4)+% 16 ν (5)+% 10 ν (12)+% 12 ν (13)+% 11 ν (14)
#11	2990.685	% 64 ν (8)+% 35 ν (9)
#12	2990.232	% 64 ν (6)+% 35 ν (7)
#13	2944.152	% 35 ν (8)+% 63 ν (9)
#14	2943.709	% 34 ν (6)+% 64 ν (7)
#15	1589.366	% 14 ν (17)+% 16 ν (18)
#16	1588.749	% 16 ν (17)+% 14 ν (18)
#17	1570.366	% 15 ν (15)+% 13 ν (19)+% 12 ν (20)+% 10 ν (22)
#18	1570.038	% 13 ν (15)+% 16 ν (19)+% 10 ν (20)+% 12 ν (22)
#19	1474.679	% 10 δ (41)+% 11 δ (42)
#20	1474.409	% 10 δ (31)+% 10 δ (32)+% 11 δ (34)
#21	1436.08	% 14 δ (44)
#22	1435.512	% 14 δ (35)
#23	1415.808	% 22 δ (37)+% 34 δ (39)
#24	1412.173	% 41 δ (37)+% 28 δ (39)
#25	1312.881	% 12 δ (32)+% 10 δ (33)+% 14 δ (40)+% 16 δ (41)
#26	1311.618	% 16 δ (32)+% 14 δ (33)+% 11 δ (40)+% 12 δ (41)
#27	1295.433	% 11 ν (20)+% 12 ν (22)
#28	1294.266	% 10 ν (17)+% 12 ν (20)+% 11 ν (22)
#29	1237.294	% 19 τ (62)+% 19 τ (64)
#30	1223.017	-
#31	1181.421	% 16 ν (25)+% 22 ν (26)
#32	1178.403	% 21 ν (25)+% 16 ν (26)
#33	1161.928	% 10 δ (33)+% 13 δ (40)+% 11 δ (41)+% 10 δ (43)
#34	1160.752	% 10 δ (31)+% 11 δ (32)+% 13 δ (33)+% 10 δ (40)
#35	1154.833	% 24 δ (36)+% 23 δ (38)+% 12 τ (62)+% 12 τ (64)
#36	1140.181	% 18 δ (35)+% 10 δ (43)+% 19 δ (44)
#37	1139.949	% 10 δ (31)+% 19 δ (35)+% 17 δ (44)
#38	1130.049	% 14 δ (36)+% 15 δ (38)+% 20 τ (62)+% 20 τ (64)
#39	1064.632	-

#40	1062.636	-
#41	1015.641	% 11 ν (15)+% 10 ν (19)+% 13 ν (21)+% 12 ν (23)
#42	1015.217	% 10 ν (15)+% 11 ν (19)+% 12 ν (21)+% 13 ν (23)
#43	985.5454	% 19 δ (47)+% 10 δ (48)+% 14 δ (51)
#44	985.4297	% 19 δ (29)+% 14 δ (45)
#45	966.1786	% 10 τ (56)+% 10 τ (59)+% 13 τ (60)+% 12 τ (67)+% 11 τ (68)+% 17 τ (69)
#46	965.6292	% 13 τ (56)+% 13 τ (59)+% 18 τ (60)+% 10 τ (67)+% 13 τ (69)
#47	947.612	% 12 τ (65)+% 14 τ (66)+% 16 τ (67)+% 16 τ (68)
#48	946.2142	% 14 τ (56)+% 12 τ (57)+% 12 τ (58)+% 15 τ (59)+% 10 τ (68)
#49	917.9883	-
#50	896.7803	% 13 τ (57)+% 12 τ (58)+% 15 τ (60)+% 13 τ (65)+% 14 τ (66)+% 16 τ (69)
#51	878.069	% 12 τ (60)+% 10 τ (69)
#52	828.7026	% 13 τ (67)+% 13 τ (68)+% 12 τ (58)+% 11 τ (59)+% 14 τ (65)+% 12 τ (66)
#53	826.3312	% 10 τ (56)+% 10 τ (58)+% 10 τ (65)
#54	822.7836	-
#55	793.4106	% 15 ν (26)+% 12 δ (45)+% 23 δ (51)
#56	793.1696	% 14 ν (25)+% 23 δ (45)+% 12 δ (51)
#57	748.6328	% 16 τ (73)
#58	741.7594	% 16 τ (73)
#59	691.082	% 10 ν (28)+% 13 τ (69)
#60	690.0312	% 11 τ (60)+% 11 τ (73)+% 18 τ (74)
#61	681.413	% 11 ν (27)+% 10 ν (28)+% 14 τ (73)+% 15 τ (74)
#62	657.3709	% 26 ν (27)+% 27 ν (28)
#63	613.4125	% 10 δ (29)+% 13 δ (46)+% 16 δ (47)+% 21 δ (48)+% 11 δ (52)
#64	613.0269	% 16 δ (29)+% 20 δ (46)+% 10 δ (47)+% 13 δ (48)+% 11 δ (49)
#65	561.8674	% 11 δ (49)+% 10 δ (52)
#66	551.3502	% 12 δ (49)+% 11 δ (52)
#67	462.6332	% 14 τ (76)+% 12 γ (81)
#68	458.9411	% 12 τ (76)+% 14 γ (81)

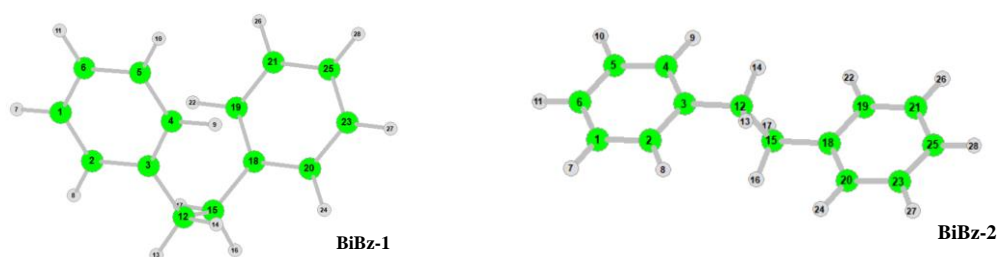


Fig. S3. The atomic number of BiBz-1 and BiBz-2 in VEDA4 (both are the same).

Table. S5. Internal coordinates and related atoms in BiBz-1 and BiBz-2 (both are the same).

Stretching	Related atoms	Bending	Related atoms
ν 1	C(1)-H(7)	δ 28	C(19)-C(21)-C(25)
ν 2	C(2)-H(8)	δ 29	C(3)-C(12)-C(15)
ν 3	C(4)-H(9)	δ 30	H(7)-C(1)-C(2)

v4	C(5)-H(10)	δ31	H(8)-C(2)-C(1)
v5	C(6)-H(11)	δ32	H(9)-C(4)-C(5)
v6	C(12)-H(13)	δ33	H(10)-C(5)-C(6)
v7	C(12)-H(14)	δ34	H(11)-C(6)-C(1)
v8	C(15)-H(16)	δ35	H(13)-C(12)-C(3)
v9	C(15)-H(17)	δ36	H(14)-C(12)-H(13)
v10	C(19)-H(22)	δ37	H(16)-C(15)-C(12)
v11	C(20)-H(24)	δ38	H(17)-C(15)-H(16)
v12	C(21)-H(26)	δ39	H(22)-C(19)-C(21)
v13	C(23)-H(27)	δ40	H(24)-C(20)-C(23)
v14	C(25)-H(28)	δ41	H(26)-C(21)-C(25)
v15	C(1)-C(6)	δ42	H(27)-C(23)-C(25)
v16	C(2)-C(1)	δ43	H(28)-C(25)-C(23)
v17	C(5)-C(4)	δ44	C(1)-C(6)-C(5)
v18	C(6)-C(5)	δ45	C(2)-C(1)-C(6)
v19	C(19)-C(21)	δ46	C(5)-C(4)-C(3)
v20	C(20)-C(23)	δ47	C(6)-C(5)-C(4)
v21	C(21)-C(25)	δ48	C(20)-C(23)-C(25)
v22	C(25)-C(23)	δ49	C(21)-C(25)-C(23)
v23	C(4)-C(3)	δ50	C(4)-C(3)-C(12)
v24	C(18)-C(20)	δ51	C(18)-C(20)-C(23)
v25	C(3)-C(12)	δ52	C(15)-C(18)-C(20)
v26	C(15)-C(18)	δ53	C(12)-C(15)-C(18)
v27	C(12)-C(15)		

Torsion	Related atoms
τ54	H(7)-C(1)-C(2)-C(3)
τ55	H(8)-C(2)-C(1)-C(6)
τ56	H(9)-C(4)-C(5)-C(6)
τ57	H(10)-C(5)-C(6)-C(1)
τ58	H(11)-C(6)-C(1)-C(2)
τ59	H(13)-C(12)-C(3)-C(4)
τ60	H(14)-C(12)-C(3)-C(4)
τ61	H(16)-C(15)-C(18)-C(19)
τ62	H(17)-C(15)-C(18)-C(19)
τ63	H(22)-C(19)-C(21)-C(25)
τ64	H(24)-C(20)-C(23)-C(25)
τ65	H(26)-C(21)-C(25)-C(23)
τ66	H(27)-C(23)-C(25)-C(21)
τ67	H(28)-C(25)-C(23)-C(20)
τ68	C(1)-C(6)-C(5)-C(4)
τ69	C(2)-C(1)-C(6)-C(5)
τ70	C(5)-C(4)-C(3)-C(12)
τ71	C(6)-C(5)-C(4)-C(3)
τ72	C(19)-C(21)-C(25)-C(23)

τ_{73}	C(21)-C(25)-C(23)-C(20)
τ_{74}	C(4)-C(3)-C(12)-C(15)
τ_{75}	C(18)-C(20)-C(23)-C(25)
τ_{76}	C(3)-C(12)-C(15)-C(18)
τ_{77}	C(12)-C(15)-C(18)-C(19)
γ_{78}	C(15)-C(19)-C(20)-C(18)

Table. S6. Assignment of normal mode of BiBz-1.

Mode	Frequency	Vibration assignment (>10%)
#1	3074.11888	%15v(4)+%20v(5)+%16v(12)+%20v(14)
#2	3074.04176	%16v(4)+%20v(5)+%15v(12)+%19v(14)
#3	3063.87156	%19v(1)+%19v(3)+%12v(4)+%14v(10)+%14v(13)
#4	3063.76552	%14v(1)+%14v(3)+%10v(4)+%19v(10)+%13v(12)+%19v(13)
#5	3055.81252	%14v(1)+%16v(3)+%12v(5)+%15v(10)+%13v(13)+%11v(14)
#6	3055.639	%13v(1)+%16v(3)+%11v(5)+%17v(10)+%14v(13)+%12v(14)
#7	3047.09796	%11v(3)+%18v(4)+%11v(5)+%13v(10)+%22v(12)+%13v(14)
#8	3047.04012	%13v(3)+%22v(4)+%13v(5)+%11v(10)+%18v(12)+%11v(14)
#9	3036.83136	%18v(1)+%71v(2)
#10	3036.83136	%71v(11)+%18v(13)
#11	2968.4452	%15v(6)+%35v(7)+%15v(8)+%35v(9)
#12	2955.74932	%29v(6)+%21v(7)+%29v(8)+%21v(9)
#13	2924.52536	%21v(6)+%29v(7)+%21v(8)+%29v(9)
#14	2919.40652	%35v(6)+%15v(7)+%35v(8)+%15v(9)
#15	1591.8532	%16v(16)+%14v(20)
#16	1590.81208	%13v(16)+%16v(20)
#17	1570.66448	%17v(18)+%11v(21)+%13v(22)
#18	1570.2114	%11v(18)+%17v(21)+%12v(23)
#19	1476.40456	%10 δ (30)
#20	1474.8236	-
#21	1443.50324	%35 δ (36)+%37 δ (38)
#22	1437.81564	%46 δ (36)+%42 δ (38)
#23	1434.06568	%15 δ (34)+%11 δ (43)
#24	1433.57404	%10 δ (34)+%14 δ (43)
#25	1323.83228	%12 δ (35)+%19 δ (37)+%17 τ (59)
#26	1318.11576	%11 τ (60)+%11 τ (62)
#27	1311.60876	%10 δ (31)+%13 δ (32)+%14 δ (39)+%11 δ (40)
#28	1300.3878	-
#29	1294.652	%10v(19)+%10v(20)+%11v(22)+%11v(23)
#30	1278.6496	%18 τ (60)+%18 τ (62)
#31	1196.806	%13v(25)+%13v(26)
#32	1180.8036	%15v(25)+%15v(26)
#33	1169.61156	%18 δ (35)+%24 δ (37)+%10 τ (61)
#34	1161.0898	%15 δ (30)+%16 δ (31)+%18 δ (32)+%17 δ (33)
#35	1160.86808	%17 δ (39)+%16 δ (40)+%17 δ (41)+%14 δ (42)

#36	1139.94928	%11 δ (30)+%21 δ (34)+%18 δ (43)
#37	1139.50584	%17 δ (34)+%10 δ (41)+%11 δ (42)+%21 δ (43)
#38	1125.58568	%15 δ (35)+%15 δ (37)
#39	1071.76556	-
#40	1056.57292	-
#41	1016.28736	%13 ν (15)+%11 ν (18)+%10 ν (24)
#42	1015.2366	%11 ν (15)+%12 ν (21)+%14 ν (24)
#43	986.13344	%10 δ (28)+%13 δ (44)+%17 δ (45)
#44	986.00812	%18 δ (28)+%10 δ (45)+%13 δ (51)
#45	976.79228	%22 ν (27)+%11 δ (35)
#46	963.65296	%12 τ (57)+%14 τ (58)+%11 τ (65)+%12 τ (67)
#47	962.86248	%11 τ (57)+%13 τ (58)+%12 τ (65)+%16 τ (67)
#48	942.5028	%15 τ (54)+%10 τ (55)+%12 τ (56)+%12 τ (57)+%12 τ (66)
#49	941.96296	%10 τ (54)+%11 τ (63)+%10 τ (64)+%13 τ (65)+%18 τ (66)
#50	921.1502	-
#51	917.18816	%39 ν (27)+%10 τ (59)
#52	886.70648	%13 τ (55)+%13 τ (56)+%16 τ (58)+%13 τ (63)+%13 τ (64)+%17 τ (67)
#53	872.62244	%13 τ (58)+%13 τ (67)
#54	825.38644	%15 τ (65)+%14 τ (66)+%11 τ (55)+%10 τ (57)+%14 τ (63)+%16 τ (64)
#55	824.59596	%15 τ (54)+%15 τ (55)+%14 τ (56)+%14 τ (57)+%11 τ (66)+%11 τ (64)
#56	758.5234	%10 ν (25)+%10 ν (26)+%19 δ (44)+%19 δ (51)
#57	753.125	%11 δ (44)+%12 δ (51)
#58	742.24144	%12 τ (71)+%12 τ (74)
#59	733.7486	%11 τ (74)
#60	690.16616	%11 τ (67)+%10 τ (71)+%16 τ (74)
#61	689.46244	%11 τ (58)+%12 τ (71)+%13 τ (74)
#62	616.16952	%10 δ (28)+%14 δ (45)+%12 δ (46)+%20 δ (47)+%16 δ (48)
#63	615.8032	%12 δ (28)+%12 δ (45)+%10 δ (46)+%18 δ (47)+%19 δ (48)
#64	574.40904	%13 δ (29)+%11 δ (53)
#65	525.54388	-
#66	498.10844	%11 δ (46)+%12 δ (50)
#67	476.92936	%12 τ (68)

Table. S7. Assignment of normal mode of BiBz-2.

Mode	Frequency	Vibration assignment (>10%)
#1	3074.35	%11 ν (1)+%11 ν (4)+%24 ν (5)+%11 ν (12)+%11 ν (13)+%24 ν (14)
#2	3074.186	%11 ν (1)+%11 ν (4)+%25 ν (5)+%11 ν (12)+%11 ν (13)+%24 ν (14)
#3	3061.915	%21 ν (1)+%21 ν (4)+%21 ν (12)+%21 ν (13)
#4	3061.818	%21 ν (1)+%21 ν (4)+%21 ν (12)+%21 ν (13)
#5	3053.422	%22 ν (5)+%22 ν (14)
#6	3053.306	%22 ν (5)+%22 ν (14)
#7	3040.302	%21 ν (2)+%22 ν (3)+%21 ν (10)+%21 ν (11)
#8	3039.887	%21 ν (2)+%22 ν (3)+%21 ν (10)+%22 ν (11)
#9	3039.058	%17 ν (2)+%16 ν (3)+%17 ν (10)+%16 ν (11)

#10	3038.904	%17v(2)+%16v(3)+%17v(10)+%16v(11)
#11	2972.851	%25v(6)+%25v(7)+%25v(8)+%25v(9)
#12	2949.927	%25v(6)+%25v(7)+%25v(8)+%25v(9)
#13	2929.307	%25v(6)+%25v(7)+%25v(8)+%25v(9)
#14	2919.522	%25v(6)+%25v(7)+%25v(8)+%25v(9)
#15	1591.121	%15v(16)+%15v(19)
#16	1590.581	%15v(16)+%15v(19)
#17	1570.25	%15v(18)+%13v(22)+%12v(23)+%10v(24)
#18	1570.25	%13v(18)+%16v(22)+%10v(23)+%12v(24)
#19	1475.151	-
#20	1474.853	-
#21	1452.43	%45δ(36)+%45δ(38)
#22	1435.733	%42δ(36)+%42δ(38)
#23	1433.873	%13δ(34)+%13δ(43)
#24	1433.053	%13δ(34)+%13δ(43)
#25	1315.976	%17τ(59)+%20τ(60)+%11τ(61)+%20τ(62)
#26	1314.366	%10δ(31)+%10δ(32)+%10δ(39)+%10δ(40)
#27	1310.23	%13δ(31)+%13δ(32)+%13δ(39)+%13δ(40)
#28	1295.703	-
#29	1295.201	%10v(17)+%10v(20)+%10v(23)+%10v(24)
#30	1250.732	%14τ(59)+%20τ(60)+%20τ(62)
#31	1248.274	%25δ(37)+%11τ(60)+%11τ(62)
#32	1185.72	%18v(25)+%17v(26)
#33	1185.431	%18v(25)+%18v(26)
#34	1159.721	%10δ(31)+%10δ(32)+%10δ(39)+%10δ(40)
#35	1159.374	%10δ(31)+%10δ(32)+%10δ(39)+%10δ(40)
#36	1140.354	%20δ(34)+%20δ(43)
#37	1139.699	%10δ(33)+%19δ(34)+%10δ(41)+%10δ(42)+%19δ(43)
#38	1122.443	%25δ(35)+%22δ(37)
#39	1072.489	-
#40	1051.435	-
#41	1015.497	%11v(15)+%11v(18)+%11v(21)+%11v(22)
#42	1015.073	%11v(15)+%11v(18)+%11v(21)+%11v(22)
#43	985.555	%14δ(28)+%10δ(44)+%14δ(45)+%10δ(49)
#44	985.0441	%14δ(28)+%10δ(44)+%14δ(45)+%10δ(49)
#45	982.7016	%60v(27)
#46	964.2892	%22δ(35)+%10δ(37)+%13τ(61)
#47	963.5469	%11τ(54)+%15τ(58)+%15τ(67)
#48	962.4576	%11τ(54)+%16τ(58)+%16τ(67)
#49	941.105	%10τ(54)+%13τ(57)+%13τ(65)+%13τ(66)
#50	940.9508	%10τ(54)+%13τ(57)+%13τ(65)+%13τ(66)
#51	890.8324	%13τ(55)+%13τ(56)+%17τ(58)+%13τ(63)+%13τ(64)+%17τ(67)
#52	890.36	%13τ(67)+%12v(27)+%10τ(56)+%13τ(58)+%10τ(63)+%10τ(64)
#53	833.3394	%10δ(44)+%10δ(49)

#54	824.1525	%12τ(54)+%13τ(55)+%14τ(56)+%12τ(57)+%13τ(63)+%13τ(64)
#55	824.1332	%12τ(65)+%13τ(55)+%13τ(56)+%12τ(66)+%14τ(63)+%14τ(64)
#56	780.493	%12ν(25)+%12ν(26)+%20δ(44)+%20δ(49)
#57	747.5627	%10δ(37)+%25τ(59)+%12τ(60)+%21τ(61)+%12τ(62)
#58	745.8082	%13τ(71)+%15τ(75)
#59	729.9312	%10τ(71)+%14τ(75)
#60	689.6938	%10τ(58)+%10τ(67)+%10τ(71)+%16τ(75)
#61	689.5588	%10τ(58)+%10τ(67)+%10τ(71)+%15τ(75)
#62	616.5166	%12δ(28)+%11δ(45)+%10δ(46)+%18δ(47)+%18δ(48)+%10δ(51)
#63	615.3501	%12δ(28)+%12δ(45)+%10δ(46)+%18δ(47)+%18δ(48)+%10δ(51)
#64	605.1028	%11δ(44)+%11δ(49)
#65	517.7355	-
#66	515.2387	-
#67	465.2746	%18τ(68)+%14γ(78)

4.3. Comparison of theoretical and experimental spectra

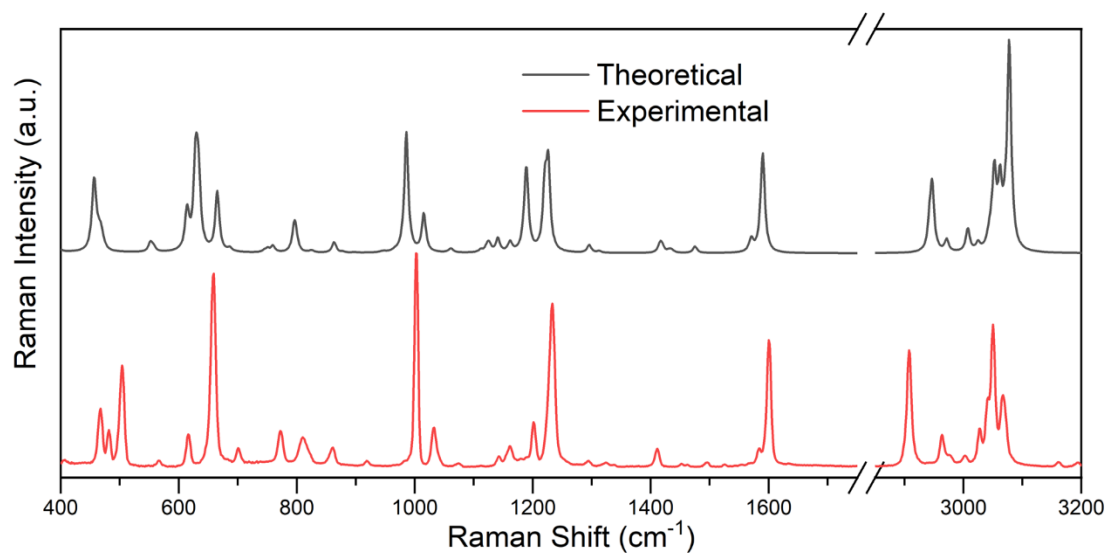


Fig. S4. Experimental measured and theoretically calculated Raman spectra of DBDS.

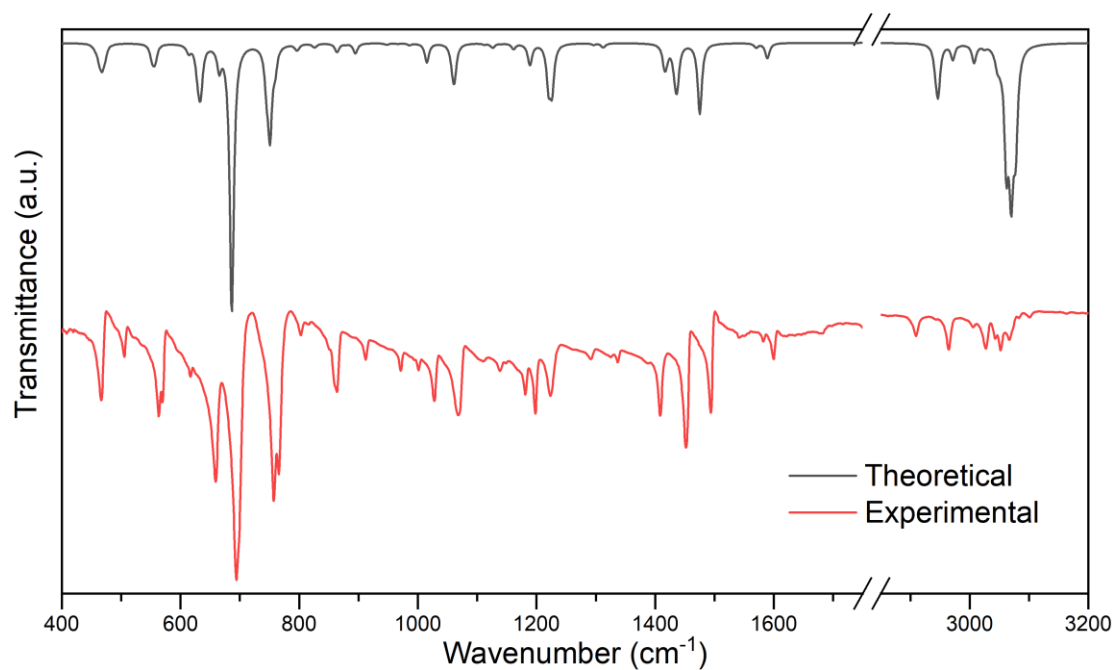


Fig. S5. Experimental measured and theoretically calculated IR spectra of DBDS.

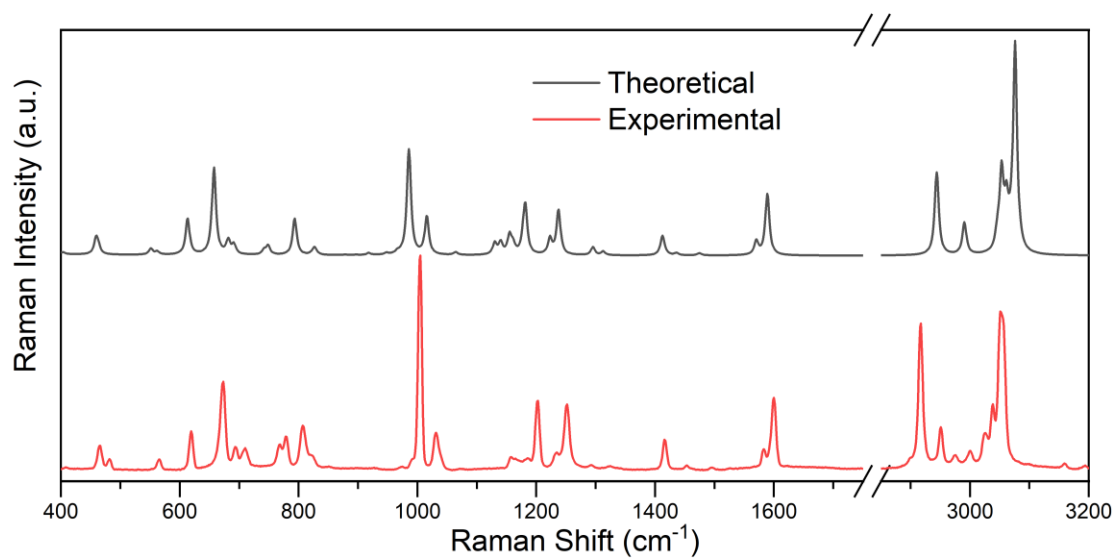


Fig. S6. Experimental measured and theoretically calculated Raman spectra of DBS.

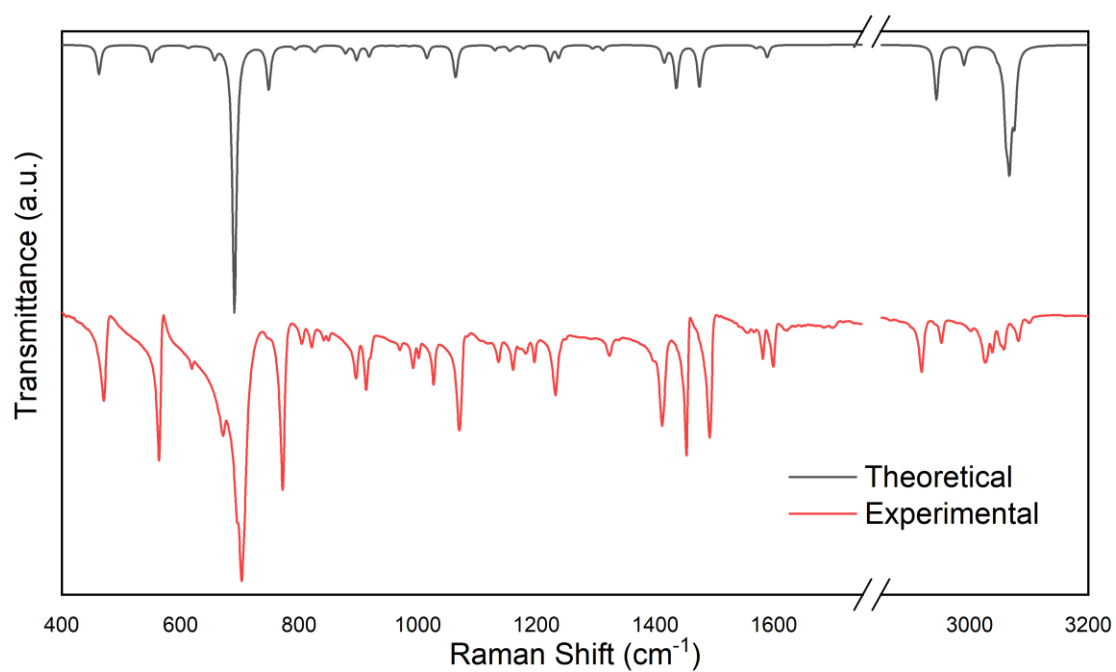


Fig. S7. Experimental measured and theoretically calculated IR spectra of DBS.

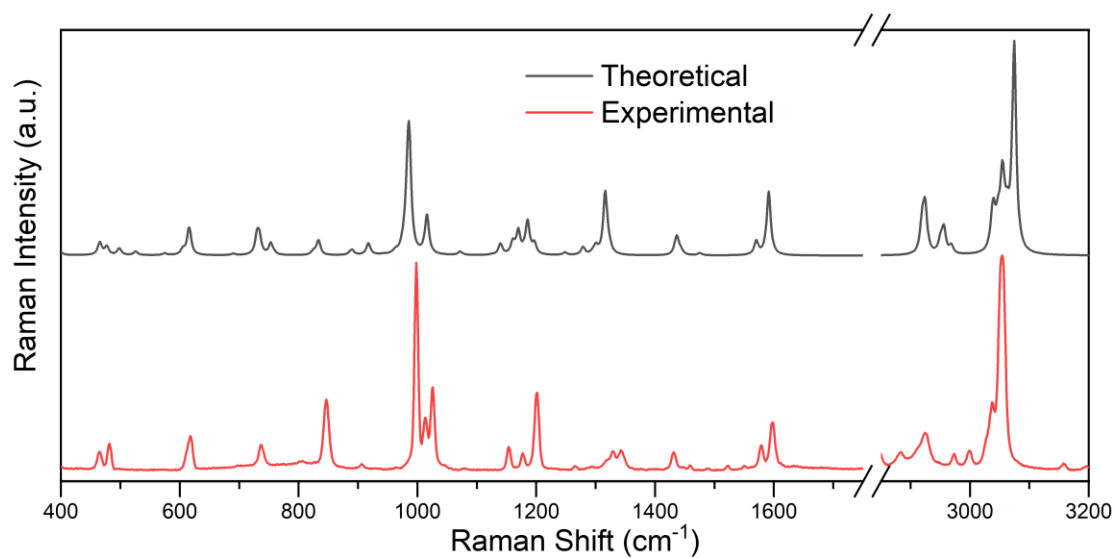


Fig. S8. Experimental measured and theoretically calculated Raman spectra of BiBz

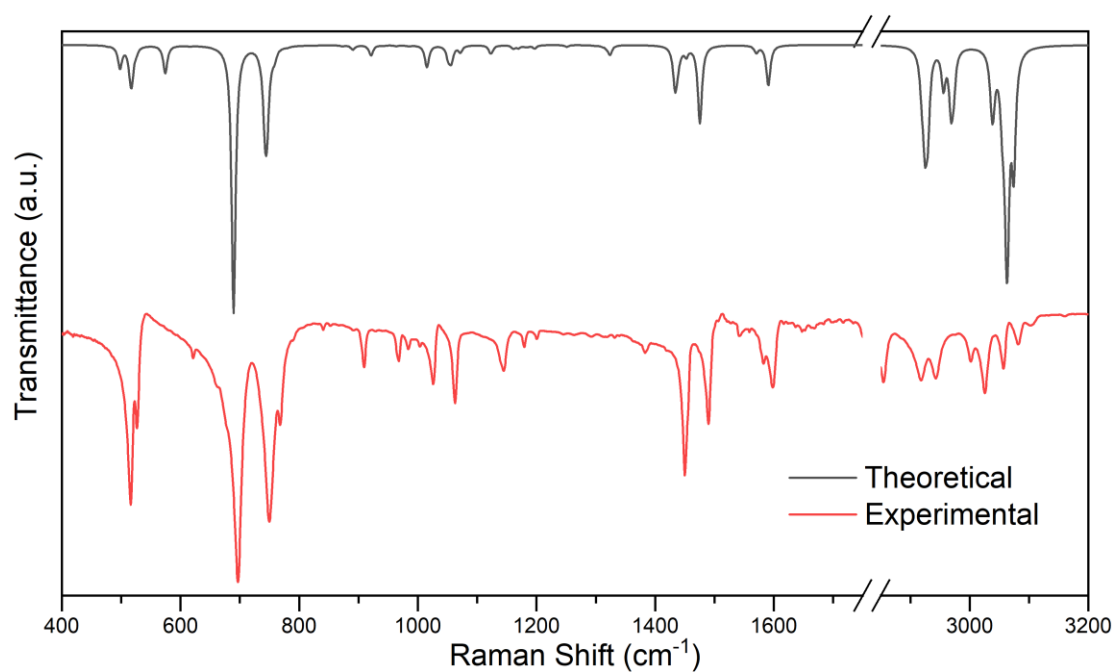


Fig. S9. Experimental measured and theoretically calculated IR spectra of BiBz