Electronic Supplementary Material (ESI) for New Journal of Chemistry.

† Electronic Supplementary Information

Spectroscopic (FT-IR, FT-Raman, ^{13}C SS-NMR) and quantum chemical investigations to explore the structural insights of nitrofurantoin-4-hydroxybenzoic acid cocrystal

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Part I. FIGURES

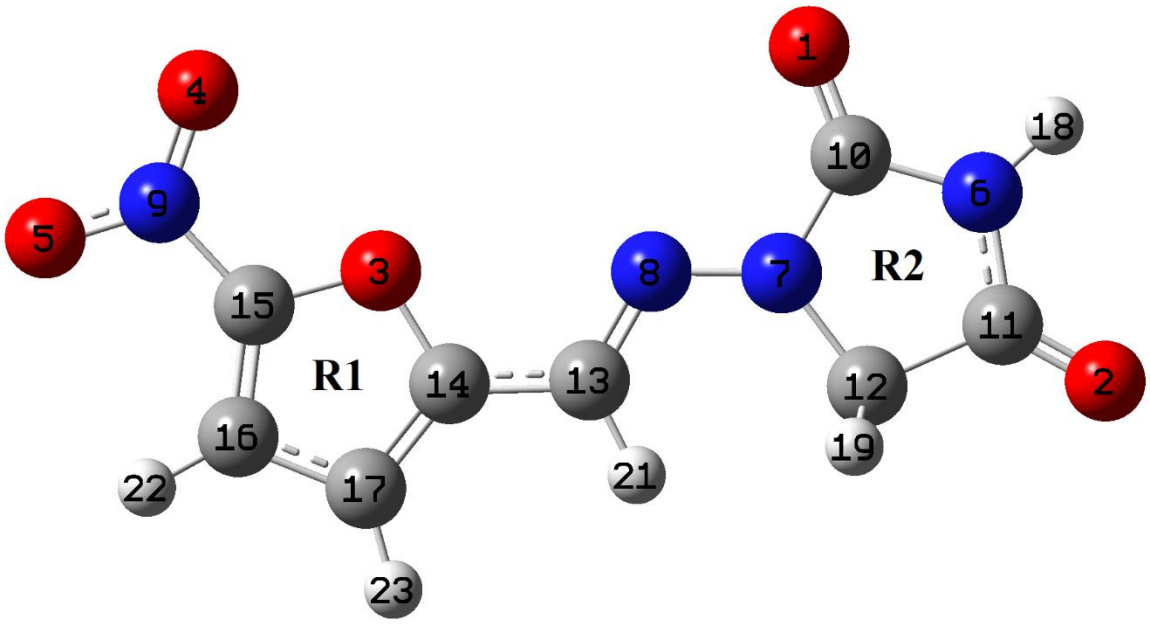

Fig. S1 Optimized structure of NF-4HBA (monomer model) with atom numbering scheme adopted in this study.

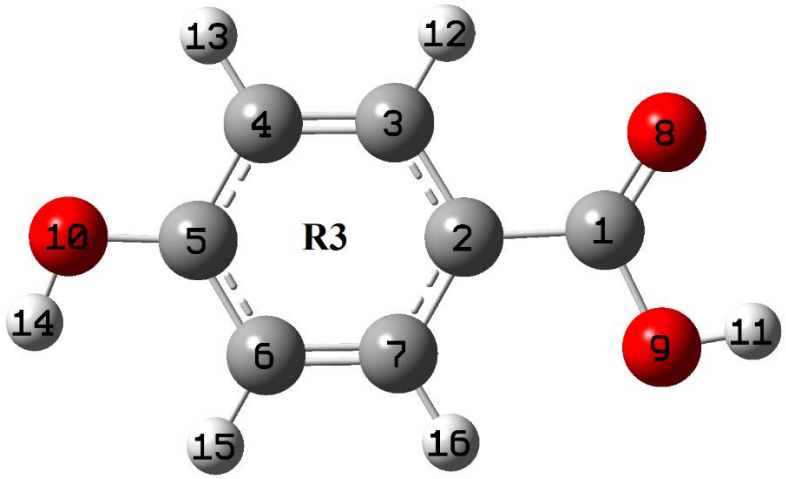

Fig. S2 Optimized structure of NF-4HBA (monomer model) with atom numbering scheme adopted in this study.

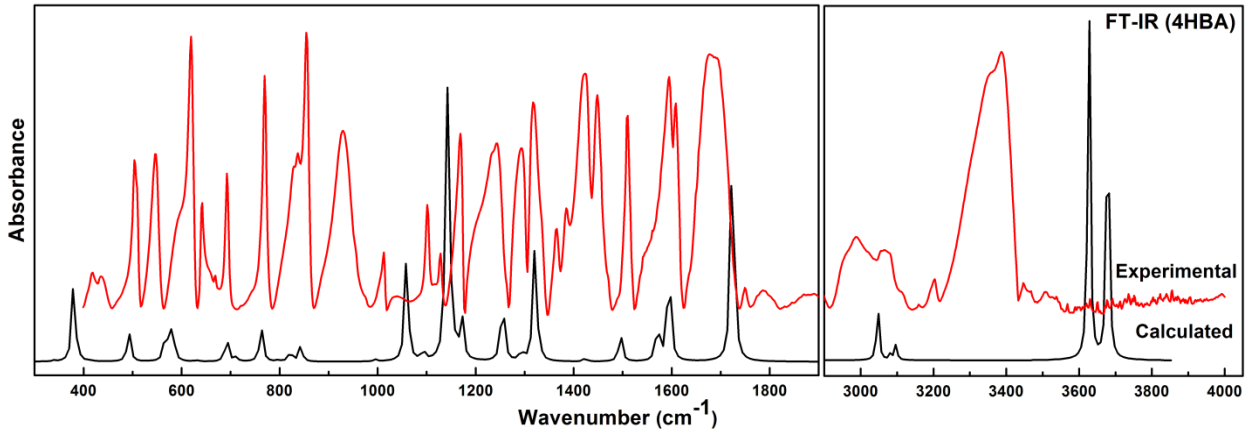

Fig. S3 Experimental and calculated FT-IR absorbance spectra of 4HBA.

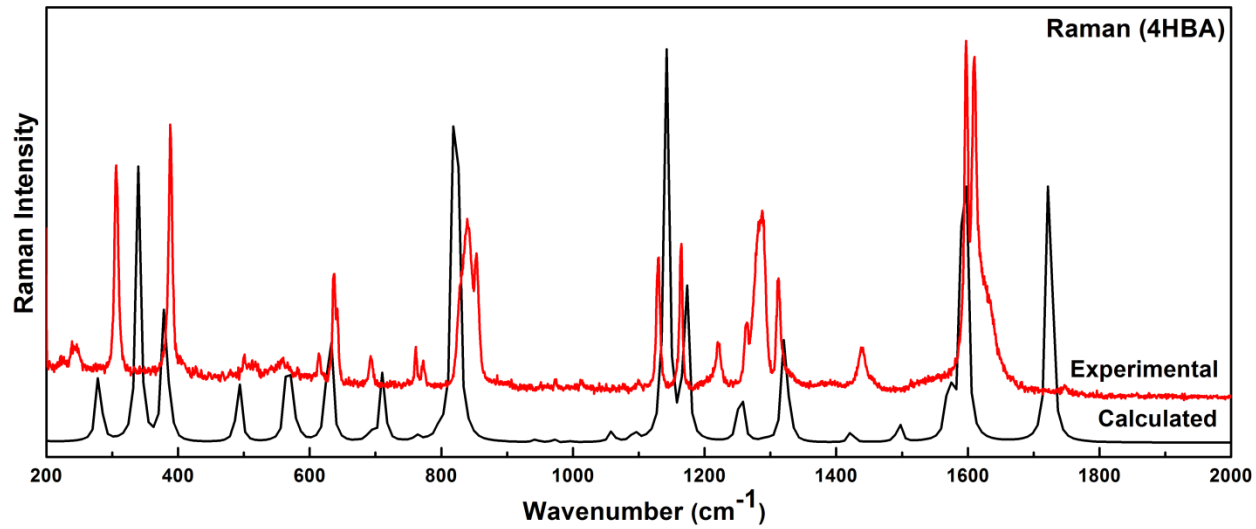

Fig. S4 Experimental and calculated Raman spectra of 4HBA.

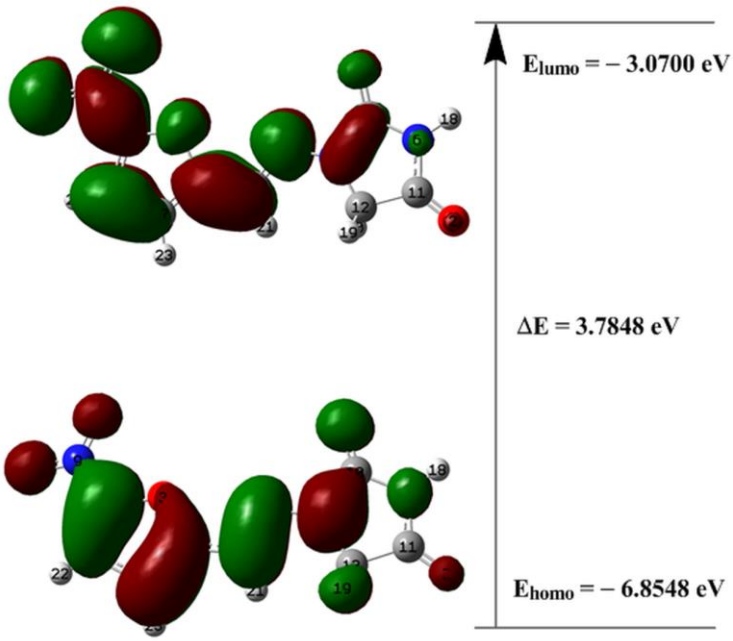

Fig. S5 HOMO–LUMO plot of the NF with orbitals involved in electronic transitions in the isolated (gaseous) phase.

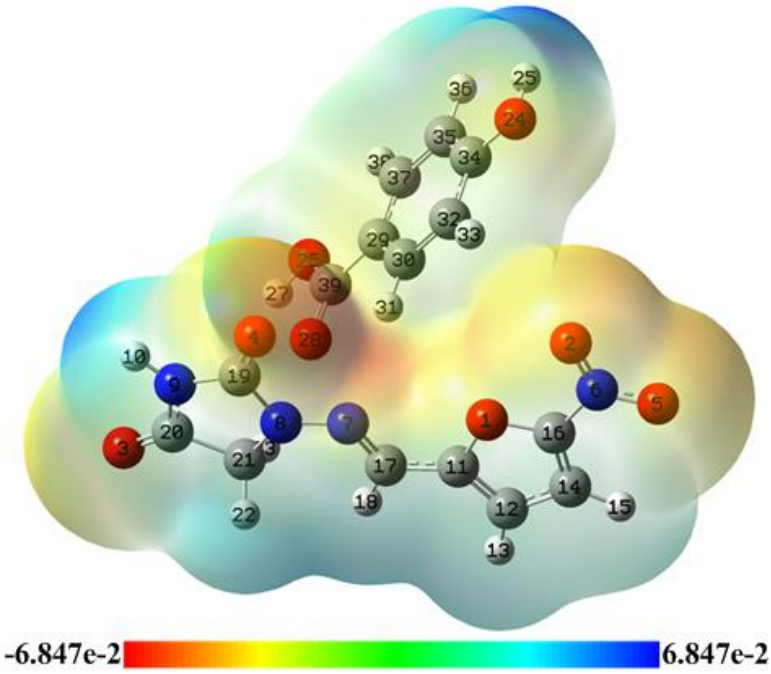

Fig. S6 Molecular electrostatic potential (MEP) formed using B3LYP/cc-pvTZ method by mapping total density over electrostatic potential in gas phase for NF-4HBA cocrystal.

Part II. TABLES

Table S1 The experimental and calculated geometric parameters of NF-4HBA and NF.

Geometrical Parameters	Experimental		Calculated Optimized Parameters		
	NF-4HBA	NF	NF-4HBA		NF
			Dimer	Monomer	Monomer
Bond length (Å)					
O1-C11	1.3737	1.3687	1.3575	1.3586	1.3582
O1-C16	1.353	1.3477	1.3472	1.3485	1.3476
O2-N6	1.2311	1.1949	1.2238	1.2221	1.1954
O3-C20	1.2237	1.2063	1.2149	1.2032	1.2023
O4-C19	1.2056	1.3626	1.1948	1.1972	1.3376
O5-N6	1.2349	1.2803	1.2305	1.2279	1.2824
N6-C16	1.4155	1.4473	1.4214	1.4283	1.4560
N7-N8	1.3629	1.3730	1.336	1.334	1.4012
N7-C17	1.2904	1.2143	1.2831	1.2829	1.2200
N7-H31	2.9439	1.3966	3.1265	2.6344	1.4041
N8-C19	1.3745	1.3531	1.3961	1.3998	1.3744
N8-C21	1.4548	0.9205	1.4574	1.4578	1.0076
N9-H10	0.8551	1.2285	1.0075	1.0076	1.2276
N9-C19	1.3995	0.9301	1.4101	1.4018	1.0924
N9-C20	1.3585	0.9856	1.3596	1.3758	1.0925
C11-C12	1.3657	1.5041	1.3763	1.3756	1.5270
C11-C17	1.4357	1.4369	1.4386	1.438	1.4388
C12-H13	0.95	0.9887	1.0762	1.0762	1.0887
C12-C14	1.4176	1.3526	1.412	1.4138	1.3751
C14-H15	0.9503	0.9226	1.0742	1.0745	1.0743
C14-C16	1.357	1.3985	1.3628	1.3621	1.4141
C17-H18	0.95	1.3391	1.0882	1.0876	1.3617
C19-O28	3.0373	1.4113	-	3.7565	1.4317
C20-C21	1.5066	0.9264	1.5191	1.5239	1.0763
C21-H22	0.9902	-	1.0917	1.0918	-
C21-H23	0.9897	-	1.0905	1.091	-
O24-H25	0.9042	-	0.9634	0.963	-
O24-C34	1.368	-	1.3682	1.3564	-
O26-H27	0.9244	-	0.9678	0.9674	-
O26-C39	1.2973	-	1.3513	1.3557	-
O28-C39	1.2582	-	1.2148	1.2155	-
C29-C30	1.3972	-	1.3986	1.4004	-
C29-C37	1.3982	-	1.3969	1.3977	-
C29-C39	1.4708	-	1.4742	1.4719	-
C30-H31	0.95	-	1.0797	1.0794	-
C30-C32	1.3824	-	1.3807	1.3798	-
C32-H33	0.9505	-	1.0816	1.0808	-
C32-C34	1.3919	-	1.3939	1.3963	-
C34-C35	1.3936	-	1.3934	1.3966	-
C35-H36	0.95	-	1.0832	1.0836	-
C35-C37	1.3882	-	1.3847	1.3836	-
C37-H38	0.9504	-	1.0795	1.0797	-
Bond Angle (°)					
C11-O1-C16	104.6143	104.8201	106.1158	106.232	106.1501
O2-N6-O5	124.7277	116.9209	125.3212	125.9622	119.1684
O2-N6-C16	118.2969	127.5844	118.3991	118.157	127.7318
O5-N6-C16	116.9754	119.2865	116.2788	115.8806	119.8737
N8-N7-C17	116.2629	112.7821	119.237	119.3025	112.3945
N8-N7-H31	107.7656	113.0228	92.8726	102.1673	114.5001
C17-N7-H31	96.2359	127.9628	88.1198	100.658	121.4838
N7-N8-C19	119.8394	118.9309	119.6907	119.6329	124.0161
N7-N8-C21	127.0192	110.1039	127.5587	127.4424	112.4628

C19-N8-C21	112.7261	108.3285	112.4218	112.3713	112.4603
H10-N9-C19	122.1132	101.6822	121.4952	121.5482	102.8274
H10-N9-C20	125.1867	114.8676	124.2668	124.0113	108.7933
C19-N9-C20	112.6928	110.0802	114.1211	114.4083	110.0875
O1-C11-C12	110.7048	110.9542	110.0246	109.9309	110.0899
O1-C11-C17	118.4285	119.0128	119.7393	119.5378	121.2521
C12-C11-C17	130.8314	126.0008	130.2324	130.525	123.7857
C11-C12-H13	126.6419	114.8383	126.0234	126.0136	114.9622
C11-C12-C14	106.7702	117.7624	106.6887	106.727	119.8172
H13-C12-C14	126.5879	109.6004	127.2871	127.2593	110.0025
C12-C14-H15	127.6007	132.6225	128.8881	128.8931	130.1803
C12-C14-C16	104.7686	132.7174	105.0764	105.1325	128.9352
H15-C14-C16	127.6306	122.5127	126.0329	125.9739	126.0010
O1-C16-N6	116.272	104.6656	117.6491	117.6031	105.0638
O1-C16-C14	113.1382	128.0744	112.0941	111.9772	128.6304
N6-C16-C14	130.5515	126.6982	130.2397	130.4149	126.6614
N7-C17-C11	119.7922	105.2273	120.9119	120.7481	104.7082
N7-C17-H18	120.1216	124.2619	123.8744	123.8637	126.2021
C11-C17-H18	120.0861	118.3036	115.2131	115.3856	118.1078
O4-C19-N8	128.6647	117.4108	129.2319	128.57	115.6901
O4-C19-N9	125.7947	107.8642	126.2131	126.6745	106.6959
O4-C19-O28	92.1125	121.4467	-	116.4812	126.0786
N8-C19-N9	105.5404	130.6543	104.5516	104.754	127.2255
N8-C19-O28	83.6457	-	-	58.5231	-
N9-C19-O28	94.1031	125.7485	-	89.4381	127.5339
O3-C20-9	125.8694	127.0593	126.5144	127.1864	126.8962
O3-C20-C21	126.6272	107.1909	127.0668	127.1391	105.5698
N9-C20-C21	107.5023	113.0483	106.4161	105.6742	112.0877
N8-C21-C20	101.476	116.1495	102.4067	102.7248	117.6940
N8-C21-H22	111.4716	130.8022	112.7034	112.6029	130.2183
N8-C21-H23	111.4774	-	111.9026	111.2108	-
C20-C21-H22	111.461	-	110.4368	110.0698	-
C20-C21-H23	111.4976	-	109.4901	109.8923	-
H22-C21-H23	109.3072	-	109.6798	110.1115	-
H25-O24-C34	110.4506	-	110.5323	109.9786	-
H27-O26-C39	111.057	-	106.79	106.3707	-
C19-O28-C39	92.9856	-	-	126.528	-
C30-C29-C37	119.5571	-	119.1489	119.0307	-
C30-C29-C39	119.4529	-	118.6092	118.8746	-
C37-C29-C39	120.9681	-	122.2418	122.0946	-
C29-C30-H31	119.7466	-	119.0563	119.046	-
C29-C30-C32	120.5462	-	121.0365	121.01	-
H31-C30-C32	119.7072	-	119.906	119.944	-
N7-H31-C30	120.1317	-	164.2131	179.9977	-
C30-C32-H33	120.3287	-	121.0604	121.1836	-
C30-C32-C34	119.3716	-	119.0683	119.4345	-
H33-C32-C34	120.2997	-	119.8712	119.3819	-
O24-C34-C32	117.3145	-	117.3166	117.4135	-
O24-C34-C35	121.7433	-	121.905	122.3823	-
C32-C34-C35	120.9417	-	120.7784	120.2042	-
C34-C35-H36	120.3279	-	120.181	119.9073	-
C34-C35-C37	119.3483	-	119.6214	119.949	-
H36-C35-C37	120.3238	-	120.1976	120.1437	-
C29-C37-C35	120.2293	-	120.3426	120.3712	-
C29-C37-H38	119.8811	-	119.8429	119.8063	-
C35-C37-H38	119.8895	-	119.8143	119.8225	-
O26-C39-O28	122.8706	-178.6492	121.3898	120.9251	179.9922
O26-C39-C29	117.0303	0.1285	113.5363	113.4857	0.0013
O28-C39-C29	120.0958	0.1232	125.0737	125.5891	0.0047
Dihedral angle (°)					
C16-O1-C11-C12	0.5608	-179.877	0.2277	-0.037	179.9624
C16-O1-C11-C17	−177.5136	−7.0713	−179.135	−179.2172	−0.032

C11-O1-C16-N6	−178.239	−179.7879	178.4844	179.1823	180.008
C11-O1-C16-C14	−0.2499	−179.7651	−0.1639	−0.1014	−180.0045
O2-N6-C16-O1	2.6936	4.9006	2.3697	−1.2169	0.0039
O2-N6-C16-C14	−174.8725	68.1898	−179.2712	177.9107	61.647
O5-N6-C16-O1	−177.3244	−58.1799	−177.3096	178.9445	−61.5926
O5-N6-C16-C14	5.1095	−175.1289	1.0496	−1.9279	−179.9737
C17-N7-N8-C19	−179.4724	−118.6982	−177.8592	−177.8793	−118.3905
C17-N7-N8-C21	−7.4338	114.9321	−4.9709	−7.0979	118.3699
H31-N7-N8-C19	−72.8964	−2.017	−88.407	−68.1264	−0.0112
H31-N7-N8-C21	99.1422	−3.1289	84.4813	102.6549	−0.0299
N8-N7-C17-C11	−179.3558	176.8326	179.41	178.5769	179.9786
N8-N7-C17-H18	0.5813	−176.8731	−0.2927	−0.8065	−179.9957
H31-N7-C17-C11	67.3041	3.0883	87.1698	67.9945	0.0128
H31-N7-C17-H18	−112.7588	176.926	−92.5328	−111.3889	179.9988
N8-N7-H31-C30	97.9005	−3.0362	88.2008	43.8189	−0.0095
C17-N7-H31-C30	−141.9389	−6.4717	−152.6126	167.1881	−0.0086
N7-N8-C19-O4	−4.553	173.5661	−3.9081	−5.6233	179.9831
N7-N8-C19-N9	175.5706	−178.5668	176.7356	174.8058	−179.982
N7-N8-C19-O28	83.0627	1.8169	-	94.7755	0.0027
C21-N8-C19-O4	−177.6669	4.4936	−177.8136	−177.7173	0.0256
C21-N8-C19-N9	2.4567	−175.1227	2.8302	2.7117	−179.9897
C21-8-C19-O28	−90.0513	−179.5106	-	−77.3186	−180.0102
N7-N8-C21-C20	−175.0364	0.0992	−175.1321	−173.6581	0.0049
N7-N8-C21-H22	66.2111	−62.8121	66.2093	67.9769	−59.9762
N7-N8-C21-H23	−56.2388	116.7978	−57.9613	−56.1544	120.039
C19-N8-C21-C20	−2.5208	65.4629	−1.8134	−2.3188	59.9576
C19-N8-C21-H22	−121.2733	−114.9273	−120.472	−120.6838	−120.0272
C19-N8-C21-H23	116.2769	−0.5219	115.3574	115.1849	0.024
H10-N9-C19-O4	−2.1396	−178.957	1.5055	0.3394	180.0129
H10-N9-C19-N8	177.7415	175.3196	−179.1126	179.9212	180.0163
H10-N9-C19-O28	−97.7226	−3.1154	-	−122.9374	0.0051
C20-N9-C19-O4	178.7969	−0.3191	177.7333	178.3536	−0.0065
C20-N9-C19-N8	−1.322	−178.3909	−2.8848	−2.0646	−179.9989
C20-N9-C19-O28	83.2138	178.211	-	55.0768	−179.9962
H10-N9-C20-O3	0.3585	0.1391	−2.6618	−1.578	0.0114
H10-N9-C20-C21	−179.2755	176.6122	177.9037	178.6112	179.9949
C19-N9-C20-O3	179.388	−5.5561	−178.7696	−179.5364	−0.0128
C19-N9-C20-C21	−0.246	0.376	1.7959	0.6528	0.0089
O1-C11-C12-H13	179.2801	178.2077	−179.9085	−179.9575	180.0012
O1-C11-C12-C14	−0.6545	−177.0324	−0.2068	0.153	−179.9951
C17-C11-C12-H13	−2.9581	2.9678	−0.6333	−0.8958	0.0540
C17-C11-C12-C14	177.1073	−0.3110	179.0684	179.2147	−0.0086
O1-C11-C17-N7	−1.0437	179.6891	−1.6394	−4.4692	−179.9595
O1-C11-C17-H18	179.0192	5.8609	178.0878	174.964	−0.0869
C12-C11-C17-N7	−178.6629	−174.1392	179.1449	176.5446	179.8617
C12-C11-C17-H18	1.4	−175.8332	−1.128	−4.0221	179.9138
C11-C12-C14-H15	−179.5719	4.1666	−179.33	−179.9363	−0.1376
C11-C12-C14-C16	0.4715	-	0.1013	−0.2048	-
H13-C12-C14-H15	0.4934	-	0.3668	0.1761	-
H13-C12-C14-C16	−179.4631	-	179.7981	179.9075	-
C12-C14-C16-O1	−0.1364	-	0.0384	0.1923	-
C12-C14-C16-N6	177.4902	-	−178.393	−178.974	-
H15-C14-C16-O1	179.9071	-	179.491	179.9341	-
H15-C14-C16-N6	−2.4663	-	1.0597	0.7677	-
O4-C19-O28-C39	−7.8567	-	-	−21.9526	-
N8-C19-O28-C39	−136.5348	-	-	−142.7317	-
N9-C19-O28-C39	118.2599	-	-	109.5325	-
O3-C20-C21-N8	−178.0329	-	−179.4174	−178.8376	-
O3-C20-C21-H22	−59.2728	-	−59.1718	−58.7055	-
O3-C20-C21-H23	63.1839	-	61.6994	62.7278	-
N9-C20-C21-N8	1.5976	-	0.013	0.9733	-
N9-C20-C21-H22	120.3576	-	120.2586	121.1054	-

N9-C20-C21-H23	−117.1856	-	−118.8701	−117.4613	-	
H25-O24-C34-C32	−174.9548	-	−177.8672	−179.6891	-	
H25-O24-C34-C35	4.8232	-	2.1185	0.309	-	
H27-O26-C39-O28	−2.9118	-	-	0.3111	-	
H27-O26-C39-C29	176.4251	-	179.1584	−179.7986	-	
C19-O28-C39-O26	−83.4186	-	-	−130.261	-	
C19-O28-C39-C29	97.2641	-	-	49.8628	-	
C37-C29-C30-H31	179.3548	-	179.2181	179.7139	-	
C37-C29-C30-C32	−0.6256	-	−0.3684	−0.2333	-	
C39-C29-C30-H31	−2.3299	-	−0.8833	−0.3753	-	
C39-C29-C30-C32	177.6897	-	179.5301	179.6775	-	
C30-C29-C37-C35	0.9071	-	−0.1799	0.09	-	
C30-C29-C37-H38	−179.1033	-	179.9717	−179.9096	-	
C39-C29-C37-C35	−177.382	-	179.9254	−179.8178	-	
C39-C29-C37-H38	2.6076	-	0.077	0.1826	-	
C30-C29-C39-O26	174.7378	-	−178.7424	179.5603	-	
C30-C29-C39-O28	−5.9059	-	1.1066	−0.5555	-	
C37-C29-C39-O26	−6.9713	-	1.1529	−0.5319	-	
C37-C29-C39-O28	172.385	-	−178.9981	179.3524	-	
C29-C30-H31-N7	−79.4984	-	−94.2454	−87.1359	-	
C32-C30-H31-N7	100.4822	-	85.346	92.8119	-	
C29-C30-C32-H33	−179.9457	-	−179.1976	−179.7785	-	
C29-C30-C32-C34	−0.0052	-	0.7086	0.2355	-	
H31-C30-C32-H33	0.0739	-	1.2193	0.2748	-	
H31-C30-C32-C34	−179.9857	-	−178.8745	−179.7112	-	
C30-C32-C34-O24	−179.8553	-	179.4738	179.9032	-	
C30-C32-C34-C35	0.3648	-	−0.5121	−0.095	-	
H33-C32-C34-O24	0.0852	-	−0.6189	−0.0831	-	
H33-C32-C34-C35	−179.6947	-	179.3952	179.9187	-	
O24-C34-C35-H36	0.0866	-	0.0285	−0.0268	-	
O24-C34-C35-C37	−179.8546	-	179.9908	179.9568	-	
C32-C34-C35-H36	179.8566	-	−179.9862	179.9713	-	
C32-C34-C35-C37	−0.0846	-	−0.024	−0.0451	-	
C34-C35-C37-C29	−0.5545	-	0.3713	0.0465	-	
C34-C35-C37-H38	179.4559	-	−179.7803	−179.9539	-	
H36-C35-C37-C29	179.5043	-	−179.6664	−179.9699	-	
H36-C35-C37-H38	−0.4853	-	0.182	0.0297	-	

Table S2 Selected reactivity descriptors as Fukui functions (f_k^+, f_k^-), local softnesses (s_k^+, s_k^-), local electrophilicity indices (ω_k^+, ω_k^-) using Hirshfeld atomic charges.

Sites	f_k^+	ω_k^+	s_k^+	f_k^-	ω_k^-	s_k^-	f_k^+/f_k^-	f_k^-/f_k^+
For NF								
O1	0.04415	0.29174	0.01145	0.06576	0.43453	0.01706	0.67139	1.48946
O2	0.04319	0.28534	0.0112	0.05523	0.36490	0.01432	0.78198	1.27880
O3	0.03651	0.24125	0.00947	0.02469	0.16312	0.00640	1.47896	0.67615
O4	0.11932	0.78839	0.03095	0.05691	0.37606	0.01476	2.09646	0.47699
O5	0.12441	0.82202	0.03227	0.06790	0.44864	0.01761	1.83225	0.54578
N6	0.01564	0.10333	0.00406	0.02640	0.17441	0.00685	0.59244	1.68794
N7	0.01846	0.12199	0.00479	0.08310	0.54911	0.02156	0.22216	4.50135
N8	0.07634	0.50444	0.01980	0.05883	0.38872	0.01526	1.29768	0.77060
N9	0.06730	0.44465	0.01746	0.01609	0.10634	0.00417	4.18137	0.23916
C10	0.03045	0.20118	0.00790	0.02506	0.16561	0.00650	1.21481	0.82317
C11	0.01572	0.10384	0.00408	0.01357	0.08969	0.00352	1.15773	0.86376
C12	0.00992	0.06553	0.00257	0.01746	0.11534	0.00453	0.56817	1.76003
C13	0.05402	0.35695	0.01401	0.06139	0.40565	0.01592	0.87995	1.13643
C14	0.05447	0.35988	0.01413	0.04859	0.32108	0.01260	1.12086	0.89217
C15	0.04028	0.26618	0.01045	0.08308	0.54896	0.02155	0.48487	2.06241
C16	0.06276	0.41466	0.01628	0.05026	0.33210	0.01304	1.24862	0.80088
C17	0.05014	0.33130	0.01301	0.08041	0.53128	0.02086	0.62359	1.60363
For 4HBA								
C1	0.0284	0.08624	0.00528	0.10734	0.32601	0.01994	0.26453	3.78031

C2	0.11817	0.35891	0.02196	0.06551	0.19895	0.01217	1.80402	0.55432
C3	0.05308	0.16122	0.00986	0.0688	0.20896	0.01278	0.77152	1.29614
C4	0.0813	0.2469	0.0151	0.05454	0.16564	0.01013	1.49058	0.67088
C5	0.09053	0.27494	0.01682	0.09507	0.28873	0.01766	0.95225	1.05014
C6	0.08062	0.24485	0.01498	0.05258	0.15969	0.00977	1.53328	0.6522
C7	0.05912	0.17954	0.01098	0.07392	0.22451	0.01373	0.79972	1.25044
O8	0.08745	0.2656	0.01625	0.12351	0.37511	0.02295	0.70807	1.41229
O9	0.03301	0.10025	0.00613	0.06105	0.18542	0.01134	0.54066	1.84959
O10	0.13165	0.39983	0.02446	0.06599	0.20043	0.01226	1.99486	0.50129

f_k^+, f_k^- (in e); s_k^+, s_k^- (in ev^{-1}) and ω_k^+, ω_k^- (in ev).

Table S3 Selected reactivity descriptors as Fukui functions (f_k^+, f_k^-), local softnesses (s_k^+, s_k^-), local electrophilicity indices (ω_k^+, ω_k^-) for monomeric model of NF-4HBA.

Sites	f_k^+	ω_k^+	s_k^+	f_k^-	ω_k^-	s_k^-
			From Hirshfeld atomic charges			
O1	0.0119	0.07428	0.00325	0.0362	0.22604	0.00988
O2	0.03283	0.20498	0.00896	0.12034	0.75137	0.03285
O3	0.04075	0.25442	0.01112	0.0394	0.24598	0.01076
O4	0.04263	0.26615	0.01164	0.04042	0.25239	0.01104
O5	0.05025	0.31375	0.01372	0.12397	0.77405	0.03384
N6	0.01103	0.06886	0.00301	0.0691	0.43145	0.01886
N7	0.03351	0.2092	0.00915	0.07214	0.45041	0.01969
N8	0.05474	0.34175	0.01494	0.01993	0.12442	0.00544
N9	0.03419	0.21346	0.00933	0.03182	0.19867	0.00869
C11	0.02595	0.16204	0.00709	0.05605	0.34996	0.0153
C12	0.0798	0.49823	0.02178	0.07749	0.48381	0.02115
C14	0.05495	0.34309	0.015	0.09625	0.60094	0.02628
C16	0.0512	0.31966	0.01398	0.03698	0.23086	0.01009
C17	0.06105	0.38115	0.01667	0.07394	0.46164	0.02018
C19	0.01578	0.09853	0.00431	0.02747	0.1715	0.0075
C20	0.0089	0.05555	0.00243	0.0136	0.08491	0.00371
C21	0.04215	0.26317	0.01151	0.02906	0.18142	0.00793
O24	0.07295	0.45545	0.01991	0.01367	0.08533	0.00373
O26	0.03397	0.21207	0.00927	0.0197	0.12298	0.00538
O28	0.01173	0.07326	0.0032	−0.0138	−0.0864	−0.0038
C29	0.03853	0.24059	0.01052	0.00023	0.00142	6.2E−05
C30	0.00837	0.05228	0.00229	−0.0227	−0.1416	−0.0062
C32	0.03654	0.22813	0.00997	−0.0157	−0.098	−0.0043
C34	0.03387	0.21145	0.00925	0.00565	0.03527	0.00154
C35	0.05702	0.35604	0.01557	0.02385	0.14892	0.00651
C37	0.04371	0.27291	0.01193	0.02133	0.13317	0.00582
C39	0.01172	0.07316	0.0032	0.00365	0.02277	0.001

f_k^+, f_k^- (in e); s_k^+, s_k^- (in ev^{-1}) and ω_k^+, ω_k^- (in ev).

Table S4 Experimental and theoretical vibrational wave numbers (cm^{-1}) of NF-4HBA with potential energy distribution (PED).

Dimer	Monomer				
Calculated Freq. (cm^{-1})	Calculated Freq.(cm^{-1})	Experimental		Potential Energy Distribution (≥5%)	Simplified description of modes
Scaled	Scaled	IR	Raman		
3674	3676	-		R3[ν(O24H)](100)	OH stretch
3628	-	-		R3[ν(O65H)](100)	OH stretch
3625	3628			R3[ν(O26H)](100)	OH stretch
3504	3503			R2[ν(NH)](99)	NH stretch
3377	-	3220		R2[ν(N48H)](89)+R3[ν(O63H)](8)	NH stretch
3376	-	3197		R3[ν(O63H)](89)+R2[ν(N48H)](7)	OH stretch
3168	3165	3160		R1[ν(CH)](99)	Ring 1 CH stretch
3168	-			R1[ν(CH)](99)	Ring 1 CH stretch
3139	3138	3147	3142	R1[ν(CH)](99)	Ring 1 CH stretch
3138	-			R1[ν(CH)](99)	Ring 1 CH stretch
3102	3106	3109	3106	R3[ν(CH)](96)	Ring 3 CH stretch

3101	-		3100	R3[ν(CH)](99)	Ring 3 CH stretch
3097	3098		3096	R3[ν(CH)](98)	Ring 3 CH stretch
3091	-	3090		R3[ν(CH)](99)	Ring 3 CH stretch
3076	3086		3087	R3[ν(CH)](98)	Ring 3 CH stretch
3076	-		3070	R3[ν(CH)](99)	Ring 3 CH stretch
3065	3047	3057	3057	R3[ν(CH)](99)	Ring 3 CH stretch
3052	-	3042	3053	R3[ν(CH)](97)	Ring 3 CH stretch
2995	3002	3026	3019	ν(C17H)(97)	CH stretch
2995	-	2996		ν(C56H)(99)	CH stretch
2989	2984	2987		R2[$\nu_a(CH_2)$](97)	Ring 2 CH_2 asym stretch
2974	-	2969	2969	R2[$\nu_a(CH_2)$](99)	Ring 2 CH_2 asym stretch
2942	2936	2952	2956	R2[$\nu_s(CH_2)$](99)	Ring 2 CH_2 sym stretch
2936	-	2928	2939	R2[$\nu_s(CH_2)$](99)	Ring 2 CH_2 sym stretch
1807	1803	1831		R2[ν(C=O)(78)+δ_{ring}(7)+ν(NC)(11)]	Ring 2 C=O stretch
1798	-	1771	1770	R2[ν(C=O)(77)+ν(NC)(11)+δ'_{ring}(5)]	Ring 2 C=O stretch
1743	1767	1745		R2[ν(C=O)(74)+ν(NC)(8)+δ_{in}(N48H)(5)]	Ring 2 C=O stretch
1729	-	1720		R2[ν(C=O)(68)+ν(NC)(9)]	Ring 2 C=O stretch
1720	-			R3[ν(C78=O)(71)+ρ(C78O65)(7)+ν(C68C78)(6)]	C=O stretch (Acid)
1696	1693	1664		R3[ν(C39=O)(71)+ρ(C39O26)(7)+ν(C29C39)(7)]	C=O stretch (Acid)
1600	-	1611	1616	ν(C56=N)(52)+R1[ρ(C56H)(16)+ν(C50C56)(16)+ν(CC)(7)]	C=N stretch
1597	1598	1597	1610	ν(C17=N)(49)+R1[ρ(C17H)(14)+ν(C11C17)(14)+ν(CC)(6)]	C=N stretch
1595	1593			R3[ν(CC)(54)+δ_a(9)+δ_{in}(CH)(14)]	Ring 3 CC stretch
1593	-			R3[ν(CC)(59)+δ_a(10)+δ_{in}(CH)(19)]	Ring 3 CC stretch
1573	1567			R3[ν(CC)(66)+δ'_a(8)+δ_{in}(CH)(6)+δ_{in}(C34O)(5)+δ(O24H)(5)]	Ring 3 CC stretch
1569	-			R3[ν(CC)(56)+δ'_a(7)+δ(O63H)(7)+δ_{in}(CH)(7)+δ_{in}(C73O)(5)]	Ring 3 CC stretch
1549	-	1564	1568	R1[ν(CC)(28)+$\nu_a(NO_2)$(24)+δ_{in}(CH)(9)]+ν(C56=N)(8)	Ring 1 CC stretch
1546	1549			R1[ν(CC)(51)+δ_{in}(CH)(12)+$\nu_a(NO_2)$(9)+ν(C17=N)(10)	Ring 1 CC stretch
1528	1525			R1[$\nu_a(NO_2)$(70)+ν(CC)(12)]	NO_2asym stretch
1512	-	1511		R1[$\nu_a(NO_2)$(76)+ν(CC)(6)]	NO_2asym stretch
1498	-	1499	1498	R3[δ_{in}(CH)(46)+ν(CC)(34)+ν(C73O)(10)+ν(C68C78)(5)]	In plane ring def + Ring 3 CC stretch
1496	1495	1494		R3[δ_{in}(CH)(52)+ν(CC)(35)+ν(C34O)(7)+ν(C29C39)(5)]	In plane ring def + Ring 3 CC stretch
1475	-		1479	R1[ν(CC)(39)+δ_{ring}(13)+ν(C50C56)(11)+ν(N45C)(5)]+ν(C56=N)(5)	Ring 1 CC stretch
1473	1476	1457		R1[ν(CC)(36)+δ_{ring}(12)+ν(C11C17)(12)+ν(N6C)(5)]	Ring 1 CC stretch
1434			1436	R3[ν(CC)(34)+δ(O63H)(15)+δ_{in}(CH)(22)+δ_{in}(C68C78)(5)]+τ(H64O3)(6)	Ring 3 CC stretch
1431	1424	1429		R2[$\delta(CH_2)$](89)	Ring 2 CH_2 deformation
1427				R3[ν(CC)(41)+δ_{in}(CH)(29)+δ(O24H)(8)+δ_{in}(C29C39)(7)+δ_{in}(C34O)(5)]	Ring 3 CC stretch +In plane ring def
1414	1424	1410	1405	R2[$\delta(CH_2)$](80)+δ(H23C21O28)(9)	Ring 2 CH_2 deformation
1380	1376	1388	1391	R1[ν(CC)(22)+ν(OC)(26)+δ_{in}(CH)(13)+δ_{in}(C11C17)(5)]	Ring CC stretch+Ring OC stretch
1378	-	1377	1378	R1[ν(CC)(20)+ν(OC)(23)+δ_{in}(CH)(12)]+R2[δ_{in}(N48H)](6)	Ring CC stretch+Ring OC stretch
1373	-			R2[δ_{in}(N48H)(45) R2[ν(NC)(6)]+δ(N48H49O24)(17)	In plane ring NH def
1361	1356			R2[ν(NC)(19)+$\omega(CH_2)$(8)+ν(NC)(8)+ν(N8N)(5)]+R1[ρ(C17H)(6)+ν(CC)(13)+ν(N6O5)(5)]	Ring 2 NC stretch
1355	1334	1346	1345	R3[δ(O63H)(17)+ν(CC)(42)+δ_{in}(CH)	Ring 3 CC stretch

				(17)]+τ(H64O3)(7)	
1351	-			R2[δ_{in}(N48H)(14)+ν(NC)(9)+ν(N47N)(5)]+R1[ρ(C56H)(9)+ν(CC)(11)+ν_s(NO_2)(9)]+δ(N48H49O24)(6)	In plane ring NH def
1339	1327			R2[ν(NC)(23)+δ_{in}(NH)(12)+ν(CC)(5)]+R1[ν_s(NO_2)(11)+ρ(C17H)(5)]	Ring NC stretch+In plane ring NH def
1335	1322			R3[ν(O26C)(16)+ν(C29C39)(15)+δ(O26H)(14)+δ(C39C29O28)(13)+ν(CC)(11)]	Ring 3 OC stretch+Ring 3 CC stretch
1325	1317	1325		R1[ρ(C56H)(8)+ρ(C17H)(7)+ν_s(NO_2)(11)+ν(N6C)(6)]	Ring 1 CH rocking
1324				R3[ν(CC)(52)+δ(O24H)(11)+δ_{in}(CH)(10)]	Ring 3 CC stretch
1322	-			R3[δ(O65H)(20)+ν(C68C78)(16)+ν(O65C)(14)+δ(C78C68O67)(8)+ν(C78O67)(6)]	OH bend (aromatic)+Ring 3 CC stretch
1319				R1[ν_s(NO_2)(21)+ρ(C56H)(12)+ν(N45C)(10)+ρ(C17H)(6)+ρ(NO_2)(5)]	NO_2sym stretch+ Ring 1 CH rocking
1315	-	1318	1321	R2[ω(CH_2)(12)+ν(NC)(18)+δ_{in}(N48H)(5)+δ_{in}(C=O)(7)]+R1[ν_s(NO_2)(14)+ν(N45C)(6)]	Ring 2 CH_2 wagging + NC stretch
1305	1301			R2[ω(CH_2)(33)+δ_{in}(NH)(13)+ν(NC)(15)]+R1[ρ(C17H)](13)	Ring 2 CH_2 wagging + In plane ring NH def
1299	-	1297		R2[δ_{in}(NH)(24)+ν(NC)(13)+ν(CC)(8)+δ_{in}(C20=O)(7)]+R1[ρ(C17H)](5)	In plane ring NHdef +Ring 2 NC stretch
1299	1295			R3[ν(CC)](26)+δ_{in}(CH)(38)+δ_{in}(C29C39)(5)]	In plane ring def+Ring 3 CC stretch
1296	1282			R2[ω(CH_2)(22)+ν(NC)(17)+ν(CC)(16)+δ_{in}(C59=O)(7)+δ_{ring}](6)]+R1[ρ(C56H)](6)	Ring 2 CH_2 wagging+NC stretch
1294	-	1281		R3[ν(CC)(40)+δ_{in}(CH)(46)+δ_{in}(C68C78)(5)]	In plane ring def+Ring 3 CC stretch
1266	1261	1257	1262	R3[ν(C73O)(48)+ν(CC)(18)+δ_{tring}(9)+δ_{in}(CH)(15)]	CO stretch (aromatic)
1247	-	1245		R1[ν(CC)(27)+ν(C50C56)(10)+ν(OC)(9)+ν_s(NO_2)(13)+δ_{in}(CH)(7)+ρ(C56H)(6)]	Ring 1 CC stretch
1244	1243		1252	R1[ν(CC)(23)+ν(C11C17)(9)+ν_s(NO_2)(8)+ν(OC)(7)+δ_{in}(CH)(7)+ρ(C17H)(6)]	Ring 1 CC stretch
1238	-	1231	1239	R3[ν(C34O)(49)+δ_{tring}(10)+ν(CC)(16)+δ_{in}(CH)(12)]	CO stretch (aromatic)
1229	1231			R2[ν(N8N)(22)+ν(NC)(11)]+R1[ν(OC)(21)+δ'_{ring}(5)+δ_{in}(CH)(5)+δ(C17C11N7)(5)]+δ(N8N7C17)(6)	Ring 2 NN stretch+Ring 1 OC stretch
1227	-			R2[ν(N47N)(24)+ν(NC)(12)]+R1[ν(OC)(20)+δ_{in}(CH)(8)+δ'_{ring}(5)]+δ(N47N46C56)(6)	Ring 2 NN stretch+Ring 1 OC stretch
1220	-	1219	1211	R3[ν(CC)](24)+δ(O63H)(15)+ν(C73O)(7)+δ_{in}(CH)(8)]+τ(H64O3)(10)+τ(O63H64)(7)	Ring 3 CC stretch+OH bend
1208	1207			R1[ν(OC)(26)+ν(N6C)(7)+δ'_{ring}(8)]+R2[ν(N8N)(18)+ν(NC)(5)]	Ring 1 OC stretch+Ring 2 NN stretch
1205	-	1188		R1[ν(OC)(29)+δ'_{ring}(9)+ν(N45C)(7)+R2[ν(N47N)(17)+ν(NC)(5)]	Ring 1 OC stretch+Ring 2 NN stretch
1181	1173			R3[δ(O26H)(21)+δ_{in}(CH)(32)+ν(CC)(16)+ν(C29C39)(7)+δ_{tring}(5)+δ(O24H)(5)]	OH bend+ In plane ring def
1178	1171	1177	1177	R2[ν(NC)(47)+ω(CH_2)(19)+δ'_{ring}(5)]	Ring 2 CH_2 wagging+NC stretch
1176	-			R2[ν(NC)(49)+ω(CH_2)(18)]	Ring 2 NC stretch+CH_2 wagging

1171	-			R3[δ(O65H)(30)+ν(C68C78)(13)+δ_{in}(CH)(24)+ν(CC)(13)+δ_{tring}(7)]	OH bend+In plane ring def
1167	1162			R2[γ(CH_2)](92)	Ring 2 CH_2 twisting
1160	1154			R3[δ(O24H)](41)+ν(CC)(21)+δ_{in}(CH)(10)+R2[γ(CH_2)](12)	OH bend+Ring 3 CC stretch
1159	-			R2[γ(CH_2)](73)+R3[δ(O24H)](6)	Ring 2 CH_2 twisting
1156	1155			R1[δ_{in}(CH)(49)+ν(N6C)(8)+δ'$_{ring}$(6)+ν(OC)(5)+ν(C11C17)(5)]	In plane ring def
1154	-			R1[δ_{in}(CH)(48)+ν(N45C)(9)+δ'$_{ring}$(7)+ν(OC)(6)+ν(C50C56)(5)]	In plane ring def
1146	1141			R3[δ(O26H)(24)+δ_{in}(CH)(35)+ν(C29C39)(12)+ν(O26C)(6)+ν(CC)(9)]	In plane ring def+OH bend
1143	-	1140		R3[δ_{in}(CH)(46)+δ(O65H)(17)+ν(C68C78)(10)+ν(CC)(11)]	In plane ring def+OH bend
1103		1120		R3[δ_{in}(CH)(53)+ν(CC)(24)]	In plane ring def+ Ring 3 CC stretch
1095	1099			R3[δ_{in}(CH)(60)+ν(CC)(25)]	In plane ring def+ Ring 3 CC stretch
1093	-			R2[ν(NC)(59)+δ_{in}(C58=O)(8)+δ_{in}(N48H)(8)]+δ(N48H49O24)(5)	Ring 2 NC stretch
1078	1080			R2[ν(NC)(57)+δ_{in}(C19=O)(12)+δ_{in}(NH)(9)+δ_{in}(N8N)(5)]	Ring 2 NC stretch
1074	1065			R3[ν(O26C)(43)+ν(CC)(17)+δ(O26H)(8)+δ(C39C29O28)(7)+δ_{in}(CH)(5)]	CO stretch (aromatic)
1059	-			R3[ν(O65C)(49)+ν(CC)(17)+δ(O65H)(10)+δ(C78C68O67)(6)+δ_{in}(CH)(9)]	CO stretch (aromatic)
1007	1004	1017		R1[δ_{in}(CH)(63)+ν(CC)(25)]	In plane ring def+ Ring 1 CC stretch
1004	-			R1[δ_{in}(CH)(62)+ν(CC)(25)]	In plane ring def+ Ring 1 CC stretch
997	-			R3[δ_{tring}(51)+ν(CC)(33)+δ_{in}(CH)(7)]	Ring 3 trigonal def.
996	993		1025	R3[δ_{tring}(51)+ν(CC)(34)+δ_{in}(CH)(9)]	Ring 3 trigonal def.
980	-		981	R2[ρ(CH_2)(65)+oop(C59=O)(16)+τ(10)]	Ring 2 CH_2 rocking
979	986	977		R2[ρ(CH_2)(63)+δ(H23C21O28)(12)+oop(C20=O)(11)+τ(5)]	Ring 2 CH_2 rocking
974	973			R3[oop(CH)(83)+puck(7)]	Ring 3 CH out of plane def
970	-			R3[oop(CH)(84)+puck(8)]	Ring 3 CH out of plane def
967	966	963	967	R1[ν(OC)(52)+δ'$_{ring}$(14)+ν(C11C17)(7)]	Ring 1 OC stretch
965				R1[ν(OC)(54)+δ'$_{ring}$(13)+ν(C50C56)(8)]	Ring 1 OC stretch
955				R3[oop(CH)(81)+puck(12)]	Ring 3 CH out of plane def
953	952			R1[δ_{ring}(42)+ν(OC)(20)+ν(CC)(13)+ν(N6C)(7)]	Ring 1 def+OC stretch
951				R1[δ_{ring}(42)+ν(OC)(18)+ν(CC)(13)+ν(N45C)(8)]	Ring 1 def+OC stretch
945	944	935	941	R3[oop(CH)(80)+puck(12)]	Ring 3 CH out of plane def
903		916		R1[ω(C56H)](57)+oop(CH)(5)+τ(C56=N)(25)	CH wagging + NC torsion
900	896	908	906	R1[ω(C17H)(50)+τ(C11C17)(6)+oop(CH)(8)]+τ(C17N)(26)	CH wagging + NC torsion
881	879		895	R1[oop(CH)(75)+τ(13)+ω(C17H)(5)]	Ring 1 CH out of plane def
879				R1[oop(CH)(79)+τ(13)]	Ring 1 CH out of plane def
877	863			R2[ν(CC)(48)+ν(NC)(13)+δ_{in}(N48H)(5)+δ_{in}(C=O)(8)]+δ(N48H49O24)(9)	Ring 2 CC stretch + NC stretch

873		875		R2[ν(CC)(55)+ν(NC)(16)+δ_{in}(NH)(7)+δ'_{ring}(5)]	Ring 2 CC stretch + NC stretch
859		862		R3[oop(CH)(67)+τ_a(11)+δ_{in}(C34O)(8)+oop(C29C39)(6)+ω(C39O26)(5)]	Ring 3 CH out of plane def
852	851	852		δ(N47N46C56)(16)+R1[δ'_{ring}(16)+δ(C56C50N46)(13)]+R2[ν(NC)(19)+δ'_{ring}(10)+ν(N47N)(7)+ν(NC)(7)]	Ring 1 def+N-N=C bend
850		847		R1[δ'_{ring}(16)+δ(C17C11N7)(14)]+δ(N8N7C17)(16)+R2[ν(NC)(19)+ν(N8N)(8)+δ_{ring}(8)]	Ring 1 def+C-C=N bend
848	848	831		R3[oop(CH)(62)+δ_{in}(C73O)(13)+τ_a(11)+ω(C78O65)(6)+oop(C68C78)(5)]	Ring 3 CH out of plane def
824		822		R3[δ_a(19)+ν(C73O)(16)+ν(CC)(49)+δ_{tring}(5)]	Ring 3 CC stretch+asym def
821	824			R3[δ_a(21)+ν(C34O)(18)+ν(CC)(42)+ν(C29C39)]	Ring 3 CC stretch+asym def
816	799	810	814	R3[oop(CH)](81)+τ(H64O3)(7)	Ring 3 CH out of plane def
804				R3[oop(CH)(82)+ω(C39O26)(5)]	Ring 3 CH out of plane def
802	800			R1[ρ(NO_2)(41)+δ'_{ring}(19)+δ(NO_2)(13)+δ_{ring}(8)]	NO_2 rocking + Ring def'
801				R1[ρ(NO_2)(42)+δ'_{ring}(19)+δ(NO_2)(14)+δ_{ring}(7)]	NO_2 rocking + Ring def'
795	792			R1[oop(CH)(78)+τ'(7)]	Ring 1 CH out of plane def
794		791		R1[oop(CH)(82)+τ'(6)]	Ring 1 CH out of plane def
767	764	775		R3[puck(32)+ω(C78O65)(28)+δ_{in}(C73O)(12)+oop(C68C78)(11)+oop(CH)(5)]	Ring 3 puckering +CO out of plane def
764				R2[ν(NC)(19)+δ'_{ring}(7)+δ_{in}(C58=O)(5)]+R1[δ'_{ring}(13)+δ_{ring}(11)+ρ(NO_2)(7)+ν(C50C56)(6)]	Ring 2 NC stretch + Ring 1 def'
763	761		788	R2[ν(NC)(18)+δ'_{ring}(6)]+R1[δ'_{ring}(14)+δ_{ring}(11)+ν(C11C17)(6)+ρ(NO_2)(6)]	Ring 2 NC stretch + Ring 1 def'
762				R3[ω(C39O26)(30)+puck(27)+δ_{in}(C34O)(13)+oop(C29C39)(10)+oop(CH)(7)]	CO out of plane def+ Ring 3 puckering
751				τ(H64O3)(40)+τ(O63H64)(21)+δ(O63H64O3)(15)+R3[τ(C73O)](11)	OH torsion
740	739	740		R1[ω(N6O5)(63)+oop(C16N)(19)+τ'(7)]	N=O wagging
739		736		R1[ω(N45O44)(67)+oop(C55N)(14)+τ'(7)]	N=O wagging
728			750	R2[oop(C58=O)(62)+τ(13)+τ'(13)+oop(N48H)(8)]	Ring 2 C=O out of plane def
725	727			R2[oop(C19=O)(65)+τ'(18)+τ(7)]	Ring 2 C=O out of plane def
716	715		739	R3[ρ(C39O26)(19)+δ_{tring}(17)+ν(C29C39)(16)+ν(O26C)(10)+ν(C34O)(8)+δ(C39C29O28)(6)+δ(O26H)(6)]	C=O (acid) rocking + CC stretch + ring trigonal def + OC stretch
713				R3[ρ(C78O65)(20)+ν(C68C78)(18)+δ_{tring}(17)+ν(O65C)(13)+ν(C73O)(6)+δ(O65H)(6)+ν(CC)(7)]	C=O (acid) rocking + CC stretch + ring trigonal def + OC stretch
699				R2[oop(N48H)](52)+δ(N48H49O24)(24)+τ(O24H49)(14)	Ring 2 NH out of plane def
696	693	693	692	R3[puck(58)+δ_{in}(C73O)(14)+ω(C78O65)(10)+oop(CH)(11)]	Ring 3 puckering
694				R3[puck](55)+δ_{in}(C34O)(14)+ω(C39O26)(7)+oop(CH)(9)]	Ring 3 puckering
674				R1[τ'(35)+oop(C50C56)(34)+τ(24)]	Ring 1 torsion + CC out

					of plane def
674	675			R1[τ'(36)+oop(C11C17)(35)+τ(21)]	Ring 1 torsion + CC out of plane def
671	668		669	R2[δ_{ring}(22)+ν(NC)(15)+δ'$_{ring}$(13)+δ_{in}(C=O)(17)+δ_{in}(N8N)(9)+ν(CC)(5)]	Ring 2 def + NC stretch
668		660		R2[δ_{ring}(23)+ν(NC)(15)+δ_{in}(C=O)(18)+δ'$_{ring}$(10)+δ_{in}(N47N)(9)+ν(CC)(5)]	Ring 2 def + NC stretch + C=O in plane def
631		636		R3[δ'$_a$(76)+δ_{in}(C73O)(6)+ν(CC)(7)]	Ring 3 asym def'
630	630	625	624	R3[δ'$_a$(74)+δ_{in}(C34O)(7)+δ_{in}(C29C39)(5)]	Ring 3 asym def'
611	603	619		R2[oop(NH)(41)+oop(C20=O)(29)+τ'(9)+ρ(CH_2)(6)]+δ(H23C21O28)(5)	Ring 2 NH out of plane def + Ring C=O out of plane def
604		605		R2[δ_{in}(C=O)(34)+δ_{ring}(14)+δ'$_{ring}$(9)+δ_{in}(N47N)(8)]+δ(N47N46C56)(5)	Ring 2 C=O out of plane def+ ring def
599	596	592		R2[δ_{in}(C=O)(32)+δ_{ring}(16)+δ_{in}(N8N)(8)+δ'$_{ring}$(7)]+δ(N8N7C17)(6)	Ring 2 C=O out of plane def+ ring def
587	584	583	583	R2[δ'$_{ring}$(29)+δ_{ring}(5)+ν(NC)(12)]	Ring 2 def'+NC stretch
587				R2[δ'$_{ring}$(29)+δ_{ring}(14)+ν(NC)(13)]	Ring 2 def'+NC stretch
582	581			R1[τ(39)+τ'(23)+oop(C16N)(21)]	Ring 1 torsion + NC out of plane def
582				R3[δ_a(23)+ρ(C78O65)(18)+δ(C78C68O67)(13)]	Ring asym def+CO rocking
582				R3[δ_a(15)+ρ(C39O26)(15)+δ(C39C29O28)(14)]+R1[τ(11)+τ'(7)+oop(C16N)(6)]	Ring asym def+CO rocking
581	581			R1[τ(51)+τ'(26)+oop(C55N)(17)]	Ring torsion
575	564	574		τ(C39O26)(65)+R3[δ_{in}(C34O)(8)+τ_a(7)+oop(C29C39)(5)]	CO torsion
570				R2[oop(C=O)(53)+τ(17)+ρ(CH_2)]13)+γ(CH_2)(6)]	Ring 2 C=O out of plane def
565		553	550	τ(C78O65)(69)+R3[δ_{in}(C73O)(9)+τ_a(8)+oop(C68C78)(6)]	CO torsion
536	540	541		R2[oop(NH)(26)+oop(C=O)(25)+ρ(CH_2)(12)]+δ(H23C21O28)(9)+R1[δ(NO_2)](5)	Ring NH out of plane def + ring C=O out of plane def
535		531		R1[δ(NO_2)(25)+δ_{in}(C16N)(15)+ρ(NO_2)(9)+δ_{in}(C11C17)(7)+R2[oop(C=O)(7)+oop(NH)(7)]	NO_2 def + NC in plane def
	534				
535				R1[δ(NO_2)(33)+δ_{in}(C55N)(20)+ρ(NO_2)(12)+δ_{in}(C50C56)(10)]	NO_2 def + NC in plane def
498		501		R3[ρ(C78O65)(15)+δ(C78C68O67)(14)+δ_{in}(C68C78)(11)+δ_{in}(C73O)(10)+δ'$_a$(8)+δ(C39C29O28)(7)]	CO rocking+C-C=O def
498	495			R3[(δ(C39C29O28)(24)+δ_{in}(C29C39)(15)+ρ(C39O26)(14)+δ_{in}(C34O)(7)+δ'$_a$(6)]	C-C=O def+CC in plane def
496				R3[δ_{in}(C73O)(31)+τ_a(29)+oop(C68C78)(12)+puck(10)+oop(CH)(5)]+τ(C78O65)(5)	CO in plane def+ Ring 3 torsion
494	494	492		R3[τ_a(37)+δ_{in}(C34O)(31)+oop(C29C39)(13)+puck(7)]	Ring 3 torsion+ CO in plane def
451	448	470	472	δ(N8N7C17)(16)+R1[δ(NO_2)(14)+ν(N6C)(14)+δ_{in}(C11C17)(10)+δ_{ring}(6)]+R2[δ_{in}(C20=O)](7)	C-C=N def+NO_2 def
448		446		δ(N47N46C56)(17)+R1[δ(NO_2)(16)+δ_{in}(C50C56)(14)+ν(N45C)(11)+δ_{ring}(6)+δ(C56C50N46)(5)]+R2[δ_{in}(N47N)(5)+δ_{in}(C=O)(9)]	N-N=C def+NO_2 def
434		439		R2[δ_{in}(C=O)](20)+ν(NC)(6)+R1[δ_{in}(C11C17)(10)+ρ(NO_2)(7)+δ(C17C11N7)(7)]	Ring 2 C=O in plane def+NC stretch

430	427			R1[ν(N45C)(14)+ρ(NO_2)(10)+δ_{in}(C50C56)(7)+δ(C56C50N46)(6)+δ'$_{ring}$(5)]+R2[δ_{in}(C=O)(23)+ν(NC)(5)]	NC stretch+NO_2 rocking
418				R3[δ_{in}(C73O)(29)+δ(C78C68O67)(7)+δ'$_a$(5)]+τ(H64O3)(12)+τ(O63H64)(7)+R1[ν(N6C)](7)	CO in plane def+C-C=O def
415	413	412	415	R3[τ'$_a$(81)+oop(CH)(7)]	Ring torsion'
410				R3[τ'$_a$(80)+oop(CH)(16)]	Ring torsion'
402	390			R3[δ_{in}(C34O)(50)+δ(C39C29O28)(10)+δ'$_a$(8)]	CO in plane def
395				R2[δ_{in}(C=O)(27)+ν(NC)(9)+R3[δ_{in}(C73O)](14)+R1[ν(N6C)](8)	Ring 2 C=O in plane def+Ring 3 CO in plane def
391	388	390	382	R2[δ_{in}(C=O)(35)+ν(NC)(11)+R1[ν(N45C)(10)+δ_{ring}(5)+R3[δ_{in}(C34O)](9)	Ring 2 C=O in plane def+NC stretch
375	376			τ(C17N)(28)+R1[τ'(14)+τ(11)+oop(C16N)(8)+oop(C11C17)(7)+ω(C17H)(7)+R2[oop(N8N)](12)	C=N torsion+Ring 1 torsion
373				τ(C56=N)(27)+R1[τ'(16)+τ(14)+oop(C50C56)(8)+ω(C56H)(8)+oop(C55N)(7)+R2[oop(N47N)](9)	C=N torsion+Ring 1 torsion
369	387			R3[τ(C34O)](90)	Ring 3 CO torsion
343				R3[δ_a(43)+ν(C68C78)(22)+ρ(C78O65)(13)]	Ring 3 asym def+CC stretch
343	342			R3[δ_a(40)+ν(C29C39)(21)+ρ(C39O26)(13)]	Ring 3 asym def+CC stretch
304	307	303	303	R2[τ(N8N)(36)+oop(N8N)(21)+τ(8)]+R1[τ(C11C17)](16)	NN torsion+NN out of plane def
302				R2[τ(N47N)(37)+oop(N47N)(23)+τ'(10)]+τ(C56=N)(6)+R1[τ(C50C56)(11)+oop(C50C56)(5)]	NN torsion+NN out of plane def
284	284			R2[δ_{in}(N8N)(16)+δ_{in}(C=O)(15)+ν(NC)(5)]+R1[δ_{in}(C16N)(13)+δ_{in}(C11C17)(11)+δ(NO_2)(6)+ν(C11C17)(5)]	NN in plane def+ Ring C=O in plane def
283				R3[oop(C68C78)(26)+τ_a(21)+puck(12)+oop(CH)(6)]	CC out of plane def+ Ring 3 asym torsion
283		280		R3[oop(C68C78)(13)+τ_a(10)+puck(6)]+R2[δ_{in}(N47N)(11)+δ_{in}(C=O)(10)]+R1[δ_{in}(C55N)(8)+δ_{in}(C50C56)(7)]	CC out of plane def+ Ring 3 asym torsion
282	279			R3[oop(C29C39)(33)+τ_a(29)+puck(13)+ω(C39O26)(5)+δ_{in}(C34O)(5)+oop(CH)(5)]	CC out of plane def+ Ring 3 asym torsion
221	216	231	232	R1[δ_{in}(C16N)(25)+δ(NO_2)(10)+δ(C17C11N7)(9)+ν(C11C17)(6)+ρ(NO_2)(5)]	CN in plane def + NO_2 def
217		209	211	R1[δ_{in}(C55N)(29)+δ(NO_2)(12)+δ(C56C50N46)(11)+ν(C50C56)(6)+ρ(NO_2)(5)+δ_{ring}(5)]	CN in plane def + NO_2 def
201	202	203		R2[τ](28)+δ(H23C21O28)(15)+ν(O28H23)(13)+R3[δ_{in}(C68C78)](12)	Ring 2 torsion+ C-HO def
200				R2[τ(31)+oop(N8N)(8)+δ(H23C21O28)(16)+ν(O28H23)(12)+R3[δ_{in}(C68C78)](11)+ R1[τ(C11C17)](5)	Ring 2 torsion+ C-HO def
197	194			R1[oop(C16N)(31)+τ(C11C17)(7)]+R2[τ(N8N)(18)+oop(N8N)(6)+τ(5)]+R3[δ_{in}(C29C39)](6)	CN out of plane def + NN torsion
195	190			R3[δ_{in}(C29C39)(41)+δ(C39C29O28)(12)]+τ(O28H23)(16)+R1[oop(C16N)](5)	CC in plane def + OH torsion
192		188		R1[oop(C55N)(42)+oop(C50C56)(6)+R2[τ(N47N)(13)+oop(N47N)(6)]+τ(C56=N)(5)	CN out of plane def + NN torsion

185	148	176		R2[τ'(66)+oop(N47N)(13)]+τ(C59O42)(7)	Ring 2 torsion
168		168		R2[τ'(54)+oop(NH)(31)]	Ring 2 torsion
156		155	159	R2[τ(52)+oop(N48H)(44)]	Ring 2 torsion
151		150		ν(O3H64)(19)+R2[δ_{in}(N8N)](15)+δ(N8N7C17)(11)+R1[δ_{in}(C16N)(11)+δ_{in}(C11C17)(5)]+R3[δ_{in}(C68C78)](5)+ν(O2H61)(5)	OH stretch+NN in plane def
144		140		ν(O42H33)(22)+R2[δ_{in}(N47N)](17)+δ(N47N46C56)(12)+R1[δ_{in}(C55N)(12)+δ_{in}(C50C56)(6)]+δ(N48H49O24)(5)	OH stretch+NN in plane def
136	134	133		R1[oop(C16N)(17)+τ(C16N)(14)+oop(C11C17)(8)+τ(C11C17)(8)+R2[oop(N8N)(14)+τ'(6)]+ν(O28H23)(8)	CN out of plane def+CN torsion
128	131			τ(C59O42)(18)+R1[oop(C55N)(15)+oop(C50C56)(10)+τ(C55N)(9)]+R2[τ(12)+oop(N47N)(10)]	CO torsion+CN out of plane def
115				R3[τ_a(27)+oop(C68C78)(16)+τ(C73O)(9)]+ν(O3H64)(12)+τ(O63H64)(6)	Ring 3 asym torsion + CC out of plane def
110	107			R3[τ_a(37)+oop(C29C39)(16)]+δ(C39O28H23)(9)+ν(O24H49)(7)+τ(O28H23)(5)	Ring 3 asym torsion + CC out of plane def
105	90			R1[τ(C16N)](18)+ν(O3H64)(13)+ν(O2H61)(10)+R2[oop(N8N)](8)+ν(O28H23)(6)+δ(N6O2H61)(5)	CN torsion+OH stretch
98				R1[τ(C16N)](31)+ν(O3H64)(15)+R2[oop(N8N)](8)	CN torsion+OH stretch
84				τ(C59O42)(34)+R1[τ(C55N)](15)+δ(N48H49O24)(12)+R2[oop(N47N)](10)+τ(O28H23)(5)	CO torsion + CN torsion
82				ν(O42H33)(20)+ν(O24H49)(20)+ν(O2H61)(10)+τ(O28H23)(8)+τ(O24H49)(6)	OH stretch
78	76			R3[τ(C29C39)](46)+δ(C39O28H23)(20)+τ(O28H23)(17)+δ(H23C21O28)(7)	CC torsion+C-HO def
75				R3[τ(C68C78)(55)+τ(C73O)(6)+τ(H64O3)(7)+ν(O28H23)(5)	CC torsion+CO torsion
74				R1[τ(C11C17)](16)+ν(O28H23)(13)+ν(O42H33)(12)+R3[τ(C68C78)](7)+δ(N6O2H61)(6)+ν(O2H61)(6)+R2[τ(5)+oop(N8N)(5)]+ν(O24H49)(5)	CC torsion+OH stretch
65				τ(H64O3)(20)+ν(O24H49)(16)+τ(O63H64)(8)+τ(C20O3)(6)+τ(O28H23)(6)+ν(O28H23)(5)	OH torsion+OH stretch
63				ν(O24H49)(29)+τ(H64O3)(14)+τ(N6O2)(8)+τ(O63H64)(6)	OH stretch+OH torsion
57				ν(O2H61)(14)+δ(N48H49O24)(13)+ν(O24H49)(11)+τ(N6O2)(11)+R1[(δ(C56C50N46)(9)+δ_{in}(C50C56)(8)]+τ(O28H23)(8)	OH stretch+NHO def
52	57			τ(C59O42)(34)+R1[τ(C55N)](11)+ν(O42H33)(11)+τ(O24H49)(7)+R2[oop(N48H)](6)	CO torsion+CN torsion
48	49			R1[(δ(C17C11N7)(16)+δ_{in}(C11C17)(13)]+δ(C20O3H64)(13)+R3[τ(C73O)](7)+δ(N8N7C17)(7)+τ(N6O2)(6)	C-C=N def + CC in plane def + C-OH def
45	39			τ(O28H23)(36)+ν(O42H33)(24)+τ(C59O42)(8)+δ(H23C21O28)(7)	OH torsion+OH stretch
42				R3[τ(C73O)(27)+τ(C68C78)(5)]+δ(C20O3H64)(9)+δ(O63H64O3)(8)+δ(N	CO torsion+C-OH def

		8N7C17)(7)+R1[(δ(C17C11N7)](7)	
39		τ(C59O42)(29)+ν(O42H33)(13)+R1[τ(C11C17)](7)+ν(O2H61)(7)+δ(C39O28H23)(7)	CO torsion+OH stretch
37	-	ν(O42H33)(19)+τ(O28H23)(12)+δ(N6O2H61)(8)+τ(H64O3)(7)+R1[τ(C16N)](5)	OH stretch+OH torsion
29	36	δ(H23C21O28)(40)+τ(C59O42)(10)+τ(O28H23)(9)+δ(C39O28H23)(8)+ν(O28H23)(7)+τ(N6O2)(5)	CHO def+CO torsion
26	-	τ(C59O42)(40)+τ(O24H49)(10)+R2[oop(N48H)](7)+δ(N48H49O24)(7)+ν(O2H61)(5)	CO torsion+OH torsion
24	29	δ(H23C21O28)(14)+τ(C59O42)(13)+δ(C39O28H23)(12)+τ(O63H64)(8)+τ(H64O3)(7)+τ(O28H23)(6)+ν(O28H23)(6)+ν(O42H33)(5)	CHO def+CO torsion
22	22	δ(C39O28H23)(52)+τ(O24H49)(8)+δ(H23C21O28)(5)	CHO def
20	-	ν(O2H61)(13)+τ(O24H49)(8)+τ(O28H23)(8)+τ(O63H64)(5)+τ(N6O2)(5)	OH stretch+OH torsion
17	-	τ(O28H23)(31)+τ(C59O42)(15)+δ(N48H49O24)(13)+ν(O42H33)(7)+τ(N6O2)(7)	OH torsion+CO torsion
15	16	δ(N48H49O24)(17)+ν(O42H33)(14)+τ(C59O42)(11)+τ(N6O2)(8)+δ(C39O28H23)(6)+ν(O24H49)(6)+τ(O63H64)(5)	NHO def+OH stretch
13	12	δ(C39O28H23)(29)+τ(N6O2)(12)+τ(O63H64)(8)+ν(O2H61)(7)+τ(O28H23)(6)+ν(O42H33)(6)+δ(N6O2H61)(5)	COH def+NO torsion
13	-	τ(O28H23)(13)+τ(C20O3)(13)+δ(H23C21O28)(10)+R1[τ(C11C17)](9)+ν(O28H23)(7)+τ(O24H49)(7)+R3[τ(C29C39)](7)+δ(C39O28H23)(5)	OH torsion+CO torsion
7	-	δ(C39O28H23)(29)+τ(N6O2)(14)+τ(O28H23)(10)+τ(C59O42)(7)+τ(O63H64)(6)+τ(C20O3)(5)+δ(H23C21O28)(5)	COH def+NO torsion
5	6	τ(C59O42)(24)+δ(N6O2H61)(18)+τ(N6O2)(18)+ν(O2H61)(9)+τ(O28H23)(7)	CO torsion+NOH def+NO torsion
4	-	δ(C39O28H23)(23)+τ(O28H23)(16)+τ(O63H64)(15)+ν(O2H61)(11)+R1[τ(C11C17)](5)	COH def+OH torsion

Table S5 Theoretical and experimental vibrational wavenumbers (in cm^{-1}) of 4HBA and their assignments.

DFT		IR	Raman	PED
Unscaled	Scaled			
3812	3679	3387		R3[ν(O10H)](100)
3758	3627	3203		R3[ν(O9H)](100)
3211	3099			R3[ν(CH)](95)
3208	3095			R3[ν(CH)](97)
3193	3081	3080		R3[ν(CH)](99)
3158	3047	3067		R3[ν(CH)](97)
1787	1724	1678		R3[ν(C1=O)(75)+ρ(C1O9)(7)+ν(C1C2)(6)
1652	1595	1609	1610	R3[ν(CC)(61)+δ_a(11)+δ_{in}(CH)(20)]
1628	1571	1595	1597	R3[ν(CC)(68)+δ'$_a$(8)+δ_{in}(CH)(6)+δ(O10H)(5)+δ_{in}(C5O)(5)]
1550	1496	1448	1440	R3[δ_{in}(CH)(48)+ν(CC)(35)+ν(C5O)(9)+ν(C1C2)(5)]
1475	1423	1423		R3[ν(CC)(42)+δ_{in}(CH)(30)+δ(O10H)(8)+δ_{in}(C2C1)(5)+δ_{in}(C5O)(5)]

1378	1329	1364		R3[ν(CC)(46)+δ_{in}(CH)(12)+δ(O9H)(8)+ν(C1C2)(8)+δ(O10H)(8)+ν(C1O9)(7)+δ(O8C1C2)(5)]
1368	1320	1317	1312	R3[δ(O9H)(13)+ν(C1C2)(10)+ν(C1O9)(9)+δ(O10H)(8)+ν(CC)(35)+δ_{in}(CH)(8)]
1340	1293	1294	1290	R3[δ_{in}(CH)(55)+ν(CC)(33)+δ_{in}(C2C1)(5)]
1300	1255	1244	1265	R3[ν(C5O)(53)+δ_{tring}(11)+ν(CC)(17)+δ_{in}(CH)(14)]
1214	1172		1220	R3[δ(O9H)(31)+δ_{in}(CH)(25)+ν(C1C2)(13)+δ_{tring}(8)+ν(CC)(13)]
1194	1152	1169	1165	R3[δ(O10H)(44)+δ_{in}(CH)(14)+ν(CC)(22)]
1183	1142	1128	1130	R3[δ_{in}(CH)(37)+δ(O9H)(16)+δ(O10H)(10)+ν(C1C2)(9)+ν(CC)(16)]
1133	1093	1101		R3[δin(CH)(55)+ν(CC)(26)]
1097	1059	1034		R3[ν(C1O9)(47)+ν(CC)(18)+δ(O9H)(9)+δ(O8C1C2)(6)+δ_{in}(CH)(9)]
1032	996	1013		R3[δ_{tring}(51)+ν(CC)(34)+δ_{in}(CH)(9)]
1007	971			R3[oop(CH)(85)+puck(9)]
979	944	930		R3[oop(CH)(81)+puck(11)]
874	843	854	853	R3[oop(CH)(64)+opp(C5O)(11)+τ_a(10)+ω(C1O9)(6)+oop(C2C1)(6)]
852	822	837	839	R3[δ_a(21)+ν(C5O)(17)+ν(CC)(47)]
827	798			R3[oop(CH)](90)
790	762	770	772	R3[puck(34)+ω(C1O9)(29)+opp(C5O)(14)+oop(C2C1)(11)+oop(CH)(7)]
737	711	694	693	R3[ρ(C1O9)(20)+ν(C1C2)(18)+δ_{tring}(17)+ν(C1O9)(13)+ν(C5O)(8)+δ(O9H)(6)+δ(O8C1C2)(5)+ν(CC)(7)]
717	692	692		R3[puck(60)+opp(C5O)(13)+ω(C1O9)(9)+oop(CH)(11)]
653	630	642	642	R3[δ'$_a$(78)+δ_{in}(C5O)(6)+ν(CC)(6)]
603	581	619	614	R3[δ_a(28)+ρ(C1O9)(26)+δ(O8C1C2)(20)+ν(C5O)(5)+δ(O9H)(5)]
588	567	548	560	R3[τ(C1O9)(71)+opp(C5O)(8)+τ_a(6)+oop(C2C1)(5)]
511	493	503	501	R3[ρ(C1O9)(25)+δ(O8C1C2)(23)+δ_{in}(C2C1)(17)+δ_{in}(C5O)(10)+δ'$_a$(8)]
510	492			R3[opp(C5O)(33)+τ_a(31)+oop(C2C1)(13)+puck(9)+oop(CH)(8)]
428	413	419		R3[τ'$_a$(82)+oop(CH)(16)]
402	388			R3[δ_{in}(C5O)(63)+δ'$_a$(11)+δ(O8C1C2)(9)]
393	379		388	R3[τ(C5O10)](95)
352	340	-	306	R3[δ_a(45)+ν(C1C2)(24)+ρ(C1O9)(14)]
290	280	-		R3[oop(C2C1)(36)+τ_a(27)+puck(16)+ω(C1O9)(6)+opp(C5O)(5)+oop(CH)(8)]
195	188	-	-	R3[δ_{in}(C2C1)(64)+δ(O8C1C2)(18)+ρ(C1O9)(6)+δ_{in}(C5O)(5)]
109	105	-	-	R3[τa(48)+oop(C2C1)(25)+ω(C1O9)(6)+oop(CH)(18)]
73	71	-	-	R3[τ(C1C2)(90)+τ'$_a$(7)]

Table S6 Second order perturbation theory analysis of Fock matrix in NBO Basis of monomeric model of NF-4HBA.

Donor NBO (i)	ED(i)/e	Acceptor NBO (j)	ED(j)/e	E(2)[a] K cal/mol	E(j)-E(i)[b] a.u.	F(i,j)[c] a.u.
within unit 1						
πO2-N6	1.98253	n(3)O5	1.47096	11.27	0.18	0.077
πO2-N6	1.98253	π*O2-N6	0.65286	7.71	0.32	0.054
πO2-N6	1.98253	π*C14-C16	0.31639	5.47	0.44	0.048
πN7-C17	1.90975	π*C11-C12	0.32703	12.10	0.34	0.061
πC11-C12	1.74906	π*N7-C17	0.24868	17.71	0.28	0.063
πC11-C12	1.74906	π*C14-C16	0.31639	19.17	0.28	0.067
σC11-C17	1.97632	σ*N7-N8	0.02727	5.25	1.10	0.068
σC12-C14	1.96998	σ*N6-C16	0.11657	8.15	0.98	0.082
σC12-C14	1.96998	σ*C11-C17	0.02912	6.21	1.14	0.075
πC14-C16	1.77585	π*O2-N6	0.65286	23.88	0.17	0.065
πC14-C16	1.77585	π*C11-C12	0.32703	14.48	0.30	0.060
σC17-H18	1.97893	σ*O1-C11	0.02826	5.82	0.89	0.064
σC20-C21	1.97360	σ*N7-N8	0.02727	5.51	1.04	0.068
n(2)O1	1.70033	π*C11-C12	0.32703	30.17	0.36	0.093
n(2)O1	1.70033	π*C14-C16	0.31639	29.09	0.35	0.090

n(2)O2	1.88800	σ*O5-N6	0.05941	19.43	0.70	0.105
n(2)O2	1.88800	σ*N6-C16	0.11657	16.61	0.57	0.087
n(2)O3	1.84575	σ*N9-C20	0.08610	28.41	0.67	0.126
n(2)O3	1.84575	σ*C20-C21	0.07982	24.64	0.59	0.110
n(2)O4	1.82269	σ*N8-C19	0.11007	31.37	0.62	0.127
n(2)O4	1.82269	σ*N9-C19	0.09265	29.35	0.63	0.124
n(2)O5	1.88972	σ*O2-N6	0.05847	19.08	0.71	0.105
n(2)O5	1.88972	σ*N6-C16	0.11657	14.61	0.57	0.082
n(3)O5	1.47096	π*O2-N6	0.65286	158.54	0.14	0.138
n(1)N7	1.90548	σ*N8-C21	0.04640	14.05	0.68	0.088
n(1)N7	1.90548	σ*C17-H18	0.03413	10.28	0.76	0.080
n(1)N8	1.63455	π*O4-C19	0.31059	51.79	0.28	0.110
n(1)N8	1.63455	π*N7-C17	0.24868	38.83	0.27	0.095
n(1)N8	1.63455	σ*C21-H22	0.02042	5.49	0.62	0.057
n(1)N8	1.63455	σ*C21-H23	0.01985	5.14	0.64	0.056
n(1)N9	1.65536	π*O3-C20	0.23905	56.83	0.28	0.116
n(1)N9	1.65536	π*O4-C19	0.31059	50.54	0.29	0.108
π*O2-N6	0.65286	π*C14-C16	0.31639	21.71	0.12	0.066
σ*N8-C19	0.11007	σ*N9-C20	0.08610	9.94	0.04	0.055
		from unit 1 to unit 2				
πN7-C17	1.90975	σ*C30-H31	0.01575	0.16	0.81	0.010
σC21-H23	1.96592	σ*O28-C39	0.01939	0.09	1.13	0.009
n(1)N7	1.90548	σ*C30-H31	0.01575	0.23	0.85	0.013
π*N7-C17	0.24868	σ*C30-H31	0.01575	0.06	0.47	0.013
		from unit 2 to unit 1				
σC30-H31	1.97611	π*N7-C17	0.24868	0.06	0.49	0.005
n(1)O28	1.97603	σ*C21-H22	0.02042	0.15	1.06	0.011
n(1)O28	1.97603	σ*C21-H23	0.01985	0.39	1.08	0.018
		within unit2				
σO24-H25	1.98716	σ*C32-C34	0.02587	5.31	1.28	0.074
πC29-C37	1.64964	π*O28-C39	0.27883	27.85	0.25	0.076
πC29-C37	1.64964	π*C30-C32	0.27569	22.09	0.29	0.073
πC29-C37	1.64964	π*C34-C35	0.38876	15.87	0.27	0.059
πC30-C32	1.68305	π*C29-C37	0.40222	16.28	0.27	0.061
πC30-C32	1.68305	π*C34-C35	0.38876	25.32	0.27	0.075
πC34-C35	1.62265	π*C29-C37	0.40222	26.55	0.29	0.078
πC34-C35	1.62265	π*C30-C32	0.27569	13.76	0.30	0.059
n(1)O24	1.97793	σ*C34-C35	0.02941	7.34	1.14	0.082
n(2)O24	1.85644	π*C34-C35	0.38876	31.17	0.34	0.099
n(1)O26	1.97794	σ*O28-C39	0.01939	6.57	1.23	0.080
n(2)O26	1.82984	π*O28-C39	0.27883	45.41	0.34	0.113
n(2)O28	1.85855	σ*O26-C39	0.09322	30.93	0.62	0.126
n(2)O28	1.85855	σ*C29-C39	0.06789	18.83	0.70	0.104
π*O28-C39	0.27883	π*C29-C37	0.40222	88.33	0.03	0.074
π*C29-C37	0.40222	π*C30-C32	0.27569	228.10	0.01	0.079
π*C34-C35	0.38876	π*C30-C32	0.27569	136.27	0.02	0.080

[a]E(2) means energy of hyperconjugative interaction (stabilization energy).
[b]Energy difference between donor (i) and acceptor (j) NBO orbitals.
[c]F(i, j) is the Fock matrix element between i and j NBO orbitals.