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Supporting information for article:

Crystal engineering of co-crystal of nicotinic acid and pyrogallol: an experimental and theoretical electron density analysis

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Table S1A: List of chemical constrains imposed between chemically equivalent atoms Constrained together for Pval, multipoles and kappas).

O2, O3, O4 (gradually deconstrained)
O5, O8 (gradually deconstrained)
O6, O7, O9, O10 (gradually deconstrained)

N1, N2

C1, C2

C2, C8

C3, C9

C4, C10

C5, C11

C6, C12

C14, C24

C15, C17, C21, C23

C16, C22

C18, C20

Table S1B.List of equivalent H atoms constrained together for dipoles and valence population while kappas were restrained to 1.16(02).

H1	H2				
H1A	H5	H7	H11		
H3	H9	H16	H22		
H4	H10				
H5A	H6	H7A	H8	H9A	H10A
H15	H17	H21	H23		
H3	H4	H15			

Table S1C. List of local symmetry constraints applied during MoPro refinement.

SYMPLM mz	O1	Finally deconstrained
SYMPLM mymz	N1	
SYMPLM mz	C1	
SYMPLM mz	O2	Finally deconstrained
SYMPLM mymz	N2	
SYMPLM mymz	C2	
SYMPLM mz	O3	Finally deconstrained
SYMPLM mymz	C3	
SYMPLM mz	O4	Finally deconstrained
SYMPLM mymz	C4	
SYMPLM mz	C5	
SYMPLM mz	O5	
SYMPLM mz	O6	
SYMPLM mymz	C6	
SYMPLM mz	C7	
SYMPLM mz	O7	
SYMPLM mz	O8	
SYMPLM mymz	C8	
SYMPLM mymz	C9	
SYMPLM mz	O9	
SYMPLM mymz	C10	
SYMPLM mz	O10	
SYMPLM mz	C11	
SYMPLM mymz	C12	
SYMPLM mz	C13	
SYMPLM mz	C14	

SYMPLM mymz	C15	
SYMPLM mymz	C16	
SYMPLM mymz	C17	
SYMPLM mymz	C18	
SYMPLM mymz	C19	
SYMPLM mymz	C20	
SYMPLM mymz	C21	
SYMPLM mymz	C22	
SYMPLM mymz	C23	
SYMPLM mz	C24	

Table S2: The optimized bond lengths for H atoms.

No.	Bond	d(Å)
1.	N1-H1	1.08298
2.	N2-H2	1.07310
3.	O5-H5A	0.99140
4.	O6-H6	0.98562
5.	O7-H7A	0.99028
6.	O8-H8	0.99065
7.	O9-H9A	0.98756
8.	O10-H10A	0.99754
9.	C1-H1A	1.08658
10.	C3-H3	1.08777
11.	C4-H4	1.08531
12.	C5-H5	1.08399
13.	C7-H7	1.08504
14.	C9-H9	1.08925
15.	C10-H10	1.08602
16.	C11-H11	1.08536
17.	C15-H15	1.08763
18.	C16-H16	1.08733
19.	C17-H17	1.08755
20.	C21-H21	1.08736
21.	C22-H22	1.08750

22.	C23-H23	1.08919

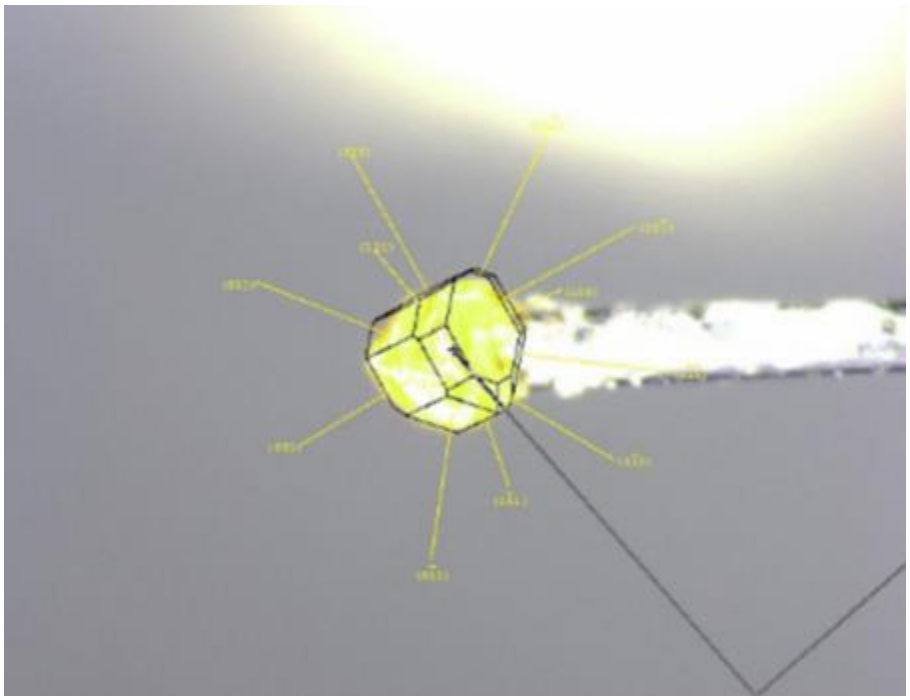

Figure S1: An image of the crystal used in experiment.

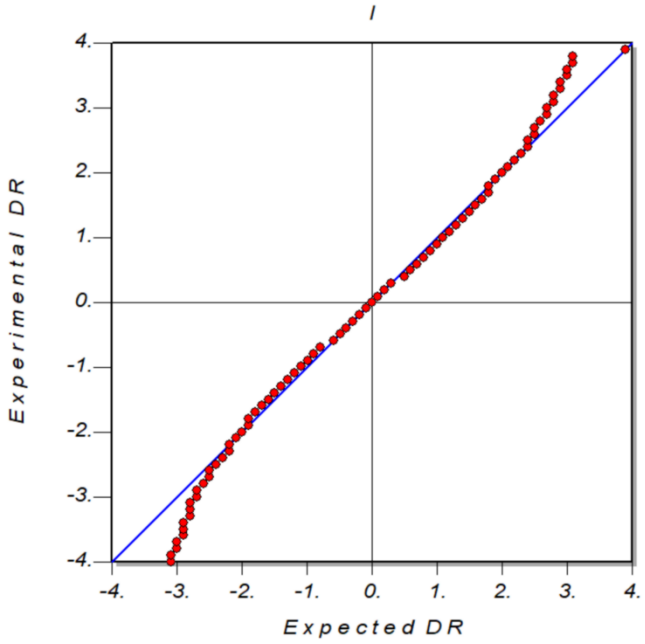

Figure S2A: Normal probability plot showing the quality of the data used.

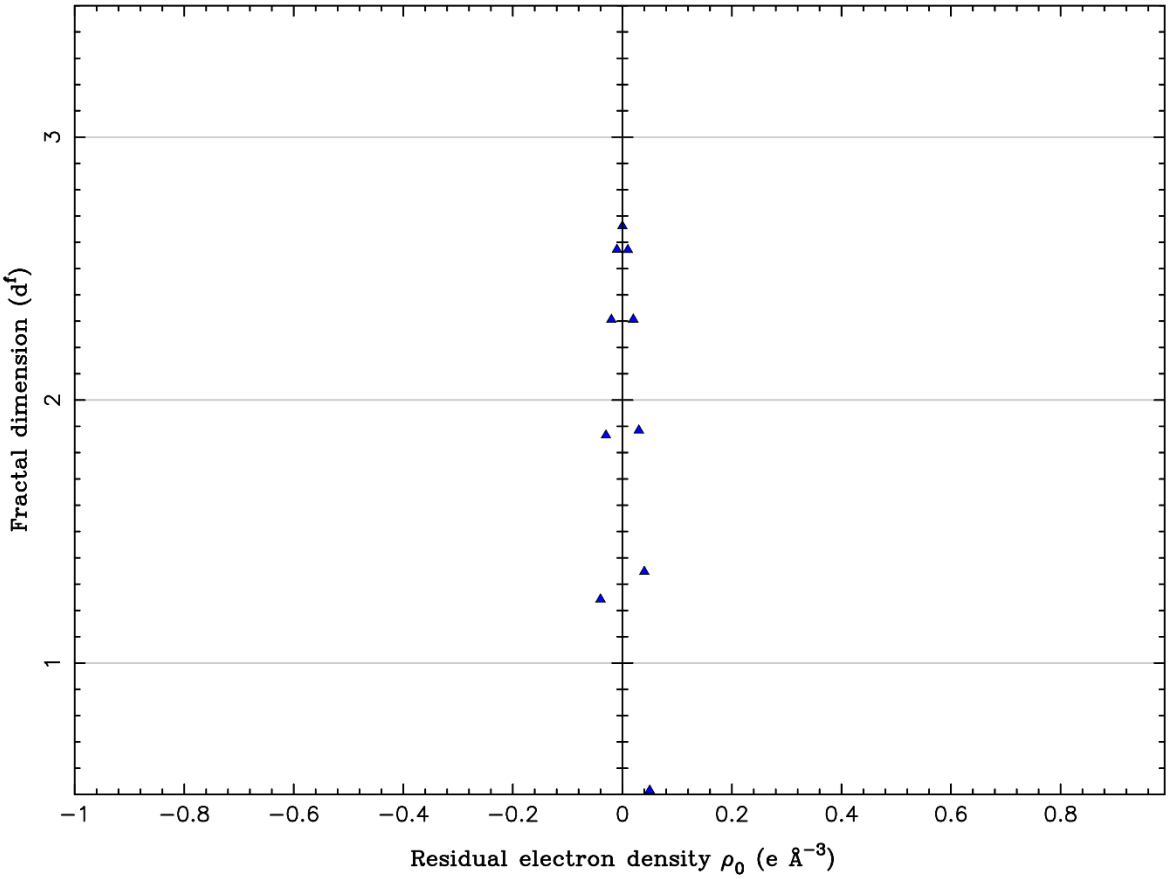

Figure S2B: Fractal dimension plot.

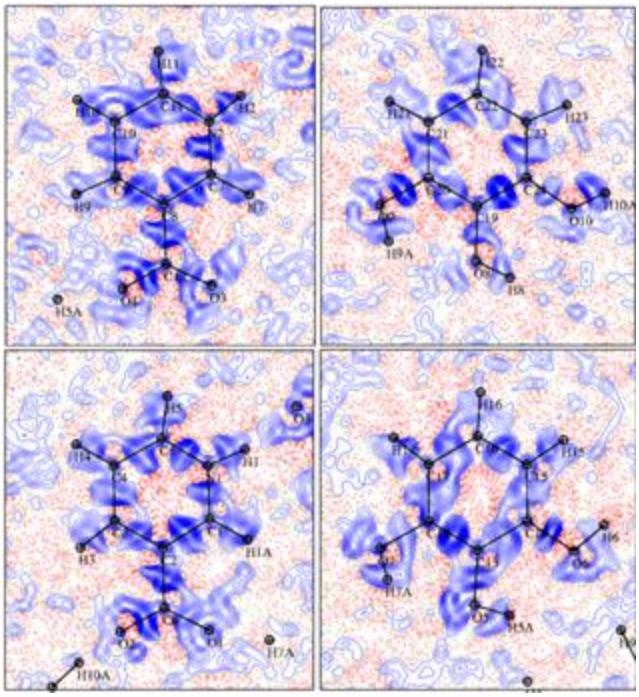

Figure S3. Deformation electron density maps of NA moiety (right), PY moiety (left), after IAM refinement with *MoPro* at 0.05eÅ^{-3} level using all data.

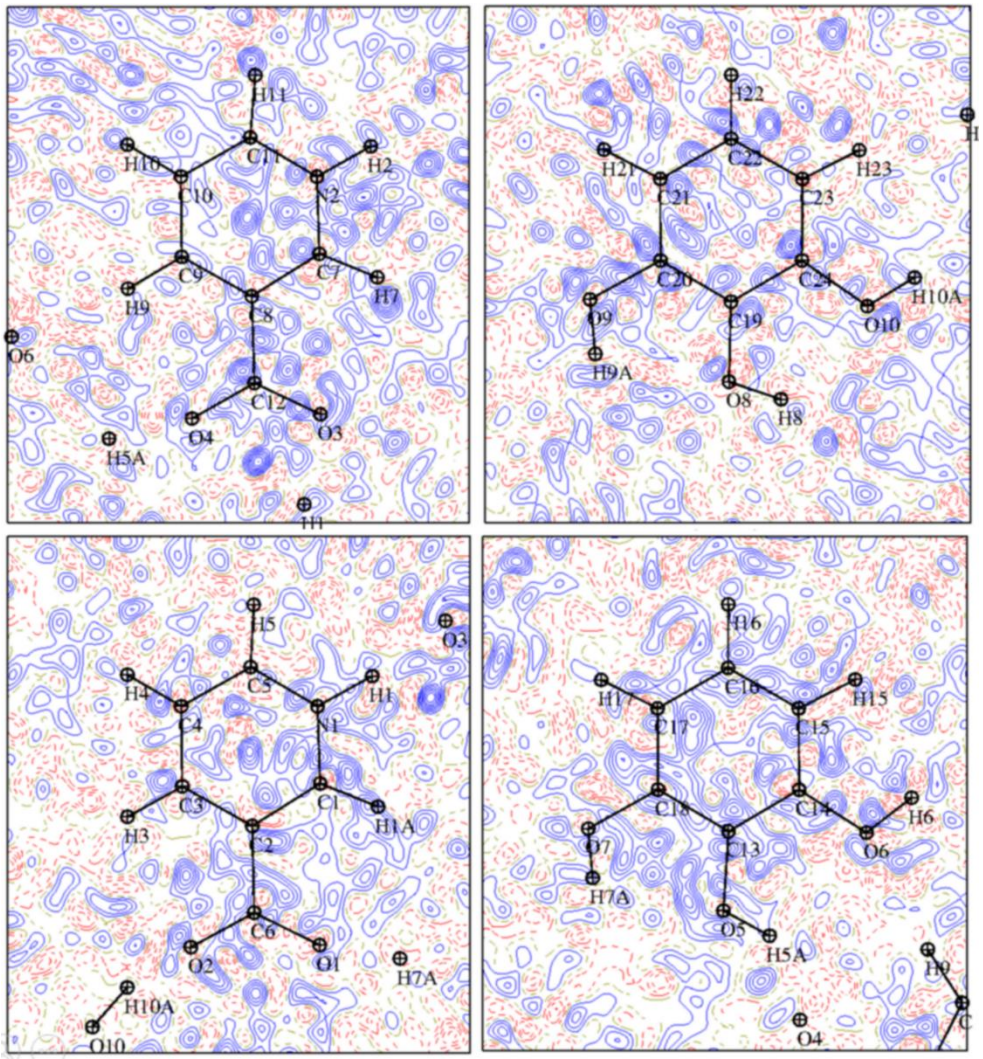

Figure S4. Residual electron density maps of NA moiety (right), PY moiety (left), after MM_{exp} with *MoPro* at 0.05eÅ^{-3} contour level using all data.

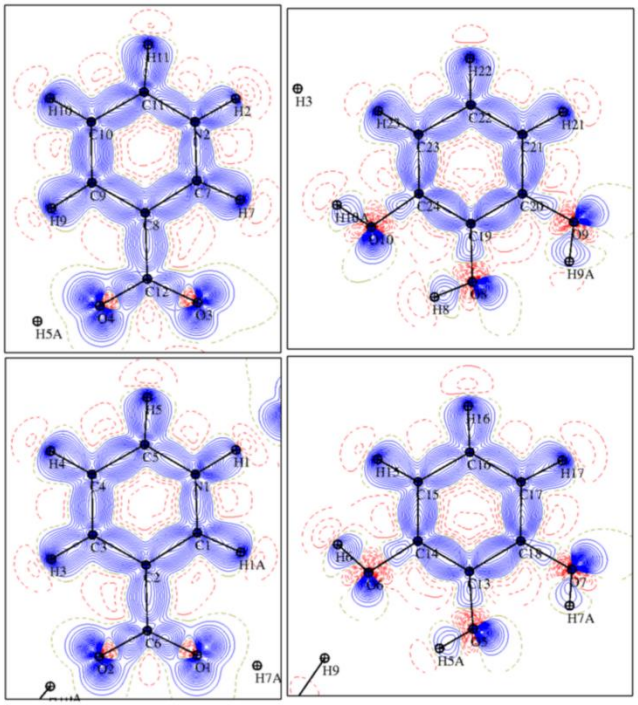

Figure S5. Static deformation electron density distribution of NA (right) and PY(left) after MM_{theo} at 0.05eÅ^{-3} contour level.

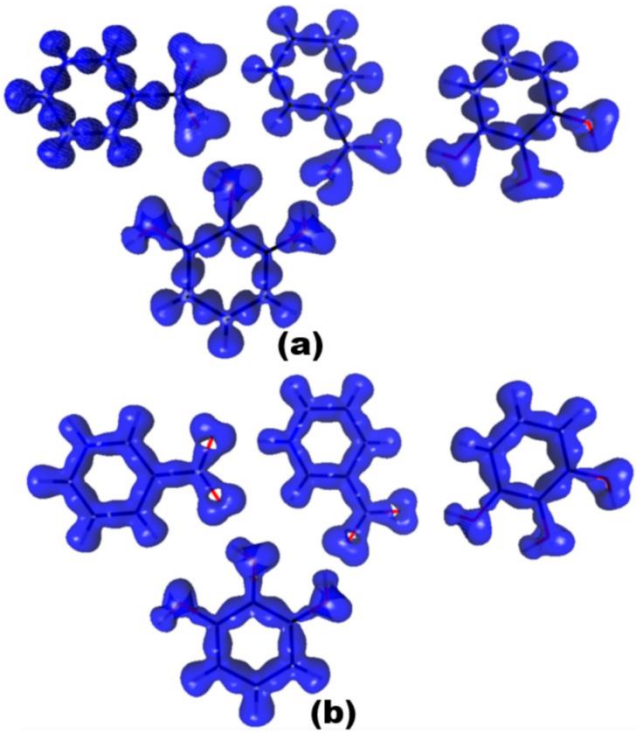

Figure S6. 3D Static deformation electron density distribution of Asymmetric unit cell of NAPY) a) after MM_{exp} and b) MM_{theo} at 0.05eÅ^{-3} contour level.

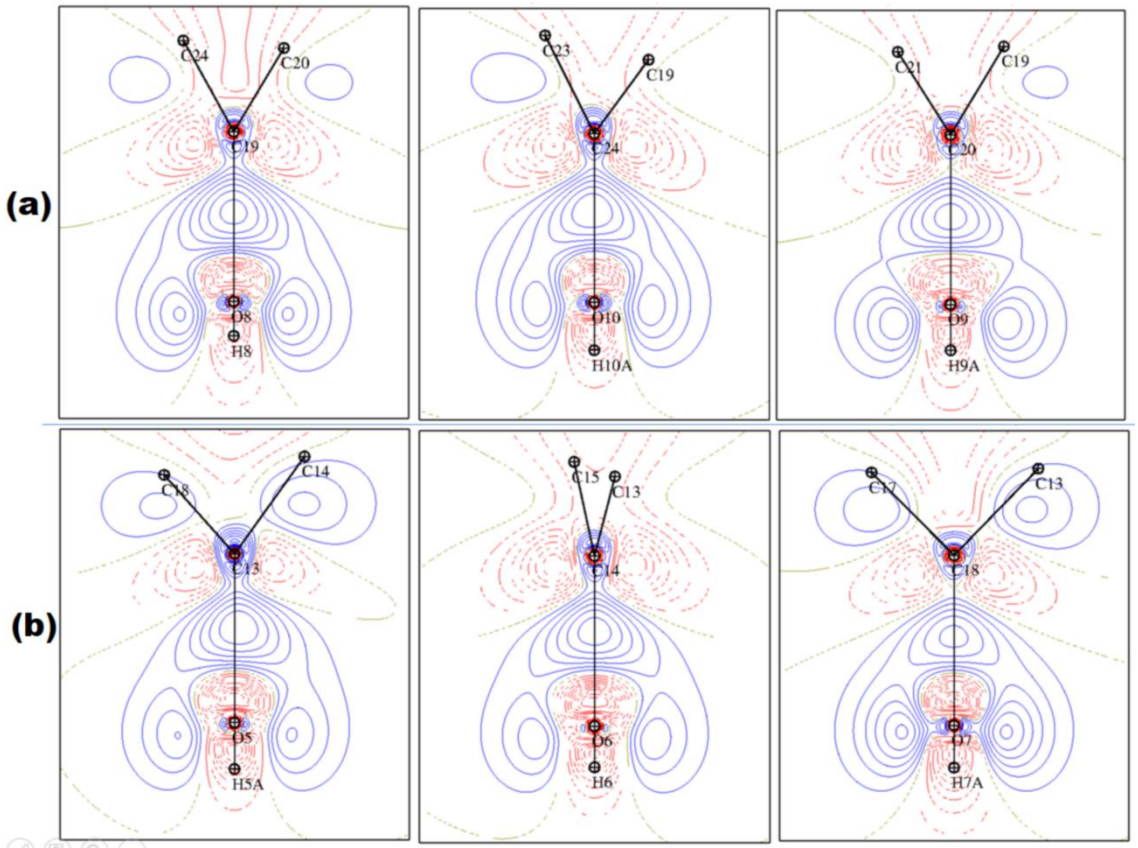

Figure S7: Lone pair electron density of PY. (a) Lone pairs of hydroxyl group of PY (1) and (b) PY (II).

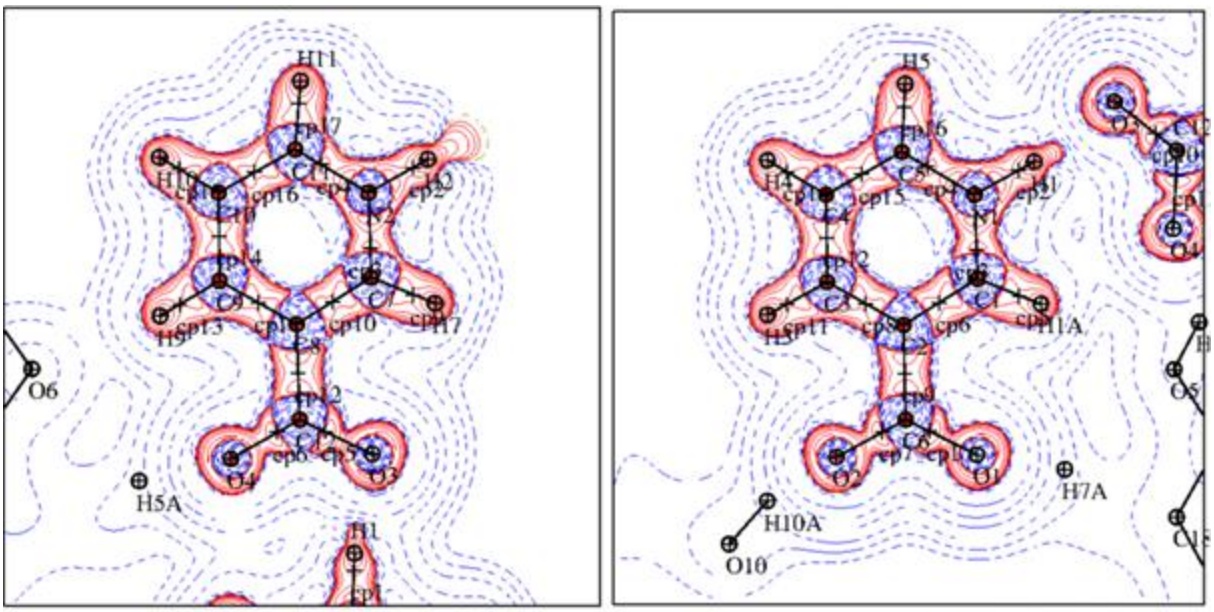

Figure S8. Contours maps of Laplacian of electron density of covalent bond critical points for (a)NA(I) and (b) NA (II) molecule calculated after MM_{exp}.

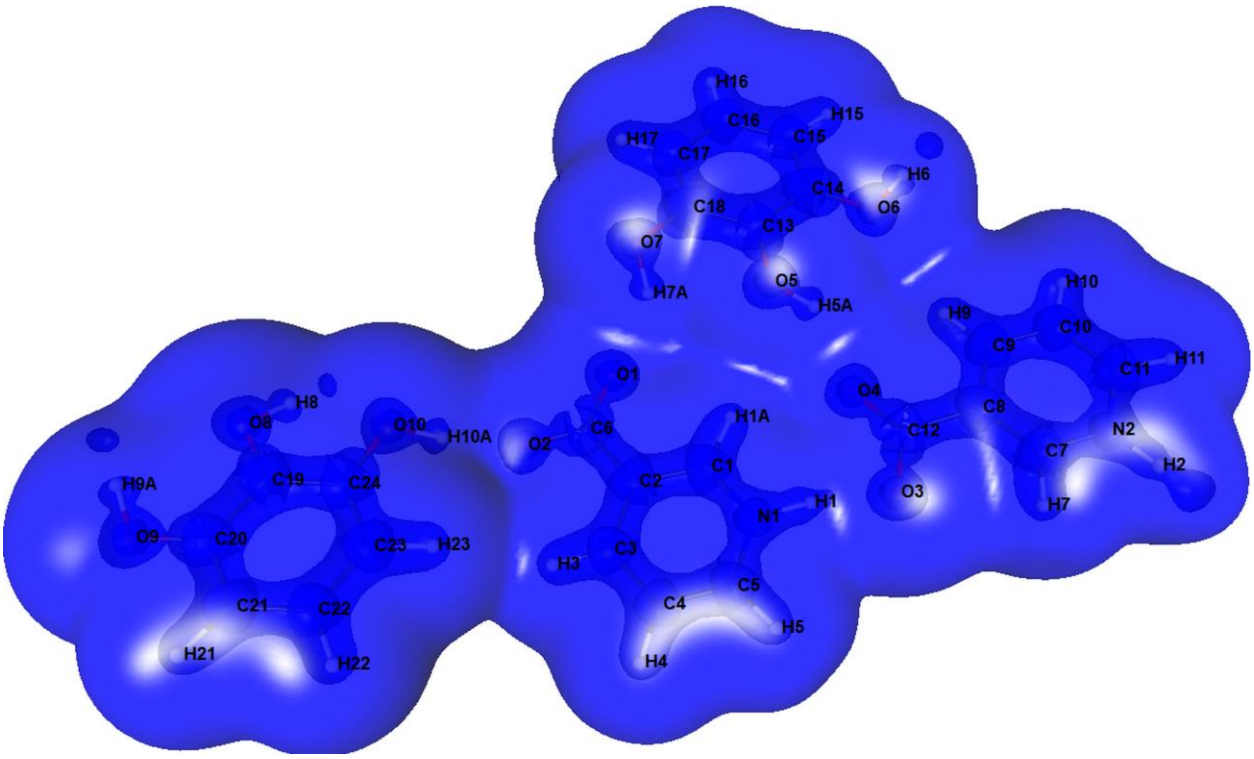

Figure S9. Contours maps of 3D Laplacian of electron density of covalent bond critical points for Asymmetric unit cell of NAPY calculated after MM_{exp}. Contours @ 0.05e/Å^3

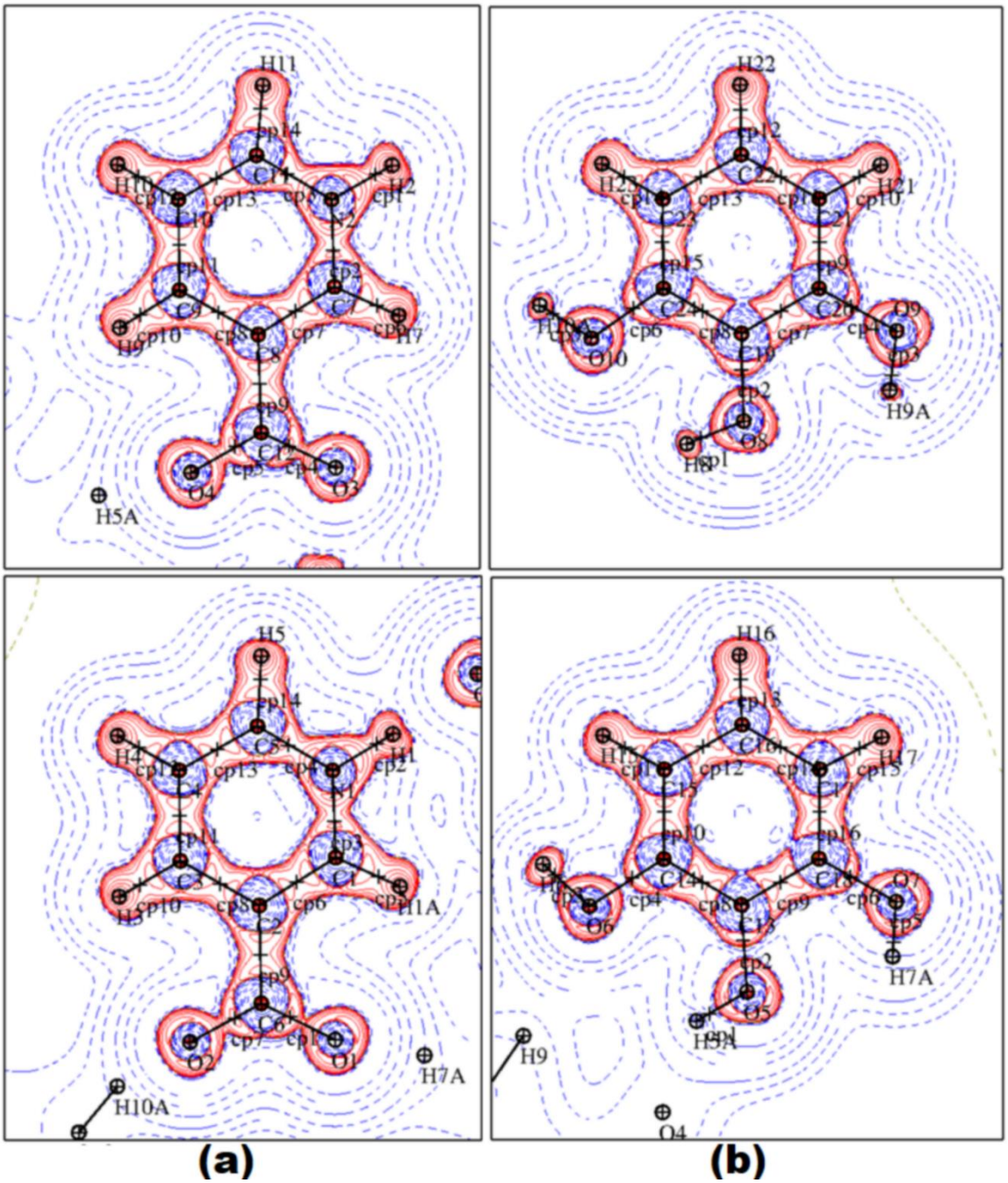

Figure S10. Contours maps of Laplacian of electron density of covalent bond critical points for (a)NA(I) and NA (II) molecule (b) PY (I) and (II) molecule calculated after MM_{theo}.

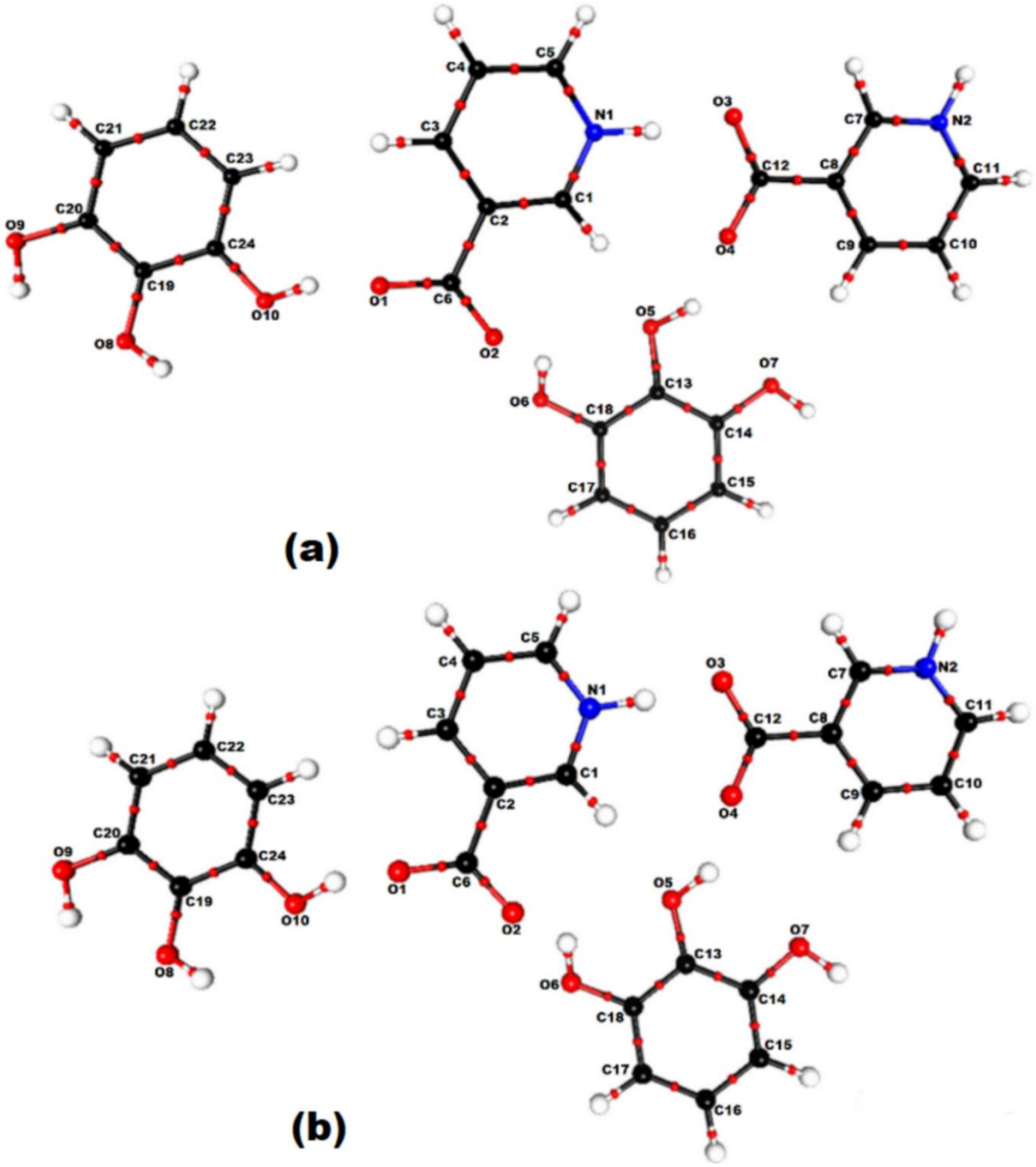

Figure S11. The molecular graph showing the (3, -1) critical points in cocrystal of NAPY. The large circles (spheres) represents the atomic positions, the small circles represent the bond critical points (red). (a) Experimental and (b) Theoretical.

Table S3. Hydrogen-bond geometry (Å, º) for Multipolar atom model (MAM).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O10—H10*A*···O2	1.00	1.68 (1)	2.6349 (4)	159 (1)
N1—H1···O3	1.08	1.59 (1)	2.6700 (4)	172 (1)
O5—H5*A*···O4	0.99	1.83 (1)	2.6854 (4)	143 (1)
O8—H8···O10	0.99	2.19 (1)	2.6925 (4)	110 (1)
O7—H7*A*···O1	0.99	1.90 (1)	2.7055 (4)	137 (1)
N2—H2···O1^{i}	1.07	1.65 (1)	2.7139 (4)	169 (1)
O8—H8···O3^{iii}	0.99	1.93 (1)	2.7515 (4)	139 (1)
O9—H9*A*···O8	0.99	2.36 (1)	2.7583 (4)	103 (1)
O9—H9*A*···O7^{vii}	0.99	1.90 (1)	2.8160 (4)	153 (1)
O6—H6···O9^{ii}	0.99	1.99 (1)	2.9711 (4)	171 (1)
C5—H5···O4^{v}	1.08	2.34 (1)	3.0356 (5)	121 (1)
C5—H5···O8^{i}	1.08	2.55 (1)	3.1304 (5)	113 (1)
C11—H11···O2^{iv}	1.09	2.51 (1)	3.1484 (5)	116 (1)
N2—H2···O2^{i}	1.07	2.43 (1)	3.1976 (5)	128 (1)
N1—H1···O4	1.08	2.46 (1)	3.2075 (5)	125 (1)
C1—H1*A*···O4	1.09	2.43 (1)	3.2167 (5)	128 (1)
C16—H16···O5^{vi}	1.09	2.44 (1)	3.2519 (5)	130 (1)
C7—H7···O2^{i}	1.09	2.51 (1)	3.2615 (5)	126 (1)
C21—H21···O10^{vii}	1.09	2.34 (1)	3.2768 (5)	143 (1)
N1—H1···C12	1.08	2.28 (1)	3.2967 (5)	156 (1)
C7—H7···O10^{i}	1.09	2.36 (1)	3.3138 (5)	146 (1)
N2—H2···C6^{i}	1.07	2.30 (1)	3.3153 (5)	158 (1)
C15—H15···O9^{ii}	1.09	2.55 (1)	3.3976 (5)	134 (1)
C17—H17···O8^{viii}	1.09	2.53 (1)	3.4591 (5)	143 (1)
C9—H9···O6	1.09	2.51 (1)	3.5076 (5)	151 (1)

Symmetry codes: (i) *x*, *y*-1, *z*; (ii) *x*, *y*-1, *z*+1; (iii) *x*, *y*+1, *z*; (iv) -*x*+3/2, *y*-1, *z*+1/2; (v) -*x*+3/2, *y*, *z*-1/2; (vi) -*x*+1, -*y*+1, *z*+1/2; (vii) -*x*+1, -*y*+2, *z*-1/2; (viii) -*x*+1, -*y*+2, *z*+1/2.

Table S4: Covalent_ CBCPs: Topological properties of (3, -1) CPs on the covalent interactions: distances (Å), electron density (e/Å^3), Laplacian (e/Å^5), Hessian eigenvalues (e/Å^5), ε = ellipticity. The upper line in each pair represents the experimental value and lower line shows the theoretical values.

N0.	Bond	d_{12}	d_{1cp}	d_{2cp}	$\rho_{cp(r)}$	$\nabla^2\rho_{(cp)}$	λ_1	λ_2	λ_3	ε
1	O1—C6	1.267	0.839	0.428	2.636	-28.977	-25.520	-22.460	19.000	0.136
		1.268	0.783	0.485	2.499	-25.192	-19.380	-18.410	12.610	0.053
2	N1—H1	1.083	0.808	0.275	2.012	-37.907	-28.750	-27.710	18.550	0.038
		1.082	0.797	0.286	1.787	-15.252	-22.160	-21.300	28.210	0.040
3	N1—C1	1.342	0.881	0.461	2.252	-24.190	-17.980	-15.490	9.280	0.161
		1.342	0.784	0.559	2.164	-17.674	-16.570	-15.000	13.890	0.105
4	N1—C5	1.344	0.878	0.466	2.257	-24.922	-17.930	-15.370	8.380	0.167
		1.343	0.784	0.560	2.209	-18.422	-16.900	-14.980	13.460	0.128
5	C1—H1A	1.086	0.720	0.367	1.909	-24.032	-18.810	-17.800	12.580	0.057
		1.085	0.723	0.363	1.839	-16.467	-18.190	-17.620	19.340	0.032
6	C1—C2	1.388	0.720	0.669	2.193	-22.877	-17.160	-13.380	7.660	0.282
		1.388	0.709	0.679	2.118	-16.946	-15.810	-13.480	12.340	0.173
7	O2—C6	1.251	0.831	0.420	2.675	-25.694	-26.610	-23.640	24.550	0.126
		1.250	0.785	0.465	2.583	-26.539	-20.680	-19.710	13.850	0.049
8	N2—H2	1.073	0.806	0.268	2.040	-40.191	-29.810	-28.910	18.530	0.031
		1.074	0.785	0.289	1.820	-16.241	-22.580	-21.680	28.020	0.041
9	N2—C7	1.344	0.881	0.463	2.247	-24.470	-17.910	-15.410	8.850	0.163
		1.344	0.777	0.567	2.221	-17.250	-17.140	-15.170	15.060	0.130
10	N2—C11	1.345	0.878	0.467	2.256	-25.021	-17.890	-15.340	8.210	0.166
		1.344	0.795	0.549	2.177	-18.249	-16.720	-14.780	13.250	0.131
11	C2—C3	1.395	0.698	0.697	2.147	-22.026	-16.270	-12.990	7.240	0.253
		1.396	0.688	0.708	2.065	-16.065	-15.170	-13.090	12.190	0.159
12	C2—C6	1.506	0.772	0.734	1.786	-15.895	-13.310	-10.800	8.220	0.232
		1.506	0.757	0.750	1.695	-10.741	-11.830	-10.690	11.780	0.107
13	O3—C12	1.269	0.832	0.438	2.610	-32.679	-24.930	-21.810	14.060	0.143
		1.270	0.795	0.476	2.460	-25.157	-19.470	-18.270	12.580	0.066
14	C3—H3	1.088	0.733	0.355	1.832	-20.947	-17.530	-16.410	12.990	0.069
		1.088	0.717	0.372	1.790	-15.124	-16.840	-16.610	18.330	0.014
15	C3—C4	1.392	0.702	0.690	2.174	-21.805	-15.640	-12.830	6.670	0.219
		1.393	0.700	0.693	2.077	-16.844	-15.270	-13.240	11.660	0.153
16	O4—C12	1.248	0.836	0.413	2.724	-21.162	-27.760	-24.620	31.220	0.127
		1.248	0.790	0.458	2.597	-26.241	-20.730	-20.040	14.530	0.034
17	C4—H4	1.085	0.726	0.359	1.808	-20.422	-16.840	-16.350	12.770	0.030

		1.087	0.713	0.373	1.822	-16.210	-16.910	-15.960	16.660	0.060
18	C4—C5	1.383	0.654	0.729	2.230	-22.882	-16.420	-13.240	6.780	0.241
		1.383	0.675	0.708	2.159	-18.256	-16.330	-13.520	11.600	0.208
19	C5—H5	1.084	0.720	0.364	1.929	-24.540	-19.090	-18.050	12.600	0.057
		1.085	0.722	0.363	1.832	-16.306	-17.880	-17.570	19.150	0.018
20	O5—H5A	0.991	0.741	0.251	2.451	-49.083	-38.940	-38.430	28.290	0.013
		0.991	0.741	0.250	2.090	-22.935	-29.600	-29.230	35.890	0.012
21	O5—C13	1.361	0.828	0.534	2.087	-21.247	-16.490	-13.940	9.180	0.183
		1.359	0.798	0.562	1.943	-9.861	-14.280	-12.720	17.140	0.123
22	O6—H6	0.986	0.739	0.247	2.470	-51.027	-39.840	-39.330	28.140	0.013
		0.985	0.732	0.253	2.177	-23.054	-30.270	-30.110	37.320	0.005
23	O6—C14	1.369	0.837	0.532	2.043	-22.313	-16.130	-14.340	8.150	0.125
		1.368	0.800	0.568	1.925	-10.321	-14.150	-12.760	16.590	0.108
24	C7—H7	1.085	0.719	0.366	1.915	-24.228	-18.900	-17.880	12.550	0.057
		1.086	0.725	0.361	1.868	-16.803	-18.380	-17.510	19.090	0.050
25	C7—C8	1.389	0.720	0.669	2.190	-22.818	-17.130	-13.360	7.680	0.282
		1.389	0.710	0.679	2.118	-16.675	-15.980	-13.510	12.810	0.183
26	O7—H7A	0.990	0.744	0.246	2.484	-51.743	-39.940	-39.780	27.970	0.004
		0.991	0.734	0.257	2.121	-21.366	-30.040	-29.560	38.240	0.016
27	O7—C18	1.373	0.860	0.512	1.943	-20.383	-14.410	-13.270	7.300	0.086
		1.372	0.809	0.563	1.859	-9.691	-13.580	-12.380	16.260	0.097
28	O8—H8	0.991	0.734	0.256	2.406	-45.464	-37.630	-36.560	28.720	0.029
		0.990	0.741	0.248	2.116	-24.456	-30.270	-29.940	35.750	0.011
29	O8—C19	1.366	0.861	0.505	2.073	-23.944	-16.110	-14.700	6.860	0.096
		1.367	0.800	0.567	1.950	-10.600	-14.610	-12.890	16.900	0.134
30	C8—C9	1.395	0.698	0.698	2.147	-22.018	-16.270	-12.990	7.240	0.253
		1.395	0.705	0.690	2.085	-16.203	-15.390	-13.320	12.510	0.155
31	C8—C12	1.512	0.774	0.738	1.775	-15.564	-13.180	-10.700	8.320	0.232
		1.512	0.760	0.752	1.682	-10.527	-11.720	-10.490	11.690	0.117
32	C9—H9	1.089	0.734	0.355	1.829	-20.870	-17.490	-16.370	12.990	0.069
		1.089	0.717	0.371	1.850	-16.522	-17.590	-17.410	18.470	0.010
33	C9—C10	1.395	0.704	0.691	2.166	-21.610	-15.580	-12.780	6.750	0.220
		1.395	0.699	0.696	2.110	-17.236	-15.910	-13.550	12.220	0.174
34	O9—H9A	0.988	0.741	0.247	2.469	-50.861	-39.720	-39.330	28.180	0.010
		0.987	0.740	0.247	2.163	-24.633	-30.280	-29.920	35.560	0.012
35	O9—C20	1.373	0.864	0.510	1.945	-20.602	-14.350	-13.450	7.200	0.067
		1.373	0.809	0.565	1.873	-9.755	-13.610	-12.230	16.090	0.113
36	C10—H10	1.086	0.727	0.359	1.808	-20.435	-16.840	-16.350	12.760	0.030
		1.085	0.714	0.371	1.791	-15.602	-16.990	-16.030	17.410	0.060
37	C10—C11	1.385	0.655	0.730	2.225	-22.774	-16.390	-13.200	6.820	0.242
		1.385	0.669	0.716	2.120	-17.668	-16.040	-13.430	11.810	0.194

38	O10—H10A	0.998	0.741	0.257	2.416	-46.139	-37.680	-37.010	28.550	0.018
		0.997	0.747	0.250	2.051	-23.958	-29.320	-29.100	34.460	0.008
39	O10—C24	1.360	0.850	0.510	2.076	-23.988	-16.430	-14.680	7.130	0.119
		1.359	0.795	0.565	1.964	-12.152	-14.660	-13.610	16.120	0.077
40	C11—H11	1.085	0.721	0.365	1.924	-24.372	-19.020	-17.980	12.630	0.058
		1.085	0.719	0.366	1.880	-17.140	-18.320	-17.560	18.740	0.043
41	C13—C14	1.402	0.696	0.706	2.174	-22.275	-16.950	-12.600	7.270	0.345
		1.403	0.704	0.699	2.104	-17.410	-16.240	-12.600	11.430	0.288
42	C13—C18	1.401	0.702	0.699	2.205	-22.820	-17.230	-13.050	7.470	0.320
		1.402	0.698	0.704	2.096	-17.116	-16.260	-12.580	11.730	0.292
43	C14—C15	1.396	0.754	0.642	2.167	-22.896	-16.620	-12.440	6.170	0.336
		1.396	0.734	0.663	2.051	-16.763	-15.330	-12.340	10.910	0.243
44	C15—H15	1.088	0.727	0.361	1.827	-20.746	-17.260	-16.210	12.730	0.065
		1.087	0.702	0.385	1.787	-15.021	-16.360	-15.460	16.800	0.058
45	C15—C16	1.395	0.671	0.724	2.126	-21.809	-15.730	-12.390	6.310	0.269
		1.394	0.700	0.695	2.021	-14.973	-14.890	-12.060	11.970	0.235
46	C16—H16	1.087	0.733	0.355	1.832	-20.999	-17.550	-16.410	12.960	0.069
		1.086	0.712	0.375	1.818	-15.482	-16.630	-15.970	17.120	0.041
47	C16—C17	1.393	0.723	0.669	2.131	-21.951	-15.770	-12.430	6.250	0.269
		1.393	0.690	0.702	2.053	-15.939	-15.040	-12.770	11.870	0.177
48	C17—H17	1.087	0.727	0.361	1.821	-20.622	-17.210	-16.140	12.730	0.066
		1.088	0.708	0.379	1.773	-14.712	-16.310	-15.360	16.960	0.062
49	C17—C18	1.391	0.654	0.738	2.138	-22.202	-16.220	-12.340	6.360	0.315
		1.391	0.665	0.726	2.101	-17.103	-15.850	-12.720	11.460	0.246
50	C19—C20	1.394	0.685	0.710	2.181	-22.779	-17.310	-12.640	7.170	0.370
		1.394	0.708	0.686	2.122	-18.340	-16.570	-12.690	10.930	0.305
51	C19—C24	1.403	0.692	0.711	2.162	-22.534	-17.250	-12.520	7.240	0.378
		1.402	0.702	0.700	2.071	-17.245	-16.250	-12.370	11.380	0.314
52	C20—C21	1.393	0.738	0.655	2.132	-22.045	-16.180	-12.290	6.430	0.316
		1.393	0.714	0.679	2.096	-17.188	-15.580	-12.710	11.100	0.225
53	C21—H21	1.087	0.727	0.361	1.823	-20.676	-17.230	-16.160	12.720	0.066
		1.089	0.706	0.383	1.794	-14.963	-16.660	-15.900	17.600	0.048
54	C21—C22	1.392	0.669	0.723	2.132	-21.997	-15.790	-12.440	6.230	0.269
		1.393	0.693	0.700	2.071	-15.716	-15.300	-12.480	12.060	0.225
55	C22—H22	1.088	0.733	0.355	1.831	-20.946	-17.460	-16.450	12.970	0.061
		1.088	0.706	0.383	1.778	-14.501	-16.460	-15.610	17.570	0.055
56	C22—C23	1.398	0.725	0.673	2.118	-21.568	-15.650	-12.330	6.410	0.269
		1.398	0.714	0.684	2.044	-15.213	-15.070	-12.470	12.330	0.208
57	C23—H23	1.089	0.728	0.361	1.822	-20.624	-17.200	-16.150	12.730	0.065
		1.089	0.698	0.391	1.769	-14.365	-15.790	-15.070	16.500	0.048
58	C23—C24	1.392	0.639	0.753	2.177	-23.229	-16.730	-12.520	6.020	0.337

		1.392	0.670	0.722	2.071	-16.384	-15.610	-12.500	11.720	0.249