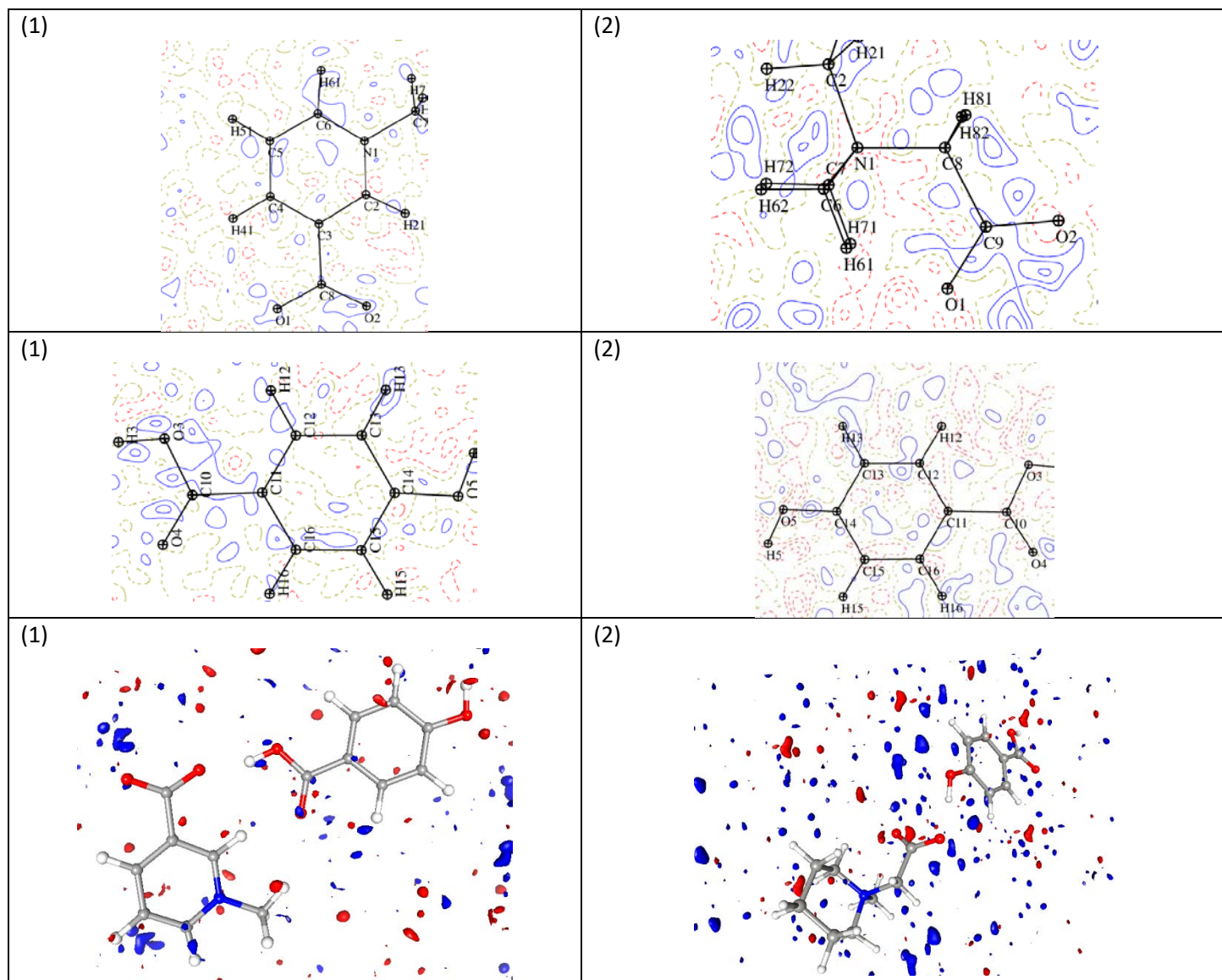
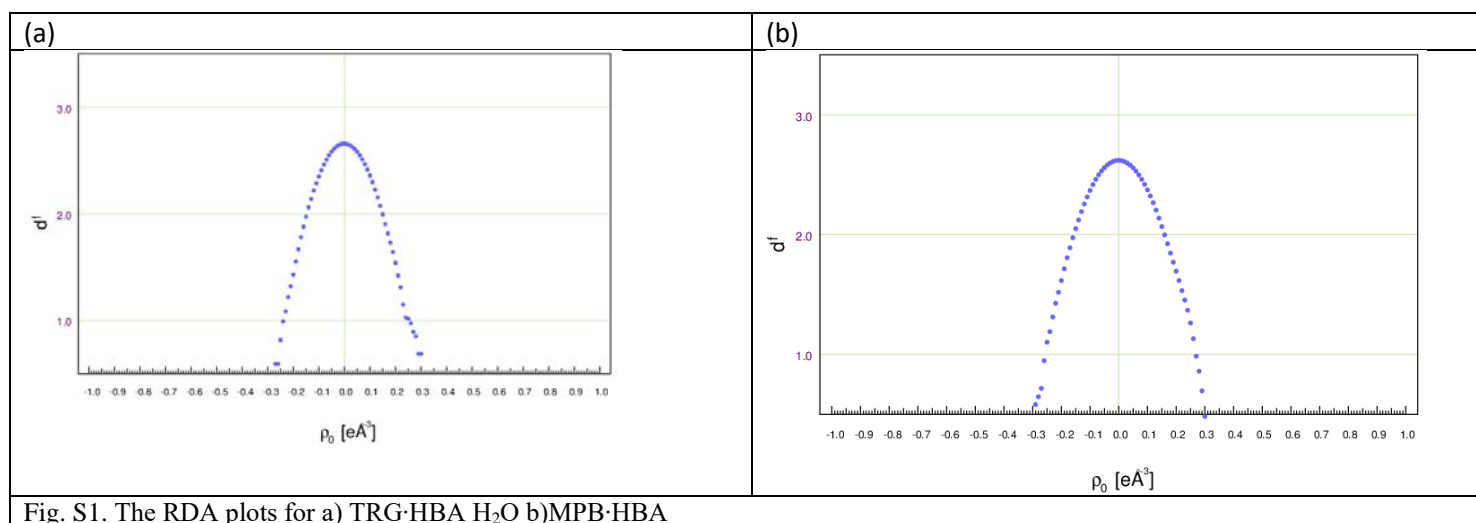


Supplementary



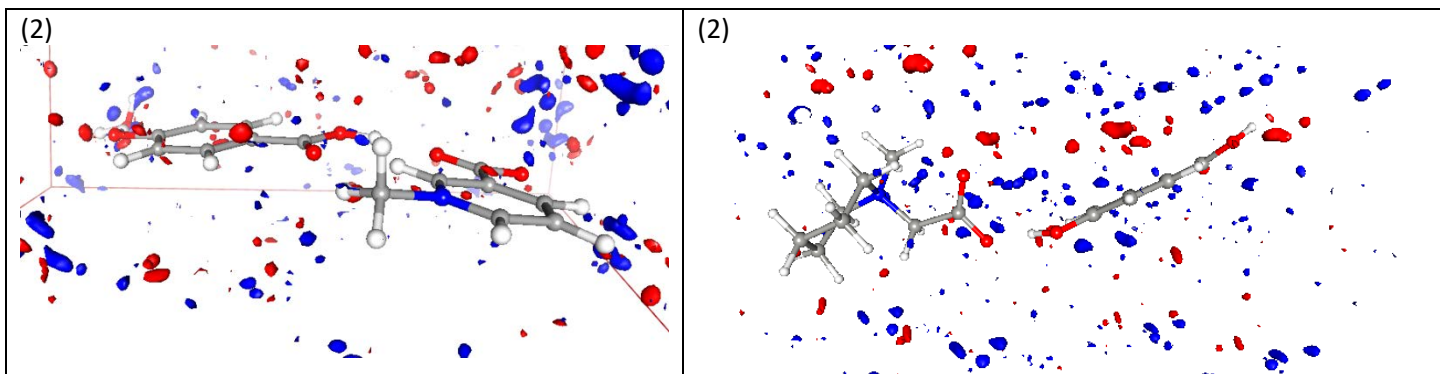


Fig.S2 The residual electron density maps for TRG·HBA·H<sub>2</sub>O (1) and MPB·HBA (2),  $\sin\theta/\lambda > 0.9 \text{ \AA}^{-1}$  contours are drawn at intervals  $0.05 \text{ e \AA}^{-3}$  (2dmaps), and  $0.1 \text{ e \AA}^{-3}$  for (1) and  $0.15 \text{ e \AA}^{-3}$  for (2) (3dmaps)

Table S1 Rigid bond test for non-hydrogen atoms of TRG·HBA·H<sub>2</sub>O

Atom1	Atom2	$Z_A^2 [\text{\AA}^2]$	$Z_B^2 [\text{\AA}^2]$	$\Delta Z_{AB}^2 [\text{\AA}^2]$
O2	C8	0.0100	0.0102	0.00026
O1	C8	0.0098	0.0097	0.00001
O4	C10	0.0124	0.0125	-0.00011
O3	C10	0.0161	0.0160	0.00007
O5	C14	0.0103	0.0105	-0.00018
N1	C2	0.0098	0.0099	-0.00011
N1	C6	0.0128	0.0131	-0.00031
N1	C7	0.0119	0.0125	-0.00062
C8	C3	0.0102	0.0099	0.00025
C3	C2	0.0102	0.0103	-0.00007
C3	C4	0.0097	0.0100	-0.00032
C11	C10	0.0102	0.0103	-0.00017
C11	C12	0.0120	0.0123	-0.00032
C11	C16	0.0154	0.0157	-0.00033
C12	C13	0.0116	0.0115	0.00005
C4	C5	0.0127	0.0129	-0.00024
C13	C14	0.0180	0.0180	0.00004
C6	C5	0.0166	0.0166	-0.00003
C15	C14	0.0151	0.0152	-0.00009
C15	C16	0.0122	0.0122	0.00006

Table S2 Rigid bond test for non-hydrogen atoms of MPB·HBA

Atom1	Atom2	$Z_A^2 [\text{\AA}^2]$	$Z_B^2 [\text{\AA}^2]$	$\Delta Z_{AB}^2 [\text{\AA}^2]$
O5	C14	0.0075	0.0075	-0.00006
O4	C10	0.0106	0.0108	-0.00015
O2	C9	0.0103	0.0105	-0.00011
O3	C10	0.0110	0.0112	-0.00013
O1	C9	0.0096	0.0097	-0.00017
N1	C8	0.0085	0.0088	-0.00027
N1	C6	0.0088	0.0093	-0.00047
N1	C2	0.0078	0.0082	-0.00042

N1	C7	0.0076	0.0081	-0.00048
C10	C11	0.0076	0.0074	0.00028
C15	C14	0.0097	0.0096	0.00011
C15	C16	0.0086	0.0087	-0.00009
C12	C11	0.0094	0.0093	0.00010
C12	C13	0.0089	0.0089	0.00005
C9	C8	0.0077	0.0079	-0.00021
C11	C16	0.0086	0.0089	-0.00031
C14	C13	0.0094	0.0094	-0.00002
C6	C5	0.0112	0.0117	-0.00046
C2	C3	0.0118	0.0120	-0.00022
C5	C4	0.0109	0.0110	-0.00015
C3	C4	0.0151	0.0153	-0.00020

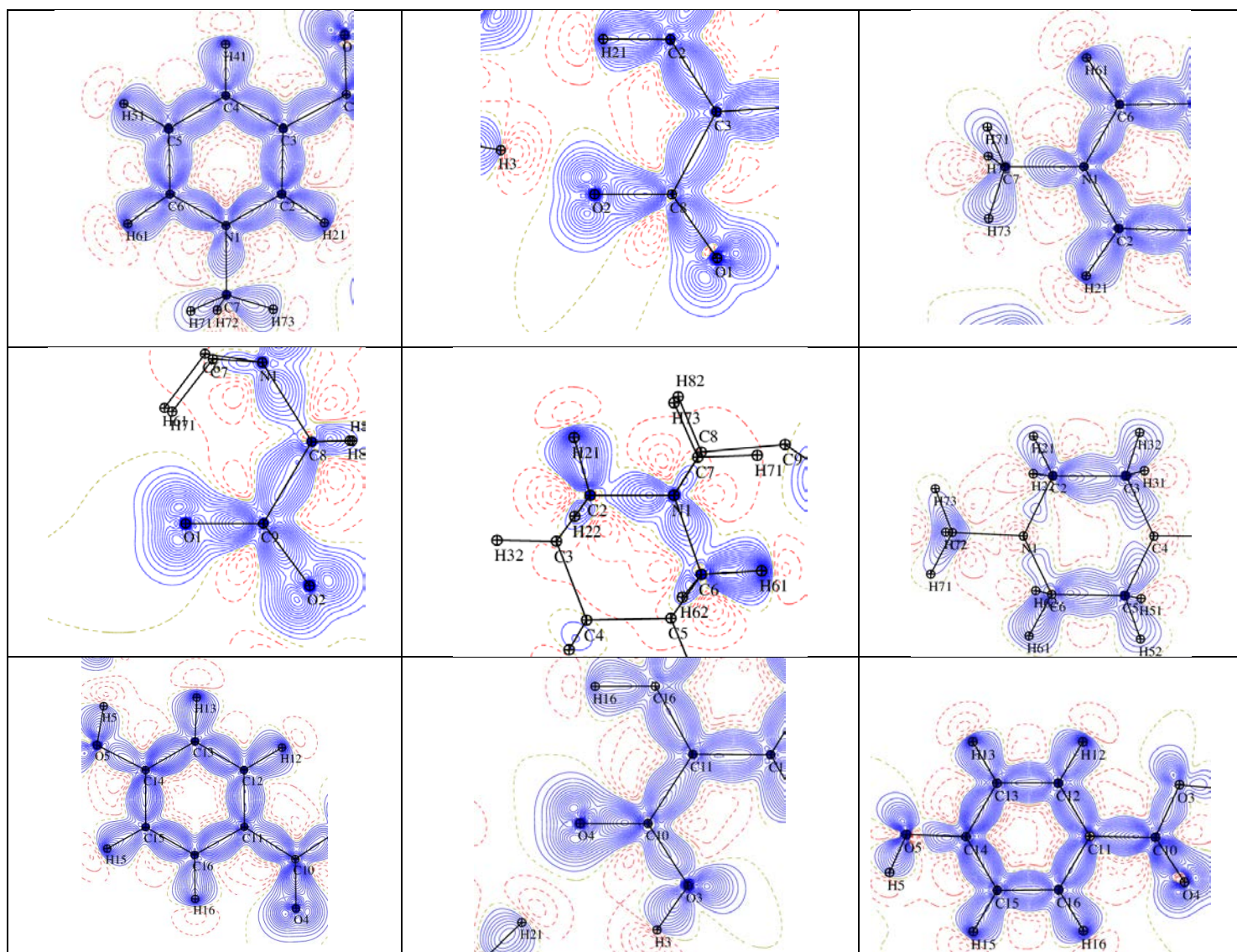


Fig. S3. The static deformation electron density distribution in plane of pyridine ring (a), carboxylate group (b), C7-N1-C2 plane (c), carboxylate group (d), C2-C3-C5 plane (e), C2-N1-C6 plane (f), in plane of hba ring (g, h) and in plane of carboxylic group of hba (i), the positive (blue) and negative (dashed red) contours are drawn at intervals  $0.05 e \text{ \AA}^{-3}$

Table S3. Characteristics of bond critical points (3,-1) for TRG·HBA·H<sub>2</sub>O

Atom 1	Atom2	D12	D1cp	D2cp	$\rho_{\text{bcp}}$	$\nabla^2$	$\lambda_1$	$\lambda_2$	$\lambda_3$	Ellip
O4	C10	1,2205	0,7842	0,4363	2,9808	-33,18	-29,5	-26,38	22,7	0,12
O1	C8	1,2591	0,7864	0,4729	2,7284	-33,13	-25,58	-22,72	15,17	0,13
O2	C8	1,2491	0,7972	0,4522	2,7258	-31,75	-26,67	-23,44	18,37	0,14
N1	C2	1,3441	0,7964	0,5477	2,3503	-23,9	-19,36	-17,07	12,53	0,13
N1	C6	1,3497	0,8029	0,5468	2,3077	-23,69	-19,24	-16,75	12,3	0,15
O3	C10	1,3301	0,8093	0,521	2,301	-23,57	-20,08	-18,23	14,75	0,1
O1W	H1W	0,983	0,7591	0,224	2,2609	-33,01	-34,8	-33,63	35,42	0,03
C6	C5	1,3792	0,7041	0,6753	2,2608	-20,42	-17,87	-14,87	12,32	0,2
O1W	H2W	0,983	0,7613	0,2219	2,2327	-32,62	-34,67	-33,09	35,14	0,05
C3	C2	1,3842	0,6678	0,7165	2,2182	-19,76	-17,92	-14,17	12,33	0,26
O5	C14	1,341	0,8076	0,5338	2,1898	-20,24	-18,78	-16,7	15,24	0,12
C15	C16	1,3841	0,6914	0,6927	2,181	-19,06	-17,34	-13,91	12,19	0,25
C3	C4	1,3922	0,7077	0,6846	2,1706	-18,67	-16,96	-14,34	12,62	0,18
C13	C14	1,4048	0,666	0,7388	2,1615	-19,23	-17,38	-13,78	11,92	0,26
C12	C13	1,3918	0,6941	0,6978	2,1511	-17,97	-16,88	-13,57	12,48	0,24
C15	C14	1,4022	0,6874	0,7149	2,1488	-19,24	-17,5	-13,76	12,02	0,27
C4	C5	1,3901	0,7026	0,6875	2,1462	-17,82	-16,64	-13,95	12,76	0,19
C11	C12	1,3991	0,6983	0,7009	2,1226	-17,69	-16,51	-13,48	12,3	0,22
C11	C16	1,4001	0,6878	0,7124	2,1222	-18,21	-16,65	-13,78	12,22	0,21
O5	H5	0,98	0,7852	0,1949	2,087	-35,42	-34,18	-33,67	32,43	0,02
O3	H3	0,98	0,7921	0,1879	2,0163	-37,93	-34,05	-34,02	30,15	0
C2	H21	1,083	0,7412	0,3419	1,8751	-19,5	-19	-18,23	17,74	0,04
C6	H61	1,083	0,7387	0,3443	1,8736	-19,9	-19,08	-18,06	17,24	0,06
C4	H41	1,083	0,7321	0,3509	1,8715	-18,68	-18,5	-17,72	17,54	0,04
C12	H12	1,083	0,7271	0,356	1,8521	-17,93	-17,94	-17,16	17,17	0,05
C13	H13	1,083	0,7125	0,3706	1,8365	-17,08	-17,43	-16,52	16,88	0,06
C11	C10	1,4788	0,7074	0,7716	1,826	-14,03	-14,25	-11,74	11,96	0,21
C15	H15	1,083	0,7105	0,3726	1,8192	-17,12	-17,37	-16,28	16,52	0,07
C5	H51	1,083	0,7217	0,3616	1,8142	-17,04	-17,19	-16,55	16,71	0,04
C16	H16	1,083	0,7279	0,3551	1,8029	-17,38	-17,55	-16,62	16,79	0,06
C7	H73	1,077	0,7257	0,3515	1,7637	-17,28	-16,91	-14,83	14,46	0,14
C8	C3	1,5125	0,7555	0,757	1,7512	-12,22	-13,3	-11,35	12,42	0,17
C7	H72	1,077	0,7207	0,3568	1,7314	-15,88	-16,2	-14,35	14,67	0,13
C7	H71	1,077	0,7201	0,3572	1,7291	-16,37	-16,32	-14,3	14,25	0,14
N1	C7	1,4717	0,8617	0,6101	1,6883	-10,13	-11,87	-11,3	13,05	0,05

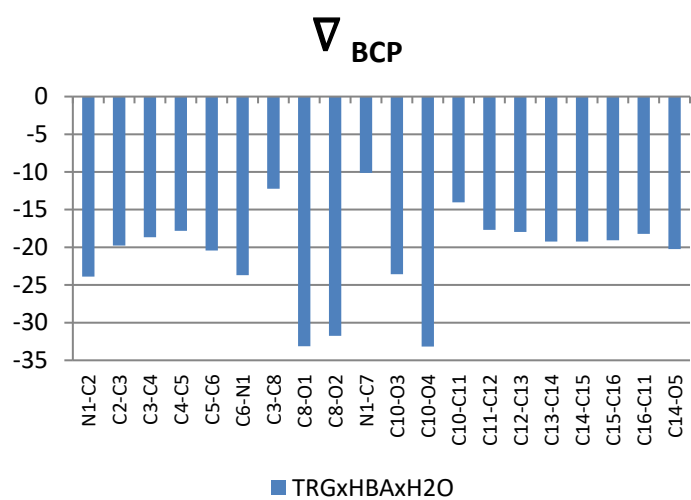
(D12: distance between two atoms, D1cp, D2cp: distance from the first and the second atom to the critical point, laplacian [ $\nabla^2(\rho_{\text{bcp}})$ ] ( $\text{e}\text{\AA}^{-5}$ ), electron density [ $\rho_{\text{bcp}}$ ] ( $\text{e}\text{\AA}^{-3}$ ) and mean curvature of the Hessian matrix  $\lambda_1, \lambda_2, \lambda_3$ .)

Table S4: Characteristics of bond critical points(3,-1) for MPB-HBA

Atom 1	Atom2	D12	D1cp	D2cp	$\rho_{\text{bcp}}$	$\nabla^2$	$\lambda_1$	$\lambda_2$	$\lambda_3$	Ellip
C14	C13	1,4012	0,7205	0,6807	2,1414	-19,29	-17,53	-13,73	11,97	0,28
C15	C14	1,4023	0,6777	0,7246	2,1397	-18,81	-17,36	-13,64	12,18	0,27
C12	C13	1,3878	0,7002	0,6876	2,131	-18,58	-16,8	-13,57	11,8	0,24
C15	C16	1,39	0,6907	0,6993	2,1364	-18,63	-16,9	-13,61	11,88	0,24
C11	C16	1,3997	0,6961	0,7036	2,12	-18,04	-16,77	-13,65	12,39	0,23
C12	C11	1,3995	0,7059	0,6936	2,1003	-17,52	-16,37	-13,58	12,43	0,21
C10	C11	1,481	0,7839	0,6971	1,8525	-14,08	-14,51	-12,08	12,51	0,2
O4	C10	1,2206	0,7743	0,4464	2,9918	-35,6	-29,26	-25,08	18,74	0,17
C9	C8	1,5356	0,7678	0,7685	1,6782	-10,73	-12,58	-10,82	12,66	0,16
O1	C9	1,2562	0,7723	0,484	2,7684	-33,46	-26,05	-22,43	15,02	0,16
O5	C14	1,3492	0,789	0,5605	2,1331	-16,43	-17,98	-15,85	17,4	0,13
O3	C10	1,3302	0,807	0,5234	2,3142	-23,63	-19,9	-18,28	14,54	0,09
O2	C9	1,256	0,7779	0,4781	2,7888	-34,64	-25,59	-23,65	14,6	0,08
C7	H72	1,077	0,7067	0,3704	1,8695	-16,25	-17,89	-16,95	18,58	0,06
C7	H73	1,077	0,71	0,367	1,8629	-16,25	-17,91	-16,92	18,59	0,06
C15	H15	1,083	0,7168	0,3662	1,8096	-17,52	-17,63	-16,67	16,78	0,06
C13	H13	1,083	0,7135	0,3695	1,8104	-17,63	-17,54	-16,6	16,51	0,06
C7	H71	1,077	0,7127	0,3643	1,9081	-17,7	-18,56	-17,6	18,46	0,05
C12	H12	1,083	0,7141	0,3689	1,8851	-18,46	-18,1	-17,28	16,92	0,05
N1	C8	1,5092	0,862	0,6474	1,5586	-5,9	-10,65	-10,25	15	0,04
C16	H16	1,083	0,7084	0,3747	1,8756	-18,15	-17,82	-17,12	16,79	0,04
N1	C7	1,5027	0,8548	0,6479	1,6285	-7,15	-11,16	-10,84	14,84	0,03
C3	H31	1,092	0,6922	0,3999	1,8887	-16,31	-16,81	-16,37	16,88	0,03
C3	C4	1,5289	0,7723	0,7568	1,6082	-8,26	-10,54	-10,39	12,67	0,02
C5	C4	1,5268	0,7683	0,7585	1,6444	-8,81	-10,89	-10,67	12,76	0,02
C2	C3	1,521	0,7769	0,7445	1,6776	-9,31	-11,35	-11,15	13,19	0,02
C3	H32	1,092	0,6963	0,3957	1,8532	-16	-16,53	-16,24	16,77	0,02
O5	H5	0,9732	0,769	0,2042	2,1061	-30,29	-34,04	-33,32	37,07	0,02
N1	C6	1,5171	0,8563	0,6608	1,5788	-5,36	-10,54	-10,43	15,62	0,01
C5	H52	1,092	0,7032	0,3888	1,8215	-15,57	-16,34	-16,22	16,99	0,01
C6	H62	1,092	0,7098	0,3822	1,8364	-15,85	-17,04	-16,92	18,1	0,01
C4	H42	1,092	0,7131	0,3789	1,8007	-16,04	-16,46	-16,28	16,69	0,01
C5	H51	1,092	0,692	0,4001	1,8701	-16,46	-16,68	-16,44	16,66	0,01
C8	H81	1,092	0,7079	0,3842	1,8765	-16,95	-17,36	-17,2	17,62	0,01
C8	H82	1,092	0,7084	0,3837	1,8621	-17,03	-17,26	-17,05	17,28	0,01
C6	H61	1,092	0,7045	0,3875	1,9116	-17,64	-17,81	-17,66	17,84	0,01
N1	C2	1,518	0,8639	0,6542	1,5737	-6,2	-10,5	-10,46	14,75	0
C6	C5	1,5216	0,7742	0,7477	1,6593	-9,01	-11,16	-11,11	13,25	0
C4	H41	1,092	0,7105	0,3815	1,7851	-16,32	-16,22	-16,2	16,1	0
C2	H22	1,092	0,7096	0,3824	1,8423	-16,6	-17,12	-17,06	17,59	0
C2	H21	1,092	0,7092	0,3828	1,8704	-17,14	-17,42	-17,4	17,69	0
O3	H3	0,9717	0,7706	0,2011	2,0488	-29,2	-33,15	-33,02	36,97	0

D12: distance between two atoms, D1cp, D2cp: distance from the first and the second atom to the critical point, laplacian [ $\nabla^2(\rho_{\text{bcp}})$ ] ( $\text{e}\text{\AA}^{-5}$ ), electron density [ $\rho_{\text{bcp}}$ ] ( $\text{e}\text{\AA}^{-3}$ )

(1)



(2)

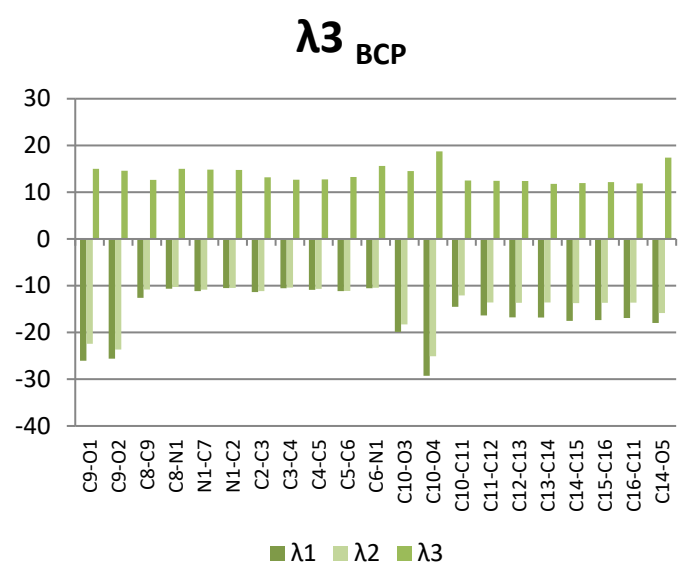
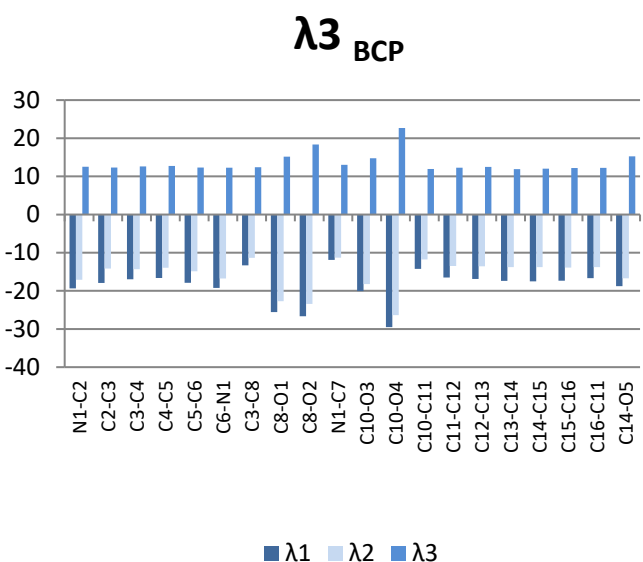
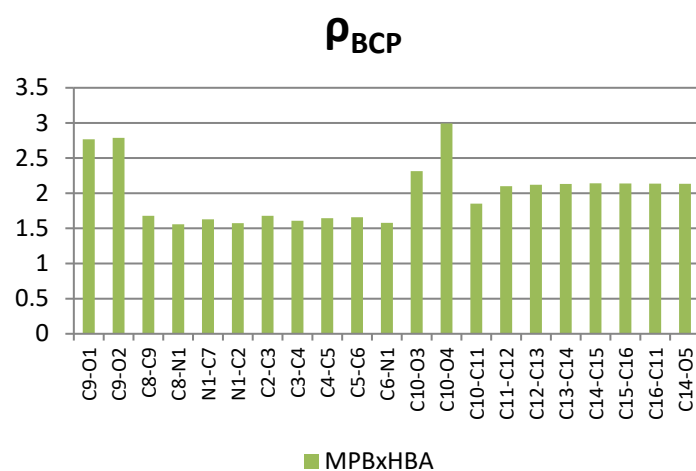
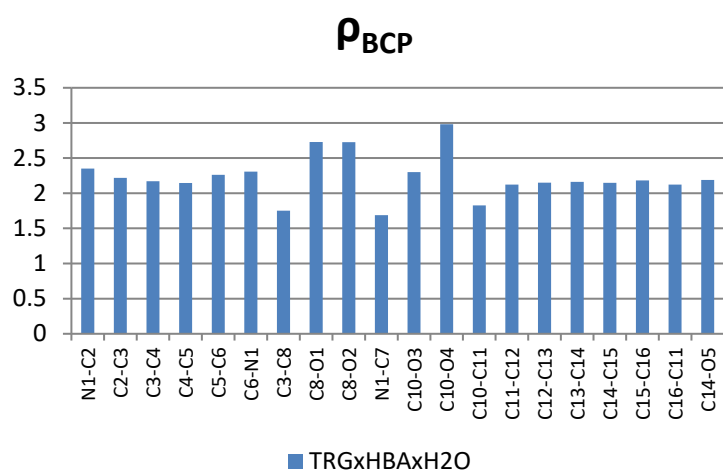
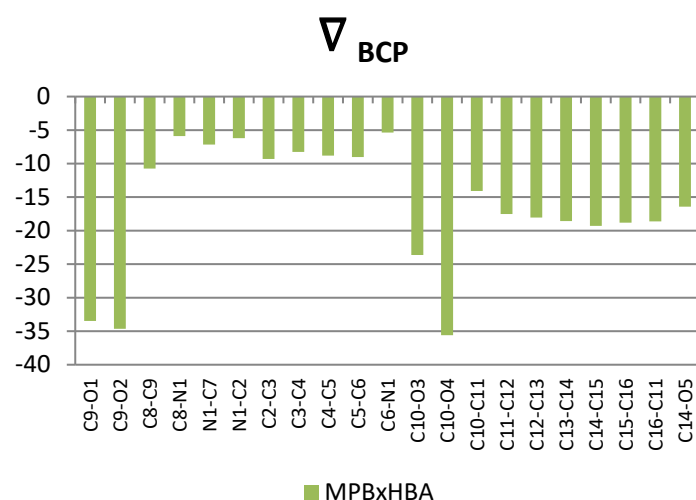


Fig. S4 Graphical representation of laplacian [ $\nabla^2(\rho_{bcp})$ ] ( $e\text{\AA}^{-5}$ ) electron density [ $\rho_{bcp}$ ] ( $e\text{\AA}^{-3}$ ) and three eigenvalues of Hessian matrix  $\lambda_3$  in bond critical points

Table S5 Atomic Charges (e) in Molecule (1) with different definition calculated as  $N_{\text{val}}-P_{\text{val}}$  and by integration over atomic basins (Inte)

	Atom	$N_{\text{val}}-P_{\text{val}}$	Inte
TRG PART	O1	-0,40318	-1,06704
	O2	-0,39143	-1,09391
	C8	0,14224	1,511275
	N1	0,00135	-0,80793
	C2	-0,02522	0,236861
	C3	-0,01836	-0,00454
	C4	0,03373	-0,04758
	C5	-0,08814	-0,11489
	C6	0,06092	0,321183
	C7	-0,03983	-0,10421
	H21	0,19934	0,231806
	H41	0,0821	0,152291
	H51	0,07982	0,131767
	H61	0,1959	0,23403
	H71	0,10678	0,194058
	H72	0,07775	0,147799
	H73	0,10504	0,191166
	sum	0,11881	0,112132
HBA PART	O5	-0,39621	-1,26634
	O4	-0,36367	-1,19165
	O3	-0,40753	-1,20219
	C10	0,17953	1,497357
	C11	0,12567	0,129594
	C12	-0,04974	-0,08631
	C13	-0,06225	-0,11707
	C14	0,08179	0,508735
	C15	-0,05866	-0,11989
	C16	-0,04669	-0,0969
	H5	0,25348	0,631237
	H3	0,27565	0,672871
	H12	0,07005	0,118481
	H13	0,08683	0,129769
	H15	0,09787	0,142667
	H16	0,09503	0,142961
	sum	-0,11885	-0,106672
WATER	O1W	-1,30670	
	H1W	0,658236	
	H2W	0,639718	

Table S6 Atomic Charges (e) in Molecule (2) with different definition as  $N_{\text{val}}-P_{\text{val}}$  and by integration over atomic basins (Inte)

	Atom	$N_{\text{val}}-P_{\text{val}}$	Inte
MPB PART	O1	-0,38586	-1,06357
	O2	-0,40162	-1,08626
	C9	-0,01178	1,381145
	C8	0,13662	0,167483
	N1	-0,27666	-0,7354
	C2	0,07548	0,198656
	C3	-0,06598	-0,13998
	C4	-0,10847	-0,06761
	C5	-0,06441	-0,11079
	C6	0,07287	0,157776
	C7	-0,08271	0,010976
	H81	0,07257	0,082322
	H82	0,07829	0,098632
	H21	0,07319	0,072342
	H22	0,06169	0,060079
	H31	-0,06877	-0,03625
	H32	-0,04413	-0,01258
	H41	0,10499	0,103689
	H42	0,09935	0,090281
	H51	-0,04656	-0,02491
H52	-0,00799	0,012628	
H61	0,05586	0,067155	
H62	0,05983	0,059858	
H71	0,08958	0,114768	
H72	0,05221	0,059643	
H73	0,05404	0,062275	
	sum	-0,47837	-0,47764
HBA PART	O5	-0,39143	-1,09022
	O4	-0,26491	-1,09864
	O3	-0,36743	-1,16481
	C10	-0,01788	1,317087
	C11	0,24418	0,133528
	C12	-0,06118	0,011569
	C13	0,08793	0,076441
	C14	0,10737	0,501249
	C15	0,08719	0,052005
	C16	-0,06073	0,049974
	H5	0,3007	0,605186
	H3	0,29171	0,608689
	H12	0,1154	0,098253
	H13	0,1462	0,145003
	H15	0,14894	0,151643
	H16	0,11215	0,081523
	sum	0,47821	0,47848

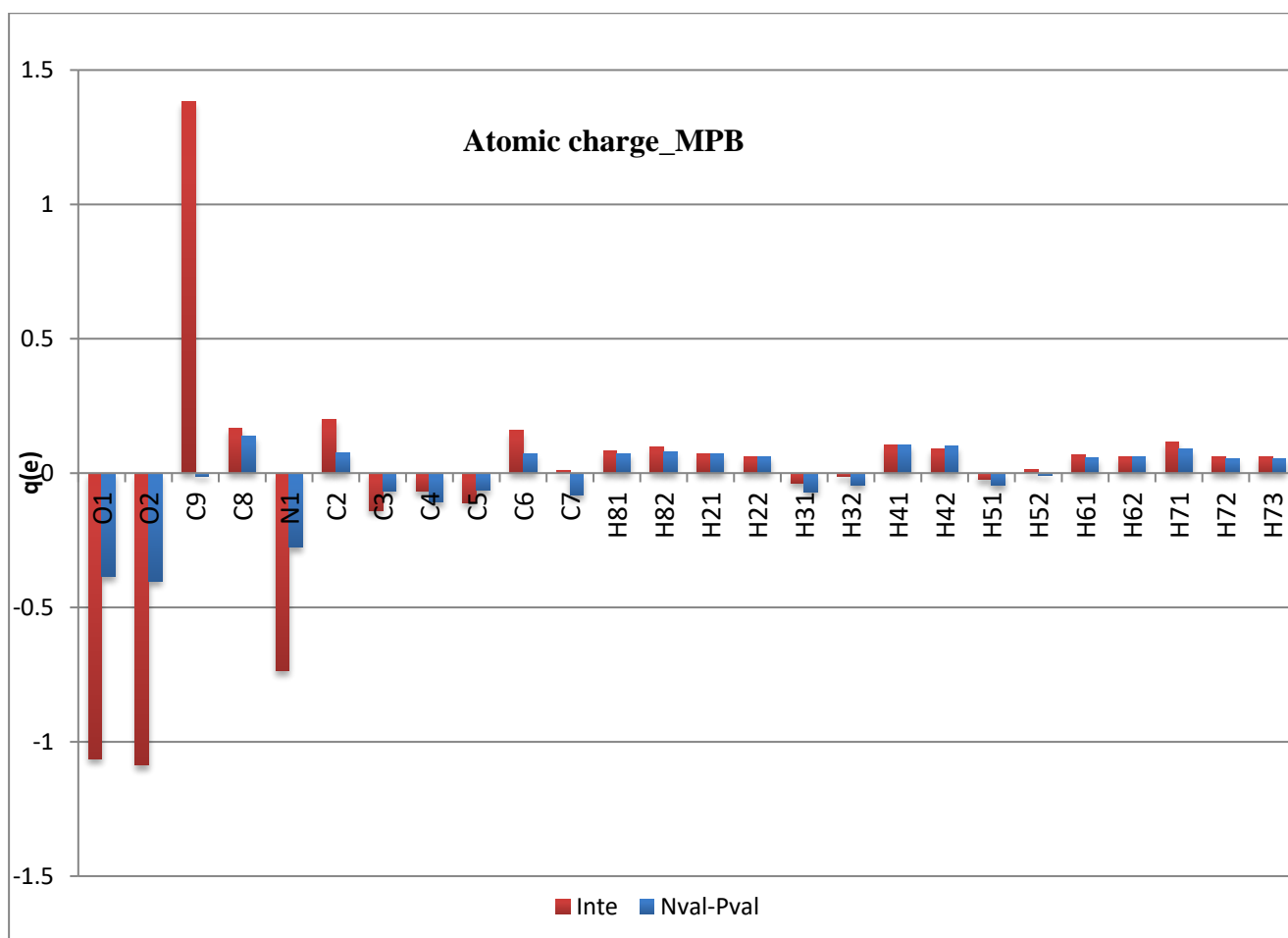
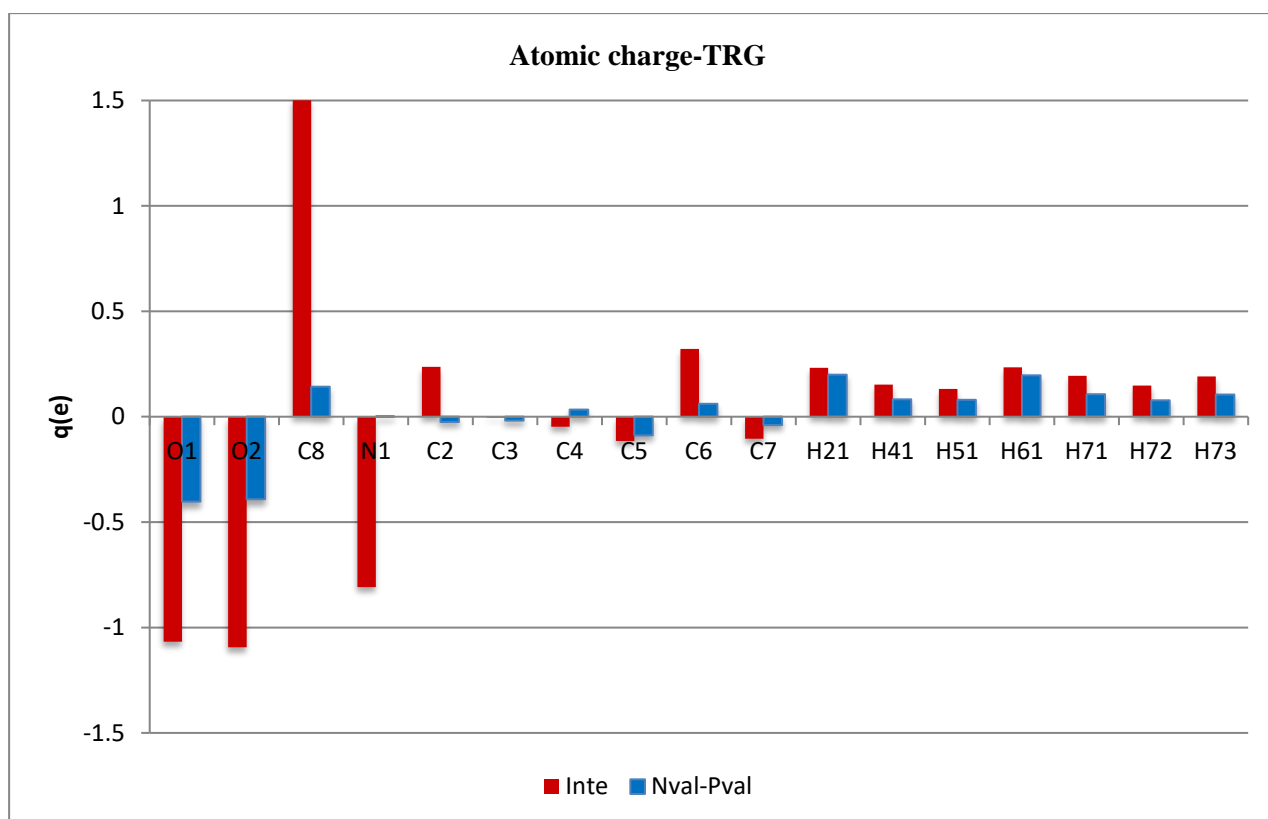


Fig. S5. Atomic charges



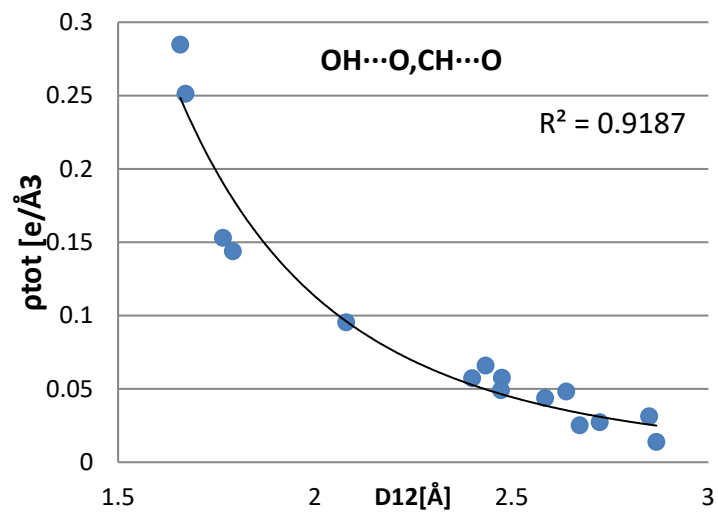
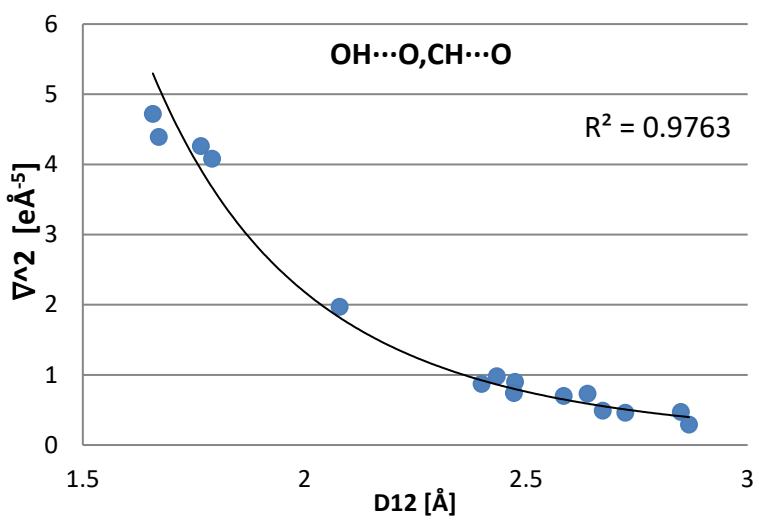
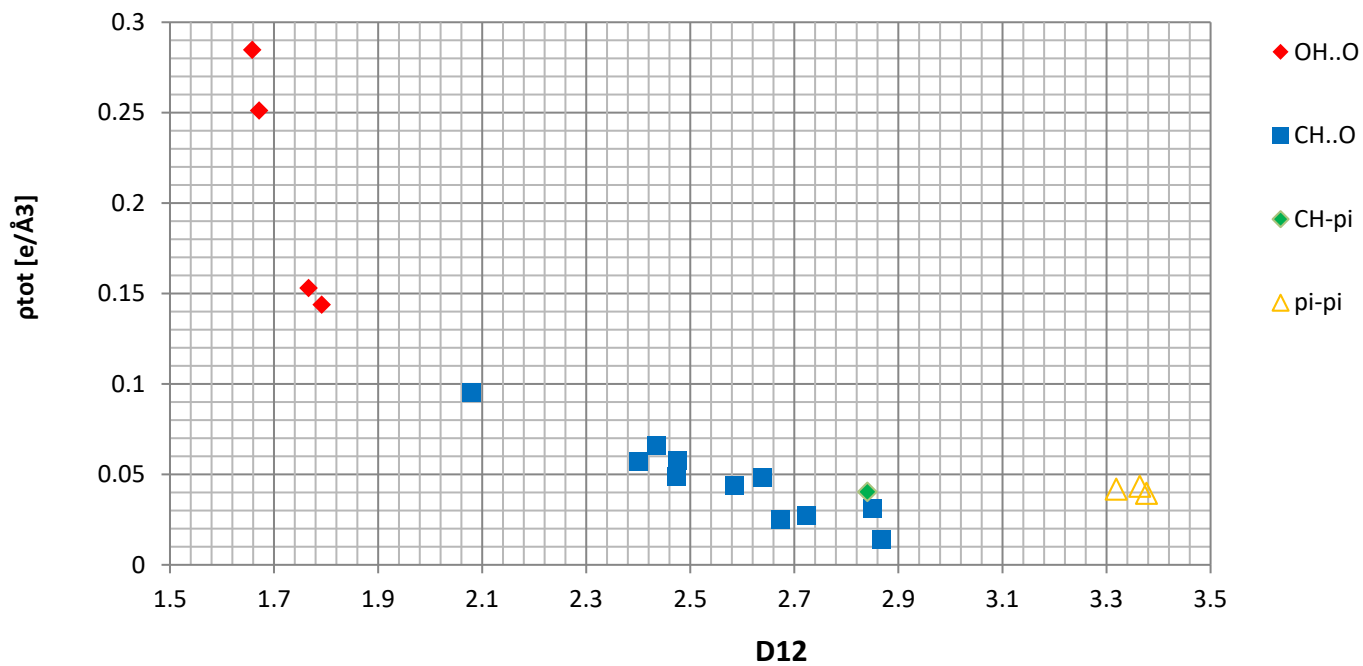
Table S7: Topological characteristic of the intermolecular critical points(3,1) in TRG·HBA·H <sub>2</sub> O												
Atom1	Atom2	Gcp	Vcp	D12	D1cp	D2cp	$\rho_{\text{bcp}}$	$\nabla^2$	$\lambda_1$	$\lambda_2$	$\lambda_3$	ELLIP
Type: OH...O hydrogen bonds												
O1W	H5	124,16	-119,75	1,658	1,118	0,5415	0,2843	4,72	-1,62	-1,4	7,74	0,16
O2	H3	110,91	-102,23	1,6714	1,1206	0,5544	0,2507	4,39	-1,3	-1,27	6,96	0,03
O1	H2W	91,07	-66,07	1,7664	1,1893	0,5958	0,1530	4,26	-0,73	-0,66	5,66	0,11
O1	H1W	86,45	-61,74	1,7917	1,1998	0,6069	0,1438	4,08	-0,70	-0,65	5,43	0,07
Type: CH...O												
O4	H21	41,83	-30,24	2,0795	1,3177	0,7708	0,0953	1,96	-0,38	-0,36	2,7	0,05
O2	H61	21,11	-15,61	2,434	1,4289	1,0379	0,066	0,98	-0,23	-0,19	1,4	0,17
O3	H71	18,54	-13,26	2,3997	1,4565	0,9597	0,0573	0,87	-0,17	-0,17	1,21	0,01
O4	H73	15,48	-10,82	2,4728	1,4745	1,0282	0,049	0,74	-0,15	-0,1	1	0,48
O1	H61	15,2	-10,6	2,639	1,5289	1,1303	0,0482	0,73	-0,14	-0,05	0,91	1,93
O2	H13	9,47	-5,76	2,6731	1,5989	1,1117	0,0253	0,48	-0,08	-0,07	0,64	0,23
O3	H12	9,11	-5,72	2,724	1,5993	1,1428	0,0273	0,46	-0,08	-0,07	0,61	0,08
O1	H51	9,51	-6,22	2,8496	1,583	1,3249	0,0314	0,47	-0,08	-0,05	0,6	0,69
O1W	H15	5,53	-3,14	2,868	1,77	1,1816	0,0139	0,29	-0,04	-0,02	0,35	0,67
O5	H41											
O1W	H41											
Another weak interactions (...)												
N1	C13	10,65	-7,68	3,3188	1,6661	1,7201	0,0418	0,5	-0,06	-0,03	0,59	1,09
C3	C15	10,29	-7,66	3,3639	1,7211	1,7727	0,0434	0,47	-0,06	-0,03	0,57	0,84
C3	C14	9,48	-6,89	3,3768	1,6952	1,6861	0,0395	0,44	-0,04	-0,02	0,5	1,44
C12	H72	9,95	-7,2	2,8404	1,6586	1,188	0,0403	0,47	-0,1	-0,05	0,62	1,1
H16	C7	10,43	-7,06	2,9164	1,0663	1,862	0,0361	0,51	-0,1	-0,06	0,67	0,69
H12	C7	6,92	-4,56	3,258	1,4294	1,8361	0,0264	0,34	-0,06	-0,03	0,43	1,23
H73	C7	10,41	-7,18	2,8935	1,2341	1,7287	0,0375	0,5	-0,14	-0,04	0,68	2,39
O4	O4	7,46	-4,91	3,5508	1,7066	1,8796	0,0276	0,37	-0,06	-0,02	0,45	2,6
O3	C16	4,49	-2,8	3,8366	1,9079	1,9651	0,0174	0,23	-0,03	-0,02	0,28	0,86
O5	C4	9,55	-6,64	3,2876	1,6694	1,6744	0,0363	0,46	-0,05	-0,02	0,53	2,35
O1W	C5	6,1	-3,86	3,4543	1,6855	1,7723	0,022	0,31	-0,04	-0,02	0,36	1,25
D12: distance between two atoms, D1cp, D2cp: distance from the first and the second atom to the critical point, Gcp- kinetic energy density [kJ/mol/Bohr <sup>3</sup> ], Vcp potential energy density [kJ/mol/Bohr <sup>3</sup> ], laplacian [ $\nabla^2(\rho_{\text{bcp}})$ ] (eÅ <sup>-5</sup> ), electron density [ $\rho_{\text{bcp}}$ ] (eÅ <sup>-3</sup> ) and eigenvalues of the Hessian matrix $\lambda_1, \lambda_2, \lambda_3$												

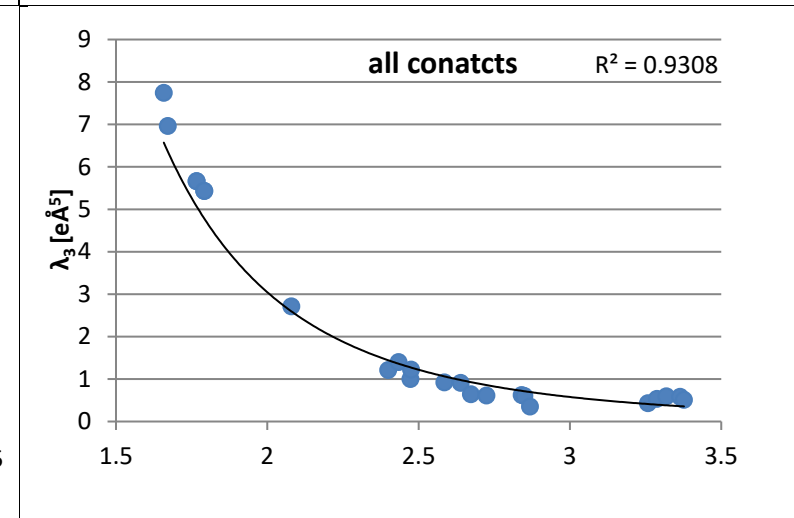
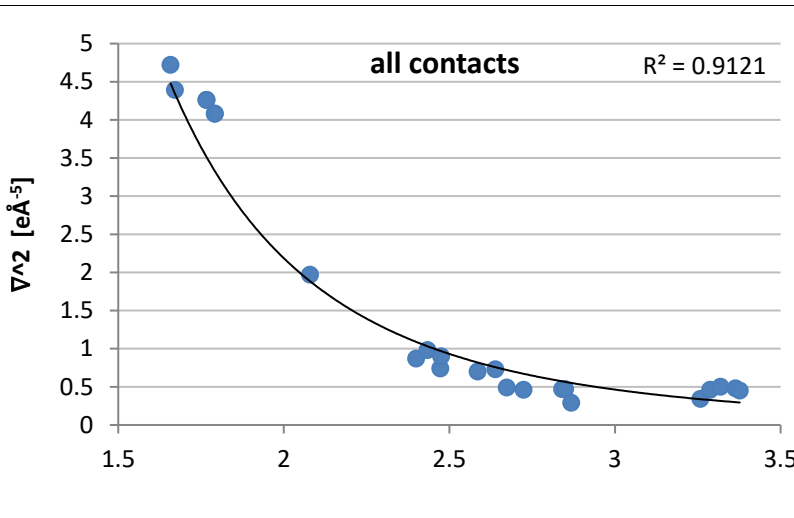
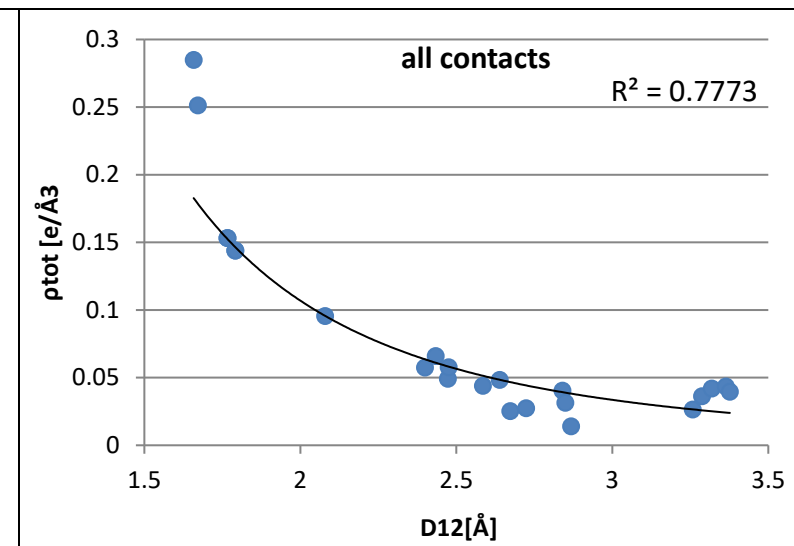
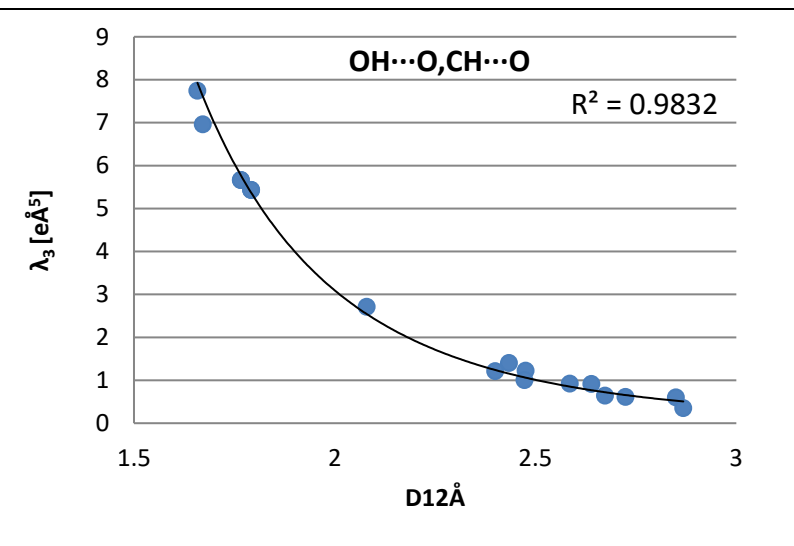
Table S8: Topological characteristic of the intermolecular critical points(3,1) in MPB·HBA

Atom1	Atom2	Gcp	Vcp	D12	D1cp	D2cp	$\rho_{\text{bcp}}$	$\nabla^2$	$\lambda_1$	$\lambda_2$	$\lambda_3$	ELLIP
Type: OH...O hydrogen bonds												
H5	O2	133,68	-133,94	1,6474	0,5371	1,111	0,3113	4,9	-1,84	-1,82	8,56	0,01
H3	O1	122,85	-121,63	1,6591	0,5541	1,1057	0,2917	4,55	-1,68	-1,63	7,87	0,03
Type: CH...O												
O1	H61	38,36	-30,99	2,2026	1,3184	0,9141	0,1097	1,68	-0,43	-0,41	2,52	0,04
O1	H71	35,69	-28,57	2,2513	1,3394	0,9383	0,1036	1,57	-0,37	-0,35	2,3	0,07
O5	H82	23,15	-15,95	2,3161	1,429	0,9132	0,0605	1,11	-0,24	-0,21	1,56	0,15
O4	H73	17,19	-12,16	2,6461	1,4505	1,2317	0,0535	0,82	-0,19	-0,1	1,11	0,82
O4	H22	17,74	-11,85	2,4316	1,4884	0,9467	0,0481	0,87	-0,14	-0,12	1,13	0,13
O2	H31	14,28	-9,95	2,6209	1,4863	1,1578	0,0464	0,68	-0,15	-0,13	0,96	0,12
O5	H81	17,88	-11,4	2,4148	1,4884	0,9346	0,0428	0,89	-0,14	-0,12	1,16	0,1
O4	H61	13,43	-9,11	2,7186	1,4933	1,2581	0,0422	0,65	-0,13	-0,11	0,89	0,19
O1	H73	13,66	-9,09	2,5623	1,4987	1,0691	0,0407	0,67	-0,13	-0,13	0,93	0,01
O2	H13	11,63	-7,61	2,6043	1,562	1,058	0,0354	0,57	-0,11	-0,08	0,76	0,45
O4	H52	10,39	-6,88	2,7762	1,5568	1,2422	0,0341	0,51	-0,09	-0,07	0,67	0,23
O1	H72	10,06	-6,48	2,7263	1,5612	1,1906	0,0312	0,5	-0,09	-0,08	0,68	0,1
O3	H62	11,14	-6,96	2,6227	1,5886	1,0397	0,0305	0,56	-0,08	-0,07	0,71	0,08
O5	H51	7,94	-5,06	2,8238	1,6745	1,2003	0,0263	0,4	-0,06	-0,04	0,5	0,53
O4	H72	8,39	-5,29	2,7806	1,6157	1,1989	0,0263	0,42	-0,07	-0,04	0,52	0,88
O2	H82	7,45	-4,7	2,991	1,6583	1,4078	0,0245	0,37	-0,05	-0,04	0,46	0,3
O3	H13	6,96	-4,34	2,8669	1,6355	1,2481	0,0228	0,35	-0,06	-0,06	0,47	0,05
Type: Weak van der Waals interactions												
C8	H82	10,14	-6,96	3,0021	1,7705	1,2634	0,0366	0,49	-0,12	-0,03	0,63	3,33
C13	H31	14,06	-10,19	2,6137	1,5459	1,0858	0,0498	0,66	-0,14	-0,06	0,86	1,59
C5	H32	7,61	-5,11	3,176	1,9176	1,308	0,0293	0,37	-0,06	-0,03	0,46	0,86
C2	H51	8,78	-5,91	3,0666	1,7523	1,348	0,0321	0,43	-0,08	-0,03	0,53	1,89
O3	C15	9,57	-6,51	3,2854	1,622	1,7682	0,0346	0,46	-0,07	-0,04	0,57	1,06
H16	H52	13,66	-10,16	2,2868	1,2019	1,0928	0,0513	0,63	-0,16	-0,16	0,95	0,03
H61	H71	8,74	-5,83	2,5116	1,2556	1,2563	0,0313	0,43	-0,09	-0,07	0,59	0,33
H12	H15	7,84	-5,19	2,6538	1,3403	1,3137	0,0288	0,39	-0,08	-0,06	0,52	0,22
H16	H12	8,11	-5,31	2,4602	1,314	1,1823	0,0287	0,4	-0,09	-0,07	0,56	0,21
H15	H13	7,93	-5,14	2,4584	1,1588	1,3323	0,0274	0,39	-0,08	-0,06	0,54	0,24
H41	H42	6,86	-4,43	2,6374	1,3471	1,3959	0,025	0,34	-0,06	-0,04	0,44	0,43
H71	H71	5,79	-3,65	2,7601	1,3801	1,3801	0,0211	0,29	-0,04	-0,03	0,37	0,35
H72	H72	5,3	-3,34	2,819	1,4095	1,4095	0,02	0,27	-0,06	-0,03	0,36	0,74
H22	H52	9,5	-6,55	2,5189	1,2877	1,3341	0,0355	0,46	-0,09	-0,06	0,6	0,4
H12	H12	11,49	-7,78	2,2027	1,1014	1,1014	0,0382	0,56	-0,14	-0,12	0,81	0,15
H15	H32	10,47	-7,24	2,3275	1,1237	1,2058	0,0379	0,5	-0,12	-0,11	0,74	0,04
H22	H52	9,5	-6,55	2,5189	1,2877	1,3341	0,0355	0,46	-0,09	-0,06	0,6	0,4

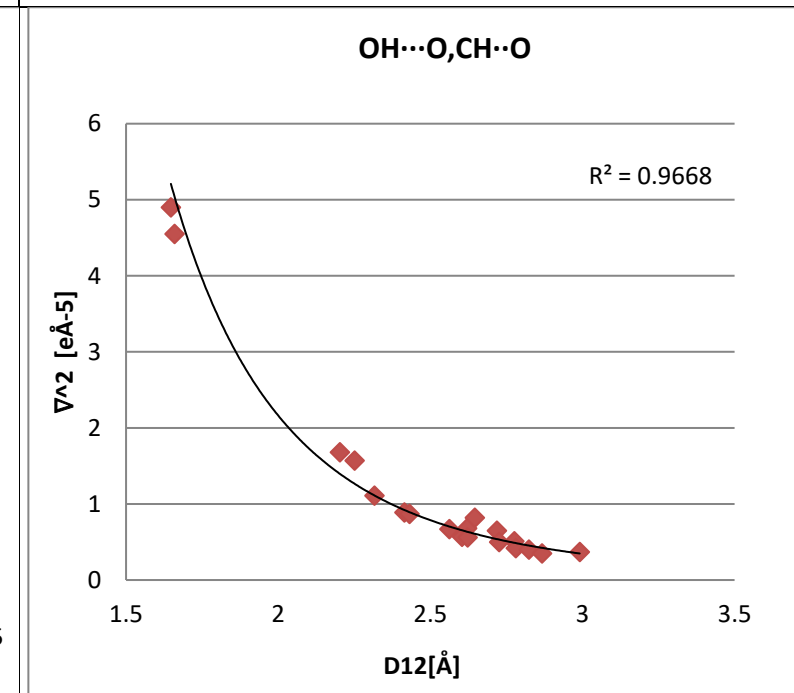
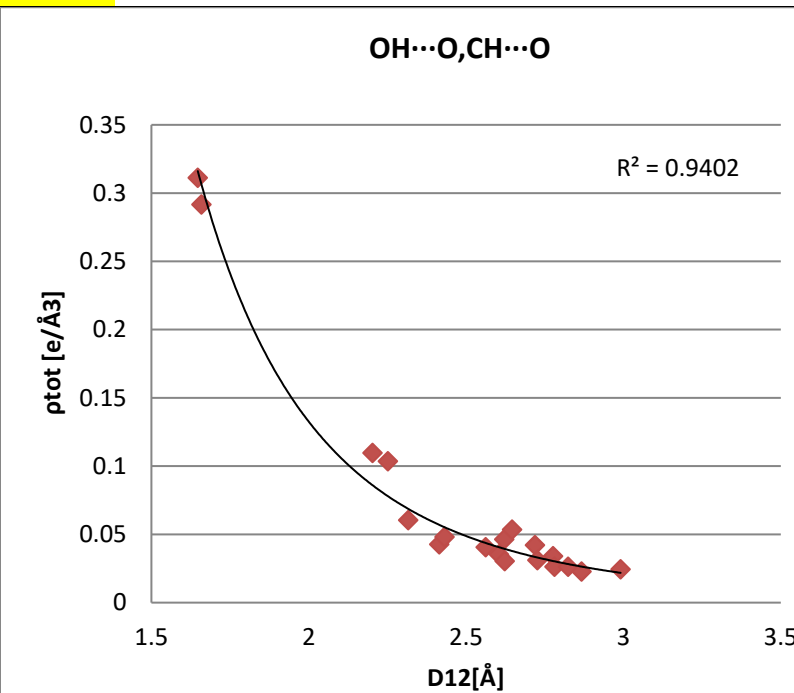
Table S8. Distances and topological characteristics of the CPs (3,1)

D12: distance between two atoms, D1cp, D2cp: distance from the first and the second atom to the critical point, Gcp- kinetic energy density [kJ/mol/Bohr<sup>3</sup>], Vcp potential energy density [kJ/mol/Bohr<sup>3</sup>] laplacian [ $\nabla^2(\rho_{\text{bcp}})$  (eÅ<sup>-5</sup>)], electron density [ $\rho_{\text{bcp}}$  (eÅ<sup>-3</sup>)] and eigenvalues of the Hessian matrix  $\lambda_1, \lambda_2, \lambda_3$





MPB-HBA



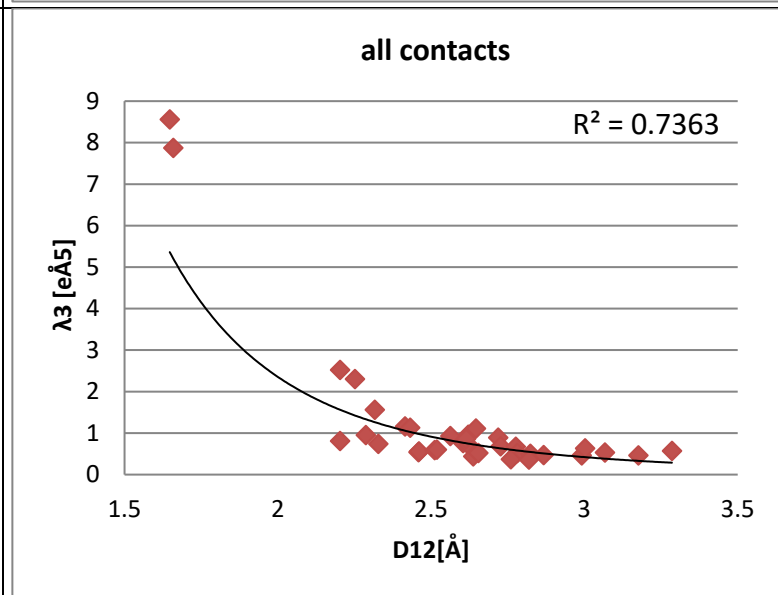
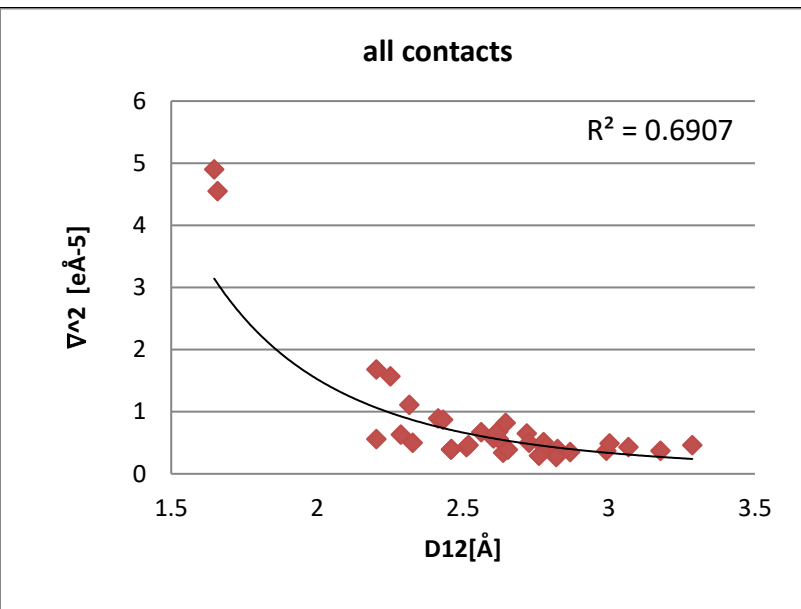
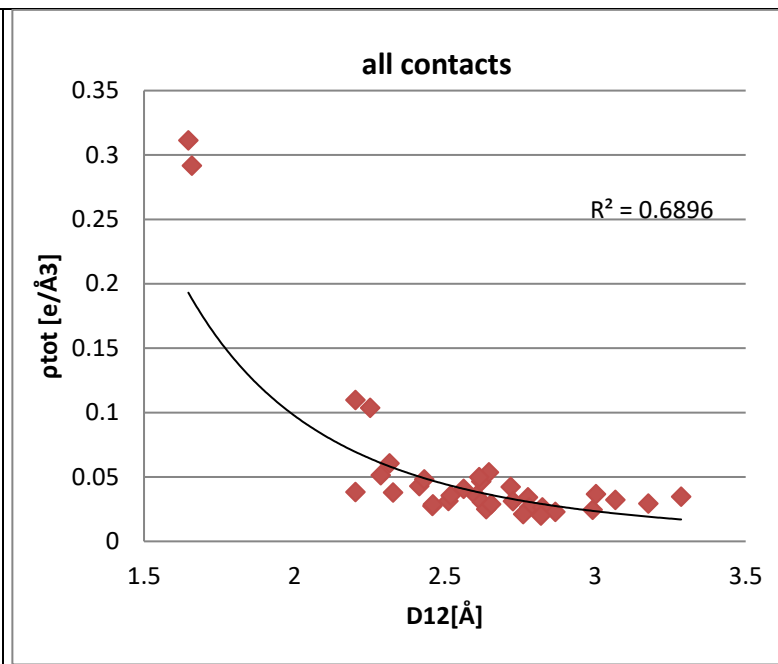
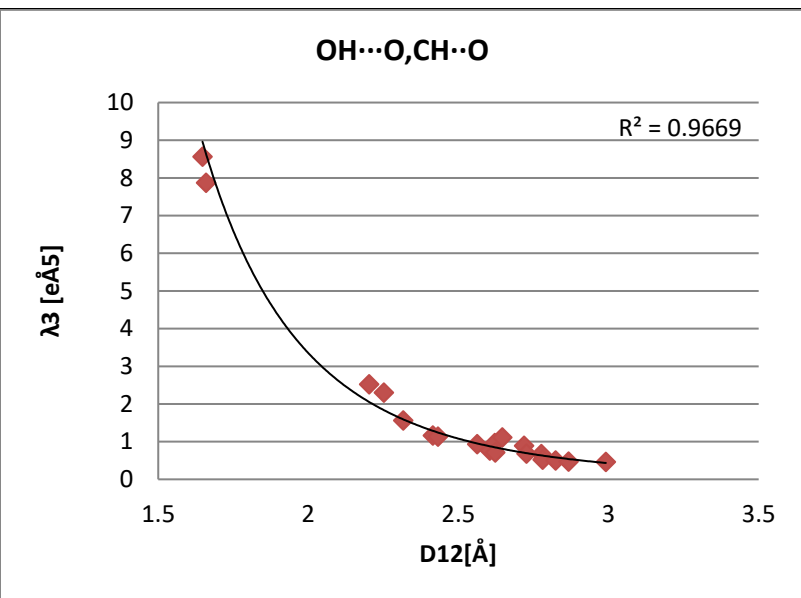


Fig. S6. Plots of CP characteristics as functions of interatomic distances for intermolecular interactions

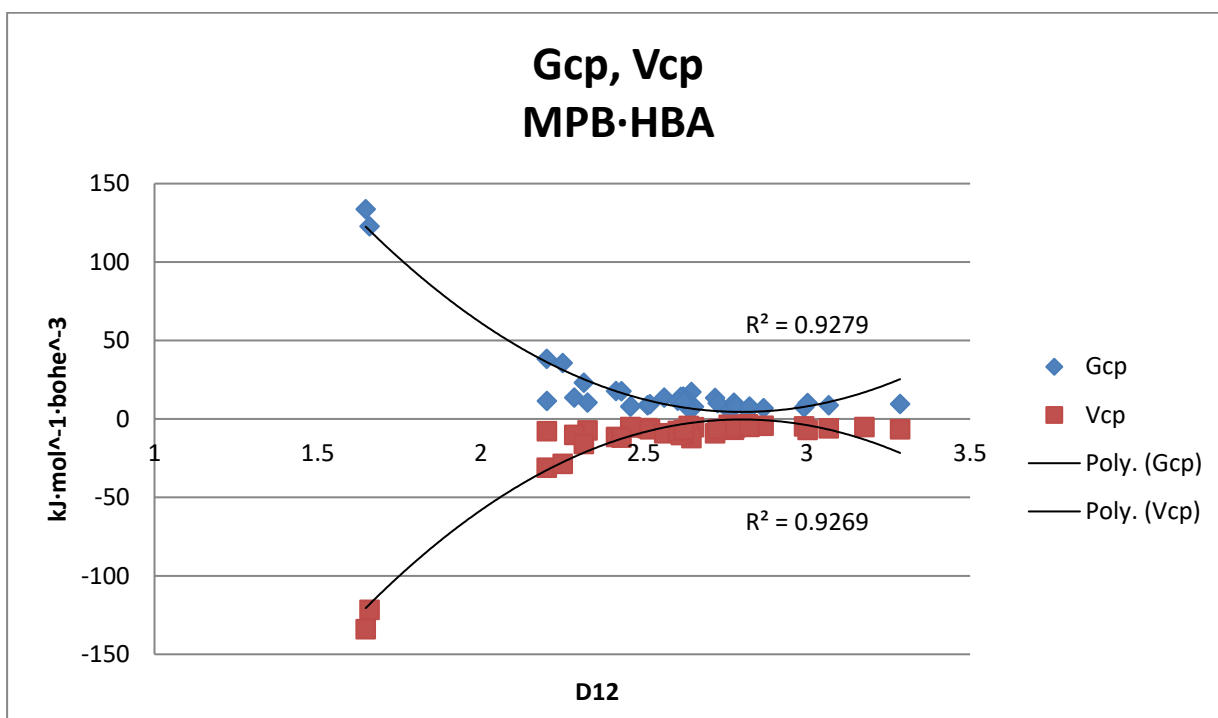
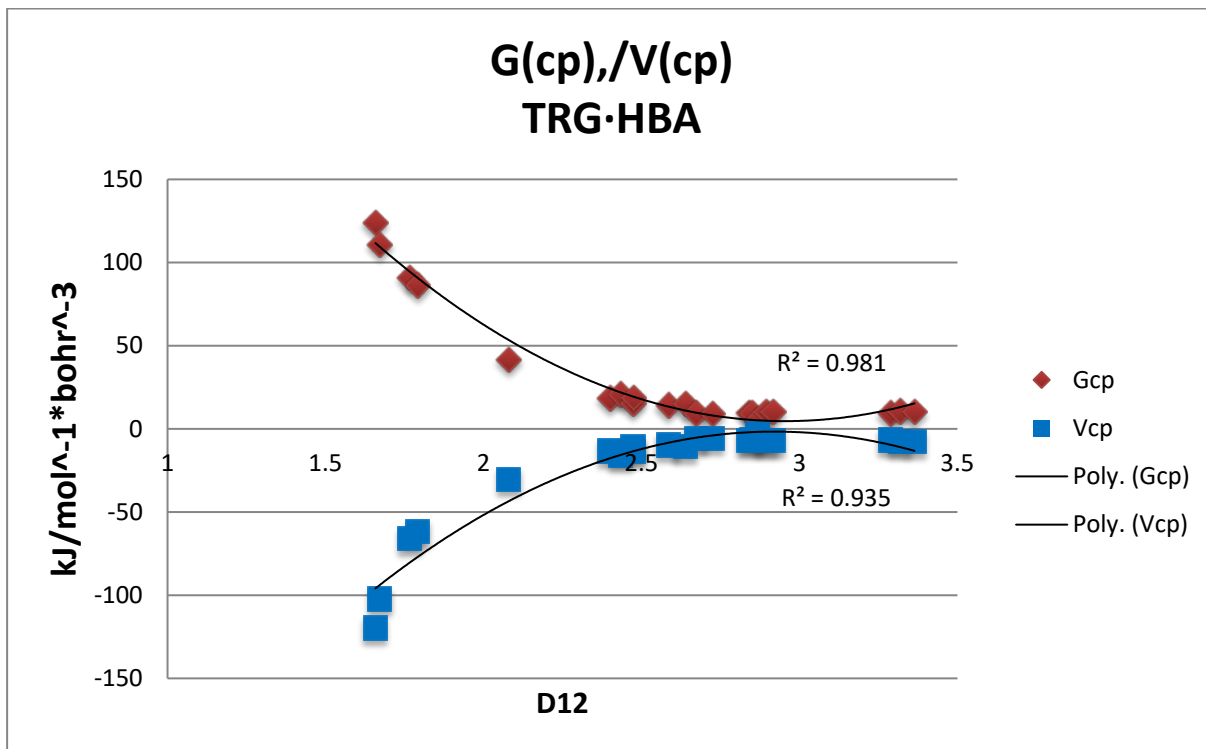


Fig. S7: Plots of kinetic and potential energies for critical points as a function of distance