Supplementary Data

Sequential approach to the synthesis of 'U and Z' shaped polycyclic heteroarenes

Hardesh K. Maurya,[a] Sanjay K. Gautam,[a] Abhinav Kumar,[a,#] Ramendra Pratap,[b] Vikas Bajpai,[c] Brijesh Kumar,[c] Vishnu K. Tandon,[a,*] Vishnu Ji Ram,[a,*]

[a]*Department of Chemistry, University of Lucknow, Lucknow 226007, India,*

[b]*Department of Chemistry, Delhi University, New Delhi 110007, India*

[c]Division of SAIF, Central Drug Research Institute , Lucknow 226001, India

Coordinates of Compound **12f**:

XYZ coordinates for dimer
Counterpoise: corrected energy = -2552.434623211921
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.045643	-1.249371	-0.860941
2	8	0	-1.891458	-1.044093	-0.438076
3	8	0	-8.104929	-0.268110	-1.901218
4	7	0	-5.042935	2.221156	1.131931
5	7	0	-2.729360	2.671024	1.607899
6	7	0	-1.050250	1.300341	0.819951
7	6	0	-4.678575	1.089541	0.476132
8	6	0	-4.051642	2.929522	1.690597
9	6	0	-2.361357	1.546451	0.949849
10	6	0	-3.342035	0.673186	0.389176
11	6	0	-3.001996	-0.556429	-0.291512
12	6	0	-5.376738	-0.818927	-0.841332
13	6	0	-6.171030	-1.754300	-1.676767
14	6	0	-5.624023	-3.003733	-2.075331
15	6	0	-6.264514	-3.884281	-2.941948
16	6	0	-7.518013	-3.516986	-3.467182
17	6	0	-8.068854	-2.297104	-3.082111
18	6	0	-7.433596	-1.434780	-2.195908
19	6	0	-8.234757	0.004595	-0.476359
20	6	0	-7.118824	0.886592	-0.004431
21	6	0	-5.726461	0.313622	-0.165031
22	6	0	-4.472600	4.131901	2.480795
23	6	0	-5.824694	4.350696	2.799881
24	6	0	-6.202830	5.463454	3.561868
25	6	0	-5.244535	6.365680	4.002669
26	6	0	-3.901979	6.167875	3.680656
27	6	0	-3.520798	5.052867	2.925733

28	6	0	-5.612260	-5.185607	-3.366676
29	6	0	-8.239888	-4.415666	-4.441152
30	1	0	-4.751338	-3.244009	-1.726197
31	1	0	-8.956315	-2.035204	-3.423064
32	1	0	-8.284263	-0.909140	-0.000947
33	1	0	-9.103620	0.488819	-0.361116
34	1	0	-7.273076	1.091005	0.974382
35	1	0	-7.157713	1.782102	-0.474544
36	1	0	-6.471294	3.677904	2.492194
37	1	0	-7.126607	5.593686	3.790226
38	1	0	-5.498643	7.147521	4.541615
39	1	0	-3.181675	6.784115	3.971809
40	1	0	-2.566393	4.898576	2.689771
41	1	0	-0.787323	0.528639	0.470061
42	1	0	-0.429398	1.883490	1.247667
43	1	0	-4.793243	-5.333595	-2.864527
44	1	0	-6.225597	-5.950276	-3.274382
45	1	0	-5.338781	-5.159872	-4.389023
46	1	0	-7.666333	-4.636797	-5.245421
47	1	0	-8.512980	-5.258654	-4.000398
48	1	0	-9.092022	-3.982808	-4.760913
49	8	0	1.797297	0.812384	0.448391
50	8	0	3.212034	-0.801958	0.952260
51	8	0	6.838162	-2.849124	2.039986
52	7	0	6.282098	0.828158	-1.267676
53	7	0	4.921758	2.723987	-1.848067
54	7	0	2.787737	2.975236	-1.010285
55	6	0	5.253155	0.324375	-0.539075
56	6	0	6.047296	1.981349	-1.909211
57	6	0	3.895174	2.227939	-1.117871
58	6	0	4.007597	0.964618	-0.462085
59	6	0	2.928619	0.375863	0.299550
60	6	0	4.465587	-1.423218	0.941146
61	6	0	4.409637	-2.580106	1.869720
62	6	0	3.159713	-3.060399	2.345286
63	6	0	3.032630	-4.068683	3.295987
64	6	0	4.203460	-4.639407	3.830277
65	6	0	5.435974	-4.181844	3.370532
66	6	0	5.553509	-3.191703	2.401863
67	6	0	7.076985	-2.853621	0.603188
68	6	0	6.876414	-1.483111	0.030986
69	6	0	5.484052	-0.910141	0.191586
70	6	0	7.161933	2.485964	-2.775400
71	6	0	8.273872	1.676200	-3.068178
72	6	0	9.296272	2.148832	-3.900741
73	6	0	9.223781	3.426378	-4.438578
74	6	0	8.133387	4.244702	-4.144189
75	6	0	7.107019	3.772046	-3.318588
76	6	0	1.671918	-4.510719	3.798322
77	6	0	4.125433	-5.709114	4.891873
78	1	0	2.355843	-2.650786	1.988613
79	1	0	6.265242	-4.586940	3.717859
80	1	0	6.461445	-3.576419	0.200629
81	1	0	8.033597	-3.121912	0.478332

82	1	0	7.099019	-1.519324	-0.955315
83	1	0	7.542478	-0.835279	0.432396
84	1	0	8.278519	0.769283	-2.690167
85	1	0	10.042241	1.581057	-4.109621
86	1	0	9.933723	3.766246	-5.027459
87	1	0	8.037027	5.163849	-4.503691
88	1	0	6.322572	4.344561	-3.101244
89	1	0	2.072671	2.634323	-0.610865
90	1	0	2.735406	3.791097	-1.500280
91	1	0	0.966051	-4.084293	3.283779
92	1	0	1.576334	-5.490551	3.783689
93	1	0	1.525444	-4.223923	4.806758
94	1	0	3.585130	-5.406157	5.692500
95	1	0	3.720548	-6.534480	4.525388
96	1	0	5.047765	-5.969228	5.203944

XYZ coordinates for monomer
Energy = -1276.21534106
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.446668	1.657484	0.156821
2	8	0	0.482037	3.638001	0.064600
3	8	0	2.340667	-2.479151	-0.625401
4	7	0	-2.130642	-0.390722	0.021211
5	7	0	-3.357403	1.666786	-0.186812
6	7	0	-2.279944	3.701042	-0.327984
7	6	0	-0.971016	0.314640	0.054602
8	6	0	-3.260051	0.326216	-0.062377
9	6	0	-2.202911	2.373566	-0.159710
10	6	0	-0.946988	1.716369	0.011817
11	6	0	0.309400	2.428678	0.082677
12	6	0	1.448830	0.258544	0.135808
13	6	0	2.861626	-0.194815	0.088401
14	6	0	3.917787	0.713092	0.370149
15	6	0	5.265638	0.390731	0.243656
16	6	0	5.608553	-0.900425	-0.200597
17	6	0	4.584083	-1.802737	-0.476482
18	6	0	3.240546	-1.480420	-0.323072
19	6	0	1.346851	-2.723665	0.410933
20	6	0	0.099605	-1.937731	0.141442
21	6	0	0.272914	-0.433702	0.116491
22	6	0	-4.536828	-0.458032	-0.016227
23	6	0	-4.536181	-1.821521	0.328360
24	6	0	-5.738353	-2.537238	0.394487
25	6	0	-6.942298	-1.906823	0.112101
26	6	0	-6.955087	-0.558657	-0.245052
27	6	0	-5.756007	0.160447	-0.304607

28	6	0	6.349599	1.415287	0.516772
29	6	0	7.053230	-1.292003	-0.392744
30	1	0	3.676524	1.607804	0.657356
31	1	0	4.807721	-2.718259	-0.766712
32	1	0	1.797632	-2.509142	1.313240
33	1	0	1.131660	-3.700697	0.368765
34	1	0	-0.579366	-2.172867	0.853736
35	1	0	-0.316945	-2.231194	-0.733099
36	1	0	-3.668204	-2.227363	0.545894
37	1	0	-5.728877	-3.463295	0.649045
38	1	0	-7.792028	-2.398758	0.159735
39	1	0	-7.788914	-0.065100	-0.455989
40	1	0	-5.750438	1.123142	-0.556715
41	1	0	-1.548646	4.193192	-0.227642
42	1	0	-3.140257	4.106016	-0.393708
43	1	0	5.963033	2.226931	0.886429
44	1	0	7.051262	1.057891	1.107837
45	1	0	6.843492	1.696094	-0.376459
46	1	0	7.535670	-0.656842	-1.016070
47	1	0	7.527313	-1.310960	0.475795
48	1	0	7.122653	-2.225809	-0.765478
