Supporting information for

Probing the aggregation behavior of 4-Aminopththalimide and 4-(N, N-dimethyl) amino-N-methylpththalimide: A combined photophysical, crystallographic, microscopic and theoretical (DFT) study

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Table S1. Crystal data and structure refinement for DMP

Identification code	sudhri_1
Empirical formula	C11 H12 N2 O2
Formula weight	204.23
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P21/n
Unit cell dimensions	a = 7.7124(4) Å
	b = 8.9272(4) Å
	c = 14.9003(7) Å
	α= 90°.
	β= 97.869(3)°.
	γ = 90°.
Volume	1016.23(8) $Å^3$
Z	4
Density (calculated)	1.335 Mg/m^3
Absorption coefficient	0.094 mm^{-1}
F(000)	432
Crystal size	0.12 x 0.09 x 0.07 mm^3
Theta range for data collection	2.67 to 29.21°.
Index ranges	-10<=h<=10, -12<=k<=12, -20<=l<=20

Reflections collected	17324
Independent reflections	2735 [R(int) = 0.0363]
Completeness to theta = 29.21°	99.1 %
Absorption correction	Empirical
Max. and min. transmission	0.9935 and 0.9888
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2735 / 0 / 136
Goodness-of-fit on F^2	1.042
Final R indices [I>2sigma(I)]	R1 = 0.0531, wR2 = 0.1471
R indices (all data)	R1 = 0.0712, wR2 = 0.1591
Largest diff. peak and hole	0.303 and -0.256 e.Å^{-3}

Table S2. Bond lengths [Å] and angles [°] for DMP

Bond lengths [Å]		Bond angles [°]		Torson angles [°]	
C(1)-C(2)	1.386(2)	C(2)-C(1)-C(6)	119.23(14)	C(6)-C(1)-C(2)-C(3)	-0.1(2)
C(1)-C(6)	1.3904(19)	C(2)-C(1)-C(8)	132.28(14)	C(8)-C(1)-C(2)-C(3)	-179.96(17)
C(1)-C(8)	1.468(2)	C(6)-C(1)-C(8)	108.49(14)	C(1)-C(2)-C(3)-C(4)	0.0(3)
C(2)-C(3)	1.376(2)	C(3)-C(2)-C(1)	118.82(14)	C(2)-C(3)-C(4)-N(2)	179.60(16)
C(3)-C(4)	1.415(2)	C(2)-C(3)-C(4)	122.46(15)	C(2)-C(3)-C(4)-C(5)	0.0(2)
C(4)-N(2)	1.365(2)	N(2)-C(4)-C(3)	121.08(15)	N(2)-C(4)-C(5)-C(6)	-179.44(15)
C(4)-C(5)	1.417(2)	N(2)-C(4)-C(5)	121.03(14)	C(3)-C(4)-C(5)-C(6)	0.1(2)
C(5)-C(6)	1.367(2)	C(3)-C(4)-C(5)	117.89(14)	C(4)-C(5)-C(6)-C(1)	-0.3(2)
C(6)-C(7)	1.490(2)	C(6)-C(5)-C(4)	118.33(13)	C(4)-C(5)-C(6)-C(7)	179.10(14)
C(7)-O(1)	1.205(2)	C(5)-C(6)-C(1)	123.27(14)	C(2)-C(1)-C(6)-C(5)	0.3(2)
C(7)-N(1)	1.388(2)	C(5)-C(6)-C(7)	129.10(13)	C(8)-C(1)-C(6)-C(5)	-179.83(14)
C(8)-O(2)	1.215(2)	C(1)-C(6)-C(7)	107.62(13)	C(2)-C(1)-C(6)-C(7)	-179.22(14)
C(8)-N(1)	1.397(2)	O(1)-C(7)-N(1)	125.23(15)	C(8)-C(1)-C(6)-C(7)	0.67(16)
C(9)-N(2)	1.444(2)	O(1)-C(7)-C(6)	128.89(15)	C(5)-C(6)-C(7)-O(1)	-0.9(3)
C(10)-N(2)	1.450(2)	N(1)-C(7)-C(6)	105.87(12)	C(1)-C(6)-C(7)-O(1)	178.60(17)
C(11)-N(1)	1.453(2)	O(2)-C(8)-N(1)	123.60(16)	C(5)-C(6)-C(7)-N(1)	179.89(15)
		O(2)-C(8)-C(1)	130.24(16)	C(1)-C(6)-C(7)-N(1)	-0.65(16)
		N(1)-C(8)-C(1)	106.15(13)	C(2)-C(1)-C(8)-O(2)	0.0(3)
		C(7)-N(1)-C(8)	111.86(13)	C(6)-C(1)-C(8)-O(2)	-179.87(17)

		C(7)-N(1)-C(11)	124.05(14)	C(2)-C(1)-C(8)-N(1)	179.42(17)
		C(8)-N(1)-C(11)	124.10(14)	C(6)-C(1)-C(8)-N(1)	-0.44(17)
		C(4)-N(2)-C(9)	121.17(15)	O(1)-C(7)-N(1)-C(8)	-178.91(16)
		C(4)-N(2)-C(10)	120.48(15)	C(6)-C(7)-N(1)-C(8)	0.38(17)
		C(9)-N(2)-C(10)	118.07(15)	O(1)-C(7)-N(1)-C(11)	1.3(3)
				C(6)-C(7)-N(1)-C(11)	-179.42(14)
				O(2)-C(8)-N(1)-C(7)	179.49(16)
				C(1)-C(8)-N(1)-C(7)	0.02(18)
				O(2)-C(8)-N(1)-C(11)	-0.7(3)
				C(1)-C(8)-N(1)-C(11)	179.82(14)
				C(3)-C(4)-N(2)-C(9)	173.92(17)
				C(5)-C(4)-N(2)-C(9)	-6.5(3)
				C(3)-C(4)-N(2)-C(10)	0.2(3)
				C(5)-C(4)-N(2)-C(10)	179.73(15)

Symmetry transformations used to generate equivalent atoms

Table S3. Distance [Å] of each atom from the mean plane in DMP and AP molecules (generated by Diamond 3.1e software)

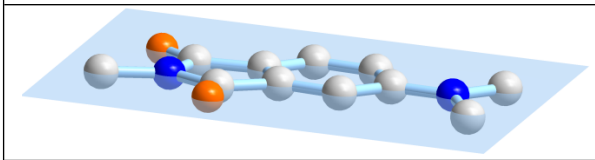
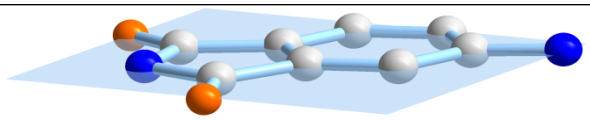
DMP		**AP**	
			
Atoms	Distance from mean plane [Å]	Atoms	Distance from mean plane [Å]
C11	-0.0106	O1	0.0007
N1	-0.0034	C1	0.0160
O1	0.0313	N1	0.0315
O2	-0.0091	C6	0.0053
C8	-0.0095	O2	-0.0388
C7	0.0055	C7	0.0136
C6	-0.0041	C8	0.0010
C1	-0.0035	C2	-0.0285
C5	-0.0025	C3	-0.0318
C2	0.0050	C4	0.0034
C3	0.0094	C5	0.0108
C4	0.0060	N2	0.0374
N2	0.0194		
C9	-0.1149		
C10	0.0336		

Table S4. Angle between two planes in DMP molecule (generated by Diamond 3.1e software)

Value	**3.355(71)°**		
Plane normal	m1=-0.9085(3) m2=0.2701(6) m3=-0.3188(6)		
Dist. from origin	d=-0.5511(26) Å		
Const. atoms	d [Å]	s [Å]	$(d/s)^2$
C5	-0.0010	0.0015	0.4181
C6	0.0014	0.0014	0.9229
C1	-0.0010	0.0015	0.4917
C2	0.0001	0.0016	0.0054
C3	0.0004	0.0016	0.0758
C4	0.0000	0.0015	0.0002
Plane normal	m1=-0.9133(4) m2=0.3039(11) m3=-0.2713(11)		
Dist. from origin	d=-0.4024(40) Å		
Const. atoms	d [Å]	s [Å]	$(d/s)^2$
C9	-0.0205	0.0023	77.6338
N2	0.0278	0.0015	324.0431
C4	-0.0091	0.0015	37.4456
C10	-0.0193	0.0023	72.1807

Table S5. Angle between two planes of AP molecule (generated by Diamond 3.1e software)

Value	**5.20(8)°**		
Plane normal	m1=-0.4073(17) m2=-0.0265(18) m3=-0.9129(8)		
Dist. from origin	d=-7.4363(230) Å		
Const. atoms	d [Å]	s [Å]	$(d/s)^2$
C4	0.0093	0.0045	4.3219
C3	-0.0050	0.0041	1.4363
C2	-0.0024	0.0048	0.2534
C8	0.0056	0.0041	1.7996
C7	-0.0025	0.0042	0.3488
C5	-0.0051	0.0045	1.3076
Plane normal	m1=-0.3376(595) m2=-0.0789(202) m3=-0.9380(198)		
Dist. from origin	d=-7.4652(2836) Å		
Const. atoms	d [Å]	s [Å]	$(d/s)^2$
H2A	0.0780	0.0727	1.1515
N2	-0.0011	0.0051	0.0465
C4	0.0002	0.0045	0.0021
H2B	0.0906	0.0727	1.5566

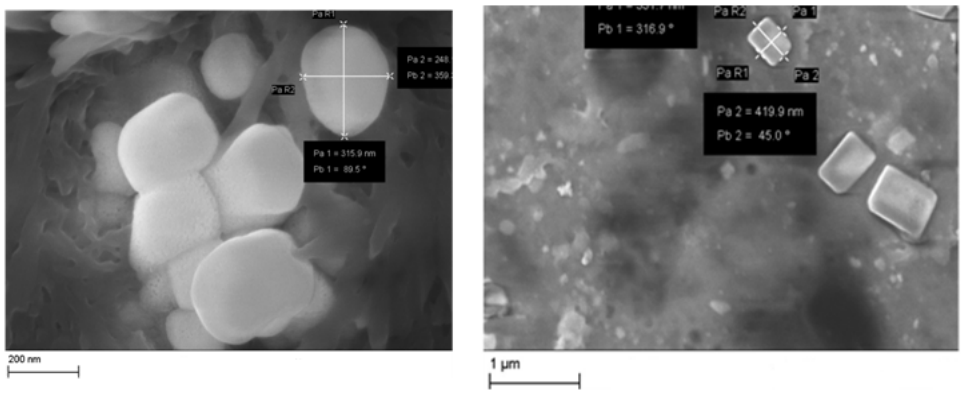


Fig. S1 FESEM (a) AP and (b) DMP aggregates at higher temperature (T= 65^0 C) in 99% water-DMSO system.

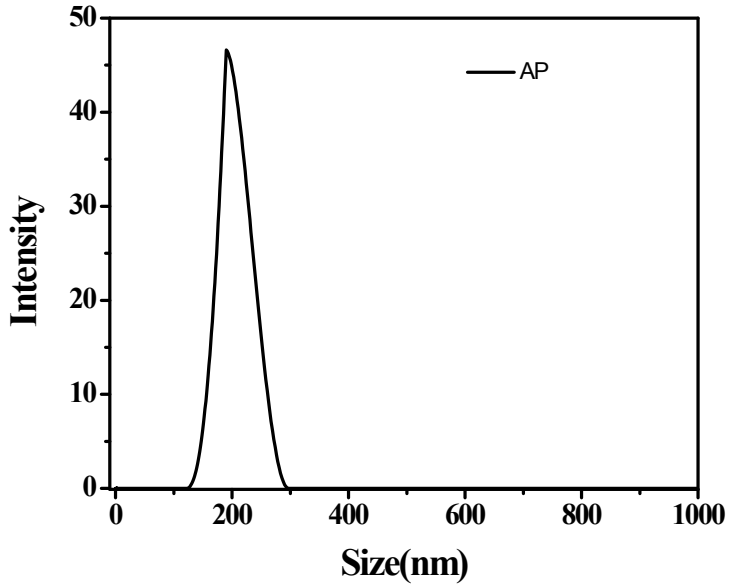


Fig. S2 The DLS data of AP aggregate at room temperature in 99% water-DMSO system.

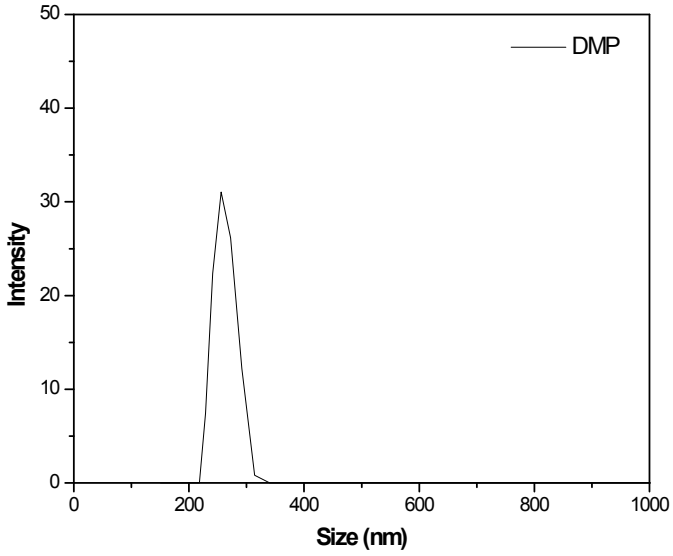


Fig. S3 The DLS data of DMP aggregate at room temperature in 99% water-DMSO system.

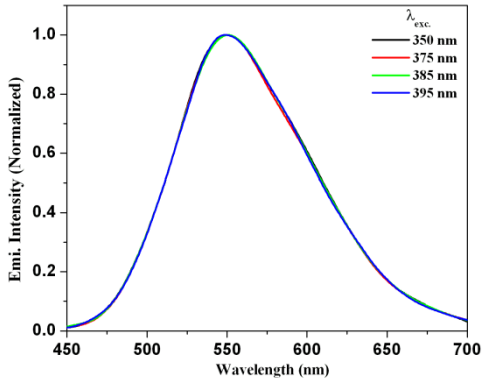


Fig. S4 Emission spectra of AP aggregates at different excitation wavelength ($\lambda_{exc.}$).

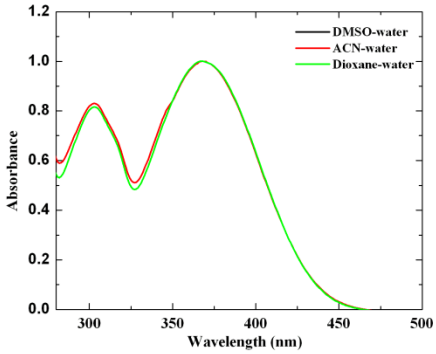


Fig. S5 Absorption spectra in aggregated form of AP in different 99% water-solvent medium at room temperature. Spectra are normalized corresponding to second peak maxima

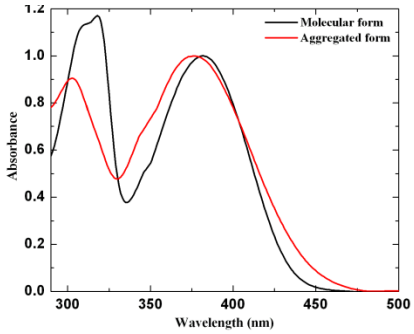


Fig. S6 Absorption spectra of 5-amino-2-methylisoindolne-1, 3-dione in molecular form in DMSO (5×10^{-6} M) solution and in aggregated form in 99% water-DMSO medium at room temperature. Spectra are normalized corresponding to second peak maxima.

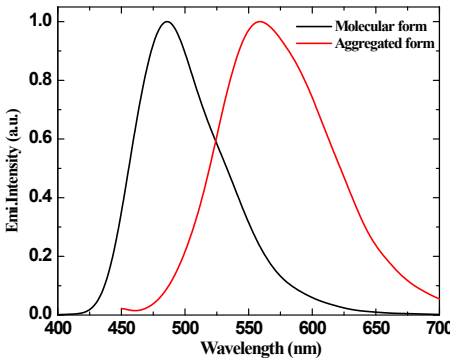


Fig. S7 Emission spectra of 5-amino-2-methylisoindolne-1, 3-dione in molecular form in DMSO (5×10^{-6} M) solution and in aggregated form in 99% water-DMSO medium at room temperature. Spectra are normalized corresponding to second peak maxima.

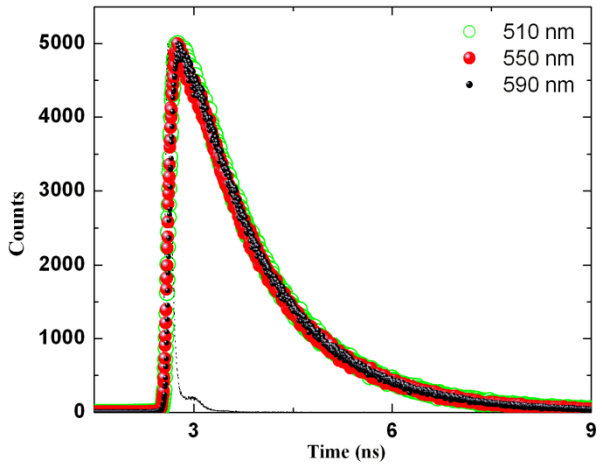


Fig. S8 Wavelength dependent fluorescence decay profiles of AP in aggregated forms at room temperature. $\lambda_{exc.}$ = 375 nm.

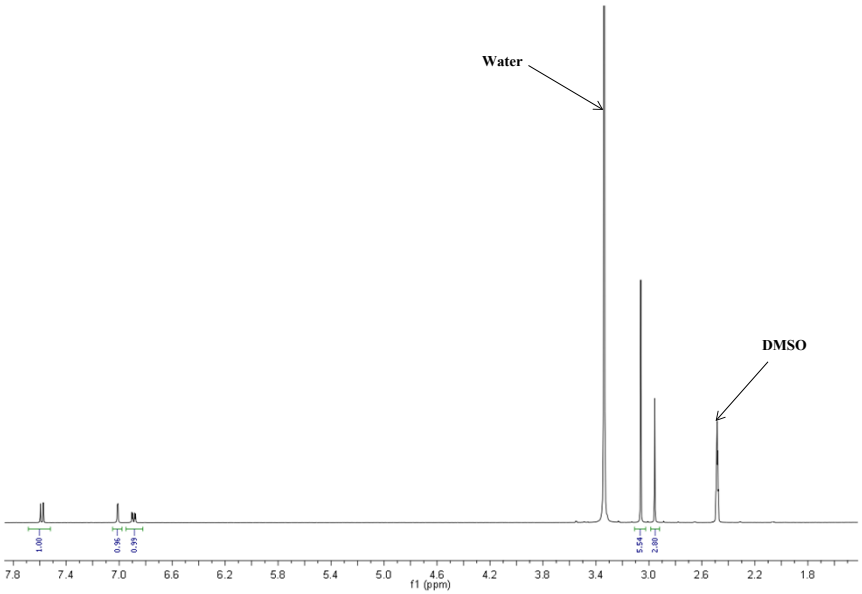


Fig. S9 ^{1}H NMR spectra of DMP in DMSO-d_6.

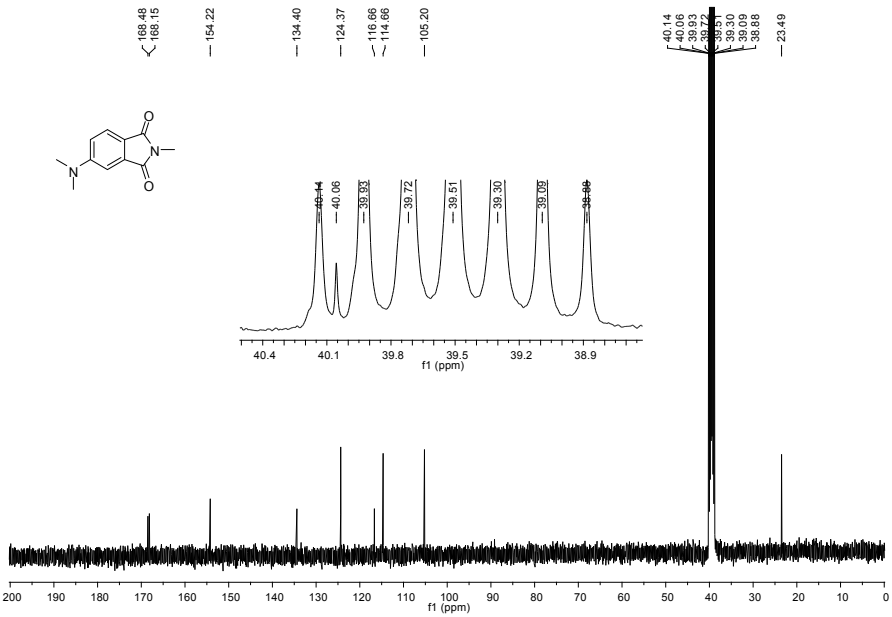
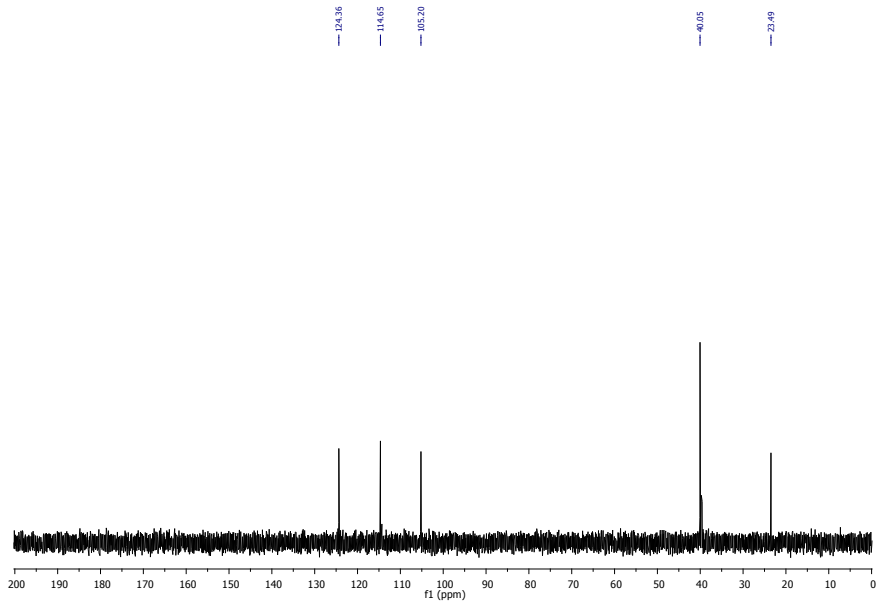


Fig. S10 ^{13}C NMR spectra of DMP in DMSO-d_6.



DEPT-135

Fig. S11 DEPT135 NMR spectra of DMP in DMSO-d_6.

Cartesian coordinates, energies and low frequencies for the optimized structures and Cartesian coordinates and energies for the hydrogen atoms optimized structures in M06-2X/6-31+G (d, p) level of theory.

AP monomer:-

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-3.586254	0.461110	-0.054174
2	1	-4.285742	-0.211761	0.219240
3	1	-3.796921	1.410206	0.214054
4	6	-0.614879	-1.740835	-0.001759
5	1	-0.372215	-2.798693	-0.000118
6	6	-1.936539	-1.307290	-0.003437
7	1	-2.742913	-2.035359	-0.009148
8	6	-2.264802	0.064977	-0.004111
9	8	2.549574	-1.911270	0.005898
10	8	1.492076	2.557453	0.001009
11	7	2.352668	0.401564	0.002118
12	1	3.336862	0.630188	0.004701
13	6	1.866353	-0.915525	0.002567
14	6	-1.237067	1.029378	-0.005740
15	1	-1.457224	2.093032	-0.012250
16	6	1.340921	1.359566	-0.000278
17	6	0.063562	0.573934	-0.003595
18	6	0.385794	-0.780171	-0.001538

Energy = -568.2568613 Hartree

Low Frequencies: -	111.6034	145.1662	165.4414
	209.0887	275.0683	332.5909
	357.9842	382.7124	427.5363

AP linear dimer:-

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.072348	2.895064	-1.148079
2	1	1.238521	3.888748	-1.164202
3	1	0.126034	2.628263	-0.921097
4	6	4.469822	1.775020	-0.400952
5	1	5.484700	2.160946	-0.392536
6	6	3.407372	2.579808	-0.746582
7	1	3.576332	3.617118	-1.020524
8	6	2.089064	2.075817	-0.763633
9	8	6.348741	-0.599837	0.472459
10	8	2.091081	-2.234902	0.580232
11	7	4.336684	-1.727214	0.578447
12	1	4.690930	-2.613323	0.909904
13	6	5.128912	-0.621200	0.340624
14	6	1.855659	0.749211	-0.394906
15	1	0.845201	0.347854	-0.397252
16	6	2.986389	-1.448640	0.386634
17	6	2.932717	-0.037863	-0.052725
18	6	4.223638	0.460361	-0.060386
19	8	-6.343179	0.601897	-0.501037
20	8	-2.687901	1.915164	1.892091

21	7	-4.660937	1.553075	0.762256
22	1	-5.177079	2.349596	1.106791
23	7	-0.708447	-2.701581	-0.368250
24	1	-0.709273	-3.554122	-0.901199
25	1	0.155701	-2.442494	0.091509
26	6	-5.197200	0.583807	-0.062604
27	6	-4.138596	-1.598979	-0.979667
28	1	-5.024992	-1.915304	-1.521552
29	6	-2.989493	-2.357471	-0.993786
30	1	-2.956214	-3.286827	-1.554731
31	6	-1.834967	-1.940975	-0.296748
32	6	-1.868605	-0.757040	0.443157
33	1	-1.005225	-0.444449	1.025469
34	6	-3.354393	1.251115	1.135708
35	6	-3.028157	-0.014032	0.443487
36	6	-4.147512	-0.420604	-0.261148

Energy = -1136.5202759 Hartree.

AP π – stacked dimer:-

Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z
1	7	4.228264	-1.056292	0.545239
2	1	5.127978	-0.835059	0.145902
3	1	4.289227	-1.508316	1.445730
4	6	2.365967	1.754877	-0.863547
5	1	2.453292	2.489851	-1.658345
6	6	3.335299	0.795503	-0.673922

7	1	4.208325	0.767328	-1.320467
8	6	3.228995	-0.148985	0.369558
9	8	-0.178370	3.606521	-0.687796
10	8	-2.927293	1.339745	-1.762732
11	8	-0.643867	0.482022	2.603651
12	8	-3.392791	-1.784752	1.528715
13	7	-0.677041	2.207731	1.080054
14	7	-3.425978	-0.059054	0.005112
15	1	-1.578115	2.600174	1.314646
16	1	-4.325339	0.331742	0.246239
17	7	1.479501	-3.322967	-0.529672
18	1	2.398060	-3.073708	-0.866543
19	1	1.487350	-3.847802	0.331711
20	6	0.106686	2.656993	0.035363
21	6	-2.642231	0.390225	-1.039565
22	6	-0.382950	-0.511894	-1.938481
23	1	-0.291697	0.227715	-2.729235
24	6	0.586413	-1.471234	-1.748850
25	1	1.461018	-1.498900	-2.393005
26	6	0.480058	-2.415769	-0.705380
27	6	2.108680	-0.128917	1.203151
28	6	-0.640279	-2.395782	0.128143
29	1	1.993451	-0.856751	2.003326
30	1	-0.748348	-3.111412	0.939249
31	6	-0.124778	1.089885	1.699030
32	6	-2.873701	-1.176888	0.624095

33	6	1.151268	0.838955	0.995509
34	6	-1.597642	-1.427803	-0.079412
35	6	1.276079	1.773877	-0.016967
36	6	-1.472840	-0.492891	-1.091897

Energy = -1136.5204623Hartree.

DMP monomer:-

Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z
1	6	0.761419	-0.934381	-0.004426
2	6	-0.225396	-1.907523	-0.004293
3	1	0.031833	-2.962129	0.000660
4	6	-1.556406	-1.502367	-0.009240
5	1	-2.327112	-2.262726	-0.007186
6	6	-1.922667	-0.129937	-0.017202
7	6	-0.893821	0.849287	-0.011122
8	6	-3.587983	1.653090	0.012369
9	1	-4.672163	1.752930	-0.021822
10	1	-3.170311	2.191744	-0.846414
11	1	-3.225740	2.132543	0.931274
12	6	-4.283023	-0.759174	0.025118
13	1	-5.253819	-0.265155	0.007845
14	1	-4.219279	-1.359782	0.942158
15	1	-4.232117	-1.436017	-0.836391
16	7	-3.240890	0.245758	-0.031719
17	1	4.345204	1.245836	0.898894
18	1	-1.103756	1.911761	-0.009094

19	6	0.410860	0.411504	-0.006598
20	6	1.675408	1.216243	-0.000922
21	6	2.241760	-1.035654	0.002147
22	6	4.111884	0.657513	0.008471
23	1	4.691535	-0.266096	0.008518
24	1	4.349971	1.248931	-0.878619
25	7	2.712462	0.289584	0.003828
26	8	1.812990	2.418775	-0.000571
27	8	2.948577	-2.017630	0.005521

Energy = -686.1250314Hartree.

Frequencies -	33.6961	56.8188	79.3615
	93.7244	122.6746	151.5639
	155.5667	173.7645	216.5212

DMP linear dimer:-

Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z
1	6	4.466207	1.903656	0.024813
2	6	5.259212	0.744243	-0.164001
3	1	6.342421	0.786878	-0.185583
4	6	4.625900	-0.457573	-0.312178
5	6	6.466398	3.314470	0.040095
6	1	6.705122	4.371754	0.141205
7	1	7.027794	2.764733	0.806417
8	1	6.816707	2.977460	-0.944510
9	6	4.218725	4.308289	0.387793
10	1	4.863196	5.167046	0.568711

11	1	3.591577	4.523596	-0.488180
12	1	3.562392	4.189937	1.257635
13	7	5.041561	3.130758	0.189946
14	8	6.375797	-2.133541	-0.553547
15	6	3.242845	-0.598579	-0.292514
16	6	-3.296550	0.683790	0.278041
17	6	2.450935	0.523871	-0.108866
18	6	-3.919781	1.790942	-0.275611
19	1	1.366188	0.455523	-0.073975
20	1	-3.371264	2.714493	-0.434622
21	6	3.060343	1.747333	0.045821
22	6	-5.248976	1.701412	-0.618369
23	1	2.425647	2.613449	0.188976
24	1	-5.728038	2.573558	-1.046013
25	6	-6.004724	0.520849	-0.427433
26	6	-5.349864	-0.600805	0.139836
27	1	-5.863215	-1.540047	0.312137
28	6	-4.028530	-0.482945	0.467845
29	6	5.214836	-1.813178	-0.503787
30	6	-3.110854	-1.500964	1.053276
31	6	2.916646	-2.017185	-0.483329
32	6	-1.923201	0.452661	0.742531
33	6	-8.128003	-0.696043	-0.474891
34	1	-9.152142	-0.516654	-0.797250
35	1	-7.762564	-1.593609	-0.989526
36	1	-8.139263	-0.903461	0.603383

37	6	-7.977272	1.613805	-1.370707
38	1	-8.994838	1.343190	-1.647174
39	1	-8.022745	2.460108	-0.671305
40	1	-7.458406	1.945672	-2.277652
41	6	4.267468	-4.116748	-0.808334
42	6	-0.697649	-1.506840	1.741036
43	1	3.260128	-4.533473	-0.819393
44	1	-0.195411	-0.802272	2.406850
45	1	4.767314	-4.317180	-1.758803
46	1	-1.024673	-2.386813	2.295684
47	1	4.851081	-4.560802	0.001093
48	1	-0.010497	-1.811769	0.945736
49	7	4.138371	-2.684425	-0.602006
50	7	-1.882011	-0.869775	1.191292
51	7	-7.320688	0.460556	-0.786158
52	8	-3.340841	-2.647321	1.346381
53	8	1.838271	-2.575622	-0.529370
54	8	-0.963453	1.197999	0.757565

Energy = -1372.2535855Hartree.

DMP π – stacked dimer:-

Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z
1	1	-4.586886	3.502514	1.511585
2	6	-2.332433	-0.081327	1.201757
3	6	2.332433	0.081327	-1.201757
4	6	-1.994215	-1.414604	1.371204

5	6	1.994215	1.414604	-1.371204
6	1	-2.177064	-1.917981	2.316055
7	1	2.177064	1.917981	-2.316055
8	6	-1.423123	-2.092714	0.319406
9	6	1.423123	2.092714	-0.319406
10	1	-1.156518	-3.132352	0.464797
11	1	1.156518	3.132352	-0.464797
12	6	-1.167242	-1.480219	-0.929880
13	6	1.167242	1.480219	0.929880
14	6	-1.519862	-0.116143	-1.083827
15	6	1.519862	0.116143	1.083827
16	1	-1.338386	0.420943	-2.008474
17	1	1.338386	-0.420943	2.008474
18	6	-2.083097	0.532061	-0.020812
19	6	2.083097	-0.532061	0.020812
20	6	-2.524155	1.951483	0.088410
21	6	2.524155	-1.951483	-0.088410
22	6	-2.942036	0.905218	2.101971
23	6	2.942036	-0.905218	-2.101971
24	6	-0.447044	-1.596183	-3.266386
25	6	0.447044	1.596183	3.266386
26	1	0.004532	-2.326257	-3.935727
27	1	-0.004532	2.326257	3.935727
28	1	0.206296	-0.714024	-3.246322
29	1	-0.206296	0.714024	3.246322
30	1	-1.417226	-1.296151	-3.684777

31	1	1.417226	1.296151	3.684777
32	6	-0.229912	-3.571772	-1.779612
33	6	0.229912	3.571772	1.779612
34	1	0.305212	-3.910418	-2.666008
35	1	-0.305212	3.910418	2.666008
36	1	-1.112398	-4.212088	-1.640592
37	1	1.112398	4.212088	1.640592
38	1	0.431482	-3.704538	-0.914046
39	1	-0.431482	3.704538	0.914046
40	6	-3.578778	3.332521	1.898727
41	6	3.578778	-3.332521	-1.898727
42	1	-3.614942	3.243056	2.985023
43	1	3.614942	-3.243056	-2.985023
44	1	4.586886	-3.502514	-1.511585
45	1	-2.940743	4.166821	1.600469
46	1	2.940743	-4.166821	-1.600469
47	7	-3.026740	2.095042	1.374601
48	7	3.026740	-2.095042	-1.374601
49	7	-0.590893	-2.177968	-1.952157
50	7	0.590893	2.177968	1.952157
51	8	-2.462101	2.828583	-0.736082
52	8	2.462101	-2.828583	0.736082
53	8	-3.312942	0.793450	3.253841
54	8	3.312942	-0.793450	-3.253841

Energy = -1372.2707277Hartree.

AP-DMP parallel:-

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	2.650998	-1.598450	1.756039
2	1	2.996379	-1.157002	2.597009
3	1	3.040178	-2.521184	1.618641
4	6	-0.807993	-0.274795	1.918196
5	1	-1.361501	0.528696	2.396759
6	6	0.551105	-0.453727	2.161574
7	1	1.072028	0.226085	2.830565
8	6	1.281145	-1.486653	1.541879
9	8	-3.758769	-0.463033	0.787739
10	8	-1.376581	-3.816093	-1.248082
11	7	-2.870098	-2.284411	-0.343284
12	1	-3.667677	-2.487993	-0.929334
13	6	-2.828140	-1.189350	0.526350
14	6	0.635248	-2.365000	0.651205
15	1	1.170529	-3.170052	0.154539
16	6	-1.629035	-2.891916	-0.513093
17	6	-0.706271	-2.157115	0.412117
18	6	-1.427893	-1.140714	1.029145
19	6	0.216643	2.289232	0.004796
20	6	1.430705	2.648944	0.563706
21	1	1.502181	3.485594	1.252228
22	6	2.560578	1.903409	0.231650
23	1	3.509094	2.180997	0.673472

24	6	2.497226	0.802815	-0.661250
25	6	1.238017	0.449853	-1.217060
26	6	3.484207	-1.169626	-1.690134
27	1	4.471861	-1.604303	-1.842421
28	1	3.030766	-1.020370	-2.674797
29	1	2.867096	-1.884238	-1.127020
30	6	4.853172	0.339929	-0.256967
31	1	5.631919	-0.321452	-0.636179
32	1	4.730727	0.157467	0.820810
33	1	5.192083	1.370786	-0.403303
34	7	3.626814	0.091076	-0.986567
35	1	-3.823059	1.455857	-1.351617
36	1	1.113936	-0.395242	-1.883699
37	6	0.145247	1.205625	-0.865009
38	6	-1.291001	1.013510	-1.247413
39	6	-1.155156	2.819672	0.198128
40	6	-3.428038	2.213249	-0.674475
41	1	-3.882937	2.088786	0.309146
42	1	-3.638527	3.214295	-1.057955
43	7	-1.994381	2.013999	-0.587667
44	8	-1.771079	0.158704	-1.961593
45	8	-1.539447	3.739637	0.884865

Energy = -1254.4009483Hartree.

Low Frequencies -	20.4952	24.2645	44.6641
	49.6486	72.5328	86.5265
	96.1554	104.0687	117.1155

AP-DMP anti parallel:-

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-3.536697	1.921465	0.047162
2	1	-4.225702	1.428728	0.597354
3	1	-3.695109	1.817831	-0.948054
4	6	-0.603271	1.033803	2.133140
5	1	-0.382587	0.564981	3.087061
6	6	-1.917082	1.215959	1.713717
7	1	-2.733385	0.891822	2.354610
8	6	-2.223103	1.770623	0.452329
9	8	2.553394	0.810770	2.274943
10	8	1.585937	2.779269	-1.754192
11	7	2.400068	1.889268	0.228048
12	1	3.388031	1.946889	0.026772
13	6	1.886387	1.310766	1.396658
14	6	-1.178905	2.192685	-0.396262
15	1	-1.386836	2.616950	-1.374609
16	6	1.404781	2.302201	-0.659307
17	6	0.114305	2.009954	0.044651
18	6	0.412776	1.435498	1.277735
19	6	-0.796962	-0.986787	-1.290372
20	6	0.189445	-0.547621	-2.161042
21	1	-0.063326	-0.046225	-3.090424
22	6	1.518968	-0.730221	-1.800086

23	1	2.286091	-0.370273	-2.474163
24	6	1.888634	-1.330185	-0.564169
25	6	0.861019	-1.786253	0.304720
26	6	3.559494	-2.067679	1.057059
27	1	4.643353	-2.051950	1.164314
28	1	3.224583	-3.112425	1.091797
29	1	3.128379	-1.517938	1.900849
30	6	4.241538	-1.017617	-1.122375
31	1	5.212384	-1.156023	-0.648547
32	1	4.137481	0.043122	-1.385284
33	1	4.223884	-1.599457	-2.053674
34	7	3.203524	-1.439106	-0.204427
35	1	-4.270223	-1.036142	1.203521
36	1	1.074221	-2.236722	1.266705
37	6	-0.443895	-1.596084	-0.090246
38	6	-1.704900	-1.902750	0.655923
39	6	-2.268813	-0.839128	-1.326871
40	6	-4.134513	-1.515804	0.228779
41	1	-4.711845	-0.996827	-0.538143
42	1	-4.471800	-2.552166	0.306328
43	7	-2.745161	-1.461672	-0.162050
44	8	-1.850021	-2.404301	1.747576
45	8	-2.972453	-0.274742	-2.139757

Energy = -1254.4070037Hartree.

Low Frequencies - 23.9044 40.4213 46.5370

66.5193 77.0071 86.7138

95.1893 110.8919 127.1189