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Supporting information for article:

Hydrogen- and halogen-bonding-directed trimeric supramolecular motifs in dihalogenated 1,2,4-triazoles

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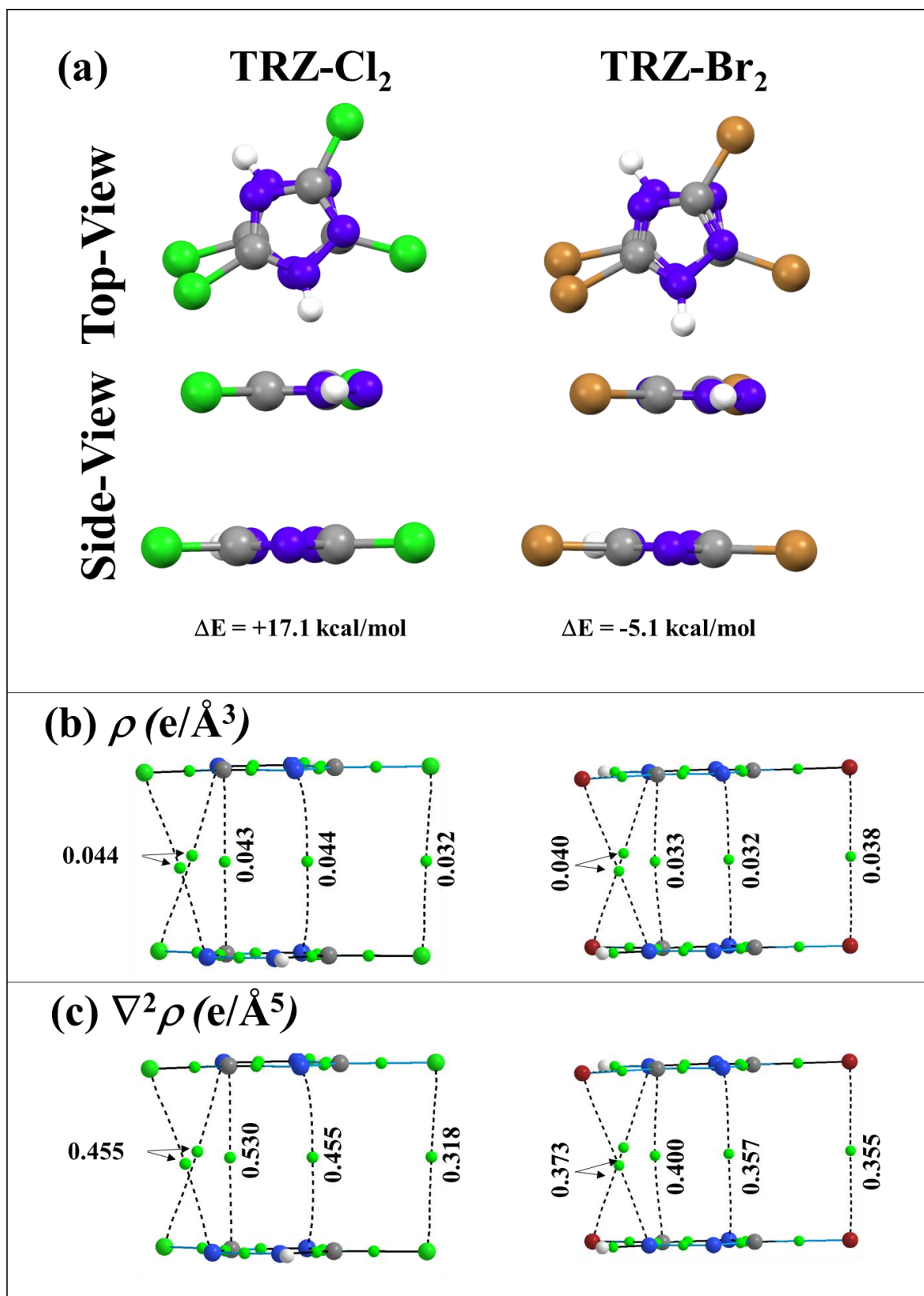


Figure S1. (a) The π -stacking dimer observed in the crystal structure of TRZ-Cl₂ and TRZ-Br₂. (b) The magnitude of ρ (e/Å³) at the BCP. (c) The magnitude of $\nabla^2\rho$ (e/Å⁵) at the BCP.

Table S1. CSD search result for Trimer-I

<i>Refcode</i>	θ_1 (°)	θ_2 (°)	θ_3 (°)	d_1 (Å)	d_2 (Å)	d_3 (Å)
GAQLIX	176.151	168.459	162.635	1.982	1.941	2.058
APURIO	163.261	167.61	161.246	2.034	2	2.042
APURIO	162.689	162.253	168.087	2.071	2.057	2.011
BECNIJ	168.587	164.227	161.699	2.088	2.128	2.106
BOKZUZ	155.396	166.183	150.429	2.01	1.999	2.246
BOKZUZ	158.37	151.908	164.128	2.122	2.162	2.01
BOKZUZ	153.904	153.326	164.566	2.123	2.085	2.07
BOKZUZ	150.257	168.818	154.183	2.226	2.001	2.15
CAYJEU	160.444	167.303	176.604	2.143	2.068	2.002
DATTAV	177.07	172.678	172.325	1.961	2.009	1.978
DATTAV	171.667	174.711	174.691	2.003	2.065	1.982
DEKWUN	167.843	173.41	161.116	2.031	1.994	2.095
DUGCUG	119.077	152.513	132.641	2.47	2.078	2.429
FITQAA	166.691	162.04	162.785	1.912	1.856	1.774
FITQAA	169.885	172.674	173.686	2.01	1.878	1.71
FUTMOZ	158.345	158.345	158.345	2.013	2.013	2.013
GARFOV	166.515	166.515	166.515	2.13	2.13	2.13
GIHJIS	169.851	166.032	172.681	2.006	1.972	1.926
HEHVAR	162.607	162.065	157.383	1.896	1.927	2.034
HOKNON	165.001	155.227	169.572	2.056	2.053	2.002
HOQHUQ	168.572	166.849	166.407	1.828	1.972	2.014
IHESIX	169.745	167.094	168.236	2.028	2.064	2.059
IHESIX	172.282	167.821	163.363	2.038	2.023	2.08
IHESIX	169.213	169.463	167.583	2.063	2.055	2.045
IJOKIB	166.552	164.533	163.526	1.959	1.954	1.972
KUYPAV	169.038	168.475	170.454	1.961	2.033	2.004
LABHEB	178.513	178.971	168.887	2.126	2.098	2.113
LABHEB	177.147	172.671	170.274	2.221	2.181	2.221
LABHEB01	170.28	170.848	164.294	2.026	1.996	2.034
LABHEB01	162.587	169.509	173.764	2.033	2.029	1.989
LEMNAT	172.969	159.884	165.9	1.974	2.039	2.041
LEPZUC	163.39	159.225	175.342	2.014	2.085	2.071

LEQBAL	163.994	167.501	171.472	2.014	2.042	1.992
LIJIY	168.762	162.475	173.197	2.006	2.044	2.105
MIGJUK	173.898	166.936	177.219	1.861	1.929	1.881
NEFCOR	170.375	168.014	172.7	2.07	1.979	1.992
NIHYEJ	173.991	169.649	170.807	1.971	1.965	1.945
PAMBEN	166.596	166.596	166.596	2.09	2.09	2.09
PAMTAY01	179.468	145.882	164.435	1.807	1.923	1.904
PESLEF	147.286	169.073	137.463	1.941	1.757	2.007
PESLEF	166.249	154.534	179.77	1.922	2.004	1.83
RIKNOO	169.703	169.757	169.667	2.014	2.009	2.062
RIKNOO	167.439	164.173	163.424	2.141	2.029	1.975
RUNJER	167.737	175.106	168.229	1.958	1.97	2.006
SAWKAD	175.009	173.281	173.55	1.992	2.022	1.83
SAWKAD	169.685	173.298	169.311	2.082	1.995	1.825
SUHVUM	148.267	146.097	148.752	2.272	2.283	2.224
SUHVUM01	154.973	157.416	157.617	2.442	2.417	2.382
UDAYUT02	172.492	172.462	165.931	2.079	2.126	2.166
UHENUQ	160.358	167.202	154.59	1.98	1.933	2.08
UHENUQ	161.123	160.25	171.991	2.062	1.972	1.991
UHENUQ01	163.181	164.277	171.198	2.014	1.991	2.051
VADVIH	174.172	177.277	175.212	1.998	1.831	1.969
VADVIH	171.865	176.531	173.354	1.833	1.877	1.952
VADVIH	163.718	173.718	166.837	2.104	1.944	1.828
VADVIH	164.184	178.055	175.392	1.859	2.077	1.922
VITRUL	149.976	149.976	149.976	1.97	1.97	1.97
VITRUL01	170.089	170.089	170.089	1.951	1.951	1.951
WIKZUL01	169.132	171.306	171.95	2.003	2.005	1.984
WUYKAD	138.468	155.288	128.722	2.011	1.863	2.108
YAXWAX	172.062	178.991	175.639	2.004	1.969	1.878
YAYGUC	171.438	178.847	173.089	2.133	2.124	2.151

Table S2. CSD search result for Trimer-II (X = Cl)

<i>Refcode</i>	θ_1 (°)	θ_2 (°)	θ_3 (°)	d_1 (Å)	d_2 (Å)	d_3 (Å)
HANDIK	163.691	167.518	175.461	2.928	3.199	3.16
KAYRUY	151.08	156.486	156.358	3.106	3.047	3.084

SIYPOI	170.479	174.669	174.669	3.195	3.133	3.133
UHAPIC	175.132	173.341	175.132	3.143	3.104	3.143
VITRUL	179.181	179.181	179.181	3.149	3.149	3.149
VITRUL01	179.361	179.361	179.361	3.086	3.086	3.086
VUGSIZ	180	172.912	172.912	3.1	3.112	3.112
VUGSIZ02	173.13	173.13	180	3.146	3.146	3.12
VUGSIZ10	180	172.912	172.912	3.1	3.112	3.112
VUGSIZ11	173.142	173.142	180	3.131	3.131	3.109
WARYAQ	170.157	173.118	173.118	3.153	3.157	3.157
XIZHIX	150.489	164.016	148.613	3.07	3.091	3.111

Table S3. CSD search result for Trimer-II (X = Br)

<i>Refcode</i>	θ_1 (°)	θ_2 (°)	θ_3 (°)	d_1 (Å)	d_2 (Å)	d_3 (Å)
NABVIV	176.706	176.706	176.706	3.072	3.072	3.072
UWUGOL	173.31	173.05	170.143	3	2.972	2.963

Table S4. CSD search result for Trimer-III (X = Cl)

<i>Refcode</i>	θ_1 (°)	θ_2 (°)	θ_3 (°)	d_1 (Å)	d_2 (Å)	d_3 (Å)
CARROE	172.774	163.014	133.952	3.381	3.452	3.49
EREQAT	166.861	166.861	166.861	3.275	3.275	3.275
HEXCET14	82.455	179.711	153.806	3.454	3.342	3.453
HEXCET14	149.661	123.835	143.444	3.353	3.384	3.444
HEXCET14	117.417	133.859	144.849	3.483	3.304	3.374
HEXCET14	159.483	144.849	153.806	3.351	3.374	3.453
HEXCET15	81.732	179.464	153.242	3.404	3.301	3.394
HEXCET15	149.302	123.462	143.502	3.312	3.339	3.393
HEXCET15	117.542	132.978	145.172	3.436	3.262	3.33
HEXCET15	159.156	145.172	153.242	3.303	3.33	3.394
ISURUL	159.05	147.766	92.396	3.448	3.263	3.486
MEQBOA	110.572	110.572	110.572	3.401	3.401	3.401
NIVSIW	112.461	112.461	112.461	3.39	3.39	3.39
NUXJUM04	130.849	98.572	86.62	3.263	3.436	3.413
PCPBPT	77.927	131.491	175.154	3.403	2.989	2.908
PUKDEH	141.189	146.931	95.853	3.418	3.49	3.38
PUKDEH	96.584	142.477	150.095	3.475	3.356	3.49

ROFHUP	173.68	173.68	173.68	3.382	3.382	3.382
UNUYOT02	115.24	121.187	103.178	3.456	3.371	3.44
UNUYOT04	113.107	121.359	101.367	3.438	3.332	3.432
UNUYOT05	115.472	119.569	101.695	3.393	3.281	3.391
UXIYOQ02	133.681	114.231	114.231	3.446	3.387	3.387
VEWJIQ	170.606	170.606	170.606	3.42	3.42	3.42
VITRUL01	172.733	172.733	172.733	3.448	3.448	3.448
VODWOB	117.172	117.172	117.172	3.342	3.342	3.342
XAXCOQ	132.406	132.406	132.406	3.366	3.366	3.366
XAXCOQ01	132.031	132.031	132.031	3.326	3.326	3.326
XAXTUL	156.741	157.035	157.874	3.495	3.488	3.48
XEHMAY	164.943	164.943	164.943	3.441	3.441	3.441
XEHMAY01	165.187	165.187	165.187	3.467	3.467	3.467
YEFNII	136.388	149.34	146.261	3.389	3.12	3.33
YEFNII	123.241	134.868	166.154	3.27	3.402	3.412
YEFNII	127.731	136.089	126.878	3.384	3.33	3.227
LEPMAY	143.212	117.766	124.242	3.419	3.365	3.382

Table S5. CSD search result for Trimer-III (X = Br)

<i>Refcode</i>	θ_1 (°)	θ_2 (°)	θ_3 (°)	d_1 (Å)	d_2 (Å)	d_3 (Å)
AZILIH	160.89	156.964	132.089	3.654	3.688	3.626
BUSFOM	153.303	174.607	175.221	3.637	3.526	3.648
CIKTOH	163.091	163.753	154.875	3.498	3.422	3.653
COCDED	121.964	123.605	125.185	3.625	3.62	3.668
COCDED01	121.503	123.261	125.426	3.623	3.616	3.659
COCGEH	123.828	123.828	123.828	3.462	3.462	3.462
DEMCEE	94.43	94.43	94.43	3.656	3.656	3.656
EQOYER	100.527	100.527	100.527	3.633	3.633	3.633
EQOYER	104.661	104.661	104.661	3.652	3.652	3.652
FEDSEN	171.403	150.743	172.173	3.637	3.638	3.561
GAPCAC	162.898	162.898	162.898	3.646	3.646	3.646
INEPIA	115.715	114.621	113.247	3.671	3.625	3.687
NABVIV	172.764	172.764	172.764	3.609	3.609	3.609
PAXREM	151.416	92.52	152.593	3.644	3.569	3.548
PEHGEP	112.237	112.237	112.237	3.44	3.44	3.44

PUZHIB	174.622	170.719	168.841	3.596	3.626	3.658
PUZHIB01	124.525	125.195	124.49	3.589	3.546	3.581
PUZHIB02	124.696	124.978	124.28	3.616	3.585	3.641
PUZHIB03	124.828	125.162	124.293	3.618	3.591	3.649
PUZHIB04	125.047	125.07	124.652	3.631	3.604	3.664
PUZHIB05	125.114	125.19	124.757	3.638	3.614	3.677
PUZHIB06	125.112	124.919	124.592	3.65	3.627	3.691
QOLWET	104.848	104.848	104.848	3.515	3.515	3.515
QOLWIX	165.296	165.296	165.296	3.558	3.558	3.558