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#### **+** Electronic Supplementary Information

# Spectroscopic (FT-IR, FT-Raman, <sup>13</sup>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. 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

Geometrical	Expe	rimental		Calculated			
Parameters	-			neters			
	NF-4HBA	NF	NF	-4HBA	NF		
			Dimer	Monomer	Monomer		
		Bond len	gth (Å)				
01-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	1.0910	_		
O24-H25	0.9042	_	0.9634	0.963	_		
024-034	1 368	_	1 3682	1 3564	-		
026-H27	0.0244		0.9678	0.9674	-		
$O_{26} C_{39}$	1 2073		1 3513	1 3557	-		
020-039	1.2573		1.3313	1.3357	-		
$C_{29}$ $C_{30}$	1.2502		1 3086	1.2155	-		
$C_{29}$ $C_{37}$	1.3082	-	1.3060	1.4004	-		
$C_{29}$ - $C_{30}$	1.3962	-	1.3909	1.3977	-		
C29-C39	1.4708	-	1.4742	1.4719	-		
C30 C22	1 2824	-	1.0797	1.0794	-		
$C_{20}$ $H_{22}$	1.3024	-	1.3607	1.3790	-		
C32-F135	0.9303	-	1.0810	1.0000	-		
C32-C34	1.3919	-	1.3939	1.3903	-		
C34-C35	1.3930	-	1.3934	1.3900	-		
C35-H30	0.95	-	1.0652	1.0650	-		
C35-C37	1.3882	-	1.3847	1.3836	-		
C37-H38	0.9504	- Donal Ar	1.0795	1.0797	-		
C11 O1 C16	104 61 42	104 9201	106 1159	106 222	106 1501		
02-N6-05	104.0145	104.8201	100.1130	100.232	110.1501		
02 - 10 - 03 02 N6 C16	118 2060	177 5944	123.3212	125.9022	117.1004		
02-100-010	116.2909	121.3044	116.3771	110.13/	121.1310		
03-100-010 Nº N7 017	110.9/34	119.2803	110.2788	110.2025	119.0/3/		
110-11/-U1/	110.2029	112.7821	119.23/	119.5025	112.3943		
INO-IN/-HOI	107.7050	115.0228	92.8/20	102.10/3	114.5001		
U1/-IN/-H31	90.2339	127.9628	88.1198	100.058	121.4838		
IN/-INÖ-UI9	119.8394	118.9309	119.690/	119.6329	124.0161		
IN/-IN8-C21	127.0192	110.1039	127.5587	127.4424	112.4628		

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

C19-N8-C2	21	112.7261	108.3285	112.4218	112.3713	112.4603
H10-N9-C	19	122.1132	101.6822	121.4952	121.5482	102.8274
H10-N9-C2	20	125.1867	114.8676	124.2668	124.0113	108.7933
C19-N9-C2	20	112.6928	110.0802	114.1211	114.4083	110.0875
01-C11-C1	12	110.7048	110.9542	110.0246	109.9309	110.0899
01-C11-C1	17	118.4285	119.0128	119.7393	119.5378	121.2521
C12-C11-C	C17	130.8314	126.0008	130.2324	130.525	123.7857
C11-C12-H	H13	126.6419	114.8383	126.0234	126.0136	114.9622
C11-C12-C	C14	106.7702	117.7624	106.6887	106.727	119.8172
H13-C12-C	C14	126.5879	109.6004	127.2871	127.2593	110.0025
C12-C14-H	115	127.6007	132.6225	128.8881	128.8931	130.1803
C12-C14-C	C16	104.7686	132.7174	105.0764	105.1325	128.9352
H15-C14-C	216	127.6306	122.5127	126.0329	125.9739	126.0010
01-C16-N	б	116.272	104.6656	117.6491	117.6031	105.0638
01-C16-C1	14	113.1382	128.0744	112.0941	111.9772	128.6304
N6-C16-C1	14	130 5515	126 6982	130 2397	130 4149	126 6614
N7-C17-C1	11	119 7922	105 2273	120 9119	120 7481	104 7082
N7-C17-H	18	120 1216	124 2619	123 8744	123 8637	126 2021
C11-C17-F	418	120.1210	118 3036	115 2131	115 3856	118 1078
04-C19-N	8	128.6647	117 4108	129 2319	128 57	115 6901
04-C19-N	0	125.0047	107 8642	126 2131	126.57	106 6050
04-C19-02	28	02 1125	107.8042	-	116 /812	126.0786
N8 C10 N0	20	92.1125 105 5404	121.4407	-	104 754	120.0780
N8 C10 O	9 10	105.5404 92.6457	130.0343	104.5510	58 5221	127.2233
No-C19-O2	20	04.1021	-	-	90 4291	-
N9-C19-O	28	94.1031	123.7463	-	09.4301 127 1964	127.3339
03-C20-9	1	125.8094	127.0393	120.3144	127.1004	120.8902
03-C20-C2	21	120.0272	107.1909	127.0008	127.1391	105.5098
N9-C20-C2	21	107.5023	115.0483	106.4161	105.6742	112.08//
N8-C21-C2	20	101.476	116.1495	102.4067	102.7248	117.6940
N8-C21-H	22	111.4/16	130.8022	112.7034	112.6029	130.2183
N8-C21-H	23	111.4774	-	111.9026	111.2108	-
C20-C21-F	122	111.461	-	110.4368	110.0698	-
C20-C21-F	123	111.4976	-	109.4901	109.8923	-
H22-C21-F	123	109.3072	-	109.6798	110.1115	-
H25-O24-O	234	110.4506	-	110.5323	109.9786	-
H2/-O26-C		111.057	-	106.79	106.3707	-
C19-O28-C	39	92.9856	-	-	126.528	-
C30-C29-C	237	119.5571	-	119.1489	119.0307	-
C30-C29-C	.39	119.4529	-	118.6092	118.8/46	-
C37-C29-C	239	120.9681	-	122.2418	122.0946	-
C29-C30-H	431	119.7466	-	119.0563	119.046	-
C29-C30-C	232	120.5462	-	121.0365	121.01	-
H31-C30-C	.32	119.7072	-	119.906	119.944	-
N7-H31-C3	30	120.1317	-	164.2131	179.9977	-
C30-C32-F	433	120.3287	-	121.0604	121.1836	-
C30-C32-C	234	119.3716	-	119.0683	119.4345	-
H33-C32-C	234	120.2997	-	119.8712	119.3819	-
O24-C34-C	232	117.3145	-	117.3166	117.4135	-
O24-C34-C	235	121.7433	-	121.905	122.3823	-
C32-C34-C	235	120.9417	-	120.7784	120.2042	-
C34-C35-H	136	120.3279	-	120.181	119.9073	-
C34-C35-C	237	119.3483	-	119.6214	119.949	-
H36-C35-C	237	120.3238	-	120.1976	120.1437	-
C29-C37-C	235	120.2293	-	120.3426	120.3712	-
C29-C37-H	138	119.8811	-	119.8429	119.8063	-
C35-C37-H	138	119.8895	-	119.8143	119.8225	-
O26-C39-C	028	122.8706	-178.6492	121.3898	120.9251	179.9922
O26-C39-C	229	117.0303	0.1285	113.5363	113.4857	0.0013
<u>028</u> -C39-C	229	120.0958	0.1232	125.0737	125.5891	0.0047
			<b>Dihedral angl</b>	e (°)		
C16-O1-C1	11-C12	0.5608	-179.877	0.2277	-0.037	179.9624
C16-O1-C1	11-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
01-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
01-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	-
04-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	62.72.78	-
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	-
С34-С35-С37-Н38	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  $(\omega_k^+, \omega_k^-)$  using Hirshfeld atomic charges.

Sites	$fk^+$	$\omega_{ m k}{}^+$	$s_k^+$	$f_k^-$	$\omega_{\rm k}$	$s_{\rm k}$	$f_k^+/f_k^-$	$f_k^-/f_k^+$	
For NF									
01	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	
08	0.08745	0.2656	0.01625	0.12351	0.37511	0.02295	0.70807	1.41229	
09	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	
$f_{k}^{+}, f_{k}^{-}$ (ir	$f_{k^{+}}, f_{k^{-}}(in e); s_{k^{+}}, s_{k^{-}}(in ev^{-1}) and \omega_{k^{+}}, \omega_{k^{-}}(in ev).$								

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

Sites	$f_k^+$	$\omega_k^+$	$s_k^+$	$f_k^-$	$\omega_{ m k}$	$s_k^-$
		Fro	m Hirshfeld atomic	charges		
01	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
$f_i + f_i - (in \rho)$	$c_{1} + c_{2} - (in \alpha v^{-1})$	and $\omega_1^+ \omega_2^-$ (in $\omega_2^-$				

 $f_k^+$ ,  $f_k^-$  (in e);  $s_k^+$ ,  $s_k^-$  (in ev<sup>-1</sup>) and  $\omega_k^+$ ,  $\omega_k^-$  (in ev).

 Table S4 Experimental and theoretical vibrational wave numbers (cm<sup>-1</sup>) of NF-4HBA with potential energy distribution (PED).

 Dimer
 Monomer

Dimer	1.1011011101				
Calculated	Calculated	Experimental		Potential Energy Distribution (≥5%)	Simplified description of
Freq. (cm <sup>-1</sup> )	Freq.(cm <sup>-1</sup> )				modes
Scaled	Scaled	IR	Raman		
3674	3676	-		R3[v(O24H)](100)	OH stretch
3628	-	-		R3[v(O65H)](100)	OH stretch
3625	3628			R3[v(O26H)](100)	OH stretch
3504	3503			R2[v(NH)](99)	NH stretch
3377	-	3220		R2[v(N48H)](89)+R3[v(O63H)](8)	NH stretch
3376	-	3197		R3[v(O63H)](89)+R2[v(N48H)](7)	OH stretch
3168	3165	3160		R1[v(CH)](99)	Ring 1 CH stretch
3168	-			R1[v(CH)](99)	Ring 1 CH stretch
3139	3138	3147	3142	R1[v(CH)](99)	Ring 1 CH stretch
3138	-			R1[v(CH)](99)	Ring 1 CH stretch
3102	3106	3109	3106	R3[v(CH)](96)	Ring 3 CH stretch

3101	-		3100	R3[v(CH)](99)	Ring 3 CH stretch
3097	3098		3096	R3[v(CH)](98)	Ring 3 CH stretch
3091	-	3090		R3[v(CH)](99)	Ring 3 CH stretch
3076	3086		3087	R3[v(CH)](98)	Ring 3 CH stretch
3076	-		3070	R3[v(CH)](99)	Ring 3 CH stretch
3065	3047	3057	3057	R3[v(CH)](99)	Ring 3 CH stretch
3052	-	3042	3053	R3[v(CH)](97)	Ring 3 CH stretch
2995	3002	3026	3019	v(C17H)(97)	CH stretch
2995	-	2996		v(C56H)(99)	CH stretch
2989	2984	2987		$R2[v_a(CH_2)](97)$	Ring 2 CH <sub>2</sub> asym stretch
2974	-	2969	2969	$R2[v_a(CH_2)](99)$	Ring 2 CH <sub>2</sub> asym stretch
2942	2936	2952	2956	$R2[v_s(CH_2)](99)$	Ring 2 CH <sub>2</sub> sym stretch
2936	-	2928	2939	$R2[v_s(CH_2)](99)$	Ring 2 CH <sub>2</sub> sym stretch
1807	1803	1831		$R2[\nu(C=O)(78)+\delta_{ring}(7)+\nu(NC)(11)]$	Ring 2 C=O stretch
1798	-	1771	1770	$R2[v(C=O)(77)+v(NC)(11)+\delta'_{ring}(5)]$	Ring 2 C=O stretch
1743	1767	1745		R2[ $\nu$ (C=O)(74)+ $\nu$ (NC)(8)+ $\delta_{in}$ (N48H)	Ring 2 C=O stretch
1729	_	1720		$R^{2}[v(C=O)(68)+v(NC)(9)]$	Ring 2 C=O stretch
1720	_	1720		$R_{2}[v(C78=0)(71)+o(C78065)(7)+v($	C=0 stretch (Acid)
1720				C(8C78)(6)	
1696	1693	1664		$B_3[v(C39=0)(71)+o(C39O26)(7)+v($	C=O stretch (Acid)
1090	1075	1004		$C_{29}C_{39}(7)$ ]	e=o succen (rield)
1600	_	1611	1616	v(C56=N)(52)+R1[o(C56H)(16)+v(C	C=N stretch
1000		1011	1010	50C56)(16)+y(CC)(7)]	C=1 ( Subtern
1597	1598	1597	1610	v(C17=N)(49)+R1[o(C17H)(14)+v(C)]	C=N stretch
1077	10,0	10,77	1010	11C17)(14)+v(CC)(6)]	
1595	1593			$R_{3}[v(CC)(54)+\delta_{a}(9)+\delta_{in}(CH)(14)]$	Ring 3 CC stretch
1593	-			$R_{3}[v(CC)(59)+\delta_{a}(10)+\delta_{in}(CH)(19)]$	Ring 3 CC stretch
1573	1567			$R_{3}[v(CC)(66)+\delta'_{2}(8)+\delta_{in}(CH)(6)+\delta_{in}(CH)(6)$	Ring 3 CC stretch
1010	1007			$C_{34O}(5) + \delta(O_{24H})(5)]$	
1569	-			$R_{3}[v(CC)(56)+\delta'_{2}(7)+\delta(O63H)(7)+\delta_{in}$	Ring 3 CC stretch
1000				$(CH)(7)+\delta_{in}(C73O)(5)]$	
1549	-	1564	1568	$R_{1}[v(CC)(28)+v_{a}(NO_{2})(24)+\delta_{in}(CH)($	Ring 1 CC stretch
10 10		1001	1000	9)]+v(C56=N)(8)	Tung I ee succen
1546	1549			$R1[v(CC)(51)+\delta_{in}(CH)(12)+v_{a}(NO_{2})($	Ring 1 CC stretch
10.10	10 17			9)+v(C17=N)(10)	Tung I ee succen
1528	1525			$R_{1}[v_{2}(NO_{2})(70)+v(CC)(12)]$	NO <sub>2</sub> asym stretch
1512	-	1511		$R_1[v_2(NO_2)(76)+v(CC)(6)]$	NO <sub>2</sub> asym stretch
1498	-	1499	1498	$R_{3}[\delta_{in}(CH)(46)+v(CC)(34)+v(C73O)($	In plane ring def + Ring 3
1100		1.,,,	1.00	10)+v(C68C78)(5)]	CC stretch
1496	1495	1494		$R_{3}[\delta_{in}(CH)(52)+v(CC)(35)+v(C34O)(52)+v(C3AO)(52)+v(C3AO)(5$	In plane ring def $+$ Ring 3
1190	11,55	1121		7)+v(C29C39)(5)]	CC stretch
1475	-		1479	$R_{1}[v(CC)(39)+\delta_{ring}(13)+v(C50C56)(1)$	Ring 1 CC stretch
1175			11/2	1)+v(N45C)(5)]+v(C56=N)(5)	rung i ee sueten
1473	1476	1457		$R_{1}[v(CC)(36)+\delta_{ring}(12)+v(C11C17)(1)$	Ring 1 CC stretch
1170	1.70	1 107		2)+v(N6C)(5)]	Tung I ee succen
1434			1436	$R_{3}[v(CC)(34)+\delta(O63H)(15)+\delta_{in}(CH)$	Ring 3 CC stretch
				$(22)+\delta_{in}(C68C78)(5)]+\tau(H64O3)(6)$	8
1431	1424	1429		$R_{2}[\delta(CH_{2})](89)$	Ring 2 CH <sub>2</sub> deformation
1427				$R_{3}[v(CC)(41)+\delta_{in}(CH)(29)+\delta(O24H)$	Ring 3 CC stretch +In
				$(8)+\delta_{in}(C29C39)(7)+\delta_{in}(C34O)(5)]$	plane ring def
1414	1424	1410	1405	$R_{2}[\delta(CH_{2})](80) + \delta(H_{2}3C_{2}1O_{2}8)(9)$	Ring 2 CH <sub>2</sub> deformation
1380	1376	1388	1391	$R1[v(CC)(22)+v(OC)(26)+\delta_{in}(CH)(13)$	Ring CC stretch+Ring OC
				$+\delta_{in}(C11C17)(5)$ ]	stretch
1378	-	1377	1378	$R1[v(CC)(20)+v(OC)(23)+\delta_{in}(CH)(12)$	Ring CC stretch+Ring OC
				$]+R2[\delta_{in}(N48H)](6)$	stretch
1373	-			$R2[\delta_{in}(N48H)(45)]$	In plane ring NH def
				$R2[v(NC)(6)]+\delta(N48H49O24)(17)$	
1361	1356			$R2[v(NC)(19)+\omega(CH_2)(8)+v(NC)(8)+$	Ring 2 NC stretch
				$v(N8N)(5)]+R1[\rho(C17H)(6)+v(CC)(1)]$	-
				3)+v(N6O5)(5)]	
1355	1334	1346	1345	$R3[\delta(O63H)(17)+v(CC)(42)+\delta_{in}(CH)$	Ring 3 CC stretch
					-

1351	-			(17)]+ $\tau$ (H64O3)(7) R2[ $\delta_{in}$ (N48H)(14)+ $\nu$ (NC)(9)+ $\nu$ (N47N)(5)]+R1[ $\rho$ (C56H)(9)+ $\nu$ (CC)(11)+ $\nu_s$ (	In plane ring NH def
1339	1327			NO <sub>2</sub> )(9)]+ $\delta$ (N48H49O24)(6) R2[v(NC)(23)+ $\delta$ <sub>in</sub> (NH)(12)+v(CC)(5) ]+R1[v <sub>s</sub> (NO <sub>2</sub> )(11)+ $\rho$ (C17H)(5)]	Ring NC stretch+In plane ring NH def
1335	1322			$R3[v(O26C)(16)+v(C29C39)(15)+\delta(O26H)(14)+\delta(C39C29O28)(13)+v(CC)(11)]$	Ring 3 OC stretch+Ring 3 CC stretch
1325	1317	1325		$R1[\rho(C56H)(8)+\rho(C17H)(7)+\nu_{s}(NO_{2})$ (11)+ $\nu(N6C)(6)$ ]	Ring 1 CH rocking
1324				$R3[v(CC)(52)+\delta(O24H)(11)+\delta_{in}(CH)$ (10)]	Ring 3 CC stretch
1322	-			R3[δ(O65H)(20)+ν(C68C78)(16)+ν( O65C)(14)+δ(C78C68O67)(8)+ν(C78 O67)(6)]	OH bend (aromatic)+Ring 3 CC stretch
1319				$R1[v_{s}(NO_{2})(21)+\rho(C56H)(12)+v(N45)$ C)(10)+ $\rho(C17H)(6)+\rho(NO_{2})(5)$ ]	NO <sub>2</sub> sym stretch+ Ring 1 CH rocking
1315	-	1318	1321	$\begin{array}{l} R2[\omega(CH_2)(12)+v(NC)(18)+\delta_{in}(N48H \\ )(5)+\delta_{in}(C=O)(7)]+R1[v_s(NO_2)(14)+v \\ (N45C)(6)] \end{array}$	Ring 2 CH <sub>2</sub> wagging + NC stretch
1305	1301			$R2[\omega(CH_2)(33)+\delta_{in}(NH)(13)+\nu(NC)(15)]+R1[\rho(C17H)](13)$	Ring 2 CH <sub>2</sub> wagging + In plane ring NH def
1299	-	1297		$R2[\delta_{in}(NH)(24)+v(NC)(13)+v(CC)(8) +\delta_{in}(C20=O)(7)]+R1[\rho(C17H)](5)$	In plane ring NHdef +Ring 2 NC stretch
1299	1295			$R3[v(CC)](26)+\delta_{in}(CH)(38)+\delta_{in}(C29)(5)]$	In plane ring def+Ring 3 CC stretch
1296	1282			$R2[\omega(CH_2)(22)+\nu(NC)(17)+\nu(CC)(16) +\delta_{in}(C59=O)(7)+\delta_{ring}](6)]+R1[\rho(C56 H)(6)]$	Ring 2 CH <sub>2</sub> wagging+NC stretch
1294	-	1281		$R3[v(CC)(40)+\delta_{in}(CH)(46)+\delta_{in}(C68C 78)(5)]$	In plane ring def+Ring 3 CC stretch
1266	1261	1257	1262	$R3[v(C73O)(48)+v(CC)(18)+\delta_{tring}(9) +\delta_{in}(CH)(15)]$	CO stretch (aromatic)
1247	-	1245		R1[v(CC)(27)+v(C50C56)(10)+v(OC)(9)+v <sub>s</sub> (NO <sub>2</sub> )(13)+ $\delta_{in}$ (CH)(7)+ $\rho$ (C56	Ring 1 CC stretch
1244	1243		1252	$R1[v(CC)(23)+v(C11C17)(9)+v_{s}(NO_{2})](8)+v(OC)(7)+\delta_{in}(CH)(7)+\rho(C17H)(6)]$	Ring 1 CC stretch
1238	-	1231	1239	$R3[v(C34O)(49)+\delta_{tring}(10)+v(CC)(16) +\delta_{v}(CH)(12)]$	CO stretch (aromatic)
1229	1231			$R2[v(N8N)(22)+v(NC)(11)]+R1[v(O C)(21)+\delta'ring(5)+\delta_{in}(CH)(5)+\delta(C17C1 1)(7)(5))+\delta(N8N7C17)(6)$	Ring 2 NN stretch+Ring 1 OC stretch
1227	-			$R2[v(N47N)(24)+v(NC)(12)]+R1[v(OC)(20)+\delta_{in}(CH)(8)+\delta_{ring}(5)]+\delta(N47)$	Ring 2 NN stretch+Ring 1 OC stretch
1220	-	1219	1211	$R3[v(CC)](24)+\delta(O63H)(15)+v(C73 O)(7)+\delta_{in}(CH)(8)]+\tau(H64O3)(10)+\tau(O63H64)(7)$	Ring 3 CC stretch+OH bend
1208	1207			$R1[v(OC)(26)+v(N6C)(7)+\delta'_{ring}(8)]+$ R2[v(N8N)(18)+v(NC)(5)]	Ring 1 OC stretch+Ring 2
1205	-	1188		$R1[v(OC)(29)+\delta'_{ring}(9)+v(N45C)(7)+R2[v(N47N)(17)+v(NC)(5)]$	Ring 1 OC stretch+Ring 2
1181	1173			$R3[\delta(026H)(21)+\delta_{in}(CH)(32)+v(CC) \\ (16)+v(C29C39)(7)+\delta_{tring}(5)+\delta(024H) \\ (5)]$	OH bend+ In plane ring def
1178	1171	1177	1177	$R2[v(NC)(47)+\omega(CH_2)(19)+\delta'_{ring}(5)]$	Ring 2 CH <sub>2</sub> wagging+NC stretch
1176	-			$R2[v(NC)(49)+\omega(CH_2)(18)]$	Ring 2 NC stretch+CH <sub>2</sub> wagging

1171	-			$R3[\delta(O65H)(30)+v(C68C78)(13)+\delta_{in}($	OH bend+In plane ring
1167	1160			CH)(24)+ $v$ (CC)(13)+ $\delta_{tring}(7)$ ]	def Ding 2 CIL twisting
116/	1162			$R_{2}[\gamma(CH_{2})](92)$ $R_{3}[\delta(O_{2}4H)](41)+\gamma(CC)(21)+\delta_{2}(CH_{2})$	OH bend+ $Ring 3 CC$
1100	1154			$(10)+R2[\gamma(CH_2)](12)$	stretch
1159	-			$R2[\gamma(CH_2)](73)+R3[\delta(O24H)](6)$	Ring 2 CH <sub>2</sub> twisting
1156	1155			$R1[\delta_{in}(CH)(49)+\nu(N6C)(8)+\delta'_{ring}(6)+$	In plane ring def
				v(OC)(5)+v(C11C17)(5)]	
1154	-			$R1[\delta_{in}(CH)(48)+v(N45C)(9)+\delta'_{ring}(7)$	In plane ring def
1146	1141			$F_{(0C)(0)}^{+}(C30C30)(3)]$ R3[ $\delta(026H)(24) + \delta_{in}(CH)(35) + v(C29)$	In plane ring def+OH
1110				C(2)(2)(2)(2)(2)(3)(3)(3)(3)(2)(2)(2)(3)(3)(3)(3)(3)(3)(3)(3)(3)(3)(3)(3)(3)	bend
1143	-	1140		$R3[\delta_{in}(CH)(46)+\delta(O65H)(17)+v(C68)$	In plane ring def+OH
				C78)(10)+v(CC)(11)]	bend
1103		1120		$R3[\delta_{in}(CH)(53)+v(CC)(24)]$	In plane ring def+ Ring 3
1095	1099			$R_{3}[\delta_{in}(CH)(60)+v(CC)(25)]$	In plane ring def+ Ring 3
1095	1077				CC stretch
1093	-			$R2[\nu(NC)(59)+\delta_{in}(C58=O)(8)+\delta_{in}(N4)$	Ring 2 NC stretch
				8H)(8)]+δ(N48H49O24)(5)	
1078	1080			$R2[v(NC)(57)+\delta_{in}(C19=O)(12)+\delta_{in}(N)$	Ring 2 NC stretch
1074	1065			H)(9)+ $\delta_{in}(N\delta N)(5)$ ] P2[ $_{1}(O26C)(42)+_{2}(CC)(17)+\delta(O26H)$	CO stratab (gramatia)
1074	1005			$(6200)(+3)^{+}((0200)(+3)^{+}((0200))(-1)^{+}(00200)(-1)^{+}$	CO stretch (aromatic)
1059	-			$R3[v(O65C)(49)+v(CC)(17)+\delta(O65H)]$	CO stretch (aromatic)
				$(10)+\delta(C78C68O67)(6)+\delta_{in}(CH)(9)]$	
1007	1004	1017		$R1[\delta_{in}(CH)(63)+v(CC)(25)]$	In plane ring def+ Ring 1
1004				$P_{1}[S_{1}(CH)(62) + (CC)(25)]$	CC stretch
1004	-			$R1[0_{m}(C11)(02) + V(CC)(23)]$	CC stretch
997	-			$R3[\delta_{tring}(51)+v(CC)(33)+\delta_{in}(CH)(7)]$	Ring 3 trigonal def.
996	993		1025	$R3[\delta_{tring}(51)+\nu(CC)(34)+\delta_{in}(CH)(9)]$	Ring 3 trigonal def.
980	-		981	$R2[\rho(CH_2)(65)+oop(C59=O)(16)+\tau(1)$	Ring 2 CH <sub>2</sub> rocking
070	986	077		$0)] \\ R_{2}[a(CH_{2})(63)+\delta(H_{2}^{2}C_{2}^{2})(0.28)(12)+$	Ring 2 CH2 rocking
)()	980	)//		$cop(C20=O)(11)+\tau(5)$	King 2 CH2 locking
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
067	066	063	067	$P_{1}[y(OC)(52)+8^{2} + (14)+y(C_{1})(12)]$	def Bing 1 OC stratch
907	900	905	907	$\frac{1}{7}$	King I OC suctori
965				$R1[v(OC)(54)+\delta'_{ring}(13)+v(C50C56)($	Ring 1 OC stretch
				8)]	-
955				R3[oop(CH)(81)+puck(12)]	Ring 3 CH out of plane
953	952			$R_{1}[\delta_{1}, (A_{2}) + y(OC)(20) + y(CC)(13) + y(CC)$	def Ring 1 def+OC stretch
955	952			(N6C)(7)]	King I del+OC suetch
951				$R1[\delta_{ring}(42)+\nu(OC)(18)+\nu(CC)(13)+\nu$	Ring 1 def+OC stretch
				(N45C)(8)]	
945	944	935	941	R3[oop(CH)(80)+puck(12)]	Ring 3 CH out of plane
003		016		$P_{1}[\omega(C56H)](57) + \alpha \alpha \mu(CH)(5) + \tau(C5)$	def CH wagging + NC torsion
903		910		6=N(25)	
900	896	908	906	$R1[\omega(C17H)(50)+\tau(C11C17)(6)+oop$	CH wagging + NC torsion
				(CH)(8)]+τ(C17N)(26)	
881	879		895	R1[oop(CH)(75)+ $\tau$ (13)+ $\omega$ (C17H)(5)]	Ring 1 CH out of plane
879				$R_{1}[000(CH)(70)+\tau(13)]$	def Ring 1 CH out of plane
017				$\operatorname{Kr}[\operatorname{oop}(\operatorname{Cii})(7) + \operatorname{tr}(10)]$	def
877	863			R2[ν(CC)(48)+ν(NC)(13)+δ <sub>in</sub> (N48H)	Ring 2 CC stretch + NC
				$(5)+\delta_{in}(C=O)(8)]+\delta(N48H49O24)(9)$	stretch

873		875		$R2[v(CC)(55)+v(NC)(16)+\delta_{in}(NH)(7) +\delta_{in}(5)]$	Ring 2 CC stretch + NC stretch
859		862		$R3[oop(CH)(67)+\tau_{a}(11)+\delta_{in}(C34O)(8)$	Ring 3 CH out of plane
852	851	852		$\delta(N47N46C56)(16)+R1[\delta'_{ring}(16)+\delta(C56C50N46)(13)]+R2[v(NC)(19)+\delta'_{r}$	Ring 1 def+N-N=C bend
850		847		$\frac{\log(10) + \sqrt{(14+11)}(7) + \sqrt{(140)}(7)}{R1[\delta_{110}(16) + \delta(C17C11N7)(14)] + \delta(N8N7C17)(16) + R2[v(NC)(19) + v(N8))(8) + \delta_{110}(8)$	Ring 1 def+C-C=N bend
848	848	831		$R3[oop(CH)(62)+\delta_{in}(C73O)(13)+\tau_a(1)+\omega(C78O(5))(6)+\omega(C78O(5)))(6)+\omega(C78O(5))(6)+\omega(C78O(5)))(6)+\omega(C78O(5))(6)+\omega(C78O(5)))(6)+\omega(C78O(5))(6)+\omega(C78O(5)))(6)+\omega(C78O(5))(6)+\omega(C78O(5)))(6)+\omega(C78O(5)))(6)+\omega(C78O(5)))(6)+\omega(C78O(5)))(6)+\omega(C78O(5)))(6)+\omega(C78O(5)))(6)+\omega(C78O(5)))(6)+\omega(C78O(5)))(6)+\omega(C78O(5)))(6)+\omega(C78O(5)))(6)+\omega(C78O(5)))(6)+\omega(C78O(5)))(6)+\omega$	Ring 3 CH out of plane
824		822		$R3[\delta_{a}(19)+v(C73O)(16)+v(CC)(49)+\delta_{trive}(5)]$	Ring 3 CC stretch+asym
821	824			$R3[\delta_a(21)+v(C34O)(18)+v(CC)(42)+v(C29C39)]$	Ring 3 CC stretch+asym
816	799	810	814	$R3[oop(CH)](81)+\tau(H64O3)(7)$	Ring 3 CH out of plane
804				R3[oop(CH)(82)+ω(C39O26)(5)]	Ring 3 CH out of plane
802	800			R1[ $\rho(NO_2)(41)+\delta'_{ring}(19)+\delta(NO_2)(13)$ )+ $\delta_{ring}(8)$ ]	NO <sub>2</sub> rocking + Ring def'
801				$R1[\rho(NO_2)(42)+\delta'_{ring}(19)+\delta(NO_2)(14)+\delta_{ring}(7)]$	NO <sub>2</sub> rocking + Ring def'
795	792			$R1[oop(CH)(78)+\tau'(7)]$	Ring 1 CH out of plane def
794		791		R1[oop(CH)(82)+τ'(6)]	Ring 1 CH out of plane
767	764	775		$\begin{array}{l} R3[puck(32)+\omega(C78O65)(28)+\delta_{in}(C7\\ 3O)(12)+oop(C68C78)(11)+oop(CH) \end{array}$	Ring 3 puckering +CO out of plane def
764				(5)] $R2[v(NC)(19)+\delta'_{ring}(7)+\delta_{in}(C58=O)(5)]+R1[\delta'_{ring}(13)+\delta_{ring}(11)+\rho(NO_2)(7)+\delta_{ring}(11)+\delta_{ri$	Ring 2 NC stretch + Ring 1 def'
763	761		788	v(C50C56)(6)] $R2[v(NC)(18)+\delta'_{ring}(6)]+R1[\delta'_{ring}(14)$ $+\delta_{virs}(11)+v(C11C17)(6)+o(NO_2)(6)]$	Ring 2 NC stretch + Ring
762				$R3[\omega(C39O26)(30) + puck(27) + \delta_{in}(C3)$ 4Q)(13) + oop(C29C39)(10) + oop(CH)	CO out of plane def+ Ring 3 puckering
751				$\begin{array}{c} 40(13) + 00p(22) + 20(10) + 00p(21) \\ (7)] \\ \tau(H64O3)(40) + \tau(O63H64)(21) + 8(O6) \\ \end{array}$	OH torsion
731	720	740		$(10403)(40)+1(003104)(21)+0(003H6403)(15)+R3[\tau(C730)](11)B1[to(N605)(62)+corr(C16N)(10)+\tau^2$	
740	139	740		$\begin{array}{c} \text{K1}[\omega(\text{NOOS})(0S) + \text{cop}(\text{C1oN})(19) + t \\ (7)] \\ \text{R1}[\omega(\text{NOOS})(0S) + \omega(\text{R1ON})(19) + t \\ (7)] \\ \end{array}$	N=O wagging
739		736		R1[ $\omega$ (N45O44)(67)+oop(C55N)(14)+ $\tau$ '(7)]	N=O wagging
728			750	R2[oop(C58=O)(62)+τ(13)+τ'(13)+o op(N48H)(8)]	Ring 2 C=O out of plane def
725	727			R2[oop(C19=O)(65)+ $\tau$ '(18)+ $\tau$ (7)]	Ring 2 C=O out of plane def
716	715		739	$R3[\rho(C39O26)(19)+\delta_{tring}(17)+\nu(C29)(16)+\nu(O26C)(10)+\nu(C34O)(8)+\nu(6)+\nu(6)+\nu(6)+\nu(6)+\nu(6)+\nu(6)+\nu(6)+\nu(6$	C=O (acid) rocking + CC stretch + ring trigonal def
713				$R_{1}^{0}(C78O65)(20)+v(C68C78)(18)+ \delta_{tring}(17)+v(O65C)(13)+v(C73O)(6)+ \delta_{0}(C65C)(13)+v(C73O)(6)+ \delta_{0}(C65C)(13)+v(C7)(13)+ \delta_{0}(C65C)(13)+v(C7)(13)+ \delta_{0}(C65C)(13)+v(C7)(13)+ \delta_{0}(C65C)(13)+v(C7)(13)+ \delta_{0}(C65C)(13)+v(C7)(13)+ \delta_{0}(C65C)(13)+v(C7)(13)+ \delta_{0}(C65C)(13)+v(C7)(13)+ \delta_{0}(C65C)(13)+v(C7)(13)+ \delta_{0}(C65C)(13)+v(C7)(13)+ \delta_{0}(C65C)(13)+v(C7)(13)+\delta_{0}(C65C)(13)+\delta_{0}($	+ OC stretch C=O (acid) rocking + CC stretch + ring trigonal def
699				$R2[oop(N48H)](52)+\delta(N48H49O24)(24)+\tau(O24H49)(14)$	Ring 2 NH out of plane
696	693	693	692	$R3[puck(58)+\delta_{in}(C73O)(14)+\omega(C78O)(14)+\omega(C78O)(10)+\omega(C78O)(11)]$	Ring 3 puckering
694				$R3[puck](55)+\delta_{in}(C34O)(14)+\omega(C39O)(26)(7)+cop(CH)(9)]$	Ring 3 puckering
674				$R1[\tau'(35)+oop(C50C56)(34)+\tau(24)]$	Ring 1 torsion + CC out

					of plane def
674	675			$R1[\tau'(36)+oop(C11C17)(35)+\tau(21)]$	Ring 1 torsion + CC out of plane def
671	668		669	R2[ $\delta_{ring}(22)+v(NC)(15)+\delta'_{ring}(13)+\delta_{in}$ (C=O)(17)+ $\delta_{in}(N8N)(9)+v(CC)(5)$ ]	Ring 2 def + NC stretch
668		660		$R2[\delta_{ring}(23)+v(NC)(15)+\delta_{in}(C=O)(18) +\delta_{ring}(10)+\delta_{in}(N47N)(9)+v(CC)(5)]$	Ring 2 def + NC stretch + $C-O$ in plane def
631		636		$R_{3}[\lambda_{0}^{2}(76)+\lambda_{0}(730)(6)+v(CC)(7)]$	Ring 3 asym def'
630	630	625	624	$R_{3}[\delta'_{a}(74)+\delta_{in}(C_{3}4O)(7)+\delta_{in}(C_{2}9C_{3}9)$	Ring 3 asym def'
				)(5)]	8 j
611	603	619		R2[oop(NH)(41)+oop(C20=O)(29)+τ '(9)+ρ(CH <sub>2</sub> )(6)]+δ(H23C21O28)(5)	Ring 2 NH out of plane def + Ring C=O out of plane def
604		605		$R2[\delta_{in}(C=O)(34)+\delta_{ring}(14)+\delta'_{ring}(9)+\delta$	Ring 2 C=O out of plane
500	504	500		$in(N4/N)(8)$ ]+ $\delta(N4/N46C56)(5)$	def+ ring def
599	596	592		$R_{2}[oin(C=O)(32)+oring(16)+oin(N8N)(8)+8^{2}(7)]+8(N8N7C17)(6)$	Ring 2 C=O out of plane $def_{\pm}$ ring def
587	584	583	583	$R_{2}[\delta'_{ring}(29) + \delta_{ring}(5) + v(NC)(12)]$	Ring 2 def'+NC stretch
587	504	505	505	$R2[\delta'_{ring}(29) + \delta_{ring}(14) + v(NC)(12)]$	Ring 2 def'+NC stretch
582	581			$R1[\tau(39)+\tau'(23)+oop(C16N)(21)]$	Ring 1 torsion $+$ NC out
				[·(··) · · () · · · · · · · · · · · · · · · · · ·	of plane def
582				R3[ $\delta_a(23)$ + $\rho(C78O65)(18)$ + $\delta(C78C6$	Ring asym def+CO
582				$R_{3}[\delta_{4}(15)+o(C_{3}9O_{2}6)(15)+\delta(C_{3}9C_{2})$	Ring asym def+CO
				$9028)(14)]+R1[\tau(11)+\tau'(7)+oop(C16)]$	rocking
				N)(6)]	0
581	581			$R1[\tau(51)+\tau'(26)+oop(C55N)(17)]$	Ring torsion
575	564	574		$\tau(C39O26)(65)+R3[\delta_{in}(C34O)(8)+\tau_a($	CO torsion
				7)+oop(C29C39)(5)]	
570				R2[oop(C=O)(53)+ $\tau$ (17)+ $\rho$ (CH <sub>2</sub> )]13)	Ring 2 C=O out of plane
ECE		550	550	$+\gamma(CH_2)(6)$ ]	def
565		553	550	$\tau(C/8065)(69)+R3[\delta in(C/30)(9)+\tau_a($	CO torsion
536	540	541		8)+00p(C08C78)(0)] R2[00p(NH)(26)+00p(C=O)(25)+0(0	Ring NH out of plane def
550	540	541		$H_2(12)]+\delta(H_2(21))+\delta(9)+R_1[\delta(N)]$	$+ \operatorname{ring} C=0$ out of plane
				$O_2)](5)$	def
535		531		$R1[\delta(NO_2)(25)+\delta_{in}(C16N)(15)+\rho(NO_2)(25)+\rho(NO_2)$	$NO_2 def + NC in plane$
				$2)(9)+\delta_{in}(C11C17)(7)+R2[oop(C=O)($	def
	534			7)+oop(NH)(7)]	
535				$R1[\delta(NO_2)(33)+\delta_{in}(C55N)(20)+\rho(NO$	$NO_2 def + NC in plane$
40.0				$_{2}(12)+\delta_{in}(C50C56)(10)]$	def
498		501		$R_{3}[\rho(C/8065)(15)+\delta(C/8C68067)(1)$	CO rocking+C-C=O def
				4)+ $\delta_{in}(C68C/8)(11)+\delta_{in}(C/3O)(10)+$ \$2(8)+\$(C20C20O28)(7)]	
408	405			$0_{a}(8) + 0(C39C29O28)(7)]$ $P_{2}[(8(C39C29O28)(24) + 8 (C29C39))$	C C-O def CC in plane
490	495			$(15) + o(C39C29C28)(14) + \delta_m(C29C39)$	def
				(15)*p(e5)020)(14)*0m(e5+0)(7)*0 ' <sub>a</sub> (6)]	dei
496				$R3[\delta_{in}(C73O)(31)+\tau_a(29)+oop(C68C)$	CO in plane def+ Ring 3
				$78)(12)+puck(10)+oop(CH)(5)]+\tau(C7)$	torsion
				8065)(5)	
494	494	492		$R3[\tau_a(37)+\delta_{in}(C34O)(31)+oop(C29C)]$	Ring 3 torsion+ CO in
				39)(13)+puck(7)]	plane def
451	448	470	472	$\delta(N8N7C17)(16)+R1[\delta(NO_2)(14)+v($	C-C=N def+NO <sub>2</sub> def
				$N6C)(14)+\delta_{in}(C11C1/)(10)+\delta_{ring}(6)]+$	
448		446		$K_{2}[0in(U_{2}U=U)](7)$ $\delta(M_{2}N_{4}GC_{5}G)(17)+P1[\delta(M_{2}U)(16)+$	N-N-C def±NO2 def
0++0		0 <del>1</del>		$\delta_{in}(C50C56)(14) + v(N45C)(11) + 8 \cdot (6)$	
				$+\delta(C56C50N46)(5)]+R2[\delta:(N47N)($	
				$5)+\delta_{in}(C=O)(9)]$	
434		439		$R2[\delta_{in}(C=O)](20)+\nu(NC)(6)+R1[\delta_{in}(C=O)](20)+\nu(NC)(6)+N1[\delta_{in}(C=O)](20)+\nu(NC)(6)+N1[\delta_{in}(C=O)](20)+\nu(NC)(6)+N1[\delta_{in}(C=O)](20)+\nu(NC)(6)+N1[\delta_{in}(C=O)](20)+\nu(NC)(6)+N1[\delta_{in}(C=O)](20)+\nu(NC)(6)+\nu(NC$	Ring 2 C=O in plane
				$C11C17)(10)+\rho(NO_2)(7)+\delta(C17C11)$	def+NC stretch
				N7)(7)]	

430	427			$\begin{array}{l} R1[\nu(N45C)(14)+\rho(NO_2)(10)+\delta_{in}(C5)\\ 0C56)(7)+\delta(C56C50N46)(6)+\delta'_{ring}(5)\\ ]+R2[\delta_{in}(C=O)(23)+\nu(NC)(5)] \end{array}$	NC stretch+NO <sub>2</sub> rocking
418				R3[δ <sub>in</sub> (C73O)(29)+δ(C78C68O67)(7) +δ' <sub>a</sub> (5)]+τ(H64O3)(12)+τ(O63H64)(7 )+R1[v(N6C)](7)	CO in plane def+C-C=O def
415	413	412	415	$R3[\tau'_{a}(81)+oop(CH)(7)]$	Ring torsion'
410				$R3[\tau'_{a}(80)+oop(CH)(16)]$	Ring torsion'
402	390			$\begin{array}{l} R3[\delta_{in}(C34O)(50) + \delta(C39C29O28)(10 \\ ) + \delta'_{a}(8)] \end{array}$	CO in plane def
395				$R2[\delta_{in}(C=0)(27)+\nu(NC)(9)+R3[\delta_{in}(C 730)](14)+R1[\nu(N6C)](8)$	Ring 2 C=O in plane def+Ring 3 CO in plane def
391	388	390	382	$\begin{array}{l} R2[\delta_{in}(C=O)(35)+\nu(NC)(11)+R1[\nu(N\\45C)(10)+\delta_{ring}(5)+R3[\delta_{in}(C34O)](9) \end{array}$	Ring 2 C=O in plane def+NC stretch
375	376			τ(C17N)(28)+R1[τ'(14)+τ(11)+oop(C 16N)(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[t(C34O)](90)	Ring 3 CO torsion
343				$R3[\delta_a(43)+\nu(C68C78)(22)+\rho(C78O6)]$	Ring 3 asym def+CC
				5)(13)]	stretch
343	342			R3[δ <sub>a</sub> (40)+v(C29C39)(21)+ρ(C39O2 6)(13)]	Ring 3 asym def+CC stretch
304	307	303	303	$R2[\tau(N8N)(36)+oop(N8N)(21)+\tau(8)] +R1[\tau(C11C17)](16)$	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			$\begin{array}{l} R2[\delta_{in}(N8N)(16)+\delta_{in}(C=O)(15)+\nu(N\\ C)(5)]+R1[\delta_{in}(C16N)(13)+\delta_{in}(C11C1\\ 7)(11)+\delta(NO_2)(6)+\nu(C11C17)(5)] \end{array}$	NN in plane def+ Ring C=O in plane def
283				R3[oop(C68C78)(26)+ $\tau_a(21)$ +puck(1	CC out of plane def+
102		200		2 + 00p(CH)(0) $P_{2}[appr(Cf_{2}^{2}C7_{2}^{2})(12) + \pi_{1}(10) + muck(f)$	CC out of plane def
203		280		$R_{100}(C000C/8)(13)+t_{a}(10)+puck(0)$ ]+ $R_{2}[\delta_{in}(N47N)(11)+\delta_{in}(C=0)(10)]+$ $R_{1}[\delta_{in}(C55N)(8)+\delta_{in}(C50C56)(7)]$	Ring 3 asym torsion
282	279			R3[oop(C29C39)(33)+ $\tau_a$ (29)+puck(1 3)+ $\omega$ (C39O26)(5)+ $\delta_{in}$ (C34O)(5)+oop (CH)(5)]	CC out of plane def+ Ring 3 asym torsion
221	216	231	232	$R1[\delta_{in}(C16N)(25)+\delta(NO_2)(10)+\delta(C1)$	CN in plane def + NO <sub>2</sub>
				7C11N7)(9)+ν(C11C17)(6)+ρ(NO <sub>2</sub> )( 5)]	def
217		209	211	$R1[\delta_{in}(C55N)(29)+\delta(NO_2)(12)+\delta(C5650N46)(11)+v(C50C56)(6)+\rho(NO_2)(5))$	CN in plane def + NO <sub>2</sub> def
201	202	203		$R_{2}[\tau](28)+\delta(H_{23}C_{21}O_{28})(15)+v(O_{28}H_{23})(13)+P_{21}\delta_{12}(C_{28}C_{28})(12)$	Ring 2 torsion+ C-HO def
200				$R2[\tau(31)+cop(N8N)(8)+\delta(H23C21O28)(16)+v(O28H23)(12)+R3[\delta_{in}(C68C70)(11)+U(C28H23)(12)+R3[\delta_{in}(C68)(12)+U(C28H23)(12)+U(C$	Ring 2 torsion+ C-HO def
197	194			$R1[oop(C16N)(31)+\tau(C11C17)](5)$ $R2[\tau(N8N)(18)+oop(N8N)(6)+\tau(5)]+$	CN out of plane def + NN torsion
195	190			$\begin{array}{l} R3[\delta_{in}(C29C39)](6) \\ R3[\delta_{in}(C29C39)(41) + \delta(C39C29O28)(6) \\ \end{array}$	CC in plane def + OH
				12)]+τ(O28H23)(16)+R1[oop(C16N) ](5)	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		$R2[\tau'(66)+oop(N47N)(13)]+\tau(C59O4)$	Ring 2 torsion
168		168		2)(7) $P_{2}[\pi^{2}(54) + con(NH)(31)]$	Ping 2 torsion
100		100	150	$R_2[t((54)+0.0p((NH)(51))]$	Ring 2 torsion
156		155	159	$R_2[t(52)+00p(N48H)(44)]$	Ring 2 torsion
151		150		$v(O3H64)(19)+R2[\delta_{in}(N8N)](15)+\delta($	OH stretch+NN in plane
				N8N7C17)(11)+R1[ $\delta_{in}$ (C16N)(11)+ $\delta_{i}$	def
				$n(C11C17)(5)]+R3[\delta_{in}(C68C78)](5)+$	
				v(O2H61)(5)	
144		140		$v(O42H33)(22)+R2[\delta_{in}(N47N)](17)+$	OH stretch+NN in plane
				$\delta(N47N46C56)(12) + R1[\delta_{in}(C55N)(1)]$	def
				$2) + \delta_{in}(C50C56)(6)] + \delta(N48H49O24)($	
				5)	
136	134	133		$R_{1000}(C_{16N})(17) + \tau(C_{16N})(14) + 00$	CN out of plane def+CN
150	134	155		$n(C_{11}C_{17})(8) + \tau(C_{11}C_{17})(8) + P_{2}[a_{2}]$	torsion
				p(C11C17)(0) + t(C11C17)(0) + t(2[00])	10131011
100	101			p(1818)(14)+t(0)]+v(028123)(8)	
128	131			t(C59042)(18) + R1[00p(C55N)(15) + (2552)(10) + (2552)(	CO torsion+CN out of
				$oop(C50C56)(10)+\tau(C55N)(9)]+R2[\tau$	plane def
				(12)+oop(N47N)(10)]	
115				$R3[\tau_a(27)+oop(C68C78)(16)+\tau(C73O)$	Ring 3 asym torsion + CC
				$(9)]+v(O3H64)(12)+\tau(O63H64)(6)$	out of plane def
110	107			$R3[\tau_a(37)+oop(C29C39)(16)]+\delta(C39)$	Ring 3 asym torsion $+$ CC
				$O28H23)(9)+v(O24H49)(7)+\tau(O28H$	out of plane def
				23)(5)	I
105	90			$R1[\tau(C16N)](18)+\nu(O3H64)(13)+\nu(O$	CN torsion+OH stretch
100	20			2H61(10)+R2[oon(N8N)](8)+v(O28)	
				$H_{23}(6) + \delta(N_{6}(0.2H_{6}))(5)$	
08				$P_1[\tau(C_1(N))](2_1) + \tau(O_2H(4))(1_5) + P_2[$	CN torsion OH stratch
90				KI[t(C10N)](51)+v(C5H04)(15)+K2[	CN IOISIOII+OH SILEICII
0.4				oop((N8N))(8)	
84				$\tau(C59O42)(34) + R1[\tau(C55N)](15) + \delta($	CO torsion + $CN$ torsion
				N48H49O24)(12)+R2[oop(N47N)](1	
				$0)+\tau(O28H23)(5)$	
82				v(O42H33)(20)+v(O24H49)(20)+v(O	OH stretch
				2H61)(10)+τ(O28H23)(8)+τ(O24H49	
				)(6)	
78	76			$R3[\tau(C29C39)](46)+\delta(C39O28H23)($	CC torsion+C-HO def
				$20)+\tau(O28H23)(17)+\delta(H23C21O28)($	
				7)	
75				$R_{3}[\tau(C68C78)(55)+\tau(C73O)(6)+\tau(H6)$	CC torsion+ $CO$ torsion
15				$AO_3(7) + v(O_28H_{23})(5)$	ce torsion co torsion
74				$P_{1}[\tau(C_{1}(C_{1}(C_{1}))](16)+\nu(C_{2}(C_{1}(C_{1})))(16)+\nu(C_{2}(C_{1}(C_{1})))(16)+\nu(C_{2}(C_{1}))(12)+\nu(C_{2}(C_{1}))(1$	CC torsion OH stratch
/4				K[(1(C11C17))(10)+v(028123)(13)+	CC torsion+OH stretch
				v(042H33)(12)+K3[t(068C/8)](/)+o	
				$(N6O2H61)(6)+v(O2H61)(6)+K2[\tau(5)]$	
				+000(N8N)(5)]+v(O24H49)(5)	
65				$\tau(H64O3)(20)+\nu(O24H49)(16)+\tau(O6)$	OH torsion+OH stretch
				$3H64)(8)+\tau(C20O3)(6)+\tau(O28H23)(6)$	
				)+v(O28H23)(5)	
63				v(O24H49)(29)+t(H64O3)(14)+t(N6	OH stretch+OH torsion
				$O2)(8)+\tau(O63H64)(6)$	
57				$v(O2H61)(14)+\delta(N48H49O24)(13)+v$	OH stretch+NHO def
				$(O24H49)(11)+\tau(N6O2)(11)+R1[(\delta($	
				$C_{56}C_{50}N_{46}(9) + \delta_{in}(C_{50}C_{56})(8)] + \tau$	
				$O_{28H23}(8)$	
52	57			$\tau(C50O(2))(34) + P1[\tau(C55N)](11) + y($	CO torsion (CN torsion
52	57			$(C_{3})^{(1)} + (C_{3})^{(1)} + (C_{3})^{(1)$	
				$(11)^{+}((0241149)(7)^{+}K2[00p]$	
40	40			$(IN4\delta\Pi)](0)$ D1[(S(G17G11)]](1() + S (G11G17))	
48	49			$K1[(o(C1/C11N/)(16)+\delta_{in}(C11C1/)($	$C-C=N \det + CC \ln plane$
				$13)$ ]+ $\delta$ (C20O3H64)(13)+R3[ $\tau$ (C73O)	det + C-OH def
				J(7)+δ(N8N7C17)(7)+τ(N6O2)(6)	
45	39			τ(O28H23)(36)+ν(O42H33)(24)+τ(C	OH torsion+OH stretch
				59O42)(8)+δ(H23C21O28)(7)	
42				$R3[\tau(C73O)(27)+\tau(C68C78)(5)]+\delta(C$	CO torsion+C-OH def
				20O3H64)(9)+δ(O63H64O3)(8)+δ(N	

		$8N7C17$ )(7)+R1[( $\delta$ (C17C11N7)](7)	
39		τ(C59O42)(29)+v(O42H33)(13)+R1[	CO torsion+OH stretch
		$\tau$ (C11C17)](7)+ $\nu$ (O2H61)(7)+ $\delta$ (C39	
		O28H23)(7)	
37	-	$v(O42H33)(19)+\tau(O28H23)(12)+\delta(N)$	OH stretch+OH torsion
		$602H61)(8)+\tau(H64O3)(7)+R1[\tau(C16)$	
		N)](5)	
29	36	$\delta(H^2(21028)(40) + \tau(C^{59}(42)(10)) +$	CHO def+CO torsion
2)	50	$\tau(\Omega^{2}8H^{2}3)(9) + \delta(C^{3}9\Omega^{2}8H^{2}3)(8) + v(10)^{10}$	
		$O(28H23)(7) + \tau(N6O2)(5)$	
26	_	$\tau(C59042)(40) + \tau(024H49)(10) + R2[$	CO torsion+OH torsion
20	-	(0.24114)(10) + 1(0.24114)(10) + 1(2)	
		(O2H61)(5)	
24	20	$\delta(H^{2}C^{2}IO^{2})(14) + \tau(C^{5}O^{2}O^{2})(13) +$	CHO def CO torsion
24	29	$\delta(1123C21028)(14) + t(C59042)(15) + \delta(C20028H22)(12) + t(C62H64)(8) + t$	CHO del+CO torsion
		(U(2))(7) + z(0)(12) + U(0)(104)(8) + U(0)(12) + z(0)(12)(6) + u(0)(104)(8) + U(0)(12)(6) + u(0)(12)(12)(12)(12)(12)(12)(12)(12)(12)(12	
		$(10403)(7) \pm i(028123)(0) \pm i(02812)(0)$	
22	22	S(0) + V(0+21155)(5) $S(C20029U22)(52) + \tau(024U40)(9) + S$	CHO dof
22		$(U_{23}^{-1})(0)^{+0}$ $(U_{23}^{-1})(0)^{+0}$	Chi dei
20		$v(O2H61)(13)+\tau(O24H40)(8)+\tau(O28)$	OH stratch OH torsion
20	-	(02101)(13) + i(0241143)(3) + i(028) (02101)(13) + i(0241143)(3) + i(028)	On stretch+On torsion
17		$\tau(028H23)(31) + \tau(059H04)(3) + \tau(1002)(3)$	OH torsion (CO torsion
17	-	(0281123)(31) + ((039042)(13) + 0(14) $48H40024)(13) + y(042H33)(7) + \tau(N6)$	
		$(13)^{+}(0421133)(7)^{+}(1004213)(7)^{+}(100421133)(7)^{+}(100421133)(7)^{+}(100421133)(7)^{+}(100421133)(7)^{+}(100421133)(7)^{+}(100421133)(7)^{+}(100421133)(7)^{+}(100421133)(7)^{+}(100421133)(7)^{+}(100421133)(7)^{+}(100421133)(7)^{+}(100421133)(7)^{+}(10042113)(7)^{+}(1004213)(7)^{+}(1004213)(7)^{+}(1004213)(7)^{+}(1004213)(7)^{+}(1004213)(7)^{+}(1004213)(7)^{+}(1004213)(7)^{+}(1004213)(7)^{+}(10042113)(7)^{+}(10042113)(7)^{+}(10042113)(7)^{+}(1004213$	
15	16	$\delta(X)/(2H40024)(17)+y(0/2H32)(1/4)+$	NHO def OH stratch
15	10	$\tau(C50042)(11) + \tau(N602)(8) + \delta(C200)$	NIIO del+OII suetell
		$28H23(6) \pm 1002(6) \pm 100$	
		)(5)	
13	12	$\lambda(-3) = \lambda(-3) + \tau(-3) + \tau(-3$	COH def+NO torsion
15	12	0(029)0201129)(29) + 1(10002)(12) + 1(10022)(12)	
		$3)(6)+y(0/2H33)(6)+\delta(N602H61)(5)$	
13	_	$\tau(028H23)(13) + \tau(02003)(13) + \delta(H2)$	OH torsion+CO torsion
15	-	$3C^{2}(0281123)(13) + R(C2003)(13) + 0(112)$	
		$(0.21020)(10) + x_1(0.01017)(9) + v_0(0.000) + x_1(0.000)(0.000) + x_1(0.000)(0.000) + x_1(0.000)(0.000) + x_1(0.000)(0$	
		0201123)(7) + 00241143)(7) + 00241143)(7) + 00201123)(7) + 8(020028H23)(5)	
7	_	$\delta(C_{39}O_{28}H_{23})(29) + \tau(N_{6}O_{2})(14) + \tau(16)$	COH def+NO torsion
7		$(23)(23)(23)(10) + \tau (C59O42)(7) + \tau (O63)$	con del into torsion
		$H(4)(6) + \tau(C^{2}(0)^{3})(5) + \delta(H^{2}(C^{2}(0)^{3})(5)) + \delta(H^{2}(0)^{3})(5)) + \delta(H^{2}(0)^{3})(5) + \delta(H^{2}(0)^{3})(5)) + \delta(H^{2}(0)^{3})(5)) + \delta(H^{2}(0)^{3})(5)) + \delta(H^{2}(0)^{3})(5) + \delta(H^{2}(0)^{3})(5) + \delta(H^{2}(0)^{3})(5)) + \delta(H^{2}(0)^{3})(5) + \delta(H^{2}(0))(5) +$	
		8)(5)	
5	6	$\tau(C59O42)(24) + \delta(N6O2H61)(18) + \tau(26)$	CO torsion+NOH
5	•	$N(02)(18)+v(02H61)(9)+\tau(02H23)$	def+NO torsion
		(7)	
4	_	$\delta(C39O28H23)(23)+\tau(O28H23)(16)+$	COH def+OH torsion
		$\tau(063H64)(15)+\nu(02H61)(11)+R1[\tau($	
		(000101)(10)(002101)(11)(11)(11)(11)(11)(11)(11)(11)(11)	

Table 55 Theoretical and experimental vibrational wavenumbers (in cin ) of 41157 and then assignment	Tε	able	S5	Theoretical	and	experimental	vibrational	wavenumbers	(in cm <sup>-</sup>	1) of	4HBA	and the	eir assignr	nents
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DFT		ID	D	DED				
Unscaled	Scaled	- IK	Kaman	PED				
3812	3679	3387		R3[v(O10H)](100)				
3758	3627	3203		R3[v(O9H)](100)				
3211	3099			R3[v(CH)](95)				
3208	3095			R3[v(CH)](97)				
3193	3081	3080		R3[v(CH)](99)				
3158	3047	3067		R3[v(CH)](97)				
1787	1724	1678		$R3[v(C1=O)(75)+\rho(C1O9)(7)+v(C1C2)(6)$				
1652	1595	1609	1610	$R3[v(CC)(61)+\delta_a(11)+\delta_{in}(CH)(20)]$				
1628	1571	1595	1597	$R3[v(CC)(68)+\delta'_{a}(8)+\delta_{in}(CH)(6)+\delta(O10H)(5)+\delta_{in}(C5O)(5)]$				
1550	1496	1448	1440	R3[δ <sub>in</sub> (CH)(48)+v(CC)(35)+v(C5O)(9)+v(C1C2)(5)]				
1475	1423	1423		$R3[v(CC)(42)+\delta_{in}(CH)(30)+\delta(O10H)(8)+\delta_{in}(C2C1)(5)+\delta_{in}(C5O)(5)]$				

$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	1378	1329	1364		$R3[v(CC)(46)+\delta_{in}(CH)(12)+\delta(O9H)(8)+v(C1C2)(8)+\delta(O10H)(8)+v(C1O9)(7)+\delta(O8C1C2)(5)]$
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	12(0	1220	1017	1212	$R_{3}[\delta(O9H)(13)+v(C1C2)(10)+v(C1O9)(9)+\delta(O10H)(8)+v(CC)(35)+\delta_{in}$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1368	1320	1317	1312	(CH)(8)]
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1340	1293	1294	1290	$R3[\delta_{in}(CH)(55)+v(CC)(33)+\delta_{in}(C2C1)(5)]$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1300	1255	1244	1265	$R3[v(C5O)(53)+\delta_{tring}(11)+v(CC)(17)+\delta_{in}(CH)(14)]$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1214	1172		1220	$R3[\delta(O9H)(31)+\delta_{in}(CH)(25)+v(C1C2)(13)+\delta_{tring}(8)+v(CC)(13)]$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1194	1152	1169	1165	$R3[\delta(O10H)(44)+\delta_{in}(CH)(14)+v(CC)(22)]$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1183	1142	1128	1130	$R3[\delta_{in}(CH)(37)+\delta(O9H)(16)+\delta(O10H)(10)+\nu(C1C2)(9)+\nu(CC)(16)]$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1133	1093	1101		R3[δin(CH)(55)+v(CC)(26)]
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1097	1059	1034		$R3[v(C1O9)(47)+v(CC)(18)+\delta(O9H)(9)+\delta(O8C1C2)(6)+\delta_{in}(CH)(9)]$
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	1032	996	1013		$R3[\delta_{tring}(51)+\nu(CC)(34)+\delta_{in}(CH)(9)]$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1007	971			R3[oop(CH)(85)+puck(9)]
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	979	944	930		R3[oop(CH)(81)+puck(11)]
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	874	843	854	853	$R3[oop(CH)(64)+opp(C5O)(11)+\tau_a(10)+\omega(C1O9)(6)+oop(C2C1)(6)]$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	852	822	837	839	$R3[\delta_a(21)+v(C5O)(17)+v(CC)(47)]$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	827	798			R3[oop(CH)](90)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	700	7(2)	770	770	R3[puck(34)+ω(C1O9)(29)+opp(C5O)(14)+oop(C2C1)(11)+oop(CH)(
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	/90 /0	/62	770	112	7)]
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	727	711	604	602	$R3[\rho(C1O9)(20)+\nu(C1C2)(18)+\delta_{tring}(17)+\nu(C1O9)(13)+\nu(C5O)(8)+\delta$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	151	/11	094	095	O9H)(6)+δ(O8C1C2)(5)+ν(CC)(7)]
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	717	692	692		R3[puck(60)+opp(C5O)(13)+ω(C1O9)(9)+oop(CH)(11)]
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	653	630	642	642	$R3[\delta'_{a}(78)+\delta_{in}(C5O)(6)+v(CC)(6)]$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	603	581	619	614	$R3[\delta_a(28) + \rho(C1O9)(26) + \delta(O8C1C2)(20) + \nu(C5O)(5) + \delta(O9H)(5)]$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	588	567	548	560	$R3[\tau(C1O9)(71)+opp(C5O)(8)+\tau_a(6)+oop(C2C1)(5)]$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	511	402	502	501	$R3[\rho(C1O9)(25)+\delta(O8C1C2)(23)+\delta_{in}(C2C1)(17)+\delta_{in}(C5O)(10)+\delta'_{a}(8)$
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	511	495	505	501	]
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	510	492			$R3[opp(C5O)(33)+\tau_a(31)+oop(C2C1)(13)+puck(9)+oop(CH)(8)]$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	428	413	419		R3[\tau'a(82)+oop(CH)(16)]
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	402	388			$R3[\delta_{in}(C5O)(63)+\delta'_{a}(11)+\delta(O8C1C2)(9)]$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	393	379		388	$R3[\tau(C5O10)](95)$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	352	340	-	306	$R3[\delta_a(45)+v(C1C2)(24)+\rho(C1O9)(14)]$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	200	290			$R3[oop(C2C1)(36)+\tau_a(27)+puck(16)+\omega(C1O9)(6)+opp(C5O)(5)+oop(C5O$
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	290	280	-		CH)(8)]
109105-R3[ $\tau a(48)+oop(C2C1)(25)+\omega(C1O9)(6)+oop(CH)(18)]$ 7371-R3[ $\tau (C1C2)(90)+\tau'a(7)]$	195	188	-	-	$R3[\delta_{in}(C2C1)(64) + \delta(O8C1C2)(18) + \rho(C1O9)(6) + \delta_{in}(C5O)(5)]$
73 71 - $R3[\tau(C1C2)(90)+\tau'_a(7)]$	109	105	-	-	R3[τa(48)+oop(C2C1)(25)+ω(C1O9)(6)+oop(CH)(18)]
	73	71	-	-	$R3[\tau(C1C2)(90)+\tau'_{a}(7)]$

#### 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	$E(2)^a$	E(j)-E(i) <sup>b</sup>	F(i,j) <sup>c</sup>						
				K cal/mol	a.u.	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 <sup>*</sup> C14-C16	0.31639	5.47	0.44	0.048						
πN7-C17	1.90975	π <sup>*</sup> C11-C12	0.32703	12.10	0.34	0.061						
πC11-C12	1.74906	π <sup>*</sup> N7-C17	0.24868	17.71	0.28	0.063						
πC11-C12	1.74906	π <sup>*</sup> 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 <sup>*</sup> N6-C16	0.11657	8.15	0.98	0.082						
σC12-C14	1.96998	σ <sup>*</sup> 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 <sup>*</sup> C11-C12	0.32703	14.48	0.30	0.060						
σC17-H18	1.97893	σ <sup>*</sup> 01-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 <sup>*</sup> C11-C12	0.32703	30.17	0.36	0.093						
n(2)O1	1.70033	π <sup>*</sup> C14-C16	0.31639	29.09	0.35	0.090						

(2).02	1 00000	*05 NG	0.05041	10.42	0.70	0.105					
n(2)O2	1.88800	σ O5-N6	0.05941	19.43	0.70	0.105					
n(2)O2	1.88800	σ No-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	1.845/5	σ C20-C21	0.07982	24.64	0.59	0.110					
n(2)O4	1.82269	σ <sup>*</sup> N8-C19	0.11007	31.37	0.62	0.127					
n(2)O4	1.82269	σ <sup>*</sup> 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	$\pi^*O2-N6$	0.65286	158.54	0.14	0.138					
n(1)N7	1.90548	σ <sup>*</sup> N8-C21	0.04640	14.05	0.68	0.088					
n(1)N7	1.90548	σ <sup>*</sup> C17-H18	0.03413	10.28	0.76	0.080					
n(1)N8	1.63455	π <sup>*</sup> O4-C19	0.31059	51.79	0.28	0.110					
n(1)N8	1.63455	π <sup>*</sup> 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 <sup>*</sup> O4-C19	0.31059	50.54	0.29	0.108					
π*O2-N6	0.65286	π <sup>*</sup> 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 <sup>*</sup> 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					
$\pi^* N7-C17$	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)028	1 97603	σ*C21-H22	0.02042	0.15	1.06	0.011					
n(1)028	1.97603	σ*C21-H23	0.01985	0.39	1.08	0.018					
<u>n(1)020</u>	1.97003	with	nin unit?	0.57	1.00	0.010					
σO24-H25	1 98716	σ*C32-C34	0.02587	5 31	1 28	0.074					
$\pi C^{29} - C^{37}$	1 64964	$\pi^* 0.28 - C.39$	0.27883	27.85	0.25	0.076					
$\pi C^{29} C^{37}$	1.64964	$\pi^*C30-C32$	0.27569	22.09	0.29	0.070					
$\pi C^{29} C^{37}$	1 64964	$\pi^*C34-C35$	0.38876	15.87	0.27	0.079					
$\pi C_{30} - C_{32}$	1.68305	$\pi^*C^{29}C^{37}$	0.40222	16.28	0.27	0.061					
$\pi C_{30} C_{32}$	1.68305	$\pi^*C34-C35$	0.38876	25.32	0.27	0.001					
$\pi C_{34}C_{35}$	1.62265	π <sup>*</sup> C29-C37	0.30070	26.52	0.27	0.075					
$\pi C_{34} - C_{35}$	1.62265	$\pi^{*}C30-C32$	0.7569	13.76	0.20	0.070					
$n(1)\Omega^{24}$	1.02203	$\pi^*C34-C35$	0.02941	7 3/	1.14	0.032					
n(1)024 n(2)024	1.97793	$\pi^{*}C34 C35$	0.38876	31.17	0.34	0.002					
n(2)024	1.03044	π C34-C33	0.38870	51.17	1.22	0.099					
n(1)020 n(2)026	1.7/174	0 020-C39 π <sup>*</sup> O28 C20	0.01939	0.57	0.24	0.000					
m(2)O20	1.02904	-*026-C39	0.27003	43.41	0.54	0.115					
II(2)028	1.83833	0 020-C39 -*C20 C20	0.09322	30.93	0.62	0.120					
II(2)U28 -*O28_C20	1.83833	σ C29-C39 -*C20 C27	0.06/89	18.83	0.70	0.104					
π 028-039	0.27883	π C29-C3/	0.40222	88.55	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					

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