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The crystalline state of rubrene materials: intermolecular recognition, isomorphism, polymorphism, and periodic bond-chain analysis of morphologies

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Appendix: crystallographic terminology

Throughout the article, the following notations/terms are extensively used:

[uvw] crystallographic direction. Any direction in a Bravais lattice is identified by a set of *N* indices (*N* dimensionality of the space), written in square brackets, called the direction indices. In three-dimensional space, the direction passing through the origin and the lattice nodes *nu*,*nv*,*nw* (*n* integer) has direction indices [*uvw*]. The indices [-*u*, -*v*, -*w*] identify the same direction as [*uvw*] observed from the opposite side.

<uvw> set of symmetry related crystallographic directions according to space group symmetry

(hkl) crystallographic plane identified by its Miller indices

{hkl} set of symmetry related crystallographic planes (form) according to space group symmetry

isomorphous crystals: two crystals are said to be isomorphous if (*a*) both have the same space group and unit-cell dimensions and (*b*) the types and the positions of atoms in both are the same except for a replacement of one or more atoms in one structure with different types of atoms in the other (diadochy), such as heavy atoms, or the presence of one or more additional atoms in one of them (*isomorphous addition*). Isomorphous crystals can form *solid solutions*

isostructural crystals: Two crystals are said to be *isostructural* if they have the same structure, but not necessarily the same cell dimensions nor the same chemical composition, and with a 'comparable' variability in the atomic coordinates to that of the cell dimensions and chemical composition. One also speaks of *isostructural series*. The term isotypic is synonymous with isostructural.

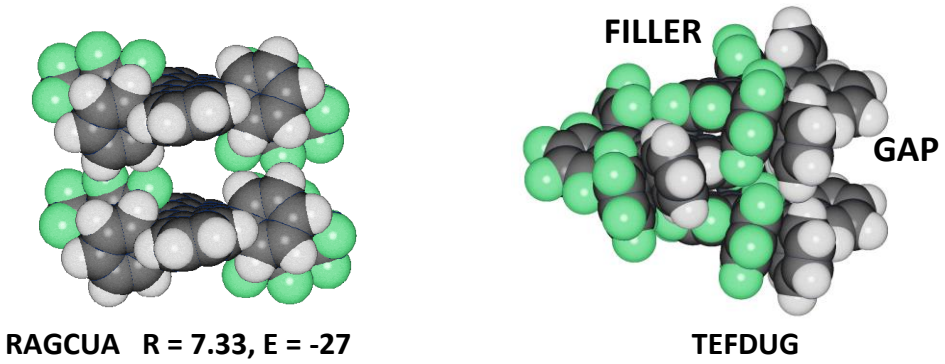

Figure S1. RAGCUA, short distance coupling with low stabilization due to parallel tetracene cores without offset. TEFDUG, close packing is restored by the insertion of another filler in the gap. These structures are outliers in the top left part of Figure 2b. Fluorine is green.

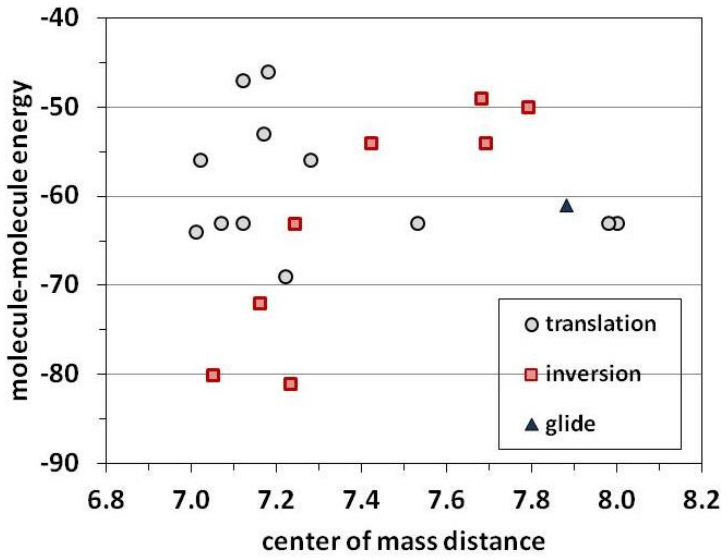

Figure S2. Molecule-Molecule energy (kJ/mol) vs. center of mass distance for the subset of slipped-cofacial pairings out of Figure 2b. No correlation

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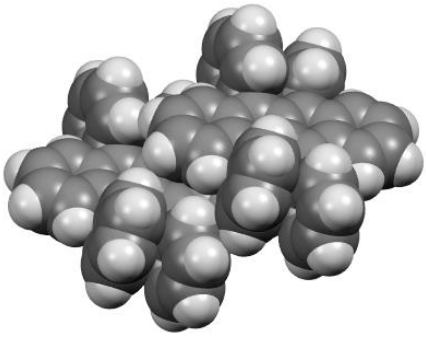
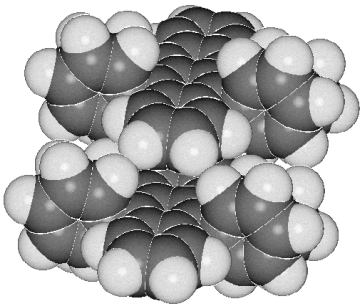


QQQCIG05



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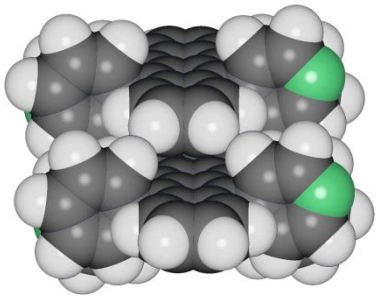
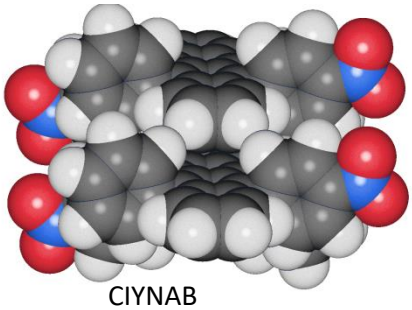
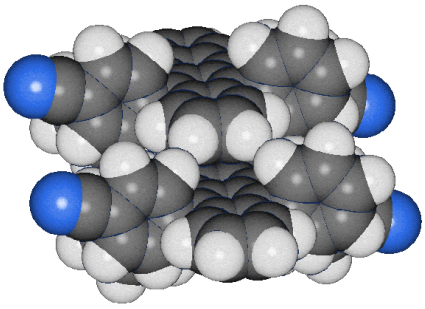


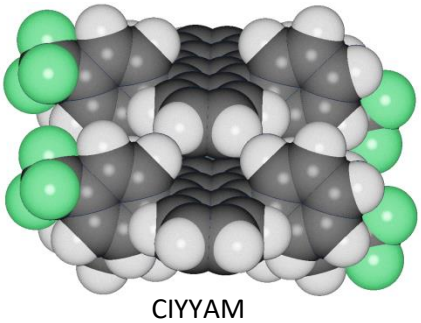
VICHAT



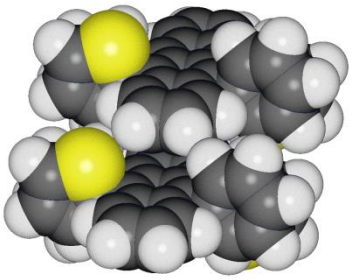
CIYNAB



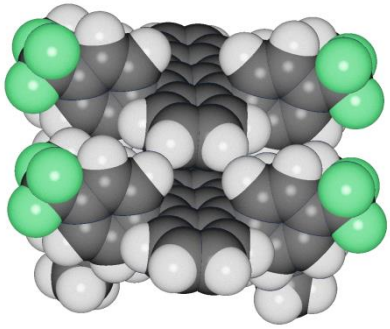
CIYXUF



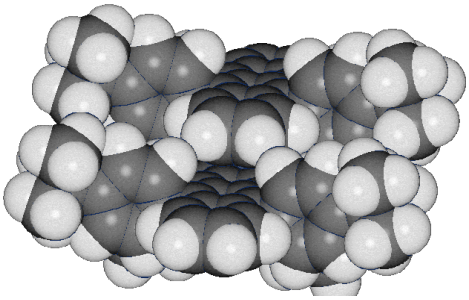
CIYYAM



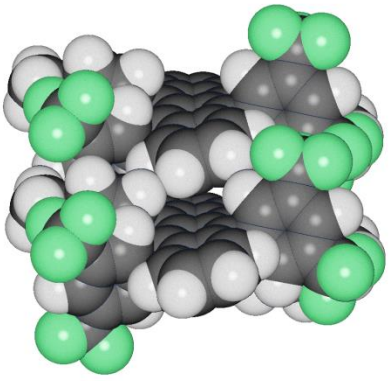
PIXPUJ



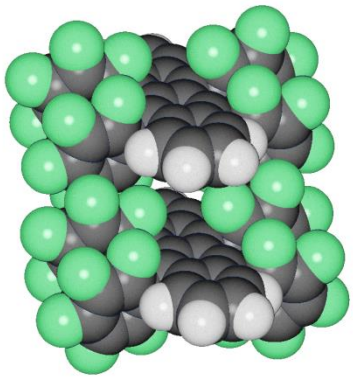
MIVDOM



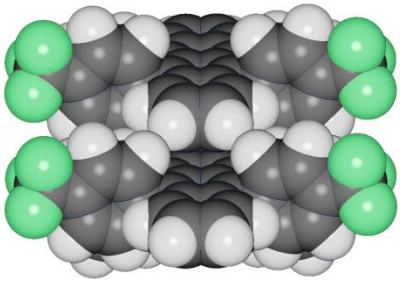
PIFHIW



RAGCEK



RAGDIP



MIVDUS

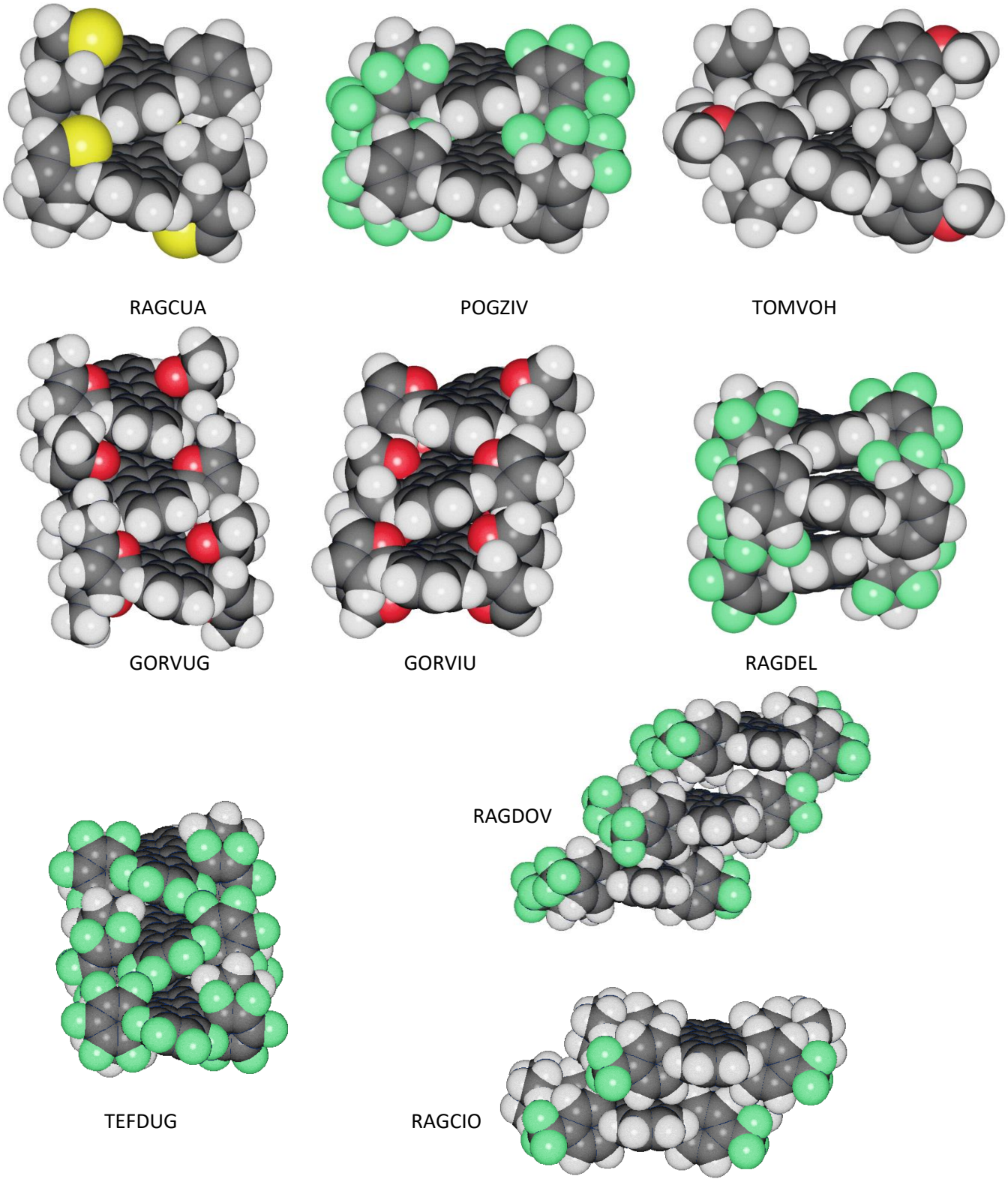


Figure S3. A gallery of slipped-cofacial arrangements with CSD refcodes (see Table 1).

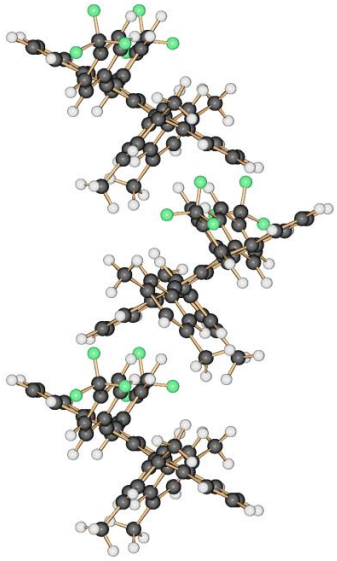


Figure S4. MIVDOM: the screw axis sequence -x, y± 1/2, 3/2-z with a very stabilizing pairwise energy; R(mm)=7.91 Å, E(mm)= -70 kJ mol^{-1}.

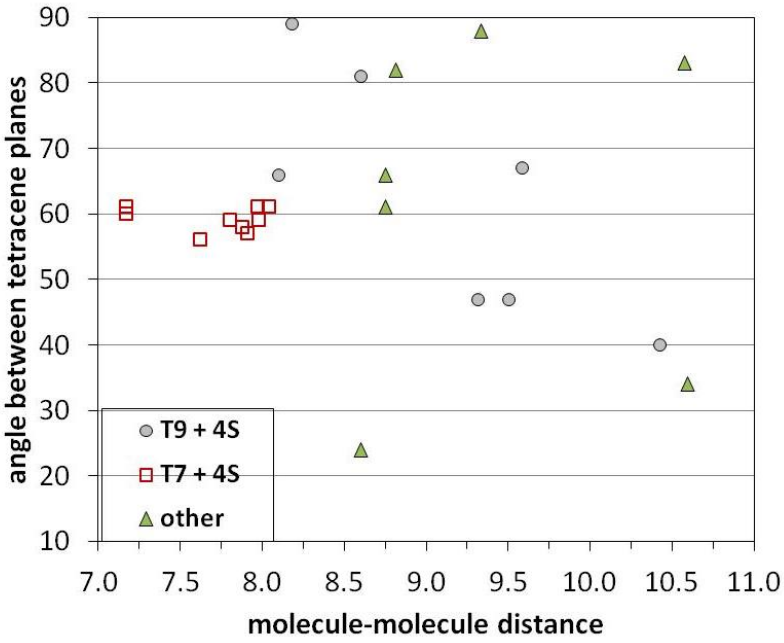
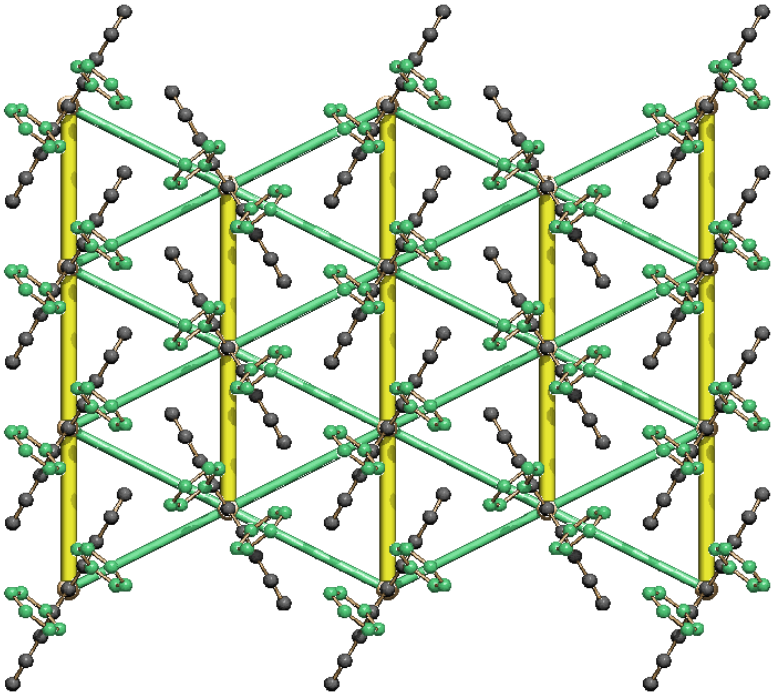
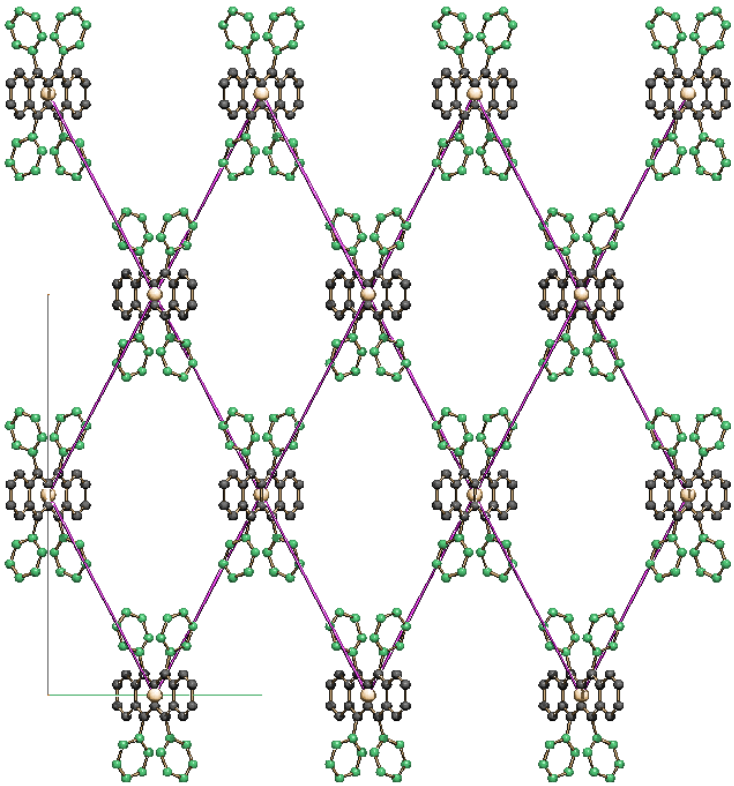


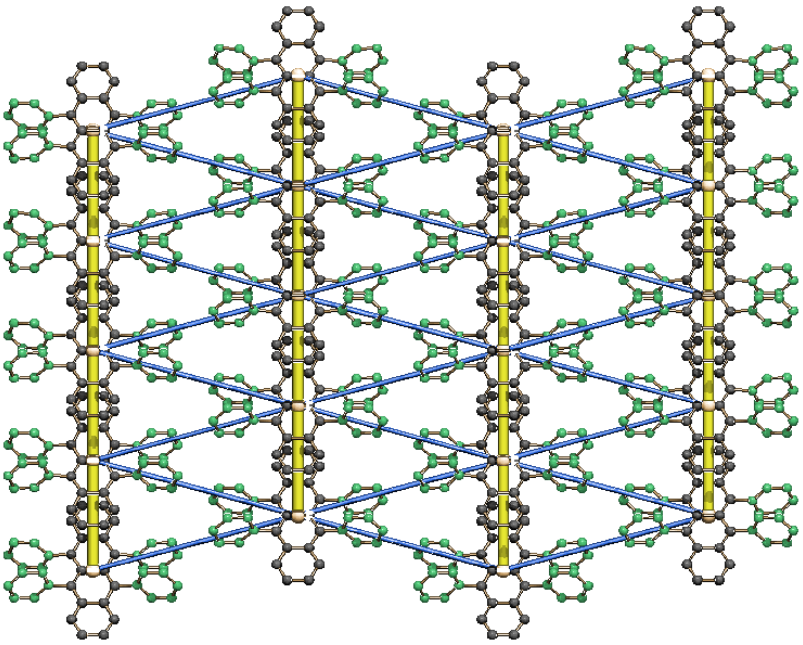
Figure S5. Plot of angles between tetracene planes in corrugated (herringbone) propagation motifs. The T7+4S cage motif (Figure 6a) has consistently a 60° angle.



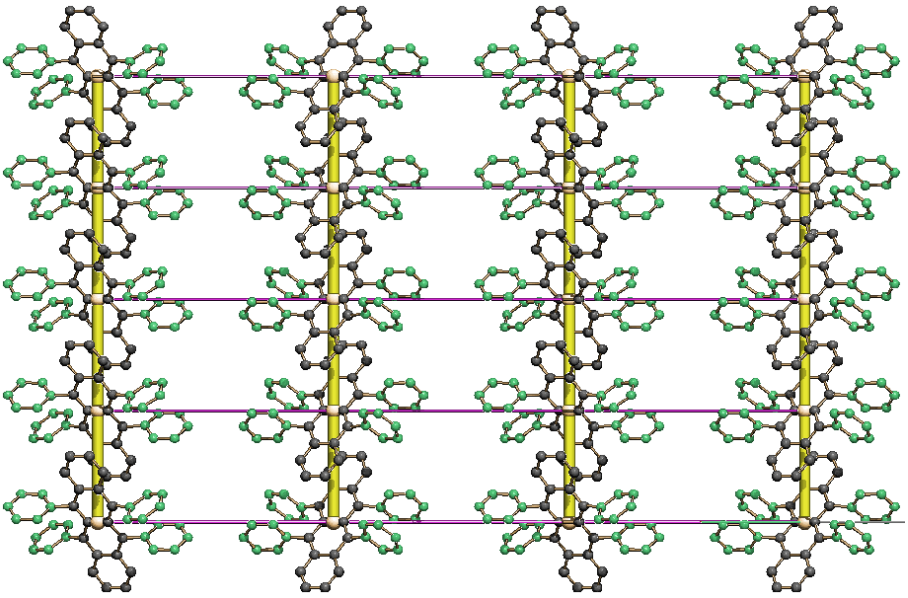
slice (200)



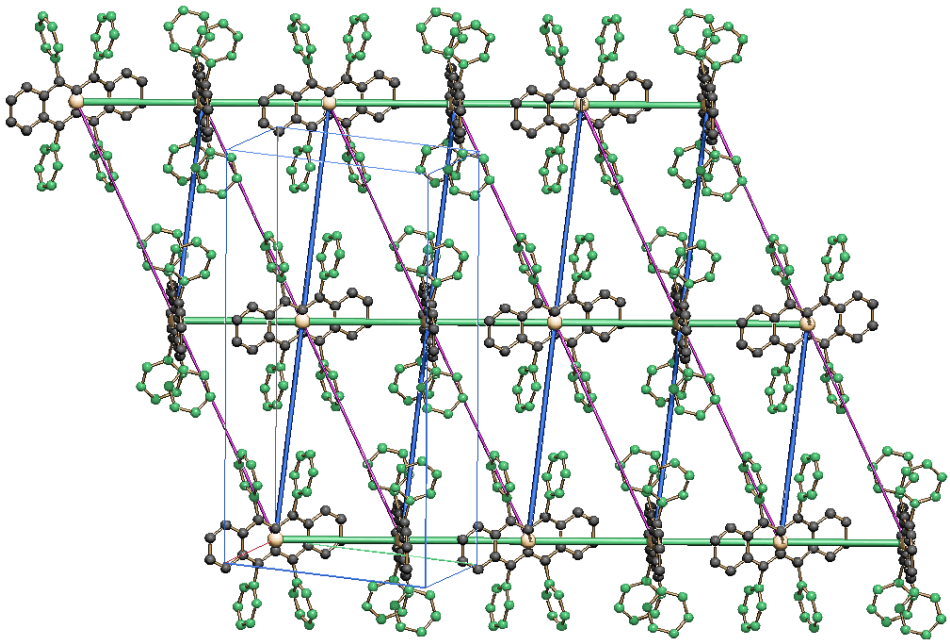
slice (020)



slice (002)

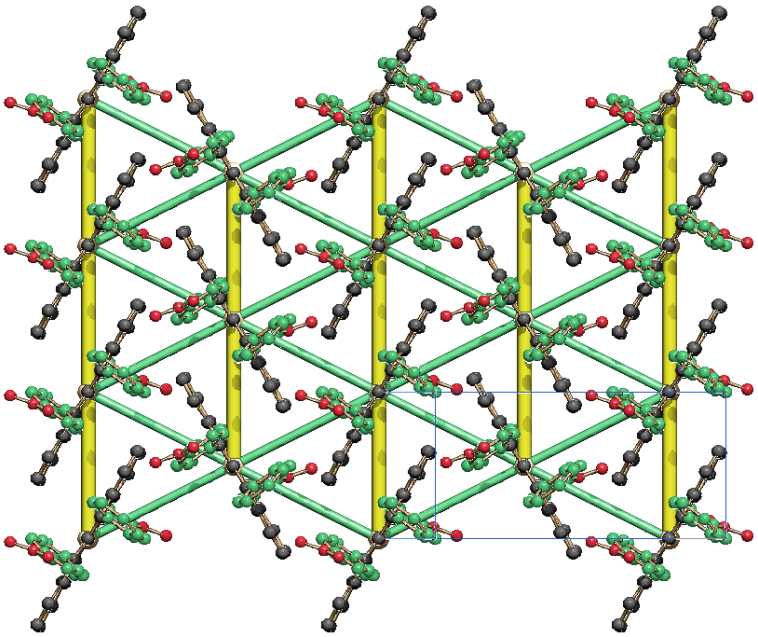


slice (202)

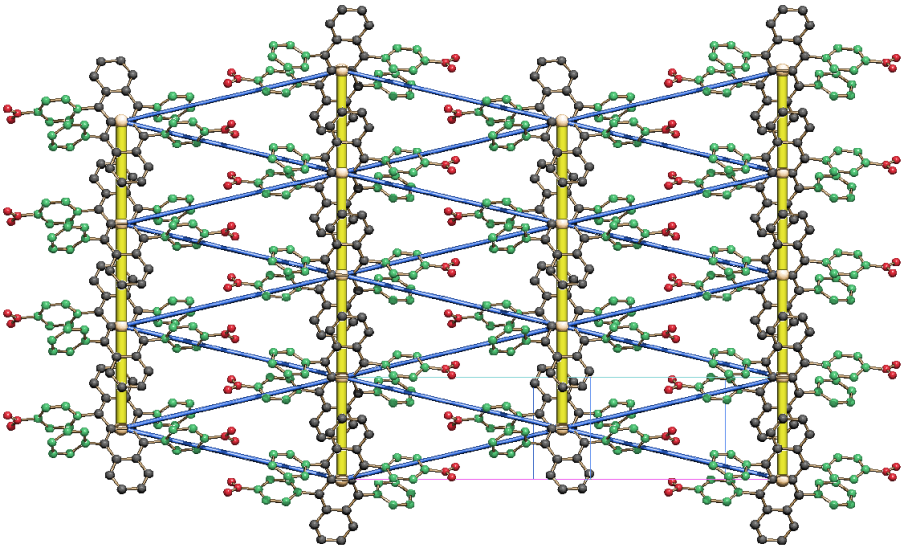


slice (111)

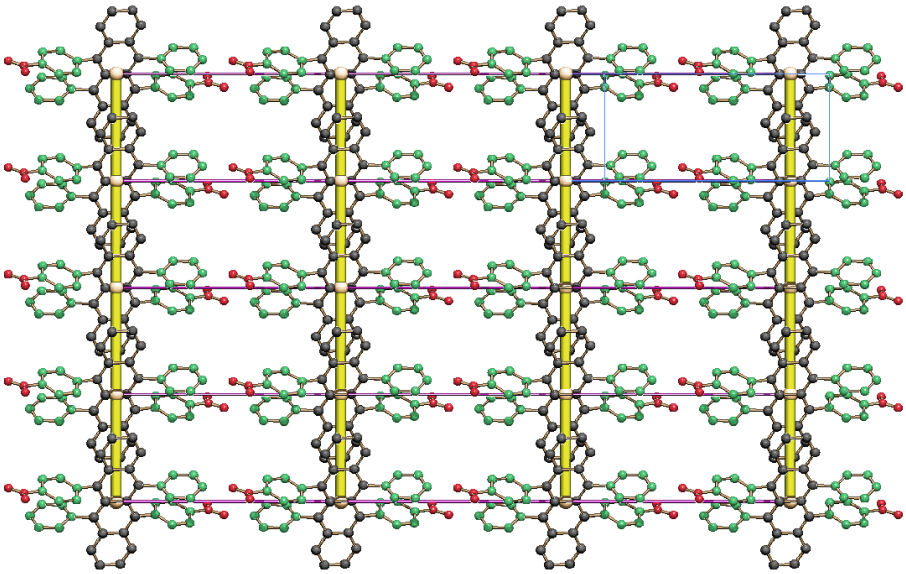
Figure S6. Energy crystal graphs in rubrene (QQQCIG05). Intermolecular bonds (see Table 3 in the manuscript) are color coded as: bond **a** yellow, bond **b** green, bond **c** cyan, bond **c** purple. All molecular plots and crystal graphs were prepared with program SCHAKAL (E. Keller SCHAKAL99, University of Freiburg - Germany, 1999).



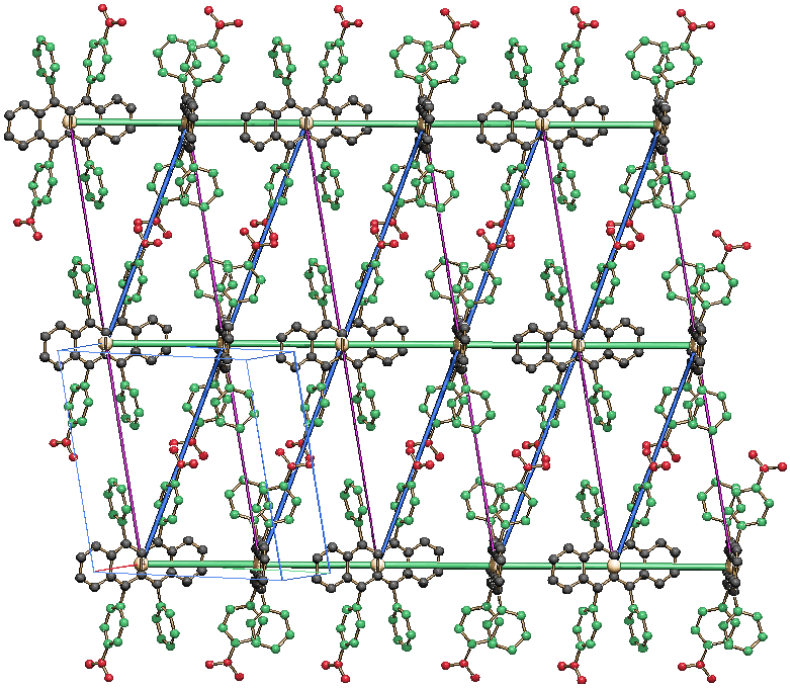
slice (100)



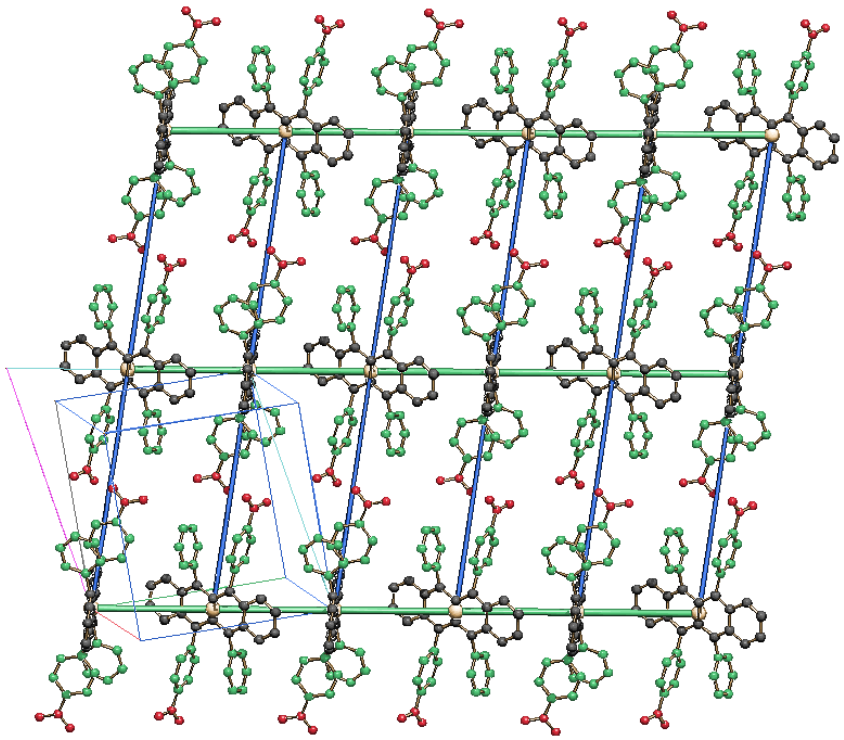
slice (10-2)



slice (002)



slice (011)



slice (11-1)

Figure S7. Energy crystal graphs in 5,11-bis(4-nitrophenyl)-6,12-diphenyltetracene (CIYNAB). Intermolecular bonds (see Table 4 in the manuscript) are color coded as: bond **a** yellow, bond **b** green, bond **c** cyan, bond **c** purple.

TABLE S1. List of all the rubrene crystal structures in the Cambridge Structural Database. From left to right: Identification code of the Cambridge Structural Database (CSD), Crystallographic *R*-factor, Spce group, Molecules in unit cell, Molecules in asymmetric unit, Temperature of data collection (K), Cell parameters (Å and degrees), Unit cell volume (Å^3), Reduced cell parameters (Å and degrees), Reduced cell volume (Å^3).

Refcode	Rfac	Space Group	Z	Z'	T	a	b	c	α	β	γ	Volume	Reduced a	Reduced b	Reduced c	Reduced α	Reduced β	Reduced γ	Reduced Volume
AXIDER	6.35	P21/c	2	0.5	293	9.0298	9.909	16.217	90	90.227	90	1451	9.0298	9.9085	16.217	90	90.227	90	1451
CIYNAB	6.73	P21/c	2	0.5	153	15.098	7.171	14.249	90	100.616	90	1516.2	7.1706	14.2489	15.0983	100.616	90	90	1516
CIYXUF	6.59	P21/c	2	0.5	123	15.978	7.276	13.981	90	102.701	90	1585.7	7.2762	13.9814	15.9782	102.701	90	90	1586
CIYYAM	6.65	P21/c	2	0.5	120	14.913	7.115	14.426	90	98.099	90	1515.4	7.1151	14.4263	14.9125	98.099	90	90	1515
GORVEQ	7.77	P212121	4	1	93	9.599	13.29	25.015	90	90	90	3190.5	9.599	13.287	25.015	90	90	90	3190
GORVIU	4.59	P-1	3	1.5	93	10.553	11.34	16.568	83.481	89.45	64.275	1772.9	10.553	11.34	16.568	83.481	89.45	64.275	1773
GORVIU01	4.6	P21/c	4	1	93	14.386	8.452	21.794	90	116.994	90	2361.2	8.452	14.386	19.9328	103.0291	90	90	2361
GORVUG	4.5	P-1	2	1	93	8.5037	13.24	14.277	62.458	80.781	74.581	1373.1	8.5037	13.244	14.277	62.458	80.781	74.581	1373
INELUK	5.62	P21/n	4	1	123	16.665	11.15	19.192	90	90.213	90	3565.8	11.1489	16.6651	19.1918	90.213	90	90	3566
INELUK01	6.87	P-1	6	3	123	12.529	17.82	24.734	90.202	101.264	90.695	5414	12.5285	17.8163	24.7339	90.202	101.264	90.695	5414
INELUK02	4.5	P21/c	2	0.5	173	8.9017	10.53	17.992	90	90.408	90	1686	8.9017	10.527	17.992	90	90.408	90	1686
INELUK03	7.34	P21/n	4	1	173	16.635	11.13	19.245	90	90.581	90	3564.1	11.1334	16.635	19.245	90.581	90	90	3564
KUSDEJ	5.27	Cmca	4	0.25	173	34.197	7.158	14.052	90	90	90	3439.5	7.1577	14.052	17.469	90	101.8218	90	1720
MIVCUR	4.75	C2/c	12	1.5	173	41.257	10.15	24.038	90	96.739	90	9993	10.1464	21.2432	24.038	96.5431	90	103.8166	4997
MIVDAY	4.31	P21	2	1	173	12.75	9.414	14.503	90	99.576	90	1716.4	9.4141	12.7495	14.5027	99.576	90	90	1716
MIVDEC	4.21	Pna21	4	1	173	15.205	13.9	14.31	90	90	90	3024.6	13.901	14.3104	15.2045	90	90	90	3025
MIVDIG	9.52	Pbcm	4	0.5	123	7.1443	14.05	34.143	90	90	90	3427.4	7.1443	14.051	34.143	90	90	90	3427
MIVDOM	7.61	Pbcm	4	0.5	123	7.5317	14.63	32.424	90	90	90	3573.7	7.5317	14.634	32.424	90	90	90	3574
MIVDUS	4.59	Pnma	4	0.5	123	7.1162	31.18	14.208	90	90	90	3152.3	7.1162	14.2075	31.179	90	90	90	3152
PIFHIW	7.42	Pnma	4	0.5	292	14.158	35.39	7.2215	90	90	90	3618.3	7.2215	14.158	35.39	90	90	90	3618
PIFHOC	9.77	P21/c	4	1	292	23.527	9.028	17.764	90	95.928	90	3752.8	9.0277	17.764	23.527	95.928	90	90	3753
PIXPOD	4.3	P21	2	1	173	11.401	8.994	13.989	90	113.59	90	1314.6	8.9944	11.401	13.989	113.59	90	90	1315
PIXPOD01	5.01	P21/c	4	1	93	13.601	9.248	20.718	90	92.771	90	2602.9	9.2479	13.601	20.718	92.771	90	90	2603
PIXPUJ	6.49	P21/c	2	0.5	173	10.173	8.915	14.751	90	95.17	90	1332.3	8.9148	10.173	14.751	95.17	90	90	1332
PIXPUJ01	6.87	P21/c	2	0.5	120	13.568	7.014	14.302	90	103.954	90	1320.9	7.0143	13.5679	14.302	103.954	90	90	1321
POGZIV	6.91	P21/c	8	2	294	22.036	8.803	30.252	90	104.921	90	5670.8	8.8034	22.036	30.252	104.921	90	90	5671

Refcode	Rfac	Space Group	Z	Z'	T	a	b	c	α	β	γ	Volume	Reduced a	Reduced b	Reduced c	Reduced α	Reduced β	Reduced γ	Reduced Volume
QQQCIG		Aba2	4	0.5	295	14.44	7.18	26.97	90	90	90	2796.2	7.18	13.9547	14.44	90	90	104.908	1398
QQQCIG01	3.2	Bbam	4	0.25	295	7.184	14.43	26.897	90	90	90	2788.9	7.184	13.9199	14.433	90	90	104.954	1394
QQQCIG02			1	0	295	9.15	11.6	7.16	103.53	112.97	90.98	675.28	0	0	0	0	0	0	0
QQQCIG03		P21/a	2	0.5	295	15.5	10.1	8.8	90	90.55	90	1377.6	8.8	10.1	15.5	90	90.55	90	1378
QQQCIG04	3.72	Cmca	4	0.25	100	26.789	7.17	14.211	90	90	90	2729.6	7.17	13.866	14.211	90	90	104.984	1365
QQQCIG05	3.77	Cmca	4	0.25	125	26.789	7.173	14.246	90	90	90	2737.5	7.173	13.8664	14.246	90	90	104.990	1369
QQQCIG06	3.87	Cmca	4	0.25	150	26.775	7.168	14.258	90	90	90	2736.4	7.168	13.8589	14.258	90	90	104.987	1368
QQQCIG07	3.88	Cmca	4	0.25	175	26.828	7.181	14.306	90	90	90	2756.1	7.181	13.8862	14.306	90	90	104.985	1378
QQQCIG08	4.07	Cmca	4	0.25	200	26.838	7.181	14.332	90	90	90	2762.1	7.181	13.8911	14.332	90	90	104.980	1381
QQQCIG09	4.05	Cmca	4	0.25	235	26.818	7.174	14.348	90	90	90	2760.4	7.174	13.8805	14.348	90	90	104.976	1380
QQQCIG10	4.19	Cmca	4	0.25	275	26.938	7.211	14.461	90	90	90	2809	7.211	13.9432	14.461	90	90	104.986	1405
QQQCIG11	4.4	Cmca	4	0.25	293	26.86	7.193	14.433	90	90	90	2788.5	7.193	13.9032	14.433	90	90	104.992	1394
QQQCIG12		Cmca	4	0.25	295	26.901	7.187	14.43	90	90	90	2789.9	7.187	13.9223	14.43	90	90	104.958	1395
QQQCIG13	4.94	P21/c	2	0.5	173	8.7397	10.13	15.635	90	90.98	90	1383.3	8.7397	10.125	15.635	90	90.98	90	1383
QQQCIG14	6.72	P-1	1	0.5	173	7.0196	8.543	11.948	93.04	105.58	96.28	683.5	7.0196	8.5432	11.948	93.04	105.58	96.28	684
QQQCIG15	4.02	Bbcm	4	0.25	293	7.175	14.44	26.812	90	90	90	2776.9	7.175	13.8777	14.435	90	90	104.981	1388
QQQCIG16	4.6	Cmca	4	0.25	100	26.797	7.162	14.194	90	90	90	2724	7.1617	13.8689	14.194	90	90	104.963	1362
QQQCIG17	2.2	Cmca	4	0.25	100	26.811	7.16	14.203	90	90	90	2726.5	7.1602	13.8751	14.2029	90	90	104.953	1363
QQQCIG18	2.2	Cmca	4	0.25	100	26.811	7.16	14.203	90	90	90	2726.5	7.1602	13.8751	14.2029	90	90	104.953	1363
QQQCIG19	4.7	Cmca	4	0.25	100	26.811	7.16	14.203	90	90	90	2726.5	7.1602	13.8751	14.2029	90	90	104.953	1363
QQQCIG20	3.3	Cmca	4	0.25	100	26.811	7.16	14.203	90	90	90	2726.5	7.1602	13.8751	14.2029	90	90	104.953	1363
QQQCIG21	2.57	Cmca	4	0.25	100	26.811	7.16	14.203	90	90	90	2726.5	7.1602	13.8751	14.2029	90	90	104.953	1363
QQQCIG22	2.2	Cmca	4	0.25	100	26.811	7.16	14.203	90	90	90	2726.5	7.1602	13.8751	14.2029	90	90	104.953	1363
QQQCIG23	2	Cmca	4	0.25	20	26.797	7.16	14.152	90	90	90	2715.2	7.1599	13.8683	14.1519	90	90	104.960	1358
QQQCIG24	5.89	P-1	1	0.5	293	7.0478	8.55	11.949	93.201	105.501	96.079	687.21	7.0478	8.5495	11.9485	93.201	105.501	96.079	687
QQQCIG25	4.5	P-1	1	0.5	293	6.8535	8.264	11.657	91.614	104.921	96.311	633.03	6.8535	8.2642	11.6573	91.614	104.921	96.311	633
QQQCIG26	6.02	P-1	1	0.5	293	6.7392	8.059	11.464	90.271	104.627	96.329	598.44	6.7392	8.0591	11.4641	90.271	104.627	96.329	598
QQQCIG27	6.56	P-1	1	0.5	293	6.6779	7.926	11.342	89.367	104.46	96.321	577.63	6.6779	7.9256	11.3415	89.367	75.54	83.679	578
QQQCIG28	6.39	P-1	1	0.5	293	6.635	7.8	11.218	88.437	104.348	96.316	559.02	6.635	7.7995	11.2182	88.437	75.652	83.684	559
QQQCIG29	5.61	P-1	1	0.5	293	6.6162	7.676	11.1	87.399	104.322	96.289	542.81	6.6162	7.6757	11.1002	87.399	75.678	83.711	543
QQQCIG30	6	P-1	2	1	293	14.24	6.774	11.281	81.264	100.378	101.773	1040.3	6.7738	11.281	14.2395	79.622	78.227	81.264	1040

Refcode	Rfac	Space Group	Z	Z'	T	a	b	c	α	β	γ	Volume	Reduced a	Reduced b	Reduced c	Reduced α	Reduced β	Reduced γ	Reduced Volume
QQQCIG31	5.24	P-1	1	0.5	293	7.0883	8.599	12.006	93.486	105.642	95.977	697.86	7.0883	8.5994	12.0059	93.486	105.642	95.977	698
QQQCIG32	5.26	P-1	1	0.5	293	7.082	8.58	11.982	93.36	105.63	96.02	694.41	7.082	8.58	11.982	93.36	105.63	96.02	694
QQQCIG33	2.56	Cmca	4	0.25	100	26.797	7.162	14.194	90	90	90	2724	7.1617	13.8689	14.194	90	90	104.963	1362
RAGCEK	5.59	P21/c	4	1	123	15.88	29.54	7.9956	90	91.745	90	3749.2	7.9956	15.88	29.5419	90	90	91.745	3749
RAGCIO	6.14	P2/c	4	1	123	31.29	7.403	17.207	90	90.524	90	3985.7	7.403	17.2071	31.2902	90.524	90	90	3986
RAGCOU	6.82	P21	4	2	123	16.408	15.28	16.446	90	97.838	90	4084	15.2768	16.4083	16.4464	97.838	90	90	4084
RAGCUA	3.74	C2/c	4	0.5	123	31.027	14.68	7.3302	90	93.322	90	3332.5	7.3302	14.6772	17.1618	115.316	93.003	90	1666
RAGDAH	3.23	P21/n	4	1	123	14.856	9.198	27.452	90	103.528	90	3647.1	9.1983	14.8556	27.4515	103.528	90	90	3647
RAGDEL	4.71	P-1	2	1	123	7.3564	14.7	15.712	65.973	88.823	89.903	1551.9	7.3564	14.7042	15.7118	65.973	88.823	89.903	1552
RAGDIP	3.89	P-1	2	1	123	7.9792	12.79	16.774	92.313	95.376	105.306	1640.5	7.9792	12.793	16.7743	92.313	95.376	105.306	1641
RAGDOV	7.13	C2/c	4	0.5	123	18.275	16.4	14.486	90	126.468	90	3490.8	12.2764	12.2764	14.2549	110.888	114.307	96.201	1745
TEFDUG	7.48	Pnna	4	0.5	173	15.521	28.08	7.3931	90	90	90	3222.2	7.3931	15.5207	28.081	90	90	90	3222
TOMVOH	4.15	Pbca	8	1	120	15.766	13.86	28.351	90	90	90	6194.7	13.859	15.766	28.351	90	90	90	6195
TOMVUN	5.49	Cmca	4	0.25	120	27.45	7.102	14.327	90	90	90	2793	7.102	14.1769	14.327	90	90	104.506	1397
TOMWAU	5.59	P21/n	4	1	120	17.677	9.424	18.571	90	103.79	90	3004.5	9.424	17.677	18.571	103.79	90	90	3005
VICHAT	4.09	P-1	1	0.5	100	7.0727	8.27	11.855	90.402	106.039	97.605	659.84	7.0727	8.2696	11.855	90.402	106.039	97.605	660

Table S2. Comparison of the CLP, LJC and Pixel force fields for some molecule-molecule energies in some isostructural rubrene derivatives. For each entry:

molecule-molecule distance (Å), symmetry operation number
LJC energies (kJ mol^{-1}), Coulombic, polarization, dispersion, repulsion, total
PIXEL energies, id.
CLP energies, id.

	symmetry operation		
1	x, y, z		cell translation
2	-x, 1/2+y, 1/2-z		screw axis

CIYXUF	7.880	2	0.00	-0.50	-0.50	
	-6.7	0.0	-73.9	27.4	-53.2	
	-17.21	-7.26	-64.40	38.08	-50.79	
	-6.1	-4.7	-58.8	18.6	-51.0	
	7.276	1	0.00	-1.00	0.00	
	8.2	0.0	-109.9	41.4	-60.4	
	-3.88	-10.47	-97.94	54.91	-57.38	
	7.7	-5.2	-87.9	29.7	-55.7	
CIYYAM	8.043	2	0.00	-0.50	-0.50	
	-5.3	0.0	-62.9	20.7	-47.4	
	-13.28	-5.98	-57.73	29.46	-47.53	
	-4.6	-4.0	-50.6	12.8	-46.4	
	7.115	1	0.00	-1.00	0.00	
	11.7	0.0	-107.8	39.6	-56.5	
	-1.09	-11.51	-97.73	54.06	-56.26	
	10.5	-5.0	-87.1	34.5	-47.2	
CIYNAB	7.976	2	0.00	-0.50	-0.50	
	-5.5	0.0	-70.2	24.7	-51.0	
	-14.71	-7.28	-62.94	34.60	-50.34	
	-4.1	-4.9	-56.0	15.6	-49.4	
	7.171	1	0.00	-1.00	0.00	
	11.6	0.0	-109.7	42.4	-55.6	
	-1.84	-12.79	-99.26	57.06	-56.84	
	11.2	-5.5	-88.5	36.7	-46.0	

Table S3. Energy (CLP) and density data for the crystal structures in the database.

For each entry:
first line: CSD refcode Cell vol (Å^3) density (g cm^{-3}) packing factor
second line: CSD refcode Ecoul Epol Edisp Erep Etot (kJ mol^{-1})

AXIDER	P21/c	1450.95	1.384	0.721		
AXIDER	P21/c	-11.8	-26.2	-228.3	69.7	-196.6
CIYNAB	P21/c	1516.24	1.364	0.738		
CIYNAB	P21/c	-19.3	-35.1	-269.3	107.8	-215.8
CIYNAB01	P-1	775.14	1.334	0.718		
CIYNAB01	P-1	-15.0	-32.1	-243.0	73.2	-216.8
CIYXUF	P21/c	1585.71	1.401	0.716		
CIYXUF	P21/c	-7.5	-29.1	-256.7	86.9	-206.5
CIYYAM	P21/c	1515.42	1.277	0.723		
CIYYAM	P21/c	-24.8	-29.5	-251.7	83.9	-222.1
GORVIU01	P21/c	2361.24	1.386	0.736		
GORVIU01	P21/c	-17.1	-26.9	-230.3	77.0	-197.2
GORVUG	P-1	1373.07	1.327	0.724		
GORVUG	P-1	-11.7	-49.5	-259.8	100.0	-221.0
INELUK	P21/n	3565.76	1.931	0.723		
INELUK	P21/n	-34.6	-35.4	-229.3	115.1	-184.2
INELUK02	P21/c	1685.96	2.042	0.765		
INELUK02	P21/c	-47.5	-38.6	-262.4	133.4	-215.1
MIVCUR	C2/c	9993.03	1.174	0.680		
MIVCUR	C2/c	-8.3	-29.7	-231.0	75.0	-194.0
MIVDOM	Pbcm	3573.74	1.347	0.704		
MIVDOM	Pbcm	-7.2	-40.5	-257.9	81.7	-223.9
PIFHOC	P21/c	3752.80	1.141	0.672		
PIFHOC	P21/c	-5.8	-35.7	-226.6	59.6	-208.5
PIXPOD01	P21/c	2602.88	1.421	0.724		
PIXPOD01	P21/c	-16.4	-40.5	-241.7	72.0	-226.6
PIXPUJ01	P21/c	1320.94	1.370	0.740		
PIXPUJ01	P21/c	-8.3	-31.2	-250.3	68.2	-221.5
POGZIV	P21/c	5670.76	1.276	0.685		
POGZIV	P21/c	-2.4	-27.7	-206.6	53.0	-183.7
RAGDAH	P21/n	3647.07	1.531	0.700		
RAGDAH	P21/n	-19.4	-37.8	-241.9	105.8	-193.2
MIVDAY	P21	1716.43	1.194	0.699		
MIVDAY	P21	-9.5	-36.4	-250.3	76.8	-219.4
MIVDEC	Pna21	3024.61	1.231	0.709		
MIVDEC	Pna21	-7.0	-26.3	-241.6	76.2	-198.7
MIVDUS	Pnma	3152.30	1.409	0.719		
MIVDUS	Pnma	-4.0	-29.1	-252.5	82.4	-203.2
PIFHIW	Pnma	3618.34	1.184	0.697		
PIFHIW	Pnma	-2.5	-37.5	-262.0	65.2	-236.9
QQQCIG05	Cmca	2737.48	1.293	0.739		
QQQCIG05	Cmca	-9.8	-22.7	-252.0	79.3	-205.1
QQQCIG13	P21/c	1383.33	1.279	0.731		
QQQCIG13	P21/c	-15.7	-22.3	-241.6	72.7	-206.8
QQQCIG14	P-1	683.50	1.294	0.740		
QQQCIG14	P-1	-4.1	-22.8	-246.4	76.9	-196.4
RAGCEK	P21/c	3749.20	1.475	0.703		

RAGCEK	P21/c	-7.1	-40.9	-252.8	97.1	-203.7
RAGCIO	P2/c	3985.71	1.301	0.696		
RAGCIO	P2/c	-9.8	-45.6	-257.1	79.7	-232.7
RAGCUA	C2/c	3332.51	1.620	0.728		
RAGCUA	C2/c	-10.4	-34.2	-254.3	113.7	-185.3
RAGDEL	P-1	1551.92	1.525	0.715		
RAGDEL	P-1	-13.8	-25.8	-230.4	105.8	-164.1
RAGDIP	P-1	1640.50	1.807	0.737		
RAGDIP	P-1	-17.0	-32.3	-245.1	108.4	-186.0
RAGDOV	C2/c	3490.80	1.531	0.718		
RAGDOV	C2/c	-17.8	-37.1	-262.9	96.2	-221.6
TEFDUG	Pnna	3222.18	1.617	0.714		
TEFDUG	Pnna	-26.6	-28.0	-231.8	108.1	-178.3
TOMVOH	Pbca	6194.72	1.271	0.718		
TOMVOH	Pbca	-10.7	-30.0	-256.7	86.8	-210.7
TOMWAU	P21/n	3004.53	1.324	0.720		
TOMWAU	P21/n	-19.5	-28.0	-250.4	98.3	-199.5
VICHAT	P-1	659.84	1.346	0.755		
VICHAT	P-1	-13.1	-24.3	-263.2	85.6	-215.0

Table S4. A summary of pairwise molecular couplings with the slipped cofacial configuration. Distances in Å, energies (AA-CLP) in kJ mol^{-1}. T, translation, Inv inversion, other operations with coordinate transformation.

translation				
CIYNAB	7.171	-46	Ty	
CIYXUF	7.276	-56	Ty	
CIYYAM	7.115	-47	Ty	
PIXPUJ	7.014	-64	Ty	
PIFHIW	7.221	-69	Tz	
MIVDOM	7.532	-63	Tx	
QQQCIG05	7.173	-53	Ty	
QQQCIG14	7.020	-56	Tx	
RAGCEK	7.996	-63	Tz	
RAGDIP	7.979	-63	Tx	
VICHAT	7.073	-63	Tx	
MIVDUS	7.116	-63	Tx	
other				
RAGCUA	7.418	-54	Inv	1 0 0
POGZIV	7.687	-54	Inv	0 1 2
TOMVOH	7.884	-61	x,y,-z	½, 0, ½
RAGDEL	7.676	-49	Inv	1 0 1
	7.791	-50	Inv	0 0 1
GORVIU	7.157	-72	Inv	1 0 0
	7.241	-63	Inv	2 0 0
GORVUG	7.051	-80	Inv	1 0 1
	7.231	-81	Inv	1 0 2
offset				
RAGCIO	7.403	-71	Ty	
RAGDOV	7.538	-77	Inv	0 1 1
	7.538	-77	Inv	0 1 2

Table S5. Extended motifs in the packing of rubrenes. Contacts with highest molecule-molecule contact energies.

Codes: SC7 (O): slipped cofacial at 7 Å distance; Operator = T, I, S

T7 = ≈7 Å translation, T9 = ≈9 Å translation; I = inversion, T = translation, S = screw, G = glide

4S: four identical screw operations, 2S: two screw related molecules

refcode	Z	SC	motif	
P-1 space groups				
CIYNAB01	1	SC7(T)		
GORVUG	2	SC7(I)		
QQQCIG14	1	SC7(T)		
RAGDEL	2	SC7(I)		
VICHAT	1	SC7(T)		
C2/c space group Z'=1/2				
RAGCUA	4	SC7(T)		
RAGDOV	4	SC7(I)		
Others				
GORVIU01	4	SC7(I)		P21/c
TOMVOH	8	SC7(S)		Pbca
CIYNAB	2	SC7(T)	T7+4S	P21/c
CIYXUF	2	SC7(T)	T7+4S	P21/c
CIYYAM	2	SC7(T)	T7+4S	P21/c
PIXPUJ01	2	SC7(T)	T7+4S	P21/c
PIFHIW	4	SC7(T)	T7+4S	Pnma
QQQCIG05	4	SC7(T)	T7+4S	Cmca
MIVDOM	4	SC7(T)	T7+2S+2S	Pbcm
MIVDUS	4	SC7(T)	T7+2S+2S	Pnma
Other fourfold cage coordinations (no SC)				
AXIDER	2	T9+4S		P21/c
INELUK02	2	T9+4S		P21/c
QQQCIG13	2	T9+4S		P21/c
PIXPOD01	4	T9+2S+2S		P21/c
MIVDAY	2	T9+2S+2S		P21
RAGDAH	4	T9+2S+2S		P21/n
PIFHOC	4	T9+2G+2G		P21/c
Approximate or no classification				
INELUK	4	2I+2S+2T		P21/n
MIVDEC	4	mix G, S		Pna21
RAGCEK	4	mix T, I,G		P21/c
RAGCIO	4	T7+4G (no SC)		P2/c
TEFDUG	4	T7+4G (no SC)		Pnna
TOMWAU	4	mix T, I, S, G		P21/n

Z' > 1: MIVCUR, POGZIV, RAGDIP not analyzed

Table S6. Surface energies (erg cm^{-2}) for selected isomorphous monoclinic rubrenes.

	CIYNAB	**CIYXUF**	**CIYYAM**	**PIXPUJ01**
Form		Surface energy		
{100}	102.5	54.5	105.2	86.4
$\{10\bar{2}\}$	86.1	78.5	86.3	89.9
{011}	107.8	89.0	103.3	88.4
{002}	86.3	79.4	85.3	92.8
$\{11\bar{1}\}$	93.7	80.6	90.5	103.0