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Supporting information for article:

Salts of purine alkaloids caffeine and theobromine with 2,6-dihydroxybenzoic acid as coformer: structural, theoretical, thermal and spectroscopic studies

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Additional information about salts formation.

After cogrinding TBR and 26DHBA with a drop of water, the obtained purple powder was dissolved in a CH₃OH:H₂O mixture. The solution, after mixing and heating, was left to evaporate for about 3 weeks in a flask. After evaporation, plate-like crystals of (TBR-H)⁺·(26DHBA)⁻ were formed and one of them was subjected to X-ray measurements. This compound was also obtained by slow evaporation from *t*BuOH:H₂O solution. In turn the crystals of (CAF-H)⁺·(26DHBA)⁻ were also obtained by slow evaporation from methanol-chloroform solution. The use of water was not conducive to the good-quality crystals formation.

Elemental analysis results.

(TBR-H)⁺·(26DHBA)⁻: calculated %C: 50.3, %H: 4.22, %N: 16.76; found: %C: 48.94, %H: 3.959, %N: 16.05.

(CAF-H)⁺·(26DHBA)⁻: calculated %C: 51.72, %H: 4.63, %N: 16.09; found: %C: 51.20, %H: 5.104, %N: 16.47.

Microwave-assisted slurry cocrystallization conditions

Tab. S1. Microwave-assisted slurry cocrystallization conditions for TBR·26DHBA.

Solvent used	Volume of solvent used	TBR	26DHBA
H ₂ O	300 µl	46.0 mg (0.256 mmol)	39.4 mg (0.256 mmol)
CH ₃ OH	400 µl	45.8 mg (0.254 mmol)	39.2 mg (0.254 mmol)
CH ₃ CN	300 µl	45.4 mg (0.252 mmol)	39.0 mg (0.253 mmol)
AcOEt	400 µl	45.1 mg (0.250 mmol)	38.7 mg (0.251 mmol)

Tab. S2. Microwave-assisted slurry cocrystallization conditions for CAF·26DHBA.

Solvent used	Volume of solvent used	CAF	26DHBA
H ₂ O	200 µl	13.8 mg (0.071 mmol)	11.0 mg (0.071 mmol)
CH ₃ OH	200 µl	13.4 mg (0.069 mmol)	10.6 mg (0.069 mmol)
CH ₃ CN	200 µl	13.4 mg (0.069 mmol)	10.6 mg (0.069 mmol)
AcOEt	200 µl	14.1 mg (0.073 mmol)	11.1 mg (0.072 mmol)

UV-vis measurements

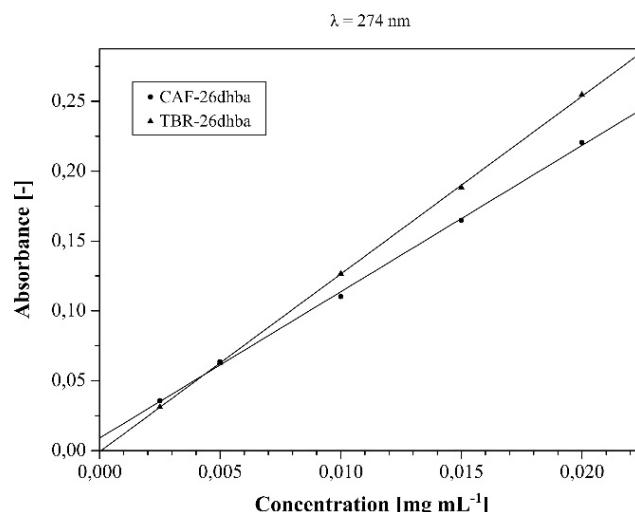


Fig. S1. Calibration curves for $(\text{TBR-H})^+ \cdot (\text{26DHBA})^-$ and $(\text{CAF-H})^+ \cdot (\text{26DHBA})^-$. Detection wavelength (λ_{det}) for both compounds are equal to 274 nm.

CSD base analysis

Tab. S3. CSD analysis for the formation of intra- and intermolecular bonds by the 2,6-dihydroxybenzoate anion in its salts (search conditions: 3D coordinations determined, structure with $R \leq 0.1$, no errors, only single crystal structures; ConQuest Version 2020.3.0). 44 deposits were found and analyzed.

REFCODE	Information on the intramolecular hydrogen bond motif	Number of intermolecular hydrogen bonds formed by <i>ortho</i> -hydroxyl groups
CAJTEP	$2S_1^1(6)$	1 – carboxyl group donor
CENRUL	$2S_1^1(6)$	
CYTRES10	$2S_1^1(6)$	
DOGDAH	$2S_1^1(6)$	
DUNSEM	$2S_1^1(6)$	
DUNSIQ	$2S_1^1(6)$	
ETAZIJ	$2S_1^1(6)^a)$	In one anion molecule in asymmetric unit each hydroxyl group accept proton from one $-\text{NH}_2$ group (2 intramolecular hydrogen bonds). In second anion 3 intermolecular hydrogen bonds were formed and $-\text{NH}_2$ group are also donors for hydroxyl groups.
EZEGUN	$2S_1^1(6)$	1 – primary amine group donor ($-\text{NH}_2$)
EZIDEX	$2S_1^1(6)$	
FABJOK	$2S_1^1(6)$	1 – secondary amine group donor
HOWLIR	$2S_1^1(6)$	1 – water donor
HUZDOV	$2S_1^1(6)^a)$	
JIQFUN	$2S_1^1(6)$	2 – each hydroxyl group accept proton from one NH_3^+ cation
JIWHUV	$2S_1^1(6)^a)$	
KEZHAZ	$2S_1^1(6)$	
KEZHED	$2S_1^1(6)$	
LAGTEV	$2S_1^1(6)^a)$	1 – primary amine group donor ($-\text{NH}_2$) ^{a)}
LAGTOF	$2S_1^1(6)$	2 – each hydroxyl group accept proton from one $-\text{NH}_2$ group
LAGTOF01		
LAGTOF02		
LEWPOS	$2S_1^1(6)$	1 – primary amine group donor ($-\text{NH}_2$)
LEWRUA	$2S_1^1(6)$	1 – primary amine group donor ($-\text{NH}_2$)
LEZJIH	$2S_1^1(6)$	
LOLDAS	$2S_1^1(6)$	1 – secondary amine group donor
LOLDEW	$2S_1^1(6)$	1 – water donor
LUTNUM	$2S_1^1(6)$	1 – primary amine group donor ($-\text{NH}_2$)
NAKZEH	$2S_1^1(6)$	1 - NH_3^+ cation as a donor
NAKZEH01		
NIJFAP	$2S_1^1(6)$	1 – secondary amine group donor
NIJFAP01		
NOWKAO	$2S_1^1(6)$	
QIRGUT	$2S_1^1(6)$	
REZHAG	$2S_1^1(6)$	
RIBLUJ	$2S_1^1(6)^a)$	
SERREP	$2S_1^1(6)$	1 – protonated primary ketimine ($=\text{NH}_2^+$ group) as a donor
TILYOF	$2S_1^1(6)^a)$	1 – protonated secondary ketimine as a donor
WINSAQ	one molecule - $2S_1^1(6)$ second molecule - $S_1^1(6)^b)$	
WINSOE	$S_1^1(6)$	
WINWAU	$2S_1^1(6)$	
WOCHED	$2S_1^1(6)$	

WOCHED01		
XABMAR	$2S_1^1(6)$	1 – protonated primary ketimine ($=NH_2^+$ group) as a donor
YUQCEV	$2S_1^1(6)$	
XOGDOO	$2S_1^1(6)^a$	

a) this motif is found in each 2,6-dihydroxybenzoate anion present in the asymmetric unit; b) two independent 2,6-dihydroxybenzoate anions in asymmetric unit.

Tab. S4. CSD analysis for the formation of intra- and intermolecular bonds by the 2,6-dihydroxybenzoic acid in its cocrystals (search conditions: 3D coordinations determined, structure with $R \leq 0.1$, no errors, only single crystal structures; ConQuest version 2020.3.0). 10 deposits were found and analyzed.

REFCOD	Information on the intramolecular hydrogen bond motif and carboxyl group conformation	Comments about intermolecular hydrogen bonds formed by <i>ortho</i> -hydroxyl groups
DEXTOQ	$2S_1^1(6)$, syn-COOH	
GEQXEH GEQXEH01	$2S_1^1(6)$, syn-COOH	
HUZDOV	$2S_1^1(6)$, anti-COOH ^a	
KEZHED	$2S_1^1(6)$, syn-COOH	
NEFGEN NEFGEN01	$2S_1^1(6)$, syn-COOH	In NEFGEN hydrogen atom of one hydroxyl group is also donor for nitrogen atom in pyrazine ring (valence angle 124.37°). In NEFGEN01 this angle is equal to 119.26°.
QIRGUT	$2S_1^1(6)$, syn-COOH	
QUGNUE	$2S_1^1(6)$, syn-COOH	
XOGDOO ^b	$2S_1^1(6)$, syn-COOH ^a	In two of the 4 acid molecules present in the asymmetric unit, the oxygen atom from one hydroxyl group accepts a proton from other hydroxyl group.

a) this motif and carboxyl group conformation is found in each 2,6-dihydroxybenzoic acid molecule present in the asymmetric unit; b) analysis based on the drawing of the structure in L. Wang *et al.* publication; the deposited structure does not contain anion molecule, the deposited structure does not contain anion molecule, which is not in accordance with the structure description in the above work.

Tab. S5. CSD analysis of crystal structure of pure 2,6-dihydroxybenzoic acid and its monohydrate.

REFCOD	Information on the intramolecular hydrogen bond motif and carboxyl group conformation	Additional notes
LEZJAB	$2S_1^1(6)$, anti-COOH	orthorhombic polymorph
LEZJAB01	$2S_1^1(6)$, syn-COOH	monoclinic polymorph
LEZJEF	$2S_1^1(6)$, anti-COOH	monohydrate, structure is disordered

Geometry of imidazole rings

Tab. S6. The comparison of selected valence angles in the imidazole ring for theobromine systems with hydroxybenzoic acid derivatives.

TBR system	REFCOD	α [°]	β [°]	γ [°]
TBR·2HBA	RUTHEV01	104.11	112.95	106.36
TBR·3HBA	POQHEL	104.14	113.02	106.11
TBR·2(4HBA)·H ₂ O	POQHIP	103.59	113.37	106.43
		103.67	113.39	106.24
TBR·23HBA·H ₂ O	HOWKUC	103.92	113.10	106.43
TBR·24HBA	HOWLAJ	104.22	112.65	106.62
TBR·25HBA	HOWLEN	104.05	113.04	106.33
TBR·26HBA·H₂O	HOWLIR	106.43	110.69	107.65
TBR·26HBA	this paper	106.85	110.22	107.63
TBR·34HBA	HOWLOX	104.09	113.24	106.04
TBR·35HBA	HOWLUD	104.06	113.22	106.14
		104.01	113.15	106.15
TBR·345HBA·H ₂ O	MUPPET	102.74	114.36	105.28

Tab. S7. The comparison of selected valence angles in the imidazole ring for caffeine systems with hydroxybenzoic acid derivatives.

CAF system	REFCOD	α [°]	β [°]	γ [°]
CAF·2HBA	XOBCAT	104.02	112.85	106.64
	XOBCAT01	104.09	112.89	106.59
CAF·3HBA	MOZCOU	103.47	113.27	106.26
CAF·2(4HBA)	MOZDAH	103.39	113.49	106.36
2CAF·4HBA	MOZCUA	103.41	113.55	105.99
CAF·4HBA·H ₂ O	LATBIT	103.28	113.61	105.75
CAF·23HBA·H ₂ O	MOZDEL	103.22	113.19	104.14
CAF·24HBA·H ₂ O	MOZCIO	103.78	113.11	105.94
CAF·25HBA	MOZDIP	103.61	113.09	106.17
CAF·26HBA	this paper	106.04	110.91	107.59
CAF·35HBA·H ₂ O	MOZCEK	103.77	113.10	106.14
2CAF·2(345HBA)·H ₂ O	MUPNOB	103.48	113.12	106.29
3CAF·345HBA·6H ₂ O	ZICGIE	103.07	113.97	106.06

Stacking geometry

Tab. S8. Stacking interactions geometry in described salts.

Compound	ArM	ArN	ArM···ArN a) [Å]	Dihedral angle b) [°]	Interplanar distance c) [Å]	Offset d) [Å]
(I), H ⁺ ·(26DHBA) ⁻	(TBR- Ar1	Ar3 ⁱⁱ	3.602(1)	1.149(1)	3.312(1)	1.417(1)
	Ar2	Ar3 ⁱⁱⁱ	3.479(1)	1.892(1)	3.285(1)	1.147(1)
	Ar1	Ar3 ⁱⁱⁱ	3.567(1)	1.149(1)	3.314(1)	1.317(1)

Symmetry codes: (ii) 1-x, 1-y, 1-z, (iii) -x, 1-y, 1-z

(II), H ⁺ ·(26DHBA) ⁻	(CAF- Ar1 Ar3 ⁱ	3.549(1)	2.19(4)	3.238(1)	1.455(1)
	Ar2 Ar3 ⁱ	3.639(1)	0.12(5)	3.288(1)	1.560(1)

Symmetry codes: (i) 1-x, 1-y, 1-z

Ar1 – pyrimidine ring in alkaloid molecule; Ar2 – imidazole ring in alkaloid molecule; Ar3 – benzene ring in 2,6-dihydroxybenzoate anion; a) The distance between the ring centroids. b) The angle between aromatic ring planes. c) The distance between ArN plane to ArM centroid. d) The distance between ArM and ArN projected onto the ring plane M.

Optimized structures

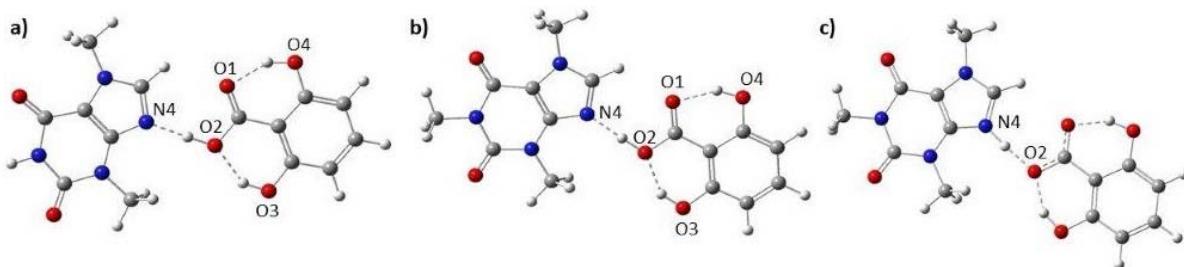


Fig. S2. The optimized at the APF-D/6-311++G(d,p) level of theory structures of (a) TBR·26DHBA (**Ia**), (b) CAF·26DHBA (**IIa**) and (c) CAF·26DHBA solvated by water.

Optimized structures of molecular complexes of TBR·26DHBA (**Ia**) and CAF·26DHBA (**IIa**) are characterized by O(2)-H···N(4) hydrogen bonds of 2.612 Å and 2.607 Å respectively. The calculated distances are about 0.06 Å longer than in the crystal. Because, the proton is not transferred from the acid to the TBR or CAF molecule, much larger differences in the length of the C7-O1 and C7-O2 bonds are observed compared to those occurring in the crystal (0.056 Å for **I**, 0.097 Å for **Ia**, and 0.041 Å for **II**, 0.096 Å for **IIa**). The dihedral angles C8-C11-C10-N4 and N3-C11-C10-N2 are determined to be 180°, which indicates the planarity of CAF and TBR rings.

As in the crystal, two hydroxyl groups of 26DHBA acid are involved in intramolecular O-H···O hydrogen bonds. But in the optimized structures **Ia** and **IIa** hydrogen bonds are longer (0.005 - 0.021 Å) compared to those in the crystals (Tab. 3).

Tab. S9. Selected experimental (**I**, **II**) and calculated (**Ia**, **IIa**) bond lengths (Å), bond and torsion angles (°), energies and dipole moments calculated by the APF-D/6-311++G(d,p) method.

	I	Ia	II	IIa
Energy (a.u.)		-1211.7674		-1251.0524
Dipole moment (D)		2.87		3.27
<i>Bond lengths</i>				
C1–C2	1.407(3)	1.423	1.4125(17)	1.422
C2–C3	1.382(3)	1.390	1.3900(18)	1.390
C3–C4	1.391(4)	1.389	1.3862(19)	1.389
C4–C5	1.376(4)	1.387	1.3865(19)	1.387

C5—C6	1.384(3)	1.392	1.3870(18)	1.392
C1—C6	1.418(3)	1.426	1.4189(17)	1.425
C1—C7	1.484(3)	1.455	1.4821(17)	1.456
C8—C11	1.446(3)	1.433	1.4369(17)	1.430
C10—C11	1.358(3)	1.376	1.3641(17)	1.372
N1—C8	1.391(3)	1.402	1.4144(15)	1.410
N1—C9	1.384(3)	1.396	1.3976(16)	1.403
N1—C15	-	-	1.4700(16)	1.459
N2—C9	1.389(3)	1.392	1.3838(16)	1.393
N2—C10	1.364(3)	1.367	1.3636(16)	1.363
N2—C13	1.469(3)	1.453	1.4631(16)	1.453
N3—C11	1.385(3)	1.380	1.3882(15)	1.381
N3—C12	1.335(3)	1.339	1.3282(16)	1.339
N3—C14	1.460(3)	1.451	1.4677(15)	1.451
N4—C10	1.361(3)	1.354	1.3608(16)	1.354
N4—C12	1.335(3)	1.331	1.3431(16)	1.331
O1—C7	1.241(3)	1.235	1.2530(16)	1.235
O2—C7	1.297(3)	1.332	1.2940(15)	1.331
O3—C2	1.361(3)	1.343	1.3545(15)	1.343
O4—C6	1.354(3)	1.337	1.3541(16)	1.337
O5—C8	1.219(3)	1.216	1.2151(16)	1.218
O6—C9	1.214(3)	1.212	1.2191(16)	1.213
MAD ^a		0.011		0.013

Bond angles

C3—C2—C1	120.4(2)	120.14	121.05(12)	120.14
C4—C3—C2	119.8(2)	119.68	119.10(12)	119.67
C5—C4—C3	121.6(2)	121.86	121.59(12)	121.86
C4—C5—C6	118.8(2)	119.42	119.64(12)	119.42
C2—C1—C6	117.99(19)	118.61	118.11(11)	118.62
C5—C6—C1	121.4(2)	120.29	120.49(12)	120.29
C2—C1—C7	122.34(19)	123.13	122.19(11)	123.11
C6—C1—C7	119.66(19)	118.26	119.69(11)	118.28
O1—C7—C1	121.53(19)	123.52	117.50(11)	123.47
O2—C7—O1	121.94(19)	120.71	121.91(11)	120.77
O2—C7—C1	116.52(18)	115.76	120.59(11)	115.77
O3—C2—C1	121.9(2)	123.17	121.83(11)	123.15
O3—C2—C3	117.7(2)	116.69	117.11(11)	116.71
O4—C6—C1	120.51(19)	122.04	121.15(11)	122.03
O4—C6—C5	118.1(2)	117.66	118.35(11)	117.68
C9—N1—C8	128.99(17)	130.36	127.35(10)	127.35
C9—N1—C15	-	-	116.09(10)	114.80
C9—N2—C13	119.92(17)	120.15	120.37(10)	120.15
C8—N1—C15	-	-	116.47(10)	117.85
C10—N2—C9	118.03(17)	119.33	118.77(10)	119.42

C10—N2—C13	122.05(17)	120.52	120.82(10)	120.43
C11—N3—C14	126.65(19)	126.12	127.02(10)	126.30
C12—N3—C11	107.63(17)	106.59	107.59(10)	106.56
C12—N3—C14	125.67(19)	127.28	125.38(11)	127.14
C12—N4—C10	106.85(17)	105.03	106.04(10)	104.90
N3—C12—N4	110.22(18)	112.41	110.91(11)	112.42
C10—C11—C8	121.95(18)	122.53	122.38(11)	123.08
N1—C8—C11	110.24(17)	109.67	110.85(10)	111.08
N2—C9—N1	116.68(17)	114.90	117.06(10)	116.60
N3—C11—C8	131.92(19)	131.94	131.80(11)	131.43
C10—C11—N3	106.05(17)	105.53	105.73(10)	105.49
N4—C10—N2	126.78(18)	126.37	126.72(11)	126.91
N4—C10—C11	109.25(18)	110.43	109.72(11)	110.63
C11—C10—N2	123.97(18)	123.19	123.53(11)	122.46
O5—C8—N1	121.97(19)	122.49	122.17(11)	123.11
O5—C8—C11	127.8(2)	127.84	126.98(11)	125.80
O6—C9—N2	121.32(19)	123.37	121.39(12)	122.21
O6—C9—N1	122.00(18)	121.73	121.55(11)	121.19
MAD ^a		0.94		0.99

Torsion angles

N3—C11—C10—N2	-179.78(18)	-180.00	177.45(11)	-180.00
N3—C11—C10—N4	0.1(2)	0.006	-0.66(14)	0.002
N3—C11—C8—O5	0.4(4)	0.003	2.1(2)	-0.009
N3—C11—C8—N1	-179.8(2)	180.00	-177.84(12)	180.00
C9—N2—C10—N4	179.22(18)	180.00	177.81(11)	180.00
C9—N2—C10—C11	-0.9(3)	-0.004	0.03(18)	-0.007
C9—N1—C8—O5	177.6(2)	179.99	-176.99(12)	180.00
C9—N1—C8—C11	-2.3(3)	0.005	2.91(17)	-0.006
C11—N3—C12—N4	0.5(2)	-0.0003	0.14(14)	0.002
C12—N4—C10—N2	-179.92(19)	179.99	-177.29(12)	180.00
C12—N4—C10—C11	0.1(2)	-0.006	0.75(14)	-0.001
C12—N3—C11—C10	-0.4(2)	-0.004	0.32(14)	-0.002
C12—N3—C11—C8	-177.1(2)	-179.99	176.88(13)	-179.98
C10—N2—C9—O6	-177.57(18)	-179.99	-178.96(12)	-179.99
C10—N2—C9—N1	2.5(3)	0.009	0.89(17)	0.016
C10—N4—C12—N3	-0.4(2)	0.004	-0.55(14)	-0.001
C10—C11—C8—O5	-176.0(2)	-179.99	178.14(12)	-179.99
C10—C11—C8—N1	3.9(3)	0.002	-1.76(17)	0.016
C8—N1—C9—O6	179.2(2)	179.99	177.25(12)	180.00
C8—N1—C9—N2	-0.8(3)	-0.01	-2.60(18)	-0.01
C8—C11—C10—N2	-2.6(3)	-0.002	0.49(19)	-0.01
C8—C11—C10—N4	177.29(18)	180.00	-177.62(11)	179.99

C15—N1—C9—O6	-	-	0.73(18)	0.001
C15—N1—C9—N2	-	-	-179.12(11)	179.99
C15—N1—C8—O5	-	-	-0.48(18)	-0.004
C15—N1—C8—C11	-	-	179.42(11)	179.99
C13—N2—C9—O6	3.2(3)	-0.004	-1.19(19)	-0.007
C13—N2—C9—N1	-176.72(18)	180.00	178.67(11)	-180.00
C13—N2—C10—N4	-1.6(3)	0.006	0.05(19)	0.012
C13—N2—C10—C11	178.3(2)	-179.99	-177.73(12)	-179.99
C14—N3—C11—C10	-177.3(2)	-179.99	-179.96(12)	179.98
C14—N3—C11—C8	5.9(4)	0.02	-3.4(2)	0.003
C14—N3—C12—N4	177.5(2)	179.98	-179.58(11)	-179.98
O4—C6—C5—C4	-179.5(2)	180.00	179.76(12)	180.00
O3—C2—C3—C4	-179.3(2)	-180.00	-178.92(12)	-180.00
C1—C6—C5—C4	0.9(3)	-0.004	0.36(19)	-0.001
C1—C2—C3—C4	0.8(4)	0.005	0.36(19)	0.000
C6—C1—C2—O3	-178.88(19)	179.98	179.98(11)	180.00
C6—C1—C2—C3	1.0(3)	-0.01	0.73(18)	-0.001
C6—C1—C7—O1	3.6(3)	-0.04	-176.21(11)	-0.012
C6—C1—C7—O2	-175.85(18)	179.95	3.39(18)	179.99
C6—C5—C4—C3	1.0(4)	-0.003	0.8(2)	-0.0003
C2—C1—C6—O4	178.56(19)	-179.99	179.52(11)	-180.00
C2—C1—C6—C5	-1.9(3)	0.01	-1.10(18)	0.001
C2—C1—C7—O1	-177.7(2)	179.97	3.42(18)	179.99
C2—C1—C7—O2	2.8(3)	-0.04	-176.98(12)	-0.005
C2—C3—C4—C5	-1.9(4)	0.002	-1.1(2)	0.001
C7—C1—C6—O4	-2.7(3)	0.02	-0.84(18)	0.004
C7—C1—C6—C5	176.86(19)	-179.98	178.55(11)	-180.00
C7—C1—C2—O3	2.4(3)	-0.03	0.35(19)	-0.007
C7—C1—C2—C3	-177.7(2)	179.98	-178.90(12)	180.00

^aMAD - mean absolute difference. MAD = 1/n $\sum |d_{\text{calc}} - d_{\text{exp}}|$; d - geometrical parameter

Infrared spectra

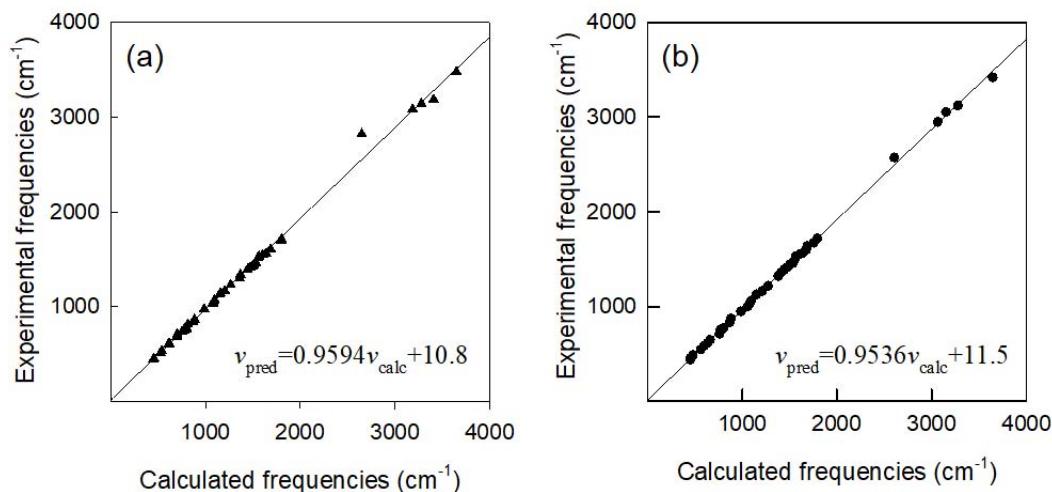


Fig. S3. Correlation between the experimental and calculated wavenumbers (cm^{-1}) for (a) TBR·26DHBA and (b) CAF·26DHBA.

In general, the calculated frequencies are higher compared to experimental ones. This is a result of the harmonic approximation assumed in the calculations. Moreover, the experimental spectrum is measured for the compound in the solid state, whereas the calculations are performed for the vibrations of the isolated molecule. The linear regression can be applied for the calculated and experimental frequencies of studied molecules to minimize differences between theoretical and calculated spectra. The new predicted frequencies were calculated from the linear function respectively for **Ia** and **IIa**:

$$\tilde{\nu}_{\text{pred}} = 0.9594 \tilde{\nu}_{\text{calc}} + 10.8; r = 0.9981$$

$$\tilde{\nu}_{\text{pred}} = 0.9536 \tilde{\nu}_{\text{calc}} + 11.5; r = 0.9996$$

The regression data are shown in the graphical representation in Fig. S3. The theoretical spectra and the analysis of PED helped to assign the frequencies to the appropriate vibration modes, and the assignment is shown in Tables S10, S12. The potential energy distribution, PED, defined and recommended by Kereszty and Jalovszky are given in Tables S11, S13.

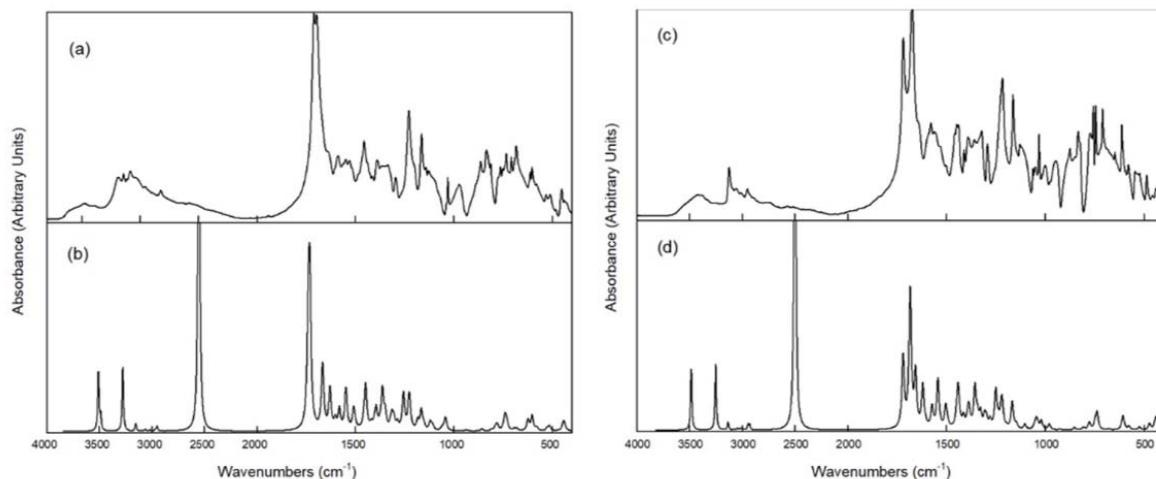


Fig. S4. The Infrared spectra of CAF·26DHBA (a) experimental and (b) computed; and of TBR·26DHBA (c) experimental and (d) computed.

Tab. S10. Experimental FTIR (**I**) and IR spectra (**Ia**) calculated by the APF-D/6-311++G(d,p) approach for TBR·26DHBA.

I	Ia				
$\tilde{\nu}_{\text{exp}}^{\text{a}}$	$\tilde{\nu}_{\text{calc}}$	$A_{\text{calc}}^{\text{b}}$	$\tilde{\nu}_{\text{pred}}^{\text{c}}$	Assignments, PED (%) ^{d,e}	Descriptions ^e
3478	3650	420	3513	$S_1 = \nu O_3 H_3$ (99)	vOH
	3627	106	3491	$S_3 = \nu N_1 H_1$ (100)	vNH
3187	3409	458	3281	$S_2 = \nu O_4 H_{4A}$ (99)	vOH
3142	3279	53	3157	$S_5 = \nu C_{12} H_{12}$ (99)	vCH
	3223	1	3103	$S_{13} = \nu C_3 H_3 + \nu C_5 H_5$ (87) $S_{14} = \nu C_4 H_4$ (10)	vCH
	3219	3	3099	$S_{12} = \nu C_3 H_3 - \nu C_5 H_5$ (97)	vCH
	3192	0.3	3073	$S_6 = \nu C_{13} H_{13B}$ (86) $S_8 = \nu C_{13} H_{13A} + \nu C_{13} H_{13C}$ (14)	vCH
3083	3186	9	3067	$S_{13} = \nu C_3 H_3 + \nu C_5 H_5$ (10) $S_{14} = \nu C_4 H_4$ (90)	vCH
	3180	3	3062	$S_{11} = \nu C_{14} H_{14B} - \nu C_{14} H_{14A} + \nu C_{14} H_{14C}$ (99)	vCH
	3166	2	3048	$S_9 = \nu C_{14} H_{14B} - \nu C_{14} H_{14C}$ (100)	vCH
	3137	9	3020	$S_7 = \nu C_{13} H_{13A} - \nu C_{13} H_{13C}$ (100)	vCH
	3082	15	2968	$S_{10} = \nu C_{14} H_{14A} + \nu C_{14} H_{14B} + \nu C_{14} H_{14C}$ (99)	vCH
	3066	34	2952	$S_6 = \nu C_{13} H_{13B}$ (14) $S_8 = \nu C_{13} H_{13A} + \nu C_{13} H_{13C}$ (86)	vCH
2823	2649	5106	2552	$S_4 = \nu O_2 H_4$ (88) $S_{15} = \nu N_4 H_4$ (10)	vOH vNH
1711	1804	684	1742	$S_{16} = \nu C_8 O_5$ (11) $S_{17} = \nu C_8 O_5 + \nu C_9 O_6$ (71)	vCO
1697	1796	981	1734	$S_{16} = \nu C_8 O_5$ (57) $S_{17} = \nu C_8 O_5 + \nu C_9 O_6$ (10)	vCO
	1727	460	1668	$S_{18} = \nu C_7 O_1$ (48) $S_{56} = \delta C_7 O_2 H_4 + \delta N_4 H_4 O_2$ (14)	vCO, δ COH, δ NHO
1605	1688	292	1630	$S_{24} = \nu C_2 C_3 + \nu C_5 C_6 + \nu C_7 O_1$ (45) $S_{25} = \nu C_3 C_4 + \nu C_4 C_5$ (12)	vCC, vCO
	1660	68	1603	$S_{19} = \nu C_{10} C_{11} - \nu C_{10} N_2$ (69)	vCC, vCN
1587 ^f					vCOO
1560	1639	145	1583	$S_{29} = \nu C_1 C_2 + \nu C_4 C_5 - \nu C_3 C_4$ (58)	vCC
1548	1604	299	1550	$S_{64} = \delta C_{11} C_{10} N_2 - \delta N_4 C_{12} N_3$ (25)	δ CCN, δ NCN

1529	1564	139	1511	$S_{21} = \nu C_{12}N_3$ (12) $S_{56} = \delta C_7O_2H_4 + \delta N_4H_4O_2$ (29)	νCN , δCOH , δNHO
1516	1556	32	1504	$S_{21} = \nu C_{12}N_3$ (28) $S_{56} = \delta C_7O_2H_4 + \delta N_4H_4O_2$ (12)	νCN , δCOH , δNHO
1456	1536	4	1484	$S_{38} = \delta C_2C_3C_4 + \delta C_3C_4C_5 + \delta C_4C_5C_6$ (14) $S_{43} = \delta C_6O_4H_{4A}$ (26) $S_{54} = \delta C_4C_3H_3^+ + \delta C_4C_5H_5^+$ (19)	δCCC , δCOH , δCCH
1433	1510	38	1459	$S_{49} = \delta H_{13A}C_{13}H_{13C} + \delta H_{14B}C_{14}H_{14A} - \delta H_{14B}C_{14}H_{14C}$ (56) $S_{81} = \tau C_9N_2C_{13}H_{13C} - \tau C_9N_2C_{13}H_{13A}$ (12) $S_{82} = \tau C_{12}N_3C_{14}H_{14B} - \tau C_{12}N_3C_{14}H_{14C}$ (10)	δHCH , $\tau CNCH$
1425	1500	314	1450	$S_{50} = \delta H_{13A}C_{13}H_{13C} + \delta H_{14B}C_{14}H_{14C} - \delta H_{14B}C_{14}H_{14A}$ (13) $S_{55} = \delta C_5C_4H_4^+ + \delta C_4C_3H_3^+$ (18)	δHCH , δCCH
	1495	14	1445	$S_{48} = \delta H_{13B}C_{13}H_{13A}$ (71) $S_{79} = \tau C_9N_2C_{13}H_{13B} - \tau C_9N_2C_{13}H_{13A}$ (29)	δHCH , $\tau CNCH$
	1491	2	1441	$S_{50} = \delta H_{13A}C_{13}H_{13C} + \delta H_{14B}C_{14}H_{14C} - \delta H_{14B}C_{14}H_{14A}$ (46)	δHCH
1415	1473	14	1424	$S_{52} = \delta H_{14A}C_{14}H_{14C} - \delta H_{14B}C_{14}H_{14A}$ (71) $S_{83} = \tau C_{12}N_3C_{14}H_{14A} - \tau C_{12}N_3C_{14}H_{14B}$ (29)	δHCH , $\tau CNCH$
	1469	28	1420	$S_{34} = \nu C_9N_1 + \nu C_{12}N_4 - \nu C_9N_2$ (19) $S_{47} = \delta H_{13B}C_{13}H_{13C} + \delta H_{13B}C_{13}H_{13A}$ (10)	νCN , δHCH
	1454	33	1406	$S_{51} = \delta H_{14B}C_{14}H_{14A} + \delta H_{14B}C_{14}H_{14C} + \delta H_{14A}C_{14}H_{14C}$ (80)	δHCH
1390	1444	149	1396	$S_{22} = \nu C_4C_5 - \nu C_1C_2$ (15) $S_{42} = \delta C_2O_3H_3$ (20) $S_{43} = \delta C_6O_4H_{4A}$ (19)	νCC , δCOH
	1433	3	1386	$S_{16} = \nu C_8O_5$ (10) $S_{44} = \delta C_8N_1H_1$ (37) $S_{47} = \delta H_{13B}C_{13}H_{13C} + \delta H_{13B}C_{13}H_{13A}$ (22)	νCO , δCNH , δHCH
	1424	23	1377	$S_{44} = \delta C_8N_1H_1$ (24) $S_{47} = \delta H_{13B}C_{13}H_{13C} + \delta H_{13B}C_{13}H_{13A}$ (31)	δCNH , δHCH
	1411	278	1365	$S_{31} = \nu C_2O_3 + \nu C_6O_4$ (10)	νCO
	1396	113	1350	$S_{31} = \nu C_2O_3 + \nu C_6O_4$ (16) $S_{34} = \nu C_9N_1 + \nu C_{12}N_4 - \nu C_9N_2$ (11)	νCO , νCN
1335	1368	35	1323	$S_{20} = \nu C_{12}N_4 + \nu C_9N_2 - \nu C_{10}N_4$ (45)	νCN

1296	1360	93	1316	$S_{31} = vC_2O_3 + vC_6O_4$ (21) $S_{38} = \delta C_2C_3C_4 + \delta C_3C_4C_5 + \delta C_4C_5C_6$ (22)	$vCO, \delta CCC$
	1350	63	1306	$S_{22} = vC_4C_5 - vC_1C_2$ (32) $S_{42} = \delta C_2O_3H_3$ (22) $S_{55} = \delta C_5C_4H_4^+ + \delta C_4C_3H_3^-$ (17)	$vCC, \delta COH,$ δCCH
	1331	48	1288	$S_{36} = vC_{13}N_2$ (17) $S_{69} = \delta C_9N_2C_{10}$ (18)	$vCN, \delta CNC$
	1300	267	1258	$S_{24} = vC_2C_3 + vC_5C_6 + vC_7O_1$ (15) $S_{28} = vC_7O_2$ (19) $S_{43} = \delta C_6O_4H_{4A}$ (14) $S_{54} = \delta C_4C_3H_3^+ + \delta C_4C_5H_5^-$ (13)	$vCC, vCO,$ $\delta COH, \delta CCH$
	1271	134	1230	$S_{37} = vC_{14}N_3$ (13) $S_{81} = \tau C_9N_2C_{13}H_{13C} - \tau C_9N_2C_{13}H_{13A}$ (16)	$vCN, \tau CNCH$
1228	1266	146	1225	$S_{23} = vC_2C_3$ (16) $S_{30} = vC_2O_3 + vC_6O_4$ (25) $S_{55} = \delta C_5C_4H_4^+ + \delta C_4C_3H_3^-$ (25)	$vCC, vCO,$ δCCH
	1224	65	1185	$S_{34} = vC_9N_1 + vC_{12}N_4 - vC_9N_2$ (10) $S_{36} = vC_{13}N_2$ (15) $S_{46} = \delta N_3C_{12}H_{12}$ (35)	$vCN, \delta NCH$
1163	1205	143	1167	$S_{26} = vC_{10}N_4 - vC_9N_1$ (24) $S_{46} = \delta N_3C_{12}H_{12}$ (12) $S_{81} = \tau C_9N_2C_{13}H_{13C} - \tau C_9N_2C_{13}H_{13A}$ (15)	$vCN, \delta NCH,$ $\tau CNCH$
	1192	35	1154	$S_{29} = vC_1C_2 + vC_4C_5 - vC_3C_4$ (11) $S_{53} = \delta C_4C_3H_3^+ - \delta C_4C_5H_5^- - \delta C_5C_4H_4^+$ (77)	$vCC, \delta CCH$
1142	1158	60	1122	$S_{33} = vC_8N_1 - vC_9N_1$ (39) $S_{44} = \delta C_8N_1H_1$ (10)	$vCN, \delta CNH$
1131	1152	0.2	1116	$S_{48} = \delta H_{13B}C_{13}H_{13A}$ (28) $S_{79} = \tau C_9N_2C_{13}H_{13B} - \tau C_9N_2C_{13}H_{13A}$ (70)	$\delta HCH, \tau CNCH$
	1148	0.01	1112	$S_{52} = \delta H_{14AC}C_{14}H_{14C} - \delta H_{14B}C_{14}H_{14A}$ (28) $S_{83} = \tau C_{12}N_3C_{14}H_{14A} - \tau C_{12}N_3C_{14}H_{14B}$ (69)	$\delta HCH, \tau CNCH$
	1145	37	1109	$S_{28} = vC_7O_2$ (26) $S_{54} = \delta C_4C_3H_3^+ + \delta C_4C_5H_5^-$ (22) $S_{66} = \delta C_1C_2C_3$ (11)	$vCO, \delta CCH,$ δCCC
1068	1096	21	1062	$S_{21} = vC_{12}N_3$ (15) $S_{49} = \delta H_{13AC}C_{13}H_{13C} + \delta H_{14B}C_{14}H_{14A} - \delta H_{14BC}C_{14}H_{14C}$ (12) $S_{82} = \tau C_{12}N_3C_{14}H_{14B} - \tau C_{12}N_3C_{14}H_{14C}$ (44)	$vCN, \delta HCH,$ $\tau CNCH$

1038	1085	6	1052	$S_{25} = \nu C_3C_4 + \nu C_4C_5$ (44) $S_{54} = \delta C_4C_3H_3 + \delta C_4C_5H_5$ (25)	$\nu CC, \delta CCH$
	1079	33	1046	$S_{23} = \nu C_2C_3$ (12) $S_{30} = \nu C_2O_3 + \nu C_6O_4$ (39)	$\nu CC, \nu CO$
1030	1076	62	1043	$S_{77} = \tau C_7O_2H_4N_4$ (73) $S_{95} = \tau C_{12}N_4H_4O_2 - \tau C_7O_2H_4N_4 - \tau C_{11}C_{10}N_4H_4 - \tau C_1C_7O_2H_4$ (14)	$\tau COHN,$ $\tau CNHO,$ $\tau CCNH,$ $\tau CCOH$
	1069	5	1036	$S_{27} = \nu C_{10}C_{11} + \nu C_{10}N_2$ (12) $S_{36} = \nu C_{13}N_2$ (13) $S_{63} = \delta C_{10}N_4C_{12}$ (18) $S_{81} = \tau C_9N_2C_{13}H_{13C} - \tau C_9N_2C_{13}H_{13A}$ (16)	$\nu CC, \nu CN,$ $\delta CNC, \tau CNCH$
973	988	0.1	959	$S_{87} = \tau C_6C_5C_4H_4$ (75) $S_{92} = \tau C_1C_2C_3C_4 + \tau C_3C_4C_5C_6 - \tau C_2C_3C_4C_5$ (10)	$\tau CCCH,$ $\tau CCCC$
	967	10	939	$S_{34} = \nu C_9N_1 + \nu C_{12}N_4 - \nu C_9N_2$ (10) $S_{63} = \delta C_{10}N_4C_{12}$ (26) $S_{81} = \tau C_9N_2C_{13}H_{13C} - \tau C_9N_2C_{13}H_{13A}$ (16)	$\nu CN, \delta CNC,$ $\tau CNCH$
862	884	16	859	$S_{78} = \tau C_{10}N_4C_{12}H_{12}$ (86)	$\tau CNCH$
834	871	0.05	846	$S_{85} = \tau C_5C_4C_3H_3 + \tau C_3C_4C_5H_5$ (84) $S_{104} = \gamma C_6C_5C_1O_4 + \gamma C_2C_3C_1O_3$ (13)	$\tau CCCH,$ $\gamma CCCO$
	833	9	810	$S_{28} = \nu C_7O_2$ (13) $S_{60} = \delta C_3C_4C_5 - \delta C_4C_5C_6 + \delta O_1C_7O_2$ (50)	$\nu CO, \delta CCC,$ δOCO
812	814	21	792	$S_{36} = \nu C_{13}N_2$ (17) $S_{37} = \nu C_{14}N_3$ (18) $S_{58} = \delta N_1C_8O_5 + \delta C_9N_1C_8$ (21)	$\nu CN, \delta NCO,$ δCNC
763	805	30	783	$S_{75} = \tau C_1C_6O_4H_{4A} - \gamma C_7O_2C_1O_1$ (10) $S_{86} = \tau C_3C_4C_5H_5 - \tau C_5C_4C_3H_3 - \tau C_6C_5C_4H_4$ (41) $S_{92} = \tau C_1C_2C_3C_4 + \tau C_3C_4C_5C_6 - \tau C_2C_3C_4C_5$ (27)	$\tau CCOH,$ $\gamma COCO,$ $\tau CCCH,$ $\tau CCCC$
	800	23	778	$S_{75} = \tau C_1C_6O_4H_{4A} - \gamma C_7O_2C_1O_1$ (11) $S_{86} = \tau C_3C_4C_5H_5 - \tau C_5C_4C_3H_3 - \tau C_6C_5C_4H_4$ (10) $S_{107} = \gamma C_7O_2C_1O_1$ (56)	$\tau CCOH,$ $\gamma COCO,$ $\tau CCCH,$
751	772	11	751	$S_{24} = \nu C_2C_3 + \nu C_5C_6 + \nu C_7O_1$ (24) $S_{31} = \nu C_2O_3 + \nu C_6O_4$ (12) $S_{40} = \delta C_2C_3C_4 + \delta C_4C_5C_6 + \delta O_1C_7O_2$ (47)	$\nu CC, \nu CO,$ $\delta CCC, \delta OCO$
	763	3	743	$S_{102} = \gamma C_8N_1C_{11}O_5 + \gamma C_9N_2N_1O_6$ (89)	$\gamma CNCO,$ $\gamma CNNO$

	762	101	742	$S_{75} = \tau C_1 C_6 O_4 H_{4A} - \gamma C_7 O_2 C_1 O_1$ (67) $S_{86} = \tau C_3 C_4 C_5 H_5 - \tau C_5 C_4 C_3 H_3 - \tau C_6 C_5 C_4 H_4$ (14)	$\tau CCOH$, $\gamma COCO$, $\tau CCCH$
733	753	42	733	$S_{101} = \tau C_{11} C_{10} N_4 C_{12} + \gamma C_{10} N_4 C_{11} N_2 + \gamma C_9 N_2 N_1 O_6$ (76)	$\tau CCNC$, $\gamma CNCN$, $\gamma CNNO$
	750	18	730	$S_{57} = \delta N_1 C_9 O_6$ (27) $S_{59} = \delta C_9 N_1 C_8 + \delta N_1 C_9 N_2 - \delta N_1 C_8 O_5$ (10) $S_{73} = \delta C_{11} C_{10} N_4 - \delta C_{11} N_3 C_{14}$ (17)	δNCO , δCNC , δNCN , δCCN
	714	14	696	$S_{101} = \tau C_{11} C_{10} N_4 C_{12} + \gamma C_{10} N_4 C_{11} N_2 + \gamma C_9 N_2 N_1 O_6$ (10) $S_{108} = \tau C_{11} C_{10} N_4 C_{12} + \gamma C_{10} N_{14} C_{11} N_2 - \gamma C_8 N_1 C_{11} O_5$ (67)	$\tau CCNC$, $\gamma CNCN$, $\gamma CNNO$, $\gamma CNCO$
707	702	7	684	$S_{86} = \tau C_3 C_4 C_5 H_5 - \tau C_5 C_4 C_3 H_3 - \tau C_6 C_5 C_4 H_4$ (24) $S_{92} = \tau C_1 C_2 C_3 C_4 + \tau C_3 C_4 C_5 C_6 - \tau C_2 C_3 C_4 C_5$ (47) $S_{107} = \gamma C_7 O_2 C_1 O_1$ (12)	$\tau CCCH$, $\tau CCCC$, $\gamma COCO$
683	698	13	680	$S_{37} = v C_{14} N_3$ (19) $S_{70} = \delta N_4 C_{12} N_3 + \delta N_1 C_9 N_2$ (34)	vCN , δNCN
	640	80	625	$S_{94} = \tau C_{11} C_8 N_1 H_1 + \tau C_{10} N_4 C_{12} N_3$ (77)	$\tau CCNH$, $\tau CNCN$
	634	1	619	$S_{85} = \tau C_5 C_4 C_3 H_3 + \tau C_3 C_4 C_5 H_5$ (14) $S_{104} = \gamma C_6 C_5 C_1 O_4 + \gamma C_2 C_3 C_1 O_3$ (69)	$\tau CCCH$, $\gamma CCCO$
	620	66	606	$S_{74} = \tau C_1 C_2 O_3 H_3$ (82)	$\tau CCOH$
	619	14	605	$S_{76} = \tau C_{10} N_4 C_{12} N_3$ (54) $S_{108} = \tau C_{11} C_{10} N_4 C_{12} + \gamma C_{10} N_{14} C_{11} N_2 - \gamma C_8 N_1 C_{11} O_5$ (13)	$\tau CNCN$, $\tau CCNC$, $\gamma CNCN$, $\gamma CNCO$
611	617	24	603	$S_{32} = v C_9 N_1 + v C_{10} N_4$ (48)	vCN
602	613	3	599	$S_{25} = v C_3 C_4 + v C_4 C_5$ (11) $S_{31} = v C_2 O_3 + v C_6 O_4$ (10) $S_{35} = v C_1 C_2$ (13) $S_{38} = \delta C_2 C_3 C_4 + \delta C_3 C_4 C_5 + \delta C_4 C_5 C_6$ (18) $S_{40} = \delta C_2 C_3 C_4 + \delta C_4 C_5 C_6 + \delta O_1 C_7 O_2$ (23)	vCC , vCO , δCCC , δOCO
	592	25	579	$S_{62} = \delta C_4 C_5 C_6 - \delta C_2 C_3 C_4 + \delta C_3 C_2 O_3 - \delta C_1 C_7 O_2 - \delta C_5 C_6 O_4$ (77)	δCCC , δCCO
531	539	22	528	$S_{71} = \delta C_4 C_5 C_6 - \delta C_2 C_3 C_4 + \delta C_1 C_7 O_1 + \delta C_5 C_6 O_4 - \delta C_3 C_2 O_3$ (63)	δCCC , δCCO

509	525	35	514	$S_{41} = \delta C_{11}C_{10}N_2 - \delta C_{11}N_3C_{14} - \delta N_1C_9N_2 + \delta N_4C_{12}N_3$ (47)	$\delta CCN, \delta CNC,$ δNCN
	480	4	471	$S_{87} = \tau C_6C_5C_4H_4$ (19) $S_{103} = \tau C_2C_3C_4C_5 - \tau C_3C_4C_5C_6 - \gamma C_6C_5C_1O_4 +$ $\gamma C_2C_3C_1O_3$ (64)	$\tau CCCH,$ $\tau CCCC,$ $\gamma CCCO$
451	455	19	447	$S_{38} = \delta C_2C_3C_4 + \delta C_3C_4C_5 + \delta C_4C_5C_6$ (11) $S_{67} = \delta C_6C_5O_4$ (59)	$\delta CCC, \delta CCO$
440	452	41	444	$S_{26} = vC_{10}N_4 - vC_9N_1$ (12) $S_{41} = \delta C_{11}C_{10}N_2 - \delta C_{11}N_3C_{14} - \delta N_1C_9N_2 + \delta N_4C_{12}N_3$ (11) $S_{58} = \delta N_1C_8O_5 + \delta C_9N_1C_8$ (12) $S_{69} = \delta C_9N_2C_{10}$ (18)	$vCN, \delta CCN,$ $\delta CNC, \delta NCN,$ $\delta NCO,$
	446	30	439	$S_{66} = \delta C_1CC$ (10) $S_{68} = \delta C_1C_7O_2 + \delta C_3C_2O_3 + \delta C_5C_6O_4$ (35)	$\delta CCC, \delta CCO$
	428	3	421	$S_{57} = \delta N_1C_9O_6$ (35)	δNCO
	398	0.3	393	$S_{35} = vC_1C_2$ (13) $S_{66} = \delta C_1C_2C_3$ (11) $S_{67} = \delta C_6C_5O_4$ (14) $S_{68} = \delta C_1C_7O_2 + \delta C_3C_2O_3 + \delta C_5C_6O_4$ (25)	$vCC, \delta CCC,$ $\delta CCO,$
	373	8	369	$S_{59} = \delta C_9N_1C_8 + \delta N_1C_9N_2 - \delta N_1C_8O_5$ (48)	$\delta CNC, \delta NCN,$ δNCO
	364	0.4	360	$S_{89} = \tau C_{11}C_{10}N_4C_{12} - \gamma C_{10}N_4C_{11}N_2$ (53) $S_{105} = \gamma C_{13}C_{10}C_9N_2 + \gamma C_{14}C_{11}C_{12}N_3$ (29)	$\tau CCNC,$ $\gamma CNCN,$ $\gamma CCCN$
	340	30	337	$S_{61} = \delta C_1C_2C_3 - \delta C_7C_1C_2$ (59)	δCCC
	318	3	316	$S_{72} = \delta C_9N_2C_{13}$ (63)	$\delta CNC,$
	260	0.04	260	$S_{90} = \tau C_1C_2C_3C_4 + \tau C_7C_1C_2C_3 + \gamma C_6C_5C_1O_4$ (57) $S_{93} = \tau C_7C_1C_2C_3$ (25)	$\tau CCCC,$ $\gamma CCCO$
	228	0.6	230	$S_{99} = \tau C_{10}N_2C_9N_1 + \tau C_8N_1C_9N_2 - \tau C_9N_2C_{10}N_4$ (16) $S_{106} = \gamma C_{14}C_{11}C_{12}N_3 - \gamma C_{13}C_{10}C_9N_2$ (67)	$\tau CNCN,$ $\gamma CCCN$
	225	0.02	227	$S_{91} = \tau C_2C_3C_4C_5 + \tau C_3C_4C_5C_6$ (80)	$\tau CCCC$
	214	18	216	$S_{39} = \delta C_{11}N_3C_{14} + \delta C_{11}C_{10}N_2$ (48) $S_{73} = \delta C_{11}C_{10}N_4 - \delta C_{11}N_3C_{14}$ (23)	$\delta CNC, \delta CCN$
	198	5	201	$S_{98} = \tau C_{10}N_2C_9N_1 + \tau C_9N_2C_{10}N_4$ (54) $S_{99} = \tau C_{10}N_2C_9N_1 + \tau C_8N_1C_9N_2 - \tau C_9N_2C_{10}N_4$ (10) $S_{105} = \gamma C_{13}C_{10}C_9N_2 + \gamma C_{14}C_{11}C_{12}N_3$ (14)	$\tau CNCN,$ $\gamma CCCN$
	149	4	154	$S_{97} = \tau C_9N_2C_{10}N_4 + \tau C_8N_1C_9N_2$ (60)	$\tau CNCN$

	121	0.005	127	$S_{88} = \tau C_1 C_7 O_2 H_4 + \tau C_{12} N_4 H_4 O_2 - \tau C_2 C_1 C_7 O_2$ (10) $S_{90} = \tau C_1 C_2 C_3 C_4 + \tau C_7 C_1 C_2 C_3 + \gamma C_6 C_5 C_1 O_4$ (23) $S_{93} = \tau C_7 C_1 C_2 C_3$ (40)	$\tau CCOH$, $\tau CNHO$, $\tau CCCO$, $\tau CCCC$
	119	0.4	125	$S_{80} = \tau C_9 N_2 C_{13} H_{13C} + \tau C_9 N_2 C_{13} H_{13A} + \tau C_9 N_2 C_{13} H_{13B}$ (73)	$\tau CNCH$
	111	7	117	$S_{15} = v N_4 H_4$ (56)	$v NH$
	107	0.7	113	$S_{80} = \tau C_9 N_2 C_{13} H_{13C} + \tau C_9 N_2 C_{13} H_{13A} + \tau C_9 N_2 C_{13} H_{13B}$ (10) $S_{99} = \tau C_{10} N_2 C_9 N_1 + \tau C_8 N_1 C_9 N_2 - \tau C_9 N_2 C_{10} N_4$ (18) $S_{105} = \gamma C_{13} C_{10} C_9 N_2 + \gamma C_{14} C_{11} C_{12} N_3$ (45) $S_{106} = \gamma C_{14} C_{11} C_{12} N_3 - \gamma C_{13} C_{10} C_9 N_2$ (10)	$\tau CNCH$, $\tau CNCN$, $\gamma CCCN$
	90	0.1	97	$S_{89} = \tau C_{11} C_{10} N_4 C_{12} - \gamma C_{10} N_4 C_{11} N_2$ (13) $S_{99} = \tau C_{10} N_2 C_9 N_1 + \tau C_8 N_1 C_9 N_2 - \tau C_9 N_2 C_{10} N_4$ (45)	$\tau CCNC$, $\tau CNNC$, $\gamma CNCN$
	78	0.4	86	$S_{15} = v N_4 H_4$ (10) $S_{65} = \delta C_7 O_2 H_4 + \delta C_{10} N_4 H_4$ (68)	$v NH$, δCOH , δCNH
	77	0.2	85	$S_{88} = \tau C_1 C_7 O_2 H_4 + \tau C_{12} N_4 H_4 O_2 - \tau C_2 C_1 C_7 O_2$ (61) $S_{93} = \tau C_7 C_1 C_2 C_3$ (11)	$\tau CCOH$, $\tau CNHO$, $\tau CCCO$, $\tau CCCC$
	58	0.005	66	$S_{84} = \tau C_{12} N_3 C_{14} H_{14A} + \tau C_{12} N_3 C_{14} H_{14B} + \tau C_{12} N_3 C_{14} H_{14C}$ (74) $S_{100} = \tau C_1 C_7 O_2 H_4 - \tau C_{11} C_{10} N_4 H_4$ (14)	$\tau CNCH$, $\tau CCOH$, $\tau CCNH$
	46	4	55	$S_{100} = \tau C_1 C_7 O_2 H_4 - \tau C_{11} C_{10} N_4 H_4$ (63)	$\tau CCOH$, $\tau CCNH$
	35	3	44	$S_{45} = \delta C_7 O_2 H_4 - \delta C_{10} N_4 H_4 + \delta N_4 H_4 O_2$ (83)	δCOH , δCNH , δNHO
	19	0.5	29	$S_{96} = \tau C_1 C_7 O_2 H_4 - \tau C_{12} N_4 H_4 O_2 + \tau C_7 O_2 H_4 N_4 + \tau C_2 C_1 C_7 O_2$ (86)	$\tau CCOH$, $\tau CNHO$, $\tau COHN$, $\tau CCCO$
	15	0.5	25	$S_{77} = \tau C_7 O_2 H_4 N_4$ (15) $S_{95} = \tau C_{12} N_4 H_4 O_2 - \tau C_7 O_2 H_4 N_4 - \tau C_{11} C_{10} N_4 H_4 - \tau C_1 C_7 O_2 H_4$ (76)	$\tau COHN$, $\tau CNHO$, $\tau CCNH$, $\tau CCOH$

^a wavenumbers (cm^{-1}); vs – very strong, s – strong, m – medium, w – weak, vw – very weak, sh – shoulder;

^b Calculated infrared intensities in $\text{km}\cdot\text{mol}^{-1}$;

^c Scaling Eqs. $\tilde{\nu}_{\text{pred}} = 0.9594\tilde{\nu}_{\text{calc}} + 10.8$; $r = 0.9981$;

^d PED – the potential energy distribution, % in bracket;

^e Abbreviations: v – stretching, δ – in-plane deformation, γ – out-of-plane deformation, τ – torsion;

^f Absent in the theoretical spectrum.

Tab. S11. Internal coordinates (PED) used in the normal modes analysis for TBR-26DHBA (Ia), calculated frequencies, PED (%) and descriptions.

Local group coordinates	Calculated frequencies (cm^{-1}), PED (%)	Descriptions ^a
$S_1 = \nu\text{O}_3\text{H}_3$	3650 (99)	vOH
$S_2 = \nu\text{O}_4\text{H}_{4A}$	3409 (99)	vOH
$S_3 = \nu\text{N}_1\text{H}_1$	3627 (100)	vNH
$S_4 = \nu\text{O}_2\text{H}_4$	2649 (88)	vOH
$S_5 = \nu\text{C}_{12}\text{H}_{12}$	3279 (99)	vCH
$S_6 = \nu\text{C}_{13}\text{H}_{13B}$	3192 (86), 3066 (14)	vCH
$S_7 = \nu\text{C}_{13}\text{H}_{13A} - \nu\text{C}_{13}\text{H}_{13C}$	3137 (100)	vCH
$S_8 = \nu\text{C}_{13}\text{H}_{13A} + \nu\text{C}_{13}\text{H}_{13C}$	3192 (14), 3066 (86)	vCH
$S_9 = \nu\text{C}_{14}\text{H}_{14B} - \nu\text{C}_{14}\text{H}_{14C}$	3166 (100)	vCH
$S_{10} = \nu\text{C}_{14}\text{H}_{14A} + \nu\text{C}_{14}\text{H}_{14B} + \nu\text{C}_{14}\text{H}_{14C}$	3082 (99)	vCH
$S_{11} = \nu\text{C}_{14}\text{H}_{14B} - \nu\text{C}_{14}\text{H}_{14A} + \nu\text{C}_{14}\text{H}_{14C}$	3180 (99)	vCH
$S_{12} = \nu\text{C}_3\text{H}_3 - \nu\text{C}_5\text{H}_5$	3219 (97)	vCH
$S_{13} = \nu\text{C}_3\text{H}_3 + \nu\text{C}_5\text{H}_5$	3223 (87), 3186 (10)	vCH
$S_{14} = \nu\text{C}_4\text{H}_4$	3223 (10), 3186 (90)	vCH
$S_{15} = \nu\text{N}_4\text{H}_4$	2649 (10), 111 (56), 78 (10)	vNH
$S_{16} = \nu\text{C}_8\text{O}_5$	1804 (11), 1796 (57), 1433 (10)	vCO
$S_{17} = \nu\text{C}_8\text{O}_5 + \nu\text{C}_9\text{O}_6$	1804 (71), 1796 (10)	vCO
$S_{18} = \nu\text{C}_7\text{O}_1$	1727 (48)	vCO
$S_{19} = \nu\text{C}_{10}\text{C}_{11} - \nu\text{C}_{10}\text{N}_2$	1660 (69)	vCO
$S_{20} = \nu\text{C}_{12}\text{N}_4 + \nu\text{C}_9\text{N}_2 - \nu\text{C}_{10}\text{N}_4$	1368 (45)	vCN
$S_{21} = \nu\text{C}_{12}\text{N}_3$	1564 (12), 1556 (28), 1096 (15)	vCN
$S_{22} = \nu\text{C}_4\text{C}_5 - \nu\text{C}_1\text{C}_2$	1444 (15), 1350 (32)	vCC
$S_{23} = \nu\text{C}_2\text{C}_3$	1266 (16), 1079 (12)	vCC
$S_{24} = \nu\text{C}_2\text{C}_3 + \nu\text{C}_5\text{C}_6 + \nu\text{C}_7\text{O}_1$	1688 (45), 1300 (15), 772 (11)	vCC, vCO
$S_{25} = \nu\text{C}_3\text{C}_4 + \nu\text{C}_4\text{C}_5$	1688 (12), 1085 (44), 613 (11)	vCC
$S_{26} = \nu\text{C}_{10}\text{N}_4 - \nu\text{C}_9\text{N}_1$	1205 (24), 452 (12)	vCN
$S_{27} = \nu\text{C}_{10}\text{C}_{11} + \nu\text{C}_{10}\text{N}_2$	1069 (12)	vCC, vCN
$S_{28} = \nu\text{C}_7\text{O}_2$	1300 (19), 1145 (26), 833 (13)	vCO
$S_{29} = \nu\text{C}_1\text{C}_2 + \nu\text{C}_4\text{C}_5 - \nu\text{C}_3\text{C}_4$	1639 (58), 1192 (11)	vCC
$S_{30} = \nu\text{C}_2\text{O}_3 + \nu\text{C}_6\text{O}_4$	1266 (25), 1079 (39)	vCO
$S_{31} = \nu\text{C}_2\text{O}_3 + \nu\text{C}_6\text{O}_4$	1411 (10), 1396 (16), 1360 (21), 772 (12), 613 (10)	vCO
$S_{32} = \nu\text{C}_9\text{N}_1 + \nu\text{C}_{10}\text{N}_4$	617 (48)	vCN
$S_{33} = \nu\text{C}_8\text{N}_1 - \nu\text{C}_9\text{N}_1$	1158 (39)	vCN
$S_{34} = \nu\text{C}_9\text{N}_1 + \nu\text{C}_{12}\text{N}_4 - \nu\text{C}_9\text{N}_2$	1469 (19), 1396 (11), 1224 (10), 967 (10)	vCN
$S_{35} = \nu\text{C}_1\text{C}_2$	613 (13), 398 (13)	vCC
$S_{36} = \nu\text{C}_{13}\text{N}_2$	1331 (17), 1224 (15), 1069 (13), 814 (17)	vCN
$S_{37} = \nu\text{C}_{14}\text{N}_3$	1271 (13), 814 (18), 698 (19)	vCN

$S_{38} = \delta C_2 C_3 C_4 + \delta C_3 C_4 C_5 + \delta C_4 C_5 C_6$	1536 (14), 1360 (22), 613 (18), 455 (11)	δCCC
$S_{39} = \delta C_{11} N_3 C_{14} + \delta C_{11} C_{10} N_2$	214 (48)	$\delta CNC, \delta CCN$
$S_{40} = \delta C_2 C_3 C_4 + \delta C_4 C_5 C_6 + \delta O_1 C_7 O_2$	772 (47), 613 (23)	$\delta CCC, \delta OCO$
$S_{41} = \delta C_{11} C_{10} N_2 - \delta C_{11} N_3 C_{14} - \delta N_1 C_9 N_2 + \delta N_4 C_{12} N_3$	525 (47), 452 (11)	$\delta CCN, \delta CNC, \delta NCN$
$S_{42} = \delta C_2 O_3 H_3$	1444 (20), 1350 (22)	δCOH
$S_{43} = \delta C_6 O_4 H_{4A}$	1536 (26), 1444 (19), 1300 (14)	δCOH
$S_{44} = \delta C_8 N_1 H_1$	1433 (37), 1424 (24), 1158 (10)	δCNH
$S_{45} = \delta C_7 O_2 H_4 - \delta C_{10} N_4 H_4 + \delta N_4 H_4 O_2$	35 (83)	$\delta COH, \delta CNH, \delta NHO$
$S_{46} = \delta N_3 C_{12} H_{12}$	1224 (35), 1205 (12)	δNCH
$S_{47} = \delta H_{13B} C_{13} H_{13C} + \delta H_{13B} C_{13} H_{13A}$	1469 (10), 1433 (22), 1424 (31)	δHCH
$S_{48} = \delta H_{13B} C_{13} H_{13A}$	1495 (71), 1152 (28)	δHCH
$S_{49} = \delta H_{13A} C_{13} H_{13C} + \delta H_{14B} C_{14} H_{14A} - \delta H_{14B} C_{14} H_{14C}$	1510 (56), 1096 (12)	δHCH
$S_{50} = \delta H_{13A} C_{13} H_{13C} + \delta H_{14B} C_{14} H_{14C} - \delta H_{14B} C_{14} H_{14A}$	1500 (13), 1491 (46)	δHCH
$S_{51} = \delta H_{14B} C_{14} H_{14A} + \delta H_{14B} C_{14} H_{14C} + \delta H_{14A} C_{14} H_{14C}$	1454 (80)	δHCH
$S_{52} = \delta H_{14A} C_{14} H_{14C} - \delta H_{14B} C_{14} H_{14A}$	1473 (71), 1148 (28)	δHCH
$S_{53} = \delta C_4 C_3 H_3 - \delta C_4 C_5 H_5 - \delta C_5 C_4 H_4$	1192 (77)	δCCH
$S_{54} = \delta C_4 C_3 H_3 + \delta C_4 C_5 H_5$	1536 (19), 1300 (13), 1145 (22), 1085 (25)	δCCH
$S_{55} = \delta C_5 C_4 H_4 + \delta C_4 C_3 H_3$	1500 (18), 1350 (17), 1266 (25)	δCCH
$S_{56} = \delta C_7 O_2 H_4 + \delta N_4 H_4 O_2$	1727 (14), 1564 (29), 1556 (12)	$\delta COH, \delta NHO$
$S_{57} = \delta N_1 C_9 O_6$	750 (27), 428 (35)	δNCO
$S_{58} = \delta N_1 C_8 O_5 + \delta C_9 N_1 C_8$	814 (21), 452 (12)	$\delta NCO, \delta CNC$
$S_{59} = \delta C_9 N_1 C_8 + \delta N_1 C_9 N_2 - \delta N_1 C_8 O_5$	750 (10), 373 (48)	$\delta CNC, \delta NCN, \delta NCO$
$S_{60} = \delta C_3 C_4 C_5 - \delta C_4 C_5 C_6 + \delta O_1 C_7 O_2$	833 (50)	$\delta CCC, \delta OCO$
$S_{61} = \delta C_1 C_2 C_3 - \delta C_7 C_1 C_2$	340 (59)	δCCC
$S_{62} = \delta C_4 C_5 C_6 - \delta C_2 C_3 C_4 + \delta C_3 C_2 O_3 - \delta C_1 C_7 O_2 - \delta C_5 C_6 O_4$	592 (77)	$\delta CCC, \delta CCO$
$S_{63} = \delta C_{10} N_4 C_{12}$	1069 (18), 967 (26)	δCNC
$S_{64} = \delta C_{11} C_{10} N_2 - \delta N_4 C_{12} N_3$	1604 (25)	$\delta CCN, \delta NCN$
$S_{65} = \delta C_7 O_2 H_4 + \delta C_{10} N_4 H_4$	78 (68)	$\delta COH, \delta CNH$
$S_{66} = \delta C_1 C_2 C_3$	1145 (11), 446 (10), 398 (11)	δCCC
$S_{67} = \delta C_6 C_5 O_4$	455 (59), 398 (14)	δCCO
$S_{68} = \delta C_1 C_7 O_2 + \delta C_3 C_2 O_3 + \delta C_5 C_6 O_4$	446 (35), 398 (25)	δCCO
$S_{69} = \delta C_9 N_2 C_{10}$	1331 (18), 452 (18)	δCNC
$S_{70} = \delta N_4 C_{12} N_3 + \delta N_1 C_9 N_2$	698 (34)	δNCN
$S_{71} = \delta C_4 C_5 C_6 - \delta C_2 C_3 C_4 + \delta C_1 C_7 O_1 + \delta C_5 C_6 O_4 - \delta C_3 C_2 O_3$	539 (63)	$\delta CCC, \delta CCO$
$S_{72} = \delta C_9 N_2 C_{13}$	318 (63)	δCNC
$S_{73} = \delta C_{11} C_{10} N_4 - \delta C_{11} N_3 C_{14}$	750 (17), 214 (23)	$\delta CCN, \delta CNC$
$S_{74} = \tau C_1 C_2 O_3 H_3$	620 (82)	τCOH
$S_{75} = \tau C_1 C_6 O_4 H_{4A} - \gamma C_7 O_2 C_1 O_1$	805 (10), 800 (11), 762 (67)	$\tau COH, \gamma COCO$
$S_{76} = \tau C_{10} N_4 C_{12} N_3$	619 (54)	$\tau CNCN$
$S_{77} = \tau C_7 O_2 H_4 N_4$	1076 (73), 15 (15)	$\tau COHN$
$S_{78} = \tau C_{10} N_4 C_{12} H_{12}$	884 (86)	$\tau CNCH$
$S_{79} = \tau C_9 N_2 C_{13} H_{13B} - \tau C_9 N_2 C_{13} H_{13A}$	1495 (29), 1152 (70)	$\tau CNCH$
$S_{80} = \tau C_9 N_2 C_{13} H_{13C} + \tau C_9 N_2 C_{13} H_{13A} + \tau C_9 N_2 C_{13} H_{13B}$	119 (73), 107 (10)	$\tau CNCH$

$S_{81} = \tau C_9 N_2 C_{13} H_{13C} - \tau C_9 N_2 C_{13} H_{13A}$	1510 (12), 1271 (16), 1205 (15), 1069 (16), 967 (16)	$\tau CNCH$
$S_{82} = \tau C_{12} N_3 C_{14} H_{14B} - \tau C_{12} N_3 C_{14} H_{14C}$	1510 (10), 1096 (44)	$\tau CNCH$
$S_{83} = \tau C_{12} N_3 C_{14} H_{14A} - \tau C_{12} N_3 C_{14} H_{14B}$	1473 (29), 1148 (69)	$\tau CNCH$
$S_{84} = \tau C_{12} N_3 C_{14} H_{14A} + \tau C_{12} N_3 C_{14} H_{14B} + \tau C_{12} N_3 C_{14} H_{14C}$	58 (74)	$\tau CNCH$
$S_{85} = \tau C_5 C_4 C_3 H_3\cdot + \tau C_3 C_4 C_5 H_5\cdot$	871 (84), 634 (14)	$\tau CCCH$
$S_{86} = \tau C_3 C_4 C_5 H_5\cdot - \tau C_5 C_4 C_3 H_3\cdot - \tau C_6 C_5 C_4 H_4\cdot$	805 (41), 800 (10), 762 (14), 702 (24)	$\tau CCCH$
$S_{87} = \tau C_6 C_5 C_4 H_4\cdot$	988 (75), 480 (19)	$\tau CCCH$
$S_{88} = \tau C_1 C_7 O_2 H_4 + \tau C_{12} N_4 H_4 O_2 - \tau C_2 C_1 C_7 O_2$	121 (10), 77 (61)	$\tau CCOH$, $\tau CNHO$, $\tau CCCO$
$S_{89} = \tau C_{11} C_{10} N_4 C_{12} - \gamma C_{10} N_4 C_{11} N_2$	364 (53), 90 (13)	$\tau CCNC$, $\gamma CNCN$
$S_{90} = \tau C_1 C_2 C_3 C_4 + \tau C_7 C_1 C_2 C_3 + \gamma C_6 C_5 C_1 O_4$	259 (57), 121 (23)	$\tau CCCC$, $\gamma CCCO$
$S_{91} = \tau C_2 C_3 C_4 C_5 + \tau C_3 C_4 C_5 C_6$	225 (80)	$\tau CCCC$
$S_{92} = \tau C_1 C_2 C_3 C_4 + \tau C_3 C_4 C_5 C_6 - \tau C_2 C_3 C_4 C_5$	988 (10), 805 (27), 702 (47)	$\tau CCCC$
$S_{93} = \tau C_7 C_1 C_2 C_3$	259 (25), 121 (40), 77 (11)	$\tau CCCC$
$S_{94} = \tau C_{11} C_8 N_1 H_1 + \tau C_{10} N_4 C_{12} N_3$	640 (77)	$\tau CCNH$, $\tau CNCN$
$S_{95} = \tau C_{12} N_4 H_4 O_2 - \tau C_7 O_2 H_4 N_4 - \tau C_{11} C_{10} N_4 H_4 - \tau C_1 C_7 O_2 H_4$	1076 (14), 15 (76)	$\tau CNHO$, $\tau COHN$, $\tau CCNH$, $\tau CCOH$
$S_{96} = \tau C_1 C_7 O_2 H_4 - \tau C_{12} N_4 H_4 O_2 + \tau C_7 O_2 H_4 N_4 + \tau C_2 C_1 C_7 O_2$	19 (86)	$\tau CCOH$, $\tau CNHO$, $\tau COHN$, $\tau CCCO$
$S_{97} = \tau C_9 N_2 C_{10} N_4 + \tau C_8 N_1 C_9 N_2$	149 (60)	$\tau CNCN$
$S_{98} = \tau C_{10} N_2 C_9 N_1 + \tau C_9 N_2 C_{10} N_4$	198 (54)	$\tau CNCN$
$S_{99} = \tau C_{10} N_2 C_9 N_1 + \tau C_8 N_1 C_9 N_2 - \tau C_9 N_2 C_{10} N_4$	228 (16), 198 (10), 107 (18), 90 (45)	$\tau CNCN$
$S_{100} = \tau C_1 C_7 O_2 H_4 - \tau C_{11} C_{10} N_4 H_4$	58 (14), 46 (63)	$\tau CCOH$, $\tau CCNH$
$S_{101} = \tau C_{11} C_{10} N_4 C_{12} + \gamma C_{10} N_4 C_{11} N_2 + \gamma C_9 N_2 N_1 O_6$	753 (76), 714 (10)	$\tau CCNC$, $\gamma CNCN$, $\gamma CNNO$
$S_{102} = \gamma C_8 N_1 C_{11} O_5 + \gamma C_9 N_2 N_1 O_6$	763 (89)	$\gamma CNCO$, $\gamma CNNO$
$S_{103} = \tau C_2 C_3 C_4 C_5 - \tau C_3 C_4 C_5 C_6 - \gamma C_6 C_5 C_1 O_4 + \gamma C_2 C_3 C_1 O_3$	480 (64)	$\tau CCCC$, $\gamma CCCO$
$S_{104} = \gamma C_6 C_5 C_1 O_4 + \gamma C_2 C_3 C_1 O_3$	871 (13), 634 (69)	$\gamma CCCO$
$S_{105} = \gamma C_{13} C_{10} C_9 N_2 + \gamma C_{14} C_{11} C_{12} N_3$	364 (29), 198 (14), 107 (45)	$\gamma CCCN$
$S_{106} = \gamma C_{14} C_{11} C_{12} N_3 - \gamma C_{13} C_{10} C_9 N_2$	228 (67), 107 (10)	$\gamma CCCN$
$S_{107} = \gamma C_7 O_2 C_1 O_1$	800 (56), 702 (12)	$\gamma COCO$
$S_{108} = \tau C_{11} C_{10} N_4 C_{12} + \gamma C_{10} N_{14} C_{11} N_2 - \gamma C_8 N_1 C_{11} O_5$	714 (67), 619 (13)	$\tau CCNC$, $\gamma CNCN$, $\gamma CNCO$

^a ν – stretching, δ – in-plane deformation, γ – out-of-plane deformation, τ – torsion.

Tab. S12. Experimental FTIR (II) and IR spectra (IIa) calculated by the APD-F/6-311++G(d,p) approach for CAF-26DHBA.

II	IIa				
$\tilde{\nu}_{\text{exp}}^{\text{a}}$	$\tilde{\nu}_{\text{calc}}$	$A_{\text{calc}}^{\text{b}}$	$\tilde{\nu}_{\text{pred}}^{\text{c}}$	Assignments, PED (%) ^{d,e}	Descriptions ^e
3420	3645	437	3487	$S_1 = \nu O_3 H_3$ (99)	vOH
	3404	467	3258	$S_2 = \nu O_4 H_{4A}$ (99)	vOH
3123	3278	52	3137	$S_4 = \nu C_{12} H_{12}$ (99)	vCH
	3223	1	3085	$S_{15} = \nu C_5 H_5$ + $\nu C_3 H_3$ (85)	vCH
	3218	3	3080	$S_{14} = \nu C_5 H_5$ – $\nu C_3 H_3$ (95)	vCH
	3197	0.5	3060	$S_6 = \nu C_{13} H_{13B}$ (81) $S_7 = \nu C_{13} H_{13A} + \nu C_{13} H_{13C}$	vCH
	3195	0.5	3058	$S_8 = \nu C_{14} H_{14A}$ (87) $S_{10} = \nu C_{14} H_{14B} + \nu C_{14} H_{14C}$ (13)	vCH
	3185	10	3049	$S_{15} = \nu C_5 H_5$ + $\nu C_3 H_3$ (15) $S_{16} = \nu C_4 H_4$ (90)	vCH
	3179	3	3043	$S_{12} = \nu C_{15} H_{15A} + \nu C_{15} H_{15B} - \nu C_{15} H_{15C}$ (99)	vCH
	3166	3	3031	$S_{11} = \nu C_{15} H_{15A} - \nu C_{15} H_{15B}$ (100)	vCH
3055	3152	10	3017	$S_5 = \nu C_{13} H_{13A} - \nu C_{13} H_{13C}$ (100)	vCH
	3136	10	3002	$S_9 = \nu C_{14} H_{14B} - \nu C_{14} H_{14C}$ (100)	vCH
	3082	15	2950	$S_{13} = \nu C_{15} H_{15A} + \nu C_{15} H_{15B} + \nu C_{15} H_{15C}$ (99)	vCH
	3080	23	2949	$S_6 = \nu C_{13} H_{13B}$ (19), $S_7 = \nu C_{13} H_{13A} + \nu C_{13} H_{13C}$ (81)	vCH
2949	3065	37	2934	$S_8 = \nu C_{14} H_{14A}$ (13) $S_{10} = \nu C_{14} H_{14B} + \nu C_{14} H_{14C}$ (87)	vCH
2573	2606	3257	2497	$S_3 = \nu O_1 H_4$ (88) $S_{17} = \nu N_4 H_4$ (10)	vOH vNH
1718	1793	503	1721	$S_{19} = \nu C_9 O_6 + \nu C_8 O_5$ (73)	vCO
1673	1756	979	1686	$S_{18} = \nu C_9 O_6 - \nu C_8 O_5$ (71)	vCO
	1728	377	1659	$S_{20} = \nu C_7 O_2$ (47) $S_{70} = \delta C_7 O_1 H_4 - \delta N_4 H_4 O_1$ (13)	vCO, δ COH, δ NHO
1639	1689	301	1622	$S_{26} = \nu C_2 C_3 + \nu C_5 C_6 + \nu C_7 O_2$ (43) $S_{27} = \nu C_3 C_4 + \nu C_4 C_5$ (12)	vCC, vCO
1598	1674	24	1608	$S_{21} = \nu C_{10} C_{11} - \nu C_{10} N_2$ (68)	vCC, vCN
1579 ^f					
1565	1639	151	1574	$S_{31} = \nu C_1 C_2 + \nu C_4 C_5 - \nu C_3 C_4$ (58)	vCC
1552	1608	353	1545	$S_{29} = \nu C_{10} C_{11} + \nu C_{10} N_2$ (13) $S_{34} = \nu C_9 N_2$ (10) $S_{42} = \delta C_{11} C_{10} N_4 - \delta C_{11} C_{10} N_2$ (20)	vCC, vCN, δ CCN
1530	1567	145	1506	$S_{23} = \nu C_{12} N_3$ (17) $S_{70} = \delta C_7 O_1 H_4 - \delta N_4 H_4 O_1$ (23)	vCN, δ COH, δ NHO
1499	1558	43	1497	$S_{23} = \nu C_{12} N_3$ (26) $S_{70} = \delta C_7 O_1 H_4 - \delta N_4 H_4 O_1$ (13)	vCN, δ COH, δ NHO
1459	1537	4	1477	$S_{41} = \delta C_2 C_3 C_4 + \delta C_3 C_4 C_5 + \delta C_4 C_5 C_6$ (15) $S_{46} = \delta C_6 O_4 H_{4A}$ (26) $S_{59} = \delta C_4 C_5 H_5 + \delta C_4 C_3 H_3$ (21)	δ CCC, δ COH, δ CCH
1447	1510	46	1451	$S_{54} = \delta H_{14B} C_{14} H_{14C} + \delta H_{15A} C_{15} H_{15C} - \delta H_{15A} C_{15} H_{15B}$ (57) $S_{88} = \tau C_{10} N_2 C_{14} H_{14B} - \tau C_{10} N_2 C_{14} H_{14C}$ (10) $S_{91} = \tau C_{11} N_3 C_{15} H_{15B} - \tau C_{11} N_3 C_{15} H_{15A}$ (11)	δ HCH, τ CNCH

1438	1503	79	1445	$S_{49} = \delta H_{13A}C_{13}H_{13C}$ (44) $S_{84} = \tau C_8N_1C_{13}H_{13A} - \tau C_8N_1C_{13}H_{13C}$ (15)	$\delta HCH, \tau CNCH$
	1501	216	1443	$S_{49} = \delta H_{13A}C_{13}H_{13C}$ (23) $S_{60} = \delta C_3C_4H_4^+$ (10)	$\delta HCH, \delta CCH$
	1496	13	1438	$S_{53} = \delta H_{14A}C_{14}H_{14B}$ (73) $S_{87} = \tau C_{10}N_2C_{14}H_{14B} - \tau C_{10}N_2C_{14}H_{14A}$ (27)	$\delta HCH, \tau CNCH$
	1493	7	1435	$S_{56} = \delta H_{15B}C_{15}H_{15C} + \delta H_{14B}C_{14}H_{14C} - \delta H_{15A}C_{15}H_{15B}$ (45)	δHCH
	1486	12	1429	$S_{51} = \delta H_{13B}C_{13}H_{13C} - \delta H_{13A}C_{13}H_{13B}$ (73) $S_{85} = \tau C_8N_1C_{13}H_{13A} - \tau C_8N_1C_{13}H_{13B} - \tau C_{10}N_2C_{14}H_{14A} + \tau C_{10}N_2C_{14}H_{14B}$ (27)	$\delta HCH, \tau CNCH$
1410	1472	61	1415	$S_{28} = vC_{10}N_4$ (13)	vCN
	1471	14	1414	$S_{55} = \delta H_{15A}C_{15}H_{15C} - \delta H_{15B}C_{15}H_{15C}$ (71) $S_{90} = \tau C_{11}N_3C_{15}H_{15C} - \tau C_{11}N_3C_{15}H_{15A}$ (29)	$\delta HCH, \tau CNCH$
	1454	29	1398	$S_{57} = \delta H_{15A}C_{15}H_{15B} + \delta H_{14B}C_{14}H_{14C} - \delta H_{15A}C_{15}H_{15C}$ (83)	δHCH
1390	1446	142	1390	$S_{24} = vC_4C_5 - vC_1C_6$ (15) $S_{45} = \delta C_2O_3H_3$ (20) $S_{46} = \delta C_6O_4H_{4A}$ (19)	$vCN, \delta COH$
	1439	30	1384	$S_{50} = \delta H_{13A}C_{13}H_{13C} + \delta H_{13A}C_{13}H_{13B}$ (50)	δHCH
	1428	4	1373	$S_{22} = vC_{12}N_4$ (10) $S_{52} = \delta H_{14A}C_{14}H_{14B} + \delta H_{14A}C_{14}H_{14C}$ (54)	$vCN, \delta HCH$
1358	1411	285	1357	$S_{23} = vC_{12}N_3$ (11) $S_{30} = vC_7O_1$ (10)	vCN, vCO
	1398	87	1345	$S_{33} = vC_2O_3 + vC_6O_4$ (33)	vCO
1322	1382	110	1329	$S_{22} = vC_{12}N_4$ (33)	vCN
	1360	83	1308	$S_{33} = vC_2O_3 + vC_6O_4$ (24) $S_{41} = \delta C_2C_3C_4 + \delta C_3C_4C_5 + \delta C_4C_5C_6$ (23) $S_{46} = \delta C_6O_4H_{4A}$ (10)	$vCO, \delta CCC, \delta COH$
	1350	58	1299	$S_{24} = vC_4C_5 - vC_1C_6$ (33) $S_{45} = \delta C_2O_3H_3$ (22) $S_{60} = \delta C_3C_4H_4^+$ (13)	$vCC, \delta COH, \delta CCH$
	1331	57	1281	$S_{28} = vC_{10}N_4$ (14) $S_{38} = vC_{14}N_2$ (16) $S_{74} = \delta C_9N_2C_{10}$ (16)	$vCN, \delta CNC$
	1301	283	1252	$S_{26} = vC_2C_3 + vC_5C_6 + vC_7O_2$ (16) $S_{30} = vC_7O_1$ (20) $S_{46} = \delta C_6O_4H_{4A}$ (13) $S_{59} = \delta C_4C_5H_5^- + \delta C_4C_3H_3^-$ (13)	$vCC, vCO, \delta COH, \delta CCH$
	1286	46	1238	$S_{37} = vC_8N_1 + vC_{12}N_4$ (16) $S_{49} = \delta H_{13A}C_{13}H_{13C}$ (10) $S_{84} = \tau C_8N_1C_{13}H_{13A} - \tau C_8N_1C_{13}H_{13C}$ (22)	$vCN, \delta HCH, \tau CNCH$
1217	1273	91	1225	$S_{64} = \delta N_4C_{12}N_3 + \delta C_9N_1C_8$ (13) $S_{88} = \tau C_{10}N_2C_{14}H_{14B} - \tau C_{10}N_2C_{14}H_{14c}$ (15)	$\delta NCN, \delta CNC, \tau CNCH$
	1267	158	1220	$S_{25} = vC_2C_3$ (17) $S_{32} = vC_6O_4 - vC_2O_3$ (25) $S_{60} = \delta C_3C_4H_4^+$ (27)	$vCC, vCO, \delta CCH$
	1244	8	1198	$S_{38} = vC_{14}N_2$ (18) $S_{39} = vC_{15}N_3$ (12) $S_{40} = vC_{13}N_1$ (14)	vCN
1163	1213	194	1168	$S_{28} = vC_{10}N_4$ (11) $S_{48} = \delta N_3C_{12}H_{12}$ (42) $S_{88} = \tau C_{10}N_2C_{14}H_{14B} - \tau C_{10}N_2C_{14}H_{14c}$ (10)	$vCN, \delta NCH, \tau CNCH$
	1191	34	1147	$S_{31} = vC_1C_2 + vC_4C_5 - vC_3C_4$ (11) $S_{58} = \delta C_4C_5H_5^- - \delta C_4C_3H_3^- - \delta C_3C_4H_4^+$ (75)	$vCN, \delta CCH$

1128	1152	0.01	1110	$S_{51} = \delta H_{13B}C_{13}H_{13C} - \delta H_{13A}C_{13}H_{13B}$ (10) $S_{53} = \delta H_{14A}C_{14}H_{14B}$ (16) $S_{87} = \tau C_{10}N_2C_{14}H_{14B} - \tau C_{10}N_2C_{14}H_{14A}$ (66)	$\delta HCH, \tau CNCH$
	1150	0.5	1108	$S_{51} = \delta H_{13B}C_{13}H_{13C} - \delta H_{13A}C_{13}H_{13B}$ (16) $S_{53} = \delta H_{14A}C_{14}H_{14B}$ (10) $S_{85} = \tau C_8N_1C_{13}H_{13A} - \tau C_8N_1C_{13}H_{13B} - \tau C_{10}N_2C_{14}H_{14A} + \tau C_{10}N_2C_{14}H_{14B}$ (66)	$\delta HCH, \tau CNCH$
	1148	0.01	1106	$S_{55} = \delta H_{15A}C_{15}H_{15C} - \delta H_{15B}C_{15}H_{15C}$ (29) $S_{90} = \tau C_{11}N_3C_{15}H_{15C} - \tau C_{11}N_3C_{15}H_{15A}$ (69)	$\delta HCH, \tau CNCH$
	1146	36	1104	$S_{30} = vC_7O_1$ (25) $S_{59} = \delta C_4C_5H_5^{\cdot} + \delta C_4C_3H_3^{\cdot}$ (22)	$vCO, \delta CCH$
1061	1098	16	1059	$S_{23} = vC_{12}N_3$ (12) $S_{54} = \delta H_{14B}C_{14}H_{14C} + \delta H_{15A}C_{15}H_{15C} - \delta H_{15A}C_{15}H_{15B}$ (14) $S_{91} = \tau C_{11}N_3C_{15}H_{15B} - \tau C_{11}N_3C_{15}H_{15A}$ (47)	$vCN, \delta HCH, \tau CNCH$
	1090	1	1051	$S_{34} = vC_9N_2$ (12) $S_{40} = vC_{13}N_1$ (13) $S_{68} = \delta C_{10}N_4C_{12}$ (11) $S_{88} = \tau C_{10}N_2C_{14}H_{14B} - \tau C_{10}N_2C_{14}H_{14C}$ (21)	$vCN, \delta CNC, \tau CNCH$
1050	1087	61	1048	$S_{103} = \tau C_{10}N_4H_4O_1 + \tau C_7O_1H_4N_4 - \tau C_1C_7O_1H_4$ (20) $S_{107} = \tau C_7O_1H_4N_4$	$\tau CNHO, \tau COHN, \tau CCOH,$
	1084	5	1045	$S_{27} = vC_3C_4 + vC_4C_5$ (43) $S_{59} = \delta C_4C_5H_5^{\cdot} + \delta C_4C_3H_3^{\cdot}$ (26)	$vCC, \delta CCH$
1031	1079	34	1040	$S_{24} = vC_4C_5 - vC_1C_6$ (10) $S_{25} = vC_2C_3$ (13) $S_{32} = vC_6O_4 - vC_2O_3$ (41) $S_{60} = \delta C_3C_4H_4^{\cdot}$ (15) $S_{76} = \delta C_4C_5C_6 - \delta C_2C_3C_4$ (10)	$vCC, vCO, \delta CCH, \delta CCC$
1000	1058	61	1020	$S_{35} = vC_9N_1$ (16) $S_{37} = vC_8N_1 + vC_{12}N_4$ (11) $S_{38} = vC_{14}N_2$ (13) $S_{68} = \delta C_{10}N_4C_{12}$ (12) $S_{84} = \tau C_8N_1C_{13}H_{13A} - \tau C_8N_1C_{13}H_{13C}$ (18)	$vCN, \delta CNC, \tau CNCH$
	1016	42	980	$S_{37} = vC_8N_1 + vC_{12}N_4$ (10) $S_{38} = vC_{14}N_2$ (21) $S_{40} = vC_{13}N_1$ (20)	vCN
947	988	0.1	954	$S_{95} = \tau C_2C_3C_4H_4^{\cdot} - \tau C_3C_4C_5H_5^{\cdot}$ (75) $S_{99} = \tau C_6C_5C_4C_3 - \tau C_2C_3C_4C_5$ (17)	$\tau CCCH, \tau CCCC$
	960	5	927	$S_{40} = vC_{13}N_1$ (15) $S_{68} = \delta C_{10}N_4C_{12}$ (16)	$vCN, \delta CNC$
874	881	16	852	$S_{83} = \tau C_{10}N_4C_{12}H_{12}$ (87)	$\tau CNCH$
833	871	0.4	842	$S_{93} = \tau C_3C_4C_5H_5^{\cdot} + \tau C_5C_4C_3H_3^{\cdot}$ (83) $S_{111} = \gamma C_6C_5C_1O_4 + \gamma C_2C_3C_1O_3$ (14)	$\tau CCCH, \gamma CCCO$
	840	5	813	$S_{42} = \delta C_{11}C_{10}N_4 - \delta C_{11}C_{10}N_2$ (11) $S_{62} = \delta N_1C_9O_6 - \delta C_9N_2C_{10}$ (20) $S_{64} = \delta N_4C_{12}N_3 + \delta C_9N_1C_8$ (10)	$\delta CCC, \delta NCO, \delta CNC, \delta NCN$
	834	13	807	$S_{30} = vC_7O_1$ (12) $S_{65} = \delta C_3C_4C_5 - \delta C_4C_5C_6 + \delta O_1C_7O_2$ (51)	$vCO, \delta CCC, \delta OCO$
772	805	32	779	$S_{81} = \gamma C_7O_1C_1O_2$ (10) $S_{94} = \tau C_2C_3C_4H_4^{\cdot} + \tau C_5C_4C_3H_3^{\cdot} - \tau C_3C_4C_5H_5^{\cdot}$ (40) $S_{100} = \tau C_2C_3C_1O_3 - \tau C_6C_5C_1O_4 - \tau C_2C_3C_4C_5$ (36)	$\gamma COCO, \tau CCCH, \tau CCCO, \tau CCCC$
	801	22	775	$S_{81} = \gamma C_7O_1C_1O_2$ (55) $S_{94} = \tau C_2C_3C_4H_4^{\cdot} + \tau C_5C_4C_3H_3^{\cdot} - \tau C_3C_4C_5H_5^{\cdot}$ (15) $S_{116} = \tau C_1C_6O_4H_{4A} + \gamma C_7O_1C_1O_2$ (15)	$\gamma COCO, \tau CCCH, \gamma CCOH$
756	774	27	750	$S_{39} = vC_{15}N_3$ (19) $S_{63} = \delta C_{11}C_8O_5$ (12)	$vCN, \delta CCO$

744	772	22	748	$S_{26} = vC_2C_3 + vC_5C_6 + vC_7O_2$ (11) $S_{33} = vC_2O_3 + vC_6O_4$ (11) $S_{67} = \delta C_2C_3C_4 + \delta C_4C_5C_6 + \delta O_1C_7O_2$ (43)	vCC, vCO, δCCC , δOCO
	766	0.3	742	$S_{110} = \gamma C_9N_1N_2O_6 + \gamma C_8N_1C_{11}O_5$ (92)	$\gamma CNNO$, $\gamma CNCO$
	763	106	739	$S_{94} = \tau C_2C_3C_4H_4^+ + \tau C_5C_4C_3H_3^- - \tau C_3C_4C_5H_5^-$ (17) $S_{116} = \tau C_1C_6O_4H_{4A} + \gamma C_7O_1C_1O_2$ (66)	$\tau CCCH$, $\gamma CCOH$, $\gamma COCO$
710	760	13	736	$S_{109} = \tau C_{11}C_{10}N_4C_{12} - \gamma C_{12}N_4C_{11}N_2 + \gamma C_9N_1N_2O_6$ (75)	$\tau CCNC$, $\gamma CNCN$, $\gamma CNCN$
	703	3	682	$S_{97} = \tau C_{11}C_{10}N_4C_{12} + \tau C_{10}N_4C_{11}N_2 - \tau C_8N_1C_{11}O_5$ (44) $S_{100} = \tau C_2C_3C_1O_3 - \tau C_6C_5C_1O_4 - \tau C_2C_3C_4C_5$ (15)	$\tau CCNC$, $\tau CNCN$, $\tau CNCO$, $\tau CCCO$, $\tau CCCC$
	702	4	681	$S_{94} = \tau C_2C_3C_4H_4^+ + \tau C_5C_4C_3H_3^- - \tau C_3C_4C_5H_5^-$ (10) $S_{97} = \tau C_{11}C_{10}N_4C_{12} + \tau C_{10}N_4C_{11}N_2 - \tau C_8N_1C_{11}O_5$ (33) $S_{100} = \tau C_2C_3C_1O_3 - \tau C_6C_5C_1O_4 - \tau C_2C_3C_4C_5$ (21)	$\tau CCCH$, $\tau CCNC$, $\tau CNCN$, $\tau CNCO$, $\tau CCCO$, $\tau CCCC$
647	660	2	641	$S_{39} = vC_{15}N_3$ (11) $S_{44} = \delta C_9N_1C_8 - \delta N_4C_{12}N_3$ (30)	vCN , δCNC , δNCN
612	634	11	616	$S_{93} = \tau C_3C_4C_5H_5^- + \tau C_5C_4C_3H_3^-$ (12) $S_{111} = \gamma C_6C_5C_1O_4 + \gamma C_2C_3C_1O_3$ (64)	$\tau CCCH$, $\gamma CCCO$
	625	79	608	$S_{80} = \tau C_1C_2O_3H_3 - \tau C_{10}N_4C_{12}N_3$ (14) $S_{102} = \tau C_1C_2O_3H_3 + \tau C_{10}N_4C_{12}N_3$ (59)	$\tau CCOH$, $\tau CNCN$
	623	16	606	$S_{80} = \tau C_1C_2O_3H_3 - \tau C_{10}N_4C_{12}N_3$ (61) $S_{102} = \tau C_1C_2O_3H_3 + \tau C_{10}N_4C_{12}N_3$ (14)	$\tau CCOH$, $\tau CNCN$
	614	3	597	$S_{27} = vC_3C_4 + vC_4C_5$ (11) $S_{33} = vC_2O_3 + vC_6O_4$ (10) $S_{36} = vC_1C_7$ (13) $S_{41} = \delta C_2C_3C_4 + \delta C_3C_4C_5 + \delta C_4C_5C_6$ (18) $S_{67} = \delta C_2C_3C_4 + \delta C_4C_5C_6 + \delta O_1C_7O_2$ (23)	vCC, vCO, δCCC , δOCO
579	593	25	577	$S_{73} = \delta C_4C_5C_6 - \delta C_2C_3C_4 - \delta C_1C_7O_1 - \delta C_5C_6O_4 + \delta C_3C_2O_3$ (73)	δCCC , δCCO
546	563	0.1	548	$S_{34} = vC_9N_2$ (10) $S_{35} = vC_9N_1$ (13) $S_{69} = \delta C_{12}N_3C_{15}$ (13)	vCN , δCNC
	539	21	525	$S_{76} = \delta C_4C_5C_6 - \delta C_2C_3C_4$ (66)	δCCC
	484	41	473	$S_{34} = vC_9N_2$ (17) $S_{75} = \delta N_1C_9N_2$ (23)	vCN , δNCN
486	480	3	469	$S_{95} = \tau C_2C_3C_4H_4^+ - \tau C_3C_4C_5H_5^-$ (16) $S_{99} = \tau C_6C_5C_4C_3 - \tau C_2C_3C_4C_5$ (66)	$\tau CCCH$, $\tau CCCCC$
457	455	6	445	$S_{35} = vC_9N_1$ (10) $S_{62} = \delta N_1C_9O_6 - \delta C_9N_2C_{10}$ (24) $S_{72} = \delta C_5C_6O_4 - \delta C_1C_7O_1$ (22)	vCN , δNCO , δCNC , δCCO
439	454	31	444	$S_{72} = \delta C_5C_6O_4 - \delta C_1C_7O_1$ (41)	δCCO
	449	67	440	$S_{41} = \delta C_2C_3C_4 + \delta C_3C_4C_5 + \delta C_4C_5C_6$ (10) $S_{43} = \delta C_3C_2O_3 + \delta C_1C_7O_1 + \delta C_5C_6O_4$ (27)	δCCC , δCCO
	435	7	426	$S_{43} = \delta C_3C_2O_3 + \delta C_1C_7O_1 + \delta C_5C_6O_4$ (16) $S_{74} = \delta C_9N_2C_{10}$ (23) $S_{79} = \delta C_{12}N_3C_{15} - \delta C_{11}C_{10}N_2$ (10)	δCCO , δCNC , δCCN
	404	9	397	$S_{43} = \delta C_3C_2O_3 + \delta C_1C_7O_1 + \delta C_5C_6O_4$ (12) $S_{63} = \delta C_{11}C_8O_5$ (35) $S_{69} = \delta C_{12}N_3C_{15}$ (10)	δCCO , δCNC
	394	8	387	$S_{36} = vC_1C_7$ (12) $S_{43} = \delta C_3C_2O_3 + \delta C_1C_7O_1 + \delta C_5C_6O_4$ (21) $S_{63} = \delta C_{11}C_8O_5$ (11) $S_{71} = \delta C_1C_2C_3 + \delta C_2C_1C_7$ (10)	vCN , δCCO , δCCC
	371	10	365	$S_{78} = \delta C_9N_1C_{13}$ (56)	δCNC

	365	0.03	360	$S_{114} = \gamma C_{15}C_{11}C_{12}N_3 - \gamma C_{14}C_9C_{10}N_2 + \gamma C_{10}N_4C_{11}N_2 - \tau C_{11}C_{10}N_4C_{12}$ (66) $S_{117} = \tau C_{11}C_{10}N_4C_{12} - \gamma C_{14}C_9C_{10}N_2 + \gamma C_{15}C_{11}C_{12}N_3 - \gamma C_{10}N_4C_{11}N_2$ (12)	$\gamma CCCN, \gamma CNCN, \tau CCNC,$
	340	30	336	$S_{66} = \delta C_2C_1C_7$ (48) $S_{71} = \delta C_1C_2C_3 + \delta C_2C_1C_7$ (16)	δCCC
	312	3	309	$S_{77} = \delta C_9N_2C_{14}$ (64) $S_{78} = \delta C_9N_1C_{13}$ (12)	$\delta CNC,$
	272	0.03	271	$S_{105} = \tau C_{10}N_2C_9N_1 + \tau C_8N_1C_9N_2$ (10) $S_{108} = \tau C_9N_2C_{10}N_4$ (11) $S_{115} = \gamma C_{13}C_8C_9N_1$ (60)	$\tau CNCN, \gamma CCCN$
	260	0.06	259	$S_{101} = \tau C_1C_2C_3C_4 - \tau C_3C_2C_1C_7$ (17) $S_{112} = \tau C_1C_2C_3C_4 + \tau C_2C_3C_4C_5 + \tau C_3C_2C_1C_7 + \gamma C_6C_5C_2O_4$ (62)	$\tau CCCC, \gamma CCCO$
	225	0.05	226	$S_{98} = \tau C_3C_4C_5C_6 + \tau C_2C_3C_4C_5$ (76)	$\tau CCCC$
	223	0.001	224	$S_{113} = \gamma C_{14}C_9C_{10}N_2 + \gamma C_{15}C_{11}C_{12}N_3$ (58)	$\gamma CCCN$
	212	16	214	$S_{69} = \delta C_{12}N_3C_{15}$ (27) $S_{79} = \delta C_{12}N_3C_{15} - \delta C_{11}C_{10}N_2$ (43)	$\delta CNC, \delta CCN$
	159	3	163	$S_{92} = \tau C_{11}N_3C_{15}H_{15A} + \tau C_{11}N_3C_{15}H_{15B} + \tau C_{11}N_3C_{15}H_{15C}$ (12) $S_{108} = \tau C_9N_2C_{10}N_4$ (42)	$\tau CNCH, \tau CNCN$
	125	8	131	$S_{101} = \tau C_1C_2C_3C_4 - \tau C_3C_2C_1C_7$ (12) $S_{106} = \tau C_8N_1C_9N_2$ (22) $S_{115} = \gamma C_{13}C_8C_9N_1$ (10) $S_{117} = \tau C_{11}C_{10}N_4C_{12} - \gamma C_{14}C_9C_{10}N_2 + \gamma C_{15}C_{11}C_{12}N_3 - \gamma C_{10}N_4C_{11}N_2$ (14)	$\tau CCCC, \tau CNCN, \tau CCNC, \gamma CCCN, \gamma CNCN$
	121	2	127	$S_{101} = \tau C_1C_2C_3C_4 - \tau C_3C_2C_1C_7$ (35) $S_{117} = \tau C_{11}C_{10}N_4C_{12} - \gamma C_{14}C_9C_{10}N_2 + \gamma C_{15}C_{11}C_{12}N_3 - \gamma C_{10}N_4C_{11}N_2$ (11)	$\tau CCCC, \tau CCNC, \gamma CCCN, \gamma CNCN$
	115	0.06	121	$S_{86} = \tau C_{10}N_2C_{14}H_{14A} + \tau C_{10}N_2C_{14}H_{14B} + \tau C_{10}N_2C_{14}H_{14C}$ (27) $S_{89} = \tau C_8N_1C_{13}H_{13A} + \tau C_8N_1C_{13}H_{13B} + \tau C_8N_1C_{13}H_{13C}$ (14) $S_{92} = \tau C_{11}N_3C_{15}H_{15A} + \tau C_{11}N_3C_{15}H_{15B} + \tau C_{11}N_3C_{15}H_{15C}$ (11) $S_{106} = \tau C_8N_1C_9N_2$ (10) $S_{117} = \tau C_{11}C_{10}N_4C_{12} - \gamma C_{14}C_9C_{10}N_2 + \gamma C_{15}C_{11}C_{12}N_3 - \gamma C_{10}N_4C_{11}N_2$ (17)	$\tau CNCH, \tau CNCN, \tau CCNC, \gamma CCCN, \gamma CNCN$
	111	8	117	$S_{17} = vN_4H_4$ (55)	vNH
	110	0.02	116	$S_{86} = \tau C_{10}N_2C_{14}H_{14A} + \tau C_{10}N_2C_{14}H_{14B} + \tau C_{10}N_2C_{14}H_{14C}$ (53) $S_{89} = \tau C_8N_1C_{13}H_{13A} + \tau C_8N_1C_{13}H_{13B} + \tau C_8N_1C_{13}H_{13C}$ (15) $S_{113} = \gamma C_{14}C_9C_{10}N_2 + \gamma C_{15}C_{11}C_{12}N_3$ (11)	$\tau CNCH, \gamma CCCN$
	88	2	95	$S_{105} = \tau C_{10}N_2C_9N_1 + \tau C_8N_1C_9N_2$ (46) $S_{108} = \tau C_9N_2C_{10}N_4$ (11)	$\tau CNCN$
	78	0.05	86	$S_{96} = \tau N_3C_{12}N_4H_4 - \tau C_{10}N_4H_4O_1 + \tau C_2C_1C_7O_1 - \tau C_7O_1H_4N_4$ (55) $S_{103} = \tau C_{10}N_4H_4O_1 + \tau C_7O_1H_4N_4 - \tau C_1C_7O_1H_4$ (11)	$\tau NCNH, \tau CNHO, \tau CCCO, \tau COHN, \tau COOH$
	77	0.4	85	$S_{47} = \delta C_{12}N_4H_4 - \delta N_4H_4O_1 - \delta C_7O_1H_4$ (68)	$\delta CNH, \delta NHO, \delta COH$
	74	0.6	82	$S_{89} = \tau C_8N_1C_{13}H_{13A} + \tau C_8N_1C_{13}H_{13B} + \tau C_8N_1C_{13}H_{13C}$ (47) $S_{106} = \tau C_8N_1C_9N_2$ (22)	$\tau CNCH, \tau CNCN$
	65	0.4	73	$S_{92} = \tau C_{11}N_3C_{15}H_{15A} + \tau C_{11}N_3C_{15}H_{15B} + \tau C_{11}N_3C_{15}H_{15C}$ (59)	$\tau CNCH$

	44	2	53	$S_{82} = \tau C_{11}O_2O_1H_4 + \tau C_{10}N_4H_4O_1 + \tau C_7C_1H_4N_4$ (57) $S_{108} = \tau C_9N_2C_{10}N_4$ (16)	$\tau COOH, \tau CNHO, \tau CCHN, \tau CNCN$
	34	2	44	$S_{61} = \delta C_{12}N_4H_4 + \delta N_4C_4O_1$ (69) $S_{70} = \delta C_7O_1H_4 - \delta N_4H_4O_1$ (15)	$\delta CNH, \delta NCO, \delta COH, \delta NHO$
	19	0.4	30	$S_{104} = \tau C_{10}N_4H_4O_1 - \tau N_3C_{12}N_4H_4 + \tau C_2C_1C_7O_1 + \tau C_7O_1H_4N_4$ (67)	$\tau CNHO, \tau NCNH, \tau CCCO, \tau COHN$
	13	0.3	24	$S_{96} = \tau N_3C_{12}N_4H_4 - \tau C_{10}N_4H_4O_1 + \tau C_2C_1C_7O_1 - \tau C_7O_1H_4N_4$ (13) $S_{103} = \tau C_{10}N_4H_4O_1 + \tau C_7O_1H_4N_4 - \tau C_1C_7O_1H_4$ (57) $S_{107} = \tau C_7O_1H_4N_4$ (14)	$\tau NCNH, \tau CNHO, \tau CCCO, \tau COHN, \tau CCOH$

^a wavenumbers (cm^{-1}); vs – very strong, s – strong, m – medium, w – weak, vw – very weak, sh – shoulder;

^b Calculated infrared intensities in $\text{km}\cdot\text{mol}^{-1}$;

^c Scaling Eqs. $\tilde{\nu}_{\text{pred}} = 0.9536\tilde{\nu}_{\text{calc}} + 11.5$; r = 0.9996;

^d PED – the potential energy distribution, % in bracket;

^e Abbreviations: v – stretching, δ – in-plane deformation, γ – out-of-plane deformation, τ – torsion;

^f Absent in the theoretical spectrum.

Tab. S13. Internal coordinates (PED) used in the normal modes analysis for CAF·26DHBA (**IIa**), calculated frequencies, PED (%) and descriptions.

Local group coordinates	Calculated frequencies (cm^{-1}), PED (%)	Descriptions ^a
$S_1 = vO_3H_3$	3645 (99)	vOH
$S_2 = vO_4H_{4A}$	3404 (99)	vOH
$S_3 = vO_1H_4$	2606 (88)	vOH
$S_4 = vC_{12}H_{12}$	3278 (99)	vCH
$S_5 = vC_{13}H_{13A} - vC_{13}H_{13C}$	3152 (100)	vCH
$S_6 = vC_{13}H_{13B}$	3197 (81), 3080 (19)	vCH
$S_7 = vC_{13}H_{13A} + vC_{13}H_{13C}$	3197 (19), 3080 (81)	vCH
$S_8 = vC_{14}H_{14A}$	3195 (87), 3065 (13)	vCH
$S_9 = vC_{14}H_{14B} - vC_{14}H_{14C}$	3136 (100)	vCH
$S_{10} = vC_{14}H_{14B} + vC_{14}H_{14C}$	3195 (13), 3065 (87)	vCH
$S_{11} = vC_{15}H_{15A} - vC_{15}H_{15B}$	3166 (100)	vCH
$S_{12} = vC_{15}H_{15A} + vC_{15}H_{15B} - vC_{15}H_{15C}$	3179 (99)	vCH
$S_{13} = vC_{15}H_{15A} + vC_{15}H_{15B} + vC_{15}H_{15C}$	3082 (99)	vCH
$S_{14} = vC_5H_5^{\cdot} - vC_3H_3^{\cdot}$	3218 (95)	vCH
$S_{15} = vC_5H_5^{\cdot} + vC_3H_3^{\cdot}$	3223 (85), 3185 (10)	vCH
$S_{16} = vC_4H_4^{\cdot}$	3185 (90)	vCH
$S_{17} = vN_4H_4$	2606 (10) 111 (55)	vNH
$S_{18} = vC_9O_6 - vC_8O_5$	1756 (71)	vCO
$S_{19} = vC_9O_6 + vC_8O_5$	1793 (73)	vCO
$S_{20} = vC_7O_2$	1728 (47)	vCO
$S_{21} = vC_{10}C_{11} - vC_{10}N_2$	1674 (68)	vCC, vCN

$S_{22} = vC_{12}N_4$	1428 (10), 1382 (33)	vCN
$S_{23} = vC_{12}N_3$	1567 (17), 1558 (26), 1411 (11), 1098 (12)	vCN
$S_{24} = vC_4C_5 - vC_1C_6$	1446 (15), 1350 (33), 1079 (10)	vCC
$S_{25} = vC_2C_3$	1267 (17), 1079 (13)	vCC
$S_{26} = vC_2C_3 + vC_5C_6 + vC_7O_2$	1689 (43), 1301 (16), 772 (11)	vCC, vCO
$S_{27} = vC_3C_4 + vC_4C_5$	1689 (12), 1084 (43), 614 (11)	vCC
$S_{28} = vC_{10}N_4$	1472 (13), 1331 (14), 1213 (11)	vCN
$S_{29} = vC_{10}C_{11} + vC_{10}N_2$	1608 (13)	vCC, vCN
$S_{30} = vC_7O_1$	1411 (10), 1301 (20), 1146 (25), 834 (12)	vCO
$S_{31} = vC_1C_2 + vC_4C_5 - vC_3C_4$	1639 (58), 1191 (11)	vCC
$S_{32} = vC_6O_4 - vC_2O_3$	1267 (25), 1079 (41)	vCN
$S_{33} = vC_2O_3 + vC_6O_4$	1398 (13), 1360 (24), 772 (11), 614 (10)	vCO
$S_{34} = vC_9N_2$	1608 (10), 1090 (12), 563 (10), 484 (17)	vCN
$S_{35} = vC_9N_1$	1058 (16), 563 (13), 455 (10)	vCN
$S_{36} = vC_1C_7$	614 (13), 394 (12)	vCC
$S_{37} = vC_8N_1 + vC_{12}N_4$	1286 (16), 1058 (11), 1016 (10)	vCN
$S_{38} = vC_{14}N_2$	1331 (16), 1244 (18), 1058 (13), 1016 (21)	vCN
$S_{39} = vC_{15}N_3$	1244 (12), 774 (19), 660 (11)	vCN
$S_{40} = vC_{13}N_1$	1244 (14), 1090 (13), 1016 (20), 960 (15)	vCN
$S_{41} = \delta C_2C_3C_4 + \delta C_3C_4C_5 + \delta C_4C_5C_6$	1537 (15), 1360 (23), 614 (18), 449 (10)	δCCC
$S_{42} = \delta C_{11}C_{10}N_4 - \delta C_{11}C_{10}N_2$	1608 (20), 840 (11)	δCCC
$S_{43} = \delta C_3C_2O_3 + \delta C_1C_7O_1 + \delta C_5C_6O_4$	449 (27), 435 (16), 404 (12), 394 (21)	δCCO
$S_{44} = \delta C_9N_1C_8 - \delta N_4C_{12}N_3$	660 (30)	$\delta CNC, \delta NCN$
$S_{45} = \delta C_2O_3H_3$	1446 (20), 1350 (22)	δCOH
$S_{46} = \delta C_6O_4H_{4A}$	1537 (26), 1446 (19), 1360 (10), 1301 (13)	δCOH
$S_{47} = \delta C_{12}N_4H_4 - \delta N_4H_4O_1 - \delta C_7O_1H_4$	77 (68)	$\delta CNH, \delta NHO, \delta COH$
$S_{48} = \delta N_3C_{12}H_{12}$	1213 (42)	δNCH
$S_{49} = \delta H_{13A}C_{13}H_{13C}$	1503 (44), 1501 (23), 1286 (10)	δHCH
$S_{50} = \delta H_{13A}C_{13}H_{13C} + \delta H_{13A}C_{13}H_{13B}$	1439 (50)	δHCH
$S_{51} = \delta H_{13B}C_{13}H_{13C} - \delta H_{13A}C_{13}H_{13B}$	1486 (73), 1152 (10), 1150 (16)	δHCH
$S_{52} = \delta H_{14A}C_{14}H_{14B} + \delta H_{14A}C_{14}H_{14C}$	1428 (54)	δHCH
$S_{53} = \delta H_{14A}C_{14}H_{14B}$	1496 (73), 1152 (16), 1150 (10)	δHCH

$S_{54} = \delta H_{14B}C_{14}H_{14C} + \delta H_{15A}C_{15}H_{15C} - \delta H_{15A}C_{15}H_{15B}$	1510 (57), 1098 (14)	δHCH
$S_{55} = \delta H_{15A}C_{15}H_{15C} - \delta H_{15B}C_{15}H_{15C}$	1471 (71), 1148 (29)	δHCH
$S_{56} = \delta H_{15B}C_{15}H_{15C} + \delta H_{14B}C_{14}H_{14C} - \delta H_{15A}C_{15}H_{15B}$	1493 (45)	δHCH
$S_{57} = \delta H_{15A}C_{15}H_{15B} + \delta H_{14B}C_{14}H_{14C} - \delta H_{15A}C_{15}H_{15C}$	1454 (83)	δHCH
$S_{58} = \delta C_4C_5H_5 - \delta C_4C_3H_3 - \delta C_3C_4H_4$	1191 (75)	δCCH
$S_{59} = \delta C_4C_5H_5 + \delta C_4C_3H_3$	1537 (21), 1301 (13), 1146 (22), 1084 (26)	δCCH
$S_{60} = \delta C_3C_4H_4$	1501 (10), 1350 (13), 1267 (27), 1079 (15)	δCCH
$S_{61} = \delta C_{12}N_4H_4 + \delta N_4C_4O_1$	34 (69)	$\delta CNH, \delta NCO$
$S_{62} = \delta N_1C_9O_6 - \delta C_9N_2C_{10}$	840 (20), 455 (24)	$\delta NCO, \delta CNC$
$S_{63} = \delta C_{11}C_8O_5$	774 (12), 404 (35), 394 (11)	δCCO
$S_{64} = \delta N_4C_{12}N_3 + \delta C_9N_1C_8$	1273 (13), 840 (10)	$\delta NCN, \delta CNC$
$S_{65} = \delta C_3C_4C_5 - \delta C_4C_5C_6 + \delta O_1C_7O_2$	834 (51)	$\delta CCC, \delta OCO$
$S_{66} = \delta C_2C_1C_7$	340 (48)	δCCC
$S_{67} = \delta C_2C_3C_4 + \delta C_4C_5C_6 + \delta O_1C_7O_2$	772 (43), 614 (23)	$\delta CCC, \delta OCO$
$S_{68} = \delta C_{10}N_4C_{12}$	1090 (11), 1058 (12), 960 (16)	δCNC
$S_{69} = \delta C_{12}N_3C_{15}$	563 (13), 404 (10), 212 (27)	δCNC
$S_{70} = \delta C_7O_1H_4 - \delta N_4H_4O_1$	1728 (13), 1567 (23), 1558 (13), 34 (15)	$\delta COH, \delta NHO$
$S_{71} = \delta C_1C_2C_3 + \delta C_2C_1C_7$	394 (10), 340 (16)	δCCC
$S_{72} = \delta C_5C_6O_4 - \delta C_1C_7O_1$	455 (22), 454 (41)	δCCO
$S_{73} = \delta C_4C_5C_6 - \delta C_2C_3C_4 - \delta C_1C_7O_1 - \delta C_5C_6O_4 + \delta C_3C_2O_3$	593 (73)	$\delta CCC, \delta CCO$
$S_{74} = \delta C_9N_2C_{10}$	1331 (16), 435 (23)	δCNC
$S_{75} = \delta N_1C_9N_2$	484 (23)	δNCN
$S_{76} = \delta C_4C_5C_6 - \delta C_2C_3C_4$	1079 (10), 539 (66)	δCCC
$S_{77} = \delta C_9N_2C_{14}$	312 (64)	δCNC
$S_{78} = \delta C_9N_1C_{13}$	371 (56), 312 (12)	δCNC
$S_{79} = \delta C_{12}N_3C_{15} - \delta C_{11}C_{10}N_2$	435 (10), 212 (43)	$\delta CNC, \delta CCN$
$S_{80} = \tau C_1C_2O_3H_3 - \tau C_{10}N_4C_{12}N_3$	625 (14), 623 (61)	$\tau CCOH, \tau CNCN$
$S_{81} = \gamma C_7O_1C_1O_2$	805 (10), 801 (55)	$\gamma COCO$
$S_{82} = \tau C_{11}O_2O_1H_4 + \tau C_{10}N_4H_4O_1 + \tau C_7C_1H_4N_4$	44 (57)	$\tau COOH, \tau CNHO, \tau CCHN$
$S_{83} = \tau C_{10}N_4C_{12}H_{12}$	881 (87)	$\tau CNCH$

$S_{84} = \tau C_8 N_1 C_{13} H_{13A} - \tau C_8 N_1 C_{13} H_{13C}$	1503 (15), 1286 (22), 1058 (18)	τ CNCH
$S_{85} = \tau C_8 N_1 C_{13} H_{13A} - \tau C_8 N_1 C_{13} H_{13B} - \tau C_{10} N_2 C_{14} H_{14A} + \tau C_{10} N_2 C_{14} H_{14B}$	1486 (27), 1150 (66)	τ CNCH
$S_{86} = \tau C_{10} N_2 C_{14} H_{14A} + \tau C_{10} N_2 C_{14} H_{14B} + \tau C_{10} N_2 C_{14} H_{14C}$	115 (27), 110 (53)	τ CNCH
$S_{87} = \tau C_{10} N_2 C_{14} H_{14B} - \tau C_{10} N_2 C_{14} H_{14A}$	1496 (27), 1152 (66)	τ CNCH
$S_{88} = \tau C_{10} N_2 C_{14} H_{14B} - \tau C_{10} N_2 C_{14} H_{14C}$	1510 (10), 1273 (15), 1213 (10), 1090 (21)	τ CNCH
$S_{89} = \tau C_8 N_1 C_{13} H_{13A} + \tau C_8 N_1 C_{13} H_{13B} + \tau C_8 N_1 C_{13} H_{13C}$	115 (14), 110 (15), 74 (47)	τ CNCH
$S_{90} = \tau C_{11} N_3 C_{15} H_{15C} - \tau C_{11} N_3 C_{15} H_{15A}$	1471 (29), 1148 (69)	τ CNCH
$S_{91} = \tau C_{11} N_3 C_{15} H_{15B} - \tau C_{11} N_3 C_{15} H_{15A}$	1510 (11), 1098 (47)	τ CNCH
$S_{92} = \tau C_{11} N_3 C_{15} H_{15A} + \tau C_{11} N_3 C_{15} H_{15B} + \tau C_{11} N_3 C_{15} H_{15C}$	159 (12), 115 (11), 65 (59)	τ CNCH
$S_{93} = \tau C_3 C_4 C_5 H_5\cdot + \tau C_5 C_4 C_3 H_3\cdot$	871 (83), 634 (12)	τ CCCH
$S_{94} = \tau C_2 C_3 C_4 H_4\cdot + \tau C_5 C_4 C_3 H_3\cdot - \tau C_3 C_4 C_5 H_5\cdot$	805 (40), 801 (15), 763 (17), 702 (10)	τ CCCH
$S_{95} = \tau C_2 C_3 C_4 H_4\cdot - \tau C_3 C_4 C_5 H_5\cdot$	988 (75), 480 (16)	τ CCCH
$S_{96} = \tau N_3 C_{12} N_4 H_4 - \tau C_{10} N_4 H_4 O_1 + \tau C_2 C_1 C_7 O_1 - \tau C_7 O_1 H_4 N_4$	78 (55), 13 (13)	τ NCNH, τ CNHO, τ CCCO, τ COHN
$S_{97} = \tau C_{11} C_{10} N_4 C_{12} + \tau C_{10} N_4 C_{11} N_2 - \tau C_8 N_1 C_{11} O_5$	703 (44), 702 (33)	τ CCNC, τ CNCN, τ CNCO
$S_{98} = \tau C_3 C_4 C_5 C_6 + \tau C_2 C_3 C_4 C_5$	225 (76)	τ CCCC
$S_{99} = \tau C_6 C_5 C_4 C_3 - \tau C_2 C_3 C_4 C_5$	988 (19), 480 (66)	τ CCCC
$S_{100} = \tau C_2 C_3 C_1 O_3 - \tau C_6 C_5 C_1 O_4 - \tau C_2 C_3 C_4 C_5$	805 (36), 703 (16), 702 (21)	τ CCCO, τ CCCC
$S_{101} = \tau C_1 C_2 C_3 C_4 - \tau C_3 C_2 C_1 C_7$	260 (17), 125 (12), 121 (35)	τ CCCC
$S_{102} = \tau C_1 C_2 O_3 H_3 + \tau C_{10} N_4 C_{12} N_3$	625 (59), 623 (14)	τ CCOH, τ CNCN
$S_{103} = \tau C_{10} N_4 H_4 O_1 + \tau C_7 O_1 H_4 N_4 - \tau C_1 C_7 O_1 H_4$	1087 (20), 78 (11), 13 (57)	τ CNHO, τ COHN, τ CCOH
$S_{104} = \tau C_{10} N_4 H_4 O_1 - \tau N_3 C_{12} N_4 H_4 + \tau C_2 C_1 C_7 O_1 + \tau C_7 O_1 H_4 N_4$	19 (67)	τ CNHO, τ NCNH, τ CCCO, τ COHN
$S_{105} = \tau C_{10} N_2 C_9 N_1 + \tau C_8 N_1 C_9 N_2$	272 (10), 88 (46)	τ CNCN
$S_{106} = \tau C_8 N_1 C_9 N_2$	125 (25), 115 (10), 74 (22)	τ CNCN
$S_{107} = \tau C_7 O_1 H_4 N_4$	1087 (72), 13 (14)	τ COHN
$S_{108} = \tau C_9 N_2 C_{10} N_4$	272 (11), 159 (42), 88 (11), 44 (16)	τ CNCN

$S_{109} = \tau C_{11}C_{10}N_4C_{12} - \gamma C_{12}N_4C_{11}N_2 + \gamma C_9N_1N_2O_6$	760 (75)	$\tau CCNC, \gamma CNCN, \gamma CNCN$
$S_{110} = \gamma C_9N_1N_2O_6 + \gamma C_8N_1C_{11}O_5$	766 (92)	$\gamma CNNO, \gamma CNCO$
$S_{111} = \gamma C_6C_5C_1O_4 + \gamma C_2C_3C_1O_3$	871 (14), 634 (64)	$\gamma CCCO$
$S_{112} = \tau C_1C_2C_3C_4 + \tau C_2C_3C_4C_5 + \tau C_3C_2C_1C_7 + \gamma C_6C_5C_2O_4$	260 (62)	$\tau CCCC, \gamma CCCC$
$S_{113} = \gamma C_{14}C_9C_{10}N_2 + \gamma C_{15}C_{11}C_{12}N_3$	223 (58), 110 (11)	$\gamma CCCN$
$S_{114} = \gamma C_{15}C_{11}C_{12}N_3 - \gamma C_{14}C_9C_{10}N_2 + \gamma C_{10}N_4C_{11}N_2 - \tau C_{11}C_{10}N_4C_{12}$	365 (66)	$\gamma CCCN, \gamma CNCN, \tau CCNC$
$S_{115} = \gamma C_{13}C_8C_9N_1$	272 (60), 125 (10)	$\gamma CCCN$
$S_{116} = \tau C_1C_6O_4H_{4A} + \gamma C_7O_1C_1O_2$	801 (15), 763 (66)	$\gamma COOH, \gamma COCO$
$S_{117} = \tau C_{11}C_{10}N_4C_{12} - \gamma C_{14}C_9C_{10}N_2 + \gamma C_{15}C_{11}C_{12}N_3 - \gamma C_{10}N_4C_{11}N_2$	365 (12), 125 (14), 121 (11), 115 (17)	$\tau CCNC, \gamma CCCN, \gamma CNCN$

^a ν – stretching, δ – in-plane deformation, γ – out-of-plane deformation, τ – torsion.

DSC curves

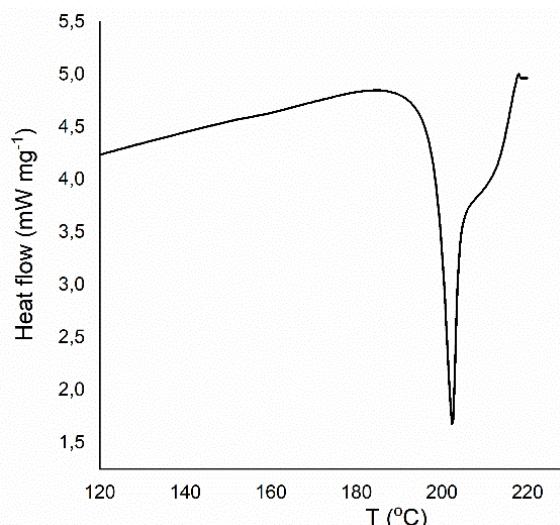


Fig. S5. DSC curve of TBR·26DHBA (**I**).

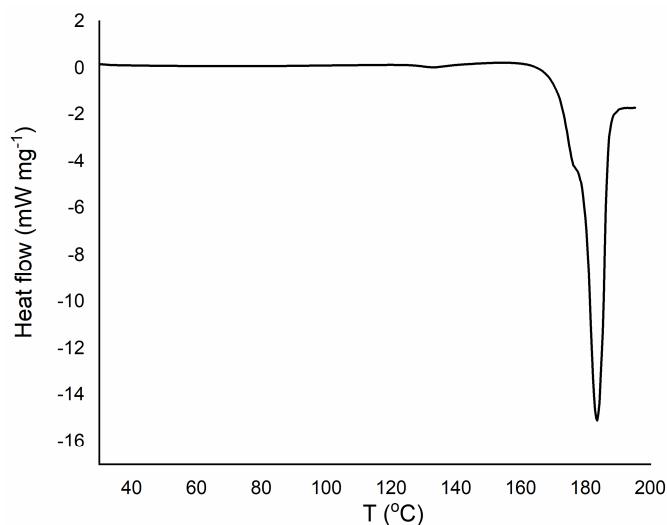


Fig. S6. DSC curve of CAF·26DHBA (**II**).