polymers

Mechanistic Insight into the Ring-Opening Polymerization of *ε*-Caprolactone and *L*-Lactide Using Ketiminate-Ligated Aluminum Catalysts

Supplementary

Theoretical Details

Table S1. Cartesian coordinate of C_{eq}**1a.**

The number of atom coordinates (angstroms)	X	Y	Z
13	−0.323482	0.337649	−0.65403
8	1.161713	0.223533	−1.820921
8	−1.394612	0.900602	0.640559
7	0.764338	−0.677639	0.682025
6	2.544291	−0.959982	−3.332665
1	3.139089	−0.058571	−3.520829
1	3.188545	−1.839713	−3.407058
1	1.777173	−1.007113	−4.114377
6	1.870645	−0.843508	−1.990405
6	2.050853	−1.808955	−1.008855
1	2.677598	−2.662678	−1.234701
6	1.593687	−1.655371	0.322813
6	2.088544	−2.648696	1.351084
1	1.237863	−3.115995	1.858173
1	2.69737	−3.426135	0.884771
1	2.685224	−2.150845	2.122173
6	0.52331	−0.494529	2.08722
6	−0.585004	−1.077837	2.709352
1	−1.274097	−1.665196	2.11676
6	−0.800923	−0.874897	4.071296
1	−1.667152	−1.328451	4.54579
6	0.079138	−0.087704	4.822273
6	1.182286	0.497525	4.198596
1	1.870375	1.115929	4.769144
6	1.403925	0.292588	2.83431
1	2.258185	0.744332	2.337666
6	−2.38566	1.879894	0.625012
1	−2.565771	2.298939	−0.378829
1	−3.344955	1.431372	0.944368
6	−2.058807	3.022349	1.574813

6	−1.421512	2.745183	2.792053
1	−1.150942	1.719927	3.016539
6	−1.114889	3.772575	3.68469
1	−0.612791	3.537861	4.620389
6	−1.446382	5.096175	3.376712
1	−1.207597	5.898017	4.070915
6	−2.087347	5.380447	2.168211
1	−2.346411	6.406545	1.917295
6	−2.384777	4.348491	1.271752
1	−2.864665	4.57824	0.322459
8	−1.340435	−0.638347	−1.716506
6	−2.590878	−1.138457	−1.323274
1	−3.103524	−1.531776	−2.218056
1	−3.246221	−0.352768	−0.914088
6	−2.495314	−2.259852	−0.297354
6	−1.419918	−3.156878	−0.332254
1	−0.650617	−3.020489	−1.085871
6	−1.316852	−4.18389	0.60712
1	−0.471341	−4.867022	0.569835
6	−2.291876	−4.332464	1.59825
1	−2.208277	−5.126833	2.335449
6	−3.371253	−3.4465	1.637802
1	−4.130366	−3.546297	2.409854
6	−3.468026	−2.417905	0.696512
1	−4.298643	−1.716649	0.74682
6	0.582842	3.161007	−0.971917
6	1.853549	2.933022	−0.190173
6	1.832515	3.592028	1.208036
6	2.109265	5.0995	1.192084
6	1.123717	5.92326	0.354015
6	1.07213	5.543124	−1.121703
1	2.70262	3.311028	−0.774614
1	0.875015	3.379261	1.694181
1	3.127575	5.271589	0.813148
1	0.111091	5.844353	0.764918
1	1.980539	1.853211	−0.107102
1	2.60258	3.09833	1.811094
1	2.091747	5.471328	2.223341
1	1.408193	6.98217	0.404073
1	0.575744	6.317146	−1.708328
1	2.069808	5.378269	−1.544566
8	−0.208464	2.256507	−1.253584

8	0.245381	4.372305	−1.382589
1	−0.098273	0.071742	5.882404

Table S2. Cartesian coordinate of **C_{eq}TS1a.**

The number of atom coordinates (angstroms)	X	Y	Z
13	−0.047683	0.376727	−0.751961
8	0.445172	−0.906732	−2.035728
8	−0.216154	2.063351	0.186357
7	0.727928	−0.658712	0.730169
6	1.254225	−1.892753	−1.915219
6	1.570972	−2.628715	−3.192175
1	0.640147	−3.009557	−3.628131
1	1.999856	−1.926861	−3.916114
1	2.263395	−3.460187	−3.040023
6	1.791569	−2.312066	−0.698238
1	2.442271	−3.177217	−0.708958
6	1.478589	−1.757604	0.559489
6	2.016539	−2.491861	1.770439
1	1.190139	−2.861125	2.387376
1	2.633041	−3.340319	1.469167
1	2.612059	−1.82958	2.406231
6	0.412554	−0.296718	2.090045
6	−0.759454	−0.782523	2.679974
1	−1.416046	−1.422152	2.102056
6	−1.067415	−0.457802	4.002704
1	−1.983257	−0.839908	4.445232
6	−0.205839	0.347657	4.750264
6	0.966276	0.83105	4.162977
1	1.642142	1.463312	4.732094
6	1.274066	0.511188	2.840261
1	2.188214	0.877894	2.388417
6	−1.354467	2.903885	0.091511
1	−1.169186	3.674024	−0.670295
1	−2.201338	2.319051	−0.281514
6	−1.727984	3.565283	1.401186
6	−1.505291	2.919447	2.62101
1	−1.022646	1.952161	2.619403
6	−1.888413	3.517001	3.822374
1	−1.700573	2.998019	4.758789
6	−2.507394	4.769496	3.820335
1	−2.804971	5.236498	4.755672
6	−2.738366	5.420392	2.605707

1	−3.215612	6.397125	2.592192
6	−2.348279	4.821583	1.405833
1	−2.525522	5.336217	0.462976
8	−1.764941	0.116602	−1.045842
6	−2.811232	−0.150066	−0.166416
1	−3.757813	0.208846	−0.606631
1	−2.704766	0.394377	0.790834
6	−2.976342	−1.62773	0.171781
6	−2.192197	−2.608676	−0.441477
1	−1.47771	−2.306322	−1.198107
6	−2.324888	−3.952321	−0.079199
1	−1.70123	−4.70202	−0.560518
6	−3.248084	−4.332868	0.895835
1	−3.348337	−5.377194	1.180185
6	−4.044228	−3.357981	1.506436
1	−4.76713	−3.642815	2.267116
6	−3.906941	−2.017669	1.145829
1	−4.517778	−1.260305	1.635038
6	1.292569	2.57349	−0.892447
6	2.373415	2.709231	0.166624
6	2.096242	3.602184	1.382327
6	2.15022	5.106218	1.101328
6	1.150602	5.577309	0.040282
6	1.383629	4.986912	−1.347489
1	3.277513	3.045885	−0.363726
1	1.12278	3.327891	1.796848
1	3.165543	5.381419	0.778242
1	0.124143	5.370258	0.360164
1	2.573469	1.686149	0.488414
1	2.846749	3.362487	2.146416
1	1.961906	5.649931	2.035105
1	1.230515	6.667079	−0.069345
1	0.849433	5.565934	−2.103061
1	2.450699	4.998149	−1.604158
8	1.239575	1.466801	−1.56423
8	0.879397	3.645619	−1.575891
1	−0.445046	0.598609	5.779875

Table S3. Cartesian coordinate of **C_{eq}2a.**

The number of atom coordinates (angstroms)	**X**	**Y**	**Z**
13	0.428558	0.22589	−0.787086
8	1.534854	−0.637712	−1.996662

8	−0.28204	1.675766	0.618848
7	0.834452	−1.035479	0.646414
6	1.779969	−1.901217	−2.007876
6	2.345568	−2.436978	−3.296375
1	1.63097	−2.251933	−4.106551
1	3.260687	−1.887325	−3.544583
1	2.568048	−3.505558	−3.247487
6	1.581985	−2.735498	−0.909464
1	1.837066	−3.781923	−1.019407
6	1.214093	−2.291371	0.380681
6	1.269626	−3.312414	1.495895
1	0.270491	−3.461003	1.918912
1	1.643489	−4.270371	1.130172
1	1.914158	−2.968964	2.311029
6	0.629633	−0.691283	2.029371
6	−0.59547	−0.941072	2.655752
1	−1.408371	−1.369278	2.082768
6	−0.752296	−0.661947	4.014498
1	−1.705617	−0.867871	4.493488
6	0.30443	−0.12245	4.752199
6	1.517367	0.157202	4.116265
1	2.340847	0.590815	4.67714
6	1.680251	−0.124293	2.758112
1	2.621352	0.078966	2.25546
6	−1.626486	2.071938	0.966572
1	−2.143198	2.420502	0.07118
1	−2.081436	1.134903	1.299239
6	−1.675501	3.113522	2.052635
6	−1.011997	2.898143	3.265835
1	−0.456998	1.979308	3.410039
6	−1.039755	3.867439	4.266948
1	−0.512597	3.692076	5.201303
6	−1.740417	5.061339	4.069126
1	−1.759983	5.818671	4.848356
6	−2.41129	5.278824	2.863888
1	−2.953041	6.206713	2.70056
6	−2.37415	4.308993	1.858883
1	−2.87376	4.489196	0.910293
8	−1.066958	−0.089725	−1.618928
6	−2.432409	−0.229062	−1.377338
1	−2.923313	−0.507691	−2.324956

1	−2.897007	0.719784	−1.067703
6	−2.763769	−1.295731	−0.343816
6	−2.093368	−2.52638	−0.370011
1	−1.322075	−2.690197	−1.116535
6	−2.387265	−3.517601	0.565903
1	−1.855418	−4.465367	0.533994
6	−3.360475	−3.294304	1.546573
1	−3.585167	−4.064004	2.280054
6	−4.037603	−2.073868	1.578335
1	−4.79166	−1.887586	2.338757
6	−3.738593	−1.082861	0.637366
1	−4.264298	−0.130689	0.672334
6	0.656607	2.617763	−0.040286
6	1.60883	3.274785	0.988172
6	1.33247	4.724467	1.413008
6	1.652661	5.771124	0.331947
6	0.657895	5.809124	−0.835585
6	0.490041	4.475204	−1.557317
1	2.609141	3.220777	0.543545
1	0.297886	4.842046	1.744678
1	2.664458	5.585898	−0.059572
1	−0.329718	6.117624	−0.467249
1	1.620936	2.616703	1.862014
1	1.961749	4.929884	2.289038
1	1.680183	6.765639	0.796792
1	0.977085	6.563099	−1.568839
1	−0.147367	4.594328	−2.439396
1	1.450542	4.06719	−1.894829
8	1.332839	1.772309	−0.860929
8	−0.178449	3.518094	−0.72303
1	0.179655	0.092723	5.80973

Table S4. Cartesian coordinate of **C_{eq}3a.**

The number of atom coordinates (angstroms)	X	Y	Z
13	−0.04825	0.527757	−0.481118
8	0.912934	−0.525644	−1.66322
8	0.735531	3.983643	0.388979
7	0.417504	−0.578612	1.056068
6	1.300557	−1.745464	−1.507686
6	1.823145	−2.417462	−2.748371
1	2.672763	−1.846062	−3.139386
1	2.132846	−3.449117	−2.567099

1	1.044177	−2.405142	−3.518511
6	1.26219	−2.413714	−0.28985
1	1.576882	−3.44866	−0.273402
6	0.862205	−1.839838	0.93317
6	0.950928	−2.724886	2.157498
1	1.700502	−2.351769	2.862656
1	−0.006758	−2.738539	2.686971
1	1.212291	−3.746501	1.877365
6	0.18505	−0.101294	2.392814
6	−1.101502	−0.11027	2.939954
1	−1.928153	−0.472964	2.338369
6	−1.30901	0.329467	4.249528
1	−2.312702	0.31738	4.66592
6	−0.23397	0.772761	5.022396
6	1.051247	0.78498	4.475555
1	1.890671	1.144725	5.063016
6	1.260084	0.353795	3.165725
1	2.255756	0.358246	2.731217
6	1.72552	3.530582	1.331992
1	1.648046	2.448827	1.456543
1	2.716247	3.756785	0.922583
6	1.504955	4.231278	2.648281
6	2.33938	5.270682	3.069698
1	3.173626	5.57541	2.441692
6	2.108722	5.920338	4.285756
1	2.765396	6.726811	4.601657
6	1.035449	5.534532	5.090809
1	0.854506	6.038251	6.036848
6	0.196692	4.494907	4.676623
1	−0.634419	4.180224	5.302553
6	0.431592	3.848953	3.464332
1	−0.205395	3.030236	3.147306
8	−1.685889	0.297682	−1.084485
6	−2.105763	−0.690214	−1.991275
1	−1.500287	−0.685194	−2.911494
1	−3.138605	−0.455398	−2.297771
6	−2.076884	−2.093548	−1.40304
6	−1.688264	−3.197573	−2.168618
1	−1.412742	−3.053892	−3.211504
6	−1.629798	−4.475148	−1.605853
1	−1.315507	−5.320027	−2.213668
6	−1.956628	−4.662734	−0.261634

1	−1.900048	−5.653097	0.18267
6	−2.360168	−3.56757	0.508592
1	−2.623493	−3.705425	1.554715
6	−2.425083	−2.297288	−0.062674
1	−2.729495	−1.439379	0.528135
6	0.072809	3.008512	−0.338999
6	−0.765983	3.707566	−1.416491
6	−1.503292	4.986129	−1.003707
6	−2.719004	4.754592	−0.100381
6	−2.414699	3.97258	1.184442
6	−2.120455	2.487442	0.971932
1	−1.455128	2.957712	−1.821937
1	−0.793905	5.654068	−0.503251
1	−3.495197	4.215246	−0.6636
1	−1.590519	4.438532	1.733668
1	−0.04552	3.939476	−2.207788
1	−1.834079	5.500747	−1.915177
1	−3.151773	5.727345	0.16784
1	−3.296352	4.016803	1.838334
1	−2.266543	1.943984	1.907707
1	−2.783254	2.055017	0.215512
8	0.869368	2.031938	−0.850312
8	−0.758311	2.164383	0.602382
1	−0.396793	1.115519	6.040042

Table S5. Cartesian coordinate of **C_{eq}TS2a.**

The number of atom coordinates (angstroms)	X	Y	Z
13	−0.046888	0.642566	−0.413124
8	1.011547	−0.368143	−1.59428
8	0.872536	4.070575	0.316745
7	0.426901	−0.567136	1.063742
6	1.329896	−1.612257	−1.517905
6	1.848996	−2.227372	−2.791178
1	2.701128	−1.643929	−3.157285
1	2.150499	−3.269425	−2.66154
1	1.068403	−2.173556	−3.559016
6	1.224365	−2.361365	−0.351331
1	1.493831	−3.408521	−0.391729
6	0.834004	−1.834506	0.894155
6	0.892197	−2.771332	2.081164
1	1.594056	−2.408452	2.83882
1	−0.090334	−2.835456	2.559454

1	1.195753	−3.772408	1.770422
6	0.238459	−0.127215	2.419428
6	−1.011126	−0.218753	3.039289
1	−1.848549	−0.61861	2.47708
6	−1.167528	0.192369	4.364767
1	−2.143749	0.119649	4.836756
6	−0.077091	0.688626	5.082211
6	1.173022	0.776881	4.465272
1	2.024003	1.173662	5.011081
6	1.329912	0.373042	3.1394
1	2.297955	0.435261	2.649872
6	1.875192	3.651327	1.285865
1	1.866459	2.5634	1.34958
1	2.847839	3.977345	0.906425
6	1.543932	4.283259	2.609388
6	2.282277	5.362523	3.103873
1	3.117596	5.752163	2.526355
6	1.953164	5.94091	4.332547
1	2.534	6.778257	4.710005
6	0.877741	5.44338	5.071303
1	0.620427	5.892312	6.027161
6	0.135553	4.36456	4.580755
1	−0.694988	3.96422	5.155764
6	0.467524	3.7865	3.356925
1	−0.091262	2.94059	2.972483
8	−1.584973	0.3852	−1.247302
6	−1.931754	−0.661372	−2.109529
1	−1.201197	−0.783886	−2.926091
1	−2.892235	−0.41085	−2.591772
6	−2.082286	−1.998192	−1.395516
6	−1.752661	−3.201524	−2.028178
1	−1.384107	−3.184022	−3.052246
6	−1.866344	−4.419756	−1.354655
1	−1.595142	−5.344123	−1.858911
6	−2.30925	−4.449204	−0.030504
1	−2.387411	−5.394643	0.500058
6	−2.651981	−3.252913	0.606853
1	−3.003771	−3.266167	1.63602
6	−2.543562	−2.040304	−0.074564
1	−2.797713	−1.105068	0.414792
6	0.356854	3.154228	−0.497078
6	−0.623698	3.736192	−1.491727

6	−1.522834	4.87369	−0.997496
6	−2.749853	4.435747	−0.18537
6	−2.466782	3.739731	1.156298
6	−2.077917	2.261465	1.070065
1	−1.209296	2.902408	−1.890833
1	−0.92392	5.580836	−0.41216
1	−3.375188	3.775498	−0.804221
1	−1.696559	4.287533	1.712632
1	0.015602	4.095901	−2.310722
1	−1.877106	5.421775	−1.879869
1	−3.352488	5.333217	0.009513
1	−3.381957	3.78366	1.763529
1	−2.181737	1.820501	2.070772
1	−2.767264	1.73379	0.397331
8	1.047411	2.11252	−0.831413
8	−0.739306	2.048193	0.646952
1	−0.200974	1.010022	6.112378

Table S6. Cartesian coordinate of **C_{eq}4a.**

The number of atom coordinates (angstroms)	X	Y	Z
13	−0.193602	0.671856	−0.169588
8	0.866953	−0.321522	−1.366233
8	1.071253	4.246577	−0.049571
7	0.2684	−0.625185	1.269638
6	1.347874	−1.512337	−1.294336
6	1.935609	−2.046537	−2.574825
1	2.729311	−1.374632	−2.920964
1	2.339097	−3.055701	−2.462314
1	1.159925	−2.054973	−3.348576
6	1.355944	−2.26885	−0.130761
1	1.785159	−3.261773	−0.168658
6	0.845437	−1.820837	1.104563
6	0.980134	−2.768855	2.277587
1	1.383475	−2.258398	3.157115
1	−0.002462	−3.162439	2.558725
1	1.627619	−3.610514	2.024156
6	−0.18609	−0.29417	2.593262
6	−1.391937	−0.805199	3.084423
1	−1.974338	−1.471426	2.45758
6	−1.834389	−0.457618	4.36201
1	−2.773965	−0.859305	4.732095
6	−1.079921	0.408525	5.15563

6	0.123678	0.922233	4.663722
1	0.71594	1.604633	5.266651
6	0.56968	0.570088	3.390181
1	1.495534	0.976335	2.995599
6	2.246034	3.955702	0.775694
1	2.39458	2.875288	0.783816
1	3.09316	4.431295	0.275696
6	2.013858	4.511066	2.153789
6	2.806254	5.545163	2.660034
1	3.599704	5.968035	2.047943
6	2.583205	6.036378	3.949425
1	3.205047	6.838551	4.337512
6	1.558547	5.501497	4.732302
1	1.381392	5.886732	5.733033
6	0.760436	4.47041	4.22559
1	−0.038792	4.048136	4.828621
6	0.988744	3.972364	2.943902
1	0.377528	3.173679	2.535318
8	−1.723059	0.453531	−1.035281
6	−2.003659	−0.507198	−2.016417
1	−1.267663	−0.487114	−2.836338
1	−2.979995	−0.263345	−2.469575
6	−2.069186	−1.924997	−1.466515
6	−1.617599	−3.019142	−2.211722
1	−1.212091	−2.855723	−3.208272
6	−1.665389	−4.313212	−1.687287
1	−1.299166	−5.150041	−2.277046
6	−2.167397	−4.52896	−0.40251
1	−2.197718	−5.533213	0.012304
6	−2.633686	−3.44324	0.345588
1	−3.035555	−3.604058	1.343664
6	−2.586485	−2.154313	−0.185841
1	−2.932536	−1.301962	0.390658
6	0.46838	3.268705	−0.689681
6	−0.74568	3.700383	−1.466202
6	−1.677526	4.731203	−0.804547
6	−2.815767	4.162901	0.06365
6	−2.454461	3.638182	1.466754
6	−1.982497	2.183539	1.543688
1	−1.28704	2.793591	−1.747813
1	−1.08304	5.445316	−0.222898
1	−3.33708	3.373675	−0.496466

1	−1.693717	4.287527	1.92101
1	−0.32843	4.127683	−2.391265
1	−2.139051	5.307219	−1.616231
1	−3.543453	4.976605	0.18748
1	−3.347867	3.717255	2.103764
1	−1.922057	1.899316	2.606226
1	−2.742443	1.53639	1.077474
8	0.984104	2.131699	−0.81132
8	−0.729128	2.009388	0.932153
1	−1.427117	0.68424	6.147568

Table S7. Cartesian coordinate of **C_{ax}1a.**

The number of atom coordinates (angstroms)	X	Y	Z
13	0.387295	−0.037568	−1.140796
8	0.725461	−1.613658	−2.102435
8	1.689917	0.832852	−1.939349
7	0.837728	−0.933194	0.570738
6	0.89951	−2.816792	−1.695564
6	0.944038	−3.865575	−2.776813
1	1.119747	−4.869528	−2.382986
1	1.730708	−3.613094	−3.496571
1	−0.007615	−3.855621	−3.319922
6	1.053301	−3.164078	−0.356341
1	1.205322	−4.209096	−0.118612
6	1.049818	−2.248927	0.713721
6	1.312626	−2.827186	2.089416
1	2.058464	−2.239105	2.632174
1	0.396534	−2.817001	2.689364
1	1.659889	−3.859334	2.014521
6	0.910588	−0.121382	1.75344
6	−0.13833	−0.102906	2.679424
6	−0.067828	0.721125	3.803274
1	−0.883456	0.720227	4.521968
6	1.042147	1.546238	4.004659
6	2.087565	1.533304	3.076631
1	2.955024	2.171124	3.223267
6	2.02461	0.701131	1.95872
6	2.245373	2.090638	−1.734692
1	2.477789	2.268861	−0.669601
1	3.212709	2.140277	−2.264642
6	1.401139	3.270566	−2.206404
6	0.185021	3.096815	−2.872988

1	−0.176991	2.092481	−3.063894
6	−0.58036	4.203221	−3.252909
1	−1.528032	4.04884	−3.763841
6	−0.139344	5.49935	−2.978013
1	−0.736921	6.358331	−3.272879
6	1.081447	5.682382	−2.320946
1	1.438399	6.686078	−2.101865
6	1.841932	4.575344	−1.941748
1	2.787583	4.723447	−1.421573
8	−1.297226	0.116151	−1.671106
6	−2.085999	−0.910396	−2.200163
1	−1.63484	−1.362307	−3.098463
1	−3.047809	−0.475217	−2.524839
6	−2.381943	−2.025883	−1.203893
6	−2.553671	−3.348605	−1.627632
1	−2.470975	−3.58506	−2.686938
6	−2.813969	−4.369114	−0.709781
1	−2.933105	−5.392357	−1.057836
6	−2.905054	−4.078317	0.653144
1	−3.098461	−4.87149	1.370892
6	−2.743456	−2.758767	1.084997
1	−2.817625	−2.522716	2.144982
6	−2.486423	−1.74235	0.163919
1	−2.33831	−0.719643	0.492689
6	−0.973949	2.290821	0.377163
6	−0.95223	3.794136	0.477734
6	−0.996861	4.305218	1.936233
6	−2.396886	4.29119	2.561886
6	−3.049945	2.904911	2.635401
6	−3.234965	2.222057	1.283716
1	−1.792001	4.206133	−0.096476
1	−0.300069	3.715851	2.545909
1	−3.050526	4.9592	1.982323
1	−2.463532	2.235082	3.275929
1	−0.037177	4.115489	−0.02003
1	−0.619909	5.33418	1.934181
1	−2.341984	4.712318	3.573232
1	−4.042929	2.99758	3.093333
1	−3.924533	1.379889	1.359557
1	−3.616874	2.9096	0.520999
8	0.002067	1.678161	−0.049989
8	−2.020495	1.594052	0.795679

1	2.825676	0.688959	1.225758
1	−1.005825	−0.72943	2.50219
1	1.094101	2.189824	4.878505

Table S8. Cartesian coordinate of **C_{ax}TS1a.**

The number of atom coordinates (angstroms)	X	Y	Z
13	0.647224	0.186784	−0.586075
8	0.530446	−1.336143	−1.656702
8	1.985409	0.937353	−1.434631
7	1.233322	−0.865122	0.958452
6	0.590853	−2.581132	−1.327721
6	0.230114	−3.550007	−2.422278
1	0.434637	−4.587845	−2.148364
1	0.779495	−3.29484	−3.334635
1	−0.839916	−3.445876	−2.639364
6	0.939814	−3.033743	−0.060347
1	0.966657	−4.103316	0.104992
6	1.292003	−2.196162	1.02099
6	1.758797	−2.866131	2.295069
1	2.804041	−2.611678	2.50107
1	1.176642	−2.516357	3.153716
1	1.671247	−3.95187	2.222784
6	1.741235	−0.107794	2.071406
6	0.889273	0.320677	3.094125
6	1.398923	1.07163	4.152485
1	0.732461	1.403669	4.944328
6	2.754707	1.410702	4.190635
6	3.599525	0.999937	3.158005
1	4.652281	1.269252	3.172537
6	3.09453	0.242732	2.098359
6	2.463066	2.233074	−1.175856
1	2.569358	2.426541	−0.097071
1	3.47428	2.317566	−1.608798
6	1.592779	3.325784	−1.775654
6	0.937899	3.117748	−2.995831
1	1.052616	2.158145	−3.491101
6	0.128645	4.11179	−3.549044
1	−0.379107	3.932013	−4.493762
6	−0.03522	5.33369	−2.889539
1	−0.669801	6.106303	−3.316192
6	0.619043	5.551798	−1.674181
1	0.49084	6.494533	−1.147659

6	1.424447	4.552237	−1.123221
1	1.90906	4.716099	−0.16305
8	−1.173883	0.511538	−0.950221
6	−2.215288	−0.11731	−1.666866
1	−1.883083	−0.259801	−2.702416
1	−3.066713	0.578578	−1.700999
6	−2.661443	−1.449088	−1.090937
6	−3.367815	−2.342124	−1.908109
1	−3.572662	−2.075499	−2.943397
6	−3.799579	−3.573026	−1.412538
1	−4.341518	−4.256689	−2.060919
6	−3.523687	−3.930131	−0.089471
1	−3.850534	−4.892027	0.296403
6	−2.819638	−3.045186	0.728007
1	−2.592158	−3.317082	1.755679
6	−2.393575	−1.810567	0.232531
1	−1.841972	−1.127327	0.867783
6	−1.18265	1.732969	0.327608
6	−1.761716	2.949608	−0.369087
6	−2.017835	4.107816	0.614747
6	−3.373862	4.012142	1.330856
6	−3.555625	2.772408	2.219479
6	−3.302225	1.440403	1.515503
1	−2.690783	2.691142	−0.889583
1	−1.195893	4.153419	1.34065
1	−4.168015	4.018815	0.569513
1	−2.879776	2.819483	3.083265
1	−1.034617	3.236062	−1.126145
1	−1.980239	5.04524	0.048401
1	−3.527195	4.910025	1.942898
1	−4.57947	2.759764	2.616386
1	−3.652458	0.604773	2.126324
1	−3.815664	1.380091	0.549167
8	0.094872	1.657811	0.508864
8	−1.890412	1.190376	1.360838
1	3.736639	−0.075266	1.281983
1	−0.168842	0.093213	3.027341
1	3.146803	2.00018	5.014987

Table S9. Cartesian coordinate of **C$_{ax}$2a.**

The number of atom coordinates (angstroms)	X	Y	Z
13	0.612868	0.286765	−0.441541

8	0.388998	−1.148796	−1.588305
8	2.000821	0.972637	−1.270174
7	1.045595	−0.869942	1.064846
6	0.736472	−2.380008	−1.425132
6	0.548461	−3.258459	−2.631949
1	0.904825	−4.278211	−2.467987
1	1.07533	−2.820595	−3.486974
1	−0.518356	−3.286327	−2.880048
6	1.221946	−2.898162	−0.228922
1	1.485345	−3.948014	−0.204093
6	1.327832	−2.171622	0.976977
6	1.768733	−2.929995	2.209697
1	2.560757	−2.388465	2.736335
1	0.937007	−3.036242	2.914317
1	2.128669	−3.926782	1.947336
6	1.091005	−0.230861	2.351014
6	0.035421	−0.387325	3.254905
6	0.056523	0.283421	4.477177
1	−0.769252	0.158725	5.172846
6	1.126354	1.122238	4.800813
6	2.176625	1.283176	3.894135
1	3.009661	1.938101	4.134909
6	2.16091	0.608897	2.672159
6	2.271615	2.344937	−1.364735
1	2.291606	2.829531	−0.375446
1	3.279502	2.470868	−1.795206
6	1.278149	3.101571	−2.237754
6	0.538577	2.437538	−3.223516
1	0.686394	1.370599	−3.359398
6	−0.388899	3.129428	−4.005876
1	−0.960847	2.596559	−4.762038
6	−0.585491	4.499896	−3.81841
1	−1.312149	5.037846	−4.421869
6	0.159334	5.173845	−2.846366
1	0.011285	6.239275	−2.687773
6	1.081827	4.476866	−2.06434
1	1.640615	5.002784	−1.292641
8	−1.322258	0.728285	−0.821903
6	−2.553839	0.193972	−1.343993
1	−2.589003	0.434532	−2.410726
1	−3.365751	0.72377	−0.837416
6	−2.670438	−1.294496	−1.117481

6	−3.074814	−2.134839	−2.158741
1	−3.281231	−1.714566	−3.140568
6	−3.201817	−3.511519	−1.951635
1	−3.516185	−4.154142	−2.769873
6	−2.906953	−4.05951	−0.702311
1	−2.989537	−5.131271	−0.542819
6	−2.501307	−3.222091	0.341452
1	−2.266976	−3.642981	1.315951
6	−2.395195	−1.847339	0.139885
1	−2.08481	−1.188331	0.94335
6	−1.291087	1.74901	0.265212
6	−1.798661	3.098739	−0.255731
6	−1.265888	4.280969	0.563641
6	−1.830269	4.383554	1.985358
6	−1.687818	3.104036	2.825492
6	−2.580907	1.950609	2.358696
1	−2.896162	3.095449	−0.282152
1	−0.176192	4.187001	0.603127
1	−2.897379	4.64962	1.935912
1	−0.648278	2.76223	2.855812
1	−1.437628	3.190164	−1.283017
1	−1.48475	5.207147	0.018098
1	−1.331445	5.212373	2.504795
1	−1.982996	3.328687	3.859408
1	−2.695384	1.2247	3.169529
1	−3.582674	2.336839	2.112345
8	0.019363	1.723214	0.548321
8	−2.103192	1.160166	1.262454
1	2.962655	0.739429	1.951059
1	−0.805197	−1.017584	2.982551
1	1.138075	1.650526	5.750097

Table S10. Cartesian coordinate of **C_{ax}3a.**

The number of atom coordinates (angstroms)	X	Y	Z
13	0.159196	0.80063	0.64081
8	−0.514693	−0.478277	−0.455646
8	1.375432	1.799189	−0.113941
7	1.280699	−0.477859	1.660154
6	−0.385476	−1.777748	−0.373589
6	−1.212316	−2.536768	−1.375514
1	−1.076447	−3.618072	−1.29968
1	−0.948803	−2.209458	−2.388144

1	−2.271922	−2.295743	−1.227355
6	0.43044	−2.424692	0.528159
1	0.45967	−3.506829	0.491402
6	1.281187	−1.784442	1.483624
6	2.204868	−2.684756	2.272672
1	3.175653	−2.750747	1.767233
1	2.382993	−2.299443	3.279004
1	1.791431	−3.694175	2.338431
6	2.220044	0.137554	2.555867
6	1.751766	0.807459	3.692621
6	2.656801	1.45608	4.534879
1	2.288399	1.9716	5.417803
6	4.023153	1.449808	4.245657
6	4.48346	0.790798	3.102991
1	5.542183	0.791562	2.85753
6	3.587718	0.137826	2.257859
6	1.986861	1.584722	−1.36464
1	1.279722	1.14906	−2.089965
1	2.298741	2.558536	−1.772247
6	3.199002	0.677561	−1.250539
6	4.466629	1.204829	−0.978974
1	4.587484	2.282774	−0.899532
6	5.567795	0.36528	−0.797157
1	6.545715	0.791458	−0.58811
6	5.411652	−1.021364	−0.878207
1	6.266413	−1.677092	−0.734449
6	4.149585	−1.559606	−1.148333
1	4.017841	−2.636814	−1.215522
6	3.055404	−0.712877	−1.336146
1	2.075649	−1.136645	−1.539504
8	−1.837921	3.446683	1.983799
6	−0.628644	4.208545	1.810912
1	0.248471	3.562194	1.897546
1	−0.618785	4.904428	2.656827
6	−0.626534	4.968583	0.502444
6	0.418929	4.826602	−0.415389
1	1.222871	4.131958	−0.195103
6	0.397211	5.529173	−1.62343
1	1.212805	5.40683	−2.332082
6	−0.671171	6.375847	−1.92674
1	−0.688797	6.919046	−2.868211
6	−1.720593	6.519561	−1.013606

1	−2.556234	7.176268	−1.242673
6	−1.694439	5.821236	0.193565
1	−2.514457	5.921317	0.900639
6	−1.812817	2.121811	1.533723
6	−3.211275	1.557964	1.814349
6	−3.607103	0.348934	0.952448
6	−4.169711	0.722176	−0.433216
6	−3.155663	1.293301	−1.436473
6	−2.358245	2.482819	−0.91466
1	−3.944683	2.36288	1.691013
1	−2.750995	−0.326454	0.843038
1	−4.984978	1.447396	−0.292124
1	−2.436846	0.517026	−1.719932
1	−3.206479	1.291735	2.875954
1	−4.380298	−0.212667	1.49103
1	−4.629295	−0.169642	−0.880115
1	−3.68269	1.603425	−2.349294
1	−1.73223	2.926579	−1.693741
1	−2.994646	3.276112	−0.508557
8	−0.797757	1.366303	2.053181
8	−1.448999	2.067293	0.116237
1	3.937471	−0.354791	1.359026
1	0.686861	0.828555	3.892877
1	4.72274	1.961372	4.901153

Table S11. Cartesian coordinate of **C_{ax}TS2a.**

The number of atom coordinates (angstroms)	X	Y	Z
13	0.462917	1.307651	0.230532
8	0.098226	0.308616	−1.318268
8	1.883042	2.179051	−0.335444
7	0.874177	−0.341791	1.239529
6	−0.086877	−0.957265	−1.468944
6	−0.586445	−1.374254	−2.82801
1	−0.707931	−2.456203	−2.919433
1	0.11342	−1.022352	−3.594678
1	−1.547959	−0.885438	−3.023863
6	0.175671	−1.895639	−0.479307
1	0.028191	−2.94125	−0.718654
6	0.718713	−1.587128	0.793641
6	1.173361	−2.755112	1.641721
1	2.248771	−2.670346	1.834436
1	0.677539	−2.762177	2.616571

1	0.979698	−3.704288	1.138696
6	1.5046	−0.159899	2.525235
6	0.766202	−0.273973	3.708033
6	1.385436	−0.072716	4.941162
1	0.803735	−0.163222	5.854846
6	2.744148	0.24856	5.002395
6	3.477044	0.367072	3.820446
1	4.5337	0.618982	3.852682
6	2.861997	0.165265	2.583453
6	2.737982	1.802356	−1.391916
1	2.177703	1.361211	−2.230168
1	3.237108	2.706122	−1.77464
6	3.788682	0.814564	−0.918229
6	4.947201	1.264267	−0.272018
1	5.120981	2.333953	−0.17978
6	5.862169	0.359375	0.270348
1	6.7551	0.725261	0.770989
6	5.626869	−1.015412	0.175199
1	6.334294	−1.721515	0.602055
6	4.478343	−1.475659	−0.473647
1	4.287643	−2.543152	−0.553853
6	3.570188	−0.564998	−1.017992
1	2.670982	−0.929022	−1.506679
8	−1.032516	4.174548	1.637917
6	−0.058366	4.856592	0.797392
1	0.868762	4.283096	0.762169
1	0.121645	5.80659	1.308814
6	−0.639873	5.072245	−0.579053
6	0.006469	4.569793	−1.712743
1	0.920561	3.998206	−1.587385
6	−0.54365	4.764875	−2.981614
1	−0.035649	4.365331	−3.855606
6	−1.747037	5.458141	−3.126518
1	−2.177224	5.606093	−4.113755
6	−2.398966	5.959816	−1.995876
1	−3.336137	6.50031	−2.101904
6	−1.84474	5.769947	−0.729812
1	−2.353714	6.152533	0.15156
6	−0.884023	2.860597	1.851452
6	−2.0169	2.333883	2.711651
6	−2.529387	0.913441	2.413297
6	−3.624951	0.799492	1.328743

6	−3.147394	0.682693	−0.127213
6	−2.366253	1.89053	−0.635567
1	−2.843698	3.049475	2.675423
1	−1.687885	0.258841	2.164435
1	−4.310892	1.654689	1.419603
1	−2.509007	−0.206511	−0.226297
1	−1.608562	2.363036	3.730773
1	−2.948273	0.52932	3.351959
1	−4.225442	−0.091987	1.552813
1	−4.01936	0.522571	−0.777432
1	−2.095841	1.759116	−1.691297
1	−2.970245	2.806774	−0.562679
8	0.274404	2.316476	1.869548
8	−1.193358	2.082638	0.119444
1	3.424754	0.262118	1.664456
1	−0.289573	−0.519208	3.656953
1	3.224704	0.408119	5.963822

Table S12. Cartesian coordinate of **C_{ax}4a.**

The number of atom coordinates (angstroms)	X	Y	Z
13	0.414909	1.108852	−0.056746
8	0.126301	0.107604	−1.622915
8	1.787686	2.055161	−0.645044
7	0.900209	−0.515651	0.963373
6	0.134185	−1.162207	−1.818418
6	−0.250026	−1.602969	−3.207588
1	−0.237697	−2.689251	−3.324841
1	0.43908	−1.154239	−3.932637
1	−1.251561	−1.224737	−3.441961
6	0.495537	−2.086785	−0.845126
1	0.504236	−3.134158	−1.119336
6	0.910446	−1.75595	0.466254
6	1.429268	−2.898974	1.313887
1	2.463031	−2.694814	1.613733
1	0.84913	−3.013915	2.233974
1	1.401942	−3.839413	0.760459
6	1.370982	−0.350736	2.316013
6	0.510418	−0.580254	3.393905
6	0.958326	−0.385534	4.70131
1	0.282635	−0.565652	5.533507
6	2.268294	0.03982	4.938165
6	3.1264	0.262686	3.858854

1	4.147752	0.592039	4.030792
6	2.682664	0.069298	2.550115
6	2.741512	1.647241	−1.59731
1	2.281538	1.073339	−2.416244
1	3.191767	2.546838	−2.045436
6	3.832733	0.810616	−0.953066
6	4.838282	1.423337	−0.193358
1	4.862702	2.508439	−0.12469
6	5.790064	0.65937	0.484211
1	6.563695	1.150462	1.069238
6	5.745266	−0.736811	0.414973
1	6.481947	−1.333954	0.94596
6	4.749192	−1.3583	−0.341475
1	4.706771	−2.44312	−0.401604
6	3.803102	−0.586953	−1.021426
1	3.021285	−1.077234	−1.595567
8	−0.563786	4.176819	1.738593
6	0.194883	4.707425	0.60107
1	1.029734	4.04439	0.372504
1	0.570049	5.668262	0.964649
6	−0.72841	4.880207	−0.577731
6	−0.416787	4.296202	−1.809163
1	0.475042	3.682941	−1.891275
6	−1.269266	4.465537	−2.901893
1	−1.021988	4.001961	−3.853286
6	−2.443316	5.210029	−2.769413
1	−3.109741	5.334954	−3.618949
6	−2.762383	5.789444	−1.537831
1	−3.676225	6.367336	−1.42698
6	−1.904765	5.629148	−0.449344
1	−2.153076	6.07491	0.510699
6	−0.37045	2.929892	2.131434
6	−1.339008	2.500347	3.203841
6	−2.404252	1.518792	2.661947
6	−3.413317	2.121853	1.647638
6	−3.546964	1.290558	0.353889
6	−2.428272	1.614432	−0.652116
1	−1.815254	3.383676	3.638739
1	−1.880675	0.678314	2.202852
1	−3.111469	3.141214	1.377594
1	−3.527338	0.221322	0.610375
1	−0.747992	1.99584	3.975499

1	−2.938545	1.11857	3.532863
1	−4.394714	2.21006	2.12991
1	−4.517912	1.478842	−0.12525
1	−2.388627	0.841001	−1.437015
1	−2.666979	2.567111	−1.15207
8	0.539424	2.205232	1.709923
8	−1.211504	1.753457	0.014495
1	3.339651	0.25103	1.708657
1	−0.50722	−0.905266	3.199336
1	2.616459	0.194385	5.955793

Table S13. Cartesian coordinate of **C_{eq}1b.**

The number of atom coordinates (angstroms)	X	Y	Z
13	−0.302745	0.335164	−0.669722
8	1.181754	0.209368	−1.83432
8	−1.351459	0.909236	0.638086
7	0.783293	−0.689489	0.665764
6	2.556018	−0.980112	−3.348434
1	3.153783	−0.080904	−3.537394
1	3.196618	−1.862343	−3.423678
1	1.787495	−1.024216	−4.128934
6	1.884526	−0.86087	−2.005657
6	2.061031	−1.828703	−1.024498
1	2.682746	−2.685576	−1.251971
6	1.606926	−1.673412	0.306562
6	2.095525	−2.668676	1.335556
1	1.242306	−3.134312	1.840135
1	2.702824	−3.448072	0.870821
1	2.692808	−2.173769	2.108257
6	0.542492	−0.501676	2.067323
6	−0.568227	−1.076671	2.69325
1	−1.258692	−1.669814	2.108853
6	−0.79925	−0.862086	4.049693
1	−1.66476	−1.300455	4.534813
6	0.084836	−0.062031	4.776425
6	1.196312	0.519221	4.17154
1	1.871456	1.14285	4.7476
6	1.418954	0.290958	2.812342
1	2.277069	0.738928	2.320282
6	−2.355566	1.877351	0.622271
1	−2.529133	2.303951	−0.379186
1	−3.312215	1.413578	0.926597

6	−2.050571	3.012384	1.587407
6	−1.45109	2.724374	2.821192
1	−1.196811	1.695771	3.047518
6	−1.162237	3.742862	3.729369
1	−0.693197	3.498426	4.679559
6	−1.474749	5.070658	3.418977
1	−1.2511	5.866507	4.124882
6	−2.078731	5.366584	2.194503
1	−2.323743	6.39594	1.942959
6	−2.358609	4.342346	1.283318
1	−2.810252	4.581351	0.322558
8	−1.331069	−0.638076	−1.721293
6	−2.584379	−1.126575	−1.321452
1	−3.100367	−1.524938	−2.21181
1	−3.234447	−0.332947	−0.919416
6	−2.494416	−2.238957	−0.285515
6	−1.429272	−3.148367	−0.319877
1	−0.663558	−3.026821	−1.079705
6	−1.331723	−4.168825	0.627251
1	−0.494919	−4.862514	0.589687
6	−2.301906	−4.298038	1.626034
1	−2.222809	−5.087523	2.368863
6	−3.370646	−3.399121	1.665685
1	−4.12561	−3.483866	2.443499
6	−3.462	−2.377081	0.716423
1	−4.284382	−1.666195	0.766127
17	−0.222199	0.23614	6.489666
6	0.592748	3.156412	−0.987995
6	1.849685	2.934461	−0.182567
6	1.798445	3.594157	1.214803
6	2.072418	5.102301	1.201778
6	1.102273	5.923412	0.343446
6	1.076916	5.539899	−1.131935
1	2.707732	3.317232	−0.750442
1	0.832293	3.378782	1.682524
1	3.097586	5.275204	0.8423
1	0.082669	5.845504	0.736379
1	1.98166	1.855211	−0.097812
1	2.558447	3.103935	1.833328
1	2.03404	5.475556	2.231853
1	1.38576	6.982434	0.395829
1	0.588353	6.311029	−1.728762

1	2.081776	5.376123	−1.537778
8	−0.188782	2.247601	−1.284053
8	0.257359	4.365822	−1.403979

Table S14. Cartesian coordinate of **C_{eq}TS1b.**

The number of atom coordinates (angstroms)	X	Y	Z
13	−0.078761	0.356129	−0.747755
8	0.37412	−0.96892	−2.002622
8	−0.213659	2.054243	0.168164
7	0.756007	−0.636903	0.729715
6	1.319261	−1.830513	−1.915613
6	1.651937	−2.556921	−3.193516
1	0.752215	−3.060509	−3.565328
1	1.947983	−1.82691	−3.955213
1	2.450191	−3.292103	−3.06688
6	1.983614	−2.13812	−0.72657
1	2.746746	−2.905333	−0.762071
6	1.639472	−1.629284	0.541447
6	2.294435	−2.283106	1.73972
1	1.537451	−2.752334	2.37759
1	3.007607	−3.047428	1.426668
1	2.815427	−1.546431	2.359201
6	0.383354	−0.337556	2.086067
6	−0.745559	−0.951019	2.639084
1	−1.319658	−1.645905	2.03855
6	−1.135387	−0.677387	3.950428
1	−2.017815	−1.14908	4.368995
6	−0.376457	0.208757	4.712185
6	0.757768	0.824727	4.184066
1	1.33328	1.519255	4.786072
6	1.130158	0.548467	2.869847
1	2.008117	1.024708	2.452317
6	−1.338657	2.916251	0.08026
1	−1.121807	3.713092	−0.643863
1	−2.184049	2.359233	−0.336977
6	−1.730645	3.527532	1.408283
6	−1.670555	2.775113	2.586504
1	−1.303126	1.758632	2.539913
6	−2.069421	3.325258	3.805057
1	−2.009547	2.727237	4.710269
6	−2.544062	4.638577	3.860557
1	−2.853626	5.068817	4.809468

6	−2.61729	5.395302	2.689031
1	−2.984144	6.418137	2.721687
6	−2.210667	4.841706	1.472485
1	−2.269248	5.436831	0.562953
8	−1.800012	0.109584	−1.008527
6	−2.849478	−0.105625	−0.118927
1	−3.786547	0.274137	−0.561792
1	−2.722166	0.453367	0.826947
6	−3.0553	−1.571219	0.244951
6	−2.323973	−2.585421	−0.380349
1	−1.619714	−2.315402	−1.159575
6	−2.489609	−3.919004	0.006143
1	−1.908855	−4.696775	−0.484232
6	−3.391289	−4.254726	1.017258
1	−3.515879	−5.291072	1.320419
6	−4.133933	−3.245582	1.639896
1	−4.83878	−3.495751	2.429117
6	−3.965078	−1.915732	1.254792
1	−4.532438	−1.131415	1.75358
17	−0.864037	0.568833	6.36814
6	1.295304	2.524194	−0.924381
6	2.376546	2.657922	0.13459
6	2.113523	3.585707	1.328231
6	2.212188	5.080987	1.015446
6	1.225659	5.556293	−0.055152
6	1.437962	4.926054	−1.428463
1	3.290647	2.96144	−0.398427
1	1.127917	3.348588	1.739286
1	3.234985	5.319121	0.686986
1	0.194726	5.385416	0.271464
1	2.55196	1.63745	0.479238
1	2.851149	3.344036	2.104366
1	2.040127	5.6498	1.937264
1	1.336025	6.640434	−0.190375
1	0.916637	5.50013	−2.196612
1	2.503943	4.902155	−1.688232
8	1.22422	1.409398	−1.581633

Table S15. Cartesian coordinate of **C_{eq}2b.**

The number of atom coordinates (angstroms)	X	Y	Z
13	0.429777	0.221383	−0.789434
8	1.533395	−0.6408	−2.002618

8	−0.282841	1.670875	0.626927
7	0.839918	−1.047361	0.638044
6	1.778312	−1.903629	−2.019631
6	2.340864	−2.434875	−3.31101
1	1.623347	−2.248406	−4.118275
1	3.254203	−1.882864	−3.560345
1	2.565012	−3.503201	−3.265925
6	1.582644	−2.742909	−0.923163
1	1.837155	−3.788885	−1.037974
6	1.218044	−2.304064	0.368065
6	1.2741	−3.326673	1.481392
1	0.276117	−3.474031	1.907829
1	1.643771	−4.285207	1.113269
1	1.923386	−2.987253	2.294647
6	0.63744	−0.702769	2.017849
6	−0.586695	−0.947177	2.647824
1	−1.400468	−1.385471	2.084329
6	−0.758778	−0.643518	3.99806
1	−1.708326	−0.833757	4.486379
6	0.300671	−0.082686	4.710349
6	1.522042	0.188643	4.093208
1	2.331819	0.638027	4.657772
6	1.683462	−0.123722	2.743133
1	2.626955	0.07676	2.244844
6	−1.628189	2.073412	0.967192
1	−2.138654	2.421739	0.068244
1	−2.088495	1.138437	1.298379
6	−1.682093	3.116768	2.051494
6	−1.031428	2.900814	3.271299
1	−0.478177	1.982239	3.418474
6	−1.067986	3.867211	4.27479
1	−0.553588	3.686532	5.21496
6	−1.765052	5.062043	4.070216
1	−1.7931	5.817957	4.850478
6	−2.422121	5.282152	2.857744
1	−2.960752	6.21105	2.689979
6	−2.376716	4.313604	1.851799
1	−2.867087	4.495468	0.898728
8	−1.06711	−0.094409	−1.616483
6	−2.432601	−0.232276	−1.371496
1	−2.925103	−0.51438	−2.317029
1	−2.895705	0.717907	−1.064489

6	−2.761233	−1.295243	−0.333361
6	−2.094662	−2.528111	−0.360712
1	−1.328978	−2.696255	−1.112062
6	−2.386024	−3.516433	0.579213
1	−1.858082	−4.466298	0.545734
6	−3.352479	−3.287795	1.565518
1	−3.575333	−4.055224	2.30186
6	−4.025772	−2.065166	1.598527
1	−4.775001	−1.875018	2.362685
6	−3.72968	−1.077285	0.653155
1	−4.253331	−0.124051	0.688449
17	0.079863	0.332105	6.408998
6	0.660501	2.610815	−0.029276
6	1.609279	3.267232	1.002729
6	1.333068	4.7176	1.425505
6	1.659143	5.763172	0.345209
6	0.66942	5.80151	−0.826536
6	0.503996	4.467573	−1.548545
1	2.611693	3.211094	0.563142
1	0.297259	4.836479	1.752777
1	2.672444	5.57673	−0.041782
1	−0.319567	6.110866	−0.462722
1	1.615846	2.61077	1.877783
1	1.958858	4.922451	2.304068
1	1.685632	6.75778	0.809744
1	0.992338	6.554869	−1.558734
1	−0.129292	4.586383	−2.433538
1	1.465723	4.058484	−1.88115
8	1.33922	1.763468	−0.84695
8	−0.169459	3.511121	−0.7168

Table S16. Cartesian coordinate of **C_{eq}3b.**

The number of atom coordinates (angstroms)	X	Y	Z
13	−0.067143	0.647997	−0.435853
8	0.904862	−0.355542	−1.612634
8	0.705038	4.071986	0.324785
7	0.408491	−0.559835	1.042579
6	1.312352	−1.593674	−1.535208
6	1.846348	−2.201388	−2.806267
1	2.690702	−1.607655	−3.166883
1	2.167197	−3.239959	−2.676313
1	1.069886	−2.154797	−3.578501

6	1.284825	−2.344111	−0.367509
1	1.616691	−3.386806	−0.406428
6	0.873382	−1.823319	0.875229
6	0.971521	−2.758549	2.063037
1	1.710899	−2.384897	2.828428
1	0.011299	−2.840492	2.53008
1	1.253222	−3.754317	1.756112
6	0.158825	−0.122501	2.393855
6	−1.13206	−0.229466	3.004892
1	−1.949035	−0.650411	2.443237
6	−1.369902	0.193706	4.321013
1	−2.371774	0.116348	4.79333
6	−0.301554	0.71765	5.026043
6	0.993938	0.822938	4.440137
1	1.811314	1.243945	4.998146
6	1.216071	0.401088	3.122604
1	2.218427	0.476073	2.648275
6	1.712438	3.650721	1.275198
1	1.63013	2.562034	1.32861
1	2.696368	3.982307	0.883798
6	1.527751	4.267389	2.611254
6	2.42116	5.295123	3.136397
1	3.268665	5.663187	2.569331
6	2.23285	5.849502	4.383811
1	2.935791	6.646294	4.785234
6	1.143179	5.380506	5.11
1	0.995929	5.808891	6.081122
6	0.243149	4.354895	4.588053
1	−0.599051	3.975927	5.155943
6	0.43734	3.800115	3.346417
1	−0.246093	2.992527	2.937345
8	−1.701051	0.377234	−1.27042
6	−2.115386	−0.686362	−2.113988
1	−1.512391	−0.824903	−2.924597
1	−3.150891	−0.445006	−2.605039
6	−2.072353	−2.00693	−1.371593
6	−1.65413	−3.223135	−1.967326
1	−1.367336	−3.228454	−2.984059
6	−1.581147	−4.425229	−1.266178
1	−1.244136	−5.35994	−1.741774
6	−1.922772	−4.424964	0.048801
1	−1.855154	−5.357566	0.600654

6	−2.356923	−3.21555	0.64957
1	−2.633788	−3.20657	1.67094
6	−2.436392	−2.019442	−0.059277
1	−2.767769	−1.073933	0.400531
17	−0.596951	1.273004	6.682272
6	0.046101	3.160436	−0.496551
6	−0.789825	3.749931	−1.490432
6	−1.530087	4.88305	−0.99136
6	−2.751757	4.436281	−0.190645
6	−2.455306	3.724474	1.143335
6	−2.155637	2.249844	1.040246
1	−1.476396	2.919554	−1.899812
1	−0.824218	5.584675	−0.395936
1	−3.523771	3.783172	−0.819884
1	−1.636869	4.271072	1.712337
1	−0.066062	4.11637	−2.303128
1	−1.854725	5.439234	−1.87057
1	−3.186973	5.330949	0.012786
1	−3.341937	3.753698	1.744322
1	−2.311572	1.794665	2.033539
1	−2.809836	1.727351	0.352644
8	0.844516	2.126334	−0.843918
8	−0.788577	2.046323	0.630613

Table S17. Cartesian coordinate of **C_{eq}TS2b.**

The number of atom coordinates (angstroms)	X	Y	Z
13	−0.048983	0.647997	−0.435853
8	1.02039	−0.355542	−1.612634
8	0.84529	4.071986	0.324785
7	0.434372	−0.559835	1.042579
6	1.357978	−1.593674	−1.535208
6	1.890519	−2.201388	−2.806267
1	2.737873	−1.607655	−3.166883
1	2.203458	−3.239959	−2.676313
1	1.11382	−2.154797	−3.578501
6	1.260913	−2.344111	−0.367509
1	1.547327	−3.386806	−0.406428
6	0.858454	−1.823319	0.875229
6	0.920312	−2.758549	2.063037
1	1.608112	−2.384897	2.828428
1	−0.066464	−2.840492	2.53008
1	1.24412	−3.754317	1.756112

6	0.2292	−0.122501	2.393855
6	−1.023488	−0.229466	3.004892
1	−1.850171	−0.650411	2.443237
6	−1.209801	0.193706	4.321013
1	−2.183252	0.116348	4.79333
6	−0.127376	0.71765	5.026043
6	1.133157	0.822938	4.440137
1	1.96172	1.243945	4.998146
6	1.303039	0.401088	3.122604
1	2.277101	0.476073	2.648275
6	1.86377	3.650721	1.275198
1	1.860945	2.562034	1.32861
1	2.829786	3.982307	0.883798
6	1.554509	4.267389	2.611254
6	2.342821	5.295123	3.136397
1	3.194896	5.663187	2.569331
6	2.042789	5.849502	4.383811
1	2.663233	6.646294	4.785234
6	0.946724	5.380506	5.11
1	0.713323	5.808891	6.081122
6	0.151881	4.354895	4.588053
1	−0.69275	3.975927	5.155943
6	0.456105	3.800115	3.346417
1	−0.140733	2.992527	2.937345
8	−1.582798	0.377234	−1.27042
6	−1.925779	−0.686362	−2.113988
1	−1.191558	−0.824903	−2.924597
1	−2.8839	−0.445006	−2.605039
6	−2.079953	−2.00693	−1.371593
6	−1.730044	−3.223135	−1.967326
1	−1.341564	−3.228454	−2.984059
6	−1.850246	−4.425229	−1.266178
1	−1.563394	−5.35994	−1.741774
6	−2.32026	−4.424964	0.048801
1	−2.404383	−5.357566	0.600654
6	−2.683093	−3.21555	0.64957
1	−3.057087	−3.20657	1.67094
6	−2.56759	−2.019442	−0.059277
1	−2.839119	−1.073933	0.400531
17	−0.360915	1.273004	6.682272
6	0.331144	3.160436	−0.496551
6	−0.646011	3.749931	−1.490432

6	−1.547933	4.88305	−0.99136
6	−2.778905	4.436281	−0.190645
6	−2.50066	3.724474	1.143335
6	−2.102067	2.249844	1.040246
1	−1.229463	2.919554	−1.899812
1	−0.952524	5.584675	−0.395936
1	−3.401386	3.783172	−0.819884
1	−1.739065	4.271072	1.712337
1	−0.002716	4.11637	−2.303128
1	−1.89717	5.439234	−1.87057
1	−3.382698	5.330949	0.012786
1	−3.420405	3.753698	1.744322
1	−2.214907	1.794665	2.033539
1	−2.780258	1.727351	0.352644
8	1.030039	2.126334	−0.843918
8	−0.756327	2.046323	0.630613

Table S18. Cartesian coordinate of **C_{eq}5b.**

The number of atom coordinates (angstroms)	X	Y	Z
13	−0.125818	0.676639	−0.345062
8	0.954605	−0.299068	−1.555787
8	1.062158	4.148168	0.224158
7	0.409588	−0.581783	1.083316
6	1.305318	−1.534766	−1.520299
6	1.823681	−2.099318	−2.817874
1	2.658589	−1.486199	−3.175245
1	2.150136	−3.137702	−2.723551
1	1.03382	−2.039931	−3.575786
6	1.236384	−2.320785	−0.374334
1	1.537401	−3.357804	−0.44512
6	0.850522	−1.833313	0.8873
6	0.954855	−2.787161	2.057135
1	1.645768	−2.407805	2.817061
1	−0.02103	−2.901287	2.540117
1	1.298644	−3.769414	1.728529
6	0.225258	−0.161657	2.442579
6	−1.006035	−0.312049	3.08672
1	−1.833311	−0.75874	2.545835
6	−1.173932	0.113592	4.404258
1	−2.13229	0.007112	4.901209
6	−0.094979	0.686016	5.076255
6	1.146204	0.830824	4.45867

1	1.97195	1.288331	4.991749
6	1.298304	0.402608	3.141203
1	2.255475	0.513096	2.639875
6	2.034984	3.724591	1.238179
1	2.043745	2.634955	1.260623
1	3.008983	4.089345	0.903296
6	1.625215	4.310489	2.558752
6	2.348685	5.353773	3.144175
1	3.22004	5.759084	2.634502
6	1.958645	5.872974	4.381388
1	2.527834	6.681031	4.832918
6	0.839043	5.352815	5.034017
1	0.537074	5.753465	5.998051
6	0.109826	4.312882	4.448955
1	−0.753239	3.896181	4.959994
6	0.501263	3.791964	3.216912
1	−0.045154	2.978383	2.752161
8	−1.617834	0.443179	−1.271785
6	−1.953025	−0.625378	−2.109549
1	−1.208007	−0.775701	−2.908686
1	−2.90313	−0.385323	−2.61731
6	−2.125252	−1.939979	−1.359091
6	−1.789729	−3.163533	−1.948588
1	−1.398235	−3.177984	−2.96412
6	−1.928407	−4.361184	−1.243654
1	−1.652235	−5.301454	−1.714656
6	−2.403481	−4.349687	0.069551
1	−2.502932	−5.279059	0.62437
6	−2.751366	−3.13319	0.664412
1	−3.129394	−3.115488	1.684235
6	−2.616429	−1.940804	−0.047739
1	−2.875909	−0.990923	0.410092
17	−0.308985	1.257385	6.730976
6	0.572782	3.25727	−0.603607
6	−0.485003	3.783062	−1.534594
6	−1.489259	4.797217	−0.96227
6	−2.738966	4.205131	−0.284838
6	−2.571243	3.60299	1.123619
6	−2.130624	2.137391	1.177888
1	−0.994884	2.916264	−1.963974
1	−0.974128	5.475171	−0.272079
1	−3.187	3.452711	−0.949512

1	−1.870965	4.212886	1.709595
1	0.086702	4.251516	−2.350521
1	−1.829153	5.414658	−1.802998
1	−3.469686	5.022392	−0.216571
1	−3.540881	3.66305	1.639411
1	−2.233976	1.791679	2.220076
1	−2.81863	1.535418	0.564482
8	1.105682	2.126917	−0.768213
8	−0.802699	1.966971	0.753621

Table S19. Cartesian coordinate of **C_{ax}1b.**

The number of atom coordinates (angstroms)	X	Y	Z
13	0.381762	−0.04108	−1.138953
8	0.709677	−1.615977	−2.106694
8	1.686894	0.822899	−1.938369
7	0.844831	−0.947067	0.56793
6	0.911043	−2.817027	−1.70986
6	0.957238	−3.85972	−2.796588
1	1.150026	−4.863209	−2.409799
1	1.733007	−3.593421	−3.523153
1	−0.000031	−3.858825	−3.329672
6	1.091329	−3.168496	−0.373791
1	1.268163	−4.21147	−0.144453
6	1.079674	−2.261608	0.701217
6	1.360284	−2.843664	2.071678
1	2.089026	−2.239424	2.619979
1	0.444981	−2.8689	2.672598
1	1.73854	−3.864012	1.987056
6	0.88276	−0.145716	1.755368
6	−0.170164	−0.173128	2.676312
6	−0.15872	0.658006	3.795216
1	−0.973539	0.63357	4.511038
6	0.90872	1.536181	3.977766
6	1.971981	1.577346	3.075563
1	2.795733	2.265221	3.232659
6	1.954613	0.728895	1.969897
6	2.245578	2.081063	−1.74486
1	2.484498	2.265751	−0.68207
1	3.210115	2.125061	−2.280027
6	1.400966	3.259806	−2.218378
6	0.18162	3.085078	−2.878647
1	−0.18308	2.080749	−3.064358

6	−0.583727	4.191195	−3.259604
1	−1.533978	4.036268	−3.765477
6	−0.139282	5.48764	−2.992131
1	−0.736885	6.346346	−3.287605
6	1.084966	5.671533	−2.341763
1	1.444527	6.675502	−2.128537
6	1.845407	4.564918	−1.961462
1	2.793704	4.713742	−1.446368
8	−1.305317	0.11683	−1.655664
6	−2.096847	−0.908187	−2.185425
1	−1.650595	−1.355339	−3.088272
1	−3.060607	−0.471675	−2.501673
6	−2.38489	−2.026825	−1.191016
6	−2.538011	−3.351971	−1.613767
1	−2.446247	−3.588829	−2.672155
6	−2.792346	−4.374136	−0.695897
1	−2.896987	−5.399227	−1.043012
6	−2.896821	−4.082168	0.665679
1	−3.087062	−4.876136	1.383311
6	−2.754426	−2.759956	1.096512
1	−2.843174	−2.523434	2.155264
6	−2.501705	−1.74224	0.175707
1	−2.367613	−0.716838	0.503089
6	−0.961093	2.29643	0.388593
6	−0.928382	3.800135	0.47827
6	−0.953278	4.322769	1.933291
6	−2.345334	4.322886	2.575538
6	−3.009425	2.942602	2.663611
6	−3.212814	2.249777	1.319756
1	−1.772197	4.213302	−0.089008
1	−0.253035	3.736835	2.541565
1	−3.000187	4.993902	2.000914
1	−2.424364	2.273825	3.306019
1	−0.017269	4.112276	−0.032282
1	−0.569641	5.348975	1.918917
1	−2.273334	4.746361	3.584469
1	−3.997647	3.047143	3.129147
1	−3.906553	1.412519	1.409765
1	−3.598048	2.932823	0.554806
8	0.007672	1.673801	−0.042879
8	−2.007005	1.608997	0.822769
1	2.762978	0.756686	1.246176

1	−1.008016	−0.838249	2.500631
17	0.901513	2.628104	5.363541

Table S20. Cartesian coordinate of **C_{ax}TS1b.**

The number of atom coordinates (angstroms)	X	Y	Z
13	0.643663	0.185684	−0.588301
8	0.526888	−1.339918	−1.654383
8	1.987725	0.930669	−1.430704
7	1.228538	−0.867582	0.958711
6	0.590279	−2.584316	−1.326532
6	0.231843	−3.553982	−2.420697
1	0.444154	−4.590747	−2.1489
1	0.775715	−3.293711	−3.334815
1	−0.839751	−3.456293	−2.632999
6	0.940557	−3.036862	−0.058297
1	0.969529	−4.106401	0.106528
6	1.289351	−2.199828	1.022575
6	1.753685	−2.867228	2.298676
1	2.799149	−2.614529	2.506234
1	1.169917	−2.516458	3.156005
1	1.665481	−3.952943	2.228538
6	1.731988	−0.108498	2.068704
6	0.876	0.33439	3.081982
6	1.370763	1.095904	4.138
1	0.710514	1.444565	4.924869
6	2.727073	1.422593	4.164982
6	3.591675	1.008784	3.154147
1	4.640761	1.282579	3.183967
6	3.084765	0.241784	2.103808
6	2.465202	2.228238	−1.179159
1	2.575169	2.425904	−0.101381
1	3.474755	2.311139	−1.615837
6	1.592007	3.318261	−1.779345
6	0.932151	3.10555	−2.99602
1	1.045494	2.144558	−3.488932
6	0.12017	4.097384	−3.549252
1	−0.391433	3.914148	−4.491192
6	−0.041078	5.321584	−2.893425
1	−0.677547	6.092541	−3.320192
6	0.618412	5.544366	−1.681737
1	0.492532	6.489047	−1.158246
6	1.426294	4.546988	−1.130485

1	1.915211	4.714814	−0.173195
8	−1.175493	0.513765	−0.948138
6	−2.220444	−0.110489	−1.664588
1	−1.894742	−0.242649	−2.703541
1	−3.072767	0.584609	−1.68666
6	−2.660445	−1.447762	−1.097064
6	−3.357855	−2.341648	−1.920835
1	−3.560046	−2.0721	−2.955833
6	−3.783812	−3.577359	−1.432059
1	−4.31881	−4.261661	−2.085458
6	−3.510903	−3.93834	−0.109468
1	−3.833137	−4.903883	0.271044
6	−2.815868	−3.052379	0.714681
1	−2.591123	−3.327254	1.742156
6	−2.395932	−1.812998	0.2261
1	−1.851259	−1.128737	0.866301
6	−1.180176	1.733179	0.333753
6	−1.757877	2.952265	−0.358653
6	−2.005498	4.109802	0.628354
6	−3.358273	4.017329	1.350854
6	−3.539779	2.776596	2.23809
6	−3.29636	1.444977	1.530163
1	−2.690058	2.697638	−0.875386
1	−1.1799	4.151994	1.3503
1	−4.156203	4.028104	0.593559
1	−2.859082	2.819436	3.098307
1	−1.033017	3.237184	−1.118438
1	−1.967619	5.047755	0.063024
1	−3.505329	4.91444	1.965409
1	−4.56134	2.767126	2.640767
1	−3.646544	0.609484	2.141111
1	−3.814723	1.388852	0.566327
8	0.098086	1.654618	0.511881
8	−1.885925	1.188512	1.366959
1	3.735934	−0.081397	1.297323
1	−0.182831	0.11309	3.014073
17	3.355699	2.391512	5.499833

Table S21. Cartesian coordinate of **C_{ax}2b.**

The number of atom coordinates (angstroms)	X	Y	Z
13	0.614776	0.282638	−0.452084
8	0.380849	−1.157396	−1.59108

8	2.000405	0.957341	−1.292139
7	1.047923	−0.875291	1.057306
6	0.743525	−2.384026	−1.433029
6	0.560366	−3.262439	−2.640301
1	0.923878	−4.279843	−2.477933
1	1.083699	−2.819735	−3.495
1	−0.506347	−3.296747	−2.88768
6	1.241586	−2.899215	−0.239277
1	1.517975	−3.945768	−0.218396
6	1.340334	−2.176176	0.967542
6	1.785557	−2.933564	2.199174
1	2.557246	−2.377808	2.740949
1	0.948293	−3.070725	2.892025
1	2.174226	−3.918168	1.932013
6	1.063865	−0.241622	2.343342
6	0.008748	−0.434495	3.240399
6	−0.019721	0.241278	4.45833
1	−0.840895	0.097511	5.152363
6	1.014753	1.123816	4.767014
6	2.074799	1.331768	3.885776
1	2.868139	2.026321	4.139725
6	2.093708	0.643576	2.673323
6	2.277129	2.328128	−1.397906
1	2.315396	2.817254	−0.411394
1	3.278721	2.445793	−1.844684
6	1.273599	3.085648	−2.258326
6	0.521435	2.422316	−3.235052
1	0.667228	1.355462	−3.37413
6	−0.415477	3.115021	−4.005352
1	−0.997121	2.582831	−4.754542
6	−0.608764	4.485566	−3.814992
1	−1.342627	5.024104	−4.409089
6	0.148711	5.158812	−2.852336
1	0.003402	6.224257	−2.691605
6	1.08041	4.460986	−2.082026
1	1.649075	4.986338	−1.317244
8	−1.31722	0.731322	−0.805528
6	−2.557969	0.204071	−1.315154
1	−2.609147	0.455978	−2.37856
1	−3.360706	0.729401	−0.789845
6	−2.670086	−1.286127	−1.100572
6	−3.056918	−2.12332	−2.150659

1	−3.256426	−1.699007	−3.13209
6	−3.174951	−3.502178	−1.952435
1	−3.476106	−4.14265	−2.777266
6	−2.888397	−4.054973	−0.703351
1	−2.964193	−5.128213	−0.550816
6	−2.500813	−3.220485	0.349708
1	−2.274529	−3.64532	1.324434
6	−2.403882	−1.843929	0.156656
1	−2.108247	−1.186033	0.966673
6	−1.268754	1.754429	0.28077
6	−1.778189	3.104912	−0.235497
6	−1.232073	4.28706	0.575837
6	−1.779451	4.395734	2.003901
6	−1.636551	3.11582	2.84308
6	−2.541127	1.9687	2.382523
1	−2.875842	3.105131	−0.249622
1	−0.142313	4.189421	0.60302
1	−2.845006	4.669462	1.96665
1	−0.598425	2.768559	2.859394
1	−1.428817	3.193579	−1.267083
1	−1.453605	5.212545	0.030333
1	−1.268527	5.221094	2.516711
1	−1.916231	3.341434	3.880735
1	−2.663542	1.246739	3.195522
1	−3.539057	2.362226	2.133202
8	0.045601	1.723308	0.545853
8	−2.067165	1.169038	1.29049
1	2.898497	0.807852	1.963315
1	−0.805083	−1.098616	2.969418
17	0.970595	2.005085	6.294513

Table S22. Cartesian coordinate of **C_{ax}3b.**

The number of atom coordinates (angstroms)	X	Y	Z
13	0.150501	0.802166	0.632281
8	−0.518963	−0.479016	−0.463561
8	1.376428	1.795562	−0.11232
7	1.273233	−0.481779	1.652296
6	−0.389624	−1.778029	−0.384494
6	−1.214849	−2.535489	−1.388567
1	−1.079069	−3.616843	−1.314248
1	−0.949902	−2.206367	−2.400202
1	−2.274545	−2.294454	−1.24131

6	0.426002	−2.426952	0.517217
1	0.455357	−3.508941	0.478254
6	1.275534	−1.789069	1.473434
6	2.199893	−2.69028	2.260502
1	3.168805	−2.759626	1.751722
1	2.381787	−2.306407	3.266754
1	1.784671	−3.698745	2.327907
6	2.212313	0.134316	2.542888
6	1.748103	0.821294	3.671068
6	2.646772	1.479277	4.510781
1	2.292103	2.009957	5.387724
6	4.007234	1.453038	4.208462
6	4.484075	0.784806	3.081569
1	5.543218	0.786772	2.84786
6	3.580827	0.12802	2.249603
6	1.997896	1.584344	−1.358951
1	1.296659	1.149897	−2.090564
1	2.312347	2.559155	−1.761737
6	3.209489	0.677496	−1.237132
6	4.47515	1.204865	−0.956116
1	4.595445	2.282721	−0.875016
6	5.575423	0.365375	−0.767762
1	6.551775	0.791662	−0.551966
6	5.420217	−1.021307	−0.851695
1	6.274231	−1.676921	−0.703419
6	4.16009	−1.559676	−1.131407
1	4.029455	−2.636794	−1.201717
6	3.066859	−0.71298	−1.325623
1	2.088752	−1.136786	−1.536996
8	−1.831182	3.444544	1.989177
6	−0.621868	4.206242	1.811889
1	0.255321	3.559525	1.895033
1	−0.608918	4.901708	2.657973
6	−0.624896	4.965849	0.503335
6	0.418707	4.826281	−0.416911
1	1.225788	4.134937	−0.197825
6	0.392123	5.528022	−1.625326
1	1.206461	5.407856	−2.335749
6	−0.679415	6.371436	−1.926422
1	−0.70085	6.914103	−2.868088
6	−1.726863	6.512995	−1.01068
1	−2.564708	7.16747	−1.237933

6	−1.695839	5.815553	0.196856
1	−2.514226	5.914	0.906007
6	−1.80986	2.120402	1.54109
6	−3.208265	1.558202	1.823869
6	−3.608389	0.350925	0.961397
6	−4.173617	0.72661	−0.422589
6	−3.160754	1.29431	−1.429028
6	−2.357516	2.480868	−0.909997
1	−3.940472	2.364546	1.703272
1	−2.754218	−0.326634	0.84945
1	−4.985934	1.454528	−0.278921
1	−2.446057	0.515473	−1.715792
1	−3.201562	1.29068	2.885156
1	−4.381448	−0.209452	1.50132
1	−4.63754	−0.163478	−0.868312
1	−3.689701	1.606974	−2.339798
1	−1.730526	2.92151	−1.689946
1	−2.989381	3.276989	−0.502733
8	−0.793742	1.362646	2.056282
8	−1.448374	2.062735	0.120957
1	3.93622	−0.374554	1.358985
1	0.684117	0.853515	3.873146
17	5.146205	2.289139	5.265439

Table S23. Cartesian coordinate of **C_{ax}TS2b.**

The number of atom coordinates (angstroms)	X	Y	Z
13	0.458092	1.311194	0.221597
8	0.08791	0.321218	−1.331168
8	1.885284	2.17514	−0.335608
7	0.867446	−0.348863	1.217994
6	−0.091477	−0.943196	−1.494477
6	−0.58922	−1.349568	−2.85709
1	−0.705608	−2.431084	−2.958845
1	0.108853	−0.986804	−3.620255
1	−1.55298	−0.86322	−3.047847
6	0.175304	−1.890572	−0.513145
1	0.032362	−2.934355	−0.762713
6	0.715373	−1.592323	0.761819
6	1.172621	−2.765355	1.601152
1	2.2482	−2.680645	1.793573
1	0.676686	−2.782594	2.575917
1	0.981006	−3.711002	1.091014

6	1.493413	−0.174475	2.50359
6	0.756346	−0.300636	3.685695
6	1.363357	−0.10306	4.924185
1	0.792932	−0.2005	5.841609
6	2.717323	0.22863	4.969945
6	3.465688	0.365322	3.803267
1	4.517157	0.626917	3.851507
6	2.847161	0.16358	2.569474
6	2.743251	1.796443	−1.389388
1	2.185326	1.353036	−2.22791
1	3.243102	2.699355	−1.772721
6	3.791838	0.81012	−0.908345
6	4.943719	1.26193	−0.251433
1	5.115658	2.331859	−0.158968
6	5.85397	0.358556	0.301594
1	6.741624	0.725882	0.810395
6	5.620556	−1.016668	0.206416
1	6.324139	−1.721446	0.641587
6	4.479258	−1.478951	−0.453791
1	4.290824	−2.546738	−0.535007
6	3.575766	−0.569836	−1.008743
1	2.682142	−0.935583	−1.506518
8	−1.015028	4.17275	1.650787
6	−0.035699	4.852639	0.814098
1	0.887516	4.273049	0.776153
1	0.150483	5.798347	1.331095
6	−0.615488	5.079509	−0.561286
6	0.035083	4.591151	−1.69872
1	0.950856	4.02132	−1.577693
6	−0.512864	4.797836	−2.966743
1	−0.001462	4.409502	−3.843785
6	−1.718332	5.48837	−3.106971
1	−2.146777	5.645369	−4.093545
6	−2.374536	5.97572	−1.972535
1	−3.31333	6.514043	−2.074973
6	−1.822503	5.774523	−0.707304
1	−2.334702	6.145959	0.176905
6	−0.878551	2.856842	1.854774
6	−2.01596	2.333449	2.710542
6	−2.531698	0.915071	2.407889
6	−3.628308	0.807716	1.323728
6	−3.152577	0.701662	−0.133649

6	−2.369829	1.911691	−0.634186
1	−2.84005	3.051938	2.671997
1	−1.691861	0.259584	2.154971
1	−4.314557	1.661783	1.421674
1	−2.515942	−0.187908	−0.240664
1	−1.611723	2.360981	3.731398
1	−2.950747	0.527992	3.34521
1	−4.227893	−0.085685	1.542245
1	−4.025608	0.548118	−0.783887
1	−2.10261	1.788567	−1.691646
1	−2.970323	2.829212	−0.551451
8	0.27606	2.302189	1.870563
8	−1.193544	2.093775	0.118908
1	3.414988	0.274349	1.655565
1	−0.297455	−0.552761	3.637138
17	3.493082	0.480358	6.535134

Table S24. Cartesian coordinate of **C_{ax}4b.**

The number of atom coordinates (angstroms)	X	Y	Z
13	0.41324	1.10878	−0.067892
8	0.126049	0.105269	−1.632844
8	1.793612	2.045882	−0.65013
7	0.895452	−0.518654	0.95255
6	0.144114	−1.162955	−1.832742
6	−0.231506	−1.602785	−3.224252
1	−0.213995	−2.688717	−3.34341
1	0.459342	−1.149749	−3.944915
1	−1.233355	−1.228052	−3.462606
6	0.508548	−2.088616	−0.86001
1	0.525475	−3.134964	−1.137469
6	0.914159	−1.759469	0.452981
6	1.43415	−2.900711	1.301961
1	2.466359	−2.693517	1.605497
1	0.850669	−3.020311	2.219464
1	1.412878	−3.84077	0.747868
6	1.357527	−0.352904	2.304899
6	0.495298	−0.585666	3.380257
6	0.926213	−0.38626	4.691453
1	0.258441	−0.565183	5.527505
6	2.231941	0.050352	4.914226
6	3.106952	0.281522	3.854073
1	4.120253	0.619559	4.042865

6	2.66397	0.07819	2.548073
6	2.756696	1.62791	−1.588981
1	2.305936	1.039698	−2.402839
1	3.206416	2.522566	−2.047058
6	3.84581	0.806097	−0.92255
6	4.833841	1.434503	−0.152392
1	4.846925	2.520268	−0.092041
6	5.781876	0.684943	0.546386
1	6.541826	1.187941	1.139087
6	5.750919	−0.712258	0.488075
1	6.484685	−1.298129	1.035286
6	4.772706	−1.34921	−0.278867
1	4.741847	−2.434789	−0.331183
6	3.830136	−0.592239	−0.979963
1	3.061876	−1.094277	−1.562381
8	−0.555793	4.178198	1.721276
6	0.206069	4.702497	0.582755
1	1.040197	4.037098	0.358545
1	0.582388	5.663886	0.943504
6	−0.715221	4.872251	−0.598096
6	−0.397738	4.291075	−1.829363
1	0.496718	3.681461	−1.909995
6	−1.247724	4.458304	−2.92436
1	−0.995799	3.997053	−3.875651
6	−2.425102	5.197915	−2.794314
1	−3.089523	5.321343	−3.645606
6	−2.750032	5.77439	−1.562892
1	−3.666485	6.348443	−1.453906
6	−1.894985	5.616207	−0.472094
1	−2.147877	6.059793	0.487714
6	−0.369182	2.933259	2.120308
6	−1.342571	2.5132	3.19205
6	−2.410326	1.534256	2.650102
6	−3.414088	2.140085	1.632043
6	−3.549566	1.307348	0.33941
6	−2.427915	1.624034	−0.66525
1	−1.816457	3.400466	3.621195
1	−1.889456	0.690571	2.193362
1	−3.106326	3.157343	1.360701
1	−3.535887	0.238369	0.597376
1	−0.756937	2.01109	3.969364
1	−2.948544	1.138413	3.52051

1	−4.395859	2.234313	2.112205
1	−4.518663	1.499955	−0.141579
1	−2.392263	0.850695	−1.450335
1	−2.65887	2.57866	−1.164677
8	0.537688	2.200675	1.703964
8	−1.210893	1.754042	0.003482
1	3.327464	0.265868	1.713608
1	−0.519789	−0.917718	3.186963
17	2.784578	0.312586	6.569793

Table S25. Cartesian coordinate of **C_{eq}1c.**

The number of atom coordinates (angstroms)	X	Y	Z
13	−0.098276	0.30334	0.104325
8	0.515018	−0.832352	−1.125019
8	−0.219085	1.670679	1.193753
7	0.332755	−1.091682	1.627065
6	0.840982	−2.073297	−0.971284
6	1.043021	−2.700503	−2.241224
1	0.066206	−2.781398	−2.73288
1	1.670942	−2.050452	−2.920587
1	1.492111	−3.695132	−2.062762
6	0.987689	−2.825869	0.27495
1	1.293901	−3.859607	0.305137
6	0.761835	−2.332417	1.508149
6	1.017453	−3.284061	2.739672
1	0.087169	−3.502187	3.022322
1	1.442478	−4.224469	2.529878
1	1.69977	−2.839836	3.599732
6	0.148041	−0.704867	2.966219
6	−1.083418	−0.961236	3.60317
6	−1.267255	−0.480041	4.895164
1	−2.216423	−0.650023	5.393386
6	−0.259255	0.212571	5.555651
6	0.96535	0.419278	4.917837
1	1.757664	0.944646	5.440862
6	1.192546	−0.031618	3.61085
6	−1.38142	2.175446	1.665741
1	−2.232462	2.167408	0.832699
1	−1.671106	1.55749	2.35459
6	−1.140545	3.59254	2.389059
6	−0.13994	3.839703	3.554047
1	0.413676	2.99771	3.938541

6	0.146143	5.13926	4.206935
1	0.928891	5.313598	5.105492
6	−0.574837	6.219766	3.710547
1	−0.352735	7.23369	4.217132
6	−1.589748	5.984327	2.565769
1	−2.162489	6.815337	2.177367
6	−1.868046	4.677222	1.911869
1	−2.654383	4.497608	1.011497
8	−1.745701	0.379696	−0.240454
6	−2.195316	0.078326	−1.49718
1	−1.516143	0.472369	−2.301776
1	−3.16214	0.588731	−1.499727
6	−2.408489	−1.403395	−1.869806
6	−2.540961	−1.854871	−3.212338
1	−2.471437	−1.140541	−3.993381
6	−2.74321	−3.207989	−3.560407
1	−2.836652	−3.54074	−4.608355
6	−2.810571	−4.13584	−2.564838
1	−2.957341	−5.191419	−2.833302
6	−2.684724	−3.692757	−1.223334
1	−2.731681	−4.40414	−0.440161
6	−2.491842	−2.336674	−0.881948
1	−2.384969	−1.987131	0.155679
6	1.535698	2.445983	−0.327057
6	2.618931	3.44704	0.181757
6	2.091954	4.571544	0.776143
6	1.29216	5.658092	−0.266648
6	0.039409	5.147418	−1.000484
6	0.299111	4.092637	−1.725222
1	3.007038	3.874599	−0.679575
1	1.479984	4.129557	1.511597
1	1.946563	6.163496	−1.003832
1	−0.670893	4.73268	−0.294429
1	3.423746	2.894426	0.899078
1	2.960269	5.029022	1.325797
1	0.984958	6.412237	0.228535
1	−0.461152	5.991064	−1.750098
1	−0.572886	3.955404	−2.357117
1	1.160161	4.336101	−2.367949
8	1.566778	1.312244	−0.850435
8	0.488795	2.760234	−0.834203
1	−0.422562	0.581974	6.563288

6	2.54878	0.209753	2.91261
1	2.522481	−0.225183	1.842068
6	3.684069	−0.482965	3.094428
1	3.511651	−1.561027	2.645639
1	4.641854	−0.338374	2.617595
1	3.783705	−0.071579	4.158892
6	2.832531	1.711921	3.353636
1	2.913198	2.21414	4.381183
1	3.780079	1.864142	2.709724
1	2.021952	2.173318	3.292199
6	−2.203552	−1.747269	2.957904
1	−1.785298	−2.225467	2.056253
6	−2.746453	−2.872448	3.882615
1	−3.44363	−3.501574	3.334803
1	−1.941869	−3.51132	4.269131
1	−3.292232	−2.473838	4.744429
6	−3.34846	−0.831167	2.51968
1	−3.745243	−0.242705	3.365664
1	−3.010489	−0.148745	1.719584
1	−4.168151	−1.433847	2.136399

Table S26. Cartesian coordinate of **C_{eq}TS1c.**

The number of atom coordinates (angstroms)	X	Y	Z
13	−0.002386	0.14608	0.104325
8	0.595077	−1.124279	−1.125019
8	−0.014573	1.776557	1.193753
7	0.458106	−1.030921	1.627065
6	0.888096	−2.365354	−0.971284
6	1.044594	−3.155573	−2.241224
1	0.066492	−3.214718	−2.73288
1	1.723074	−2.628617	−2.920587
1	1.416495	−4.167516	−2.062762
6	1.041279	−2.963425	0.27495
1	1.317264	−4.010169	0.305137
6	0.83419	−2.312484	1.508149
6	1.006448	−3.179753	2.739672
1	0.037736	−3.606373	3.022322
1	1.686219	−4.008776	2.529878
1	1.376448	−2.620818	3.599732
6	0.218644	−0.539153	2.966219
6	−1.013788	−0.80376	3.60317
6	−1.213827	−0.295919	4.895164

1	−2.162707	−0.472596	5.393386
6	−0.216107	0.410461	5.555651
6	1.000934	0.646894	4.917837
1	1.770762	1.204888	5.440862
6	1.233042	0.205549	3.61085
6	−1.259137	2.304261	1.665741
1	−1.960555	2.403479	0.832699
1	−1.666263	1.55619	2.35459
6	−1.099823	3.618324	2.389059
6	−0.325866	3.699121	3.554047
1	0.139466	2.798656	3.938541
6	−0.148231	4.918451	4.206935
1	0.462012	4.966647	5.105492
6	−0.756502	6.075971	3.710547
1	−0.616952	7.027398	4.217132
6	−1.55205	6.000383	2.565769
1	−2.035517	6.893218	2.177367
6	−1.720887	4.776632	1.911869
1	−2.327304	4.720214	1.011497
8	−1.726291	0.105872	−0.240454
6	−2.298837	−0.127877	−1.49718
1	−1.749095	0.388782	−2.301776
1	−3.31406	0.305304	−1.499727
6	−2.418544	−1.599455	−1.869806
6	−2.50027	−1.989168	−3.212338
1	−2.44396	−1.233066	−3.993381
6	−2.637539	−3.334933	−3.560407
1	−2.693764	−3.619529	−4.608355
6	−2.685152	−4.315246	−2.564838
1	−2.780927	−5.364158	−2.833302
6	−2.602174	−3.934382	−1.223334
1	−2.63214	−4.688304	−0.440161
6	−2.476022	−2.586871	−0.881948
1	−2.403375	−2.283708	0.155679
6	0.812283	2.524596	−0.327057
6	2.037476	3.256491	0.181757
6	1.874919	4.658632	0.776143
6	1.643386	5.760939	−0.266648
6	0.301157	5.665286	−1.000484
6	0.065913	4.345083	−1.725222
1	2.721594	3.290692	−0.679575
1	1.067976	4.66102	1.511597

1	2.460232	5.735931	−1.003832
1	−0.521853	5.819013	−0.294429
1	2.500582	2.579542	0.899078
1	2.79655	4.887577	1.325797
1	1.702676	6.738319	0.228535
1	0.236753	6.466148	−1.750098
1	−0.82315	4.408562	−2.357117
1	0.914759	4.078119	−2.367949
8	1.037084	1.357709	−0.850435
8	−0.229826	3.240494	−0.834203
1	−0.383967	0.781182	6.563288
6	2.555385	0.506877	2.91261
1	2.341591	0.583599	1.842068
6	3.5748	−0.634952	3.094428
1	3.224972	−1.568122	2.645639
1	4.527189	−0.374254	2.617595
1	3.766654	−0.817336	4.158892
6	3.180135	1.841328	3.353636
1	3.559175	1.794795	4.381183
1	4.033619	2.08291	2.709724
1	2.459592	2.662978	3.292199
6	−2.118405	−1.637948	2.957904
1	−1.707823	−2.097994	2.056253
6	−2.592461	−2.77678	3.882615
1	−3.26375	−3.448174	3.334803
1	−1.75556	−3.368687	4.269131
1	−3.148505	−2.390451	4.744429
6	−3.316255	−0.774072	2.51968
1	−3.715672	−0.201399	3.365664
1	−3.026639	−0.089745	1.719584
1	−4.120317	−1.414618	2.136399

Table S27. Cartesian coordinate of **C_{eq}2c.**

The number of atom coordinates (angstroms)	X	Y	Z
13	0.07619	0.091962	0.124663
8	0.688216	−1.096445	−1.142702
8	−0.041861	1.849915	1.351445
7	0.494017	−1.069933	1.637535
6	0.933299	−2.354334	−1.002687
6	1.10154	−3.12219	−2.283094
1	0.13737	−3.136783	−2.804897
1	1.818278	−2.604502	−2.929469

1	1.432624	−4.14987	−2.116071
6	1.03161	−2.981167	0.2346
1	1.273595	−4.036651	0.244495
6	0.833102	−2.357025	1.48581
6	0.985147	−3.252524	2.697763
1	0.007651	−3.661544	2.975354
1	1.645767	−4.092495	2.471787
1	1.371689	−2.714995	3.56461
6	0.259313	−0.585541	2.980486
6	−0.982	−0.830407	3.607372
6	−1.188	−0.308263	4.893
1	−2.142977	−0.469828	5.384755
6	−0.192125	0.403343	5.54921
6	1.032523	0.622649	4.919152
1	1.79845	1.182418	5.444648
6	1.278965	0.155992	3.623477
6	−1.278028	2.378479	1.896201
1	−2.031894	2.393282	1.109498
1	−1.557065	1.626421	2.636377
6	−1.10678	3.725405	2.544475
6	−0.231058	3.880017	3.626625
1	0.305198	3.012485	3.999567
6	−0.047873	5.130962	4.214326
1	0.640029	5.24197	5.048664
6	−0.751877	6.240302	3.735093
1	−0.609921	7.21556	4.193247
6	−1.639296	6.090182	2.667451
1	−2.188628	6.948635	2.289965
6	−1.809905	4.837834	2.072231
1	−2.474784	4.723508	1.220459
8	−1.654696	0.114105	−0.149378
6	−2.280558	−0.027491	−1.39678
1	−1.781124	0.569018	−2.178642
1	−3.302938	0.378454	−1.314574
6	−2.381367	−1.468118	−1.878735
6	−2.426676	−1.763965	−3.246219
1	−2.355515	−0.955454	−3.971303
6	−2.547752	−3.083207	−3.689712
1	−2.576391	−3.294771	−4.755816
6	−2.614048	−4.129888	−2.765693
1	−2.697376	−5.158064	−3.10815
6	−2.564275	−3.843047	−1.399054

1	−2.608301	−4.649964	−0.671443
6	−2.453911	−2.522246	−0.962307
1	−2.405892	−2.292803	0.096129
6	0.649497	2.518335	0.218863
6	1.797834	3.431859	0.702755
6	1.581897	4.951642	0.685459
6	1.560793	5.576046	−0.720117
6	0.290347	5.286698	−1.529494
6	−0.005661	3.801239	−1.710885
1	2.662208	3.185747	0.075554
1	0.668197	5.216387	1.223294
1	2.43768	5.222025	−1.28322
1	−0.575379	5.743858	−1.032068
1	2.045449	3.107803	1.714067
1	2.412231	5.398466	1.248106
1	1.673528	6.664416	−0.627379
1	0.371079	5.749191	−2.523369
1	−0.862929	3.659417	−2.377426
1	0.846024	3.264494	−2.146565
8	1.126892	1.435691	−0.453166
8	−0.379115	3.193859	−0.466419
1	−0.366084	0.791702	6.549106
6	2.608604	0.443438	2.927419
1	2.378917	0.689512	1.88446
6	3.545685	−0.782194	2.920142
1	3.140225	−1.610898	2.336529
1	4.512086	−0.51259	2.478318
1	3.727972	−1.135489	3.942455
6	3.363565	1.641556	3.527603
1	3.792384	1.398633	4.507381
1	4.192535	1.921985	2.869147
1	2.71909	2.517819	3.651072
6	−2.101399	−1.636554	2.952352
1	−1.707064	−2.082705	2.036499
6	−2.587681	−2.785007	3.858263
1	−3.284203	−3.427044	3.306866
1	−1.759568	−3.405854	4.217063
1	−3.119274	−2.405164	4.738186
6	−3.28537	−0.740637	2.54272
1	−3.682416	−0.196306	3.408174
1	−2.978643	−0.030504	1.772399

1	−4.09559	−1.354536	2.130019

Table S28. Cartesian coordinate of **C_{eq}3c.**

The number of atom coordinates (angstroms)	X	Y	Z
13	−0.045658	0.383742	−0.578478
8	0.904745	−0.849991	−1.576439
8	0.672402	4.001313	−0.567215
7	0.361198	−0.504676	1.120965
6	1.135898	−2.080983	−1.263564
6	1.683171	−2.938416	−2.372074
1	2.686211	−2.582425	−2.637423
1	1.740051	−3.992767	−2.092543
1	1.053407	−2.832341	−3.259812
6	0.956647	−2.588232	0.015879
1	1.154062	−3.641089	0.174391
6	0.675076	−1.809475	1.160359
6	0.819319	−2.555426	2.476521
1	1.879413	−2.701518	2.70574
1	0.364892	−2.0416	3.320562
1	0.368953	−3.547589	2.378394
6	0.332001	0.186129	2.391803
6	−0.881021	0.290933	3.112327
6	−0.830591	0.848123	4.397788
1	−1.742034	0.933153	4.980173
6	0.370556	1.282141	4.951413
6	1.542798	1.216993	4.204547
1	2.46148	1.603429	4.631825
6	1.548905	0.694352	2.905377
6	1.640743	3.887902	0.491462
1	1.785819	2.837577	0.73347
1	2.58556	4.283043	0.103317
6	1.186022	4.670881	1.699306
6	1.508033	6.026645	1.833972
1	2.122216	6.507395	1.075699
6	1.045779	6.763262	2.926538
1	1.303125	7.815261	3.018582
6	0.257017	6.146952	3.901433
1	−0.100593	6.718287	4.754195
6	−0.064636	4.792844	3.777859
1	−0.668063	4.298529	4.53447
6	0.394896	4.062273	2.682436

1	0.143119	3.013427	2.585452
8	−1.697821	0.082716	−1.109946
6	−2.086812	−0.750051	−2.175387
1	−1.412998	−0.651453	−3.041125
1	−3.081374	−0.420132	−2.519132
6	−2.168623	−2.218506	−1.791991
6	−1.784806	−3.226897	−2.681599
1	−1.420847	−2.957524	−3.671144
6	−1.84762	−4.572435	−2.308557
1	−1.534664	−5.342667	−3.009198
6	−2.29906	−4.925201	−1.035307
1	−2.341267	−5.970373	−0.739758
6	−2.697352	−3.923684	−0.144292
1	−3.054097	−4.186638	0.848665
6	−2.633837	−2.583902	−0.524471
1	−2.92986	−1.800711	0.163382
6	0.041893	2.834512	−0.967902
6	−0.878404	3.190875	−2.144454
6	−1.672225	4.495847	−2.034178
6	−2.803495	4.46163	−1.001459
6	−2.348416	4.115852	0.423143
6	−1.995296	2.648102	0.651354
1	−1.541974	2.334073	−2.301623
1	−0.981919	5.311796	−1.794381
1	−3.565209	3.732944	−1.316546
1	−1.510614	4.749711	0.728545
1	−0.206492	3.242179	−3.007804
1	−2.099494	4.72069	−3.020175
1	−3.299051	5.441268	−0.987704
1	−3.173527	4.327263	1.117124
1	−1.966494	2.450494	1.722786
1	−2.738817	1.990009	0.1887
8	0.870359	1.790083	−1.248906
8	−0.692797	2.216543	0.194857
1	0.388555	1.696219	5.955853
6	2.833496	0.729694	2.069823
1	2.534575	0.870497	1.02436
6	3.751098	1.907788	2.453282
1	4.2802	1.713323	3.393826
1	4.511115	2.047914	1.677086
1	3.199803	2.84551	2.568741
6	3.654067	−0.576115	2.128109

1	3.824744	−0.883297	3.166961
1	3.16582	−1.393969	1.595595
1	4.63173	−0.421346	1.65722
6	−2.209861	−0.223362	2.55266
1	−2.182737	−0.102127	1.464851
6	−3.434645	0.54729	3.082567
1	−4.312808	0.29491	2.478353
1	−3.665122	0.272812	4.118741
1	−3.300646	1.632278	3.048508
6	−2.424023	−1.72463	2.845441
1	−3.443142	−2.018851	2.56727
1	−1.740144	−2.358542	2.280928
1	−2.294237	−1.93297	3.914112

Table S29. Cartesian coordinate of **C_{eq}TS2c.**

The number of atom coordinates (angstroms)	X	Y	Z
13	−0.12611	0.508519	−0.489562
8	0.90302	−0.69211	−1.490075
8	0.73052	4.067664	−0.705804
7	0.281167	−0.489013	1.1735
6	1.136607	−1.934583	−1.239375
6	1.716695	−2.727319	−2.38069
1	2.706079	−2.325387	−2.630473
1	1.810644	−3.789854	−2.144824
1	1.083868	−2.608556	−3.265098
6	0.932513	−2.512922	0.005309
1	1.139062	−3.570057	0.116832
6	0.617864	−1.786708	1.174442
6	0.765526	−2.575763	2.465034
1	1.82665	−2.695542	2.705395
1	0.283483	−2.107122	3.320051
1	0.349449	−3.577848	2.324796
6	0.223991	0.161685	2.462595
6	−0.99384	0.207654	3.180385
6	−0.97359	0.754106	4.470561
1	−1.890889	0.794345	5.048759
6	0.203699	1.243428	5.029768
6	1.38179	1.231812	4.288304
1	2.281198	1.654757	4.72213
6	1.41715	0.710571	2.989003
6	1.81258	4.009838	0.261319

1	2.037278	2.966495	0.471782
1	2.680807	4.467769	−0.220706
6	1.404484	4.76543	1.498442
6	1.774063	6.102908	1.67706
1	2.378587	6.598719	0.92082
6	1.372794	6.80239	2.817566
1	1.666202	7.840771	2.9468
6	0.599256	6.165913	3.791046
1	0.290285	6.708566	4.680671
6	0.229219	4.828803	3.620469
1	−0.361756	4.318719	4.376059
6	0.626518	4.13461	2.478808
1	0.340976	3.099506	2.338692
8	−1.714565	0.137208	−1.171936
6	−2.013474	−0.728484	−2.234745
1	−1.272778	−0.653063	−3.047031
1	−2.97912	−0.417585	−2.66942
6	−2.1233	−2.189163	−1.82464
6	−1.739903	−3.214114	−2.696181
1	−1.353451	−2.961277	−3.681688
6	−1.831582	−4.554244	−2.311833
1	−1.518265	−5.336618	−2.998849
6	−2.313353	−4.886404	−1.043986
1	−2.378705	−5.927556	−0.738447
6	−2.711789	−3.869097	−0.171684
1	−3.091995	−4.116494	0.816382
6	−2.618764	−2.533638	−0.562791
1	−2.914528	−1.739529	0.112749
6	0.211216	2.93054	−1.170947
6	−0.864639	3.190308	−2.207243
6	−1.785053	4.389936	−1.968498
6	−2.872667	4.175904	−0.907575
6	−2.374671	3.942834	0.5291
6	−1.944697	2.512437	0.857151
1	−1.436154	2.265132	−2.31677
1	−1.180076	5.265394	−1.70566
1	−3.51052	3.331285	−1.206938
1	−1.557489	4.632849	0.76873
1	−0.300887	3.333771	−3.139904
1	−2.27582	4.624156	−2.921991
1	−3.518348	5.064383	−0.912412
1	−3.194765	4.177359	1.222254

1	−1.846598	2.426274	1.945892
1	−2.723954	1.812753	0.527562
8	0.937411	1.862387	−1.280967
8	−0.696712	2.138358	0.29548
1	0.199405	1.652455	6.036675
6	2.704653	0.788598	2.160677
1	2.405785	0.95342	1.118438
6	3.611177	1.962779	2.576322
1	4.127375	1.754605	3.521128
1	4.383353	2.116442	1.814328
1	3.055763	2.896464	2.69634
6	3.540815	−0.508961	2.181635
1	3.708015	−0.847332	3.211263
1	3.066811	−1.314601	1.619252
1	4.519951	−0.327062	1.723449
6	−2.300238	−0.334604	2.596533
1	−2.248643	−0.208031	1.510981
6	−3.548234	0.416794	3.09732
1	−4.411591	0.140074	2.482209
1	−3.790804	0.149868	4.132854
1	−3.431003	1.502699	3.048975
6	−2.495693	−1.840562	2.873344
1	−3.503169	−2.148371	2.568452
1	−1.788973	−2.457823	2.318631
1	−2.386858	−2.057548	3.942748

Table S30. Cartesian coordinate of **C_{eq}4c.**

The number of atom coordinates (angstroms)	X	Y	Z
13	0.07619	0.091962	0.124663
8	0.688216	−1.096445	−1.142702
8	−0.041861	1.849915	1.351445
7	0.494017	−1.069933	1.637535
6	0.933299	−2.354334	−1.002687
6	1.10154	−3.12219	−2.283094
1	0.13737	−3.136783	−2.804897
1	1.818278	−2.604502	−2.929469
1	1.432624	−4.14987	−2.116071
6	1.03161	−2.981167	0.2346
1	1.273595	−4.036651	0.244495
6	0.833102	−2.357025	1.48581
6	0.985147	−3.252524	2.697763

1	0.007651	−3.661544	2.975354
1	1.645767	−4.092495	2.471787
1	1.371689	−2.714995	3.56461
6	0.259313	−0.585541	2.980486
6	−0.982	−0.830407	3.607372
6	−1.188	−0.308263	4.893
1	−2.142977	−0.469828	5.384755
6	−0.192125	0.403343	5.54921
6	1.032523	0.622649	4.919152
1	1.79845	1.182418	5.444648
6	1.278965	0.155992	3.623477
6	−1.278028	2.378479	1.896201
1	−2.031894	2.393282	1.109498
1	−1.557065	1.626421	2.636377
6	−1.10678	3.725405	2.544475
6	−0.231058	3.880017	3.626625
1	0.305198	3.012485	3.999567
6	−0.047873	5.130962	4.214326
1	0.640029	5.24197	5.048664
6	−0.751877	6.240302	3.735093
1	−0.609921	7.21556	4.193247
6	−1.639296	6.090182	2.667451
1	−2.188628	6.948635	2.289965
6	−1.809905	4.837834	2.072231
1	−2.474784	4.723508	1.220459
8	−1.654696	0.114105	−0.149378
6	−2.280558	−0.027491	−1.39678
1	−1.781124	0.569018	−2.178642
1	−3.302938	0.378454	−1.314574
6	−2.381367	−1.468118	−1.878735
6	−2.426676	−1.763965	−3.246219
1	−2.355515	−0.955454	−3.971303
6	−2.547752	−3.083207	−3.689712
1	−2.576391	−3.294771	−4.755816
6	−2.614048	−4.129888	−2.765693
1	−2.697376	−5.158064	−3.10815
6	−2.564275	−3.843047	−1.399054
1	−2.608301	−4.649964	−0.671443
6	−2.453911	−2.522246	−0.962307
1	−2.405892	−2.292803	0.096129
6	0.649497	2.518335	0.218863
6	1.797834	3.431859	0.702755

6	1.581897	4.951642	0.685459
6	1.560793	5.576046	−0.720117
6	0.290347	5.286698	−1.529494
6	−0.005661	3.801239	−1.710885
1	2.662208	3.185747	0.075554
1	0.668197	5.216387	1.223294
1	2.43768	5.222025	−1.28322
1	−0.575379	5.743858	−1.032068
1	2.045449	3.107803	1.714067
1	2.412231	5.398466	1.248106
1	1.673528	6.664416	−0.627379
1	0.371079	5.749191	−2.523369
1	−0.862929	3.659417	−2.377426
1	0.846024	3.264494	−2.146565
8	1.126892	1.435691	−0.453166
8	−0.379115	3.193859	−0.466419
1	−0.366084	0.791702	6.549106
6	2.608604	0.443438	2.927419
1	2.378917	0.689512	1.88446
6	3.545685	−0.782194	2.920142
1	3.140225	−1.610898	2.336529
1	4.512086	−0.51259	2.478318
1	3.727972	−1.135489	3.942455
6	3.363565	1.641556	3.527603
1	3.792384	1.398633	4.507381
1	4.192535	1.921985	2.869147
1	2.71909	2.517819	3.651072
6	−2.101399	−1.636554	2.952352
1	−1.707064	−2.082705	2.036499
6	−2.587681	−2.785007	3.858263
1	−3.284203	−3.427044	3.306866
1	−1.759568	−3.405854	4.217063
1	−3.119274	−2.405164	4.738186
6	−3.28537	−0.740637	2.54272
1	−3.682416	−0.196306	3.408174
1	−2.978643	−0.030504	1.772399
1	−4.09559	−1.354536	2.130019

Table S31. Cartesian coordinate of **C_{ax}1c.**

The number of atom coordinates (angstroms)	**X**	**Y**	**Z**
13	0.277016	−0.110945	−0.653733

8	0.47808	−1.779598	−1.480675
8	1.405712	0.588569	−1.820673
7	0.927237	−0.833175	1.085021
6	0.932138	−2.891977	−1.045728
6	0.836659	−4.049233	−2.003655
1	1.317905	−4.953485	−1.622485
1	1.286114	−3.769769	−2.962472
1	−0.225013	−4.254573	−2.186324
6	1.447779	−3.055824	0.239783
1	1.842333	−4.028469	0.507408
6	1.412467	−2.074326	1.249421
6	1.899949	−2.530194	2.612067
1	2.346046	−1.72128	3.191545
1	1.057846	−2.919786	3.195023
1	2.627891	−3.337771	2.503363
6	0.821951	−0.00809	2.267873
6	−0.26526	−0.18055	3.152861
6	−0.363684	0.674342	4.259939
1	−1.200374	0.562384	4.943891
6	0.592294	1.653854	4.505308
6	1.668249	1.800515	3.630751
1	2.41346	2.563481	3.832363
6	1.797856	0.990701	2.497626
6	1.932536	1.854062	−2.045259
1	2.43558	2.251594	−1.149174
1	2.718754	1.775569	−2.816727
6	0.947014	2.924854	−2.504144
6	−0.382909	2.631729	−2.815322
1	−0.728533	1.60834	−2.737657
6	−1.268774	3.647371	−3.186559
1	−2.302709	3.399542	−3.415471
6	−0.833777	4.972136	−3.263654
1	−1.523008	5.761836	−3.551868
6	0.50074	5.2728	−2.972376
1	0.854127	6.299509	−3.03242
6	1.379218	4.256027	−2.596937
1	2.414052	4.498081	−2.357609
8	−1.479339	−0.015226	−0.867215
6	−2.200724	−0.643267	−1.888578
1	−1.71219	−0.526055	−2.872151
1	−3.178413	−0.13703	−1.980086
6	−2.475061	−2.130668	−1.693663

6	−2.894229	−2.912278	−2.777701
1	−2.997294	−2.45419	−3.7601
6	−3.163042	−4.273329	−2.618976
1	−3.480096	−4.865053	−3.474499
6	−3.011381	−4.8778	−1.367218
1	−3.211214	−5.939059	−1.243143
6	−2.592259	−4.104991	−0.281597
1	−2.4595	−4.563127	0.695939
6	−2.332476	−2.743695	−0.447238
1	−1.986036	−2.143651	0.382497
6	−0.694887	2.515154	0.589901
6	−0.440402	4.000434	0.54797
6	−0.31808	4.630174	1.954154
6	−1.660487	4.870882	2.657066
6	−2.501997	3.6065	2.872323
6	−2.883083	2.882812	1.584875
1	−1.238235	4.48735	−0.026876
1	0.32491	3.995158	2.575854
1	−2.246867	5.589898	2.066628
1	−1.972897	2.892564	3.515762
1	0.480403	4.134144	−0.018647
1	0.199974	5.589238	1.840505
1	−1.473777	5.345572	3.628084
1	−3.433541	3.875569	3.38618
1	−3.689302	2.16925	1.757506
1	−3.19546	3.574255	0.794358
8	0.170304	1.724691	0.20945
8	−1.816271	2.035917	1.085277
1	0.504244	2.298933	5.375809
6	2.973998	1.182787	1.545009
1	2.666962	0.819276	0.561038
6	4.19145	0.345396	1.981974
1	3.965329	−0.724629	1.97956
1	5.033055	0.509711	1.298689
1	4.513263	0.624095	2.993117
6	3.373815	2.658238	1.379448
1	3.828761	3.068178	2.288944
1	4.112608	2.755842	0.576373
1	2.50654	3.274862	1.122135
6	−1.327183	−1.25956	2.958306
1	−0.977448	−1.942544	2.180054
6	−1.544884	−2.096761	4.233581

1	−2.199211	−2.948574	4.01471
1	−0.601925	−2.483567	4.635529
1	−2.025723	−1.510611	5.025364
6	−2.661299	−0.661772	2.472599
1	−3.033198	0.080705	3.190228
1	−2.535716	−0.180408	1.500745
1	−3.418086	−1.44995	2.37882

Table S32. Cartesian coordinate of **C_{ax}TS1c.**

The number of atom coordinates (angstroms)	X	Y	Z
13	0.777623	0.111364	−0.380736
8	0.569348	−1.48934	−1.325597
8	2.14914	0.632858	−1.355941
7	1.353148	−0.862972	1.220991
6	1.374236	−2.496983	−1.207527
6	1.379221	−3.448429	−2.374998
1	2.040921	−4.304042	−2.21985
1	1.691264	−2.909797	−3.277215
1	0.359325	−3.810129	−2.553772
6	2.14822	−2.733823	−0.08149
1	2.779044	−3.614717	−0.07218
6	2.036878	−2.00032	1.12881
6	2.689032	−2.624146	2.34315
1	2.850972	−1.905099	3.146008
1	2.052643	−3.426754	2.733197
1	3.644653	−3.075491	2.060003
6	1.078232	−0.313671	2.528523
6	−0.011884	−0.820405	3.266195
6	−0.280006	−0.255778	4.520037
1	−1.116711	−0.632414	5.102325
6	0.504091	0.771968	5.032842
6	1.571863	1.262238	4.285044
1	2.1826	2.064959	4.68854
6	1.872149	0.74323	3.021502
6	2.576975	1.94775	−1.568068
1	2.699459	2.501396	−0.625411
1	3.57291	1.917969	−2.042617
6	1.642769	2.750268	−2.462135
6	0.823241	2.108378	−3.398334
1	0.872602	1.026687	−3.479319
6	−0.062594	2.841175	−4.191117

1	−0.700671	2.326301	−4.905545
6	−0.135483	4.230976	−4.064809
1	−0.830497	4.801502	−4.675467
6	0.690803	4.882106	−3.14444
1	0.63875	5.962618	−3.034518
6	1.571086	4.144339	−2.350144
1	2.190713	4.653045	−1.614187
8	−1.04429	0.488455	−0.693915
6	−2.029301	0.099262	−1.653739
1	−1.487652	−0.338266	−2.497901
1	−2.538295	1.000647	−2.013398
6	−3.021782	−0.890846	−1.092881
6	−4.318018	−0.497212	−0.745742
1	−4.623202	0.53617	−0.896733
6	−5.227315	−1.419354	−0.22095
1	−6.231515	−1.099457	0.044446
6	−4.846845	−2.751035	−0.047459
1	−5.553523	−3.472032	0.354851
6	−3.553193	−3.153786	−0.394555
1	−3.252585	−4.189924	−0.261493
6	−2.646333	−2.228932	−0.909355
1	−1.636512	−2.529493	−1.171042
6	−0.916363	1.867186	0.318153
6	−1.380476	3.034656	−0.532421
6	−1.364825	4.355893	0.259889
6	−2.646036	4.589612	1.074651
6	−2.925052	3.536796	2.157098
6	−2.954897	2.093723	1.654255
1	−2.386512	2.856005	−0.927883
1	−0.482217	4.374974	0.912058
1	−3.498498	4.615022	0.379361
1	−2.164421	3.588763	2.946583
1	−0.702209	3.083665	−1.381003
1	−1.241595	5.177984	−0.454713
1	−2.603142	5.580024	1.545545
1	−3.892201	3.754249	2.630106
1	−3.371673	1.431173	2.416367
1	−3.567177	1.981214	0.751528
8	0.370392	1.720267	0.508228
8	−1.628149	1.582591	1.444586
1	0.284165	1.191486	6.011334
6	3.052235	1.304471	2.236188

1	3.011851	0.899456	1.221439
6	4.391125	0.859873	2.855968
1	4.478637	−0.231717	2.885949
1	5.233096	1.249836	2.271407
1	4.491192	1.232377	3.882976
6	2.986054	2.837306	2.117184
1	3.093768	3.327512	3.092255
1	3.799622	3.200263	1.477474
1	2.032306	3.138644	1.676593
6	−0.909655	−1.944319	2.754669
1	−0.539865	−2.266758	1.776886
6	−0.87781	−3.166494	3.69292
1	−1.453713	−3.993219	3.26014
1	0.144328	−3.517482	3.870808
1	−1.319142	−2.930099	4.66841
6	−2.356855	−1.46085	2.550963
1	−2.775979	−1.06507	3.484316
1	−2.393454	−0.676397	1.794289
1	−2.993203	−2.285586	2.215555

Table S33. Cartesian coordinate of **C_{ax}2c.**

The number of atom coordinates (angstroms)	X	Y	Z
13	0.584859	0.298107	0.180144
8	0.181982	−1.173617	−0.825917
8	1.926984	1.145455	−0.555826
7	1.586361	−0.787925	1.482054
6	1.012027	−2.162778	−1.019827
6	0.726935	−2.972241	−2.255243
1	1.437554	−3.789776	−2.397344
1	0.748686	−2.312098	−3.130305
1	−0.288189	−3.382434	−2.193292
6	2.050524	−2.478506	−0.164265
1	2.675832	−3.325999	−0.416732
6	2.245544	−1.872941	1.112716
6	3.192111	−2.55323	2.074406
1	3.86935	−1.825609	2.531341
1	2.630921	−3.019167	2.891563
1	3.777468	−3.326029	1.572117
6	1.622223	−0.374854	2.864318
6	0.690948	−0.944692	3.759155
6	0.704001	−0.51082	5.089416

1	−0.007933	−0.934286	5.792832
6	1.601614	0.461416	5.523463
6	2.499099	1.023245	4.620288
1	3.187347	1.793537	4.957634
6	2.526367	0.622901	3.278394
6	1.946715	2.287515	−1.359645
1	1.429236	3.136634	−0.88118
1	2.995605	2.607079	−1.480826
6	1.342747	2.071473	−2.738759
6	1.456787	0.826668	−3.370648
1	1.981113	0.026974	−2.857314
6	0.882645	0.609487	−4.623957
1	0.972011	−0.36498	−5.09847
6	0.189607	1.639054	−5.268421
1	−0.265346	1.468199	−6.240465
6	0.084458	2.888041	−4.652152
1	−0.455649	3.693796	−5.143157
6	0.657284	3.098963	−3.395437
1	0.55204	4.067127	−2.909275
8	−1.023195	1.230531	−0.676753
6	−1.847582	1.31503	−1.848673
1	−1.188196	0.990143	−2.656506
1	−2.092802	2.367292	−2.032329
6	−3.100277	0.469025	−1.812972
6	−4.303702	0.994137	−2.292814
1	−4.337649	2.022128	−2.648633
6	−5.46444	0.215232	−2.314095
1	−6.393173	0.638186	−2.688227
6	−5.429324	−1.097257	−1.843097
1	−6.330793	−1.704398	−1.848879
6	−4.227114	−1.626999	−1.360824
1	−4.19486	−2.648475	−0.9901
6	−3.068511	−0.852934	−1.350636
1	−2.135435	−1.25836	−0.975601
6	−1.42231	1.718576	0.690547
6	−1.405183	3.248124	0.690547
6	−1.749932	3.847819	2.06456
6	−3.258374	3.989768	2.317576
6	−4.03885	2.66854	2.325895
6	−3.862882	1.826252	1.062926
1	−2.075188	3.646083	−0.081537
1	−1.282646	3.23105	2.842037

1	−3.682238	4.645006	1.541457
1	−3.73495	2.050503	3.180517
1	−0.387526	3.521963	0.400658
1	−1.29111	4.841564	2.13507
1	−3.416651	4.504355	3.274107
1	−5.108945	2.884092	2.450305
1	−4.616059	1.035425	1.016188
1	−3.97903	2.43069	0.154892
8	−0.41068	1.172516	1.405747
8	−2.618795	1.114804	1.060001
1	1.595076	0.786154	6.560828
6	3.485988	1.297137	2.305884
1	3.41518	0.788092	1.342885
6	4.949311	1.218142	2.774964
1	5.263159	0.179812	2.935605
1	5.612318	1.659274	2.021231
1	5.108066	1.762209	3.713615
6	3.056556	2.756611	2.063131
1	3.133329	3.350052	2.982886
1	3.694388	3.221275	1.301689
1	2.020964	2.797306	1.713721
6	−0.343651	−1.974458	3.314965
1	−0.154852	−2.221616	2.266429
6	−0.242494	−3.282317	4.121661
1	−0.95449	−4.021949	3.736609
1	0.761872	−3.718038	4.065985
1	−0.474964	−3.119761	5.180623
6	−1.765945	−1.386968	3.391156
1	−2.027408	−1.128576	4.425017
1	−1.846951	−0.487467	2.776197
1	−2.499553	−2.120974	3.034175

Table S34. Cartesian coordinate of **C_{ax}3c.**

The number of atom coordinates (angstroms)	X	Y	Z
13	0.078781	0.114999	0.426592
8	0.090086	−1.409709	−0.55
8	1.313077	1.289642	0.03931
7	0.948704	−0.716965	1.998153
6	0.797084	−2.488862	−0.351637
6	0.781043	−3.453585	−1.504346
1	1.348626	−4.364182	−1.297928

1	1.20013	−2.95582	−2.386564
1	−0.255796	−3.718962	−1.741995
6	1.496873	−2.747683	0.806098
1	2.031613	−3.687819	0.876093
6	1.520959	−1.907836	1.961978
6	2.250799	−2.48805	3.154391
1	3.30061	−2.65645	2.888455
1	2.209591	−1.8483	4.034074
1	1.822766	−3.4653	3.402751
6	1.014409	0.063959	3.215778
6	−0.046041	−0.027457	4.142834
6	0.057905	0.697036	5.33501
1	−0.742289	0.63303	6.066211
6	1.164987	1.496619	5.601056
6	2.185382	1.596961	4.661301
1	3.044596	2.229221	4.868699
6	2.134439	0.889891	3.452903
6	1.565448	1.927618	−1.180733
1	0.680171	2.475272	−1.543802
1	2.350039	2.684014	−1.013103
6	2.031872	0.977108	−2.274376
6	2.793446	−0.153731	−1.955194
1	3.026376	−0.354679	−0.913771
6	3.225772	−1.02676	−2.954023
1	3.813638	−1.901919	−2.687666
6	2.903244	−0.781026	−4.292191
1	3.235402	−1.463512	−5.070098
6	2.150485	0.348048	−4.621449
1	1.89126	0.547477	−5.658201
6	1.72036	1.219017	−3.617282
1	1.130616	2.095478	−3.880206
8	−2.639033	2.394901	0.265371
6	−1.625894	3.30234	0.720979
1	−1.847368	4.244651	0.205634
1	−0.633565	2.972382	0.400345
6	−1.660571	3.512629	2.218103
6	−0.481002	3.763553	2.924572
1	0.474628	3.725984	2.407319
6	−0.520482	4.038756	4.292211
1	0.405386	4.219991	4.829013
6	−1.739051	4.043956	4.972532
1	−1.768042	4.24599	6.040233

6	−2.919231	3.771538	4.275852
1	−3.871587	3.760964	4.800355
6	−2.879685	3.513489	2.905481
1	−3.791789	3.292254	2.359276
6	−2.259036	1.049552	0.187454
6	−3.556017	0.249045	0.040942
6	−3.39036	−1.151346	−0.567728
6	−3.387046	−1.162645	−2.107872
6	−2.154345	−0.535066	−2.775067
6	−1.823438	0.877631	−2.306655
1	−4.272385	0.835519	−0.545617
1	−2.47607	−1.618566	−0.184127
1	−4.291623	−0.643984	−2.4594
1	−1.270253	−1.152704	−2.587972
1	−3.955361	0.184711	1.058215
1	−4.226711	−1.773031	−0.225049
1	−3.475397	−2.200178	−2.456404
1	−2.307049	−0.503833	−3.862822
1	−1.015359	1.298246	−2.910247
1	−2.683467	1.555669	−2.361644
8	−1.457989	0.616952	1.199838
8	−1.338112	0.884304	−0.953842
1	1.225667	2.050085	6.534501
6	3.297852	1.006861	2.473552
1	3.057466	0.420411	1.585419
6	4.6001	0.452173	3.08161
1	4.480431	−0.585539	3.411438
1	5.410196	0.48466	2.343085
1	4.91754	1.041006	3.950492
6	3.486812	2.458168	1.998218
1	3.738662	3.128021	2.829175
1	4.301789	2.513136	1.265953
1	2.57258	2.813919	1.517156
6	−1.255326	−0.926355	3.912301
1	−1.234228	−1.263713	2.874344
6	−1.187987	−2.171607	4.817426
1	−2.042247	−2.832565	4.626852
1	−0.26947	−2.744379	4.646145
1	−1.210601	−1.887926	5.876739
6	−2.58	−0.169481	4.105823
1	−2.727518	0.138064	5.148046
1	−2.602827	0.721067	3.474831

1	−3.422303	−0.817079	3.831556

Table S35. Cartesian coordinate of **C_{ax}TS2c.**

The number of atom coordinates (angstroms)	X	Y	Z
13	−0.031196	0.058608	0.391858
8	0.007498	−1.50685	−0.529699
8	1.30778	1.153196	0.067111
7	0.891924	−0.778219	1.97579
6	0.926858	−2.433116	−0.437306
6	0.996555	−3.348773	−1.628003
1	1.735929	−4.144022	−1.504122
1	1.248901	−2.75471	−2.514012
1	0.010758	−3.795111	−1.803326
6	1.762083	−2.586554	0.647197
1	2.474818	−3.402996	0.627938
6	1.675243	−1.830284	1.85881
6	2.538324	−2.322474	2.999615
1	3.590984	−2.13562	2.754622
1	2.310458	−1.825766	3.942137
1	2.42215	−3.403818	3.123691
6	0.737326	−0.115799	3.248587
6	−0.351731	−0.494032	4.065178
6	−0.546618	0.189123	5.269193
6	−1.372293	−0.094042	5.915779
6	0.296634	1.230483	5.651818
1	1.362849	1.588769	4.833653
6	2.025149	2.394056	5.140011
6	1.610879	0.92591	3.622969
1	1.501008	1.935362	−1.076143
1	0.585642	2.481997	−1.358657
6	2.261566	2.700835	−0.845705
6	1.971188	1.133535	−2.281219
1	2.738547	−0.024041	−2.106467
6	2.963366	−0.355627	−1.097559
1	3.183147	−0.755658	−3.209096
6	3.775613	−1.654693	−3.056093
1	2.868144	−0.33837	−4.505586
6	3.210561	−0.910495	−5.363959
1	2.106317	0.817729	−4.689467
6	1.850037	1.14817	−5.693025
1	1.662081	1.545564	−3.58298

8	1.0606	2.440792	−3.731482
6	−2.419807	2.503626	0.788138
1	−1.261169	3.195156	1.336077
1	−0.361543	2.834988	0.834752
6	−1.183411	2.946793	2.398945
6	−1.45602	4.666761	1.10771
1	−0.844545	5.298129	0.018454
6	−0.215737	4.71511	−0.650473
1	−1.032615	6.662716	−0.207752
6	−0.548788	7.143678	−1.05371
1	−1.839702	7.40794	0.654802
6	−1.985658	8.470932	0.481923
1	−2.455975	6.784778	1.743642
6	−3.081991	7.362016	2.418897
1	−2.262526	5.42152	1.968042
6	−2.738444	4.935029	2.816232
6	−2.30798	1.164105	0.669925
6	−3.665394	0.547707	0.408547
6	−3.659124	−0.860168	−0.208071
6	−3.706596	−0.882644	−1.748107
6	−2.406956	−0.516726	−2.478527
1	−1.814565	0.842521	−2.112718
1	−4.25164	1.241609	−0.202821
1	−2.792053	−1.422719	0.15755
1	−4.513048	−0.211128	−2.079635
1	−1.641134	−1.272184	−2.276268
1	−4.141036	0.525862	1.397379
1	−4.545956	−1.388065	0.162879
1	−4.002338	−1.890616	−2.068428
1	−2.595558	−0.525495	−3.561567
1	−0.977256	1.074945	−2.782203
8	−2.558793	1.645496	−2.220345
8	−1.460728	0.538991	1.457272
1	−1.318193	0.883253	−0.78432
6	0.125657	1.755781	6.587994
1	2.823852	1.324882	2.789793
6	2.818877	0.73312	1.87346
1	4.133524	1.038275	3.550036
1	4.199186	−0.011147	3.857431
1	4.999784	1.263018	2.916059
6	4.213365	1.653983	4.454074
1	2.756978	2.799591	2.356029

1	2.77737	3.479093	3.21681
1	3.614818	3.043678	1.71762
6	1.846513	2.985474	1.781962
1	−1.277633	−1.642373	3.679785
1	−1.126971	−1.850096	2.617857
6	−0.915517	−2.918056	4.464815
1	−1.560418	−3.753355	4.16573
1	0.125141	−3.21333	4.292684
1	−1.043286	−2.759958	5.542769
6	−2.76336	−1.291953	3.86055
1	−3.034162	−1.177206	4.916747
1	−2.998242	−0.360912	3.338669
1	−3.390568	−2.09109	3.447445

Table S36. Cartesian coordinate of **C_{ax}4c.**

The number of atom coordinates (angstroms)	X	Y	Z
13	0.021267	0.328316	0.466658
8	0.594477	0.889354	−1.23079
8	−2.468802	0.818255	3.244519
7	1.834991	−0.336038	0.879042
6	1.512951	0.355481	−1.959607
6	1.495968	0.738164	−3.415093
1	0.567959	0.376533	−3.870353
1	2.349871	0.333884	−3.964294
1	1.49447	1.830836	−3.498482
6	2.490076	−0.495162	−1.449151
1	3.23324	−0.885395	−2.133649
6	2.70101	−0.710543	−0.067041
6	4.040916	−1.305346	0.315542
1	4.424977	−1.931281	−0.493939
1	4.763901	−0.497749	0.482814
1	3.993173	−1.889237	1.235117
6	2.288585	−0.349635	2.249146
6	1.886616	−1.399282	3.099872
6	2.263198	−1.356343	4.457272
6	3.018123	−0.273402	4.919263
6	3.418287	0.746218	4.061886
1	4.010305	1.567184	4.45604
6	3.075493	0.728624	2.705698
6	−3.289689	−0.136856	2.497361
1	−3.898522	−0.626623	3.262407

1	−2.641109	−0.864395	2.008872
6	−4.12931	0.61939	1.502138
6	−4.038529	0.314879	0.141428
1	−3.343604	−0.45411	−0.17728
6	−4.799046	1.023392	−0.791911
1	−4.713575	0.779505	−1.847644
6	−5.651216	2.044664	−0.368784
1	−6.238948	2.60159	−1.093811
6	−5.746307	2.352339	0.992643
1	−6.408262	3.14717	1.326118
6	−4.992559	1.639274	1.924321
1	−5.059428	1.882716	2.981824
8	−1.047247	−0.995072	−0.020672
6	−0.802804	−1.937835	−1.024298
1	0.254228	−2.255888	−1.039331
1	−1.383033	−2.84842	−0.79578
6	−1.177271	−1.498526	−2.436258
6	−1.892647	−0.323537	−2.683305
1	−2.150396	0.319998	−1.852081
6	−2.237746	0.040811	−3.987231
1	−2.787344	0.963358	−4.158852
6	−1.865143	−0.763264	−5.066728
1	−2.12811	−0.477461	−6.081879
6	−1.140945	−1.935646	−4.829901
1	−0.835787	−2.565321	−5.662149
6	−0.802128	−2.296347	−3.525159
1	−0.231381	−3.206845	−3.348741
6	−1.158932	0.832513	3.053672
6	−0.47177	1.927656	3.824456
6	−1.175823	3.299383	3.862696
6	−1.01374	4.248731	2.654853
6	−1.785546	3.919413	1.355296
6	−0.985528	3.090585	0.347311
1	0.54827	1.993837	3.448247
1	−2.242688	3.144727	4.061879
1	0.053477	4.366473	2.426124
1	−2.710626	3.379775	1.59552
1	−0.402564	1.542537	4.853483
1	−0.776117	3.824548	4.739971
1	−1.351269	5.232676	3.007672
1	−2.084659	4.857245	0.866032
1	−1.600409	2.898937	−0.546881

1	−0.103946	3.666259	0.01441
8	−0.569552	−0.065523	2.43383
8	−0.594103	1.899718	0.966207
1	3.300934	−0.231425	5.968751
6	3.529332	1.857606	1.781303
1	3.429518	1.517876	0.746987
6	2.620314	3.091814	1.920528
1	2.6301	3.471005	2.950226
1	2.960404	3.898096	1.259109
1	1.590304	2.8414	1.654222
6	5.006895	2.232608	1.990616
1	5.323733	2.949464	1.224412
1	5.175325	2.702949	2.96608
1	5.657758	1.35281	1.927453
6	1.057165	−2.556031	2.571942
1	0.368137	−2.887643	3.355829
1	0.426395	−2.221577	1.746919
6	1.89663	−3.75795	2.101529
1	2.604476	−4.087914	2.870595
1	1.247043	−4.605138	1.852905
1	2.471511	−3.509195	1.2042
6	1.841006	−2.437531	5.427882
1	0.752159	−2.449574	5.568353
1	2.12615	−3.438056	5.08381
1	2.298174	−2.279861	6.409647

Table S37. Cartesian coordinate of **L_{ax}1a.**

The number of atom coordinates (angstroms)	X	Y	Z
13	0.262125	1.030969	−0.416931
8	−1.032341	2.039628	−1.308447
8	−0.350145	−0.559267	−0.926117
7	−0.255679	1.815554	1.321494
6	−3.015389	3.186476	−1.88893
1	−2.478302	3.785743	−2.632364
1	−3.823124	3.781062	−1.455726
1	−3.448014	2.327067	−2.413417
6	−2.04489	2.686684	−0.851794
6	−2.248997	2.932945	0.500865
1	−3.131693	3.489384	0.788097
6	−1.365381	2.540574	1.525279
6	−1.719575	2.987037	2.928193

1	−0.880479	3.507972	3.399371
1	−2.587533	3.648484	2.918155
1	−1.949487	2.121162	3.558012
6	0.579641	1.56663	2.469051
6	1.71567	2.352341	2.677572
6	2.57484	2.072385	3.741035
1	3.460689	2.683867	3.89067
6	2.303814	1.007655	4.602958
6	1.161276	0.228726	4.400476
1	0.940809	−0.600192	5.068248
6	0.30091	0.507185	3.338614
6	−1.614886	−0.803511	−1.481447
1	−1.804478	−0.177625	−2.366907
1	−1.641277	−1.850646	−1.828684
6	−2.7551	−0.594216	−0.49273
6	−2.545658	−0.752115	0.882067
1	−1.552224	−1.013649	1.231496
6	−3.58192	−0.543271	1.793197
1	−3.397394	−0.661412	2.858658
6	−4.852069	−0.178663	1.340335
1	−5.659136	−0.009039	2.048221
6	−5.075962	−0.030954	−0.030784
1	−6.059516	0.256168	−0.394315
6	−4.033766	−0.236846	−0.93687
1	−4.211883	−0.106457	−2.002781
8	1.649085	1.757601	−1.214872
6	2.672773	1.106565	−1.909206
1	2.326753	0.168713	−2.380541
1	2.995212	1.751071	−2.74486
6	3.903139	0.791381	−1.065659
6	4.746645	−0.274799	−1.402506
1	4.506057	−0.901456	−2.258959
6	5.887829	−0.553403	−0.643843
1	6.524809	−1.391286	−0.914618
6	6.189913	0.228188	0.474473
1	7.072876	0.011207	1.070473
6	5.343736	1.285283	0.824389
1	5.561539	1.88782	1.702808
6	4.214139	1.566094	0.056516
1	3.537534	2.365948	0.335048
6	2.284318	−1.128129	0.722762
6	2.052931	−2.281189	−0.231812

6	4.202746	−3.19001	0.443524
6	4.102563	−2.373049	1.725067
1	1.764034	−1.848127	−1.188654
1	5.090788	−1.936738	1.876155
8	1.593403	−0.123121	0.709489
8	3.225119	−1.221816	1.646101
1	2.976332	0.787164	5.427357
8	5.126874	−3.949955	0.276712
8	3.249514	−3.051113	−0.492954
6	3.711131	−3.22848	2.927013
1	4.450556	−4.022167	3.061217
1	2.725956	−3.683838	2.791996
1	3.686762	−2.600219	3.821375
6	0.92774	−3.189122	0.26574
1	1.144671	−3.598964	1.256588
1	0.810467	−4.017324	−0.438236
1	0.005383	−2.607224	0.295464
1	1.923258	3.167315	1.990913
1	−0.581523	−0.101062	3.163562

Table S38. Cartesian coordinate of **L$_{ax}$TS1a.**

The number of atom coordinates (angstroms)	X	Y	Z
13	1.228224	0.116953	1.217193
8	1.592918	1.424072	−0.022912
8	−0.091897	−0.931106	0.706947
7	0.311248	1.434025	2.400665
6	1.460019	3.302632	−1.450211
1	2.551402	3.336164	−1.546763
1	1.059617	4.317319	−1.510291
1	1.072879	2.717273	−2.291226
6	1.089363	2.612328	−0.165811
6	0.273074	3.216087	0.768907
1	−0.128475	4.193479	0.535378
6	−0.113036	2.629936	2.001332
6	−1.070332	3.432186	2.858024
1	−0.558749	3.87117	3.720735
1	−1.518379	4.23924	2.275282
1	−1.865749	2.79152	3.249208
6	−0.110323	0.961191	3.691139
6	0.425363	1.513765	4.85884
6	0.033431	1.030642	6.107771

1	0.455412	1.467555	7.008982
6	−0.887624	−0.015304	6.199417
6	−1.405002	−0.582274	5.031862
1	−2.111635	−1.405978	5.092788
6	−1.01693	−0.102025	3.780777
6	−0.814647	−0.898506	−0.501904
1	−0.162025	−1.085309	−1.364107
1	−1.546819	−1.722315	−0.479597
6	−1.562855	0.406882	−0.722236
6	−2.42549	0.906769	0.26289
1	−2.553076	0.350207	1.186543
6	−3.104248	2.110044	0.0761
1	−3.768005	2.483166	0.852371
6	−2.931763	2.837198	−1.106091
1	−3.458652	3.776712	−1.252308
6	−2.078267	2.347869	−2.095417
1	−1.934642	2.907087	−3.016902
6	−1.398948	1.14139	−1.901067
1	−0.725112	0.765655	−2.667263
8	2.824766	−0.740918	0.746444
6	3.529552	−0.8307	−0.485487
1	4.351567	−1.547078	−0.354839
1	3.97778	0.147282	−0.700705
6	2.662439	−1.260053	−1.651307
6	2.222468	−2.585671	−1.766781
1	2.525035	−3.315917	−1.021835
6	1.408883	−2.973331	−2.832086
1	1.074209	−4.004602	−2.908449
6	1.031047	−2.041659	−3.803501
1	0.39986	−2.34443	−4.634765
6	1.470468	−0.720156	−3.700147
1	1.184544	0.010361	−4.453038
6	2.276056	−0.333687	−2.626183
1	2.601145	0.697961	−2.533388
6	2.633838	−1.67762	2.428106
6	2.11418	−3.017495	1.945677
6	4.429133	−3.583469	1.48091
6	4.865276	−2.551451	2.519058
1	1.329157	−2.821448	1.216431
1	5.600513	−1.917254	2.015248
8	1.799933	−0.81017	2.823585
8	3.837157	−1.6559	3.001609

1	−1.191393	−0.392259	7.172186
8	5.265147	−4.221144	0.88329
8	3.123649	−3.780667	1.240704
6	5.504421	−3.237671	3.723697
1	6.353928	−3.839216	3.39191
1	4.783319	−3.88727	4.229458
1	5.850753	−2.480114	4.431608
6	1.574481	−3.824166	3.124349
1	2.350772	−3.997727	3.876587
1	1.207802	−4.789444	2.764929
1	0.750383	−3.276059	3.589352
1	1.156315	2.313441	4.779143
1	−1.372539	−0.563603	2.86628

Table S39. Cartesian coordinate of **L_{ax}2a.**

The number of atom coordinates (angstroms)	X	Y	Z
13	0.90318	−0.224732	1.379194
8	1.598102	0.94614	0.188421
8	−0.486247	−1.189587	0.976765
7	0.125974	1.183898	2.511531
6	1.857036	2.826922	−1.216118
1	2.949961	2.740443	−1.194128
1	1.580974	3.878493	−1.321658
1	1.504363	2.269411	−2.089966
6	1.280943	2.203815	0.024311
6	0.493312	2.926692	0.8945
1	0.270545	3.953344	0.63419
6	−0.052394	2.433385	2.113083
6	−0.861223	3.404022	2.945028
1	−0.255718	3.824012	3.755617
1	−1.218585	4.229182	2.325166
1	−1.71723	2.903742	3.405633
6	−0.331738	0.767711	3.804239
6	0.30172	1.23837	4.961012
6	−0.117302	0.798638	6.216122
1	0.381263	1.167999	7.108278
6	−1.163744	−0.120833	6.326
6	−1.782093	−0.604029	5.170833
1	−2.589155	−1.327841	5.24669
6	−1.368188	−0.167879	3.911147
6	−1.437123	−1.13856	−0.058274
1	−1.079391	−1.703986	−0.931364

1	−2.35468	−1.635934	0.293444
6	−1.783701	0.272831	−0.499286
6	−2.611968	1.081822	0.290626
1	−3.024745	0.679059	1.21291
6	−2.908615	2.39013	−0.091596
1	−3.556066	3.003257	0.530465
6	−2.378794	2.909187	−1.276767
1	−2.612329	3.926787	−1.579331
6	−1.547236	2.114573	−2.067405
1	−1.128451	2.511666	−2.988862
6	−1.248875	0.806106	−1.677646
1	−0.593099	0.192812	−2.290044
8	2.306124	−1.645339	0.584517
6	3.186111	−1.4957	−0.544513
1	3.84317	−2.371604	−0.590131
1	3.794339	−0.59538	−0.423982
6	2.345499	−1.425317	−1.793815
6	1.377197	−2.40543	−2.042635
1	1.214095	−3.187901	−1.307495
6	0.615315	−2.364322	−3.210558
1	−0.136987	−3.127225	−3.391201
6	0.817853	−1.344496	−4.145339
1	0.22438	−1.312637	−5.054949
6	1.781553	−0.363446	−3.90114
1	1.940871	0.436391	−4.619501
6	2.537692	−0.403445	−2.727434
1	3.275115	0.369384	−2.530084
6	2.823514	−1.730164	1.979264
6	2.703117	−3.186101	2.435902
6	4.912186	−3.584285	1.531622
6	5.239124	−2.110406	1.782182
1	1.731129	−3.54832	2.098615
1	5.6875	−1.764781	0.843079
8	1.980731	−0.923205	2.645064
8	4.13019	−1.245004	2.075415
1	−1.487639	−0.464934	7.304335
8	5.766428	−4.331118	1.108302
8	3.662292	−4.030431	1.73894
6	6.276077	−1.966823	2.896556
1	7.171161	−2.540144	2.642197
1	5.881678	−2.326238	3.851207
1	6.54015	−0.911517	3.00637

6	2.845999	−3.349077	3.941448
1	3.79778	−2.942194	4.294909
1	2.794902	−4.409553	4.203953
1	2.037444	−2.810403	4.440722
1	1.13	1.934188	4.864792
1	−1.815778	−0.559983	3.005281

Table S40. Cartesian coordinate of **L_{ax}3a.**

The number of atom coordinates (angstroms)	X	Y	Z
13	4.652025	−2.240079	−3.858678
8	6.401227	−2.693652	−3.776159
8	3.860932	−2.576011	−5.372491
7	5.011865	−0.338823	−4.138592
6	8.63659	−2.858906	−4.513082
1	8.964982	−3.207455	−3.526975
1	9.444251	−2.293693	−4.983804
1	8.417081	−3.750979	−5.111739
6	7.3758	−2.054088	−4.364708
6	7.285951	−0.75077	−4.815276
1	8.162602	−0.318706	−5.28185
6	6.155681	0.101641	−4.639484
6	6.313997	1.549185	−5.048388
1	5.403154	1.925167	−5.522164
1	6.506456	2.178473	−4.172488
1	7.153928	1.664174	−5.736925
6	3.928631	0.567766	−3.890273
6	4.008811	1.504395	−2.853623
6	2.931517	2.351761	−2.595721
1	2.999159	3.075727	−1.78819
6	1.768161	2.263339	−3.364159
6	1.685172	1.316734	−4.387863
1	0.779905	1.236071	−4.983396
6	2.758788	0.465392	−4.652505
6	3.366785	−3.792841	−5.868913
1	2.721418	−4.293068	−5.13533
1	2.736777	−3.573728	−6.746623
6	4.460853	−4.763981	−6.285202
6	5.699911	−4.295721	−6.739076
1	5.873282	−3.224931	−6.784745
6	6.707868	−5.190787	−7.103767
1	7.665982	−4.812092	−7.452229

6	6.489348	−6.569103	−7.022332
1	7.276688	−7.265744	−7.297788
6	5.25265	−7.044039	−6.579425
1	5.075037	−8.113793	−6.502795
6	4.247071	−6.146193	−6.214021
1	3.295095	−6.522395	−5.846326
8	2.125282	−3.553631	−1.936969
6	1.442862	−4.684906	−1.37067
1	0.439463	−4.29737	−1.164604
1	1.878958	−4.98962	−0.415248
6	1.35351	−5.857603	−2.322977
6	0.943145	−5.641766	−3.645343
1	0.707584	−4.631294	−3.966022
6	0.853944	−6.705692	−4.541309
1	0.538909	−6.525189	−5.565758
6	1.173641	−8.002688	−4.12359
1	1.111533	−8.831446	−4.823673
6	1.571116	−8.226589	−2.804869
1	1.826571	−9.228935	−2.47301
6	1.655594	−7.1579	−1.90752
1	1.988045	−7.336042	−0.88875
6	3.51504	−3.390241	−1.893611
6	4.158411	−3.706199	−0.52899
6	4.555327	−6.010162	−1.244911
6	4.644937	−5.546508	−2.695006
1	3.496097	−3.323899	0.25111
1	3.974579	−6.205981	−3.254339
8	3.777407	−2.129449	−2.300117
8	4.199122	−4.194307	−2.918816
1	0.928632	2.921988	−3.160004
8	4.764078	−7.167808	−0.95919
8	4.205432	−5.14017	−0.276475
6	6.074841	−5.725383	−3.204464
1	6.346366	−6.779521	−3.108405
1	6.776684	−5.114372	−2.632891
1	6.132602	−5.429609	−4.250878
6	5.553364	−3.117805	−0.374038
1	6.195645	−3.401944	−1.212062
1	5.994845	−3.479218	0.559131
1	5.493959	−2.028029	−0.348064
1	2.704705	−0.289151	−5.430646

1	4.909676	1.55182	−2.248645

Table S41. Cartesian coordinate of **L_{ax}TS2a.**

The number of atom coordinates (angstroms)	X	Y	Z
13	4.821561	−3.426514	−3.975671
8	6.630763	−3.840977	−4.10109
8	4.251197	−4.126542	−5.473376
7	5.1949	−1.51566	−4.308736
6	8.933784	−3.892014	−4.622352
1	9.210634	−4.290115	−3.638708
1	9.748715	−3.267911	−4.996403
1	8.798657	−4.750444	−5.290011
6	7.633435	−3.141211	−4.509759
6	7.547692	−1.792485	−4.822679
1	8.44286	−1.29304	−5.170872
6	6.364391	−1.024925	−4.733673
6	6.464887	0.422991	−5.167432
1	6.330592	1.099149	−4.317197
1	7.437326	0.625094	−5.619948
1	5.678392	0.664426	−5.889199
6	4.07114	−0.614834	−4.290673
6	3.922257	0.317896	−3.260012
6	2.814325	1.16625	−3.239131
1	2.705799	1.889368	−2.435099
6	1.848816	1.084195	−4.245374
6	1.996342	0.146435	−5.270457
1	1.246004	0.071835	−6.052939
6	3.102281	−0.703836	−5.294617
6	3.224545	−5.063708	−5.649323
1	2.270075	−4.697593	−5.239749
1	3.06625	−5.204543	−6.731825
6	3.512863	−6.425364	−5.027034
6	4.822925	−6.842081	−4.762661
1	5.645889	−6.173667	−4.994849
6	5.069886	−8.086276	−4.176909
1	6.093521	−8.390719	−3.970773
6	4.009437	−8.936973	−3.852484
1	4.20142	−9.90161	−3.38968
6	2.699907	−8.5335	−4.125376
1	1.86214	−9.176946	−3.869712
6	2.457642	−7.287973	−4.708067

1	1.433517	−6.972781	−4.891052
8	1.945157	−4.691477	−2.648701
6	1.468441	−5.741401	−1.774104
1	1.256188	−5.337899	−0.780168
1	2.258411	−6.491658	−1.683011
6	0.227454	−6.339604	−2.387581
6	−0.632677	−5.581791	−3.188836
1	−0.386274	−4.548472	−3.410968
6	−1.785638	−6.160185	−3.723551
1	−2.441725	−5.566158	−4.354039
6	−2.094606	−7.494872	−3.452933
1	−2.990961	−7.943852	−3.871814
6	−1.241852	−8.251925	−2.645837
1	−1.470512	−9.293076	−2.435207
6	−0.084197	−7.67739	−2.12025
1	0.588648	−8.275242	−1.510231
6	2.789228	−3.729008	−2.290904
6	2.996993	−3.413303	−0.806329
6	4.462992	−5.385639	−0.251672
6	5.252724	−5.331885	−1.565937
1	2.004896	−3.178601	−0.398178
1	5.205435	−6.358993	−1.958229
8	3.053933	−2.880984	−3.18486
8	4.64706	−4.454242	−2.461321
1	0.98569	1.743841	−4.228362
8	4.7325	−6.193161	0.608
8	3.394481	−4.56464	−0.025564
6	6.718521	−4.997283	−1.257281
1	7.098047	−5.675427	−0.48842
1	6.809958	−3.965046	−0.901312
1	7.307535	−5.101172	−2.168598
6	3.917336	−2.227916	−0.56847
1	4.914245	−2.428289	−0.965357
1	3.987512	−2.040603	0.506453
1	3.516684	−1.342084	−1.066093
1	4.675696	0.369836	−2.478994
1	3.218258	−1.456606	−6.068137

Table 42. Cartesian coordinate of **L$_{ax}$4a.**

The number of atom coordinates (angstroms)	**X**	**Y**	**Z**
13	4.855023	−3.511808	−4.003204

8	6.330985	−4.555138	−3.995386
8	3.913935	−3.690444	−5.427362
7	5.777421	−1.82755	−4.184879
6	8.50742	−5.327727	−4.492763
1	8.581035	−5.831665	−3.522148
1	9.499639	−4.992847	−4.802649
1	8.134809	−6.068549	−5.209885
6	7.522313	−4.197987	−4.39102
6	7.881746	−2.89446	−4.690805
1	8.89817	−2.723661	−5.023545
6	7.052104	−1.746126	−4.555469
6	7.696607	−0.411229	−4.854951
1	8.167591	0.002155	−3.955828
1	8.479489	−0.537869	−5.606836
1	6.967332	0.318296	−5.212973
6	4.999798	−0.657901	−3.895867
6	5.388152	0.232297	−2.8844
6	4.578338	1.321207	−2.565697
1	4.885253	2.005822	−1.779921
6	3.371383	1.520579	−3.241529
6	2.977229	0.62091	−4.233454
1	2.031699	0.756283	−4.750024
6	3.783741	−0.468414	−4.56247
6	2.738749	−4.400748	−5.748309
1	1.890097	−4.006981	−5.177242
1	2.524857	−4.218697	−6.813645
6	2.836105	−5.900108	−5.526249
6	4.059945	−6.57695	−5.596508
1	4.96823	−6.014598	−5.787889
6	4.118504	−7.960045	−5.40837
1	5.077799	−8.470037	−5.458111
6	2.952104	−8.686457	−5.157242
1	2.998582	−9.761753	−5.003949
6	1.726377	−8.019465	−5.092117
1	0.814611	−8.565171	−4.867693
6	1.673892	−6.637437	−5.272634
1	0.721902	−6.121756	−5.187078
8	1.275933	−4.546679	−2.622428
6	1.308368	−5.581818	−1.618544
1	0.960958	−5.189076	−0.659058
1	2.342144	−5.916859	−1.492749
6	0.425134	−6.721659	−2.061704

6	−0.759712	−6.490981	−2.769018
1	−1.019358	−5.476363	−3.054924
6	−1.582932	−7.557722	−3.131393
1	−2.494728	−7.368311	−3.691669
6	−1.238881	−8.864836	−2.774957
1	−1.881783	−9.694715	−3.055763
6	−0.062197	−9.098222	−2.060053
1	0.218533	10.111644	−1.786143
6	0.767937	−8.031433	−1.71236
1	1.694725	−8.22015	−1.17571
6	1.626383	−3.261192	−2.415068
6	1.898061	−2.720123	−1.001028
6	3.827538	−4.051978	−0.036687
6	4.768857	−3.962122	−1.243636
1	0.902852	−2.622244	−0.546789
1	5.202875	−4.971577	−1.297981
8	1.535095	−2.48877	−3.346161
8	4.095194	−3.654413	−2.433786
1	2.73775	2.365407	−2.986932
8	4.212507	−4.573968	0.987522
8	2.544048	−3.611665	−0.062496
6	5.909077	−2.983676	−0.903956
1	6.359686	−3.251472	0.055659
1	5.535411	−1.956995	−0.850484
1	6.680234	−3.029956	−1.678737
6	2.555707	−1.348697	−1.036798
1	3.49301	−1.386825	−1.588877
1	2.735341	−1.009035	−0.012456
1	1.904606	−0.635327	−1.544016
1	3.47489	−1.1864	−5.314513
1	6.310846	0.055059	−2.340877

Table S43. Cartesian coordinate of **L_{ax}5a.**

The number of atom coordinates (angstroms)	X	Y	Z
13	0.856223	−0.394274	1.391754
8	1.069247	0.473149	−0.190581
8	−0.703501	−1.164894	1.661408
7	0.388819	1.269664	2.365355
6	0.670507	1.931346	−2.002587
1	1.702656	1.79734	−2.343042
1	0.33161	2.940941	−2.247354

1	0.056679	1.201441	−2.543253
6	0.590282	1.635348	−0.529941
6	0.044143	2.545784	0.355878
1	−0.322245	3.481927	−0.047227
6	−0.003004	2.382905	1.771473
6	−0.519842	3.550324	2.585166
1	−1.200483	3.20699	3.369808
1	0.30631	4.069228	3.083218
1	−1.03887	4.269263	1.947684
6	0.392685	1.186585	3.79603
6	1.38026	1.840266	4.541708
6	1.398207	1.722713	5.931348
1	2.169408	2.231801	6.503472
6	0.436178	0.947593	6.584355
6	−0.539678	0.284205	5.836926
1	−1.286298	−0.327499	6.33673
6	−0.563706	0.397105	4.445697
6	−1.262364	−2.262883	0.994606
1	−0.622168	−3.157664	1.061834
1	−2.208443	−2.524902	1.497823
6	−1.56378	−2.000785	−0.475272
6	−1.949367	−0.725632	−0.905277
1	−1.993453	0.082422	−0.181431
6	−2.25465	−0.487722	−2.246639
1	−2.552648	0.509131	−2.563007
6	−2.181183	−1.525167	−3.181034
1	−2.414448	−1.339857	−4.226222
6	−1.795395	−2.800617	−2.76159
1	−1.720178	−3.611426	−3.481758
6	−1.486516	−3.031537	−1.418908
1	−1.173459	−4.024251	−1.100541
8	5.31498	−4.207034	−1.557179
6	4.02737	−4.406635	−2.212801
1	3.312836	−4.89546	−1.551239
1	4.277415	−5.099012	−3.021599
6	3.483732	−3.108289	−2.754208
6	2.146713	−2.754954	−2.553132
1	1.498155	−3.386911	−1.956114
6	1.641168	−1.566472	−3.084117
1	0.606747	−1.299919	−2.896366
6	2.473188	−0.726607	−3.824069
1	2.082176	0.198854	−4.237859

6	3.813924	−1.071211	−4.025544
1	4.46618	−0.415457	−4.596305
6	4.316985	−2.257407	−3.494319
1	5.36018	−2.524328	−3.64011
6	5.516599	−3.94275	−0.258487
6	4.416219	−4.138126	0.801766
6	2.57485	−2.531415	0.927389
6	3.036837	−1.862764	2.229744
1	4.780569	−3.602325	1.675392
1	4.116062	−1.65175	2.159515
8	6.629935	−3.656014	0.123829
8	2.319731	−0.689742	2.369157
1	0.452413	0.8555	7.666955
8	1.5643	−2.088667	0.384703
8	3.14352	−3.596426	0.369983
6	2.771108	−2.809892	3.419778
1	3.365699	−3.728995	3.391563
1	1.708474	−3.072056	3.447959
1	3.010988	−2.264122	4.335592
6	4.220427	−5.615248	1.129579
1	3.861277	−6.17128	0.259672
1	3.49105	−5.720247	1.937897
1	5.172489	−6.045843	1.453004
1	2.135826	2.422783	4.022891
1	−1.294924	−0.132663	3.844793

Table S44. Cartesian coordinate of **L$_{ax}$1b.**

The number of atom coordinates (angstroms)	X	Y	Z
13	0.244316	1.017588	−0.448719
8	−1.073228	2.030764	−1.300211
8	−0.372784	−0.575849	−0.938497
7	−0.251126	1.787046	1.312791
6	−3.027556	3.242254	−1.842734
1	−2.4869	3.826515	−2.595448
1	−3.808612	3.860124	−1.393566
1	−3.495057	2.3968	−2.359523
6	−2.052447	2.712698	−0.82505
6	−2.221353	2.968599	0.532007
1	−3.079654	3.553964	0.835216
6	−1.3398	2.537376	1.540391
6	−1.667344	2.96516	2.95528

1	−0.80446	3.437513	3.434913
1	−2.505668	3.663713	2.966765
1	−1.933934	2.09514	3.565114
6	0.572272	1.462268	2.445779
6	1.756414	2.169397	2.667859
6	2.640314	1.77569	3.670915
1	3.572894	2.307146	3.826021
6	2.322585	0.669629	4.45595
6	1.129813	−0.029015	4.275281
1	0.896116	−0.883098	4.902098
6	0.256142	0.375656	3.267774
6	−1.636983	−0.814156	−1.500558
1	−1.814592	−0.195262	−2.393231
1	−1.669928	−1.864307	−1.837364
6	−2.781931	−0.584794	−0.522165
6	−2.590997	−0.766136	0.852483
1	−1.609267	−1.063912	1.206087
6	−3.629838	−0.540544	1.756503
1	−3.460683	−0.679974	2.822
6	−4.884669	−0.133781	1.296231
1	−5.693665	0.049082	1.99854
6	−5.090525	0.037764	−0.074744
1	−6.061955	0.357012	−0.443946
6	−4.045601	−0.186434	−0.973644
1	−4.209597	−0.038661	−2.039464
8	1.600452	1.762336	−1.285807
6	2.627763	1.108019	−1.974614
1	2.288381	0.156406	−2.422213
1	2.935504	1.739185	−2.825639
6	3.867128	0.8245	−1.133265
6	4.688244	−0.274661	−1.41384
1	4.427838	−0.946757	−2.229136
6	5.832255	−0.529289	−0.65036
1	6.451091	−1.393609	−0.876584
6	6.161232	0.312121	0.415164
1	7.046077	0.11459	1.014887
6	5.340225	1.406322	0.706956
1	5.583494	2.059275	1.541639
6	4.206636	1.660684	−0.064278
1	3.55114	2.493023	0.168167
6	2.319498	−1.083458	0.724526
6	2.124008	−2.293232	−0.163068

6	4.25689	−3.141358	0.636222
6	4.120627	−2.236587	1.854179
1	1.873113	−1.917513	−1.155009
1	5.103238	−1.787102	2.002609
8	1.606303	−0.098702	0.634892
8	3.243144	−1.09722	1.666833
8	5.188393	−3.904735	0.545685
8	3.326288	−3.077258	−0.332152
6	3.692818	−3.002271	3.103264
1	4.413805	−3.799528	3.30168
1	2.700811	−3.44615	2.977986
1	3.667395	−2.31646	3.954349
6	0.976532	−3.164606	0.348741
1	1.154535	−3.50812	1.372253
1	0.882577	−4.037357	−0.302856
1	0.057585	−2.577437	0.303387
1	2.000768	3.004854	2.020195
1	−0.664225	−0.17191	3.092562
17	3.463123	0.123948	5.688353

Table S45. Cartesian coordinate of **L$_{ax}$TS1b.**

The number of atom coordinates (angstroms)	X	Y	Z
13	1.236028	0.121135	1.210665
8	1.599192	1.430698	−0.026308
8	−0.090429	−0.924789	0.713758
7	0.315159	1.440087	2.393973
6	1.47164	3.310831	−1.45119
1	2.563175	3.342423	−1.546063
1	1.072978	4.326161	−1.510738
1	1.084891	2.726796	−2.293301
6	1.098367	2.619652	−0.168308
6	0.281542	3.22445	0.766619
1	−0.118112	4.202523	0.533025
6	−0.108143	2.63799	1.996308
6	−1.066929	3.438288	2.852787
1	−0.557976	3.874374	3.718677
1	−1.51187	4.248142	2.271809
1	−1.865595	2.798118	3.238336
6	−0.108288	0.961189	3.678093
6	0.416615	1.509241	4.852585
6	0.033955	1.017765	6.099925

1	0.441594	1.442798	7.010809
6	−0.872892	−0.038905	6.161769
6	−1.390707	−0.614596	5.001956
1	−2.084475	−1.446	5.06819
6	−1.001623	−0.11388	3.760823
6	−0.823585	−0.896955	−0.489784
1	−0.178431	−1.09325	−1.355344
1	−1.559521	−1.71666	−0.455046
6	−1.565821	0.411365	−0.711815
6	−2.433018	0.911971	0.269018
1	−2.571962	0.35177	1.189004
6	−3.104897	2.119083	0.082004
1	−3.77303	2.49215	0.854496
6	−2.92088	2.849371	−1.096544
1	−3.442774	3.791538	−1.243286
6	−2.063277	2.359246	−2.081856
1	−1.911457	2.920503	−3.000738
6	−1.390804	1.148986	−1.887079
1	−0.714212	0.772294	−2.650265
8	2.827731	−0.740122	0.738452
6	3.526734	−0.841132	−0.496479
1	4.345363	−1.560952	−0.364996
1	3.978958	0.133276	−0.719173
6	2.650891	−1.272763	−1.654567
6	2.206608	−2.597697	−1.761193
1	2.5125	−3.325488	−1.015138
6	1.385055	−2.98773	−2.819466
1	1.04727	−4.018416	−2.889324
6	1.003522	−2.059176	−3.792456
1	0.366417	−2.363895	−4.61844
6	1.446946	−0.73837	−3.6977
1	1.158295	−0.010535	−4.452117
6	2.260438	−0.349316	−2.630619
1	2.589266	0.68183	−2.544667
6	2.645895	−1.664347	2.425645
6	2.124142	−3.007877	1.955724
6	4.437113	−3.577233	1.486285
6	4.876741	−2.539955	2.517673
1	1.335223	−2.817662	1.229131
1	5.613408	−1.910874	2.009706
8	1.812491	−0.794106	2.819923
8	3.850801	−1.637544	2.993831

8	5.270807	−4.218743	0.889882
8	3.13051	−3.774297	1.250429
6	5.514147	−3.219675	3.726854
1	6.36249	−3.82491	3.398794
1	4.792079	−3.864803	4.236842
1	5.862132	−2.458331	4.429851
6	1.590794	−3.806661	3.142713
1	2.369907	−3.973313	3.893449
1	1.224449	−4.775168	2.791861
1	0.767357	−3.257122	3.607194
1	−1.349982	−0.577227	2.844701
1	1.139401	2.316851	4.786897
17	−1.362419	−0.669133	7.735668

Table S46. Cartesian coordinate of **L_{ax}2b.**

The number of atom coordinates (angstroms)	X	Y	Z
13	0.907363	−0.209679	1.36681
8	1.595919	0.963965	0.175165
8	−0.510319	−1.136947	0.958682
7	0.142464	1.204136	2.511575
6	1.817536	2.840881	−1.243924
1	2.910404	2.752684	−1.243913
1	1.54083	3.892866	−1.342518
1	1.445136	2.28649	−2.111563
6	1.264062	2.217596	0.006563
6	0.47772	2.93841	0.880153
1	0.241293	3.960529	0.614229
6	−0.05122	2.450314	2.107102
6	−0.860822	3.423281	2.935683
1	−0.235966	3.90605	3.69541
1	−1.277033	4.204679	2.295903
1	−1.676225	2.915551	3.456864
6	−0.290239	0.788759	3.809122
6	0.3145	1.30774	4.960581
6	−0.070331	0.865868	6.224525
1	0.399356	1.265794	7.116668
6	−1.060241	−0.110911	6.3287
6	−1.660292	−0.654358	5.193814
1	−2.420524	−1.421705	5.293016
6	−1.269978	−0.204619	3.933042
6	−1.352936	−1.093059	−0.169458

1	−0.872723	−1.57541	−1.032687
1	−2.258561	−1.675426	0.061079
6	−1.760287	0.317943	−0.556231
6	−2.579472	1.073967	0.293948
1	−2.934943	0.62959	1.220744
6	−2.933512	2.382379	−0.032803
1	−3.572507	2.954334	0.63554
6	−2.470476	2.956483	−1.221249
1	−2.747537	3.975434	−1.479179
6	−1.650194	2.214665	−2.071984
1	−1.282627	2.655075	−2.995646
6	−1.295101	0.904182	−1.738144
1	−0.646325	0.331996	−2.396937
8	2.291101	−1.636892	0.587789
6	3.189598	−1.522436	−0.533882
1	3.832829	−2.408672	−0.550905
1	3.808821	−0.62882	−0.420425
6	2.366964	−1.465943	−1.794527
6	1.469273	−2.499724	−2.088114
1	1.35854	−3.321982	−1.386763
6	0.711555	−2.465495	−3.25879
1	0.014503	−3.270405	−3.474935
6	0.84873	−1.398182	−4.151622
1	0.259214	−1.371692	−5.063979
6	1.74498	−0.365945	−3.865122
1	1.855274	0.468226	−4.553031
6	2.496586	−0.399918	−2.688361
1	3.180997	0.410595	−2.456831
6	2.796262	−1.738588	1.988333
6	2.655871	−3.195179	2.436515
6	4.875389	−3.613047	1.567797
6	5.211921	−2.142403	1.823845
1	1.685226	−3.547113	2.08494
1	5.678275	−1.801042	0.891986
8	1.954893	−0.92501	2.648234
8	4.105609	−1.266372	2.097225
8	5.729387	−4.368635	1.160567
8	3.616112	−4.045461	1.748848
6	6.231384	−2.006811	2.955051
1	7.12521	−2.588595	2.715984
1	5.818187	−2.36147	3.903473
1	6.50341	−0.953873	3.067958

6	2.776729	−3.365276	3.943354
1	3.726488	−2.967296	4.311957
1	2.713859	−4.4264	4.200357
1	1.965472	−2.822918	4.434185
1	1.102196	2.04799	4.861169
1	−1.697044	−0.636923	3.035148
17	−1.551779	−0.677017	7.925015

Table S47. Cartesian coordinate of **L_{ax}3b.**

The number of atom coordinates (angstroms)	X	Y	Z
13	4.977647	−3.24924	−3.824582
8	6.752438	−3.506705	−3.603375
8	4.274996	−4.033526	−5.208855
7	5.186779	−1.423966	−4.500764
6	9.101535	−3.301302	−3.668121
1	9.190635	−3.539838	−2.601576
1	9.91049	−2.625297	−3.953633
1	9.207251	−4.244491	−4.216498
6	7.740949	−2.719809	−3.935577
6	7.588993	−1.459307	−4.480637
1	8.487155	−0.90422	−4.720454
6	6.341416	−0.828286	−4.751893
6	6.370139	0.560165	−5.349125
1	5.683773	0.628255	−6.198925
1	6.04099	1.302655	−4.614162
1	7.376251	0.825157	−5.679232
6	3.948876	−0.746027	−4.749633
6	3.486575	0.234322	−3.8652
6	2.254605	0.850182	−4.0765
1	1.891038	1.608892	−3.39209
6	1.485272	0.467729	−5.175208
6	1.922734	−0.519364	−6.057123
1	1.305652	−0.811064	−6.900021
6	3.157381	−1.129716	−5.838129
6	3.065839	−4.759311	−5.223572
1	2.322413	−4.322284	−4.540893
1	2.640516	−4.688808	−6.238047
6	3.236433	−6.226326	−4.868668
6	4.401159	−6.919174	−5.216729
1	5.193492	−6.383996	−5.731713
6	4.55568	−8.265472	−4.878736

1	5.470204	−8.788568	−5.147458
6	3.544104	−8.938984	−4.187047
1	3.669274	−9.983335	−3.913869
6	2.373791	−8.25573	−3.844758
1	1.580714	−8.762148	−3.300039
6	2.223547	−6.909671	−4.186735
1	1.319823	−6.379845	−3.899081
8	2.445309	−4.337041	−1.828381
6	1.889353	−5.430567	−1.09605
1	1.971473	−5.252079	−0.015775
1	2.420547	−6.361835	−1.322505
6	0.439332	−5.586252	−1.493488
6	−0.288304	−4.529867	−2.0511
1	0.204338	−3.579387	−2.225301
6	−1.629802	−4.707185	−2.398385
1	−2.183683	−3.88152	−2.837444
6	−2.257253	−5.936364	−2.187276
1	−3.300009	−6.072491	−2.461017
6	−1.534295	−6.993621	−1.628415
1	−2.011414	−7.95659	−1.466893
6	−0.192955	−6.819064	−1.287451
1	0.37082	−7.648327	−0.864995
6	3.78988	−3.974629	−1.707531
6	4.317998	−3.900876	−0.262974
6	4.911809	−6.278774	−0.396653
6	5.064284	−6.166675	−1.912086
1	3.559229	−3.418252	0.357738
1	4.413818	−6.935655	−2.342093
8	3.968153	−2.825478	−2.39245
8	4.658124	−4.895536	−2.441336
8	5.151565	−7.324857	0.162792
8	4.456554	−5.229829	0.318774
6	6.506476	−6.437821	−2.330822
1	6.797302	−7.432285	−1.984382
1	7.182736	−5.688665	−1.911773
1	6.574143	−6.395883	−3.419109
6	5.646471	−3.16626	−0.15784
1	6.379506	−3.594396	−0.848378
1	6.025355	−3.245541	0.864913
1	5.51053	−2.11342	−0.413226
1	3.508245	−1.920671	−6.490925
1	4.088214	0.499924	−3.001665

17	−0.076296	1.239693	−5.446088

Table S48. Cartesian coordinate of **Lax TS2b.**

The number of atom coordinates (angstroms)	X	Y	Z
13	4.824145	−3.427695	−3.968968
8	6.632935	−3.838718	−4.101346
8	4.241988	−4.110827	−5.469248
7	5.199486	−1.514948	−4.304426
6	8.939645	−3.886294	−4.605304
1	9.210366	−4.29089	−3.622641
1	9.756796	−3.259822	−4.970243
1	8.80819	−4.74023	−5.279364
6	7.638877	−3.136297	−4.495462
6	7.556104	−1.784065	−4.797947
1	8.454114	−1.282409	−5.135299
6	6.372056	−1.019068	−4.717842
6	6.471713	0.429862	−5.14772
1	6.328105	1.104732	−4.29782
1	7.447737	0.636142	−5.590236
1	5.692467	0.670694	−5.877643
6	4.071631	−0.623967	−4.299381
6	3.903821	0.313552	−3.276403
6	2.788035	1.149446	−3.256919
1	2.655411	1.878099	−2.464424
6	1.838286	1.032978	−4.271108
6	1.985175	0.098763	−5.295848
1	1.232179	0.017261	−6.072257
6	3.105348	−0.730743	−5.304155
6	3.216608	−5.050675	−5.645275
1	2.262766	−4.687534	−5.231713
1	3.056021	−5.187635	−6.727768
6	3.510507	−6.413095	−5.028042
6	4.823449	−6.832876	−4.78343
1	5.644514	−6.16616	−5.027152
6	5.076284	−8.078034	−4.202348
1	6.102112	−8.385007	−4.011615
6	4.018714	−8.926506	−3.862941
1	4.215324	−9.891929	−3.403807
6	2.706206	−8.519872	−4.116029
1	1.870884	−9.161849	−3.848945
6	2.458067	−7.273389	−4.694235

1	1.43216	−6.955972	−4.862411
8	1.948194	−4.674768	−2.633967
6	1.465403	−5.725188	−1.762046
1	1.255364	−5.32237	−0.767375
1	2.251373	−6.479695	−1.67293
6	0.221783	−6.31478	−2.378054
6	−0.638763	−5.547067	−3.169443
1	−0.391283	−4.511853	−3.381461
6	−1.794238	−6.117686	−3.706948
1	−2.450883	−5.515929	−4.329418
6	−2.105184	−7.454432	−3.44888
1	−3.003609	−7.897256	−3.869828
6	−1.252047	−8.221367	−2.651637
1	−1.482445	−9.264045	−2.450783
6	−0.09182	−7.654553	−2.123285
1	0.581147	−8.259756	−1.520709
6	2.800748	−3.721854	−2.273847
6	3.019358	−3.417038	−0.788679
6	4.47305	−5.404044	−0.25464
6	5.253023	−5.352002	−1.574785
1	2.031688	−3.176365	−0.373433
1	5.18985	−6.375694	−1.973415
8	3.067899	−2.869085	−3.163705
8	4.651219	−4.461022	−2.460268
8	4.742653	−6.216855	0.599734
8	3.411952	−4.576102	−0.017747
6	6.725166	−5.037195	−1.276546
1	7.102302	−5.723725	−0.514059
1	6.83225	−4.00786	−0.916509
1	7.305766	−5.144187	−2.192901
6	3.951122	−2.240724	−0.548888
1	4.943566	−2.446005	−0.954443
1	4.030514	−2.061898	0.526766
1	3.552933	−1.347806	−1.035881
1	4.648855	0.383664	−2.489478
1	3.228217	−1.486651	−6.073012
17	0.421394	2.083297	−4.252333

Table S49. Cartesian coordinate of **L$_{ax}$4b.**

The number of atom coordinates (angstroms)	**X**	**Y**	**Z**
13	5.095466	−3.499157	−4.17376

8	6.763416	−4.171915	−4.402403
8	4.089173	−3.874563	−5.524576
7	5.585794	−1.645864	−4.339039
6	9.065141	−4.370245	−4.890241
1	9.250383	−4.943306	−3.974145
1	9.954523	−3.786597	−5.136778
1	8.875035	−5.096611	−5.688793
6	7.846213	−3.512618	−4.700764
6	7.90094	−2.134899	−4.837897
1	8.855456	−1.699359	−5.104855
6	6.810827	−1.24012	−4.672314
6	7.085114	0.228198	−4.905195
1	7.1364	0.769741	−3.954638
1	8.033773	0.366233	−5.426892
1	6.282186	0.685378	−5.490704
6	4.532376	−0.684812	−4.15985
6	4.52127	0.159647	−3.045974
6	3.469894	1.051729	−2.849584
1	3.454231	1.70728	−1.985671
6	2.427662	1.08223	−3.775713
6	2.42002	0.241149	−4.886494
1	1.594118	0.27107	−5.588507
6	3.476248	−0.647381	−5.074759
6	2.995828	−4.763653	−5.594497
1	2.127489	−4.342219	−5.070411
1	2.714835	−4.866215	−6.654629
6	3.278665	−6.146276	−5.025188
6	4.576041	−6.671148	−4.980693
1	5.403298	−6.092234	−5.379281
6	4.818244	−7.928274	−4.419331
1	5.834401	−8.313255	−4.381347
6	3.762364	−8.687975	−3.911886
1	3.950975	−9.661818	−3.467874
6	2.460752	−8.183441	−3.979111
1	1.626634	−8.758271	−3.58544
6	2.224944	−6.923632	−4.530113
1	1.213906	−6.527949	−4.549706
8	1.544694	−4.554022	−2.543519
6	1.123445	−5.604602	−1.64752
1	0.937641	−5.203908	−0.64716
1	1.923893	−6.344952	−1.570667
6	−0.134723	−6.234968	−2.196137

6	−1.037775	−5.510153	−2.981147
1	−0.808783	−4.482368	−3.244129
6	−2.208773	−6.113714	−3.444275
1	−2.899305	−5.544025	−4.060492
6	−2.492452	−7.442412	−3.121095
1	−3.403116	−7.910885	−3.484266
6	−1.595392	−8.168437	−2.333856
1	−1.804013	−9.204899	−2.082582
6	−0.420895	−7.568124	−1.878157
1	0.282053	−8.139837	−1.276401
6	2.141126	−3.402257	−2.165801
6	2.6196	−3.24488	−0.716999
6	4.201272	−5.224144	−0.52237
6	5.126445	−4.860134	−1.6886
1	1.704523	−3.103045	−0.125517
1	5.314177	−5.8248	−2.180904
8	2.160019	−2.477994	−2.948121
8	4.545353	−3.949914	−2.577823
8	4.411848	−6.227311	0.124627
8	3.15883	−4.446813	−0.122444
6	6.450322	−4.349143	−1.089014
1	6.856547	−5.07765	−0.38141
1	6.293201	−3.397965	−0.56967
1	7.173593	−4.193333	−1.893249
6	3.504891	−2.02583	−0.512247
1	4.394019	−2.092102	−1.136811
1	3.786554	−1.959764	0.542893
1	2.955374	−1.125983	−0.797052
1	3.47552	−1.337396	−5.911351
1	5.328372	0.104565	−2.322163
17	1.089919	2.202773	−3.528906

Table S50. Cartesian coordinate of **L$_{ax}$5a.**

The number of atom coordinates (angstroms)	X	Y	Z
13	0.849442	0.849442	1.376941
8	1.060621	1.060621	−0.19927
8	−0.713645	−0.713645	1.650009
7	0.381579	0.381579	2.358735
6	0.651888	0.651888	−2.00654
1	1.684358	1.684358	−2.348036
1	0.308216	0.308216	−2.24853

1	0.040833	0.040833	−2.548052
6	0.574908	0.574908	−0.534875
6	0.024326	0.024326	0.354743
1	−0.348958	−0.348958	−0.04581
6	−0.017437	−0.017437	1.769118
6	−0.536669	−0.536669	2.585346
1	−1.182074	−1.182074	3.397404
1	0.291879	0.291879	3.044897
1	−1.095089	−1.095089	1.955154
6	0.404849	0.404849	3.785256
6	1.371458	1.371458	4.528516
6	1.423267	1.423267	5.915047
1	2.173572	2.173572	6.492769
6	0.502635	0.502635	6.552239
6	−0.458229	−0.458229	5.827916
1	−1.160989	−1.160989	6.340362
6	−0.502437	−0.502437	4.440822
6	−1.272365	−1.272365	0.98732
1	−0.634137	−0.634137	1.064039
1	−2.221099	−2.221099	1.488181
6	−1.565375	−1.565375	−0.485335
6	−1.955783	−1.955783	−0.922948
1	−2.010261	−2.010261	−0.20263
6	−2.25335	−2.25335	−2.267295
1	−2.55582	−2.55582	−2.589744
6	−2.166932	−2.166932	−3.196955
1	−2.394291	−2.394291	−4.244395
6	−1.776124	−1.776124	−2.769879
1	−1.690982	−1.690982	−3.486256
6	−1.475144	−1.475144	−1.424207
1	−1.158211	−1.158211	−1.099749
8	5.304909	5.304909	−1.53876
6	4.01909	4.01909	−2.200768
1	3.298377	3.298377	−1.543986
1	4.268266	4.268266	−3.010419
6	3.486292	3.486292	−2.74093
6	2.148389	2.148389	−2.552614
1	1.490995	1.490995	−1.966224
6	1.652695	1.652695	−3.083052
1	0.617183	0.617183	−2.905084
6	2.495571	2.495571	−3.809733
1	2.112266	2.112266	−4.22338

6	3.837213	3.837213	−3.99827
1	4.497925	4.497925	−4.558664
6	4.330435	4.330435	−3.467595
1	5.374179	5.374179	−3.603497
6	5.502162	5.502162	−0.239569
6	4.395299	4.395299	0.815696
6	2.563208	2.563208	0.928344
6	3.021105	3.021105	2.232033
1	4.758451	4.758451	1.689921
1	4.101439	4.101439	2.167612
8	6.615464	6.615464	0.148082
8	2.307729	2.307729	2.364168
8	1.557176	1.557176	0.3796
8	3.128299	3.128299	0.375506
6	2.743617	2.743617	3.42277
1	3.333387	3.333387	3.400207
1	1.679472	1.679472	3.445541
1	2.981351	2.981351	4.338792
6	4.186922	4.186922	1.145758
1	3.828405	3.828405	0.275155
1	3.45278	3.45278	1.950622
1	5.134217	5.134217	1.475074
1	2.09574	2.09574	4.013144
1	−1.219045	−1.219045	3.847528
17	0.563399	0.563399	8.307874

Table S51. Cartesian coordinate of **L_{ax}1c.**

The number of atom coordinates (angstroms)	X	Y	Z
13	0.837864	0.301025	1.087225
8	0.420948	1.524609	−0.251647
8	−0.433232	−0.890408	0.783961
7	0.474737	1.616683	2.515383
6	−0.520109	3.294296	−1.500345
1	0.347174	3.319051	−2.170287
1	−0.922744	4.304331	−1.393378
1	−1.276252	2.650783	−1.96331
6	−0.12096	2.688911	−0.18307
6	−0.330978	3.357923	1.015866
1	−0.764728	4.349042	0.972593
6	−0.023682	2.840925	2.293582
6	−0.33677	3.75284	3.463452

1	0.449095	3.729188	4.220831
1	−0.477122	4.780799	3.123293
1	−1.260173	3.427714	3.954875
6	0.682519	1.248406	3.901941
6	1.988817	1.312888	4.43262
6	2.172557	0.965503	5.774446
1	3.165523	1.017692	6.209896
6	1.106889	0.529291	6.559604
6	−0.164324	0.428011	6.004222
1	−0.986031	0.062361	6.613293
6	−0.403757	0.785871	4.670823
6	−1.080224	−1.146184	−0.435559
1	−0.362555	−1.250097	−1.262271
1	−1.588141	−2.1229	−0.3487
6	−2.123677	−0.113517	−0.828579
6	−2.774653	0.656515	0.140117
1	−2.498122	0.524528	1.180501
6	−3.743399	1.592401	−0.225423
1	−4.229465	2.192407	0.540264
6	−4.086691	1.761333	−1.569331
1	−4.840293	2.490438	−1.855572
6	−3.447609	0.989405	−2.543995
1	−3.701419	1.118371	−3.593491
6	−2.468897	0.063862	−2.173953
1	−1.954118	−0.517468	−2.936196
8	2.491061	−0.031922	0.526411
6	3.005398	0.30683	−0.744529
1	4.095692	0.156035	−0.718091
1	2.830129	1.364672	−0.987971
6	2.408826	−0.561184	−1.839348
6	2.662142	−1.940987	−1.850124
1	3.332375	−2.366431	−1.106859
6	2.057237	−2.772815	−2.792691
1	2.260336	−3.840708	−2.780727
6	1.198822	−2.231384	−3.755294
1	0.728194	−2.876555	−4.49264
6	0.952757	−0.856985	−3.764437
1	0.286258	−0.427253	−4.508291
6	1.549091	−0.031114	−2.807196
1	1.322917	1.030511	−2.789709
6	2.023813	−2.054118	2.483989
6	1.705389	−3.003239	1.348542

6	3.633737	−4.341231	1.972408
6	3.579087	−3.69723	3.353129
1	1.559944	−2.387956	0.464329
1	4.614189	−3.482561	3.625964
8	1.449477	−0.983979	2.629914
8	2.932504	−2.396007	3.384821
1	1.271667	0.256953	7.599029
6	−1.801334	0.614495	4.083395
1	−1.843509	1.16398	3.139091
6	−2.067505	−0.86803	3.756363
1	−3.075627	−0.993361	3.341759
1	−1.351642	−1.232332	3.015826
1	−1.992547	−1.481486	4.662736
6	−2.908857	1.180441	4.989969
1	−3.017946	0.59699	5.911283
1	−2.709558	2.219247	5.277255
1	−3.872329	1.148966	4.468244
6	3.173236	1.726182	3.563847
1	2.932322	1.471179	2.528129
6	3.415514	3.246184	3.622716
1	3.611463	3.570483	4.652369
1	4.281853	3.521041	3.008972
1	2.552363	3.806084	3.249132
6	4.459782	0.956048	3.904052
1	4.876864	1.251455	4.874396
1	4.274144	−0.122823	3.922404
1	5.22372	1.16151	3.145601
8	4.411881	−5.236678	1.747169
8	2.816315	−3.87248	1.015827
6	2.950033	−4.61509	4.398003
1	3.512432	−5.551653	4.435753
1	1.907102	−4.839019	4.157817
1	2.988223	−4.131011	5.377156
6	0.440904	−3.815586	1.621725
1	0.527609	−4.424382	2.526355
1	0.264969	−4.476544	0.768767
1	−0.39593	−3.121346	1.718241

Table S52. Cartesian coordinate of **L$_{ax}$TS1c.**

The number of atom coordinates (angstroms)	**X**	**Y**	**Z**
13	0.910619	0.104662	1.381513

8	1.262082	1.454627	0.162339
8	−0.436746	−0.783132	0.692767
7	0.254637	1.418518	2.705666
6	0.778918	3.256024	−1.294543
1	1.836066	3.339292	−1.570905
1	0.319201	4.246557	−1.315557
1	0.287575	2.61886	−2.039079
6	0.653072	2.591849	0.047938
6	−0.072001	3.174649	1.074774
1	−0.537743	4.133166	0.88501
6	−0.207743	2.624551	2.369887
6	−0.918319	3.472386	3.40169
1	−0.279809	3.653199	4.270706
1	−1.221769	4.432304	2.979977
1	−1.807551	2.952072	3.771829
6	0.178354	1.042559	4.101316
6	1.261828	1.361817	4.946189
6	1.198766	0.958912	6.284857
1	2.02379	1.196381	6.951359
6	0.102718	0.252985	6.774238
6	−0.953897	−0.056811	5.922685
1	−1.804793	−0.613539	6.305979
6	−0.940261	0.329726	4.577001
6	−0.817436	−0.931796	−0.649149
1	0.042427	−1.149643	−1.29796
1	−1.481069	−1.811233	−0.718633
6	−1.564707	0.259098	−1.230452
6	−2.304112	1.117599	−0.412054
1	−2.309928	0.941368	0.657995
6	−3.001125	2.19876	−0.95503
1	−3.560534	2.862623	−0.300104
6	−2.975276	2.433157	−2.331272
1	−3.514193	3.276964	−2.754583
6	−2.247836	1.574026	−3.160368
1	−2.217289	1.748668	−4.233325
6	−1.54723	0.498161	−2.611522
1	−0.96771	−0.15769	−3.256162
8	2.538947	−0.718049	0.950904
6	3.429101	−0.642121	−0.165753
1	4.273459	−1.312641	0.032979
1	3.822501	0.379589	−0.212084
6	2.78231	−1.005335	−1.485549

6	2.534644	−2.343236	−1.823652
1	2.831334	−3.133905	−1.141824
6	1.913795	−2.666224	−3.031002
1	1.726059	−3.707548	−3.279261
6	1.544675	−1.656109	−3.923692
1	1.065594	−1.908184	−4.86619
6	1.800001	−0.321708	−3.600416
1	1.515739	0.470689	−4.287763
6	2.410375	−0.001341	−2.386805
1	2.58725	1.036001	−2.124669
6	2.225633	−1.858338	2.398531
6	1.841476	−3.161035	1.720384
6	4.224339	−3.59776	1.494112
6	4.48936	−2.643394	2.656266
1	1.134485	−2.92735	0.92573
1	5.216718	−1.916161	2.281368
8	1.297679	−1.11365	2.843797
8	3.356791	−1.880492	3.121485
1	0.072992	−0.055681	7.816057
6	−2.108538	−0.045454	3.67245
1	−1.958541	0.443435	2.707202
6	−2.132403	−1.561184	3.401662
1	−2.973906	−1.816781	2.746497
1	−1.21113	−1.868338	2.903685
1	−2.243391	−2.124418	4.336677
6	−3.459658	0.433563	4.234277
1	−3.715956	−0.082913	5.166664
1	−3.455501	1.509714	4.443099
1	−4.260703	0.230238	3.513892
6	2.489716	2.116679	4.444607
1	2.341693	2.341868	3.384396
6	2.676708	3.45812	5.178383
1	2.859082	3.303946	6.248375
1	3.536853	4.000657	4.768328
1	1.794711	4.100731	5.080486
6	3.761227	1.254915	4.555164
1	3.991456	1.022522	5.602136
1	3.641216	0.310467	4.019183
1	4.621532	1.791453	4.136049
8	5.149223	−4.155959	0.950535
8	2.967071	−3.797838	1.066139
6	5.073355	−3.391164	3.851794

1	5.987789	−3.906754	3.549679
1	4.35834	−4.124919	4.236619
1	5.303727	−2.677262	4.646959
6	1.229114	−4.122261	2.735642
1	1.931874	−4.333072	3.548083
1	0.972842	−5.060599	2.236493
1	0.324311	−3.680914	3.160569

Table S53. Cartesian coordinate of **L$_{ax}$2c.**

The number of atom coordinates (angstroms)	**X**	**Y**	**Z**
13	0.771796	−0.211804	1.432724
8	1.511908	0.971574	0.279769
8	−0.650828	−1.079548	0.97391
7	0.107386	1.194417	2.644165
6	1.74193	2.867359	−1.11162
1	2.83555	2.877202	−1.024894
1	1.385538	3.890155	−1.25306
1	1.491676	2.268154	−1.991816
6	1.156112	2.220363	0.112026
6	0.352245	2.920524	0.984598
1	0.109746	3.946589	0.735957
6	−0.094402	2.439298	2.251116
6	−0.81183	3.443817	3.123245
1	−0.928008	3.100769	4.150901
1	−0.28354	4.401864	3.11852
1	−1.809332	3.618979	2.701271
6	−0.184519	0.791756	4.000461
6	0.856408	0.858842	4.953113
6	0.583256	0.430473	6.256482
1	1.364314	0.486404	7.009219
6	−0.670851	−0.065644	6.60691
6	−1.678098	−0.134139	5.649886
1	−2.655962	−0.519608	5.925779
6	−1.458623	0.290348	4.332656
6	−1.489347	−1.187729	−0.148475
1	−1.00659	−1.796196	−0.927408
1	−2.403153	−1.716472	0.160238
6	−1.870553	0.156505	−0.74173
6	−2.961079	0.880976	−0.242676
1	−3.576774	0.444665	0.539652
6	−3.270509	2.146444	−0.744311

1	−4.119788	2.695068	−0.344489
6	−2.497262	2.699549	−1.768493
1	−2.73975	3.681491	−2.166745
6	−1.418402	1.978315	−2.284622
1	−0.819434	2.395925	−3.090067
6	−1.105446	0.718306	−1.770755
1	−0.258494	0.166293	−2.165948
8	2.201238	−1.640666	0.575747
6	3.129283	−1.452352	−0.508538
1	3.802029	−2.3168	−0.543059
1	3.716599	−0.546309	−0.338682
6	2.354765	−1.364478	−1.797684
6	1.424397	−2.357359	−2.128291
1	1.238979	−3.165233	−1.426344
6	0.732157	−2.301559	−3.338327
1	0.007109	−3.073335	−3.581451
6	0.969354	−1.255583	−4.235011
1	0.428985	−1.211493	−5.176484
6	1.897275	−0.263334	−3.911326
1	2.082623	0.556623	−4.600068
6	2.581881	−0.316848	−2.694724
1	3.291435	0.464085	−2.435921
6	2.679421	−1.781137	1.972783
6	2.626769	−3.259981	2.363253
6	4.897443	−3.50504	1.56576
6	5.127282	−2.024037	1.874178
1	1.69125	−3.662601	1.973172
1	5.59868	−1.62688	0.966879
8	1.785908	−1.051427	2.659301
8	3.958552	−1.23226	2.135605
1	−0.861268	−0.396247	7.624711
6	−2.591746	0.221996	3.318134
1	−2.203657	0.573717	2.361629
6	−3.068521	−1.224405	3.101419
1	−3.870348	−1.251964	2.352748
1	−2.242396	−1.841568	2.739442
1	−3.464663	−1.661917	4.025565
6	−3.763344	1.137408	3.719227
1	−4.234247	0.800238	4.650341
1	−3.432896	2.171087	3.868545
1	−4.533234	1.135814	2.937656
6	2.229306	1.425637	4.607533

1	2.310203	1.470892	3.519324
6	2.370752	2.861323	5.149915
1	2.293574	2.874247	6.24407
1	3.344204	3.284496	4.873861
1	1.589257	3.519119	4.75347
6	3.379869	0.533067	5.099956
1	3.426601	0.488655	6.194578
1	3.267325	−0.478819	4.705893
1	4.338027	0.931885	4.746006
8	5.81419	−4.194258	1.177845
8	3.659721	−4.018384	1.673273
6	6.099893	−1.851939	3.041263
1	7.039662	−2.362654	2.816721
1	5.683173	−2.26094	3.965913
1	6.291929	−0.786133	3.191893
6	2.722029	−3.479813	3.86572
1	3.641191	−3.04679	4.270936
1	2.711802	−4.551655	4.082755
1	1.873253	−2.999206	4.357092

Table S54. Cartesian coordinate of **L$_{ax}$3c.**

The number of atom coordinates (angstroms)	X	Y	Z
13	4.869034	−3.196208	−3.85189
8	6.61806	−3.615902	−3.965925
8	3.822919	−3.894538	−5.038539
7	5.075502	−1.358307	−4.461085
6	8.962242	−3.38756	−3.795888
1	8.995262	−3.88688	−2.820017
1	9.774664	−2.659774	−3.852842
1	9.115236	−4.162111	−4.556057
6	7.609639	−2.760192	−3.99013
6	7.465633	−1.402257	−4.187643
1	8.364323	−0.796688	−4.197955
6	6.239083	−0.735531	−4.491795
6	6.351122	0.722681	−4.868881
1	5.392009	1.156798	−5.148996
1	6.75822	1.283074	−4.019129
1	7.054602	0.840186	−5.699928
6	3.857118	−0.708261	−4.890573
6	3.048686	−0.044575	−3.944614
6	1.84019	0.508801	−4.388827

1	1.205159	1.03111	−3.678814
6	1.444082	0.408383	−5.718623
6	2.260977	−0.248172	−6.635832
1	1.952062	−0.315644	−7.675111
6	3.47558	−0.822347	−6.245291
6	2.62452	−4.599607	−4.815903
1	2.104356	−4.24172	−3.916078
1	1.951364	−4.401907	−5.665963
6	2.823495	−6.100328	−4.688589
6	3.923283	−6.733882	−5.275257
1	4.644229	−6.129836	−5.817482
6	4.108009	−8.111628	−5.136404
1	4.973635	−8.588623	−5.58976
6	3.192026	−8.875793	−4.40815
1	3.342048	−9.945576	−4.289571
6	2.083071	−8.25092	−3.830009
1	1.364842	−8.831399	−3.256144
6	1.90052	−6.873745	−3.97403
1	1.044286	−6.39253	−3.508185
8	2.721404	−4.165442	−1.358579
6	2.148646	−5.349075	−0.813176
1	2.369544	−5.428313	0.260038
1	2.560783	−6.236696	−1.307125
6	0.653933	−5.330621	−1.045126
6	0.000087	−4.237373	−1.620447
1	0.572329	−3.3601	−1.899865
6	1.379846	−4.280556	−1.842024
1	1.876376	−3.425564	−2.29352
6	2.116844	−5.411892	−1.491091
1	3.188596	−5.444181	−1.667524
6	1.466492	−6.506632	−0.913271
1	2.030394	−7.394282	−0.638953
6	0.090615	−6.46469	−0.693144
1	0.413949	−7.32222	−0.252065
6	4.113259	−4.054436	−1.530756
6	4.900595	−4.136602	−0.210959
6	5.131951	−6.547553	−0.520791
6	5.072117	−6.34933	−2.032457
1	4.343609	−3.579777	0.545479
1	4.350198	−7.085063	−2.402883
8	4.330007	−2.887942	−2.176734
8	4.612591	−5.053506	−2.448248

1	0.502818	0.845099	−6.041899
6	4.359635	−1.498944	−7.287526
1	5.189074	−1.986143	−6.768615
6	3.614474	−2.597726	−8.063305
1	4.294891	−3.080671	−8.775099
1	3.24381	−3.356903	−7.371288
1	2.771491	−2.193595	−8.635823
6	4.959427	−0.451558	−8.246633
1	4.171251	0.056931	−8.814813
1	5.523688	0.314663	−7.703174
1	5.636446	−0.930182	−8.964231
6	3.462299	0.13117	−2.487273
1	4.384156	−0.429876	−2.322173
6	3.749375	1.613921	−2.178819
1	2.847491	2.226223	−2.297551
1	4.098518	1.728931	−1.14565
1	4.517667	2.021185	−2.845794
6	2.414437	−0.442582	−1.517071
1	1.451854	0.074779	−1.607662
1	2.266005	−1.509581	−1.698862
1	2.758031	−0.322713	−0.48226
8	5.328228	−7.64728	−0.055223
8	4.923148	−5.4993	0.301954
6	6.430479	−6.635055	−2.671647
1	6.725569	−7.661997	−2.441449
1	7.196581	−5.946696	−2.306708
1	6.343546	−6.513692	−3.752504
6	6.322029	−3.605516	−0.330018
1	6.846162	−4.08074	−1.163723
1	6.865519	−3.804135	0.597984
1	6.30028	−2.529638	−0.514979

Table S55. Cartesian coordinate of **L_{ax}TS2c.**

The number of atom coordinates (angstroms)	**X**	**Y**	**Z**
13	4.791073	−3.383855	−3.8334
8	6.620973	−3.742369	−3.888776
8	4.30176	−4.21982	−5.28654
7	5.116663	−1.526278	−4.405489
6	8.67206	−4.098108	−5.012849
1	9.210011	−4.175201	−4.060669
1	9.333238	−3.661951	−5.765387

1	8.405376	−5.11771	−5.31529
6	7.413797	−3.297798	−4.811196
6	7.154949	−2.154021	−5.549535
1	7.870697	−1.862164	−6.308103
6	6.080286	−1.267305	−5.291386
6	6.065652	0.012235	−6.100053
1	5.616478	0.84523	−5.558932
1	7.074805	0.287651	−6.414645
1	5.466953	−0.156591	−7.002892
6	4.193173	−0.468891	−4.063227
6	4.493766	0.331082	−2.935925
6	3.589491	1.341207	−2.587008
1	3.795266	1.975577	−1.731129
6	2.419693	1.545374	−3.317403
6	2.13797	0.736772	−4.413288
1	1.220708	0.895803	−4.973834
6	3.012165	−0.283716	−4.809219
6	3.353451	−5.211821	−5.540841
1	2.343323	−4.891677	−5.242607
1	3.312054	−5.382699	−6.630134
6	3.640043	−6.547353	−4.86358
6	4.902951	−6.851208	−4.342316
1	5.697035	−6.115363	−4.41592
6	5.137629	−8.076277	−3.711917
1	6.123283	−8.292259	−3.305869
6	4.11404	−9.020743	−3.600478
1	4.294903	−9.970378	−3.103532
6	2.855065	−8.731499	−4.133345
1	2.044385	−9.450186	−4.046799
6	2.623982	−7.505464	−4.759318
1	1.633292	−7.2802	−5.146628
8	1.960339	−4.686285	−2.730695
6	1.471351	−5.800677	−1.950237
1	1.169544	−5.465128	−0.954533
1	2.291548	−6.516247	−1.842089
6	0.308887	−6.419532	−2.686455
6	−0.43915	−5.703213	−3.625389
1	−0.168754	−4.678988	−3.860185
6	−1.511879	−6.312925	−4.280575
1	−2.079684	−5.751007	−5.017266
6	−1.851995	−7.636214	−3.994934
1	−2.684728	−8.109602	−4.507723

6	−1.112175	−8.350872	−3.048649
1	−1.365676	−9.383207	−2.823413
6	−0.035207	−7.746029	−2.401719
1	0.554214	−8.3128	−1.684935
6	2.694799	−3.687404	−2.2579
6	2.72288	−3.411206	−0.753362
6	4.317887	−5.243353	−0.072602
6	5.237328	−5.077332	−1.288417
1	1.679341	−3.276316	−0.440009
1	5.384125	−6.101151	−1.663781
8	3.012364	−2.80404	−3.100463
8	4.612365	−4.294715	−2.254281
1	1.729164	2.33334	−3.028093
6	2.657278	−1.148626	−6.015537
1	3.464902	−1.867745	−6.174569
6	1.37568	−1.968945	−5.769629
1	1.168164	−2.609135	−6.635557
1	1.489671	−2.602547	−4.888125
1	0.507605	−1.314523	−5.620998
6	2.505725	−0.301485	−7.294358
1	1.644436	0.373737	−7.224655
1	3.39057	0.314592	−7.485447
1	2.347681	−0.951264	−8.163072
6	5.774832	0.116075	−2.127866
1	5.983239	−0.961134	−2.125156
6	6.991056	0.811337	−2.776164
1	6.798147	1.883815	−2.899181
1	7.876026	0.6967	−2.138913
1	7.235468	0.393695	−3.754526
6	5.667522	0.576491	−0.66359
1	5.661319	1.670142	−0.586454
1	4.765433	0.201476	−0.173134
1	6.536404	0.218596	−0.100253
8	4.580828	−6.025683	0.811322
8	3.139919	−4.554687	0.029396
6	6.593218	−4.520183	−0.833109
1	7.014635	−5.156969	−0.050336
1	6.481303	−3.503214	−0.440949
1	7.266092	−4.487397	−1.691078
6	3.510125	−2.162791	−0.405712
1	4.54924	−2.268101	−0.718332
1	3.469447	−1.997287	0.674163

1	3.085072	−1.300218	−0.924193

Table S56. Cartesian coordinate of **L_{ax}4c.**

The number of atom coordinates (angstroms)	X	Y	Z
13	4.838081	−3.415035	−3.853415
8	6.567112	−3.962608	−4.008908
8	3.938367	−4.184026	−5.096087
7	5.140111	−1.619843	−4.456669
6	8.550514	−4.382659	−5.228655
1	9.122692	−4.509789	−4.302302
1	9.200484	−3.964344	−6.000222
1	8.216077	−5.379721	−5.538671
6	7.350042	−3.522514	−4.955809
6	7.124001	−2.344217	−5.647104
1	7.834992	−2.072504	−6.416922
6	6.100092	−1.40019	−5.354848
6	6.136956	−0.096903	−6.117946
1	5.938627	0.757171	−5.467465
1	7.099281	0.041801	−6.613833
1	5.351874	−0.107109	−6.881974
6	4.243603	−0.534391	−4.112462
6	4.555961	0.245429	−2.975384
6	3.709656	1.316128	−2.669463
1	3.923712	1.943265	−1.810889
6	2.579796	1.585793	−3.440202
6	2.272409	0.777921	−4.528266
1	1.374861	0.97698	−5.106797
6	3.094154	−0.297436	−4.889224
6	3.029878	−5.22572	−5.303575
1	2.03937	−4.950048	−4.919653
1	2.913854	−5.364144	−6.390714
6	3.416569	−6.564967	−4.691168
6	4.699678	−6.827073	−4.199024
1	5.472086	−6.069197	−4.274626
6	5.003911	−8.062523	−3.618908
1	6.003651	−8.241665	−3.230979
6	4.032354	−9.060901	−3.538228
1	4.265968	10.018715	−3.081004
6	2.755503	−8.816874	−4.052156
1	1.985598	−9.581665	−3.992558
6	2.453132	−7.581164	−4.623265

1	1.449298	−7.394087	−4.995815
8	1.705064	−4.300749	−2.492817
6	1.384757	−5.567668	−1.89485
1	1.104879	−5.445659	−0.845071
1	2.271699	−6.208682	−1.93476
6	0.24741	−6.197956	−2.665792
6	−0.470638	−5.505592	−3.64416
1	−0.217863	−4.473733	−3.862167
6	−1.493944	−6.145904	−4.349918
1	−2.039196	−5.60029	−5.115606
6	−1.814055	−7.476125	−4.07689
1	−2.607232	−7.973034	−4.628921
6	−1.107638	−8.166456	−3.086505
1	−1.349075	−9.202853	−2.865803
6	−0.083386	−7.530537	−2.388006
1	0.481544	−8.078204	−1.637063
6	2.19691	−3.228103	−1.833018
6	2.475139	−3.318413	−0.328472
6	4.29981	−5.049679	−0.1611
6	5.159619	−4.50316	−1.304419
1	1.488664	−3.354169	0.152313
1	5.479001	−5.414202	−1.830515
8	2.195434	−2.158624	−2.40599
8	4.433636	−3.652692	−2.15979
1	1.932956	2.419704	−3.180372
6	2.695485	−1.187535	−6.06176
1	3.504847	−1.896548	−6.251391
6	1.450601	−2.022825	−5.702332
1	1.221634	−2.727542	−6.510751
1	1.613259	−2.581501	−4.778887
1	0.576919	−1.375249	−5.556205
6	2.454431	−0.385869	−7.354233
1	1.58836	0.279512	−7.260542
1	3.317708	0.234492	−7.621086
1	2.255762	−1.068515	−8.188573
6	5.769547	−0.073214	−2.100236
1	5.832816	−1.165797	−2.029581
6	7.095077	0.432345	−2.707871
1	7.043357	1.511306	−2.897221
1	7.921404	0.25172	−2.010082
1	7.345962	−0.068396	−3.645033
6	5.648294	0.473203	−0.667074

1	5.781918	1.561293	−0.639924
1	4.679648	0.24198	−0.216856
1	6.43172	0.035158	−0.038477
8	4.697137	−5.980404	0.504844
8	3.068193	−4.554905	0.129455
6	6.411371	−3.828922	−0.720212
1	6.934492	−4.518953	−0.052055
1	6.14456	−2.927701	−0.159635
1	7.077937	−3.548112	−1.539608
6	3.224393	−2.098251	0.179058
1	4.166283	−1.991714	−0.355956
1	3.409395	−2.201534	1.252033
1	2.629992	−1.200335	−0.002939

Table S57. Cartesian coordinate of **L_{ax}5c.**

The number of atom coordinates (angstroms)	X	Y	Z
13	0.769012	−0.608368	1.359333
8	0.843464	0.100162	−0.303068
8	−0.685771	−1.46358	1.820611
7	0.368054	1.130329	2.243108
6	0.410175	1.461058	−2.185523
1	1.407188	1.238073	−2.57929
1	0.119227	2.474086	−2.47414
1	−0.287554	0.745398	−2.634479
6	0.410354	1.267498	−0.69477
6	−0.012178	2.269297	0.154086
1	−0.341266	3.201076	−0.291176
6	0.010935	2.213796	1.579349
6	−0.400482	3.489356	2.282362
1	−0.2945	3.429622	3.364665
1	0.197939	4.327205	1.909343
1	−1.447019	3.710675	2.04288
6	0.421289	1.143044	3.687005
6	1.647036	1.448031	4.320486
6	1.694454	1.413413	5.718675
1	2.624698	1.656771	6.22419
6	0.571816	1.081586	6.473098
6	−0.626853	0.789008	5.830735
1	−1.504862	0.54345	6.421908
6	−0.730752	0.813096	4.433408
6	−1.419812	−2.402444	1.077293

1	−0.859367	−3.340514	0.941838
1	−2.326091	−2.652165	1.651968
6	−1.829871	−1.873541	−0.28685
6	−2.571436	−0.687372	−0.378878
1	−2.851358	−0.168164	0.534371
6	−2.935105	−0.167357	−1.620017
1	−3.509115	0.754284	−1.674598
6	−2.560943	−0.829503	−2.794759
1	−2.846163	−0.427221	−3.76347
6	−1.815433	−2.007526	−2.714518
1	−1.512244	−2.524215	−3.621845
6	−1.449962	−2.520726	−1.466183
1	−0.851424	−3.426527	−1.406351
8	5.528583	−3.507081	−0.993994
6	4.578383	−4.039097	−1.971981
1	3.826541	−4.66433	−1.497861
1	5.194126	−4.658699	−2.63018
6	3.932609	−2.907171	−2.723817
6	2.569159	−2.639376	−2.567911
1	1.973235	−3.235036	−1.88542
6	1.971619	−1.586459	−3.263217
1	0.916459	−1.382947	−3.113156
6	2.736547	−0.797308	−4.122734
1	2.27314	0.021109	−4.667652
6	4.102238	−1.05722	−4.281431
1	4.700291	−0.442511	−4.948724
6	4.696915	−2.108217	−3.585661
1	5.75866	−2.310353	−3.703889
6	5.474836	−3.654713	0.33554
6	4.327935	−4.416474	1.028654
6	2.449525	−2.869682	0.985624
6	2.914476	−2.106407	2.231745
1	4.431049	−4.167085	2.082623
1	4.008336	−1.989408	2.199946
8	6.368373	−3.206227	1.022153
8	2.297762	−0.869085	2.218717
1	0.63013	1.059105	7.558353
6	−2.081375	0.532324	3.782963
1	−1.936101	0.506504	2.701963
6	−2.634947	−0.845643	4.184755
1	−3.566925	−1.048523	3.642429
1	−1.913682	−1.625635	3.931795

1	−2.858975	−0.897721	5.257209
6	−3.095194	1.645159	4.112462
1	−3.302788	1.685752	5.188651
1	−2.727332	2.631048	3.809136
1	−4.045426	1.461975	3.595869
6	2.882818	1.872517	3.534539
1	2.709908	1.63816	2.482749
6	3.103981	3.393415	3.656365
1	3.289606	3.67909	4.699157
1	3.970754	3.705412	3.061134
1	2.232018	3.957068	3.308051
6	4.145878	1.106474	3.960632
1	4.449997	1.352116	4.985231
1	3.976664	0.029363	3.893963
1	4.981805	1.365368	3.299987
8	1.462261	−2.462244	0.384811
8	3.023242	−3.997225	0.545954
6	2.506216	−2.898327	3.494896
1	2.990262	−3.877207	3.580646
1	1.420111	−3.034717	3.495857
1	2.77465	−2.293901	4.365209
6	4.419348	−5.929564	0.870052
1	4.327925	−6.245927	−0.171188
1	3.621419	−6.401615	1.450342
1	5.384383	−6.272232	1.255172