Electronic Supplementary Material (ESI) for RSC Advances

On differences in electron densities of phenoxazine and phenothiazine derivatives – charge density studies*

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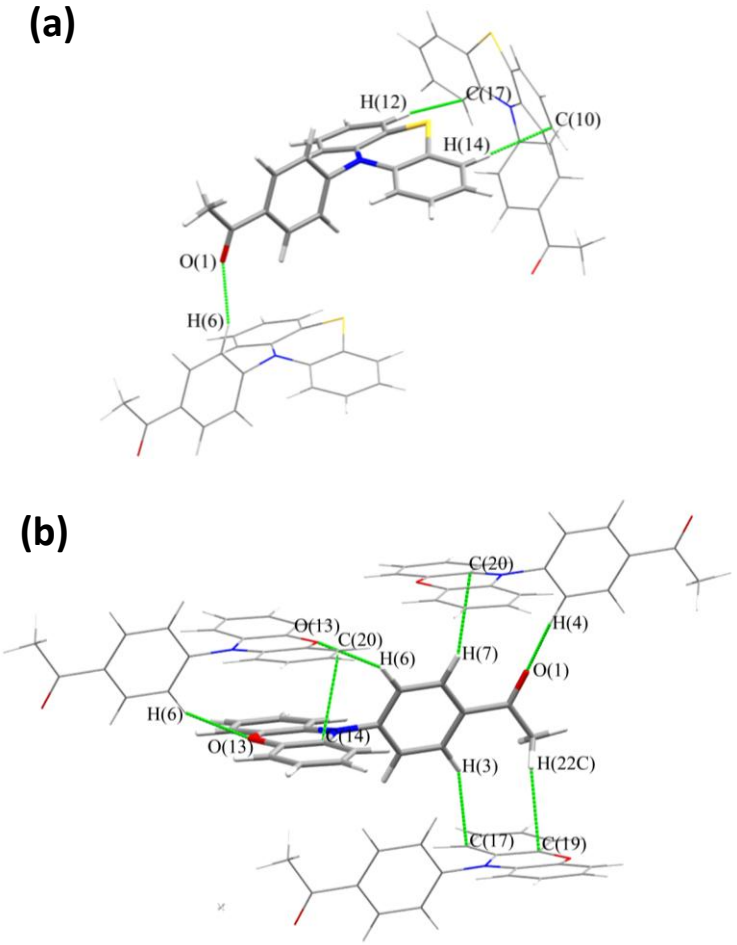
Keywords:
experimental charge density, phenoxazine and phenothiazine derivatives, X-ray structural studies

In honour of Prof. Richard F. W. Bader on the occasion of His 80th Birthday



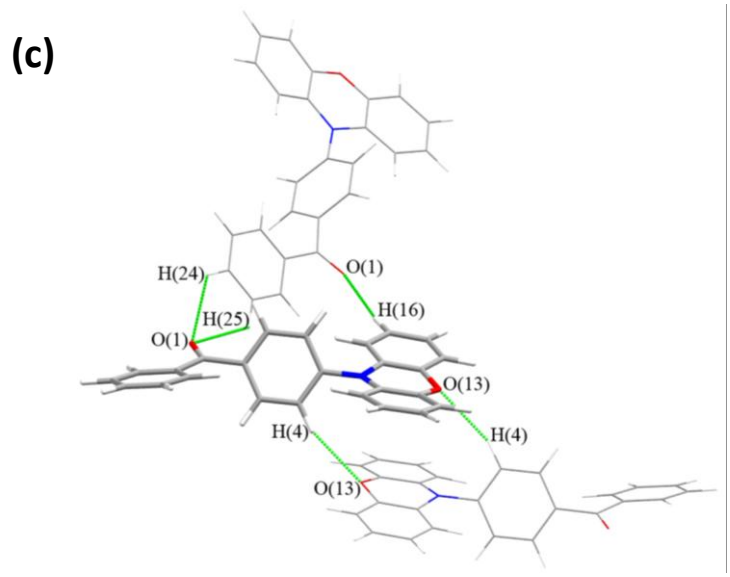
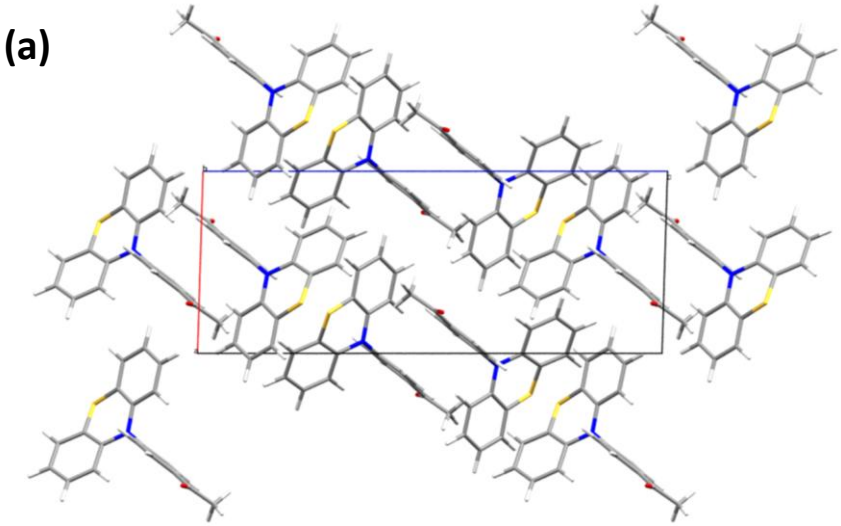
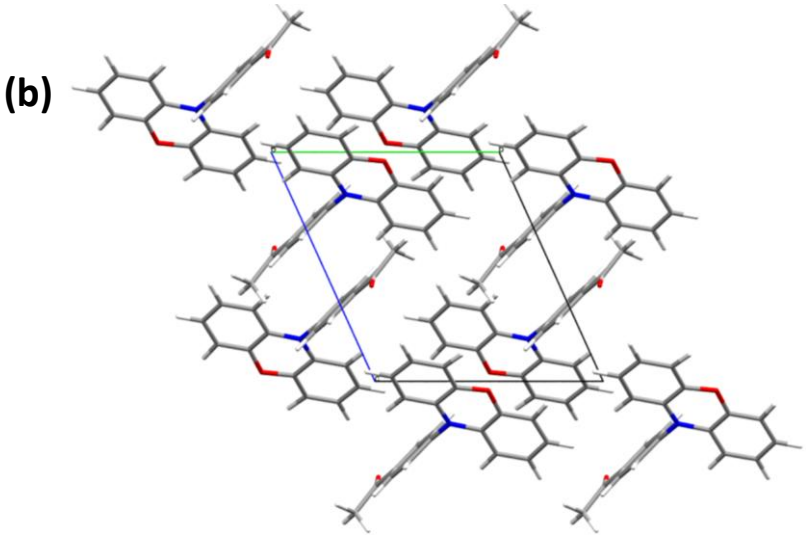


Figure 1S. Intermolecular interactions in the crystal lattice of: (a) **PAS**, (b) **PAO**, (c) **PBO.**





(c)

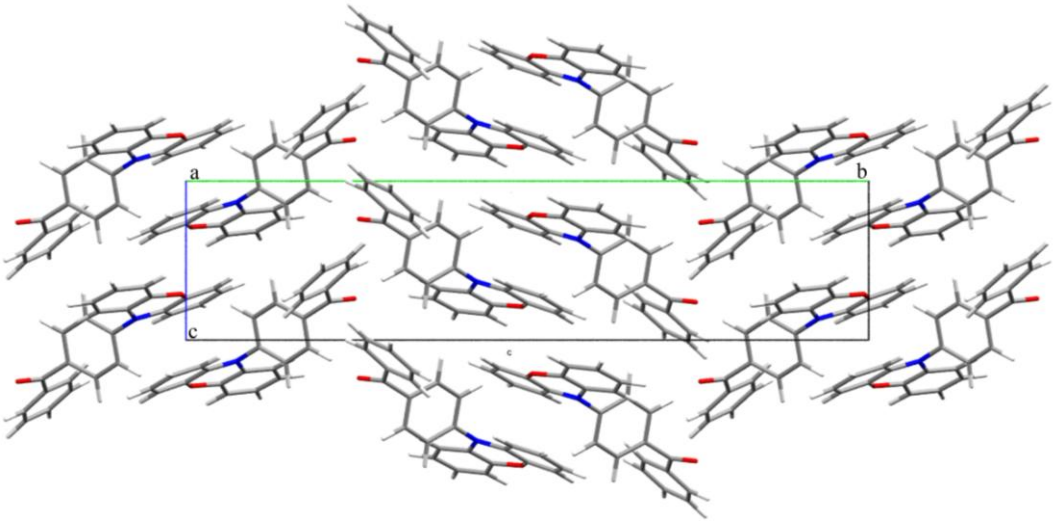
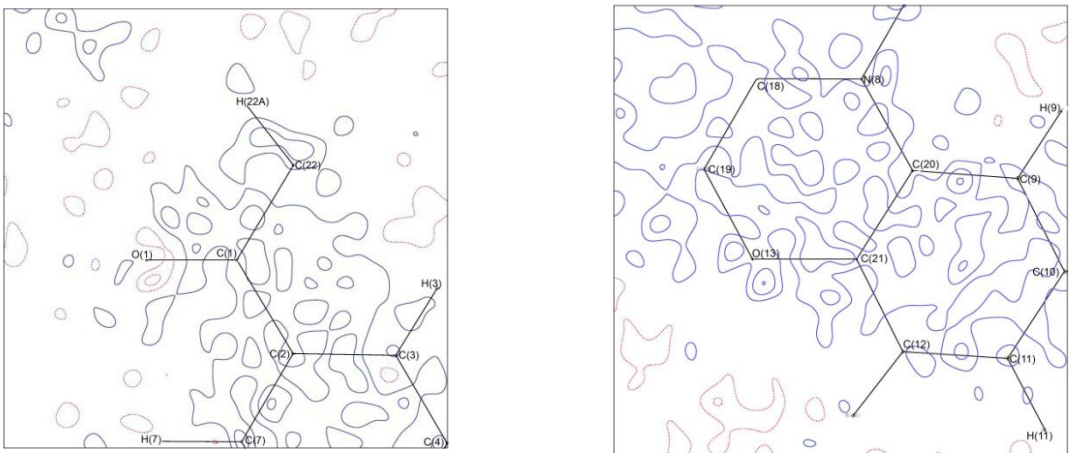
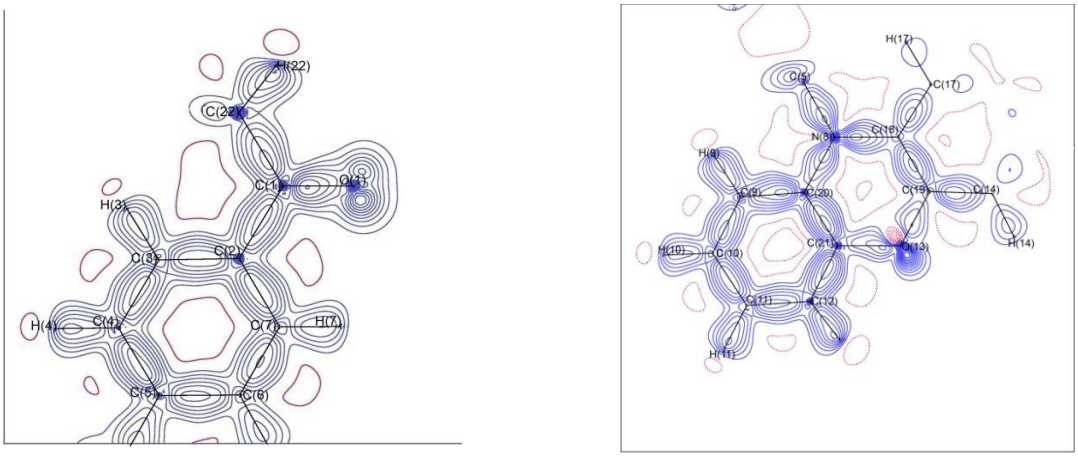


Figure 2S. The crystal packing of molecules: (a) **PAS** – view along the Y-axis, (b) **PAO –** view along the X-axis**,** and (c) **PBO** -view along the X-axis.



(*a*) (*b*)

Figure 3S. Residual density maps for the **PAO** molecule: (*a*) the O(1)C(1)C(2) plane; (*b*) the O(13)C(20)C(21) plane. Blue solid line – the positive values, red dashed lines – the negative ones. Contours at ± n·0.05 e·Å^{-3} (n = 1, 2, …).



(*a*) (*b*)

Figure 4S. Static deformation density maps for **PAO**: (*a*) the O(1)C(1)C(2) plane; (*b*) the O(13)C(20)C(21) plane. Blue solid line – the positive values, red dashed lines – the negative ones. Contours at ± n·0.1 e·Å^{-3} (n =0, 1, 2, …).

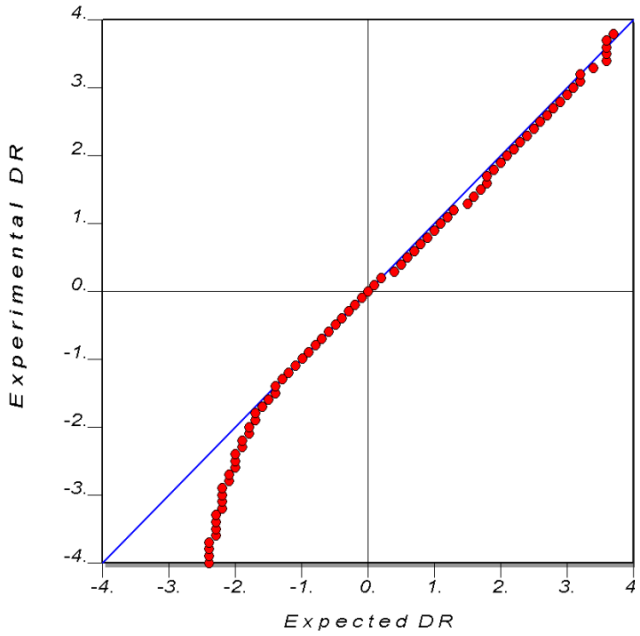


Figure 5S. Normal probability plot for the final multipole refinement of **PAO**.

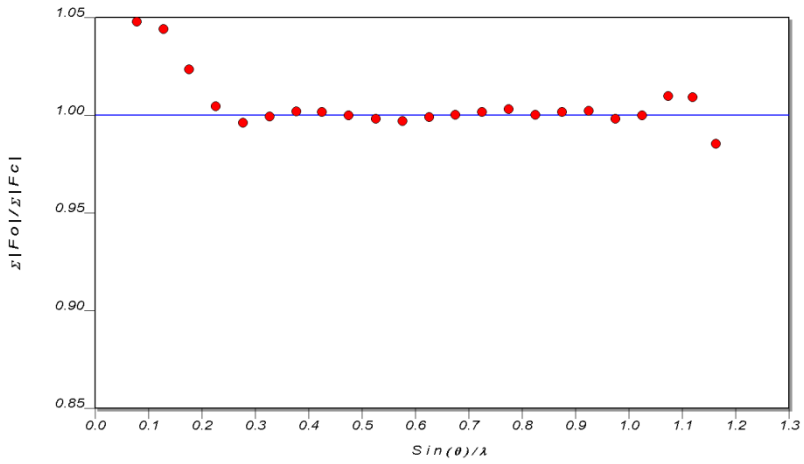


Figure 6S. Scale plot for the final multipole refinement of **PAO**.

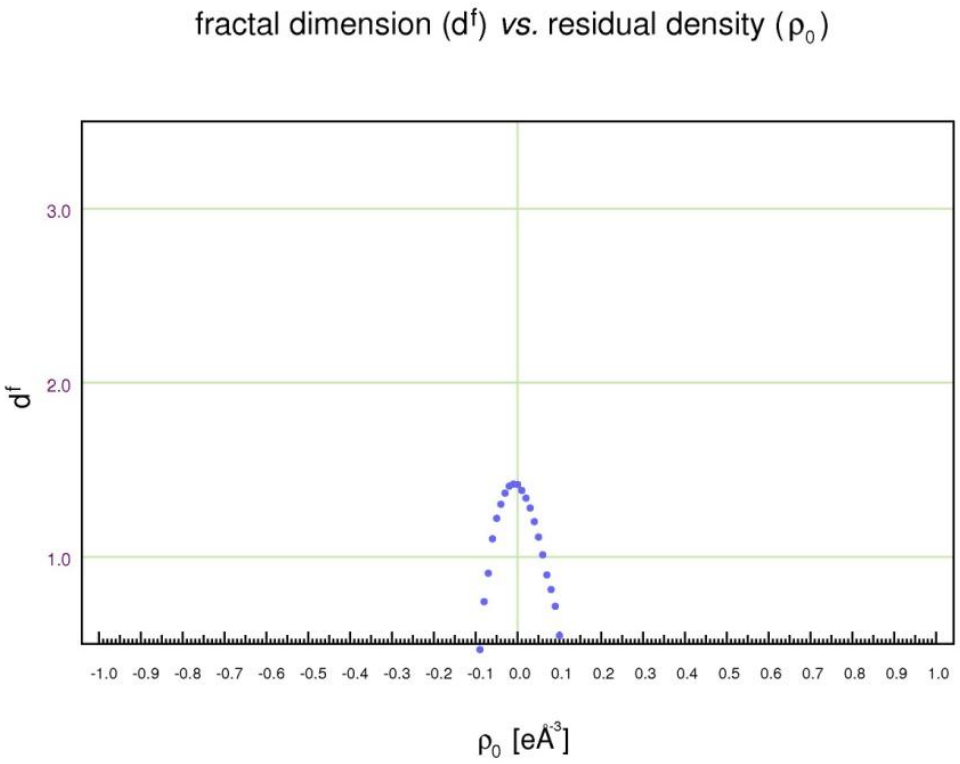


Figure 7S. Fractional dimension vs. residual density for **PAO** - the O(1)C(1)C(2) plane.

Table 1S. Minima and maxima of residual density for **PAO**.

Highest peaks	*Height / e·Å^{-3}*	*Remarks*
1	0.2	is 0.50 A from C(22)
2	0.17	is 0.35 A from C(1)
3	0.17	Random position
4	0.17	is 0.49 A from C(14)
5	0.16	is 0.37 A from C(3)
6	0.16	is 0.61 A from C(17)
7	0.15	Random position
8	0.15	is 0.70 A from C(2)
9	0.15	is 0.46 A from C(14)
10	0.15	is 0.41 A from C(18)
Deepest holes	*Height / e·Å^{-3}*	*Remarks*
1	-0.13	Random position
2	-0.12	Random position
3	-0.12	Random position
4	-0.12	Random position
5	-0.12	Random position
6	-0.12	Random position
7	-0.12	Random position
8	-0.12	Random position
9	-0.11	Random position
10	-0.11	Random position

Table 2S. Selected topological parameters (ρ_{BCP}) and $L_{(BCP)}$ at BCPs for **PAO** (ρ – electron density, L – negative Laplacian, d_1 – distance from the first atom to BCP, d_2 – distance from BCP to the second atom).

Bond	$\rho_{(BCP)}$ / e·Å^{-3}	$L_{(BCP)}$ / e·Å^{-5}	d_1 / Å	d_2 / Å
O(1) -C(1)	2.965(18)	-27.16(9)	0.7878	0.4347
O(13) -C(19)	2.058(16)	-15.91(6)	0.8190	0.5611
O(13) -C(21)	2.070(16)	-15.95(5)	0.8247	0.5582
N(8) -C(5)	2.038(14)	-14.49(4)	0.8180	0.6056
N(8) -C(18)	2.121(14)	-18.00(5)	0.8199	0.5826
N(8) -C(20)	2.025(14)	-14.17(5)	0.8181	0.5855
C(1) -C(2)	1.899(11)	-15.15(3)	0.7517	0.7409
C(1) -C(22)	1.829(11)	-13.67(3)	0.7787	0.7286
C(2) -C(3)	2.179(12)	-18.44(4)	0.6943	0.7035
C(2) -C(7)	2.186(12)	-18.80(4)	0.7030	0.6997
C(3) -C(4)	2.165(12)	-17.80(4)	0.7022	0.6907
C(3) -H(3)	1.925(33)	-22.5(1)	0.7225	0.3608
C(4) -C(5)	2.242(12)	-19.35(4)	0.6859	0.7097
C(4) -H(4)	1.922(33)	-20.4(1)	0.7099	0.3738
C(5) -C(6)	2.177(12)	-18.70(4)	0.7015	0.6988
C(6) -C(7)	2.224(12)	-19.79(4)	0.6982	0.6908
C(6) -H(6)	1.884(34)	-19.7(1)	0.7219	0.3616
C(7) -H(7)	1.878(34)	-20.5(1)	0.7184	0.3653
C(9) -C(10)	2.129(12)	-17.38(4)	0.6849	0.7107
C(9) -C(20)	2.157(12)	-17.55(4)	0.6717	0.7265
C(9) -H(9)	1.882(33)	-19.7(1)	0.7231	0.3603
C(10) -C(11)	2.239(12)	-20.62(4)	0.6951	0.6943
C(10) -H(10)	1.883(36)	-19.9(1)	0.7262	0.3579
C(11) -C(12)	2.139(12)	-17.33(4)	0.7071	0.6871
C(11) -H(11)	1.881(35)	-19.5(1)	0.7176	0.3657
C(12) -C(21)	2.242(12)	-20.21(4)	0.6740	0.7117
C(12) -H(12)	1.907(33)	-21.2(1)	0.7211	0.3634
C(14) -C(15)	2.134(12)	-17.94(4)	0.7009	0.6952
C(14) -C(19)	2.262(12)	-21.05(4)	0.6547	0.7310
C(14) -H(14)	1.864(34)	-20.2(1)	0.7180	0.3655
C(15) -C(16)	2.183(12)	-18.81(4)	0.7145	0.6762
C(15) -H(15)	1.870(36)	-20.2(1)	0.7278	0.3618
C(16) -C(17)	2.189(12)	-19.42(4)	0.6969	0.6996
C(16) -H(16)	1.865(35)	-19.8(1)	0.7295	0.3540
C(17) -C(18)	2.164(12)	-18.20(4)	0.6846	0.7126
C(17) -H(17)	1.862(33)	-19.9(1)	0.7192	0.3648
C(18) -C(19)	2.205(12)	-20.66(4)	0.7063	0.6956
C(20) -C(21)	2.181(12)	-20.13(4)	0.6812	0.7219
C(22) -H(22A)	1.882(46)	-19.8(1)	0.6952	0.3669
C(22) -H(22B)	1.784(53)	-17.6(2)	0.7114	0.3496
C(22) -H(22C)	1.717(49)	-16.4(2)	0.7207	0.3432

Table 3S. The integrated atomic charges (*Q*) for **PAO**. *I* stands for the integrated Laplacian.

Atom	*Q* / *e*	*I* / *e*·Å^{-2}
Donor		
O(1)	-1.286	2.50E-04
C(1)	0.856	8.45E-04
C(2)	-0.036	-7.67E-04
C(3)	-0.014	5.84E-04
H(3)	0.139	-3.91E-04
C(4)	-0.082	-2.79E-05
H(4)	0.094	5.72E-04
C(5)	0.192	-4.38E-04
C(6)	-0.096	2.66E-04
H(6)	0.103	5.77E-04
C(7)	0.035	5.73E-04
H(7)	0.074	-1.78E-04
C(22)	-0.207	8.22E-04
H(22A)	0.088	1.98E-05
H(22B)	0.188	-8.78E-05
H(22C)	0.176	4.83E-04
Acceptor		
N(8)	-1.101	-7.11E-05
C(9)	-0.036	-1.88E-04
H(9)	0.108	1.16E-04
C(10)	-0.076	4.18E-04
H(10)	0.096	2.72E-04
C(11)	-0.067	1.47E-04
H(11)	0.084	3.28E-04
C(12)	-0.015	9.08E-04
H(12)	0.118	7.22E-04
C(13)	-0.015	9.08E-04
O(13)	-1.065	3.34E-04
C(14)	0.073	2.39E-04
H(14)	0.064	4.87E-05
C(15)	-0.080	9.89E-04
H(15)	0.104	-1.89E-03
C(16)	0.031	2.99E-04
H(16)	0.107	1.16E-04
C(17)	-0.062	-1.20E-04
H(17)	0.133	-4.35E-04
C(18)	0.319	-2.11E-04
C(19)	0.338	-5.89E-05
C(20)	0.319	-7.46E-04
C(21)	0.390	4.59E-06
SUM	-0.008	

Table 4S. Dipole moment values for the **PAO** molecule from Gaussian calculation and from topological analysis (TOPXD). The dipole moment from Gaussian03 for the **PAO3** geometry.

PAO				
	x	y	z	d [D]
Gaussian03 (yellow)	0,2856	0,1362	-2,3795	2,3935
TopXD (blue)	-1,0021	1,4488	-2,7810	3,2920

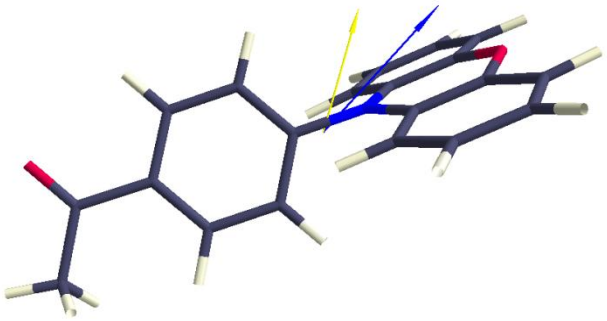


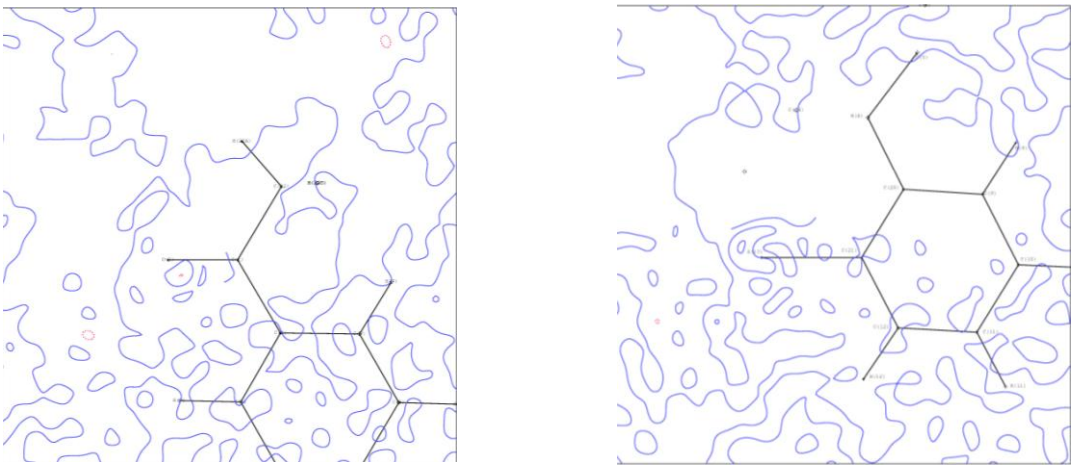
Table 5S. Cartesian coordinates for **PAO0, PAO8, PAO9** and **PAO12** used in theoretical calculations.

	PAO0			PAO8			PAO9			PAO12		
	X	Y	Z	X	Y	Z	X	Y	Z	X	Y	Z
O1	-5.53497	-0.12052	-1.23519	-5.64034	0.76284	0.65002	-5.56002	-1.26256	-0.27732	5.61474	-1.08582	-0.17405
O13	3.55189	0.01088	0.19065	3.47150	0.31170	0.51347	2.63644	0.07602	-1.36638	-2.71403	0.18952	1.28489
N8	0.73918	-0.00019	0.08318	0.72357	-0.07639	0.46468	0.69746	-0.01912	0.56133	-0.72696	-0.07749	-0.61859
C1	-4.99226	-0.01937	-0.15181	-5.01409	-0.06316	0.01084	-4.98320	-0.18774	-0.29036	4.95126	-0.17250	0.28550
C2	-3.49199	-0.01006	-0.05084	-3.52117	-0.12167	0.09839	-3.50995	-0.10467	-0.08609	3.47381	-0.11744	0.07417
C3	-2.74397	-0.12251	-1.23117	-2.85543	0.77920	0.94326	-2.77800	-1.28496	0.10482	2.85576	-1.13449	-0.66543
C4	-1.35630	-0.11911	-1.19174	-1.47737	0.76257	1.05643	-1.40953	-1.26697	0.30814	1.49059	-1.12761	-0.90189
C5	-0.69165	-0.00341	0.03314	-0.69998	-0.18905	0.37031	-0.69748	-0.05002	0.33036	0.67871	-0.10241	-0.38713
C6	-1.42570	0.10800	1.21346	-1.35817	-1.04052	-0.52833	-1.42573	1.13553	0.11808	1.29401	0.91897	0.35517
C7	-2.81768	0.10565	1.17087	-2.74609	-1.01950	-0.64060	-2.79848	1.10121	-0.08348	2.66444	0.90951	0.57669
C9	0.83009	-2.46267	-0.02915	0.54025	2.27964	-0.42880	1.44951	-2.33002	1.13408	-1.47155	-2.44397	-0.95103
C10	1.58304	-3.63834	-0.05704	1.15264	3.49478	-0.73372	2.25842	-3.42423	0.83310	-2.27392	-3.50905	-0.54376
C11	2.97059	-3.58486	-0.02174	2.52521	3.65521	-0.57858	3.16042	-3.35912	-0.22848	-3.19453	-3.34036	0.48737
C12	3.60629	-2.34357	0.04697	3.28848	2.57116	-0.15577	3.28409	-2.18772	-0.97194	-3.33623	-2.09481	1.09395
C14	3.58958	2.36243	-0.00167	3.90802	-1.94125	-0.02222	3.14995	2.35803	-0.88036	-3.09068	2.47057	0.69468
C15	2.94495	3.59665	-0.10590	3.48375	-3.25633	-0.19057	2.94748	3.49142	-0.09664	-2.78137	3.57236	-0.09896
C16	1.55734	3.63850	-0.15369	2.12486	-3.53786	-0.11989	2.03078	3.46442	0.95507	-1.81213	3.46778	-1.09818
C18	1.44617	1.21759	0.01380	1.59342	-1.17470	0.16213	1.44225	1.19039	0.39443	-1.41422	1.16574	-0.48270
C17	0.81301	2.45831	-0.09844	1.19471	-2.51506	0.06579	1.29010	2.31221	1.20958	-1.13990	2.26503	-1.29746
C19	2.85002	1.19325	0.06073	2.97854	-0.93408	0.18790	2.40166	1.21637	-0.62192	-2.40445	1.27836	0.49518
C20	1.45443	-1.21426	0.03862	1.28016	1.20242	0.07218	1.51512	-1.17568	0.35330	-1.55117	-1.20862	-0.30599
C21	2.85824	-1.17865	0.08263	2.66843	1.36812	0.14865	2.46953	-1.10506	-0.66709	-2.52461	-1.04355	0.68933
C22	-5.81313	0.09911	1.11780	-5.73485	-1.05161	-0.88777	-5.76412	1.09621	-0.51775	5.61764	0.93234	1.08681
H3	-3.27449	-0.21003	-2.17135	-3.44501	1.49351	1.50470	-3.31062	-2.22824	0.08831	3.47525	-1.92649	-1.06850
H4	-0.77672	-0.20468	-2.10359	-0.98549	1.45657	1.72665	-0.89073	-2.20534	0.43115	1.06110	-1.91605	-1.50029
H6	-0.90051	0.19521	2.15720	-0.79737	-1.69341	-1.17903	-0.91983	2.08902	0.09152	0.69471	1.71823	0.77023
H7	-3.37020	0.19251	2.09825	-3.21324	-1.69938	-1.34280	-3.31207	2.04101	-0.24792	3.09582	1.71134	1.16394
H9	-0.25022	-2.51657	-0.05532	-0.52438	2.18635	-0.57785	0.76166	-2.36801	1.96942	-0.79094	-2.57487	-1.77983
H10	1.07173	-4.59238	-0.10712	0.54281	4.31221	-1.09979	2.18718	-4.32364	1.43291	-2.18384	-4.46565	-1.04435
H11	3.56060	-4.49291	-0.04480	3.00227	4.60091	-0.80558	3.78750	-4.21100	-0.46337	-3.81895	-4.16700	0.80478
H12	4.68592	-2.26010	0.08148	4.36616	2.63003	-0.06377	4.00393	-2.09532	-1.77598	-4.06576	-1.91982	1.87530
H14	4.66971	2.28791	0.03734	4.95827	-1.67654	-0.01094	3.87925	2.34055	-1.68097	-3.84908	2.51823	1.46663
H15	3.52832	4.50819	-0.15004	4.20805	-4.04692	-0.34425	3.52279	4.38822	-0.29399	-3.30696	4.50741	0.05463
H16	1.03949	4.58665	-0.23749	1.77186	-4.55962	-0.19490	1.89611	4.33774	1.58200	-1.58430	4.32036	-1.72680
H17	-0.26731	2.50216	-0.14017	0.15750	-2.78399	0.18320	0.58132	2.27910	2.02803	-0.38395	2.17218	-2.06832
H22A	-5.59618	1.03692	1.63773	-5.53015	-2.08142	-0.58069	-5.39982	1.62579	-1.40298	5.20541	0.98520	2.09882
H22B	-6.86907	0.06854	0.85501	-6.80523	-0.86253	-0.82670	-6.81472	0.84538	-0.65465	6.68542	0.72729	1.14277
H22C	-5.58720	-0.71906	1.80793	-5.40826	-0.94729	-1.92675	-5.66237	1.77318	0.33565	5.46022	1.90742	0.61647

Table 6S. Integrated atomic charges for **PAO0, PAO2, PAO4, PAO8, PAO9** and **PAO12**.

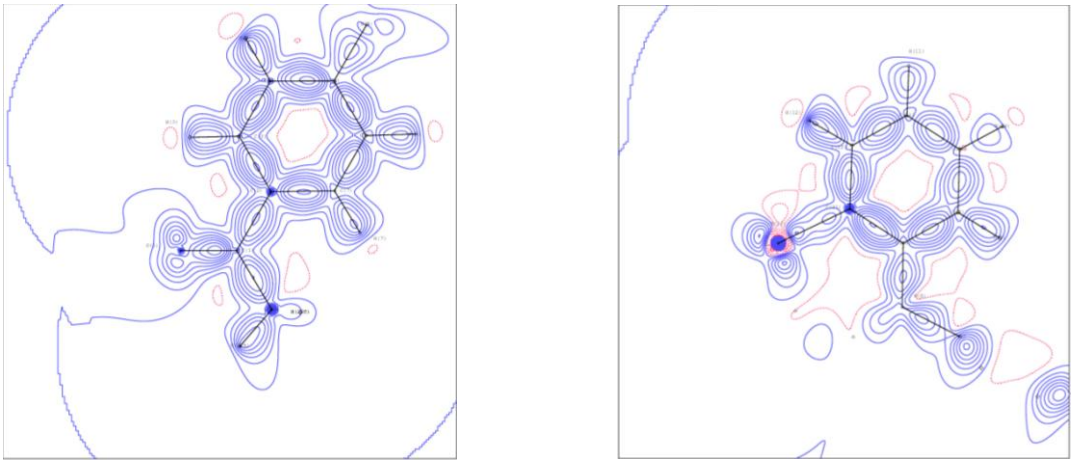
	PAO0		**PAO2**		**PAO4**		**PAO8**		**PAO9**		**PAO12**	
	rho [r] integral	charge	rho [r] integral	charge	rho [r] integral	charge	rho [r] integral	charge	rho [r] integral	charge	rho [r] integral	charge
O1	9.035	-1.035	9.193	-1.193	9.171	-1.171	9.144	-1.144	9.152	-1.152	9.124	-1.124
O13	9.023	-1.023	8.993	-0.993	8.967	-0.967	9.018	-1.018	9.117	-1.117	9.034	-1.034
N8	8.167	-1.167	8.103	-1.103	8.083	-1.083	8.163	-1.163	8.122	-1.122	8.158	-1.158
C1	5.027	0.973	4.962	1.039	4.981	1.019	5.019	0.981	4.971	1.030	4.965	1.035
C2	6.067	-0.066	6.008	-0.008	6.031	-0.031	6.005	-0.005	6.051	-0.051	6.026	-0.026
C3	5.991	0.009	5.989	0.011	6.013	-0.013	6.049	-0.049	5.980	0.020	5.980	0.020
C4	5.961	0.039	5.962	0.038	5.959	0.041	5.983	0.017	6.058	-0.058	5.998	0.002
C5	5.653	0.347	5.632	0.368	5.621	0.379	5.647	0.353	5.650	0.351	5.635	0.365
C6	5.920	0.080	5.994	0.006	6.016	-0.016	6.026	-0.026	5.979	0.021	5.966	0.034
C7	6.025	-0.025	5.991	0.009	5.991	0.009	6.010	-0.010	6.032	-0.032	5.970	0.030
C9	6.001	-0.001	6.071	-0.071	6.070	-0.070	5.981	0.019	5.987	0.013	5.990	0.010
C10	6.005	-0.005	6.124	-0.124	6.123	-0.123	6.006	-0.006	5.986	0.014	5.987	0.013
C11	6.005	-0.005	6.058	-0.058	6.028	-0.028	5.996	0.004	5.997	0.003	6.033	-0.033
C12	5.972	0.028	5.993	0.007	5.976	0.024	5.973	0.027	5.965	0.035	5.986	0.014
C14	6.001	-0.001	6.032	-0.032	5.966	0.035	5.969	0.031	5.993	0.007	6.048	-0.048
C15	5.975	0.025	5.987	0.013	6.006	-0.006	6.001	-0.001	6.043	-0.043	6.045	-0.045
C16	6.018	-0.018	6.063	-0.063	5.988	0.012	5.952	0.048	5.986	0.014	6.010	-0.010
C17	6.029	-0.029	6.013	-0.013	5.986	0.014	6.038	-0.038	6.011	-0.011	5.967	0.033
C18	5.662	0.338	5.622	0.378	5.651	0.349	5.740	0.260	5.746	0.254	5.689	0.311
C19	5.568	0.432	5.507	0.493	5.531	0.469	5.510	0.490	5.539	0.461	5.531	0.469
C20	5.651	0.349	5.647	0.354	5.646	0.354	5.763	0.237	5.660	0.340	5.655	0.345
C21	5.601	0.399	5.524	0.476	5.506	0.494	5.545	0.455	5.545	0.455	5.540	0.460
C22	5.994	0.006	5.939	0.061	5.995	0.005	5.969	0.031	5.975	0.025	5.982	0.018
H3	0.976	0.025	0.929	0.071	0.929	0.071	0.938	0.062	0.969	0.031	0.948	0.052
H4	0.955	0.045	0.981	0.019	0.968	0.032	0.963	0.037	0.978	0.022	0.983	0.017
H6	0.985	0.016	0.963	0.038	0.962	0.038	0.969	0.031	1.000	0.000	0.976	0.024
H7	0.929	0.071	0.985	0.015	0.980	0.020	0.984	0.016	0.993	0.007	1.006	-0.006
H9	0.978	0.022	0.984	0.016	0.980	0.020	0.978	0.023	0.964	0.036	0.983	0.017
H10	0.985	0.015	0.994	0.006	0.993	0.007	0.986	0.014	0.977	0.024	0.995	0.005
H11	0.988	0.012	0.995	0.005	0.994	0.006	0.989	0.011	0.977	0.023	0.976	0.024
H12	0.956	0.044	0.992	0.008	0.989	0.011	0.952	0.048	0.959	0.042	0.960	0.040
H14	0.989	0.011	0.970	0.030	0.965	0.035	0.987	0.013	0.954	0.046	0.958	0.042
H15	0.995	0.005	0.988	0.012	0.997	0.003	0.965	0.035	0.980	0.021	0.981	0.019
H16	0.990	0.010	1.008	-0.008	0.983	0.017	1.002	-0.002	0.980	0.020	0.983	0.017
H17	0.985	0.016	0.985	0.015	0.992	0.008	0.976	0.024	0.966	0.034	0.966	0.034
H22A	0.971	0.029	0.968	0.032	0.966	0.034	0.988	0.012	0.957	0.043	0.957	0.043
H22B	0.988	0.012	1.012	-0.012	0.992	0.008	0.995	0.005	0.998	0.002	0.997	0.003
H22C	0.991	0.009	0.989	0.012	0.991	0.009	0.992	0.008	0.998	0.002	1.000	0.000
SUM		-0.011		-0.146		0.015		-0.169		-0.193		0.012

PAS



(*a*) (*b*)

Figure 8S. Residual density maps for **PAS** molecule: (*a*) the O(1)C(1)C(2) plane; (*b*) the S(13)C(20)C(21) plane. Blue solid line – the positive values, red dashed lines – the negative ones. Contours at ± n·0.1 e·Å^{-3} (n = 1, 2, …).



(*a*) (*b*)

Figure 9S. Static deformation density maps for **PAS**: (*a*) the O(1)C(1)C(2) plane; (*b*) the O(13)C(20)C(21) plane. Blue solid line – the positive values, red dashed lines – the negative ones. Contours at ± n·0.1 e·Å^{-3} (n =0, 1, 2, …).

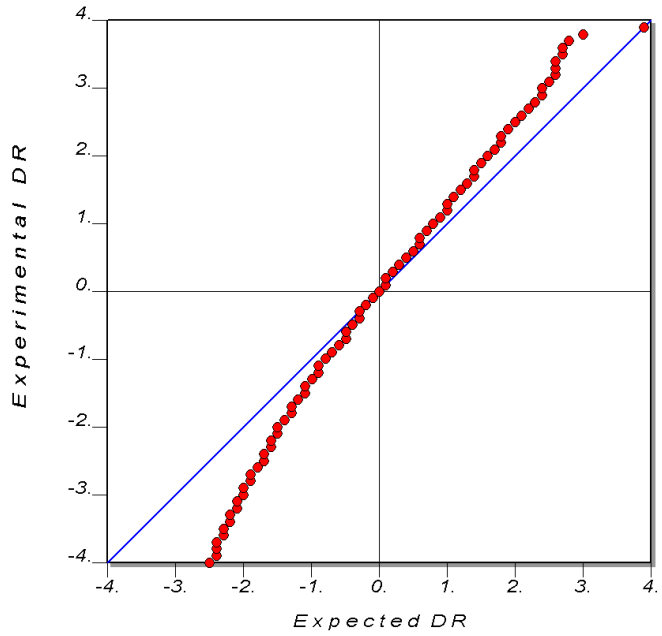


Figure 10. Normal probability plot for final multipole refinement of **PAS**.

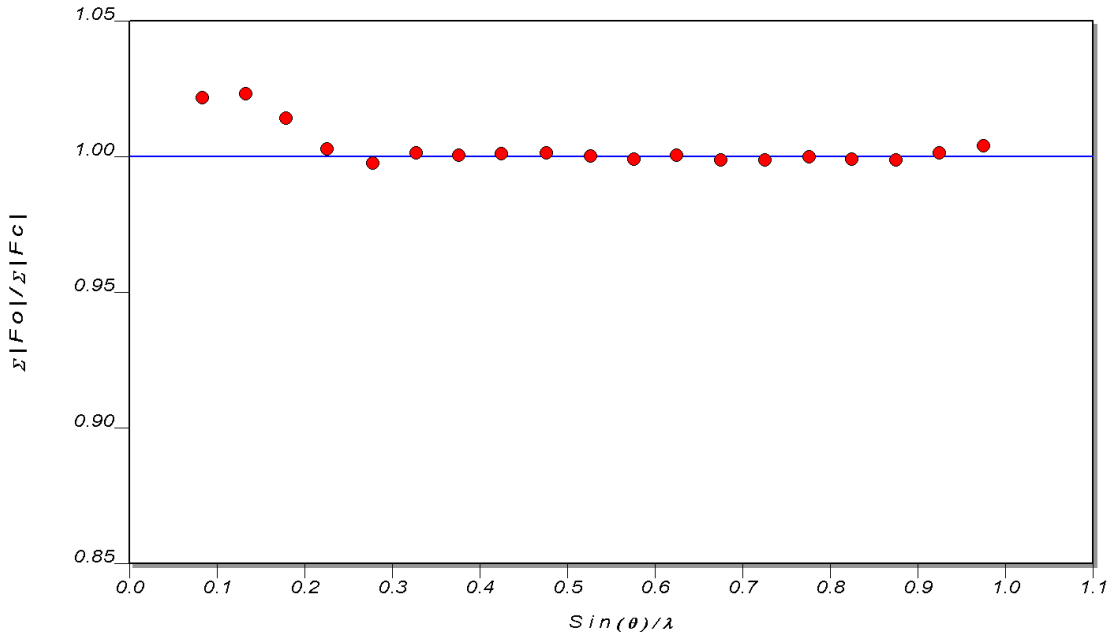


Figure 11S. Scale plot for final multipole refinement of **PAS**.

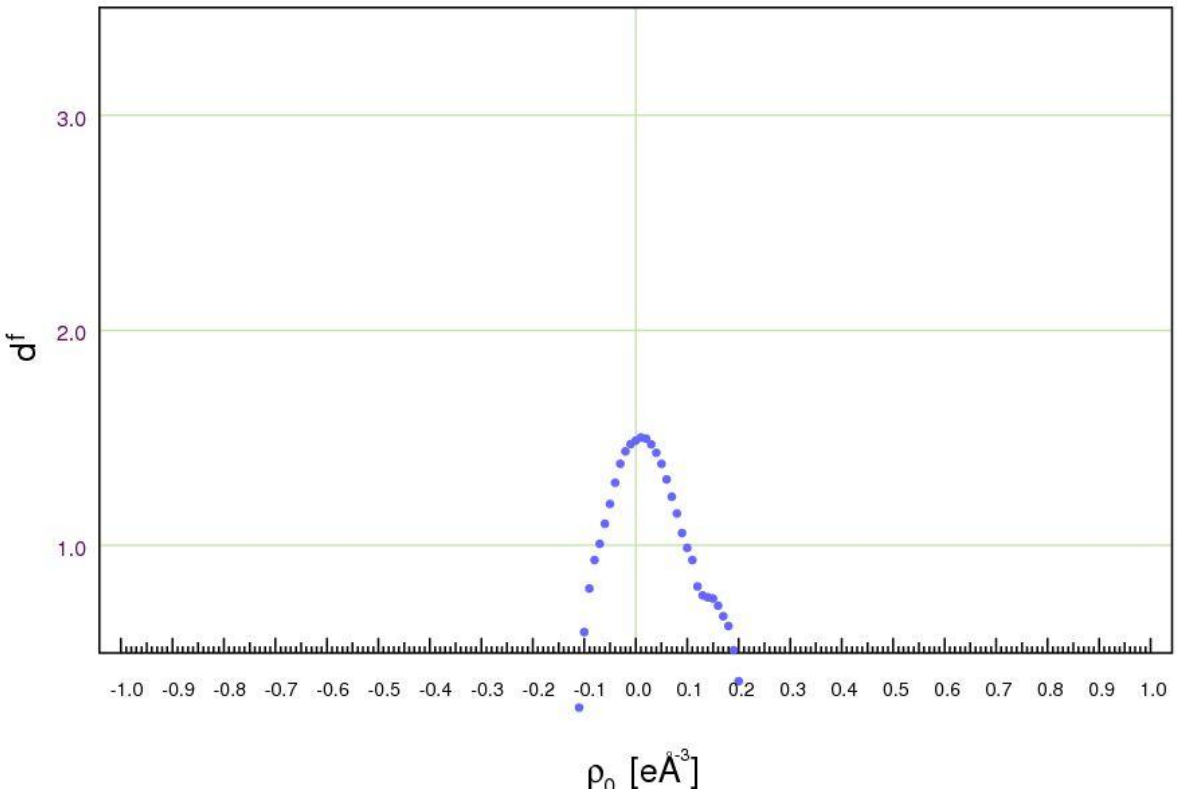


Figure 12S. Fractional dimension vs. residual density for **PAS**, the S(13)C(20)C(21) plane

Table 7S. Minima and maxima of residual density (**PAS**).

Highest peaks	**Height / e·Å^{-3}**	**Remarks**
1	0.26	is 0.41 A from S(13)
2	0.18	is 0.37 A from C(1)
3	0.18	is 0.89 A from S(13)
4	0.16	is 0.37 A from O(1)
5	0.14	Random position
6	0.13	is 0.47 A from C(14)
7	0.13	is 0.49 A from C(9)
8	0.13	is 0.41 A from C(11)
9	0.13	is 0.37 A from C(17)
10	0.13	is 1.02 A from S(13)
Deepest holes	Height / e·Å–3	Remarks
1	-0.14	is 1.02 A from S(13)
2	-0.13	is 0.87 A from S(13)
3	-0.12	Random position
4	-0.11	is 0.46 A from S(13)
5	-0.11	Random position
6	-0.11	Random position
7	-0.11	Random position
8	-0.11	Random position
9	-0.10	Random position
10	-0.10	Random position

Table 8S. Selected topological parameters (ρ_{BCP}) and $L(_{BCP})$] at BCPs for **PAS** (ρ – electron density, L – negative Laplacian, d_1 – distance from the first atom to BCP, d_2 – distance from BCP to the second atom).

Bond	ρ(BCP) / e·Å^{-3}	L(rBCP) / e·Å^{-5}	d1 / Å	d2 / Å
S(13) -C(19)	1.333(15)	-3.69(3)	0.9127	0.8461
S(13) -C(21)	1.321(15)	-3.96(3)	0.9169	0.8420
O(1) -C(1)	2.929(16)	-22.50(10)	0.8000	0.4213
N(8) -C(5)	1.974(13)	-13.81(4)	0.8193	0.6186
N(8) -C(18)	2.032(13)	-16.81(5)	0.8081	0.6035
N(8) -C(20)	2.013(13)	-16.33(5)	0.8107	0.6025
C(1) -C(2)	1.867(12)	-14.38(4)	0.7415	0.7529
C(1) -C(22)	1.835(12)	-15.15(4)	0.76115	0.74515
C(2) -C(3)	2.190(13)	-21.09(4)	0.71525	0.68861
C(2) -C(7)	2.206(12)	-19.90(4)	0.69813	0.69822
C(3) -C(4)	2.227(13)	-21.00(4)	0.68941	0.69862
C(3) -H(3)	1.847(21)	-19.25(7)	0.74386	0.3392
C(4) -C(5)	2.201(13)	-20.60(4)	0.67434	0.7274
C(4) -H(4)	1.848(22)	-19.66(7)	0.7402	0.3434
C(5) -C(6)	2.279(13)	-22.41(4)	0.6991	0.6894
C(6) -C(7)	2.223(13)	-20.21(4)	0.7182	0.6763
C(6) -H(6)	1.878(22)	-19.82(7)	0.7316	0.3515
C(7) -H(7)	1.877(24)	-20.45(8)	0.7343	0.3494
C(9) -C(10)	2.164(13)	-19.36(4)	0.6784	0.7161
C(9) -C(20)	2.136(12)	-18.53(4)	0.7040	0.6974
C(9) -H(9)	1.872(2)	-19.38(7)	0.7467	0.3363
C(10) -C(11)	2.209(13)	-19.54(4)	0.7077	0.6826
C(10) -H(10)	1.787(22)	-18.15(7)	0.7271	0.3567
C(11) -C(12)	2.133(13)	-18.88(4)	0.7167	0.6754
C(11) -H(11)	1.793(23)	-17.43(7)	0.7214	0.3619
C(12) -C(21)	2.156(13)	-18.19(4)	0.6833	0.7108
C(12) -H(12)	1.864(24)	-20.05(8)	0.7335	0.3497
C(14) -C(15)	2.155(13)	-19.26(4)	0.6867	0.7074
C(14) -C(19)	2.183(13)	-18.68(4)	0.6795	0.7176
C(14) -H(14)	1.854(25)	-20.68(8)	0.7439	0.3402
C(15) -C(16)	2.319(14)	-21.43(4)	0.6808	0.7099
C(15) -H(15)	1.816(36)	-17.73(7)	0.7331	0.3516
C(16) -C(17)	2.121(12)	-18.04(4)	0.6926	0.7048
C(16) -H(16)	1.876(23)	-20.21(8)	0.7319	0.3517
C(17) -C(18)	2.121(12)	-18.29(4)	0.6914	0.7109
C(17) -H(17)	1.876(23)	-20.21(8)	0.7575	0.3256
C(18) -C(19)	2.185(13)	-19.95(4)	0.6848	0.7222
C(20) -C(21)	2.179(13)	-19.13(4)	0.6909	0.7126
C(22) -H(22A)	1.833(22)	-18.45(7)	0.7256	0.3350
C(22) -H(22B)	1.844(23)	-19.24(8)	0.7236	0.3362
C(22) -H(22C)	1.805(25)	-18.44(8)	0.7096	0.3498

Table 9S. PAS – the integrated atomic charges (*Q*). *I* stands for the integrated Laplacian.

Atom	*Q* / *e*	*I* / *e*·Å^{-2}
O(1)	-1.034	3.19E-04
C(1)	0.933	6.62E-04
C(2)	-0.123	4.53E-04
C(3)	-0.015	5.12E-04
H(3)	0.128	-6.80E-04
C(4)	-0.021	6.81E-04
H(4)	0.127	-1.38E-04
C(5)	0.195	9.73E-04
C(6)	-0.126	9.77E-04
H(6)	0.104	-1.44E-04
C(7)	-0.069	1.43E-04
H(7)	0.089	4.25E-04
C(22)	-0.138	5.94E-04
H(22A)	0.093	1.35E-04
H(22B)	0.088	8.11E-05
H(22C)	0.083	-8.02E-06
Acceptor		
S(13)	0.183	3.93E-05
N(8)	-0.844	-8.70E-06
C(9)	-0.144	1.72E-04
H(9)	0.124	1.16E-03
C(10)	-0.107	2.34E-05
H(10)	0.126	7.15E-04
C(11)	-0.027	-4.50E-04
H(11)	0.063	-4.22E-04
C(12)	-0.021	3.55E-05
H(12)	0.087	7.25E-04
C(14)	-0.064	4.89E-04
H(14)	0.160	6.18E-04
C(15)	-0.091	-3.09E-04
H(15)	0.100	7.96E-04
C(16)	-0.241	6.71E-04
H(16)	0.075	-9.38E-05
C(17)	-0.180	3.58E-04
H(17)	0.155	4.58E-04
C(18)	0.328	1.98E-04
C(19)	-0.130	1.90E-04
C(20)	0.291	4.03E-04
C(21)	-0.157	6.23E-04
SUM	0.003	

Table 10S. Dipole moment values for the **PAS** molecule from Gaussian calculation and from topological analysis from TOPXD. The dipole moment from Gaussian03 for **PAS0** geometry.

PAS				
	x	y	z	d[D}
Gaussian03 (yellow)	-0,2557	0,0238	1,5245	1,5460
TopXD (blue)	-0,6508	2,0340	0,6925	2,2455

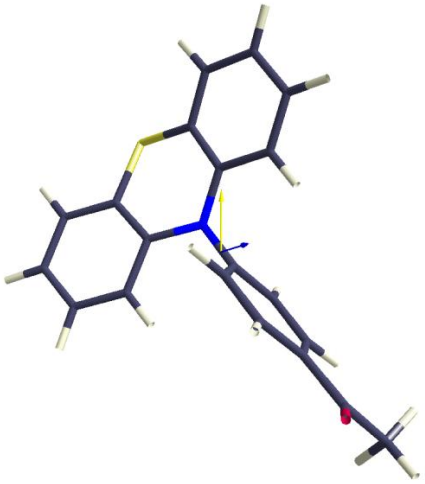


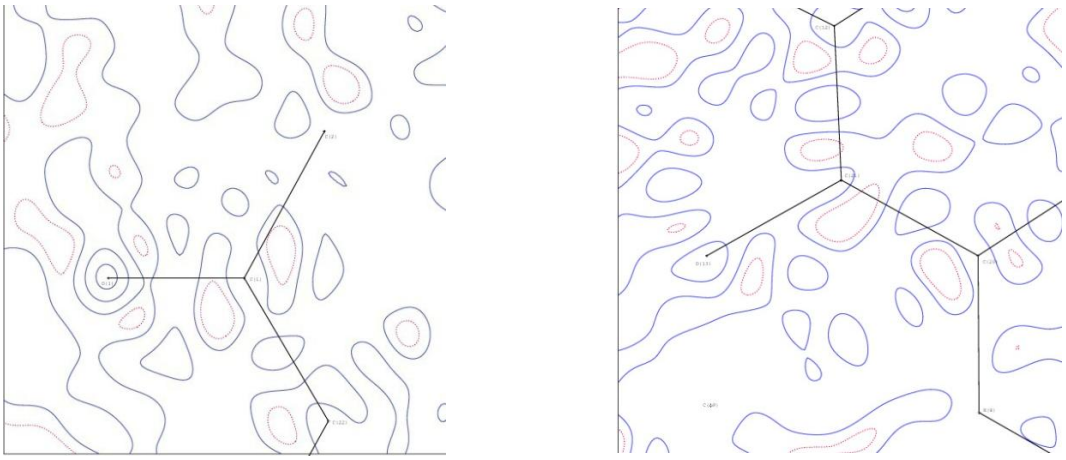
Table 11S. Cartesian coordinates for **PAS0, PAS5, PAS8** and **PAS13** used in theoretical calculations.

	PAS0			PAS5			PAS8			PAS13		
	X	Y	Z	X	Y	Z	X	Y	Z	X	Y	Z
S13	3.47806	0.00566	1.04948	2.79699	0.25497	1.56548	2.60062	0.21638	1.71858	2.24541	-0.04149	1.81325
O1	-5.71324	-0.01531	-1.04458	-5.76817	-0.85777	-0.43051	-5.72624	-1.22839	-0.03190	-5.50584	-1.25052	0.68735
N8	0.61609	-0.00113	0.06378	0.62189	-0.08783	-0.50411	0.58746	-0.07024	-0.43233	0.63781	0.03376	-0.70961
C1	-5.12820	-0.00383	0.02159	-5.07080	-0.16660	0.29006	-5.10823	-0.21768	0.25891	-5.00032	-0.19155	0.35402
C2	-3.62572	-0.00278	0.06447	-3.58575	-0.12462	0.10473	-3.62809	-0.15052	0.09942	-3.54112	-0.09290	0.06942
C3	-2.92405	-0.01571	-1.14919	-3.01377	-0.88516	-0.92206	-2.94216	-1.27606	-0.37689	-2.73843	-1.23276	0.21895
C4	-1.53604	-0.01545	-1.16378	-1.64331	-0.87719	-1.14288	-1.56924	-1.26875	-0.55724	-1.37677	-1.19636	-0.02540
C5	-0.82124	-0.00207	0.03969	-0.79552	-0.11882	-0.32334	-0.80954	-0.12313	-0.24889	-0.75337	-0.00661	-0.45094
C6	-1.51052	0.01091	1.25100	-1.36567	0.65293	0.69962	-1.49395	1.00606	0.23986	-1.55108	1.14281	-0.59034
C7	-2.90317	0.01058	1.26320	-2.73790	0.65187	0.90730	-2.87042	0.98789	0.40640	-2.91401	1.09339	-0.33328
C9	0.64633	-2.37614	-0.60175	1.22398	-2.42991	-1.04159	1.37810	-2.28674	-1.22315	1.39015	-2.15418	-1.53846
C10	1.32894	-3.58209	-0.74928	2.00816	-3.55818	-0.81282	2.20778	-3.39300	-1.05424	2.11222	-3.33073	-1.36036
C11	2.68055	-3.67307	-0.43480	3.05151	-3.51450	0.10743	3.14042	-3.41798	-0.01910	2.88033	-3.51086	-0.20912
C12	3.34022	-2.54666	0.05156	3.30734	-2.33257	0.79585	3.26769	-2.32017	0.82756	2.93897	-2.51088	0.75742
C14	3.33032	2.55517	0.04467	2.94261	2.72106	0.32310	2.93613	2.67265	0.46211	2.85404	2.52439	0.96689
C15	2.66616	3.67701	-0.44615	2.49657	3.70057	-0.55955	2.62463	3.62545	-0.50365	2.79470	3.58776	0.07058
C16	1.31524	3.57920	-0.76176	1.44076	3.42285	-1.42797	1.65657	3.35124	-1.47143	2.06908	3.46502	-1.11395
C17	0.63764	2.37093	-0.61031	0.83853	2.16897	-1.41718	0.99113	2.12923	-1.46869	1.37889	2.28682	-1.38825
C18	1.29118	1.23669	-0.10947	1.25754	1.18662	-0.51303	1.26629	1.18450	-0.47748	1.37792	1.23939	-0.46585
C19	2.64845	1.35587	0.23900	2.31387	1.47497	0.36038	2.25053	1.45654	0.48141	2.14718	1.35024	0.70031
C20	1.29545	-1.23700	-0.10636	1.43340	-1.24979	-0.32006	1.43899	-1.21496	-0.32859	1.40829	-1.16445	-0.55509
C21	2.65343	-1.34957	0.24209	2.49674	-1.21437	0.59842	2.42115	-1.22214	0.67414	2.19797	-1.33911	0.58804
C22	-5.89886	0.00945	1.32763	-5.69445	0.66888	1.39343	-5.84299	0.99984	0.79472	-5.85768	1.05704	0.22633
H3	-3.49066	-0.02574	-2.07224	-3.66975	-1.46769	-1.55747	-3.51586	-2.16362	-0.61532	-3.20743	-2.15183	0.54922
H4	-0.99749	-0.02482	-2.10447	-1.23917	-1.43542	-1.97497	-1.08801	-2.16463	-0.91815	-0.78912	-2.09211	0.11997
H6	-0.94723	0.02107	2.17645	-0.72014	1.24385	1.33767	-0.94024	1.89623	0.50520	-1.10731	2.08099	-0.89080
H7	-3.41842	0.02071	2.21570	-3.14189	1.25132	1.71402	-3.35032	1.87775	0.79602	-3.48996	2.00317	-0.45398
H9	-0.40166	-2.32861	-0.86213	0.44467	-2.47333	-1.78733	0.68749	-2.24831	-2.05530	0.79030	-1.99712	-2.42728
H10	0.79480	-4.44759	-1.12414	1.81140	-4.46453	-1.37352	2.13608	-4.22608	-1.74360	2.08290	-4.10133	-2.12166
H11	3.21781	-4.60531	-0.56110	3.67374	-4.38522	0.27708	3.79122	-4.27489	0.10983	3.45131	-4.42191	-0.07244
H12	4.39253	-2.59497	0.30774	4.13178	-2.27246	1.49711	4.02771	-2.30658	1.60009	3.56061	-2.63215	1.63692
H14	4.38233	2.60880	0.30099	3.77093	2.92080	0.99323	3.70785	2.86650	1.19797	3.45674	2.59592	1.86486
H15	3.19958	4.61104	-0.57544	2.97856	4.67103	-0.57565	3.15088	4.57286	-0.51246	3.33959	4.49998	0.28431
H16	0.77799	4.44097	-1.14074	1.09642	4.17679	-2.12630	1.42914	4.08445	-2.23639	2.05029	4.27916	-1.82891
H17	-0.40975	2.31731	-0.87221	0.02957	1.94134	-2.10137	0.24217	1.90356	-2.21858	0.83004	2.16964	-2.31496
H22A	-6.96432	0.00616	1.10444	-6.77232	0.51638	1.38004	-6.90548	0.76869	0.85075	-6.88757	0.79827	0.46683
H22B	-5.65475	0.89808	1.91723	-5.47647	1.73136	1.25101	-5.69521	1.86614	0.14311	-5.81400	1.46197	-0.78903
H22C	-5.65320	-0.86599	1.93601	-5.30012	0.38122	2.37260	-5.47852	1.27098	1.78998	-5.51264	1.84021	0.90792

Table 12S. Integrated atomic charges for **PAS0, PAS5, PAS8** and **PAS13**.

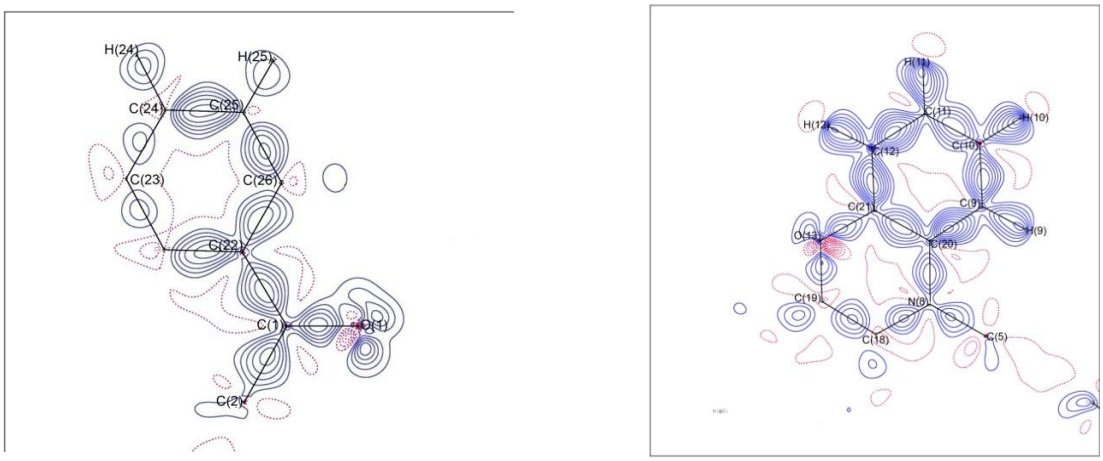
	PAS0		PAS5		PAS8		PAS13	
	rho [r] integral	charge	rho [r] integral	charge	rho [r] integral	charge	rho [r] integral	charge
O1	9.2665	-1.2665	9.0742	-1.0742	9.2696	-1.2696	9.0796	-1.0796
S13	15.6991	0.3009	15.809	0.191	15.8115	0.1885	15.369	0.631
N8	8.1602	-1.1602	8.0979	-1.0979	8.1289	-1.1289	8.097	-1.097
C1	4.9571	1.0429	5.0067	0.9933	4.8778	1.1222	4.9813	1.0187
C2	6.0713	-0.0713	6.0158	-0.0158	6.0783	-0.0783	6.0418	-0.0418
C3	5.9183	0.0817	6.0025	-0.0025	6.0186	-0.0186	5.9392	0.0608
C4	6.0578	-0.0578	5.9931	0.0069	5.9704	0.0296	6.0257	-0.0257
C5	5.6288	0.3712	5.6548	0.3452	5.5032	0.4968	5.631	0.369
C6	5.9711	0.0289	5.9823	0.0177	5.9223	0.0777	5.9736	0.0264
C7	6.0649	-0.0649	5.9842	0.0158	6.0164	-0.0164	5.9877	0.0123
C9	6.0161	-0.0161	5.9799	0.0201	5.9942	0.0058	5.9482	0.0518
C10	5.9918	0.0082	5.9964	0.0036	6.0076	-0.0076	6.0072	-0.0072
C11	0.9919	0.0081	5.9765	0.0235	6.0927	-0.0927	5.9798	0.0202
C12	6.0078	-0.0078	5.9766	0.0234	5.945	0.055	5.9586	0.0414
C14	5.9913	0.0087	6.0236	-0.0236	6.093	-0.093	6.0253	-0.0253
C15	5.9526	0.0474	5.985	0.015	5.972	0.028	6.0239	-0.0239
C16	5.9742	0.0258	6.0703	-0.0703	5.96	0.04	6.02	-0.02
C17	6.0381	-0.0381	5.9807	0.0193	5.9311	0.0689	5.9528	0.0472
C18	5.6226	0.3774	5.6533	0.3467	5.6287	0.3713	5.6424	0.3576
C19	6.1471	-0.1471	6.1123	-0.1123	6.1161	-0.1161	6.2063	-0.2063
C20	5.6192	0.3808	5.6945	0.3055	5.6492	0.3508	5.6886	0.3114
C21	6.1467	-0.1467	6.095	-0.095	6.1151	-0.1151	6.1132	-0.1132
C22	5.9632	0.0368	5.9505	0.0495	5.9041	0.0959	5.9636	0.0364
H3	0.9342	0.0658	0.9367	0.0633	0.9444	0.0556	0.9441	0.0559
H4	0.9622	0.0378	0.9865	0.0135	0.9803	0.0197	0.975	0.025
H6	0.9569	0.0431	0.9858	0.0142	0.9796	0.0204	1.0024	-0.0024
H7	0.9831	0.0169	0.9975	0.0025	0.9871	0.0129	0.9937	0.0063
H9	0.9792	0.0208	0.9819	0.0181	0.9718	0.0282	0.9653	0.0347
H10	0.9866	0.0134	0.9838	0.0162	0.9849	0.0151	0.9814	0.0186
H11	0.9842	0.0158	0.9802	0.0198	0.9812	0.0188	0.9804	0.0196
H12	0.9766	0.0234	0.9753	0.0247	0.9681	0.0319	0.9771	0.0229
H14	0.9758	0.0242	0.978	0.022	0.9877	0.0123	0.9694	0.0306
H15	0.9954	0.0046	0.9793	0.0207	0.974	0.026	0.9779	0.0221
H16	5.9902	0.0098	0.9802	0.0198	0.9733	0.0267	0.9813	0.0187
H17	0.9804	0.0196	0.9724	0.0276	0.966	0.034	0.9914	0.0086
H22A	0.9868	0.0132	0.9649	0.0351	0.9633	0.0367	0.9919	0.0081
H22B	0.9887	0.0113	1.0037	-0.0037	0.9999	1E-04	1.0008	-0.0008
H22C	0.991	0.009	0.9889	0.0111	1.0213	-0.0213	0.9986	0.0014
		0.071		0.1898		0.3113		0.6135

PBO



(*a*) (*b*)

Figure 13S. Residual density maps for the **PBO** molecule: (*a*) the O(1)C(1)C(2) plane; (*b*) the O(13)C(20)C(21) plane. Blue solid line – the positive values, red dashed lines – the negative ones. Contours at ± n·0.1 e·Å^{-3} (n = 1, 2, …).



(*a*) (*b*)

Figure 14S. Static deformation density maps for **PBO:** (*a*) the O(1)C(1)C(2) plane; (*b*) the O(13)C(20)C(21) plane. Blue solid line – the positive values, red dashed lines – the negative ones. Contours at ± n·0.1 e·Å^{-3} (n =0, 1, 2, …).

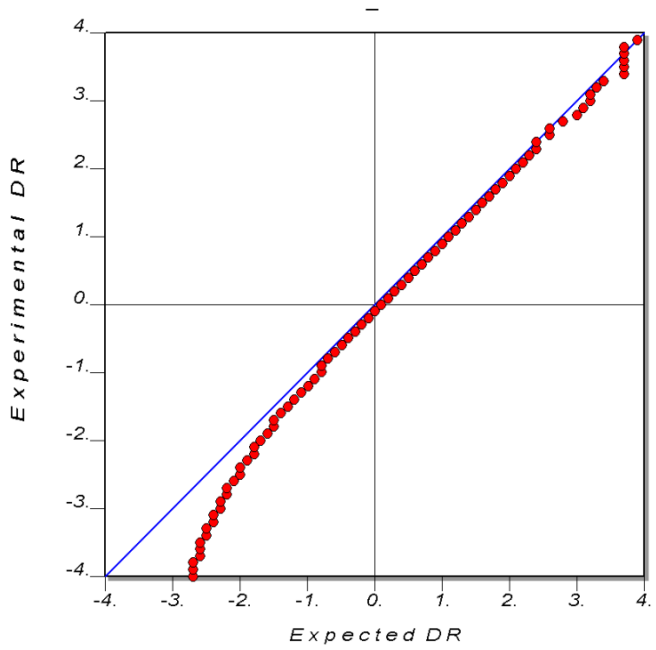


Figure 15S. Normal probability plot for final multipole refinement of **PBO**.

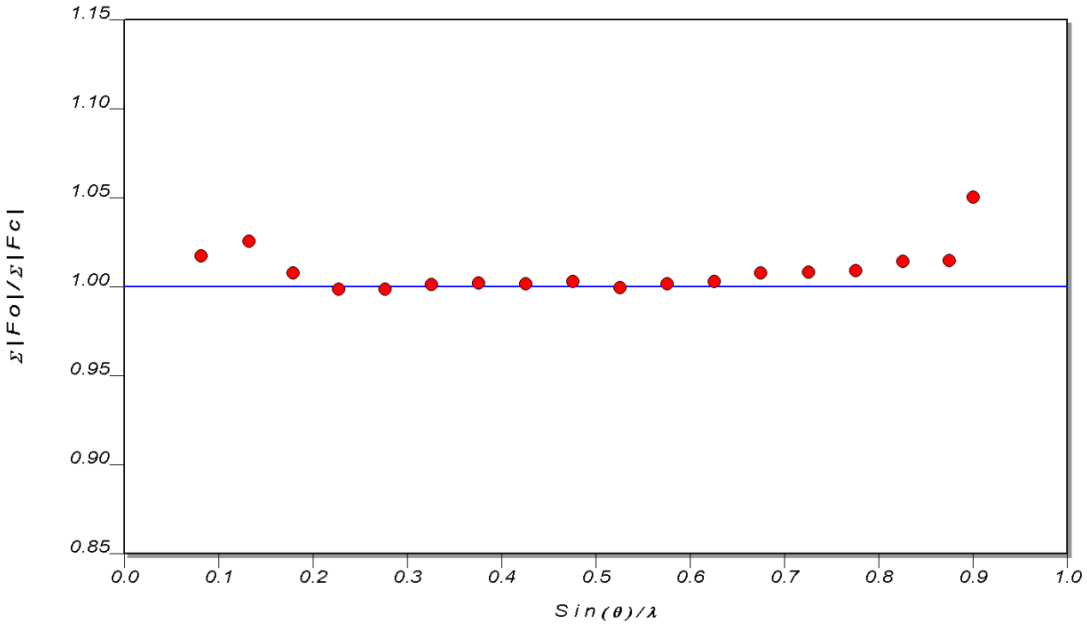


Figure 16S. Scale plot for final multipole refinement of **PBO**.

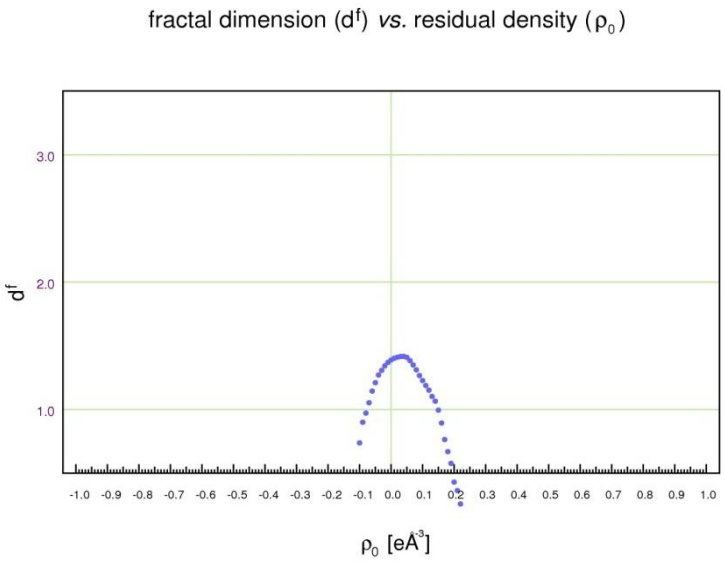


Figure 17S. Fractional dimension vs. residual density for **PBO** in the O(1)C(1)C(2) plane.

Table 13S. Minima and maxima of residual density for **PBO**.

Highest peaks	***Height / e·Å^{-3}***	***Remarks***
1	0.22	is 0.05 A from O(1)
2	0.21	is 0.75 A from C(11)
3	0.21	is 0.72 A from C(25)
4	0.20	is 0.67 A from C(14)
5	0.20	is 0.73 A from C(26)
6	0.20	is 0.65 A from C(9)
7	0.18	is 0.44 A from C(4)
8	0.18	Random position
9	0.18	is 0.46 A from C(5)
10	0.18	Random position
Deepest holes	*Height / e·Å^{-3}*	*Remarks*
1	-0.17	Random position
2	-0.17	Random position
3	-0.17	Random position
4	-0.16	Random position
5	-0.15	Random position
6	-0.15	Random position
7	-0.15	Random position
8	-0.15	Random position
9	-0.15	is 0.37 A from C(4)
10	-0.15	Random position

Table 14S. Selected topological parameters (ρ_{BCP}) and $L(_{BCP})$] at BCPs for **PBO** (ρ – electron density, L – negative Laplacian, d_1 – distance from the first atom to BCP, d_2 – distance from BCP to the second atom).

Bond	ρ(BCP) / e·Å^{-3}	L(BCP) / e·Å^{-5}	d_1 / Å	d_2 / Å
O(1) -C(1)	2.601(31)	-4.30(16)	0.8187	0.4079
O(13) -C(19)	2.002(26)	-20.73(11)	0.8776	0.5025
O(13) -C(21)	2.018(32)	-18.77(11)	0.8819	0.4994
N(8) -C(5)	1.835(22)	-14.99(13)	0.8661	0.5586
N(8) -C(18)	2.055(23)	-22.93(9)	0.8359	0.5693
N(8) -C(20)	2.023(24)	-21.02(10)	0.8593	0.5465
C(1) -C(2)	1.732(18)	-13.95(55)	0.7903	0.7069
C(1) -C(22)	1.824(18)	-17.16(5)	0.7580	0.7270
C(2) -C(3)	2.132 (20)	-20.50(6)	0.7242	0.6730
C(2) -C(7)	2.056(20)	-19.43(6)	0.6647	0.7317
C(3) -C(4)	2.045(19)	-17.66(6)	0.7087	0.6845
C(3) -H(3)	1.834(48)	-19.22(14)	0.7043	0.3805
C(4) -C(5)	2.048(20)	-18.42(6)	0.6999	0.6965
C(4) -H(4)	1.877(51)	-20.89(17)	0.7307	0.3531
C(5) -C(6)	2.110(20)	-20.13(6)	0.7301	0.6660
C(6) -C(7)	2.083(20)	-18.83(6)	0.7020	0.6911
C(6) -H(6)	1.781(47)	-17.55(13)	0.6982	0.3865
C(7) -H(7)	1.807(48)	-18.26(15)	0.7138	0.3694
C(9) -C(10)	2.117(21)	-21.42(7)	0.7370	0.6612
C(9) -C(20)	2.129(22)	-23.13(9)	0.5797	0.8177
C(9) -H(9)	1.776(49)	-17.87(15)	0.7124	0.3712
C(10) -C(11)	2.062(21)	-17.73(6)	0.6828	0.7047
C(10) -H(10)	1.816(54)	-20.51(17)	0.7275	0.3575
C(11) -C(12)	2.157(22)	-21.60(7)	0.6303	0.7635
C(11) -H(11)	1.909(52)	-21.64(17)	0.7329	0.3527
C(12) -C(21)	2.223(22)	-23.43(7)	0.6463	0.7384
C(12) -H(12)	1.844(61)	-20.35(15)	0.7141	0.3695
C(14) -C(15)	2.110(21)	-20.88(6)	0.6921	0.7037
C(14) -C(19)	2.169(21)	-22.07(7)	0.6567	0.7270
C(14) -H(14)	1.733(5)	-16.18(16)	0.7162	0.3673
C(15) -C(16)	2.076(21)	-19.05(6)	0.7155	0.6716
C(15) -H(15)	1.786(50)	-18.72(15)	0.7059	0.3781
C(16) -C(17)	2.090(25)	-18.61(8)	0.6944	0.7049
C(16) -H(16)	1.834(51)	-19.09(17)	0.7258	0.3572
C(17) -C(18)	2.077(20)	-20.14(6)	0.6861	0.7144
C(17) -H(17)	1.843(51)	-19.26(16)	0.7116	0.3716
C(18) -C(19)	2.080(20)	-20.40(6)	0.6971	0.7112
C(20) -C(21)	2.019(20)	-17.65(6)	0.7005	0.6991
C(22) -C(26)	2.037(20)	-18.57(6)	0.6992	0.7041
C(22) -C(27)	2.087(21)	-20.65(7)	0.7753	0.6265
C(23) -C(24)	1.992(20)	-17.57(7)	0.6395	0.7545
C(23) -C(27)	2.087(20)	-21.57(6)	0.7077	0.6876
C(23) -H(23)	1.819(50)	-20.29(17)	0.7346	0.3493

C(24)	-C(25)	2.066(20)	-19.27(6)	0.7265	0.6830
C(24)	-H(24)	1.830(51)	-20.34(16)	0.7215	0.3624
C(25)	-C(26)	2.166(21)	-23.39(6)	0.7092	0.6773
C(25)	-H(25)	1.809(47)	-19.40(13)	0.6916	0.3919
C(26)	-H(26)	1.793(48)	-16.39(14)	0.6984	0.3861
C(27)	-H(27)	1.801(47)	-18.57(14)	0.7076	0.3766

Table 15S. Integrated atomic charges (*Q*) for **PBO**. *I* stands for the integrated Laplacian values.

Atom	*Q / e*	*I / e·Å^{-2}*
Donor		
O(1)	-1.0719	5.00E-04
C(1)	1.0428	2.15E-03
C(2)	-0.0289	1.13E-04
C(3)	-0.0759	7.81E-04
H(3)	0.1028	2.77E-04
C(4)	-0.1981	-2.33E-04
H(4)	0.1592	-9.59E-05
C(5)	0.2268	-8.65E-05
C(6)	-0.0263	1.44E-03
H(6)	0.0790	6.33E-04
C(7)	-0.1555	-4.41E-04
H(7)	0.1298	1.70E-04
C(22)	-0.0796	4.00E-05
C(23)	0.0117	-3.73E-04
H(23)	0.2108	3.64E-04
C(24)	-0.1838	4.43E-04
H(24)	0.1793	-2.20E-04
C(25)	-0.0060	-4.14E-04
H(25)	0.1198	5.05E-04
C(26)	-0.0519	3.95E-04
H(26)	0.0733	-7.56E-05
C(27)	0.1428	-8.52E-04
H(27)	0.1154	1.67E-04
Acceptor		
N(8)	-1.0599	4.60E-04
C(9)	0.0519	7.13E-04
H(9)	0.1307	1.01E-03
C(10)	0.0131	3.93E-04
H(10)	0.1505	1.67E-03
C(11)	-0.0793	4.20E-04
H(11)	0.1343	1.26E-03
C(12)	-0.2970	1.47E-03
H(12)	0.1386	6.22E-04
O(13)	-1.0650	-3.74E-04
C(14)	-0.1171	9.09E-05
H(14)	0.1665	-1.13E-04
C(15)	-0.0980	4.38E-04
H(15)	0.1412	1.74E-04
C(16)	-0.0977	5.41E-04
H(16)	0.1028	-2.08E-04
C(17)	-0.1038	8.33E-04
H(17)	0.0989	-3.84E-04

C(18)	0.3116	1.11E-03
C(19)	0.3831	1.19E-03
C(20)	0.1077	-2.31E-03
C(21)	0.2905	1.34E-03

Table 16S. Dipole moment valuesfor **PBO** molecule from Gaussian calculation and from topological analysis by using TOPXD. The dipole moment from Gaussian03 for the **PBO0** geometry.

Dipole moment				
	x	y	z	d[D]
Gaussian03 (yellow)	-0.6273	2.6976	1.1183	2.9869
TopXD (blue)	2.9374	2.0194	4.9568	6.1055

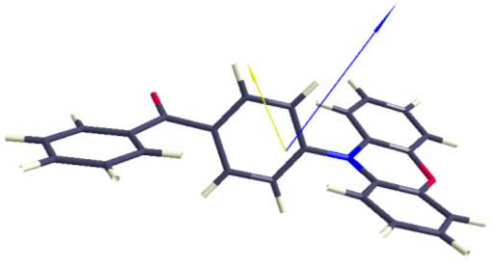


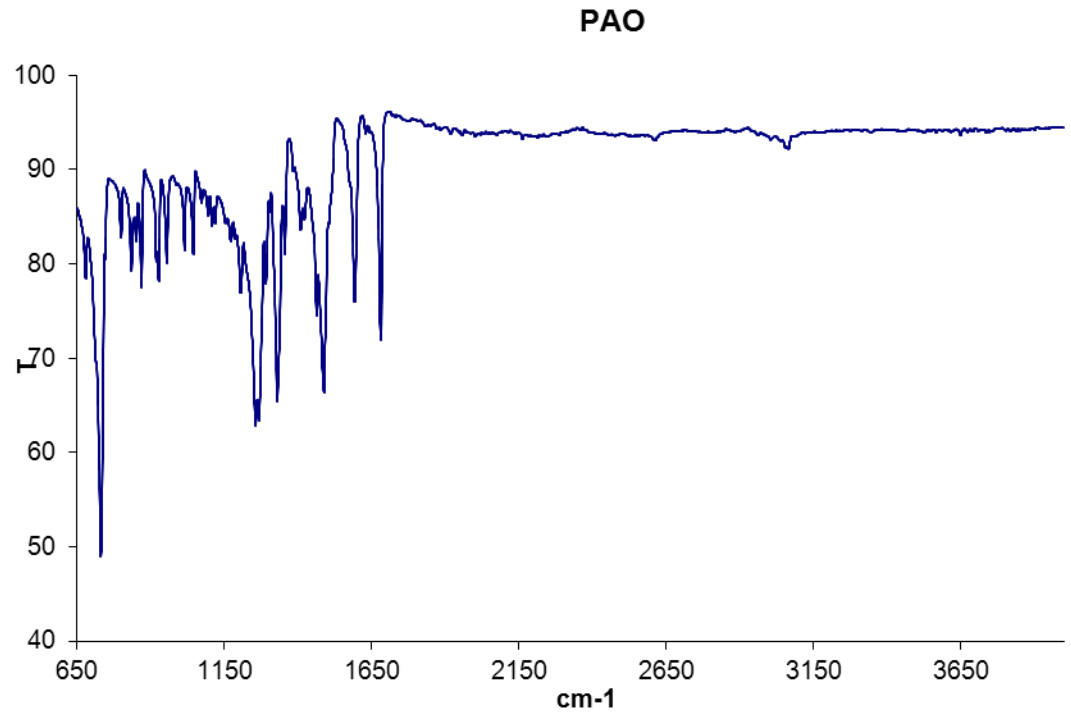
Table 17S. Cartesian coordinates for **PBO0, PBO8, PBO9** and **PBO12** used in theoretical calculations.

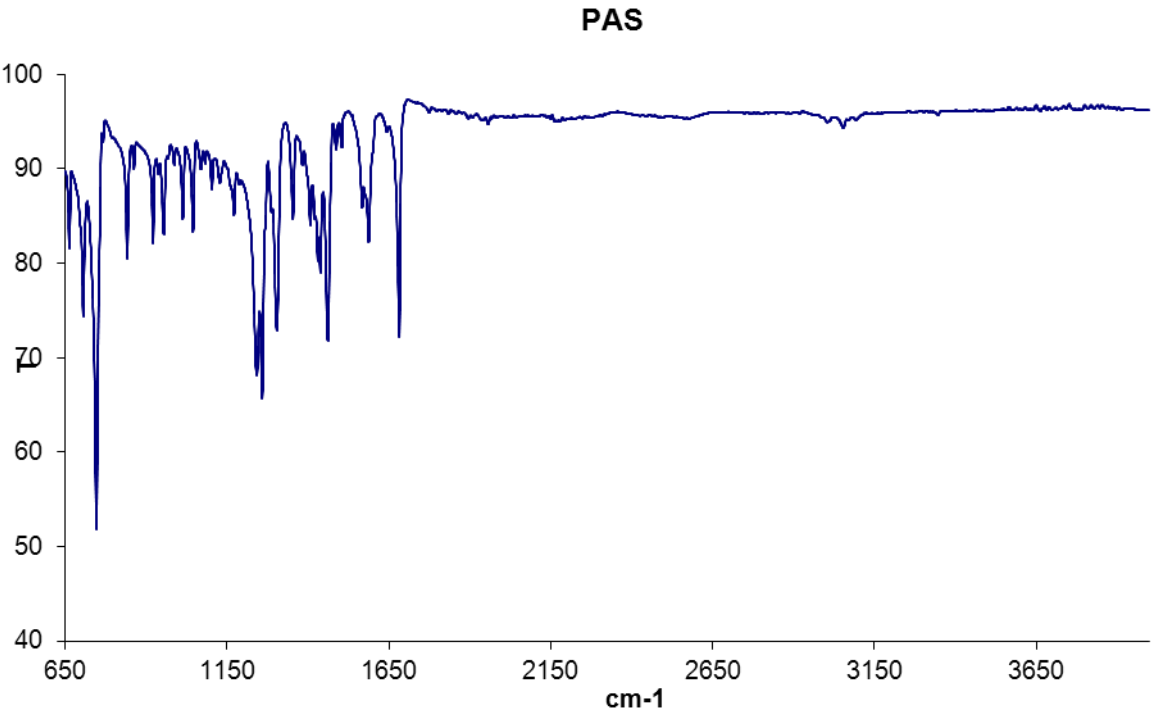
	PBO0			PBO8			PBO9			PBO12		
	X	Y	Z	X	Y	Z	X	Y	Z	X	Y	Z
O1	3.96645	-1.74488	1.73155	3.93662	-2.43229	0.49320	4.00245	-2.41752	-0.77469	4.11458	-1.59146	-1.81361
O13	-4.72570	0.36577	-0.28988	-4.70728	0.27643	0.43914	-3.59284	0.63466	1.45573	-3.55131	0.58481	1.49901
N8	-1.96486	-0.02714	0.13097	-1.94896	0.06417	0.46777	-1.97000	-0.10303	-0.61866	-2.03081	-0.14209	-0.69783
C1	3.64633	-0.91843	0.89336	3.64846	-1.26036	0.30309	3.64017	-1.31641	-0.38379	3.66748	-0.87743	-0.92807
C2	2.19144	-0.61889	0.66387	2.21769	-0.82575	0.35227	2.19593	-0.95132	-0.38443	2.19323	-0.66785	-0.80271
C3	1.30754	-0.77160	1.74035	1.31166	-1.58863	1.10441	1.24130	-1.97799	-0.36549	1.33307	-1.64287	-1.32461
C4	-0.05522	-0.56213	1.57001	-0.03160	-1.26272	1.14409	-0.11520	-1.71017	-0.42227	-0.04322	-1.48198	-1.29267
C5	-0.55830	-0.22480	0.31074	-0.53303	-0.14255	0.45437	-0.58677	-0.38582	-0.52901	-0.61657	-0.32530	-0.73913
C6	0.31126	-0.09443	-0.77242	0.35522	0.55714	-0.37479	0.36911	0.64644	-0.55303	0.24323	0.66521	-0.23856
C7	1.67996	-0.27921	-0.59469	1.71154	0.23993	-0.39655	1.72627	0.36467	-0.47568	1.62106	0.49272	-0.26641
C9	-2.32562	-2.43154	-0.27667	-1.86857	2.54727	0.04102	-2.19548	2.19420	-1.55485	-2.31145	2.15136	-1.57739
C10	-3.19256	-3.48515	-0.57346	-2.55409	3.74288	-0.17634	-2.67284	3.49494	-1.40974	-2.79526	3.44634	-1.41293
C11	-4.54617	-3.24560	-0.77340	-3.93913	3.75801	-0.28295	-3.42881	3.84441	-0.29010	-3.52963	3.78135	-0.27405
C12	-5.03214	-1.94033	-0.67560	-4.63922	2.56581	-0.11908	-3.73552	2.88877	0.67553	-3.79177	2.81887	0.69768
C14	-4.46907	2.69612	-0.03958	-5.00064	-1.96155	-0.27201	-4.69720	-1.48196	1.47983	-4.42779	-1.60878	1.73629
C15	-3.68934	3.82772	0.20768	-4.47509	-3.17630	-0.70204	-4.89215	-2.74035	0.91512	-4.53762	-2.92324	1.28974
C16	-2.32690	3.67931	0.43372	-3.09617	-3.31084	-0.82449	-4.16363	-3.12451	-0.21009	-3.86516	-3.32208	0.13751
C17	-1.74173	2.41166	0.40972	-2.24608	-2.26112	-0.47843	-3.20979	-2.26648	-0.75456	-3.05979	-2.41861	-0.55472
C18	-2.51040	1.27144	0.15976	-2.75269	-1.06066	0.03229	-2.95555	-1.03222	-0.15579	-2.88368	-1.11679	-0.08220
C19	-3.88830	1.43891	-0.05929	-4.14513	-0.92539	0.07268	-3.74065	-0.63691	0.93274	-3.61329	-0.72005	1.04741
C20	-2.80072	-1.12147	-0.17075	-2.54664	1.32395	0.13448	-2.44808	1.24357	-0.56568	-2.53594	1.18841	-0.59241
C21	-4.17194	-0.89658	-0.37793	-3.95208	1.38638	0.12245	-3.24891	1.59633	0.52430	-3.29144	1.53294	0.52997
C22	4.69651	-0.20814	0.09370	4.73031	-0.26070	0.01683	4.66754	-0.33022	0.09818	4.60885	-0.21202	0.03490
C23	5.57019	1.74378	-1.04677	5.72164	1.94288	0.20849	5.44661	1.37846	1.63119	5.22519	0.55035	2.25175
C24	6.76954	1.07410	-1.28104	6.86092	1.49242	-0.45544	6.69378	1.37435	1.00952	6.48626	0.91175	1.78172
C25	6.93964	-0.23308	-0.82108	6.94285	0.16347	-0.87535	6.93450	0.51120	-0.06082	6.81567	0.70257	0.44131
C26	5.91535	-0.86519	-0.12666	5.89074	-0.71040	-0.62843	5.93299	-0.34553	-0.50352	5.88826	0.13164	-0.42250
C27	4.53349	1.10343	-0.37107	4.65610	1.07398	0.43598	4.43423	0.53759	1.17231	4.28631	-0.00020	1.38139
H3	1.70623	-1.05846	2.70575	1.68247	-2.44573	1.65318	1.58552	-3.00336	-0.30253	1.76567	-2.52778	-1.77551
H4	-0.74021	-0.66441	2.40358	-0.70605	-1.84761	1.75685	-0.80901	-2.53518	-0.37026	-0.66819	-2.25024	-1.72114
H6	-0.09014	0.14917	-1.74913	-0.00447	1.31854	-1.04873	0.05666	1.67789	-0.61910	-0.16885	1.57245	0.18273
H7	2.34466	-0.18662	-1.44471	2.36521	0.80115	-1.05306	2.42631	1.19047	-0.50876	2.25310	1.28057	0.12466
H9	-1.27282	-2.62884	-0.12420	-0.80205	2.59263	0.18626	-1.61341	1.91174	-2.42367	-1.73853	1.87997	-2.45624
H10	-2.79633	-4.49100	-0.64662	-1.98858	4.66445	-0.24853	-2.45895	4.23264	-2.17389	-2.60450	4.19121	-2.17630
H11	-5.22431	-4.05806	-1.00410	-4.47306	4.68333	-0.46169	-3.79954	4.85646	-0.17831	-3.90963	4.78815	-0.14714
H12	-6.08051	-1.71237	-0.82643	-5.72169	2.53150	-0.13578	-4.34871	3.12404	1.53684	-4.37127	3.04612	1.58421
H14	-5.53546	2.76980	-0.21613	-6.06811	-1.78982	-0.20601	-5.27728	-1.14114	2.32869	-4.96238	-1.25609	2.60990
H15	-4.15027	4.80772	0.22427	-5.13683	-3.99402	-0.96085	-5.63191	-3.40881	1.33945	-5.16509	-3.62351	1.82815
H16	-1.70594	4.54492	0.63216	-2.66617	-4.23327	-1.19641	-4.34076	-4.08913	-0.67044	-3.97399	-4.33324	-0.23602
H17	-0.68013	2.30632	0.59010	-1.18214	-2.39537	-0.60035	-2.65753	-2.55078	-1.64136	-2.57672	-2.72795	-1.47011
H23	5.44159	2.76467	-1.38795	5.66280	2.96946	0.55209	5.26177	2.03355	2.47517	4.97230	0.69425	3.29617
H24	7.57196	1.57012	-1.81558	7.68547	2.17197	-0.64002	7.47788	2.03572	1.36116	7.21266	1.34887	2.45780
H25	7.87346	-0.75402	-0.99955	7.83029	-0.19010	-1.38801	7.90569	0.50217	-0.54286	7.79798	0.97817	0.07437
H26	6.04039	-1.87082	0.25605	5.94939	-1.75023	-0.92635	6.11403	-1.03943	-1.31553	6.13821	-0.06048	-1.45891
H27	3.60886	1.63525	-0.18277	3.77968	1.42792	0.96499	3.47118	0.53693	1.66842	3.31268	-0.29053	1.75712

Table 18S. Integrated atomic charges for **PBO0, PBO2, PBO4, PBO8, PBO9** and **PBO12**.

	PBO0		PBO2		PBO4		PBO8		PBO9		PBO12	
	rho [r] integral	charge	rho [r] integral	charge	rho [r] integral	charge	rho [r] integral	charge	rho [r] integral	charge	rho [r] integral	charge
O1	9.351	-1.351	9.052	-1.052	9.071	-1.071	9.044	-1.044	9.044	-1.044	9.304	-1.304
O13	8.959	-0.959	9.088	-1.088	9.097	-1.097	8.954	-0.954	9.051	-1.051	9.032	-1.032
N8	8.077	-1.077	8.081	-1.081	8.023	-1.023	8.037	-1.037	8.088	-1.088	8.043	-1.043
C1	4.988	1.012	4.960	1.040	4.991	1.009	5.086	0.914	5.013	0.987	5.016	0.984
C2	6.005	-0.005	6.002	-0.002	6.029	-0.029	6.016	-0.016	6.045	-0.045	6.009	-0.009
C3	5.991	0.009	6.044	-0.044	5.985	0.015	5.978	0.022	5.975	0.025	5.942	0.058
C4	5.987	0.013	6.120	-0.120	6.013	-0.013	6.003	-0.003	6.001	-0.001	6.008	-0.008
C5	5.730	0.270	5.653	0.347	5.628	0.372	5.645	0.355	5.620	0.380	5.653	0.348
C6	6.021	-0.021	5.978	0.022	6.002	-0.002	6.023	-0.023	6.061	-0.061	6.024	-0.024
C7	5.981	0.019	5.987	0.013	6.081	-0.081	5.989	0.011	5.979	0.021	5.991	0.009
C9	5.984	0.016	6.020	-0.020	6.011	-0.011	5.989	0.011	5.968	0.032	6.066	-0.066
C10	6.001	-0.001	5.957	0.043	6.040	-0.040	6.006	-0.006	5.993	0.007	5.988	0.012
C11	6.013	-0.013	5.999	0.001	5.999	0.001	5.538	0.462	5.963	0.037	5.960	0.040
C12	5.937	0.064	6.005	-0.005	5.999	0.001	5.956	0.044	5.979	0.021	5.987	0.013
C14	5.960	0.040	5.980	0.020	6.008	-0.008	5.981	0.019	5.974	0.026	6.004	-0.004
C15	5.992	0.008	5.993	0.007	6.001	-0.001	6.005	-0.005	5.950	0.050	6.017	-0.017
C16	5.953	0.047	6.007	-0.007	6.008	-0.008	5.987	0.013	5.974	0.026	5.983	0.017
C17	6.024	-0.024	6.002	-0.002	5.984	0.016	6.000	0.000	5.969	0.031	5.974	0.026
C18	5.664	0.336	5.739	0.261	5.680	0.321	5.681	0.319	5.705	0.295	5.689	0.312
C19	5.593	0.407	5.524	0.476	5.562	0.438	5.529	0.471	5.570	0.430	5.528	0.472
C20	5.669	0.331	5.643	0.357	5.681	0.319	5.660	0.340	5.672	0.328	5.666	0.335
C21	5.528	0.472	5.625	0.375	5.525	0.475	5.973	0.027	5.553	0.447	5.517	0.484
C22	6.026	-0.026	6.010	-0.010	6.034	-0.034	6.012	-0.012	6.048	-0.048	6.016	-0.016
C23	6.055	-0.055	6.029	-0.029	6.011	-0.011	5.975	0.025	5.991	0.009	5.993	0.007
C24	5.984	0.016	5.990	0.010	5.990	0.010	5.986	0.014	5.967	0.033	5.972	0.028
C25	5.983	0.017	6.103	-0.103	5.974	0.026	6.006	-0.006	5.974	0.026	5.991	0.009
C26	5.965	0.035	5.974	0.026	5.972	0.028	6.052	-0.052	5.965	0.035	5.980	0.020
C27	6.026	-0.026	5.985	0.015	6.020	-0.020	5.982	0.018	6.014	-0.014	6.000	0.000
H3	0.952	0.048	0.941	0.059	0.937	0.063	0.944	0.056	0.946	0.054	0.975	0.025
H4	0.962	0.038	0.963	0.038	0.957	0.043	0.964	0.036	0.975	0.025	0.985	0.015
H6	0.960	0.040	0.960	0.041	0.968	0.032	0.987	0.014	0.978	0.022	0.968	0.032
H7	0.971	0.029	0.973	0.027	0.968	0.032	0.967	0.033	0.981	0.019	0.978	0.022
H9	0.980	0.020	0.984	0.016	0.985	0.016	0.975	0.026	0.969	0.031	0.972	0.028
H10	1.005	-0.005	0.991	0.009	1.006	-0.006	0.973	0.027	0.996	0.004	0.982	0.018
H11	0.974	0.026	0.996	0.004	0.992	0.008	0.996	0.004	0.986	0.014	0.984	0.016
H12	0.988	0.012	0.967	0.033	0.963	0.037	0.959	0.041	0.958	0.042	0.961	0.039
H14	0.982	0.018	0.970	0.030	0.984	0.016	0.966	0.034	0.961	0.039	0.970	0.030
H15	0.987	0.013	0.989	0.011	1.006	-0.006	0.983	0.017	0.976	0.024	0.975	0.025
H16	0.991	0.009	1.014	-0.014	0.985	0.015	0.980	0.020	0.984	0.016	0.998	0.002
H17	0.979	0.021	0.979	0.021	0.970	0.030	0.959	0.041	0.975	0.025	0.981	0.020

H23	0.983	0.017	0.997	0.003	0.982	0.018	0.989	0.011	0.986	0.014	0.999	0.001
H24	0.977	0.023	0.983	0.017	0.983	0.017	0.984	0.016	0.989	0.011	0.991	0.009
H25	0.997	0.003	0.982	0.018	0.977	0.024	0.979	0.021	0.984	0.016	0.986	0.014
H26	0.946	0.054	0.951	0.049	0.962	0.038	0.952	0.048	0.973	0.027	0.965	0.035
H27	0.977	0.023	0.983	0.018	0.977	0.023	0.980	0.020	0.993	0.007	1.006	-0.006
		-0.060		-0.171		-0.018		0.371		0.285		-0.025





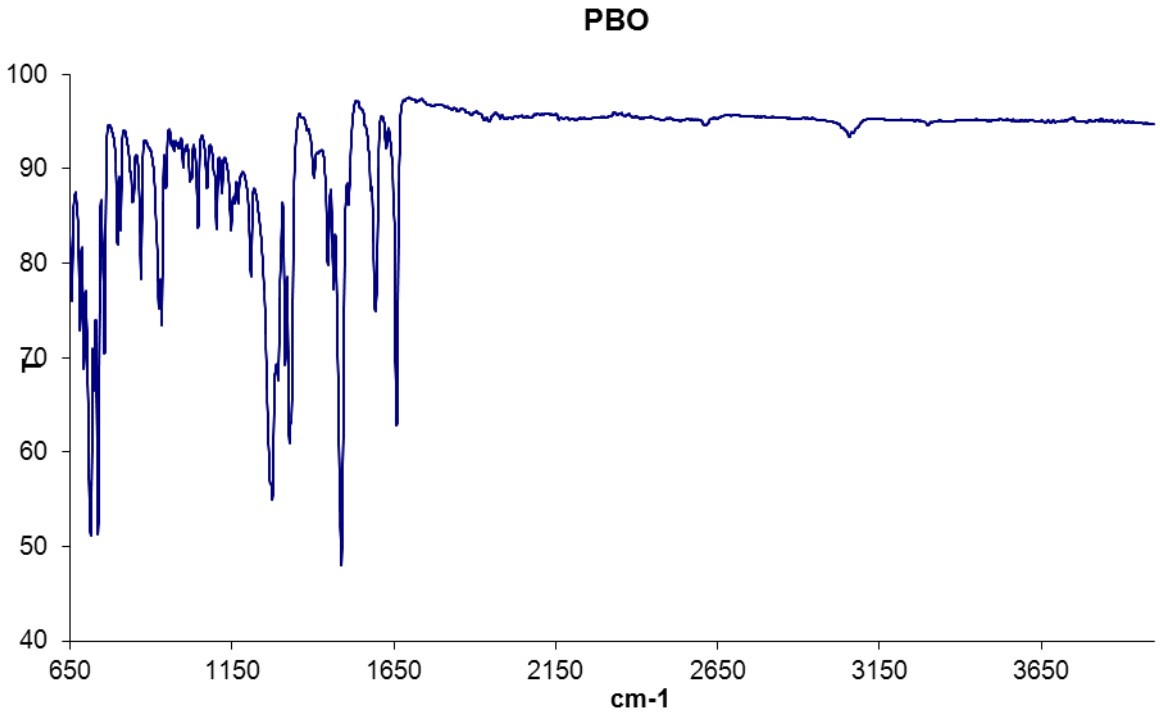


Figure 18S. IR spectra of **PAO, PAS** and **PBO**.

Table 19S. List of torsion angles for which geometry optimization was done for PAO, PAS and PBO.

i	PAO	PAS	PBO
0	81	-168	-88
1	91	-158	-78
2	101	-148	-68
3	111	-138	112
4	121	-128	122
5	131	-118	132
6	141	-108	142
7	151	-98	152
8	161	82	162
9	171	92	172
10	-179	102	-178
11	-169	112	-168
12	-159	122	-158
13	-149	132	-148
14	-139	142	-138
15	-129	152	-128
16	-119	162	-118
17	-109	172	-108
18	-99	-178	-98