

## ДОПОЛНИТЕЛЬНЫЕ МАТЕРИАЛЫ К СТАТЬЕ

**ГАЛОГЕННАЯ СВЯЗЬ В ПОРИСТЫХ МАТЕРИАЛАХ:  
РАЦИОНАЛЬНЫЙ ВЫБОР СТРОИТЕЛЬНЫХ БЛОКОВ****А.С. Новиков<sup>1,2</sup>, И.Ф. Сахапов<sup>3,4</sup>, А.С. Загузин<sup>3,5</sup>, В.П. Федин<sup>5</sup>, С.А. Адонин<sup>3,5</sup>**<sup>1</sup>Санкт-Петербургский государственный университет, Санкт-Петербург, Россия<sup>2</sup>Российский университет дружбы народов, Москва, Россия<sup>3</sup>Южно-Уральский государственный университет, Челябинск, Россия<sup>4</sup>Институт органической и физической химии им. А.Е. Арбузова РАН, Казань, Россия<sup>5</sup>Институт неорганической химии им. А.В. Николаева СО РАН, Новосибирск, Россия

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**Таблица S1.** Атомные координаты для оптимизированных модельных структур

Модельная структура	Заряд	X	Y	Z
<b>2-amino-5-iodo-14-benzenedicarboxylate_2-</b>				
	6	-2.148119	-0.329224	0.014712
	6	-2.285966	1.091970	0.000028
	6	-1.112314	1.888479	-0.003032
	6	0.190750	1.356414	0.008696
	6	0.301023	-0.054850	0.014805
	6	-0.847259	-0.868495	0.014111
	6	-3.347154	-1.293021	0.019852
	8	-3.095961	-2.548338	0.035374
	8	-4.530463	-0.752143	0.007362
	6	1.356799	2.390456	0.035053
	8	2.523921	1.950018	0.320946
	8	1.022239	3.609824	-0.212126
	53	2.163814	-1.126794	-0.032328
	7	-3.540300	1.686994	-0.009525
	1	-1.178993	2.973546	-0.028467
	1	-0.778459	-1.951916	0.014073
	1	-3.619010	2.687147	-0.032936
	1	-4.328043	1.037082	-0.010423
<b>2-amino-5-iodoisophthalate_2-</b>				
	6	-2.036825	-2.631425	-0.000153
	6	-1.363226	-1.243340	-0.000147
	6	-2.099766	-0.000072	-0.000186
	6	-1.363367	1.243193	-0.000144

	6	-2.037730	2.630877	-0.000148
	6	0.041273	1.222688	-0.000084
	6	0.728898	0.000123	-0.000068
	6	0.041422	-1.222532	-0.000087
	8	-1.260620	-3.654450	0.000302
	8	-3.332660	-2.662383	0.000230
	8	-1.262240	3.654456	0.000304
	8	-3.333590	2.660695	0.000223
	53	2.887594	0.000254	0.000006
	7	-3.465583	0.000271	-0.000272
	1	0.538540	2.187955	-0.000064
	1	0.538861	-2.187713	-0.000069
	1	-3.905727	0.917218	-0.000336
	1	-3.906292	-0.916441	-0.000338
<b>2-bromo-5-iodoisophthalate_2-</b>				
	6	-1.372272	2.676408	0.042720
	6	-0.761195	1.240360	-0.012920
	6	-1.447578	0.000065	0.000165
	6	-0.761326	-1.240309	0.013496
	6	-1.372549	-2.676326	-0.042306
	6	0.652435	-1.221694	0.054520
	6	1.330819	-0.000036	0.000166
	6	0.652566	1.221661	-0.054085
	8	-0.733845	3.552248	-0.653721
	8	-2.369525	2.865085	0.816289
	8	-0.735044	-3.552095	0.655039
	8	-2.369201	-2.865011	-0.816689
	53	3.486100	-0.000104	-0.000136
	35	-3.398165	0.000083	-0.000317
	1	1.153952	-2.179376	0.140090
	1	1.154028	2.179380	-0.139661
<b>2-bromo-3,5- trifluoroterephthalate_2-</b>				
	6	-3.299210	-0.695281	-0.000935
	6	-1.844658	-0.127511	0.005827
	6	-0.711492	-0.952461	-0.000960
	6	0.600888	-0.451629	-0.005282
	6	0.854036	0.931157	0.008712
	6	2.290617	1.539323	0.013490
	6	-0.274779	1.757396	0.024645
	6	-1.579920	1.245933	0.012737
	8	-3.945271	-0.508357	-1.086401
	8	-3.662107	-1.271612	1.078865
	8	2.823256	1.674720	-1.138934

	8	2.754003	1.818608	1.169804
	9	-2.630542	2.152514	0.035552
	9	-0.117220	3.139025	0.044408
	35	2.080095	-1.709968	-0.028559
	9	-0.893934	-2.329269	-0.028462
<b>2-bromoterephthalate_2-</b>				
	6	-3.512175	-0.220506	0.026340
	6	-2.038159	0.243023	0.017474
	6	-0.995938	-0.701996	0.004135
	6	0.346208	-0.275828	0.004763
	6	0.713569	1.085595	0.008891
	6	2.151134	1.680736	0.047737
	6	-0.359346	2.013951	-0.000180
	6	-1.704457	1.612373	0.010731
	8	-4.398881	0.712509	0.038709
	8	-3.712636	-1.491364	0.020414
	8	2.246938	2.896715	-0.368374
	8	3.085034	0.944058	0.518243
	35	1.671120	-1.735815	-0.067481
	1	-1.264369	-1.752970	-0.007764
	1	-0.071214	3.060271	-0.032252
	1	-2.522274	2.326771	0.010566
<b>2-fluoro-5-iodoisophthalate_2-</b>				
	6	-2.049127	2.655659	-0.034591
	6	-1.389734	1.243394	0.010369
	6	-2.063661	0.000016	0.000051
	6	-1.389741	-1.243366	-0.010344
	6	-2.049258	-2.655615	0.034569
	6	0.021854	-1.224145	-0.036776
	6	0.700122	0.000038	-0.000009
	6	0.021868	1.224236	0.036745
	8	-3.208227	2.755195	-0.558043
	8	-1.304918	3.603124	0.426328
	8	-3.208486	-2.755076	0.557716
	8	-1.305109	-3.603172	-0.426263
	53	2.855887	-0.000051	0.000001
	9	-3.444097	0.000079	0.000216
	1	0.517434	-2.187197	-0.096897
	1	0.517433	2.187297	0.096908
<b>2-hydroxy-5-iodoisophthalate_2-</b>				
	6	1.966537	2.690260	-0.015059
	6	1.360218	1.259386	0.025745
	6	2.090535	0.031567	0.037013
	6	1.381304	-1.216008	0.009253

	6	2.125421	-2.554857	0.026046
	6	-0.024770	-1.240896	-0.022536
	6	-0.720484	-0.028388	-0.005398
	6	-0.047200	1.204744	0.030945
	8	1.253536	3.590968	0.579518
	8	3.042130	2.869046	-0.678629
	8	1.452870	-3.634091	-0.021406
	8	3.430672	-2.465432	0.093005
	53	-2.876923	-0.052148	-0.025697
	8	3.450550	0.006862	0.114115
	1	-0.506954	-2.213023	-0.049110
	1	-0.565614	2.156886	0.085935
	1	3.722051	-0.993704	0.116213
<b>2-iodo-11-biphenyl-44-dicarboxylate_2-</b>				
	6	-1.015976	-0.766661	0.042542
	6	-1.758255	-1.462049	-0.940788
	6	-3.165554	-1.439547	-0.932025
	6	-3.864733	-0.732279	0.064581
	6	-3.130475	-0.043973	1.050790
	6	-1.723882	-0.058812	1.042311
	6	0.481268	-0.855975	0.050126
	6	1.370064	0.246955	0.015098
	6	2.767895	0.086748	0.042970
	6	3.329661	-1.201908	0.100263
	6	2.473097	-2.317690	0.119395
	6	1.080119	-2.143636	0.094518
	6	-5.409998	-0.718554	0.080734
	8	-5.957389	-0.058534	1.038135
	8	-5.988466	-1.371078	-0.863847
	6	4.866204	-1.378953	0.132216
	8	5.555859	-0.296478	0.112606
	8	5.284710	-2.592370	0.175007
	53	0.643087	2.257627	-0.188669
	1	-1.221999	-2.005852	-1.715636
	1	-3.756902	-1.958506	-1.680663
	1	-3.696670	0.485857	1.811093
	1	-1.167553	0.467536	1.813895
	1	3.453554	0.927578	0.010908
	1	2.933841	-3.299868	0.159193
	1	0.417786	-3.005318	0.129099
<b>2-iodoterephthalate_2-</b>				
	6	1.478998	2.288291	0.032810
	6	0.177886	1.434205	0.005671

	6	0.083557	0.025557	0.009252
	6	-1.160610	-0.641687	0.007298
	6	-2.362490	0.090669	0.010549
	6	-3.725111	-0.638908	0.017175
	6	-2.293950	1.497978	0.001515
	6	-1.049281	2.145764	-0.005414
	8	2.567631	1.687557	0.334999
	8	1.322567	3.538710	-0.231384
	8	-4.769247	0.114124	0.020857
	8	-3.686901	-1.924523	0.018508
	53	1.793588	-1.284647	-0.029993
	1	-1.233750	-1.724578	0.003722
	1	-3.231985	2.045069	-0.001585
	1	-0.960818	3.227647	-0.029491
<b>3-bromo-3-iodo-44-bipyridine_0</b>				
	6	1.347886	0.159871	-2.274529
	6	2.585489	-0.466755	-2.500306
	7	3.437401	-0.777396	-1.496786
	6	3.087583	-0.470042	-0.230687
	6	1.865236	0.158678	0.075183
	6	0.961273	0.480871	-0.955919
	6	-2.701313	1.125959	-0.048104
	6	-1.491302	0.430215	-0.261090
	6	-0.354201	1.142903	-0.697979
	6	-0.493311	2.531010	-0.911295
	6	-1.735029	3.145105	-0.675696
	7	-2.817208	2.454667	-0.250854
	53	-1.438793	-1.658312	0.070223
	35	1.463012	0.567540	1.920714
	1	0.684231	0.385978	-3.102184
	1	2.905370	-0.730508	-3.502563
	1	3.789865	-0.725560	0.555576
	1	-3.590171	0.602767	0.289491
	1	0.357579	3.115517	-1.244563
	1	-1.871477	4.210660	-0.826576
<b>3-bromo-35-diiodo-44-bipyridine_0</b>				
	6	-0.000431	1.085235	-2.067327
	6	-0.000676	2.442442	-2.430751
	7	-0.000656	3.440843	-1.517599
	6	-0.000364	3.123301	-0.206854
	6	-0.000063	1.786619	0.235627
	6	-0.000065	0.737154	-0.700764
	6	1.163067	-2.759888	0.323977

	6	1.206213	-1.407038	-0.071264
	6	0.000071	-0.697602	-0.280345
	6	-1.206075	-1.407150	-0.071161
	6	-1.162764	-2.759945	0.323947
	7	0.000226	-3.415242	0.513975
	53	3.094600	-0.483522	-0.312825
	35	0.000291	1.424972	2.132797
	53	-3.094583	-0.483753	-0.312519
	1	-0.000643	0.308619	-2.824647
	1	-0.000901	2.743081	-3.472765
	1	-0.000388	3.942288	0.504408
	1	2.076273	-3.320060	0.491703
	1	-2.075868	-3.320311	0.491541
<b>3-chloro-3-iodo-44-bipyridine_0</b>				
	6	1.860105	0.762005	-1.635311
	6	3.163172	0.246508	-1.750105
	7	3.830935	-0.284348	-0.700609
	6	3.224110	-0.316605	0.503721
	6	1.923148	0.180805	0.692194
	6	1.205903	0.729776	-0.386428
	6	-2.589768	1.067281	-0.007848
	6	-1.320771	0.462323	-0.139174
	6	-0.175332	1.281130	-0.237872
	6	-0.365474	2.679390	-0.213646
	6	-1.664559	3.198294	-0.082350
	7	-2.755004	2.405757	0.021337
	53	-1.199569	-1.647546	-0.213761
	17	1.206184	0.115608	2.338812
	1	1.351538	1.173487	-2.500437
	1	3.686575	0.254544	-2.699892
	1	3.777290	-0.741515	1.334300
	1	-3.485955	0.461166	0.073422
	1	0.489369	3.343380	-0.285268
	1	-1.841508	4.268204	-0.056781
<b>3-chloro-35-diiodo-44-bipyridine_0</b>				
	6	0.000491	1.529446	-1.619222
	6	0.000631	2.930238	-1.730879
	7	0.000333	3.747395	-0.652391
	6	-0.000126	3.197928	0.579137
	6	-0.000247	1.804955	0.766394
	6	0.000053	0.938925	-0.339595
	6	1.162906	-2.684863	0.047785
	6	1.206270	-1.282825	-0.097929
	6	0.000007	-0.547570	-0.177064

	6	-1.206240	-1.282848	-0.098056
	6	-1.162875	-2.684881	0.047681
	7	0.000012	-3.363355	0.116691
	53	3.095079	-0.333838	-0.173648
	17	-0.000777	1.148956	2.438539
	53	-3.095000	-0.333809	-0.173957
	1	0.000725	0.903278	-2.504851
	1	0.001021	3.413863	-2.701480
	1	-0.000389	3.869822	1.430648
	1	2.075797	-3.266632	0.112075
	1	-2.075774	-3.266644	0.111927
<b>3-iodo-3-methyl-44-bipyridine_0</b>				
	6	1.961537	0.602557	-1.444622
	6	3.267664	0.081218	-1.476125
	7	3.911741	-0.322155	-0.359396
	6	3.269574	-0.217578	0.824707
	6	1.957835	0.284077	0.969395
	6	1.292948	0.701340	-0.209754
	6	-2.519508	1.082862	-0.013020
	6	-1.249869	0.467226	-0.075264
	6	-0.090647	1.269001	-0.148409
	6	-0.274177	2.670007	-0.166706
	6	-1.572577	3.202755	-0.103309
	7	-2.674923	2.422592	-0.024553
	53	-1.144234	-1.647901	-0.092791
	6	1.302308	0.364705	2.330704
	1	1.471760	0.915672	-2.360728
	1	3.810330	-0.015494	-2.410774
	1	3.822779	-0.545430	1.701025
	1	-3.423644	0.485417	0.043531
	1	0.588995	3.324639	-0.225983
	1	-1.740979	4.274439	-0.115008
	1	2.028831	0.167815	3.122894
	1	0.862042	1.351899	2.502903
	1	0.496033	-0.372296	2.422115
<b>3-iodo-35-dimethyl-44-bipyridine_0</b>				
	6	-1.889089	0.343035	1.225067
	6	-3.182357	-0.216720	1.159896
	7	-3.816269	-0.489600	0.000064
	6	-3.182331	-0.217003	-1.159832
	6	-1.889079	0.342762	-1.225105
	6	-1.240668	0.625924	-0.000048
	6	2.566361	1.078759	0.000027

	6	1.304472	0.444912	-0.000001
	6	0.130362	1.226864	-0.000097
	6	0.289912	2.630579	-0.000194
	6	1.581269	3.183788	-0.000173
	7	2.698925	2.420928	-0.000052
	53	1.217585	-1.671188	0.000071
	6	-1.216895	0.604477	-2.555591
	6	-1.216901	0.604968	2.555506
	1	-3.720883	-0.454024	2.073478
	1	-3.720829	-0.454573	-2.073360
	1	3.481624	0.495611	0.000120
	1	-0.586013	3.271427	-0.000283
	1	1.732269	4.258211	-0.000245
	1	-1.882586	0.349599	-3.383663
	1	-0.304047	0.005614	-2.655331
	1	-0.926924	1.655440	-2.657432
	1	-1.882709	0.350535	3.383620
	1	-0.926609	1.655872	2.657033
	1	-0.304241	0.005856	2.655475
<b>3-iodo-44-bipyridine_0</b>				
	6	2.389494	0.930368	-0.934825
	6	3.659311	0.323775	-0.904577
	7	4.027264	-0.558728	0.050814
	6	3.129530	-0.868219	1.014914
	6	1.836518	-0.317335	1.060936
	6	1.450209	0.601743	0.063478
	6	-2.332408	1.295891	0.093794
	6	-1.122967	0.565266	0.054609
	6	0.108066	1.260107	0.083133
	6	0.045620	2.673034	0.129417
	6	-1.199164	3.320290	0.161545
	7	-2.369493	2.642357	0.149431
	53	-1.263156	-1.542210	-0.132168
	1	2.134726	1.629009	-1.725033
	1	4.401629	0.547453	-1.664042
	1	3.460197	-1.574467	1.769507
	1	1.153251	-0.593156	1.856614
	1	-3.288002	0.782095	0.072336
	1	0.964580	3.249182	0.157212
	1	-1.268788	4.402101	0.202029
<b>5-iodoisophthalate_2-</b>				
	6	-2.291458	-2.593041	0.000044
	6	-1.557534	-1.227916	0.000042
	6	-2.253789	0.000001	0.000059

	6	-1.557533	1.227917	0.000057
	6	-2.291456	2.593042	0.000080
	6	-0.145158	1.231102	0.000036
	6	0.525893	0.000000	0.000021
	6	-0.145159	-1.231103	0.000022
	8	-1.534968	-3.637789	-0.000080
	8	-3.572646	-2.555332	-0.000028
	8	-1.534965	3.637790	-0.000093
	8	-3.572644	2.555334	-0.000051
	53	2.691474	0.000000	-0.000005
	1	-3.338292	0.000001	0.000077
	1	0.354552	2.194199	0.000037
	1	0.354551	-2.194200	0.000009
<b>22-diiodo-11-biphenyl-44-dicarboxylate_2-</b>				
	6	0.746944	-0.068396	0.987284
	6	1.604335	0.649007	0.121807
	6	3.002659	0.515018	0.178917
	6	3.585855	-0.349253	1.124677
	6	2.754031	-1.071855	1.999560
	6	1.357661	-0.930625	1.930986
	6	-0.746997	0.068188	0.987298
	6	-1.604281	-0.648788	0.121347
	6	-3.002627	-0.514963	0.178459
	6	-3.585974	0.348626	1.124747
	6	-2.754270	1.070618	2.000244
	6	-1.357885	0.929574	1.931656
	6	5.125748	-0.488475	1.200420
	8	5.566140	-1.295018	2.097224
	8	5.793563	0.218151	0.362778
	6	-5.125881	0.487686	1.200498
	8	-5.793621	-0.218783	0.362664
	8	-5.566359	1.293984	2.097479
	53	-0.780863	-2.001499	-1.317149
	53	0.780993	2.002219	-1.316231
	1	3.670494	1.060990	-0.479173
	1	3.236609	-1.728662	2.716545
	1	0.710580	-1.490048	2.602160
	1	-3.670373	-1.060634	-0.479971
	1	-3.236957	1.726868	2.717666
	1	-0.710927	1.488492	2.603367
<b>22-diiodobiphenyl-4455-tetracarboxylate_4-</b>				
	6	-0.748115	0.592071	0.112625

	6	-1.410313	-0.324202	0.960194
	6	-2.806098	-0.340923	1.104778
	6	-3.626560	0.564874	0.393516
	6	-3.007128	1.472654	-0.506931
	6	-1.592696	1.481492	-0.601369
	6	0.749313	0.599272	-0.074790
	6	1.413063	-0.270542	-0.969707
	6	2.810271	-0.298971	-1.092417
	6	3.630332	0.558075	-0.321887
	6	3.003588	1.490343	0.547585
	6	1.590301	1.472253	0.662584
	6	-5.129772	0.516094	0.777470
	8	-5.726240	1.633788	0.956543
	8	-5.611076	-0.664640	1.011382
	6	5.153007	0.283826	-0.452150
	8	5.565234	-0.038518	-1.638281
	8	5.842189	0.270014	0.625654
	6	-3.766870	2.384794	-1.503933
	8	-3.295051	3.576306	-1.658808
	8	-4.718095	1.836990	-2.167681
	6	3.740747	2.612791	1.321700
	8	3.357175	2.810272	2.538471
	8	4.579415	3.313993	0.650893
	53	0.278977	-1.647099	-2.177926
	53	-0.278392	-1.768305	2.088216
	1	-3.304862	-1.055943	1.750933
	1	-1.142502	2.209398	-1.271253
	1	3.310155	-0.966084	-1.787117
	1	1.139381	2.159985	1.373101
<b>25-difluoro-36- diiodoterephthalate_2-</b>				
	6	1.811231	2.398405	0.000134
	6	0.891198	1.138853	0.000115
	6	-0.503964	1.271299	0.000072
	6	-1.385749	0.178097	0.000014
	6	-0.891185	-1.138829	-0.000055
	6	-1.811240	-2.398359	-0.000084
	6	0.503972	-1.271274	-0.000055
	6	1.385763	-0.178074	0.000056
	8	2.134658	2.830982	-1.157018
	8	2.138124	2.828411	1.157286
	8	-2.137099	-2.829123	-1.157239
	8	-2.135727	-2.830150	1.157073
	53	3.476666	-0.540822	-0.000161

	9	1.038486	-2.557491	-0.000208
	53	-3.476662	0.540788	0.000118
	9	-1.038489	2.557505	0.000238
<b>25-diiodoterephthalate_2-</b>				
	6	1.651138	2.509539	0.061889
	6	0.857409	1.167537	0.027888
	6	1.388228	-0.139378	0.019302
	6	0.552707	-1.270770	0.012320
	6	-0.857417	-1.167497	0.027851
	6	-1.651161	-2.509564	0.061873
	6	-1.388217	0.139394	0.019311
	6	-0.552704	1.270800	0.012359
	8	0.954138	3.563343	-0.173332
	8	2.897489	2.437606	0.338876
	8	-2.897616	-2.437566	0.338314
	8	-0.954054	-3.563384	-0.172859
	53	-3.488662	0.578849	-0.038409
	53	3.488671	-0.578856	-0.038458
	1	0.949990	-2.279981	-0.015435
	1	-0.950009	2.280003	-0.015418
<b>33-dibromo-44-bipyridine_0</b>				
	6	-1.185269	1.977173	1.139185
	6	-2.536086	1.960048	1.527856
	7	-3.420952	1.059104	1.043778
	6	-2.991542	0.144283	0.150282
	6	-1.654194	0.097547	-0.287631
	6	-0.716439	1.022227	0.212481
	6	2.991579	0.144319	-0.150135
	6	1.654204	0.097529	0.287693
	6	0.716464	1.022225	-0.212415
	6	1.185322	1.977199	-1.139079
	6	2.536150	1.960090	-1.527706
	7	3.421015	1.059163	-1.043591
	35	1.145891	-1.241362	1.585358
	35	-1.145940	-1.241174	-1.585499
	1	-0.500544	2.708604	1.554809
	1	-2.922012	2.678097	2.243311
	1	-3.721471	-0.564239	-0.226315
	1	3.721509	-0.564173	0.226514
	1	0.500608	2.708641	-1.554703
	1	2.922083	2.678123	-2.243173
<b>33-diiodo-44-bipyridine_0</b>				
	6	-0.520907	1.577105	-2.188949
	6	-1.566241	2.515782	-2.190734

	7	-2.618115	2.433039	-1.345087
	6	-2.665110	1.410165	-0.467562
	6	-1.656861	0.423964	-0.397463
	6	-0.552767	0.503512	-1.272516
	6	2.665129	-1.410148	-0.467537
	6	1.656869	-0.423956	-0.397446
	6	0.552789	-0.503505	-1.272514
	6	0.520954	-1.577087	-2.188961
	6	1.566303	-2.515746	-2.190750
	7	2.618163	-2.433004	-1.345083
	53	1.850318	1.133478	1.020409
	53	-1.850345	-1.133494	1.020374
	1	0.311949	1.676251	-2.876889
	1	-1.566749	3.353480	-2.879929
	1	-3.523193	1.371302	0.194952
	1	3.523211	-1.371273	0.194978
	1	-0.311893	-1.676233	-2.876914
	1	1.566826	-3.353439	-2.879950
<b>35-diiodo-3-methyl-44-bipyridine_0</b>				
	6	-0.030437	1.664764	-1.418086
	6	-0.029370	3.071050	-1.445892
	7	-0.002544	3.816952	-0.319577
	6	0.024588	3.181816	0.872552
	6	0.026626	1.778021	1.014799
	6	-0.002077	1.010594	-0.173325
	6	-1.166166	-2.637114	0.001311
	6	-1.207170	-1.228905	-0.063271
	6	-0.002815	-0.485084	-0.103864
	6	1.200632	-1.230529	-0.066650
	6	1.158045	-2.638589	-0.001430
	7	-0.004481	-3.320855	0.029887
	53	-3.100096	-0.281290	-0.079243
	6	0.059449	1.122906	2.377290
	53	3.094872	-0.285798	-0.094381
	1	-0.053044	1.094712	-2.341029
	1	-0.050422	3.612944	-2.385611
	1	0.045434	3.816017	1.754924
	1	-2.080077	-3.220128	0.030904
	1	2.071264	-3.222800	0.025897
	1	0.080927	1.873471	3.170852
	1	0.945507	0.486475	2.483695
	1	-0.821368	0.488716	2.529665
<b>35-diiodo-35-dimethyl-44-</b>				

<b>bipyridine_0</b>				
	6	-0.030831	1.686147	1.225328
	6	-0.029201	3.095152	1.159944
	7	-0.000108	3.784437	0.000065
	6	0.029045	3.095191	-1.159858
	6	0.030788	1.686203	-1.225294
	6	0.000013	0.982105	0.000010
	6	-1.162145	-2.671460	-0.003734
	6	-1.202937	-1.262012	-0.004061
	6	0.000033	-0.515643	-0.000010
	6	1.203004	-1.262003	0.004059
	6	1.162244	-2.671447	0.003769
	7	0.000052	-3.355175	0.000028
	53	-3.094088	-0.310966	-0.012731
	6	0.065431	0.959663	-2.551503
	53	3.094099	-0.310901	0.012697
	6	-0.065454	0.959558	2.551511
	1	-0.052033	3.683615	2.073164
	1	0.051823	3.683705	-2.073044
	1	-2.075812	-3.255704	-0.006832
	1	2.075920	-3.255678	0.006883
	1	0.089441	1.668260	-3.382712
	1	0.950678	0.317293	-2.623547
	1	-0.815824	0.319364	-2.673232
	1	-0.950695	0.317176	2.623521
	1	0.815806	0.319263	2.673218
	1	-0.089477	1.668122	3.382748
<b>36-diiodobenzene-1245-tetracarboxylate_4-</b>				
	6	0.679951	1.226819	-0.313747
	6	-0.680008	1.226861	0.314411
	6	-1.354607	-0.056167	0.160342
	6	-0.751486	-1.262059	-0.076522
	6	0.751477	-1.262125	0.076458
	6	1.354562	-0.056182	-0.160239
	6	1.184401	2.388425	-0.907909
	8	2.221320	2.696303	-1.586935
	8	0.293839	3.556516	-0.677823
	6	-1.184735	2.388832	0.907538
	8	-2.222283	2.697520	1.585274
	8	-0.293210	3.556469	0.677879
	6	-1.492832	-2.544281	-0.560597
	8	-1.577985	-2.714794	-1.834859
	8	-1.976594	-3.320888	0.344710

	6	1.493100	-2.544294	0.560234
	8	1.977867	-3.320039	-0.345263
	8	1.577525	-2.715548	1.834455
	53	3.623302	-0.004750	0.082234
	53	-3.623354	-0.005048	-0.081843
<b>46-difluoro-5-iodo-isophthalate_2-</b>				
	6	2.412990	-2.561611	0.030085
	6	1.583268	-1.246257	0.034303
	6	2.247613	-0.000010	-0.000008
	6	1.583280	1.246239	-0.034334
	6	2.413033	2.561576	-0.030093
	6	0.180228	1.211532	-0.048108
	6	-0.532843	0.000013	-0.000014
	6	0.180229	-1.211528	0.048097
	8	1.875347	-3.577299	-0.535284
	8	3.572458	-2.470536	0.570466
	8	1.875360	3.577282	0.535215
	8	3.572556	2.470484	-0.570355
	53	-2.650932	0.000010	0.000010
	9	-0.578084	-2.370085	0.139471
	9	-0.578038	2.370116	-0.139522
	1	3.331944	0.000025	0.000000
<b>235-trifluoro-6-iodoterephthalate_2-</b>				
	6	-3.393645	-1.223680	0.001363
	6	-2.096517	-0.355024	0.001589
	6	-0.811196	-0.914580	0.000729
	6	0.367991	-0.149178	-0.005109
	6	0.309912	1.258483	0.003788
	6	1.573251	2.172331	0.013934
	6	-0.970134	1.822974	0.014017
	6	-2.134324	1.042548	0.001908
	8	-4.039994	-1.229204	-1.099888
	8	-3.648408	-1.816654	1.102845
	8	2.103815	2.375778	-1.130024
	8	1.924849	2.593447	1.166978
	9	-3.356531	1.699933	0.016500
	9	-1.113563	3.206260	0.023963
	53	2.240763	-1.146251	-0.013833
	9	-0.702632	-2.301623	-0.015960
<b>246-triiodo-135-benzenetricarboxylate_3-</b>				
	6	-0.761810	-1.221024	-0.000188
	6	-1.384766	0.047383	-0.000189

	6	-0.676504	1.270099	-0.000203
	6	0.733481	1.175521	-0.000241
	6	1.438204	-0.049213	0.000069
	6	0.651275	-1.223036	0.000033
	6	-1.585519	-2.541449	-0.000408
	8	-1.880779	-3.015666	1.153163
	8	-1.881677	-3.014391	-1.154270
	6	-1.408741	2.643320	0.000043
	8	-1.671600	3.135605	1.153870
	8	-1.671025	3.136556	-1.153460
	6	2.993827	-0.102013	0.000339
	8	3.551561	-0.122028	1.154052
	8	3.551836	-0.119814	-1.153349
	53	1.663668	-3.121259	-0.000047
	53	1.872106	3.000877	-0.000055
	53	-3.535458	0.120388	0.000185
<b>335-triiodo-44-bipyridine_0</b>				
	6	-0.000182	-0.235975	2.450376
	6	-0.000195	-1.412768	3.217035
	7	-0.000044	-2.644287	2.657175
	6	0.000104	-2.746528	1.312646
	6	0.000093	-1.615642	0.467446
	6	-0.000025	-0.329206	1.042911
	6	1.163490	2.726519	-0.943028
	6	1.206305	1.540171	-0.181742
	6	-0.000055	0.919451	0.219299
	6	-1.206475	1.540112	-0.181784
	6	-1.163702	2.726440	-0.943041
	7	-0.000099	3.301720	-1.309117
	53	3.090307	0.710268	0.305857
	53	0.000260	-1.898144	-1.626586
	53	-3.090464	0.710025	0.305672
	1	-0.000290	0.737336	2.929683
	1	-0.000320	-1.376051	4.301055
	1	0.000242	-3.748359	0.896494
	1	2.076107	3.217906	-1.263127
	1	-2.076315	3.217806	-1.263176
<b>2356-tetraiodoterephthalate_2-</b>				
	6	0.000382	-2.996501	-0.000257
	6	0.000049	-1.433933	-0.000106
	6	1.210727	-0.706649	-0.000150
	6	1.210666	0.707004	-0.000210
	6	-0.000084	1.434168	-0.000186
	6	-0.000137	2.996838	-0.000038

	6	-1.210715	0.706879	-0.000099
	6	-1.210630	-0.706793	-0.000131
	8	-0.000709	-3.536833	1.156726
	8	0.001868	-3.536168	-1.157624
	8	-0.000592	3.536999	-1.157121
	8	0.000169	3.536760	1.157160
	53	-3.020098	-1.849129	-0.000325
	53	-3.020502	1.848748	0.000401
	53	3.020272	1.849211	-0.000378
	53	3.020188	-1.849059	0.000565
<b>3355-tetrabromo-44-bipyridine_0</b>				
	6	0.847747	0.847635	-1.487596
	6	0.823478	0.823271	-2.893866
	7	0.000054	0.000086	-3.574798
	6	-0.823404	-0.823122	-2.893925
	6	-0.847714	-0.847547	-1.487660
	6	0.000007	0.000027	-0.746341
	6	-0.823563	0.823055	2.893903
	6	-0.847827	0.847488	1.487636
	6	-0.000015	-0.000014	0.746341
	6	0.847772	-0.847556	1.487620
	6	0.823454	-0.823204	2.893888
	7	-0.000072	-0.000100	3.574799
	35	-2.056322	2.055813	0.591256
	35	-2.056127	-2.055979	-0.591317
	35	2.056300	-2.055838	0.591229
	35	2.056165	2.056002	-0.591168
	1	1.471622	1.471127	-3.473085
	1	-1.471515	-1.470966	-3.473194
	1	-1.471759	1.470831	3.473154
	1	1.471619	-1.471023	3.473126
<b>3355-tetraiodo-44-bipyridine_0</b>				
	6	0.852356	0.854745	1.484168
	6	0.821474	0.824214	2.893240
	7	0.000005	-0.000116	3.574880
	6	-0.821478	-0.824394	2.893195
	6	-0.852374	-0.854826	1.484120
	6	-0.000012	-0.000022	0.747989
	6	0.823645	-0.822117	-2.893221
	6	0.854476	-0.852665	-1.484146
	6	0.000024	0.000030	-0.747988
	6	-0.854319	0.852842	-1.484139
	6	-0.823214	0.822587	-2.893212
	7	0.000292	0.000313	-3.574880

	53	2.186583	-2.180316	-0.519881
	53	-2.181398	-2.185498	0.519779
	53	-2.186675	2.180219	-0.519849
	53	2.181376	2.185517	0.519950
	1	1.465165	1.470683	3.480023
	1	-1.465160	-1.470904	3.479941
	1	1.468937	-1.467001	-3.479989
	1	-1.468391	1.467591	-3.479974
<b>tetraiodoisophthalate_2-</b>				
	6	-1.854207	2.592478	-0.000021
	6	-1.078557	1.239704	0.000111
	6	-1.751216	-0.000353	0.000014
	6	-1.078118	-1.240190	0.000001
	6	-1.853344	-2.593201	-0.000079
	6	0.334934	-1.222199	-0.000032
	6	1.051868	0.000157	0.000015
	6	0.334542	1.222263	0.000094
	8	-2.115905	3.064811	-1.157422
	8	-2.114681	3.065895	1.157202
	8	-2.113530	-3.066482	-1.157438
	8	-2.115076	-3.065841	1.157172
	53	-3.885507	-0.000555	-0.000018
	53	1.316231	-3.125950	0.000175
	53	3.198389	0.000479	-0.000151
	53	1.315003	3.126422	0.000056