J. Braz. Chem. Soc., Vol. 21, No. 9, S1-S6, 2010.
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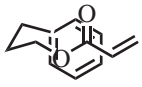
0103 - 5053 $6.00+0.00

Revisiting the Origin of the Preferential π–π Stacking Conformation of the (+)–8–Phenylmenthyl Acrylate

Saulo L. Capim, Sidney R. Santana, Boaz G. de Oliveira, Gerd B. Rocha* and Mário L. A. A. Vasconcellos*

Departamento de Química, Universidade Federal da Paraíba, Campus I, 58059–900 João Pessoa–PB, Brazil

Table S1. Cartesian coordinates and energies of HF/6–311++G(2d,2p) geometry optimized structures 2 and 3 (conformations **2***S*, **2***T*,**3***S* and **3***T*).

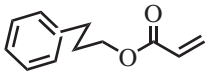


Stacking (*S*)

3*S*

Standard orientation: opt RHF/6–311++g(2d,2p)6d E = –612.47937340 a.u.					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.205188	1.945146	–0.015940
2	6	0	–0.137280	2.498597	–0.450446
3	6	0	–1.349391	2.064574	0.386618
4	6	0	2.366553	–0.088480	–0.022114
5	6	0	2.292837	–1.508206	–0.456294
6	8	0	3.275064	0.398184	0.564463
7	6	0	3.295279	–2.331948	–0.241203
8	6	0	–1.782755	0.621205	0.244542
9	6	0	–2.356035	0.168010	–0.936100
10	6	0	–2.763168	–1.143724	–1.071673
11	6	0	–2.610096	–2.032474	–0.021770
12	6	0	–2.050434	–1.592011	1.160281
13	6	0	–1.643202	–0.275330	1.289776
14	1	0	1.348487	2.041734	1.050826
15	1	0	2.009272	2.474791	–0.505628
16	1	0	–0.294792	2.262492	–1.496072
17	1	0	–0.061957	3.578950	–0.384358
18	1	0	–2.182964	2.699761	0.108767
19	1	0	–1.146249	2.273135	1.430401
20	1	0	1.390096	–1.815774	–0.944390
21	1	0	3.248347	–3.357345	–0.552214
22	1	0	4.185885	–1.995478	0.252300
23	1	0	–2.488522	0.846560	–1.758011
24	1	0	–3.204807	–1.471878	–1.992862
25	1	0	–2.929383	–3.051294	–0.124166
26	1	0	–1.930842	–2.268921	1.984078
27	1	0	–1.209951	0.052017	2.215888
28	8	0	1.282736	0.574203	–0.374292

Table S2. Cartesian coordinates and energies of HF/6–311++G(2d,2p) geometry optimized structures 2 and 3 (conformations **2***S*, **2***T*, **3***S* and **3***T*).



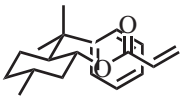
Trans (*T*)

3*T*

Standard orientation: opt RHF/6–311++g(2d,2p)6d E = –612.48328199 a.u.					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	–1.391617	0.722918	–0.002296
2	6	0	–0.033663	0.054653	–0.000267
3	6	0	1.100880	1.083531	–0.003888
4	6	0	–3.643853	0.077859	–0.000295
5	6	0	–4.556002	–1.095844	0.003549
6	8	0	–3.993900	1.210135	–0.004088
7	6	0	–5.861439	–0.935776	0.003433
8	6	0	2.471488	0.446802	–0.001633
9	6	0	3.111800	0.141229	1.189866
10	6	0	4.353261	–0.466711	1.194760
11	6	0	4.978808	–0.778992	0.002733
12	6	0	4.352938	–0.475935	–1.191447
13	6	0	3.111436	0.132050	–1.190880
14	1	0	–1.529032	1.341280	–0.877672
15	1	0	–1.528901	1.346849	0.869141
16	1	0	0.050052	–0.588362	–0.868197
17	1	0	0.050333	–0.582573	0.871892
18	1	0	1.004604	1.727822	0.862534
19	1	0	1.004606	1.721675	–0.874849
20	1	0	–4.097690	–2.064295	0.006406
21	1	0	–6.524830	–1.778501	0.006175
22	1	0	–6.293519	0.045630	0.000474
23	1	0	2.639555	0.383780	2.123417
24	1	0	4.832048	–0.691979	2.128058
25	1	0	5.943407	–1.247769	0.004427
26	1	0	4.831422	–0.708395	–2.123135
27	1	0	2.638953	0.367385	–2.126158
28	8	0	–2.379253	–0.298541	0.001049

*e–mail: mlaav@quimica.ufpb.br, gbr@quimica.ufpb.br

Table S3. Cartesian coordinates and energies of HF/6–311++G(2d,2p) geometry optimized structures 2 and 3 (conformations **2***S*, **2***T*,**3***S* and **3***T*).



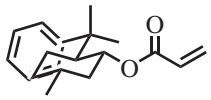
Stacking (*S*)

2*S*

Standard orientation: : opt RHF/6–311++g(2d,2p) 6d
E = −884.62474366 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.225330	–1.804189	0.366358
2	6	0	3.425739	–1.320553	–0.445397
3	6	0	3.664485	0.177400	–0.290432
4	6	0	2.378738	0.925684	–0.628427
5	6	0	1.193801	0.443615	0.199221
6	6	0	0.923313	–1.055714	0.017136
7	6	0	–0.339122	–1.597926	0.784647
8	6	0	–0.330827	–3.144055	0.815190
9	6	0	–0.329079	–1.127830	2.247581
10	6	0	–1.644825	–1.199000	0.065059
11	6	0	–1.840774	–1.541425	–1.270719
12	6	0	–3.018916	–1.256581	–1.928045
13	6	0	–4.054440	–0.621999	–1.265211
14	6	0	–3.884503	–0.284615	0.059397
15	6	0	–2.696603	–0.571091	0.713418
16	6	0	4.837349	0.664696	–1.134985
17	8	0	0.041905	1.179819	–0.209186
18	1	0	2.099684	–2.860893	0.188895
19	1	0	2.448169	–1.692302	1.422721
20	1	0	4.308538	–1.873626	–0.143204
21	1	0	3.264269	–1.547622	–1.496626
22	1	0	3.901107	0.372592	0.753394
23	1	0	2.505939	1.987396	–0.460637
24	1	0	2.143025	0.792374	–1.680495
25	1	0	1.380899	0.661064	1.237375
26	1	0	0.750046	–1.216088	–1.039793
27	1	0	–1.279103	–3.501880	1.193643
28	1	0	–0.189518	–3.570901	–0.169325
29	1	0	0.446763	–3.525560	1.462335
30	1	0	–1.116613	–1.612537	2.809628
31	1	0	–0.457596	–0.060180	2.349765
32	1	0	0.606760	–1.393650	2.719957
33	1	0	–1.067547	–2.043080	–1.817294
34	1	0	–3.130017	–1.534900	–2.958477
35	1	0	–4.973225	–0.401434	–1.772700
36	1	0	–4.674029	0.205689	0.595885
37	1	0	–2.610304	–0.285507	1.740350
38	1	0	5.008376	1.725220	–0.992823
39	1	0	5.750318	0.142933	–0.872338
40	1	0	4.652451	0.497359	–2.190902
41	6	0	–0.216884	2.340085	0.358913
42	6	0	–1.417403	2.975189	–0.247236
43	8	0	0.424602	2.812875	1.238687
44	1	0	–1.931560	2.411781	–0.999071
45	1	0	–2.674169	4.635909	–0.303190
46	6	0	–1.811556	4.170975	0.132933
47	1	0	–1.277642	4.710285	0.890522

Table S4. Cartesian coordinates and energies of HF/6–311++G(2d,2p) geometry optimized structures 2 and 3 (conformations **2***S*, **2***T*,**3***S* and **3***T*).



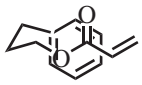
Trans (*T*)

2*T*

Standard orientation: HF/6–311++G(2d,2p) 6d
E = −884.62473753 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.751393	1.679884	0.504564
2	6	0	0.112285	2.956074	–0.034386
3	6	0	–1.392536	2.980079	0.206987
4	6	0	–2.007975	1.708196	–0.366647
5	6	0	–1.360612	0.435459	0.170674
6	6	0	0.150415	0.393423	–0.099328
7	6	0	0.918924	–0.897455	0.373339
8	6	0	0.667307	–1.179572	1.862422
9	6	0	0.481660	–2.164665	–0.398369
10	6	0	2.420359	–0.704861	0.075366
11	6	0	3.391935	–0.685531	1.063221
12	6	0	4.734672	–0.525628	0.755933
13	6	0	5.141074	–0.379532	–0.551642
14	6	0	4.186087	–0.398683	–1.553071
15	6	0	2.852850	–0.561106	–1.241740
16	6	0	–2.053122	4.229492	–0.366427
17	8	0	–2.001121	–0.667199	–0.479113
18	1	0	1.812406	1.708516	0.314225
19	1	0	0.632879	1.663940	1.583223
20	1	0	0.580386	3.816757	0.430950
21	1	0	0.305965	3.037773	–1.101291
22	1	0	–1.558327	2.978384	1.282224
23	1	0	–3.067140	1.670405	–0.146388
24	1	0	–1.905661	1.711335	–1.448246
25	1	0	–1.552999	0.358100	1.227382
26	1	0	0.273288	0.452154	–1.175752
27	1	0	1.206474	–2.063900	2.176874
28	1	0	0.963803	–0.363851	2.506582
29	1	0	–0.382267	–1.371031	2.035130
30	1	0	1.201633	–2.954567	–0.225727
31	1	0	0.423821	–1.995286	–1.464599
32	1	0	–0.481460	–2.517646	–0.070018
33	1	0	3.122153	–0.790842	2.092780
34	1	0	5.457714	–0.515488	1.548762
35	1	0	6.179127	–0.255156	–0.790699
36	1	0	4.480531	–0.289933	–2.579211
37	1	0	2.142767	–0.575149	–2.044165
38	1	0	–3.117337	4.239981	–0.162035
39	1	0	–1.623909	5.127861	0.061752
40	1	0	–1.921482	4.280267	–1.442183
41	6	0	–3.101857	–1.169420	0.043025
42	6	0	–3.644199	–2.264819	–0.805177
43	8	0	–3.592030	–0.801585	1.058768
44	1	0	–3.103537	–2.495925	–1.700880
45	1	0	–5.132483	–3.699828	–1.066877
46	6	0	–4.737208	–2.909479	–0.459045
47	1	0	–5.259847	–2.657736	0.442762

Table S5. Cartesian coordinates and energies of HF/6–311++G(2d,2p) geometry optimized structures 2 and 3 (conformations **2***S*, **2***T*,**3***S* and **3***T*).



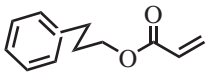
Stacking (*S*)

3*S*

Standard orientation: opt MP2/6–311++g(2d,2p) 6d
E = –614.68988216 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	–2.716864	0.048546	–0.301562
2	6	0	–2.326814	–1.413931	–0.211465
3	6	0	–1.190743	–1.715953	0.770320
4	6	0	–0.845288	1.478996	0.006501
5	6	0	0.305841	2.073205	–0.706862
6	8	0	–1.052387	1.546940	1.201535
7	6	0	1.291319	2.657562	–0.019283
8	6	0	0.199580	–1.283801	0.356375
9	6	0	0.670988	–1.445629	–0.951931
10	6	0	1.984946	–1.116414	–1.288035
11	6	0	2.856300	–0.623387	–0.316695
12	6	0	2.398486	–0.451926	0.989797
13	6	0	1.082658	–0.779256	1.317609
14	1	0	–2.966351	0.452948	0.675748
15	1	0	–3.557250	0.183253	–0.976237
16	1	0	–2.085251	–1.783076	–1.207425
17	1	0	–3.215832	–1.959174	0.110600
18	1	0	–1.168200	–2.794532	0.937968
19	1	0	–1.422735	–1.258153	1.732747
20	1	0	0.328229	1.979662	–1.782053
21	1	0	2.152363	3.073364	–0.519652
22	1	0	1.235141	2.713982	1.058140
23	1	0	0.014336	–1.830553	–1.720437
24	1	0	2.327225	–1.251342	–2.305060
25	1	0	3.874938	–0.370816	–0.576051
26	1	0	3.061349	–0.064754	1.751569
27	1	0	0.728643	–0.628314	2.329235
28	8	0	–1.643744	0.824238	–0.873748

Table S6. Cartesian coordinates and energies of MP2/6–311++G(2d,2p) geometry optimized structures 3 (conformations **3***S* and **3***T*).



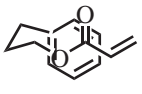
Trans (*T*)

3*T*

Standard orientation: opt MP2/6–311++g(2d,2p) 6d
E = –614.68553739 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.375147	0.702327	–0.007998
2	6	0	0.008177	0.060489	–0.000146
3	6	0	–1.100321	1.116671	–0.013442
4	6	0	3.639497	0.061496	–0.000637
5	6	0	4.562645	–1.099159	0.014014
6	8	0	3.967100	1.230525	–0.016015
7	6	0	5.884445	–0.908442	0.010781
8	6	0	–2.463867	0.481861	–0.005976
9	6	0	–3.098174	0.137680	–1.204154
10	6	0	–4.338250	–0.500960	–1.200654
11	6	0	–4.962356	–0.806667	0.009285
12	6	0	–4.340936	–0.467193	1.211566
13	6	0	–3.100842	0.171344	1.199942
14	1	0	1.530383	1.334744	0.864259
15	1	0	1.530650	1.312681	–0.895779
16	1	0	–0.096586	–0.567407	0.884159
17	1	0	–0.096358	–0.589246	–0.868557
18	1	0	–0.992739	1.745930	–0.898178
19	1	0	–0.993226	1.767527	0.855580
20	1	0	4.122752	–2.084919	0.027130
21	1	0	6.569511	–1.741830	0.021278
22	1	0	6.283642	0.095198	–0.002546
23	1	0	–2.620742	0.378134	–2.146138
24	1	0	–4.816381	–0.754615	–2.136514
25	1	0	–5.924691	–1.298413	0.015101
26	1	0	–4.821145	–0.694573	2.153098
27	1	0	–2.625477	0.438079	2.135872
28	8	0	2.352826	–0.360270	0.005483

Table S7. Cartesian coordinates and energies of MP2/6–311++G(2d,2p) geometry optimized structures 3 (conformations **3***S* and **3***T*).



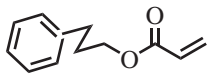
Stacking (*S*)

3*S*

Standard orientation: opt MPWB95/6–311++g(2d,2p) 6d
iop(3/76=0690003100)
E = –616.04311982 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	–2.609503	–0.405898	–0.299849
2	6	0	–2.009479	–1.789759	–0.232784
3	6	0	–0.862739	–1.946122	0.758964
4	6	0	–1.106478	1.396528	–0.012543
5	6	0	–0.126584	2.233052	–0.727717
6	8	0	–1.358837	1.470921	1.160490
7	6	0	0.581035	3.135353	–0.071208
8	6	0	0.456107	–1.333726	0.368475
9	6	0	0.988534	–1.475937	–0.906323
10	6	0	2.219681	–0.934492	–1.227611
11	6	0	2.947549	–0.242328	–0.276311
12	6	0	2.430956	–0.096562	0.997466
13	6	0	1.197545	–0.636920	1.311928
14	1	0	–2.912375	–0.057986	0.683009
15	1	0	–3.467736	–0.395475	–0.965527
16	1	0	–1.701191	–2.096138	–1.230878
17	1	0	–2.814236	–2.465274	0.057256
18	1	0	–0.705140	–3.012612	0.926260
19	1	0	–1.166187	–1.529154	1.718700
20	1	0	–0.013561	2.059479	–1.785685
21	1	0	1.312288	3.751685	–0.568765
22	1	0	0.435541	3.263562	0.990664
23	1	0	0.437702	–2.013711	–1.663359
24	1	0	2.612383	–1.056223	–2.225615
25	1	0	3.907607	0.180851	–0.527767
26	1	0	2.984908	0.445660	1.748303
27	1	0	0.788587	–0.498199	2.301736
28	8	0	–1.683455	0.529630	–0.854647

Table S8. Cartesian coordinates and energies of MPW1B95/6–311++G(2d,2p) geometry optimized structures 2 and 3 (conformations **2***S*, **2***T*, **3***S* and **3***T*).



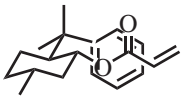
Trans (*T*)

3*T*

Standard orientation: opt MPWB95/6–311++g(2d,2p) 6d
iop(3/76=0690003100)
E = –616.04509962 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.378431	–0.519547	–0.439116
2	6	0	0.021948	0.050079	–0.124766
3	6	0	–1.090115	–0.836749	–0.671428
4	6	0	3.627879	–0.063060	–0.019085
5	6	0	4.568974	0.903826	0.577835
6	8	0	3.933895	–1.096864	–0.549874
7	6	0	5.867413	0.656882	0.574700
8	6	0	–2.454908	–0.352406	–0.283084
9	6	0	–3.128323	–0.931211	0.782341
10	6	0	–4.372039	–0.470619	1.175088
11	6	0	–4.965169	0.580915	0.502012
12	6	0	–4.306147	1.165137	–0.565624
13	6	0	–3.062363	0.701394	–0.952646
14	1	0	1.544481	–0.612023	–1.510983
15	1	0	1.510061	–1.508845	–0.005227
16	1	0	–0.062110	1.052256	–0.541922
17	1	0	–0.085401	0.148595	0.954170
18	1	0	–0.953501	–1.851305	–0.298211
19	1	0	–1.011081	–0.891196	–1.757128
20	1	0	4.147038	1.798497	1.007510
21	1	0	6.575370	1.346313	1.005589
22	1	0	6.239944	–0.255135	0.133099
23	1	0	–2.672705	–1.756484	1.310448
24	1	0	–4.879407	–0.935899	2.006084
25	1	0	–5.936618	0.941377	0.802291
26	1	0	–4.763916	1.981861	–1.102385
27	1	0	–2.557465	1.159364	–1.791532
28	8	0	2.365083	0.356211	0.106228

Table S9. Cartesian coordinates and energies of MPW1B95/6–311++G(2d,2p) geometry optimized structures 2 and 3 (conformations **2***S*, **2***T*, **3***S* and **3***T*).



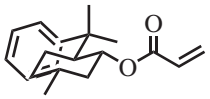
Stacking (*S*)

2*S*

Standard orientation: opt MPWB95/6–311++g(2d,2p) 6d iop(3/76=0690003100)
E = – 889.95725590 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.331005	–1.627212	0.455650
2	6	0	3.507622	–1.130442	–0.366033
3	6	0	3.653796	0.378438	–0.308342
4	6	0	2.343372	1.014901	–0.735864
5	6	0	1.189533	0.522705	0.108701
6	6	0	1.010548	–0.984163	0.034725
7	6	0	–0.218328	–1.500643	0.842150
8	6	0	–0.132532	–3.021380	1.019936
9	6	0	–0.238204	–0.878701	2.232940
10	6	0	–1.515384	–1.228604	0.086112
11	6	0	–1.690385	–1.733447	–1.198849
12	6	0	–2.867359	–1.543190	–1.895247
13	6	0	–3.913868	–0.845043	–1.317764
14	6	0	–3.761782	–0.346477	–0.039299
15	6	0	–2.577049	–0.537811	0.651888
16	6	0	4.811959	0.868937	–1.154230
17	8	0	–0.011678	1.149651	–0.358136
18	1	0	2.261577	–2.706405	0.357936
19	1	0	2.517015	–1.421030	1.512003
20	1	0	4.424885	–1.609965	–0.025842
21	1	0	3.370578	–1.426568	–1.409313
22	1	0	3.840484	0.659440	0.731871
23	1	0	2.398303	2.099639	–0.657332
24	1	0	2.144420	0.773277	–1.782194
25	1	0	1.351799	0.830703	1.138932
26	1	0	0.846639	–1.237400	–1.014861
27	1	0	–1.065259	–3.391368	1.437935
28	1	0	0.032505	–3.530182	0.072396
29	1	0	0.671270	–3.294853	1.698859
30	1	0	–1.011603	–1.337774	2.844414
31	1	0	–0.416427	0.193592	2.212433
32	1	0	0.713517	–1.047652	2.731845
33	1	0	–0.892623	–2.289475	–1.668868
34	1	0	–2.969550	–1.945180	–2.891741
35	1	0	–4.835826	–0.696858	–1.858107
36	1	0	–4.566671	0.199725	0.428417
37	1	0	–2.488863	–0.126661	1.643985
38	1	0	4.918019	1.949771	–1.093272
39	1	0	5.750612	0.420917	–0.835093
40	1	0	4.658769	0.608365	–2.200880
41	6	0	–0.460660	2.212812	0.312062
42	6	0	–1.690968	2.736291	–0.312544
43	8	0	0.067027	2.671449	1.292019
44	1	0	–2.069952	2.197855	–1.166271
45	1	0	–3.178163	4.215578	–0.264265
46	6	0	–2.279285	3.814588	0.175675
47	1	0	–1.860438	4.314354	1.035933

Table S10. Cartesian coordinates and energies of MPW1B95/6–311++G(2d,2p) geometry optimized structures 2 and 3 (conformations **2***S*, **2***T*, **3***S* and **3***T*).



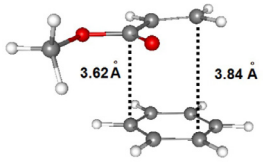
Trans (*T*)

2*T*

Standard orientation: opt MPWB95/6–311++g(2d,2p) 6d iop(3/76=0690003100)
E = –889.95629860 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.821841	1.591542	0.398574
2	6	0	0.205070	2.908760	–0.031916
3	6	0	–1.282062	2.963247	0.261273
4	6	0	–1.948187	1.760405	–0.380121
5	6	0	–1.318472	0.461235	0.074057
6	6	0	0.161885	0.379122	–0.262641
7	6	0	0.856243	–0.963863	0.133734
8	6	0	0.429509	–1.396728	1.530168
9	6	0	0.497517	–2.099024	–0.834413
10	6	0	2.364530	–0.767029	0.038666
11	6	0	3.204442	–0.821085	1.140957
12	6	0	4.571130	–0.629263	1.013264
13	6	0	5.128850	–0.375028	–0.223285
14	6	0	4.304665	–0.315095	–1.334140
15	6	0	2.944506	–0.510268	–1.200794
16	6	0	–1.910956	4.260598	–0.206043
17	8	0	–2.024237	–0.619795	–0.557264
18	1	0	1.882937	1.595474	0.172637
19	1	0	0.738811	1.492783	1.483582
20	1	0	0.716865	3.735352	0.459822
21	1	0	0.355207	3.044860	–1.106137
22	1	0	–1.414830	2.882377	1.343562
23	1	0	–3.009211	1.733772	–0.137528
24	1	0	–1.860748	1.831997	–1.466523
25	1	0	–1.454966	0.362341	1.148696
26	1	0	0.265505	0.489956	–1.345795
27	1	0	0.974094	–2.286609	1.836911
28	1	0	0.597187	–0.624719	2.278399
29	1	0	–0.629006	–1.644158	1.538751
30	1	0	1.156006	–2.947012	–0.659990
31	1	0	0.614726	–1.794619	–1.871350
32	1	0	–0.524794	–2.428098	–0.698504
33	1	0	2.798769	–1.011082	2.121180
34	1	0	5.198865	–0.678559	1.889876
35	1	0	6.192477	–0.225508	–0.323625
36	1	0	4.723789	–0.116873	–2.308800
37	1	0	2.320278	–0.456402	–2.080025
38	1	0	–2.973936	4.291895	0.022887
39	1	0	–1.439864	5.119335	0.267453
40	1	0	–1.799235	4.373568	–1.283932
41	6	0	–3.098297	–1.092146	0.081383
42	6	0	–3.729225	–2.179898	–0.692510
43	8	0	–3.485592	–0.688779	1.146166
44	1	0	–3.276335	–2.435603	–1.637432
45	1	0	–5.275618	–3.596385	–0.770898
46	6	0	–4.799854	–2.797937	–0.224725
47	1	0	–5.217154	–2.504755	0.726639

Table S11. Cartesian coordinates and energies of MPW1B95/6–311++G(2d,2p) geometry optimized structures 2 and 3 (conformations **2***S*, **2***T*, **3***S* and **3***T*).



4

Standard orientation: opt MPWB95/6–311++g(2d,2p) 6d
iop(3/76=0690003100)
E = –538.63055147 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	–3.051402	–1.352407	–0.011567
2	6	0	–1.711069	0.543924	–0.002474
3	6	0	–0.881434	1.435478	–0.830656
4	8	0	–1.912665	0.663865	1.176038
5	6	0	–0.309025	2.498546	–0.294047
6	8	0	–2.232194	–0.447186	–0.736330
7	1	0	–3.893472	–0.830604	0.432357
8	1	0	–3.392957	–2.086629	–0.729660
9	1	0	–2.481858	–1.828228	0.781063
10	1	0	–0.763621	1.170501	–1.868951
11	1	0	0.308695	3.162493	–0.876644
12	1	0	–0.450999	2.713996	0.754138
13	6	0	0.965065	–1.304899	0.799157
14	6	0	1.199605	–1.542082	–0.543669
15	6	0	2.129853	–0.779156	–1.228682
16	6	0	2.825814	0.217782	–0.569072
17	6	0	2.590012	0.454514	0.774096
18	6	0	1.655620	–0.303000	1.457294
19	1	0	0.235547	–1.893598	1.333474
20	1	0	0.656612	–2.320164	–1.057517
21	1	0	2.313812	–0.964411	–2.275780
22	1	0	3.554326	0.810019	–1.101253
23	1	0	3.132793	1.233051	1.287800
24	1	0	1.461752	–0.112047	2.501026

Table S12. Cartesian coordinates and energies of MPW1B95/6–311++G(2d,2p) geometry optimized structures to the complex **4**.

BENZENE

Standard orientation: opt MPWB95/6–311++g(2d,2p) 6d
iop(3/76=0690003100)
E = –232.19609986

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	–0.215622	1.366749	0.000000
2	6	0	–1.291600	0.496640	–0.000011
3	6	0	–1.076046	–0.870020	0.000011
4	6	0	0.215634	–1.366748	–0.000001
5	6	0	1.291596	–0.496651	–0.000010
6	6	0	1.076038	0.870030	0.000008
7	1	0	–0.384603	2.432500	0.000006
8	1	0	–2.299044	0.883216	–0.000010
9	1	0	–1.914544	–1.549198	0.000014
10	1	0	0.384583	–2.432503	0.000000
11	1	0	2.299051	–0.883197	–0.000003
12	1	0	1.914557	1.549182	0.000011

Table S13. Cartesian coordinates and energies of MPW1B95/6–311++G(2d,2p) geometry optimized structures to the complex 4.

METHYL ACRYLATE

Standard orientation: opt MPWB95/6–311++g(2d,2p) 6d
iop(3/76=0690003100)
E = – 306.43239576 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	–0.040557	0.105756	–0.000047
2	6	0	–1.310024	–0.644225	–0.000044
3	1	0	–1.244640	–1.720576	–0.000118
4	6	0	–2.462937	0.001994	0.000059
5	1	0	–2.473278	1.081509	0.000132
6	1	0	–3.405133	–0.521743	0.000069
7	6	0	2.274613	–0.078066	0.000043
8	1	0	2.380204	0.545210	0.882364
9	1	0	3.012300	–0.869703	0.000133
10	1	0	2.380313	0.545106	–0.882339
11	8	0	1.008010	–0.724008	0.000001
12	8	0	0.064948	1.302438	–0.000040