Supporting information for:

Molecular structures, polymorphism and the role of F…F interactions in crystal packing of fluorinated tosylates

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Crystallographic data

Single crystal X-ray studies of **1–4** were carried out in Center for molecule composition studies of INEOS RAS using Bruker APEX II and Bruker APEX DUO diffractometers. All crystal samples were colorless crystals with low melting point. To prevent damage of the samples and decrease of thermal movement of atoms the measurements were carried out at 120 K.

The structures were solved by direct method and refined in anisotropic approximation for non-hydrogen atoms. Hydrogens atoms of methyl, methylene and aromatic fragments were calculated according to those idealized geometry and refined with constraints applied to C-H bond lengths and equivalent displacement parameters ($U_{iso}(H) = 1.2U_{eq}(C)$ for CH_2, CH and CH_{Ar} groups; $U_{iso}(H) = 1.5U_{eq}(C)$ for CH3 group. All structures were solved with the ShelXT [1] program and refined with the ShelXL [2] program. Molecular graphics was drawn using OLEX2 [3] program. The structure **3a** was refined as inversion twin using TWIN and BASF instructions (Flack parameter is equal to 0.11(17)).

Table S1. Crystallographic data for **1–4**.

	1	**2a**	**2b**	**3a**	**3b**	**4**
Brutto formula	$C_{10}H_9F_5O_3S$	$C_{10}H_{10}F_4O_3S$	$C_{10}H_{10}F_4O_3S$	$C_{14}H_{10}F_{12}O_3S$	$C_{14}H_{10}F_{12}O_3S$	$C_{16}H_{10}F_{16}O_3S$
Formula weight	304.23	286.24	286.24	486.28	486.28	586.30
Diffractometer	Bruker APEX DUO	Bruker APEX-II CCD	Bruker APEX DUO	Bruker APEX-II CCD	Bruker APEX DUO	Bruker APEX-II CCD
Anode [Wavelength, Å]	CuKα [1.54178] sealed tube	MoKα [0.71073] sealed tube	MoKα [0.71073] sealed tube	MoKα [0.71073] sealed tube	CuKα [1.54178] sealed tube	MoKα [0.71073] sealed tube
Crystal Dimensions, mm	0.14 × 0.35 × 0.46	0.31 × 0.34 × 0.39	0.24 × 0.27 × 0.39	0.22 × 0.25 × 0.4	0.24 × 0.29 × 0.33	0.16 × 0.26 × 0.31
a, Å	10.7844(5)	24.4055(17)	20.638(2)	12.276(4)	16.8565(8)	18.473(3)
b, Å	5.3625(2)	5.7862(4)	5.3458(5)	5.0713(15)	5.7460(3)	5.7169(9)
c, Å	20.6018(10)	18.9225(12)	22.241(3)	14.808(4)	18.1583(8)	19.623(3)
β, °	93.403(3)	117.353(2)	106.746(2)	107.241(6)	90.094(3)	95.081(4)
Volume, Å^3	1189.33(9)	2373.4(3)	2349.7(4)	880.5(4)	1758.76(15)	2064.1(6)
Density, gcm^{-3}	1.699	1.602	1.618	1.834	1.836	1.887
T_{min}/T_{max}	0.5215/0.7535	0.6579/0.7461	0.6457/0.7453	0.5400/0.7461	0.4113/0.7536	0.6133/0.7461
μ, mm^{-1}	3.120	0.322	0.326	0.321	2.985	0.319
Space group	$P2_1/c$	C2/c	$P2_1/c$	$P2_1$	$P2_1/n$	$P2_1/n$
Z	4	8	8	2	4	4
F(000)	616	1168	1168	484	968	1160
Reflections collected	7933	10487	16579	5769	19041	44143
Independent reflections	2339	3608	7219	4764	3363	6406
Reflections (I>2σ(I))	2074	2771	4009	3542	2992	4819
Parameters	173	164	327	273	272	365

R_{int}	0.0471	0.0377	0.0670	0.0285	0.0543	0.0688
$2\theta_{min}$ - $2\theta_{max}$, °	11.542 - 144.658	3.758 - 61.002	3.824 - 61.172	3.798 - 61.448	23.808 - 144.144	4.168 - 61.630
wR_2 (all reflections)	0.1109	0.1088	0.1268	0.1430	0.1409	0.1497
$R_1(I>\sigma(I))$	0.0393	0.0425	0.0581	0.0596	0.0517	0.0465
GOF	1.050	1.050	0.998	1.017	1.107	1.015
ρ_{min}/ρ_{max}, eÅ^{-3}	-0.355/0.418	-0.411/0.453	-0.505/0.359	-0.627/0.427	-0.409/0.554	-0.448/0.522

Figure S1. Molecular structure of **2b**. Atoms are presented as thermal ellipsoids.

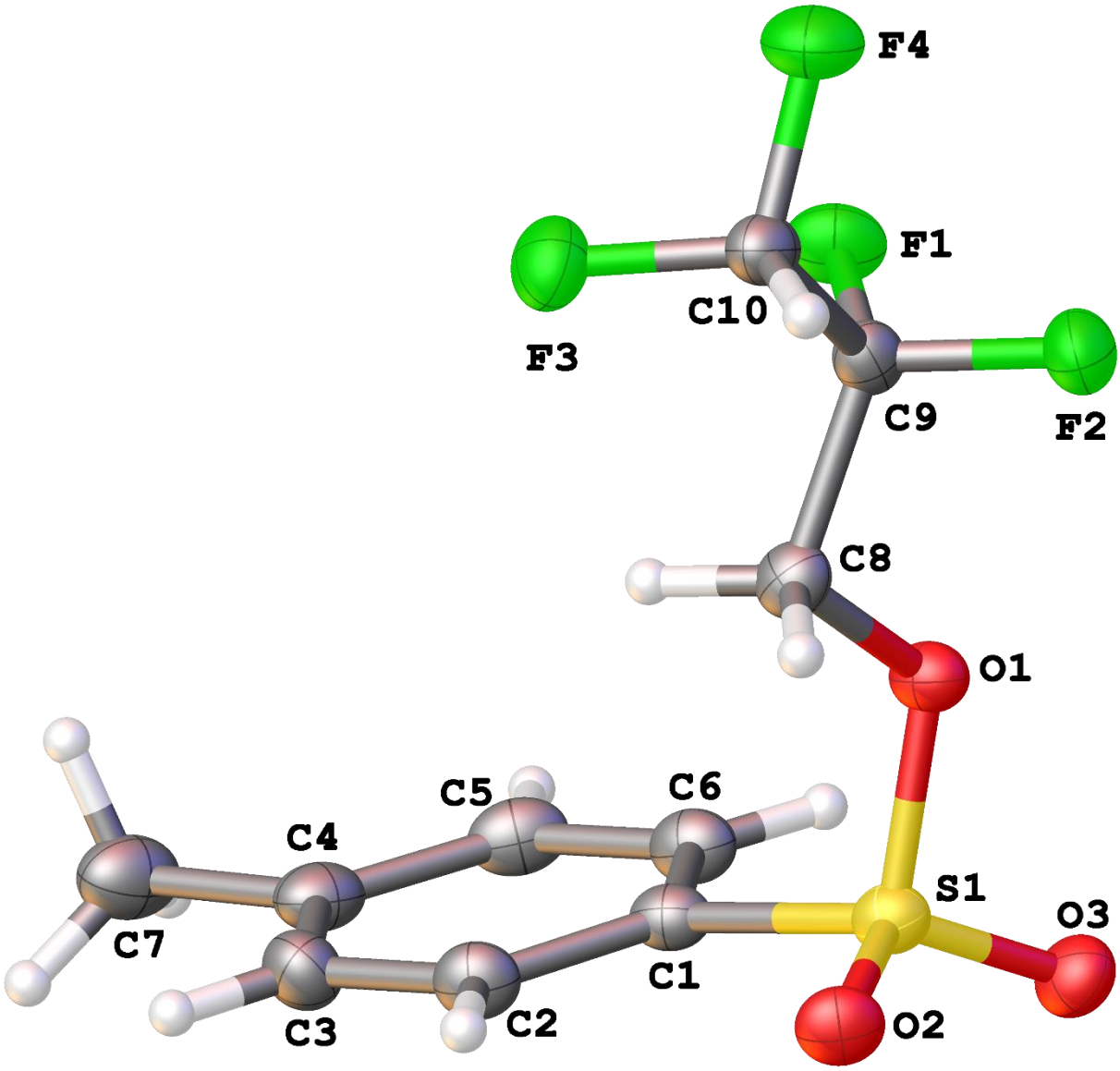
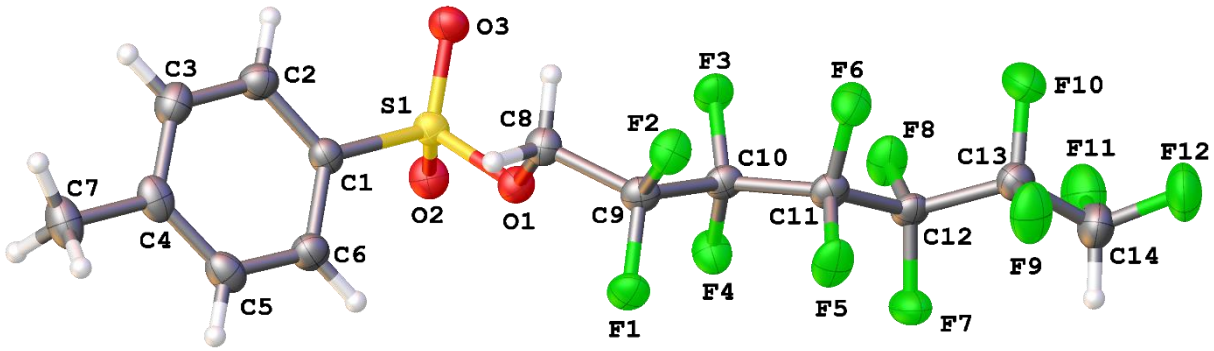


Figure S2. Molecular structure of **3b**. Atoms are presented as thermal ellipsoids.



VASP calculations output

Parameters of unit cell and optimized fractional coordinates (CONTCAR files)

Compound **1**

C10 H9 F5 O3 S
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10.7653839999999992 0.0000000000000000 -0.6401470000000000
0.0000000000000000 5.3624999999999998 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.6018000000000008
S F O C H
4 20 12 40 36
Direct
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0.2660083350309216 0.0045009602173901 0.2467215759741156
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0.6656347547531574 -0.0008581099721092 0.2109609746699035

Compound **2a**

C10 H10 F4 O3 S
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21.6767840000000014 0.0000000000000000 -11.2136279999999999
0.0000000000000000 5.7862000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 18.9224999999999994
S F O C H
8 32 24 80 80
Direct
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0.5726095635954686 0.8693102961618002 0.1133530706611987
0.5726095635954686 0.1306897038382003 0.6133530706611988
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Compound **2b**

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0.7926371330793505	0.5569533301322852	0.5955776522664027
0.2073628669206489	0.0569533301322854	0.9044223477335973
0.2073628669206489	0.4430466698677145	0.4044223477335974
0.7926371330793505	0.9430466698677149	0.0955776522664027
0.3549604988564285	0.7034077001090573	0.3814339131424420
0.6450395011435716	0.2034077001090571	0.1185660868575583
0.6450395011435716	0.2965922998909435	0.6185660868575587
0.3549604988564285	0.7965922998909427	0.8814339131424413
0.2806424865721980	0.0270874371540545	0.3149129806532914
0.7193575134278022	0.5270874371540546	0.1850870193467089
0.7193575134278022	0.9729125628459454	0.6850870193467087
0.2806424865721980	0.4729125628459450	0.8149129806532913
0.3770180641002074	0.8994354018017866	0.1697422334031020
0.6229819358997934	0.3994354018017855	0.3302577665968979
0.6229819358997934	0.1005645981982146	0.8302577665968984
0.3770180641002074	0.6005645981982134	0.6697422334031016
0.4511151324485808	0.5810515266622964	0.2355081610182330
0.5488848675514192	0.0810515266622971	0.2644918389817666
0.5488848675514192	0.4189484733377032	0.7644918389817670
0.4511151324485808	0.9189484733377036	0.7355081610182330
0.3080291546005043	0.3696333315714596	0.2081527368533101
0.6919708453994959	0.8696333315714598	0.2918472631466899
0.6919708453994959	0.6303666684285402	0.7918472631466897
0.3080291546005043	0.1303666684285399	0.7081527368533103
0.2330616501947374	0.2106200110955946	0.2097211862872403
0.7669383498052623	0.7106200110955948	0.2902788137127599
0.7669383498052623	0.7893799889044052	0.7902788137127594
0.2330616501947374	0.2893799889044053	0.7097211862872406
0.2713091006629895	0.1508960284232995	0.1486165877450488
0.7286908993370104	0.6508960284232994	0.3513834122549512
0.7286908993370104	0.8491039715767006	0.8513834122549510
0.2713091006629895	0.3491039715767004	0.6486165877450490
0.5347836198833155	0.6500093089736086	0.4733734886045449
0.4652163801166844	0.1500093089736091	0.0266265113954554
0.4652163801166844	0.3499906910263907	0.5266265113954551
0.5347836198833155	0.8499906910263914	0.9733734886045449
0.5076920401227196	0.8914870174444398	0.4149739771985432
0.4923079598772800	0.3914870174444394	0.0850260228014565

0.4923079598772800	0.1085129825555604	0.5850260228014564
0.5076920401227196	0.6085129825555602	0.9149739771985436
0.6359373600419896	0.8815148798271060	0.5475991471866051
0.3640626399580106	0.3815148798271056	0.9524008528133949
0.3640626399580106	0.1184851201728943	0.4524008528133948
0.6359373600419896	0.6184851201728940	0.0475991471866053
0.0307627702984404	0.2132161469829668	0.5192839759839956
0.9692372297015591	0.7132161469829673	0.9807160240160044
0.9692372297015591	0.7867838530170327	0.4807160240160044
0.0307627702984404	0.2867838530170336	0.0192839759839955
0.1119601079899773	0.5161991656477830	0.4988456634754049
0.8880398920100230	0.0161991656477836	0.0011543365245956
0.8880398920100230	0.4838008343522165	0.5011543365245956
0.1119601079899773	0.9838008343522170	-0.0011543365245955
0.1571882044507604	0.7851157153893416	0.6891002018120916
0.8428117955492397	0.2851157153893412	0.8108997981879084
0.8428117955492397	0.2148842846106587	0.3108997981879077
0.1571882044507604	0.7148842846106584	0.1891002018120923
0.0763538928567701	0.4793814819856170	0.7105697253052313
0.9236461071432306	0.9793814819856169	0.7894302746947687
0.9236461071432306	0.5206185180143831	0.2894302746947696
0.0763538928567701	0.0206185180143826	0.2105697253052309
0.1943853408721120	0.0232274966223144	0.6087192306211289
0.8056146591278880	0.5232274966223144	0.8912807693788711
0.8056146591278880	-0.0232274966223144	0.3912807693788704
0.1943853408721120	0.4767725033776858	0.1087192306211294
0.1746420189428258	0.9143052642580983	0.5299941941007666
0.8253579810571743	0.4143052642580986	0.9700058058992334
0.8253579810571743	0.0856947357419017	0.4700058058992338
0.1746420189428258	0.5856947357419017	0.0299941941007666
0.2406083904000565	0.7722945015139119	0.5895383786554771
0.7593916095999436	0.2722945015139127	0.9104616213445229
0.7593916095999436	0.2277054984860875	0.4104616213445225
0.2406083904000565	0.7277054984860881	0.0895383786554777
0.9348201281395631	0.6555873659475910	0.6501555276546158
0.0651798718604370	0.1555873659475913	0.8498444723453842
0.0651798718604370	0.3444126340524087	0.3498444723453844
0.9348201281395631	0.8444126340524090	0.1501555276546155
0.9449163392430719	0.4143440266603844	0.7086169893835325
0.0550836607569282	0.9143440266603848	0.7913830106164675
0.0550836607569282	0.5856559733396151	0.2913830106164678
0.9449163392430719	0.0856559733396153	0.2086169893835322
0.7871234281272689	0.3980913833391072	0.5631523351773987
0.2128765718727311	0.8980913833391078	0.9368476648226013
0.2128765718727311	0.6019086166608922	0.4368476648226010
0.7871234281272689	0.1019086166608925	0.0631523351773989

Compound **3a**

C10 H9 F5 O3 S
1.00000000000000
11.7243969999999997 0.0000000000000000 -3.6385030000000000
0.0000000000000000 5.0712999999999999 0.0000000000000000
0.0000000000000000 0.0000000000000000 14.8079999999999998
S F O C H
2 24 6 28 20
Direct
0.3425877668142540 0.7775986338863931 0.8409963819408877
0.6574122331857453 0.2775986338863929 0.1590036180591125
0.6934425524128209 0.3595639711362545 0.8516450619642165
0.3065574475871787 0.8595639711362544 0.1483549380357840
0.6324553251501696 0.7735331690957007 0.8308699389284496
0.3675446748498309 0.2735331690957012 0.1691300610715495
0.5269658455384225 0.6968970919447131 0.6483171321182991
0.4730341544615779 0.1968970919447134 0.3516828678817007
0.5461765151692424 0.2651313617515728 0.6615639894870409
0.4538234848307581 0.7651313617515733 0.3384360105129595
0.7654462137341328 0.2763732507664198 0.6943347621158299
0.2345537862658664 0.7763732507664199 0.3056652378841699
0.7807296674292862 0.6995298136813946 0.7303687185466012
0.2192703325707133 0.1995298136813945 0.2696312814533983
0.6677379707626013 0.8405747831095355 0.5519447246484764
0.3322620292373996 0.3405747831095352 0.4480552753515233
0.6270696089518365 0.4252358282312224 0.5094842415318258
0.3729303910481631 0.9252358282312219 0.4905157584681744
0.8584391599912500 0.3119390011688395 0.5567314470304000
0.1415608400087491 0.8119390011688388 0.4432685529695999
0.8981092599150299 0.7288570234274787 0.5966384043196369
0.1018907400849706 0.2288570234274792 0.4033615956803630
0.9069237152744949 0.5820885646409465 0.4199533040498628
0.0930762847255055 0.0820885646409462 0.5800466959501372
0.7744676387082590 0.8814131875332386 0.4154367704331409
0.2255323612917414 0.3814131875332382 0.5845632295668585
0.4062692402082917 0.6015499281530557 0.7796451046359294
0.5937307597917081 0.1015499281530561 0.2203548953640705
0.4242186578795650 0.8409356987057406 0.9310476863995384
0.5757813421204356 0.3409356987057397 0.0689523136004612
0.2903136375335763 0.9830815348631917 0.7750648405829593
0.7096863624664236 0.4830815348631930 0.2249351594170405
0.2379926580953955 0.5629348909745043 0.8577722788647195
0.7620073419046048 0.0629348909745049 0.1422277211352808
0.1397025621517805 0.5165263783658938 0.7826087239425249
0.8602974378482195 0.0165263783658936 0.2173912760574746
0.0595094520976365 0.3383946219007939 0.7953881426539463
0.9404905479023632 0.8383946219007935 0.2046118573460535
0.0753894707994941 0.2083424257966996 0.8819915187365809
0.9246105292005048 0.7083424257967001 0.1180084812634194
0.1747962153273700 0.2600721392564559 0.9559069211174336
0.8252037846726298 0.7600721392564572 0.0440930788825667
0.2569651474720023 0.4352397792739208 0.9445609904697244
0.7430348525279974 0.9352397792739220 0.0554390095302749
-0.0112654563688369 0.0159407649427307 0.8954830675657414
0.0112654563688368 0.5159407649427306 0.1045169324342579
0.4989802217700489 0.4329139305544270 0.8276888724476053
0.5010197782299513 0.9329139305544274 0.1723111275523952
0.6053030088147340 0.5188457375757327 0.8023870582101637
0.3946969911852666 0.0188457375757326 0.1976129417898359
0.5958206732723705 0.5000721926954401 0.6946098168344238
0.4041793267276303 0.0000721926954405 0.3053901831655764

0.7140950168827465	0.5151645759967990	0.6731168812414690
0.2859049831172533	0.0151645759967988	0.3268831187585307
0.7050933529633927	0.5881976374504774	0.5679186830913823
0.2949066470366074	0.0881976374504777	0.4320813169086180
0.8188859666185864	0.5637955837395849	0.5408647830361522
0.1811140333814140	0.0637955837395852	0.4591352169638480
0.8038621896586896	0.6235387740501237	0.4348140929083433
0.1961378103413105	0.1235387740501239	0.5651859070916572
0.1263149411468410	0.6181621837242114	0.7154206327456371
0.8736850588531589	0.1181621837242045	0.2845793672543620
0.9832512242994556	0.2987601185005612	0.7369553472461330
0.0167487757005450	0.7987601185005617	0.2630446527538676
0.1879685471988622	0.1613549028476484	0.0236079061319971
0.8120314528011373	0.6613549028476489	0.9763920938680024
0.3345217901528452	0.4729731269882232	0.0018640594541928
0.6654782098471541	0.9729731269882229	-0.0018640594541928
0.9025563590648906	0.0646625084656362	0.8509591765128174
0.0974436409351095	0.5646625084656363	0.1490408234871827
0.9883760041771986	0.0103577742821364	0.9694215951585194
0.0116239958228013	0.5103577742821374	0.0305784048414807
0.0082728130817418	0.8155706520998596	0.8761869318373501
0.9917271869182583	0.3155706520998590	0.1238130681626502
0.4765602794357026	0.2295652657387275	0.8048848354674644
0.5234397205642972	0.7295652657387278	0.1951151645325360
0.5190408155686891	0.4471138157108930	0.9049779847510494
0.4809591844313107	0.9471138157108934	0.0950220152489508
0.7396670170867814	0.4962973769728119	0.3871464600400635
0.2603329829132185	-0.0037026230271881	0.6128535399599364

Compound **3b**

C16 H10 F16 O3 S
1.00000000000000
16.8564770000000017 0.0000000000000000 -0.0276550000000000
0.0000000000000000 5.7460000000000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 18.1583000000000006
S F O C H
4 48 12 56 40
Direct
0.5722859885673156 0.4999534273540449 0.3516633484818328
0.9277140114326844 -0.0000465726459553 0.1483366515181677
0.4277140114326852 0.5000465726459554 0.6483366515181674
0.0722859885673153 0.0000465726459555 0.8516633484818326
0.4026240586361985 0.0904880650914435 0.3465992907620619
0.0973759413638014 0.5904880650914435 0.1534007092379379
0.5973759413638017 0.9095119349085565 0.6534007092379379
0.9026240586361983 0.4095119349085563 0.8465992907620621
0.3790452360765875 0.0261553498268649 0.4646115400469847
0.1209547639234128 0.5261553498268650 0.0353884599530152
0.6209547639234125 0.9738446501731350 0.5353884599530149
0.8790452360765875 0.4738446501731352 0.9646115400469851
0.3461667965945324 0.5394534582872673 0.4117059249337872
0.1538332034054674 0.0394534582872674 0.0882940750662130
0.6538332034054676 0.4605465417127326 0.5882940750662129
0.8461667965945324 0.9605465417127327 0.9117059249337871
0.3355827210110365 0.7107969041658690 0.3029589790959096
0.1644172789889636 0.2107969041658684 0.1970410209040907
0.6644172789889637 0.2892030958341314 0.6970410209040908
0.8355827210110363 0.7892030958341310 0.8029589790959092
0.2389468654991834 0.0566841320737780 0.3839924978864681
0.2610531345008168 0.5566841320737783 0.1160075021135317
0.7610531345008165 0.9433158679262217 0.6160075021135315
0.7389468654991835 0.4433158679262219 0.8839924978864685
0.2351153037316104 0.7884066500111706 0.4708071517069898
0.2648846962683902 0.2884066500111708 0.0291928482930103
0.7648846962683898 0.2115933499888291 0.5291928482930111
0.7351153037316102 0.7115933499888294 0.9708071517069889
0.1700023230425195 0.7988164914660086 0.2868547238106335
0.3299976769574807 0.2988164914660081 0.2131452761893661
0.8299976769574804 0.2011835085339918 0.7131452761893659
0.6700023230425196 0.7011835085339914 0.7868547238106341
0.2003161981373349 0.4704750471017364 0.3434712876933069
0.2996838018626647 0.9704750471017365 0.1565287123066929
0.7996838018626660 0.5295249528982635 0.6565287123066932
0.7003161981373340 0.0295249528982636 0.8434712876933068
0.0806528745726915 0.9180621430630024 0.4171170405795830
0.4193471254273086 0.4180621430630026 0.0828829594204170
0.9193471254273090 0.0819378569369976 0.5828829594204175
0.5806528745726909 0.5819378569369976 0.9171170405795825
0.0972878442872888 0.5513208190558130 0.4516204172375741
0.4027121557127115 0.0513208190558132 0.0483795827624255
0.9027121557127121 0.4486791809441868 0.5483795827624252
0.5972878442872879 0.9486791809441870 0.9516204172375748
0.0380404004052000 0.4042938819041741 0.3167258941361584
0.4619595995948002 0.9042938819041740 0.1832741058638416
0.9619595995947992 0.5957061180958260 0.6832741058638411
0.5380404004052008 0.0957061180958263 0.8167258941361589
0.9585908393070436 0.6325284738249554 0.3813359759085208
0.5414091606929564 0.1325284738249558 0.1186640240914794
0.0414091606929565 0.3674715261750438 0.6186640240914790
0.4585908393070436 0.8674715261750446 0.8813359759085210

0.4990792485350686	0.6807254907624318	0.3453600743664053
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0.5009207514649316	0.3192745092375681	0.6546399256335952
-0.0009207514649316	0.8192745092375682	0.8453600743664048
0.5710601607208154	0.3854513334513855	0.2808784131714169
0.9289398392791846	0.8854513334513854	0.2191215868285834
0.4289398392791847	0.6145486665486146	0.7191215868285835
0.0710601607208158	0.1145486665486146	0.7808784131714165
0.5643658618908255	0.3631639456219407	0.4181993448844462
0.9356341381091745	0.8631639456219393	0.0818006551155535
0.4356341381091743	0.6368360543780607	0.5818006551155533
0.0643658618908257	0.1368360543780597	0.9181993448844467
0.6549751246092811	0.6852929494341289	0.3596714227195252
0.8450248753907189	0.1852929494341279	0.1403285772804751
0.3450248753907184	0.3147070505658718	0.6403285772804749
0.1549751246092817	0.8147070505658711	0.8596714227195251
0.7134321448889537	0.6330752873383676	0.4115842713006182
0.7865678551110463	0.1330752873383681	0.0884157286993823
0.2865678551110467	0.3669247126616323	0.5884157286993821
0.2134321448889535	0.8669247126616324	0.9115842713006179
0.7795958646321389	0.7770222232135466	0.4167910265708240
0.7204041353678611	0.2770222232135473	0.0832089734291761
0.2204041353678609	0.2229777767864532	0.5832089734291755
0.2795958646321390	0.7229777767864534	0.9167910265708245
0.7879705339114228	0.9730993509932138	0.3715411643066686
0.7120294660885772	0.4730993509932137	0.1284588356933316
0.2120294660885770	0.0269006490067862	0.6284588356933312
0.2879705339114227	0.5269006490067862	0.8715411643066688
0.7276306404884416	0.0221419526918625	0.3203320927573566
0.7723693595115584	0.5221419526918627	0.1796679072426435
0.2723693595115584	-0.0221419526918626	0.6796679072426436
0.2276306404884417	0.4778580473081379	0.8203320927573564
0.6613737390229233	0.8797662172376932	0.3137084622596281
0.8386262609770767	0.3797662172376941	0.1862915377403721
0.3386262609770766	0.1202337827623060	0.6862915377403723
0.1613737390229230	0.6202337827623068	0.8137084622596277
0.8593064356453920	0.1275454354786023	0.3773631445501443
0.6406935643546080	0.6275454354786025	0.1226368554498555
0.1406935643546078	0.8724545645213975	0.6226368554498556
0.3593064356453924	0.3724545645213979	0.8773631445501444
0.4801070585479918	0.8107303105665425	0.4108729747056701
0.0198929414520082	0.3107303105665415	0.0891270252943295
0.5198929414520086	0.1892696894334582	0.5891270252943299
0.9801070585479914	0.6892696894334575	0.9108729747056701
0.3991195799200945	0.9217403319482985	0.3992585011253254
0.1008804200799055	0.4217403319482986	0.1007414988746744
0.6008804200799052	0.0782596680517012	0.6007414988746744
0.8991195799200948	0.5782596680517015	0.8992585011253256
0.3319980610934203	0.7451486572688325	0.3767756590721240
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Compound **4**

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0.0000000000000000 5.7168999999999999 0.0000000000000000
0.0000000000000000 0.0000000000000000 19.6219999999999999
S F O C H
4 64 12 64 40
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0.5837852236912493	0.0665977358510194	0.5369353847560919
0.9162147763087507	0.5665977358510190	0.9630646152439081
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0.8070011420351012	0.7544934804155640	0.5252211076134145

Table S2. Total energy of unit cell (OUTCAR file)

Compound	**Total Energy; eV**
1	-678.92560789
2a	-1353.33111345
2b	-1353.44311667
3a	-475.52413940
3b	-951.15082313
4	-1088.29245063

CrystalExplorer17 output

Compound **1**

Interaction Energies (kJ/mol)
R is the distance between molecular centroids (mean atomic position) in Å.

Total energies, only reported for two benchmarked energy models, are the sum of the four energy components, scaled appropriately (see the scale factor table below)

	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	1	x, y, z	5.36	B3LYP/6-31G(d,p)	-9.4	-4.8	-42.3	25.2	-34.7
	0	x, -y+1/2, z+1/2	11.35	B3LYP/6-31G(d,p)	-2.6	-0.4	-7.5	2.3	-8.1
	0	-x, -y, -z	15.02	B3LYP/6-31G(d,p)	2.4	-0.3	-5.9	3.3	-0.8
	1	-x, y+1/2, -z+1/2	6.04	B3LYP/6-31G(d,p)	-6.4	-3.3	-20.7	13.2	-19.1
	0	-x, -y, -z	9.88	B3LYP/6-31G(d,p)	-0.6	-0.1	-11.2	1.8	-9.3
	2	x, -y+1/2, z+1/2	10.32	B3LYP/6-31G(d,p)	-3.0	-0.4	-10.4	3.3	-10.4
	1	-x, y+1/2, -z+1/2	6.50	B3LYP/6-31G(d,p)	-11.0	-3.5	-25.4	15.6	-26.8
	1	-x, -y, -z	13.21	B3LYP/6-31G(d,p)	1.5	-0.8	-9.9	2.6	-6.0
	1	-x, -y, -z	10.20	B3LYP/6-31G(d,p)	0.5	-0.1	-4.6	0.7	-3.1

Scale factors for benchmarked energy models
See Mackenzie et al. IUCrJ (2017)

Energy Model	k_ele	k_pol	k_disp	k_rep
CE-HF ... HF/3-21G electron densities	1.019	0.651	0.901	0.811
CE-B3LYP ... B3LYP/6-31G(d,p) electron densities	1.057	0.740	0.871	0.618

Compound **2a**

Interaction Energies (kJ/mol)
R is the distance between molecular centroids (mean atomic position) in Å.

Total energies, only reported for two benchmarked energy models, are the sum of the four energy components, scaled appropriately (see the scale factor table below)

	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	1	x, y, z	5.79	B3LYP/6-31G(d,p)	-14.8	-5.5	-30.6	20.4	-33.7
	1	-x, y, -z+1/2	7.38	B3LYP/6-31G(d,p)	-4.1	-0.8	-10.6	4.4	-11.4
	1	-x+1/2, y+1/2, -z+1/2	9.35	B3LYP/6-31G(d,p)	-5.2	-2.1	-24.6	13.6	-20.1
	0	x+1/2, -y+1/2, z+1/2	12.34	B3LYP/6-31G(d,p)	0.1	-0.5	-5.2	1.4	-3.9
	2	x+1/2, -y+1/2, z+1/2	11.58	B3LYP/6-31G(d,p)	-4.3	-0.4	-5.7	3.4	-7.8
	0	-x+1/2, -y+1/2, -z	11.89	B3LYP/6-31G(d,p)	2.8	-0.8	-6.1	2.7	-1.3
	0	-x, -y, -z	5.99	B3LYP/6-31G(d,p)	-49.3	-9.7	-25.0	37.4	-58.1
	1	-x, y, -z+1/2	4.58	B3LYP/6-31G(d,p)	-9.5	-2.1	-42.9	17.3	-38.3
	1	-x, -y, -z	7.15	B3LYP/6-31G(d,p)	8.6	-2.5	-10.5	2.2	-0.6

Scale factors for benchmarked energy models
See Mackenzie et al. IUCrJ (2017)

Energy Model	k_ele	k_pol	k_disp	k_rep
CE-HF ... HF/3-21G electron densities	1.019	0.651	0.901	0.811
CE-B3LYP ... B3LYP/6-31G(d,p) electron densities	1.057	0.740	0.871	0.618

Compound **2b**

Interaction Energies (kJ/mol)
R is the distance between molecular centroids (mean atomic position) in Å.

Total energies, only reported for two benchmarked energy models, are the sum of the four energy components, scaled appropriately (see the scale factor table below)

	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	1	-	10.13	B3LYP/6-31G(d,p)	-2.0	-0.2	-5.7	2.4	-5.8
	0	-	9.37	B3LYP/6-31G(d,p)	-2.0	-0.7	-11.4	5.7	-9.0
	0	x, y, z	5.35	B3LYP/6-31G(d,p)	-10.2	-4.1	-36.6	22.5	-31.8
	0	-x, y+1/2, -z+1/2	6.01	B3LYP/6-31G(d,p)	-9.9	-3.6	-19.4	14.0	-21.5
	0	-x, -y, -z	7.84	B3LYP/6-31G(d,p)	-20.3	-4.2	-12.5	13.4	-27.2
	1	-	9.63	B3LYP/6-31G(d,p)	-4.4	-0.6	-10.6	5.1	-11.2
	0	-	13.02	B3LYP/6-31G(d,p)	0.5	-0.0	-0.3	0.0	0.3
	0	-	12.28	B3LYP/6-31G(d,p)	0.8	-0.1	-0.8	0.0	0.1
	1	-	10.27	B3LYP/6-31G(d,p)	-4.0	-0.6	-7.4	2.6	-9.5
	0	-x, -y, -z	17.96	B3LYP/6-31G(d,p)	0.1	-0.0	-0.0	0.0	0.1
	0	-x, -y, -z	6.36	B3LYP/6-31G(d,p)	-7.7	-2.3	-36.5	19.4	-29.7
	0	x, -y+1/2, z+1/2	20.71	B3LYP/6-31G(d,p)	-0.2	-0.0	-0.0	0.0	-0.2
	0	-x, -y, -z	8.76	B3LYP/6-31G(d,p)	-1.5	-0.4	-5.3	0.8	-6.1
	0	-	11.83	B3LYP/6-31G(d,p)	0.2	-0.0	-0.4	0.0	-0.1
	0	-x, -y, -z	18.94	B3LYP/6-31G(d,p)	0.0	-0.0	-0.0	0.0	-0.0
	0	x, -y+1/2, z+1/2	22.22	B3LYP/6-31G(d,p)	-0.1	-0.0	-0.0	0.0	-0.1
	1	-	11.37	B3LYP/6-31G(d,p)	-2.6	-0.3	-2.3	0.1	-4.9
	1	-	12.12	B3LYP/6-31G(d,p)	-2.5	-0.3	-4.7	0.9	-6.5
	0	-	11.10	B3LYP/6-31G(d,p)	-0.4	-1.1	-15.3	7.4	-10.0
	1	-	13.02	B3LYP/6-31G(d,p)	2.2	-0.6	-6.8	5.3	-0.7

Scale factors for benchmarked energy models
See Mackenzie et al. IUCrJ (2017)

Energy Model	k_ele	k_pol	k_disp	k_rep
CE-HF ... HF/3-21G electron densities	1.019	0.651	0.901	0.811
CE-B3LYP ... B3LYP/6-31G(d,p) electron densities	1.057	0.740	0.871	0.618

Compound **3a**

Interaction Energies (kJ/mol)
R is the distance between molecular centroids (mean atomic position) in Å.

Total energies, only reported for two benchmarked energy models, are the sum of the four energy components, scaled appropriately (see the scale factor table below)

	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	1	x, y, z	13.28	B3LYP/6-31G(d,p)	-3.0	-0.4	-7.4	2.5	-8.3
	1	x, y, z	5.07	B3LYP/6-31G(d,p)	-11.1	-5.2	-63.2	29.3	-52.5
	0	-x, y+1/2, -z	18.05	B3LYP/6-31G(d,p)	2.4	-0.8	-9.7	5.5	-3.1
	1	x, y, z	12.28	B3LYP/6-31G(d,p)	-1.9	-0.8	-16.4	7.1	-12.5
	0	-x, y+1/2, -z	6.46	B3LYP/6-31G(d,p)	-10.3	-3.3	-32.9	15.1	-32.7
	1	-x, y+1/2, -z	9.34	B3LYP/6-31G(d,p)	-5.7	-3.7	-24.8	14.3	-21.6
	1	-x, y+1/2, -z	14.58	B3LYP/6-31G(d,p)	1.1	-0.1	-5.5	0.3	-3.5

Scale factors for benchmarked energy models
See Mackenzie et al. IUCrJ (2017)

Energy Model	k_ele	k_pol	k_disp	k_rep
CE-HF ... HF/3-21G electron densities	1.019	0.651	0.901	0.811
CE-B3LYP ... B3LYP/6-31G(d,p) electron densities	1.057	0.740	0.871	0.618

Compound **3b**

Interaction Energies (kJ/mol)
R is the distance between molecular centroids (mean atomic position) in Å.

Total energies, only reported for two benchmarked energy models, are the sum of the four energy components, scaled appropriately (see the scale factor table below)

	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	1	-x, -y, -z	13.73	B3LYP/6-31G(d,p)	1.1	-0.1	-3.6	0.0	-2.1
	0	-x+1/2, y+1/2, -z+1/2	6.76	B3LYP/6-31G(d,p)	-10.6	-3.5	-32.1	15.9	-32.0
	1	x, y, z	16.86	B3LYP/6-31G(d,p)	-0.3	-0.4	-9.0	3.2	-6.6
	1	x, y, z	17.81	B3LYP/6-31G(d,p)	-1.9	-0.2	-5.2	2.0	-5.5
	1	-x, -y, -z	6.80	B3LYP/6-31G(d,p)	-27.9	-4.9	-41.4	28.2	-51.7
	0	x, y, z	5.75	B3LYP/6-31G(d,p)	-11.9	-4.4	-43.7	22.5	-39.9
	1	-x, -y, -z	6.98	B3LYP/6-31G(d,p)	-4.4	-2.1	-50.3	18.0	-38.8
	0	-x+1/2, y+1/2, -z+1/2	13.72	B3LYP/6-31G(d,p)	-5.8	-3.4	-19.4	13.8	-17.0

Scale factors for benchmarked energy models
See Mackenzie et al. IUCrJ (2017)

Energy Model	k_ele	k_pol	k_disp	k_rep
CE-HF ... HF/3-21G electron densities	1.019	0.651	0.901	0.811
CE-B3LYP ... B3LYP/6-31G(d,p) electron densities	1.057	0.740	0.871	0.618

Compound **4**

Interaction Energies (kJ/mol)
R is the distance between molecular centroids (mean atomic position) in Å.

Total energies, only reported for two benchmarked energy models, are the sum of the four energy components, scaled appropriately (see the scale factor table below)

	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	1	-x, -y, -z	8.48	B3LYP/6-31G(d,p)	-22.9	-4.5	-43.7	22.9	-51.5
	1	x, y, z	5.72	B3LYP/6-31G(d,p)	-13.9	-4.7	-49.7	25.6	-45.6
	0	-x+1/2, y+1/2, -z+1/2	6.68	B3LYP/6-31G(d,p)	-11.0	-3.5	-39.6	17.3	-38.1
	1	x, y, z	19.62	B3LYP/6-31G(d,p)	0.4	-0.5	-8.1	2.5	-5.4
	0	-x+1/2, y+1/2, -z+1/2	16.52	B3LYP/6-31G(d,p)	-5.4	-3.1	-18.6	12.7	-16.3
	1	-x, -y, -z	8.76	B3LYP/6-31G(d,p)	-4.1	-1.6	-46.1	14.5	-36.7
	1	-x, -y, -z	14.01	B3LYP/6-31G(d,p)	0.7	-0.2	-12.8	1.9	-9.4
	0	x, y, z	20.44	B3LYP/6-31G(d,p)	-1.7	-0.2	-5.1	1.8	-5.3
	0	-x, -y, -z	14.19	B3LYP/6-31G(d,p)	-0.1	-0.1	-3.8	0.0	-3.5

Scale factors for benchmarked energy models
See Mackenzie et al. IUCrJ (2017)

Energy Model	k_ele	k_pol	k_disp	k_rep
CE-HF ... HF/3-21G electron densities	1.019	0.651	0.901	0.811
CE-B3LYP ... B3LYP/6-31G(d,p) electron densities	1.057	0.740	0.871	0.618

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