Electronic Supplementary Material (ESI) for RSC Advances.
This journal is © The Royal Society of Chemistry 2016

Fractional coordinates and lattice parameters of all the optimized structures and transition states (TS) all listed as following,

1. Single-layer graphyne, P6/*MMM*, hexagonal, *a*=0.689 Å, *b*=0.689 Å, *c*=0.810 Å, α=90°, β=90°, γ=60°

Element	Atom Number	Fractional coordinates of atoms u	v	w
C	1	1.588275	1.588275	0.500000
C	2	1.794320	1.794320	0.500000
C	3	-1.588275	0.000000	0.500000
C	4	-1.794320	-0.000000	0.500000
C	5	0.000000	-1.588275	0.500000
C	6	0.000000	-1.794320	0.500000
C	7	-1.588275	-1.588275	0.500000
C	8	-1.794320	-1.794320	0.500000
C	9	1.588275	-0.000000	0.500000
C	10	1.794320	-0.000000	0.500000
C	11	0.000000	1.588275	0.500000
C	12	-0.000000	1.794320	0.500000

2. Single-layer graphdiyne, P6/MMM, hexagonal, *a*=0.945 Å, *b*=0. 945 Å, *c*=0.833 Å, α=90°, β=90°, γ=60°

Element	Atom Number	Fractional coordinates of atoms u	v	w
C	1	0.571058	0.571058	-0.500000
C	2	0.700951	0.700951	-0.500000
C	3	0.849317	0.849317	-0.500000
C	4	-0.571058	0.000000	-0.500000
C	5	-0.700951	0.000000	-0.500000
C	6	-0.849317	0.000000	-0.500000
C	7	-0.000000	-0.571058	-0.500000
C	8	0.000000	-0.700951	-0.500000
C	9	-0.000000	-0.849317	-0.500000
C	10	-0.571058	-0.571058	-0.500000
C	11	-0.700951	-0.700951	-0.500000
C	12	-0.849317	-0.849317	-0.500000
C	13	0.571058	0.000000	-0.500000
C	14	0.700951	-0.000000	-0.500000
C	15	0.849317	0.000000	-0.500000
C	16	0.000000	0.571058	-0.500000

C	17	0.000000	0.700951	-0.500000
C	18	-0.000000	0.849317	-0.500000

3. Double-layers graphyne, P6/MMM, hexagonal, *a*=0.685 Å, *b*=0. 685 Å, *c*=0.656 Å, α=90°, β=90°, γ=60°

Element	Atom Number	Fractional coordinates of atoms u	v	w
C	1	-0.755342	-0.170225	-0.250000
C	2	-0.958226	-0.171158	-0.250000
C	3	-0.166554	-0.581364	-0.250000
C	4	-0.165715	-0.378344	-0.250000
C	5	-0.577232	0.240121	-0.250000
C	6	-0.372482	0.035784	-0.250000
C	7	-0.576240	-0.171661	-0.250000
C	8	-0.373239	-0.170786	-0.250000
C	9	-0.165002	-0.760564	-0.250000
C	10	-0.165876	-0.963497	-0.250000
C	11	-0.754807	0.417524	-0.250000
C	12	-0.959099	0.622290	-0.250000
C	13	0.755342	0.170225	0.250000
C	14	0.958226	0.171158	0.250000
C	15	0.166554	0.581364	0.250000
C	16	0.165715	0.378344	0.250000
C	17	0.577232	-0.240121	0.250000
C	18	0.372482	-0.035784	0.250000
C	19	0.576240	0.171661	0.250000
C	20	0.373239	0.170786	0.250000
C	21	0.165002	0.760564	0.250000
C	22	0.165876	0.963497	0.250000
C	23	0.754807	-0.417524	0.250000
C	24	0.959099	-0.622290	0.250000

4. Double-layers graphdiyne, P6/MMM, hexagonal, *a*=0.943 Å, *b*=0. 943 Å, *c*=0.697 Å, α=90°, β=90°, γ=60°

Element	Atom Number	Fractional coordinates of atoms u	v	w
C	1	0.762105	0.250000	0.833918
C	2	0.631335	0.250000	0.833708
C	3	0.484571	0.250000	0.833227
C	4	0.333294	0.250000	0.404010

C	5	0.331965	0.250000	0.535525
C	6	0.332516	0.250000	0.682223
C	7	0.903074	0.250000	0.262810
C	8	0.033667	0.250000	0.133299
C	9	0.181448	0.250000	0.985406
C	10	0.903093	0.250000	0.834034
C	11	0.033630	0.250000	0.834653
C	12	0.180609	0.250000	0.834631
C	13	0.333899	0.250000	0.262701
C	14	0.333329	0.250000	0.132131
C	15	0.332586	0.250000	0.985548
C	16	0.761170	0.250000	0.404123
C	17	0.631262	0.250000	0.534300
C	18	0.483691	0.250000	0.682369
C	19	-0.762105	0.750000	-0.833918
C	20	-0.631335	0.750000	-0.833708
C	21	-0.484571	0.750000	-0.833227
C	22	-0.333294	0.750000	-0.404010
C	23	-0.331965	0.750000	-0.535525
C	24	-0.332516	0.750000	-0.682223
C	25	-0.903074	0.750000	-0.262810
C	26	-0.033667	0.750000	-0.133299
C	27	-0.181448	0.750000	-0.985406
C	28	-0.903093	0.750000	-0.834034
C	29	-0.033630	0.750000	-0.834653
C	30	-0.180609	0.750000	-0.834631
C	31	-0.333899	0.750000	-0.262701
C	32	-0.333329	0.750000	-0.132131
C	33	-0.332586	0.750000	-0.985548
C	34	-0.761170	0.750000	-0.404123
C	35	-0.631262	0.750000	-0.534300
C	36	-0.483691	0.750000	-0.682369

5. One Na absorbed on the B site of single-layer graphyne, P6/MMM, hexagonal, *a*=0.689 Å, *b*=0. 689 Å, *c*=0.444 Å, α=90°, β=90°, γ=60°

Element	Atom Number	Fractional coordinates of atoms u	v	w
C	1	0.590857	0.590857	0.488960
C	2	0.790768	0.790768	0.489050
C	3	-0.590857	0.000000	0.488960
C	4	-0.790768	0.000000	0.489050
C	5	0.000000	-0.590857	0.488960

C	6	-0.000000	-0.790768	0.489050
C	7	-0.590857	-0.590857	0.488960
C	8	-0.790768	-0.790768	0.489050
C	9	0.590857	0.000000	0.488960
C	10	0.790768	-0.000000	0.489050
C	11	0.000000	0.590857	0.488960
C	12	0.000000	0.790768	0.489050
Na	1	0.000000	1.000000	0.945604

6. Two Na absorbed on the A sites of single-layer graphyne, P6/MMM, hexagonal, *a*=0.689 Å, *b*=0. 689 Å, *c*=0.384 Å, α=90°, β=90°, γ=60°

Element	Atom Number	Fractional coordinates of atoms u	v	w
C	1	0.593367	0.590032	0.453553
C	2	0.792200	0.789100	0.453136
C	3	0.411058	-0.001487	0.453358
C	4	0.211015	-0.000784	0.453380
C	5	0.001497	0.408049	0.454441
C	6	0.002046	0.207942	0.453682
C	7	0.411421	0.408706	0.452864
C	8	0.212522	0.209671	0.453509
C	9	0.593721	0.000359	0.452386
C	10	0.793697	-0.000452	0.452957
C	11	0.003279	0.590705	0.452550
C	12	0.002673	0.790795	0.453028
Na	1	0.337901	0.664018	0.954366
Na	2	0.667130	0.334765	0.953179

7. Six Na absorbed on the A and B sites of double-layer graphyne, P6/MMM, hexagonal, *a*=0.692 Å, *b*=0. 692 Å, *c*=0.773 Å, α=90°, β=90°, γ=60°

Element	Atom Number	Fractional coordinates of atoms u	v	w
C	1	0.226667	0.862445	0.740942
C	2	0.040499	0.831370	0.742525
C	3	0.790536	0.439323	0.743379
C	4	0.830733	0.620452	0.742813
C	5	0.424197	0.244107	0.743428
C	6	0.618846	0.042936	0.742971
C	7	0.439877	0.790206	0.743291
C	8	0.621085	0.830136	0.742777

C	9	0.862789	0.226112	0.741169
C	10	0.831655	0.040047	0.742643
C	11	0.244337	0.423838	0.743529
C	12	0.043345	0.618553	0.743005
C	13	0.755429	0.172141	0.239210
C	14	0.957056	0.169372	0.243532
C	15	0.170420	0.576343	0.244294
C	16	0.165603	0.378517	0.241886
C	17	0.574488	0.755829	0.245697
C	18	0.378240	0.956572	0.243835
C	19	0.575082	0.171375	0.243999
C	20	0.377169	0.166767	0.241863
C	21	0.170993	0.756752	0.238633
C	22	0.168423	0.958137	0.243406
C	23	0.754814	0.575502	0.245593
C	24	0.955528	0.379262	0.243782
Na	1	0.496823	0.496850	0.495257
Na	2	0.835735	0.836392	0.453055
Na	3	0.169223	0.169880	0.533448
Na	4	0.496193	0.496691	0.990554
Na	5	0.832195	0.832936	1.032690
Na	6	0.166898	0.166764	0.952169

8. One Na absorbed on the B site of single-layer graphdiyne, P6/MMM, hexagonal, *a*=0.948 Å, *b*=0. 948 Å, *c*=0.459 Å, α=90°, β=90°, γ=60°

Element	Atom Number	Fractional coordinates of atoms u	v	w
C	1	1.570469	1.570469	0.500263
C	2	1.700454	1.700454	0.501091
C	3	1.847478	1.847478	0.501956
C	4	-1.570469	0.000000	0.500263
C	5	-1.700454	0.000000	0.501091
C	6	-1.847478	0.000000	0.501956
C	7	-0.000000	-1.570469	0.500263
C	8	-0.000000	-1.700454	0.501091
C	9	-0.000000	-1.847478	0.501956
C	10	-1.570469	-1.570469	0.500263
C	11	-1.700454	-1.700454	0.501091
C	12	-1.847478	-1.847478	0.501956
C	13	1.570469	-0.000000	0.500263
C	14	1.700454	-0.000000	0.501091
C	15	1.847478	-0.000000	0.501956

C	16	0.000000	1.570469	0.500263
C	17	0.000000	1.700454	0.501091
C	18	0.000000	1.847478	0.501956
Na	1	1.000000	1.000000	1.002008

9. One Na absorbed on the A site of single-layer graphdiyne, P6/MMM, hexagonal, *a*=0.944 Å, *b*=0. 944 Å, *c*=0.823 Å, α=90°, β=90°, γ=60°

Element	Atom Number	Fractional coordinates of atoms u	v	w
C	1	0.568880	0.569362	0.503154
C	2	0.700657	0.700171	0.502715
C	3	0.847240	0.845619	0.502582
C	4	0.426578	-0.006452	0.503019
C	5	0.295392	-0.006119	0.502973
C	6	0.150467	-0.002262	0.502801
C	7	0.002428	0.429363	0.503199
C	8	0.000429	0.296792	0.503131
C	9	-0.001323	0.149938	0.502952
C	10	0.428157	0.428600	0.503529
C	11	0.297224	0.296933	0.503331
C	12	0.151833	0.150253	0.502990
C	13	0.567643	-0.005958	0.503046
C	14	0.700555	-0.003236	0.502998
C	15	0.847476	-0.001232	0.502796
C	16	0.002885	0.570401	0.502974
C	17	0.003182	0.701882	0.502786
C	18	-0.000288	0.847050	0.502619
Na	1	0.333739	0.662360	0.504942

10. Six Na absorbed on the C sites of single-layer graphdiyne, P6/MMM, hexagonal, *a*=0.95 Å, *b*=0. 95 Å, *c*=1.549 Å, α=90°, β=90°, γ=60°

Element	Atom Number	Fractional coordinates of atoms u	v	w
C	1	0.567908	0.573907	0.093982
C	2	0.699538	0.705821	0.091993
C	3	0.845196	0.851963	0.092682
C	4	0.427718	0.005218	0.092727
C	5	0.295530	0.004657	0.091169
C	6	0.149662	0.004170	0.092527
C	7	-0.003325	0.433697	0.092694

C	8	-0.002814	0.301996	0.091471
C	9	-0.002651	0.156449	0.092684
C	10	0.427387	0.433504	0.093774
C	11	0.295368	0.301951	0.091889
C	12	0.149353	0.156183	0.092639
C	13	0.568070	0.005484	0.092635
C	14	0.699442	0.004355	0.091414
C	15	0.844854	0.003939	0.092607
C	16	-0.002953	0.574101	0.093315
C	17	-0.003027	0.705988	0.091776
C	18	-0.002785	0.851724	0.092717
Na	1	0.433672	0.223463	0.218060
Na	2	0.214846	0.443826	1.217289
Na	3	0.561078	0.789120	1.217555
Na	4	0.213901	0.790448	1.217754
Na	5	0.779532	0.223017	1.217818
Na	6	0.780171	0.570029	1.218646

11. Six Na absorbed on the C sites of double-layer graphdiyne, P6/MMM, hexagonal, *a*=0.95 Å, *b*=0. 95 Å, *c*=0.859 Å, α=90°, β=90°, γ=60°

Element	Atom Number	Fractional coordinates of atoms u	v	w
C	1	0.756235	0.263168	0.840885
C	2	0.629400	0.233193	0.834819
C	3	0.482663	0.231965	0.834255
C	4	0.338166	0.263576	0.400477
C	5	0.329777	0.238798	0.534911
C	6	0.329235	0.234940	0.680930
C	7	0.898010	0.262214	0.261299
C	8	0.032481	0.242654	0.133069
C	9	0.177402	0.235772	0.987327
C	10	0.897293	0.265951	0.840701
C	11	0.031046	0.240039	0.833617
C	12	0.177090	0.235268	0.833123
C	13	0.338608	0.259419	0.259337
C	14	0.332022	0.231911	0.132419
C	15	0.331007	0.231519	0.985991
C	16	0.757391	0.262144	0.401769
C	17	0.629210	0.242117	0.535958
C	18	0.483563	0.235700	0.680896
C	19	0.236823	0.746485	0.170450
C	20	0.369754	0.737238	0.167658

C	21	0.514987	0.737153	0.169119
C	22	0.668437	0.744419	0.599158
C	23	0.666855	0.739375	0.468007
C	24	0.667933	0.739033	0.322167
C	25	0.096933	0.740313	0.738495
C	26	0.965180	0.740457	0.870612
C	27	0.820015	0.738741	0.016265
C	28	0.097085	0.748246	0.170730
C	29	0.966286	0.741407	0.168437
C	30	0.820463	0.739755	0.169595
C	31	0.668068	0.743090	0.738961
C	32	0.665396	0.733651	0.871745
C	33	0.666887	0.735593	0.017093
C	34	0.236755	0.740496	0.598942
C	35	0.369191	0.739726	0.467448
C	36	0.514571	0.738944	0.322028
Na	1	0.497319	0.489362	0.501785
Na	2	0.498610	0.483689	1.004270
Na	3	0.002419	0.491256	0.998878
Na	4	0.309177	0.976305	0.350640
Na	5	0.845482	0.979131	0.349675
Na	6	0.833798	0.979767	0.828388

Transition states (TS), corresponding lattice parameters are same to above single-layer GY and GDY

1. TS of B site to A site on the single-layer graphyne

Element	Atom Number	Fractional coordinates of atoms u	v	w
C	1	0.590522	0.590619	0.499448
C	2	0.791758	0.791349	0.500934
C	3	0.410734	0.000095	0.493602
C	4	0.209029	0.000034	0.492537
C	5	0.000391	0.410973	0.490195
C	6	-0.000155	0.208599	0.487490
C	7	0.411017	0.411219	0.491259
C	8	0.209876	0.209441	0.488700
C	9	0.590110	0.001069	0.497710
C	10	0.791800	0.000578	0.496954
C	11	0.001303	0.590635	0.498982
C	12	0.000381	0.792293	0.497777
Na	1	0.099717	0.211929	0.798713

2. TS of A site to A site on the single-layer graphyne

Element	Atom Number	Fractional coordinates of atoms u	v	w
C	1	0.589523	0.589523	0.500000
C	2	0.791471	0.791471	0.500000
C	3	0.410477	-0.000000	0.500000
C	4	0.208529	-0.000000	0.500000
C	5	0.000000	0.410477	0.500000
C	6	0.000000	0.208529	0.500000
C	7	0.410477	0.410477	0.500000
C	8	0.208529	0.208529	0.500000
C	9	0.589523	0.000000	0.500000
C	10	0.791471	0.000000	0.500000
C	11	-0.000000	0.589523	0.500000
C	12	-0.000000	0.791471	0.500000
Na	1	0.491980	0.490774	0.707900

3. TS of A site to A site on the single-layer graphdiyne

Element	Atom Number	Fractional coordinates of atoms u	v	w
C	1	0.568684	0.570676	0.456544
C	2	0.701173	0.700885	0.466203
C	3	0.847147	0.846192	0.480984
C	4	0.426215	-0.006393	0.504964
C	5	0.295306	-0.005791	0.495559
C	6	0.150284	-0.002023	0.489461
C	7	0.002392	0.429493	0.507088
C	8	0.000336	0.297027	0.499455
C	9	-0.001405	0.150282	0.491713
C	10	0.427301	0.429297	0.456164
C	11	0.296772	0.296978	0.466464
C	12	0.151574	0.150517	0.480781
C	13	0.567232	-0.006208	0.507178
C	14	0.700154	-0.003263	0.499476
C	15	0.847171	-0.000938	0.491791
C	16	0.002703	0.570571	0.504596
C	17	0.003326	0.702123	0.495293
C	18	-0.000577	0.847157	0.489456
Na	1	0.511103	0.480314	0.776388

4. TS of A site to C site on the single-layer graphdiyne

Element	Atom Number	Fractional coordinates of atoms u	v	w
C	1	0.567910	0.573908	0.093982
C	2	0.699540	0.705821	0.091993
C	3	0.845199	0.851964	0.092682
C	4	0.427720	0.005218	0.092727
C	5	0.295531	0.004657	0.091169
C	6	0.149662	0.004170	0.092527
C	7	-0.003326	0.433697	0.092694
C	8	-0.002814	0.301996	0.091471
C	9	-0.002651	0.156449	0.092684
C	10	0.427388	0.433505	0.093774
C	11	0.295369	0.301951	0.091889
C	12	0.149354	0.156183	0.092639
C	13	0.568072	0.005484	0.092635
C	14	0.699445	0.004355	0.091414
C	15	0.844857	0.003939	0.092607
C	16	-0.002954	0.574101	0.093315
C	17	-0.003027	0.705988	0.091776
C	18	-0.002786	0.851724	0.092717
Na	1	0.755545	0.245829	1.192667

5. TS of C site to B site on the single-layer graphdiyne

Element	Atom Number	Fractional coordinates of atoms u	v	w
C	1	0.567910	0.573908	0.093982
C	2	0.699540	0.705821	0.091993
C	3	0.845199	0.851964	0.092682
C	4	0.427720	0.005218	0.092727
C	5	0.295531	0.004657	0.091169
C	6	0.149662	0.004170	0.092527
C	7	-0.003326	0.433697	0.092694
C	8	-0.002814	0.301996	0.091471
C	9	-0.002651	0.156449	0.092684
C	10	0.427388	0.433505	0.093774
C	11	0.295369	0.301951	0.091889
C	12	0.149354	0.156183	0.092639
C	13	0.568072	0.005484	0.092635

C	14	0.699445	0.004355	0.091414
C	15	0.844857	0.003939	0.092607
C	16	-0.002954	0.574101	0.093315
C	17	-0.003027	0.705988	0.091776
C	18	-0.002786	0.851724	0.092717
Na	1	0.908946	0.093274	1.232441

6. TS of C site to C site on the single-layer graphdiyne

Element	Atom Number	Fractional coordinates of atoms u	v	w
C	1	0.568880	0.569362	0.503154
C	2	0.700657	0.700171	0.502715
C	3	0.847240	0.845619	0.502582
C	4	0.426578	-0.006452	0.503019
C	5	0.295392	-0.006119	0.502973
C	6	0.150467	-0.002262	0.502801
C	7	0.002428	0.429363	0.503199
C	8	0.000429	0.296792	0.503131
C	9	-0.001323	0.149938	0.502952
C	10	0.428157	0.428600	0.503529
C	11	0.297224	0.296933	0.503331
C	12	0.151833	0.150253	0.502990
C	13	0.567643	-0.005958	0.503046
C	14	0.700555	-0.003236	0.502998
C	15	0.847476	-0.001232	0.502796
C	16	0.002885	0.570401	0.502974
C	17	0.003182	0.701882	0.502786
C	18	-0.000288	0.847050	0.502619
Na	1	0.684228	0.672752	0.778883